# ADVANCED ECONOMETRIC METHODS (R300)

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Last revised on November 25, 2020

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## ESTIMATION IN PARAMETRIC PROBLEMS

## Reading

Evaluation of estimators:

Casella and Berger, Chapters 7 and 10

Hansen I, Chapter 6

Asymptotics for the sample mean:

Goldberger, Chapter 9

Hansen I, Chapters 7 and 8

Maximum likelihood:

Davidson and MacKinnon, Chapter 8

Hansen I, Chapter 10

Wooldridge, Chapter 13

Linear regression:

Goldberger, Chapters 14–16

Hansen II, Chapters 2–5

## Estimation

We are interested in saying something about a population based on a sample

 $x_1,\ldots,x_n$ 

from it. The  $x_i$  may be scalars or vectors.

Want to learn some feature of the population, say  $\theta$ ; the estimand. For that we use an estimator

$$\theta_n = \theta_n(x_1, \ldots, x_n);$$

this is just a function of the sample (it can be any function).

Some questions:

- How do we evaluate estimators, i.e., what is a good estimator?
- How do we construct good estimators?
- Does there exist a best estimator and, if so, is it unique?

This inferential aim is different from a descriptive data analysis that gives means, variances, correlations, regression coefficients, and so on.

A way to formalize sampling is to see  $x_1, \ldots, x_n$  as a draw from an (*n*-variate) probability (mass or density) function, g.

We begin with the random sampling and the parametric framework.

The sample is a random sample if

- 1 the  $x_i$  are independent across i, so that  $g(x_1, \ldots, x_n) = \prod_{i=1}^n f_i(x_i)$  for probability functions  $f_1, \ldots, f_n$ ; and
- **2** all  $x_i$  are identically distributed, so that  $f_i = f$  for some f and all i.

We say that the  $x_i$  are i.i.d.

The parametric framework says that  $f = f_{\theta}$  is known up to parameter  $\theta$  which is finite dimensional (and so is a vector, in general).

That is, we know the class

$$\{f_{\theta}: \theta \in \Theta\},\$$

but not the particular  $\theta$  that generated the data.

We know the whole probability distribution once we know the parameter  $\theta$ .

We may calculate  $P_{\theta}(x_i \in A) = \int_A f_{\theta}(x) dx$  for any set A. For example,

$$F_{\theta}(x) = P_{\theta}(x_i \in (-\infty, x]) = P_{\theta}(x_i \le x)$$

for any x (the cumulative distribution function).

We know all raw and centered moments; for example, the mean and variance  $E_{\theta}(x_i) = \int x f_{\theta}(x) dx, \quad \operatorname{var}_{\theta}(x_i) = \int (x - E_{\theta}(x_i)) (x - E_{\theta}(x_i))' f_{\theta}(x) dx,$ 

and so on.

We know  $E_{\theta}(\varphi(x_i))$  for any chosen function  $\varphi$  and so also parameters  $\psi$  defined through

$$E_{\theta}(\varphi(x_i;\psi)) = 0,$$

(which we call moment conditions). Obvious example is  $\psi = E_{\theta}(x_i)$ , which has  $\varphi(x_i; \psi) = x_i - \psi$ .

For univariate  $x_i$  the  $\tau$ th-quantile is  $q_{\tau} = \inf_q \{q : F_{\theta}(q) \ge \tau\}$ , for  $\tau \in (0, 1)$ . It is a solution to the moment condition  $E_{\theta}(\{x_i \le \psi\} - \tau) = 0$  and so has  $\varphi(x_i; \psi) = \{x_i \le \psi\} - \tau$ .

### Examples

Let  $x_1, \ldots, x_n$  be a sequence of zeros and ones with  $P_{\theta}(x_i = 1) = \theta$ . Then  $x_i$  is Bernoulli with mass function

$$f_{\theta}(x) = \theta^x \left(1 - \theta\right)^{1 - x}, \qquad \theta \in (0, 1),$$

for  $x \in \{0, 1\}$ .

One possible (and sensible) estimator of  $\theta$  would be the sample frequency of ones, i.e.,  $\overline{x}_n = n^{-1} \sum_{i=1}^n x_i$ 

Another simple example has  $x_1, \ldots, x_n$  representing the number of arrivals per unit of time. The Poisson distribution has

$$f_{\theta}(x) = P_{\theta}(x_i = x) = \frac{\theta^x e^{-\theta}}{x!}, \qquad \theta > 0$$

for  $x \in \mathbb{N}$ .

 $\theta$  is the arrival rate, i.e., the expected number of arrivals per time unit. A sensible estimator of  $\theta$  is again the sample mean. We have data on the number of births per hour over a 24 hour period in Addenbrooke's.

Fitting a Poisson model to such data we estimate the number of births per hour by the sample mean, here 1.875 births/hour.

Given an estimate of  $\theta$  we can estimate the mass function.



The hospital data also tell us that, of the 44 babies, 18 were boys and 26 where girls.

The maximum likelihood estimator of the probability of giving birth to a boy is 18/44 = .409.

The estimator is a random variable.

Using arguments to be developed later we can test whether there is a gender bias at Addenbrooke's.

The standard error on our estimate is  $\sqrt{(18/44) \times (26/44)/44} = .074$  which gives us the value

$$\frac{.409 - .500}{.074} = -1.23$$

for a test statistic which is (asymptotically) standard normal under the null of no gender bias.

Using a Neyman-Pearson argument (see later) we cannot reject the absence of gender bias (at conventional significance levels).

A continuous example with two parameters is the normal distribution.

The univariate standard-normal density is

$$\phi(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2};$$

it has mean zero and variance one. The corresponding distribution function is

$$\Phi(x) = \int_{-\infty}^{x} \phi(u) \, du.$$

The normal distribution is a location/scale family:

If  $z_i \sim N(0, 1)$ , then

$$x_i = \mu + \sigma z_i \sim N(\mu, \sigma^2).$$

Its cumulative distribution function is

$$P(x_i \le x) = P\left(z_i \le \frac{x-\mu}{\sigma}\right) = \Phi\left(\frac{x-\mu}{\sigma}\right)$$

and its density function is

$$\frac{1}{\sigma}\phi\left(\frac{x-\mu}{\sigma}\right) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{1}{2}(x-\mu)^2/\sigma^2}.$$

Obvious estimators for  $\mu, \sigma^2$  would be the sample mean and sample variance.

Less obvious is when

$$x_i^* \sim N(\mu, \sigma^2)$$

but we observe

$$x_i = \begin{cases} x_i^* & \text{if } x_i^* \ge 0\\ 0 & \text{if } x_i^* < 0 \end{cases}$$

This is a **censored** normal variable.

How would we estimate the parameters here?

Some obvious candidates would be

- the sample mean and variance of the  $x_i$ ;
- the sample mean and variance of the positive  $x_i$ .

These turn out not to be very attractive and should not be used.

We will construct a better estimator later on.

As a final example, suppose that  $x_i \sim \chi_{\theta}^2$ .

The Chi-squared distribution with (integer)  $\theta$  degrees of freedom has density

$$f_{\theta}(x) = \frac{x^{\theta/2 - 1} e^{-x/2}}{2^{\theta/2} \Gamma(\theta/2)},$$

where  $\Gamma(\theta) = \int_0^\infty x^{\theta-1} e^{-x} dx$  denotes the Gamma function at  $\theta$ . We note without proof that

- $\bullet E_{\theta}(x_i) = \theta,$
- $\operatorname{var}_{\theta}(x_i) = 2\theta$ ,
- $E_{\theta}(x_i^p) = 2^p \Gamma(p + \theta/2) / \Gamma(\theta/2).$

It follows that the sample mean is an obvious candidate estimator of  $\theta$ .

But there is also information in higher-order moments so the sample mean may be inefficient (it is here but it need not be, a priori; see the Poisson example).

## Change of variable

Let x be a random variable with density f. Let  $y = \varphi(x)$  for an invertible function  $\varphi$ .

The density of y is

$$f(\varphi^{-1}(y)) \left| \det \left( \frac{\partial \varphi^{-1}(y)}{\partial y'} \right) \right|.$$

Easiest to see in the univariate case:

If  $\varphi$  is increasing,

$$P(y \le a) = P(\varphi(x) \le a) = P(x \le \varphi^{-1}(a)),$$

and differentiation with respect to a gives

$$f(\varphi^{-1}(a)) \left. \frac{\partial \varphi^{-1}(y)}{\partial y} \right|_{y=a}$$

by the chain rule.

If  $\varphi$  is decreasing,  $P(y \le a) = 1 - P(x \le \varphi^{-1}(a))$ , and differentiation gives  $-f(\varphi^{-1}(a)) \left( \left. \partial \varphi^{-1}(y) / \partial y \right|_{y=a} \right)$ .

Let x be a continuous univariate random variable with density f. Then

$$\varphi(t) = E(e^{\iota tx}) = \int e^{\iota tx} f(x) \, dx$$

is its characteristic function. (Here,  $\iota$  is the imaginary unit, i.e.,  $\iota^2 = -1$ ) So,  $\varphi$  is the Fourier transform of f.

Like  $f, \varphi$  completely characterizes the random variable.

f can be recovered from  $\varphi$  through the inverse Fourier transform

$$f(x) = \frac{1}{2\pi} \int e^{-\iota tx} \varphi(t) \, dt.$$

Further, raw moments equal

$$E(x^{p}) = \iota^{-p} \left. \frac{\partial^{p} \varphi(t)}{\partial t^{p}} \right|_{t=0}$$

.

For multivariate x,  $\varphi(t) = E(e^{\iota t'x})$  for a vector t of conformable dimension.

An example is the standard normal case. Here,

$$f(x) = \frac{e^{-x^2/2}}{\sqrt{2\pi}}, \qquad \varphi(t) = e^{-t^2/2}.$$

We have, using the definition of the cosine function,

$$\varphi(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{\iota tx} e^{-x^2/2} dx = \frac{2}{\sqrt{2\pi}} \int_{0}^{+\infty} \frac{1}{2} (e^{\iota tx} + e^{-\iota tx}) e^{-x^2/2} dx$$
$$= \frac{2}{\sqrt{2\pi}} \int_{0}^{+\infty} \cos(tx) e^{-x^2/2} dx.$$

Next,

$$\begin{aligned} \varphi'(t) &= \frac{2}{\sqrt{2\pi}} \int_0^{+\infty} \frac{\partial \cos(tx)}{\partial t} e^{-x^2/2} \, dx \\ &= -\frac{2}{\sqrt{2\pi}} \int_0^{+\infty} \sin(tx) \, x \, e^{-x^2/2} \, dx \\ &= \frac{2}{\sqrt{2\pi}} \left( e^{-x^2/2} \sin(tx) \right) \Big|_0^{+\infty} - \frac{2}{\sqrt{2\pi}} \int_0^{+\infty} t \, \cos(tx) \, e^{-x^2/2} \, dx \\ &= -t \, \varphi(t). \end{aligned}$$

This implies that  $\varphi \propto e^{-t^2/2}$ . But because  $\int f(x) dx = 1$  we must have that  $\varphi(0) = 1$  so that, indeed,  $\varphi = e^{-t^2/2}$ .

To see that

$$\phi(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-\iota t x} e^{-t^2/2} dt,$$

we can use the same calculations.

Moreover, note that

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-\iota tx} e^{-t^2/2} dt = \frac{1}{\pi} \int_{0}^{+\infty} \cos(tx) e^{-t^2/2} dt$$

by the same argument as before. We have already computed the last integral.

Moreover,

$$\frac{1}{\pi} \int_0^{+\infty} \cos(tx) e^{-t^2/2} dt = \frac{1}{\pi} \left( \frac{\sqrt{2\pi}}{2} \varphi(x) \right) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} = \phi(x),$$

as claimed.

Let  $z \sim N(0, 1)$ . Then the density of  $x = z^2$  at a > 0 is

$$\frac{\phi(\sqrt{a}) + \phi(-\sqrt{a})}{2\sqrt{a}} = \frac{1}{2\sqrt{a}} \left( \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}a} + \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}a} \right) = \frac{1}{\sqrt{2\pi}\sqrt{a}} e^{-\frac{1}{2}a}.$$

This is the density of a  $\chi_1^2$  random variable. Indeed, use that  $\Gamma(1/2) = \sqrt{\pi}$  to rewrite the density as

$$\frac{1}{\sqrt{2\pi}\sqrt{a}}e^{-\frac{1}{2}a} = \frac{a^{1/2-1}e^{-a/2}}{2^{1/2}\sqrt{\pi}} = \frac{a^{1/2-1}e^{-a/2}}{2^{1/2}\Gamma(1/2)},$$

which co-incides with the definition given above.

The characteristic function of a  $\chi^2_p\text{-variable}$  is

$$\varphi_p(t) = (1 - 2\iota t)^{-p/2}$$

So, if

$$z_i \sim N(0, 1),$$
  
then  $z_i^2 \sim \chi_1^2$  has  $\varphi_1(t) = (1 - 2\iota t)^{-1/2}.$ 

The characteristic function of  $\sum_{i=1}^{n} z_i^2$  is (by independence) equal to

$$\prod_{i=1}^{n} \varphi_1(t) = \left( (1 - 2\iota t)^{-1/2} \right)^n = (1 - 2\iota t)^{-n/2} = \varphi_n(t).$$

Hence,

$$\sum_{i=1}^n z_i^2 \sim \chi_n^2.$$

## Sum of independent normal variables

The characteristic function of a  $N(\mu,\sigma^2)$  variable is

$$\varphi_{\mu,\sigma^2}(t) = e^{\iota t\mu - \sigma^2 \frac{t^2}{2}}.$$

So, if

$$z_i \sim N(0,1)$$

are independent the characteristic function of  $\sum_{i=1}^{n} z_i$  is

$$\prod_{i=1}^{n} \varphi_{0,1}(t) = \prod_{i=1}^{n} (e^{-t^2/2}) = (e^{-t^2/2})^n = e^{-n t^2/2} = \varphi_{0,n}(t),$$
  
i.e.,  $\sum_{i=1}^{n} z_i \sim N(0, n).$ 

By the location/scale properties of the normal we then have that

$$\overline{z}_n \sim N(0, n^{-1})$$

and

$$\overline{x}_n = \mu + \sigma \,\overline{z}_n \sim N(\mu, \sigma^2/n).$$

Sampling distributions of several estimators.

#### Blue is better than red.



An estimator  $\theta_n$  is best unbiased if  $E_{\theta}(\theta_n) = \theta$  and

$$\operatorname{var}_{\theta}(\theta_n) \leq \operatorname{var}_{\theta}(\theta_*)$$

for any other unbiased estimator  $\theta_*$ .

Here and later, the inequality is to be interpreted in the matrix sense:  $A \ge 0$  means that matrix A is positive semi-definite, i.e.,  $x'Ax \ge 0$  for any real non-zero vector x.

A lower bound on the variance can be found.

This is called an efficiency bound; here: Cramér-Rao bound.

Very often such an estimator will not exist.

If it exists, it is unique.

The Cauchy distribution with location  $\mu$  and scale  $\gamma$  has the symmetric density

$$\frac{1}{\pi\gamma\left(1+\left(\frac{x-\mu}{\gamma}\right)^2\right)}$$

It has no moments.

For example, with  $\mu = 0$  and  $\gamma = 1$  we have

$$E(|x|) = \lim_{M \to \infty} 2 \int_0^M \frac{1}{\pi} \frac{x}{1+x^2} \, dx = \lim_{M \to \infty} \frac{\log(1+M^2)}{\pi} = +\infty$$

So it is not useful to estimate the location parameter  $\mu$  via the sample mean. A sensible estimator would be the sample median, which is well defined in spite of the non-existence of moments.

So, if an estimator is Cauchy distributed its bias does not exist.

An example where this happens is with ratios of normal variates, as these are Cauchy.

## Ratio of normals

Take independent scalar normal variates  $x \sim N(0, \sigma_1^2)$  and  $y \sim N(0, \sigma_2^2)$ .

Consider the transformation  $(x, y) \rightarrow (u, v) = (x/y, y)$ . The Jacobian of the transformation is v and so the density of u is

$$f_{\sigma_1,\sigma_2}(u) = \int_{-\infty}^{+\infty} \frac{\phi((uv)/\sigma_1)}{\sigma_1} \frac{\phi(v/\sigma_2)}{\sigma_2} |v| dv.$$

This is (using that  $\phi(u) = e^{-u^2/2}/\sqrt{2\pi}$  and that  $\phi(u) = \phi(-u)$  for all u)

$$\begin{split} f_{\sigma_1,\sigma_2}(u) &= \frac{1}{\pi \sigma_1 \sigma_2} \int_0^{+\infty} e^{-\frac{1}{2}v^2 ((1/\sigma_2)^2 + (u/\sigma_1)^2)} v \, dv \\ &= \frac{1}{\pi \sigma_1 \sigma_2} \int_0^{+\infty} e^{-\frac{1}{2}v^2 (1+u^2 (\sigma_2/\sigma_1)^2)/\sigma_2^2} v \, dv \\ &= \frac{1}{\pi \sigma_1 \sigma_2 \left( (1+u^2 (\sigma_2/\sigma_1)^2)/\sigma_2^2 \right)} \int_0^{+\infty} \left( -e^{-\frac{1}{2}v^2 (1+u^2 (\sigma_2/\sigma_1)^2)/\sigma_2^2} \right)' dv \\ &= \frac{1}{\pi \frac{\sigma_1}{\sigma_2} \left( 1 + \left( \frac{u}{\sigma_1/\sigma_2} \right)^2 \right)}, \end{split}$$

which is a Cauchy distribution with location zero and scale  $\sigma_1/\sigma_2$ .

Let

$$\frac{\partial \log f_{\theta}(x)}{\partial \theta}$$

be the score.

The score has mean zero:

$$E_{\theta}\left(\frac{\partial \log f_{\theta}(x_i)}{\partial \theta}\right) = \int \frac{\partial \log f_{\theta}(x)}{\partial \theta} f_{\theta}(x) \, dx = \int \frac{\partial f_{\theta}(x)}{\partial \theta} \, dx = 0$$

(where the last step follows from  $f_{\theta}$  integrating to one.) The variance of the score,

$$I_{\theta} = \operatorname{var}_{\theta} \left( \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right),$$

is called the Fisher information.

When the score is a vector the information is a (variance-covariance) matrix.

#### Theorem 1 (Cramér-Rao bound)

Under regularity conditions,

$$\operatorname{var}_{\theta}(\theta_n) \ge I_{\theta}^{-1}/n$$

for any unbiased estimator  $\theta_n$  of  $\theta$ .

More information reduces the variance bound.

The bound shrinks like  $n^{-1}$ .

From the proof (to follow) we have that  $\theta_n$  attains the bound if and only if

$$n I_{\theta} (\theta_n - \theta) = \sum_{i=1}^n \left. \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right|_{\theta}$$

#### Proof (for the scalar case).

Differentiating the zero-bias condition

$$E_{\theta}(\theta_n - \theta) = \int \dots \int (\theta_n(x_1, \dots, x_n) - \theta) \prod_i f_{\theta}(x_i) \, dx_1 \dots dx_n = 0,$$

gives

$$\int \dots \int \left\{ \left( \theta_n(x_1, \dots, x_n) - \theta \right) \frac{\partial \prod_i f_\theta(x_i)}{\partial \theta} - \prod_i f_\theta(x_i) \right\} \, dx_1 \dots dx_n = 0.$$

Because densities integrate to one and an identity below we can re-write as

$$\int \cdots \int (\theta_n(x_1, \dots, x_n) - \theta) \sum_i \frac{\partial \log f_\theta(x_i)}{\partial \theta} \prod_i f_\theta(x_i) \, dx_1 \dots dx_n = 1.$$

But this is just

$$E_{\theta}\left(\left(\theta_{n}-\theta\right)\sum_{i}\frac{\partial\log f_{\theta}(x_{i})}{\partial\theta}\right)=1.$$

Furthermore, this is a covariance (as both terms have zero mean), and so

$$1 = \operatorname{cov}_{\theta} \left( \theta_n, \sum_i \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right)^2 \le \operatorname{var}_{\theta}(\theta_n) \times \operatorname{var}_{\theta} \left( \sum_i \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right)^2$$

(by Cauchy-Schwarz). The result then follows from

$$\operatorname{var}_{\theta}\left(\sum_{i} \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta}\right) = n I_{\theta}.$$

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#### Proof Annex: Identity used in Step 2.

Above we used the following:

$$\sum_{i=1}^{n} \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} = \sum_{i=1}^{n} \frac{1}{f_{\theta}(x_i)} \frac{\partial f_{\theta}(x_i)}{\partial \theta}$$
$$= \sum_{i=1}^{n} \left( \frac{\prod_{j \neq i} f_{\theta}(x_j)}{\prod_j f_{\theta}(x_j)} \right) \frac{\partial f_{\theta}(x_i)}{\partial \theta}$$
$$= \frac{\sum_{i=1}^{n} \prod_{j \neq i} f_{\theta}(x_j) \frac{\partial f_{\theta}(x_i)}{\partial \theta}}{\prod_i f_{\theta}(x_j)} = \frac{\frac{\partial \prod_i f_{\theta}(x_i)}{\partial \theta}}{\prod_i f_{\theta}(x_j)}$$

(using the chain rule on the differentiation of a product), so that we obtain

$$\frac{\partial \prod_{i=1}^{n} f_{\theta}(x_{i})}{\partial \theta} = \left(\sum_{i=1}^{n} \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta}\right) \left(\prod_{j=1}^{n} f_{\theta}(x_{j})\right),$$

the integral of which is an expectation.

#### Theorem 2 (Cauchy-Schwarz)

For scalar random variables  $x_i$  and  $y_i$ 

$$E(x_i y_i)^2 \le E(x_i^2) \ E(y_i^2).$$

Equally, for a sample of size n,

$$\left(n^{-1}\sum_{i=1}^{n} x_i y_i\right)^2 \le \left(n^{-1}\sum_{i=1}^{n} x_i^2\right) \left(n^{-1}\sum_{i=1}^{n} y_i^2\right).$$

A useful result is the following alternative characterization of the information.

### Theorem 3 (Information equality)

$$\operatorname{var}_{\theta}\left(\frac{\partial \log f_{\theta}(x_{i})}{\partial \theta}\right) = I_{\theta} = -E_{\theta}\left(\frac{\partial^{2} \log f_{\theta}(x_{i})}{\partial \theta \partial \theta'}\right).$$

We will need this later when establishing optimality of maximum likelihood.

### **Proof.**

Differentiating

$$\int \frac{\partial \log f_{\theta}(x)}{\partial \theta} f_{\theta}(x) \, dx = 0$$

under the integral sign gives

$$\int \frac{\partial^2 \log f_{\theta}(x)}{\partial \theta \partial \theta'} f_{\theta}(x) \, dx + \int \frac{\partial \log f_{\theta}(x)}{\partial \theta} \, \frac{\partial f_{\theta}(x)}{\partial \theta'} \, dx = 0.$$

Because

$$\frac{\partial \log f_{\theta}(x)}{\partial \theta} = \frac{1}{f_{\theta}(x)} \frac{\partial f_{\theta}(x)}{\partial \theta},$$

we have  $\frac{\partial f_{\theta}(x)}{\partial \theta} = \frac{\partial \log f_{\theta}(x)}{\partial \theta} f_{\theta}(x)$  and so we obtain

$$E_{\theta}\left(\frac{\partial^2 \log f_{\theta}(x_i)}{\partial \theta \partial \theta'}\right) + E_{\theta}\left(\frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \ \frac{\partial \log f_{\theta}(x_i)}{\partial \theta'}\right) = 0.$$

Re-arrangement then yields the result.

## Theorem 4 (Uniqueness)

If  $\theta_n^A$  and  $\theta_n^B$  are such that

$$E_{\theta}(\theta_n^A) = E_{\theta}(\theta_n^B) = \theta, \qquad \operatorname{var}_{\theta}(\theta_n^A) = \operatorname{var}_{\theta}(\theta_n^B) = I_{\theta}^{-1}/n,$$

then  $\theta_n^A = \theta_n^B$ .

#### Proof (for the scalar case).

Define a third estimator  $\theta_n^C$  through the linear combination

$$\theta_n^c = \lambda \, \theta_n^A + (1 - \lambda) \, \theta_n^B, \qquad \lambda \in (0, 1).$$

Then  $E_{\theta}(\theta_n^C) = \lambda E_{\theta}(\theta_n^A) + (1 - \lambda) E_{\theta}(\theta_n^B) = \theta$ , so  $\theta_n^C$  is also unbiased, and

$$\operatorname{var}_{\theta}(\theta_n^C) = \lambda^2 \operatorname{var}_{\theta}(\theta_n^A) + (1-\lambda)^2 \operatorname{var}_{\theta}(\theta_n^B) + 2 \lambda(1-\lambda) \operatorname{cov}_{\theta}(\theta_n^A, \theta_n^B).$$

Now,  $\operatorname{var}_{\theta}(\theta_n^A) = \operatorname{var}_{\theta}(\theta_n^B) = I_{\theta}^{-1}/n$  by efficiency and

$$|\operatorname{cov}_{\theta}(\theta_n^A, \theta_n^B)| \le \operatorname{std}_{\theta}(\theta_n^A) \operatorname{std}_{\theta}(\theta_n^B) = I_{\theta}^{-1}/n$$

by Cauchy-Schwarz. Thus,

$$\operatorname{var}_{\theta}(\theta_n^C) \leq I_{\theta}^{-1}/n.$$

The inequality cannot be strict because  $\theta_n^A$  and  $\theta_n^B$  are best-unbiased. So we must have that  $|\operatorname{corr}_{\theta}(\theta_n^A, \theta_n^B)| = 1$  which happens iff

$$\theta_n^A = a + b \, \theta_n^E$$

for constants a, b. Now we have that b = 1 as  $\operatorname{var}_{\theta}(\theta_n^A) = \operatorname{var}_{\theta}(\theta_n^B)$  and a = 0 as  $E_{\theta}(\theta_n^A) = E_{\theta}(\theta_n^B)$ .

## Bernoulli

With binary data we have

$$\log f_{\theta}(x) = x \log(\theta) + (1 - x) \log(1 - \theta),$$

so that

$$\frac{\partial \log f_{\theta}(x)}{\partial \theta} = \frac{x}{\theta} - \frac{1-x}{1-\theta} = \frac{x-\theta}{\theta(1-\theta)},$$
$$\frac{\partial^2 \log f_{\theta}(x)}{\partial \theta^2} = -\frac{\theta(1-\theta) + (x-\theta)(1-2\theta)}{\theta^2(1-\theta)^2} = -\frac{(x-\theta)^2}{\theta^2(1-\theta)^2}.$$

Clearly,

$$E_{\theta}\left(\frac{\partial \log f_{\theta}(x_i)}{\partial \theta}\right) = \frac{E_{\theta}(x_i - \theta)}{\theta(1 - \theta)} = \frac{P_{\theta}(x_i = 1) - \theta}{\theta(1 - \theta)} = 0.$$

Further note that, here,

$$\left(\frac{\partial \log f_{\theta}(x)}{\partial \theta}\right)^2 = -\frac{\partial^2 \log f_{\theta}(x)}{\partial \theta^2},$$

and so the same holds on taking expectations. This immediately verifies the information equality.

Note that

$$E_{\theta}(x_i^2) = E_{\theta}(x_i)$$

when  $x_i \in \{0, 1\}$ .

So,

$$\operatorname{var}_{\theta}(x_i) = E_{\theta}((x_i - \theta)^2) = E_{\theta}(x_i^2 - 2x_i\theta + \theta^2) = \theta(1 - \theta)$$

The information thus is

$$I_{\theta} = \frac{\operatorname{var}_{\theta}(x_i)}{\theta^2 (1-\theta)^2} = \frac{1}{\theta(1-\theta)}.$$

The efficiency bound for  $\theta$  is

$$\frac{\theta(1-\theta)}{n}.$$

Note that this is a concave function in  $\theta$  (and so is maximized at  $\theta = 1/2$ ).

The sample-mean theorem immediately implies that  $\overline{x}_n$  is the best unbiased estimator of  $\theta$ .

## Sample-mean theorem

#### Theorem 5 (Sample-mean theorem)

Let  $\overline{x}_n$  be the mean of a random sample  $x_1, \ldots, x_n$  from a distribution with finite mean and variance  $\mu, \sigma^2$ . Then

$$E(\overline{x}_n) = \mu, \qquad \operatorname{var}(\overline{x}_n) = \sigma^2/n,$$

no matter the distribution of the  $x_i$ .

#### Proof.

By linearity of the expectations operator in the first step and by random sampling in the second step,

$$E(\overline{x}_n) = E\left(\frac{1}{n}\sum_{i=1}^n x_i\right) = \frac{1}{n}\sum_{i=1}^n E(x_i) = \mu.$$

Next,

$$\operatorname{var}(\overline{x}_n) = \operatorname{var}\left(\frac{1}{n}\sum_{i=1}^n x_i\right) = \frac{\operatorname{var}(\sum_{i=1}^n x_i)}{n^2} = \frac{\sum_{i=1}^n \operatorname{var}(x_i)}{n^2} = \frac{\sigma^2}{n}$$

again by random sampling.

#### Poisson

Here we have

$$\log f_{\theta}(x) = x \log(\theta) - \theta + \text{constant.}$$

So,

$$\frac{\partial \log f_{\theta}(x)}{\partial \theta} = \frac{x}{\theta} - 1, \qquad \frac{\partial^2 \log f_{\theta}(x)}{\partial \theta^2} = -\frac{x}{\theta^2}.$$

We note the mean/variance equality of a Poisson distribution:

$$\begin{split} E_{\theta}(x_i) &= \sum_{x=0}^{\infty} x \, \frac{e^{-\theta} \theta^x}{x!} = \sum_{x=1}^{\infty} \frac{e^{-\theta} \theta^x}{(x-1)!} = \sum_{x=0}^{\infty} \frac{e^{-\theta} \theta^{x+1}}{x!} = \theta \sum_{x=0}^{\infty} \frac{e^{-\theta} \theta^x}{x!} = \theta \\ \text{(because } \sum_{x=0}^{\infty} \frac{e^{-\theta} \theta^x}{x!} = \sum_{x=0}^{\infty} f_{\theta}(x) = 1\text{), and similarly,} \\ E_{\theta}(x_i^2) &= \sum_{x=0}^{\infty} x^2 \, \frac{e^{-\theta} \theta^x}{x!} = \theta \sum_{x=0}^{\infty} (x+1) \, \frac{e^{-\theta} \theta^x}{x!} = \theta^2 + \theta, \\ \text{so that } \operatorname{var}_{\theta}(x_i) &= E_{\theta}(x_i^2) - E_{\theta}(x_i)^2 = \theta. \\ \text{Then } I_{\theta} = 1/\theta \text{ and} \\ \theta/n \end{split}$$

is the efficiency bound.

It is again immediate (by the sample-mean theorem) that  $\overline{x}_n$  will be best unbiased.
# Normal distribution

Here,

$$\log f_{\theta}(x) = -\frac{1}{2} \left( \log \sigma^2 + \frac{(x-\mu)^2}{\sigma^2} \right) + \text{constant.}$$

So,

$$\frac{\partial \log f_{\theta}(x)}{\partial \mu} = \frac{(x-\mu)}{\sigma^2},$$
$$\frac{\partial \log f_{\theta}(x)}{\partial \sigma^2} = -\frac{1}{2} \left(\frac{1}{\sigma^2} - \frac{(x-\mu)^2}{\sigma^4}\right),$$

and

$$\frac{\partial^2 \log f_\theta(x)}{\partial \theta \partial \theta'} = - \begin{pmatrix} \frac{1}{\sigma^2} & \frac{(x-\mu)}{\sigma^4} \\ \frac{(x-\mu)}{\sigma^4} & -\frac{1}{2\sigma^4} + \frac{(x-\mu)^2}{\sigma^6} \end{pmatrix}.$$

The information now is the (diagonal) matrix

$$I_{\theta} = -E_{\theta} \left( \frac{\partial^2 \log f_{\theta}(x_i)}{\partial \theta \partial \theta'} \right) = \begin{pmatrix} \frac{1}{\sigma^2} & 0\\ 0 & \frac{1}{2\sigma^4} \end{pmatrix},$$

so that the efficiency bounds for  $\mu$  and  $\sigma^2$  are  $\sigma^2/n$  and  $2\sigma^4/n$ , respectively.

The sample mean is again best unbiased for  $\mu$ .

An unbiased estimator of  $\sigma^2$  is

$$\frac{1}{n-1}\sum_{i=1}^n (x_i - \overline{x}_n)^2.$$

However, it does not hit the efficiency bound (see below).

In fact, as

$$\sum_{i=1}^{n} \frac{\partial \log f_{\theta}(x)}{\partial \sigma^{2}} = -\frac{1}{2} \left( \frac{n}{\sigma^{2}} - \frac{\sum_{i=1}^{n} (x_{i} - \mu)^{2}}{\sigma^{4}} \right) = \frac{n}{2\sigma^{4}} \left( \sum_{i=1}^{n} \frac{(x_{i} - \mu)^{2}}{n} - \sigma^{2} \right)$$

depends on  $\mu$  we cannot have proportionality of the sampling error of any estimator when  $\mu$  is unknown; the best unbiased estimator is  $n^{-1} \sum_{i} (x_i - \mu)^2$ , which is infeasible.

It follows that the efficiency bound is not attainable for  $\sigma^2$ . Moreover, a best unbiased estimator of  $\sigma^2$  does not exist.

First start with the obvious estimator of  $\sigma^2$  that is

$$\hat{\sigma}_n^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \overline{x}_n)^2.$$

This estimator is biased:

$$E\left(n^{-1}\sum_{i=1}^{n}(x_{i}-\overline{x}_{n})^{2}\right) = E((x_{i}-\overline{x}_{n})^{2})$$

$$= E(((x_{i}-\mu)-(\overline{x}_{n}-\mu))^{2})$$

$$= E((x_{i}-\mu)^{2}) - 2E((x_{i}-\mu)(\overline{x}_{n}-\mu)) + E((\overline{x}_{n}-\mu)^{2})$$

$$= \operatorname{var}_{\theta}(x_{i}) - 2\operatorname{cov}_{\theta}(x_{i},\overline{x}_{n}) + \operatorname{var}_{\theta}(\overline{x}_{n})$$

$$= \sigma^{2} - 2\sigma^{2}/n + \sigma^{2}/n$$

$$= \frac{n-1}{n}\sigma^{2}.$$

The bias arises from estimating the population mean by the sample mean.

The estimator  $\overline{x}_n$  has a variance,  $\sigma^2/n$ , and covaries with each datapoint  $x_i$ , with covariance  $\sigma^2/n$ .

An unbiased estimator is therefore

$$\tilde{\sigma}^2 = \frac{n}{n-1}\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^n (x_i - \overline{x}_n)^2;$$

the change in the numerator is called a degrees of freedom correction. We can show (see below) that

$$(n-1)\frac{\tilde{\sigma}^2}{\sigma^2} = \frac{\sum_{i=1}^n (x_i - \overline{x}_n)^2}{\sigma^2} \sim \chi_{n-1}^2,$$

and we know the variance of a  $\chi^2_{n-1}$  is 2(n-1).

Hence,

$$\operatorname{var}(\tilde{\sigma}^2) = \left(\frac{\sigma^2}{n-1}\right)^2 \operatorname{var}\left((n-1)\frac{\tilde{\sigma}^2}{\sigma^2}\right) = \frac{2\sigma^4}{n-1}$$

which exceeds the efficiency bound  $2\sigma^4/n$ .

# Sampling distribution of normal variance

First,

$$(n-1)\frac{\tilde{\sigma}^2}{\sigma^2} = \frac{\sum_{i=1}^n (x_i - \overline{x}_n)^2}{\sigma^2}$$
$$= \sum_{i=1}^n \left(\frac{(x_i - \mu) - (\overline{x}_n - \mu)}{\sigma}\right)^2 = \sum_{i=1}^n \left(\frac{x_i - \mu}{\sigma}\right)^2 - \sum_{i=1}^n \left(\frac{\overline{x}_n - \mu}{\sigma}\right)^2$$
$$= \sum_{i=1}^n \left(\frac{x_i - \mu}{\sigma}\right)^2 - n\left(\frac{\overline{x}_n - \mu}{\sigma}\right)^2 = \sum_{i=1}^n \left(\frac{x_i - \mu}{\sigma}\right)^2 - \left(\frac{\overline{x}_n - \mu}{\sigma/\sqrt{n}}\right)^2.$$

The right-hand side terms are  $\chi_n^2$  and  $\chi_1^2$ , respectively. The characteristic function of a  $\chi_p^2$  is  $(1 - 2\iota t)^{-p/2}$ .

Second,  $\overline{x}_n$  and  $\tilde{\sigma}^2$  are independent by Basu's theorem.

Third, the characteristic function of the sum of independent variables is the product of their characteristic functions, so  $(n-1)\tilde{\sigma}^2/\sigma^2$  has characteristic function

$$(1 - 2\iota t)^{-n/2} (1 - 2\iota t)^{1/2} = (1 - 2\iota t)^{-(n-1)/2},$$

so it is  $\chi^2_{n-1}$ .

### Tobit

 $x_i^* \sim N(\mu, \sigma^2).$ 

The data are top-coded at c, i.e.,

$$x_i = \begin{cases} x_i^* & \text{if } x_i^* < c \\ c & \text{if } x_i^* \ge c \end{cases}$$

The density is

$$f_{\theta}(x) = \left(\frac{1}{\sigma}\phi\left(\frac{x-\mu}{\sigma}\right)\right)^{\{x$$

Let us focus on the mean parameter  $\mu$  here. So we assume that  $\sigma$  is known. Note that

$$\frac{\partial \log f_{\theta}(x)}{\partial \mu} = \{x < c\} \frac{(x-\mu)}{\sigma^2} + \{x = c\} \frac{\phi((c-\mu)/\sigma)/\sigma}{1 - \Phi((c-\mu)/\sigma)};$$

both coded and non-coded observations will contribute to the likelihood.

The probability of not being top-coded and being top coded are

$$\Phi\left(\frac{c-\mu}{\sigma}\right), \qquad 1-\Phi\left(\frac{c-\mu}{\sigma}\right),$$

respectively.

Further,

$$f_{\theta}(x \mid x < c) = \frac{1}{\sigma} \frac{\phi((x-\mu)/\sigma)}{\Phi((c-\mu)/\sigma)};$$

so that the deviation of the mean (from  $\mu$ ) of this truncated distribution is

$$\frac{\int_{-\infty}^{c} \frac{(x-\mu)}{\sigma} \phi\left(\frac{(x-\mu)}{\sigma}\right) dx}{\Phi\left(\frac{c-\mu}{\sigma}\right)} = \frac{-\sigma^2 \int_{-\infty}^{c} \frac{\partial(\phi((x-\mu)/\sigma)/\sigma)}{\partial x} dx}{\Phi\left(\frac{c-\mu}{\sigma}\right)} = -\sigma \frac{\phi(\frac{c-\mu}{\sigma})}{\Phi\left(\frac{c-\mu}{\sigma}\right)}.$$

Using these results it is immediate that

$$E_{\theta}\left(\frac{\partial \log f_{\theta}(x_i)}{\partial \mu}\right) = 0.$$

After some more calculus,  $\partial^2 \log f_{\theta}(x) / \partial^2 \mu$  is found to be

$$-\{x < c\} \frac{1}{\sigma^2} - \{x = c\} \frac{1}{\sigma^2} \frac{\phi((c-\mu)/\sigma)}{1 - \Phi(c-\mu)/\sigma} \left(\frac{\phi((c-\mu)/\sigma)}{1 - \Phi(c-\mu)/\sigma} - \frac{c-\mu}{\sigma}\right)$$

The information on  $\mu$  then becomes

$$\frac{1}{\sigma^2}\Phi\left(\frac{c-\mu}{\sigma}\right) + \frac{1}{\sigma^2}\phi\left(\frac{c-\mu}{\sigma}\right)\left(\frac{\phi((c-\mu)/\sigma)}{1-\Phi(c-\mu)/\sigma)} - \frac{c-\mu}{\sigma}\right).$$

The mean of the underlying random variable is  $\mu$ .

The mean of the coded data is c.

The mean of the non-coded data is

$$\mu - \sigma \frac{\phi((c-\mu)/\sigma)}{\Phi((c-\mu)/\sigma)}$$

The marginal mean is

$$\left(\mu - \sigma \frac{\phi((c-\mu)/\sigma)}{\Phi((c-\mu)/\sigma)}\right) \Phi\left(\frac{c-\mu}{\sigma}\right) + c \left(1 - \Phi\left(\frac{c-\mu}{\sigma}\right)\right).$$

# Probit

Again take  $x_i^* \sim N(\mu, \sigma^2)$ .

Now only observe

$$x_i = \begin{cases} 1 & \text{if } x_i^* \ge 0 \\ 0 & \text{if } x_i^* < 0 \end{cases},$$

which is Bernoulli.

The probability of success and failure are

$$\Phi(\mu/\sigma), \qquad 1 - \Phi(\mu/\sigma),$$

respectively.

These probabilities depend on  $\mu, \sigma$  only through the ratio  $\theta = \mu/\sigma$ , implying a scale indeterminacy; we can only learn  $\theta$ .

The mass function becomes

$$f_{\theta}(x) = \Phi(\theta)^{x} \times (1 - \Phi(\theta))^{1-x}$$

(Could further just focus on success probability  $p = \Phi(\theta)$  but this would not extend to the model with covariates.)

Then

$$\frac{\partial \log f_{\theta}(x)}{\partial \theta} = (x - \Phi(\theta)) \frac{\phi(\theta)}{\Phi(\theta)(1 - \Phi(\theta))},$$

which has mean zero and variance

$$rac{\phi( heta)^2}{\Phi( heta)(1-\Phi( heta))},$$

so the efficiency bound for  $\theta$  becomes

$$\frac{1}{n} \frac{\Phi(\theta)(1 - \Phi(\theta))}{\phi(\theta)^2}.$$

A sensible way to estimate  $\theta$  would be to first estimate the success probability  $p = \Phi(\theta)$  by the sample mean  $\overline{x}_n$  and then construct

$$\theta_n = \Phi^{-1}(\overline{x}_n).$$

This estimator is not unbiased (an unbiased estimator of  $\theta$  does not exist here) but it will hit the efficiency bound in large samples.

Derivation of best unbiased estimator above required regularity conditions:

- Differentiability of the density/mass function,
- Conditions for interchanging order of differentiation and integration.

An example where this fails is

 $x_i \sim (\text{continuous}) \text{ uniform}[0, \theta],$ 

that is,

$$f_{\theta}(x) = \frac{\{0 \le x \le \theta\}}{\theta}.$$

Nonetheless, a best unbiased estimator exists.

This follows from the Lehmann-Sheffé theorem, which builds on complete sufficient statistics.

<sup>▶</sup> Skip the remainder of this section

### Sufficiency

A statistic  $\gamma_n = \gamma(x_1, \ldots, x_n)$  is sufficient for  $\theta$  if

$$f_{\theta}(x_1,\ldots,x_n|\gamma_n)=f(x_1,\ldots,x_n|\gamma_n),$$

i.e., the conditional distribution does not depend on  $\theta$ .

An obvious example is the Bernoulli distribution, where  $P_{\theta}(x_i = 1) = \theta$ . Here,

$$f_{\theta}(x_1, \dots, x_n) = \theta^{\sum_{i=1}^n x_i} (1-\theta)^{n-\sum_{i=1}^n x_i}$$

so a sufficient statistic will be  $\sum_{i=1}^{n} x_i$ , the number of successes in the sample. Indeed,  $\sum_{i=1}^{n} x_i$  is binomial with

$$f_{\theta}\left(\sum_{i=1}^{n} x_{i}\right) = \binom{n}{\sum_{i=1}^{n} x_{i}} \theta^{\sum_{i=1}^{n} x_{i}} (1-\theta)^{n-\sum_{i=1}^{n} x_{i}},$$

and so

$$f_{\theta}(x_1, \dots, x_n | \sum_{i=1}^n x_i) = {n \choose \sum_{i=1}^n x_i} = \frac{n!}{(\sum_{i=1}^n x_i)!(n - \sum_{i=1}^n x_i)!}$$

is free of  $\theta$ .

# Sufficiency of the sample mean for a normal population

As another illustration, take  $x_i \sim N(\theta, \sigma^2)$  with  $\sigma^2$  known.

Then the sample mean  $\overline{x}_n$  is sufficient for the unknown population mean  $\theta$ . We have

$$f_{\theta}(x_1, \dots, x_n) = \prod_{i=1}^n \frac{1}{\sigma} \phi\left(\frac{x_i - \theta}{\sigma}\right)$$
  
=  $\frac{1}{(2\pi\sigma^2)^{n/2}} e^{\left(-\frac{1}{2}\frac{\sum_{i=1}^n (x_i - \theta)^2}{\sigma^2}\right)}$   
=  $\frac{1}{(2\pi\sigma^2)^{n/2}} e^{\left(-\frac{1}{2}\frac{\sum_{i=1}^n (x_i - \overline{x}_n)^2 + n(\overline{x}_n - \theta)^2}{\sigma^2}\right)}$   
=  $\frac{1}{(2\pi\sigma^2)^{(n-1)/2}} e^{\left(-\frac{1}{2}\frac{\sum_{i=1}^n (x_i - \overline{x}_n)^2}{\sigma^2}\right)} \frac{1}{(2\pi\sigma^2)^{1/2}} e^{\left(-\frac{1}{2}\frac{n(\overline{x}_n - \theta)^2}{\sigma^2}\right)}$ 

and

$$f_{\theta}(\overline{x}_n) = \frac{1}{\sigma/\sqrt{n}} \phi\left(\frac{\overline{x}_n - \theta}{\sigma/\sqrt{n}}\right) = \frac{n^{1/2}}{(2\pi\sigma^2)^{1/2}} e^{\left(-\frac{1}{2}\frac{n}{\sigma}\frac{(\overline{x}_n - \theta)^2}{\sigma^2}\right)}.$$

It follows that

$$f_{\theta}(x_1, \dots, x_n | \overline{x}_n) = \frac{f_{\theta}(x_1, \dots, x_n)}{f_{\theta}(\overline{x}_n)} = \frac{n^{-1/2}}{(2\pi\sigma^2)^{(n-1)/2}} e^{\left(-\frac{1}{2}\frac{\sum_{i=1}^n (x_i - \overline{x}_n)^2}{\sigma^2}\right)},$$

which does not depend on  $\theta$ .

When  $\sigma^2$  is unknown a sufficient statistic for both  $\mu$  and  $\sigma^2$  is the pair

$$\overline{x}_n, \qquad \frac{1}{n-1} \sum_{i=1}^n (x_i - \overline{x}_n)^2,$$

i.e., the sample mean and sample variance.

# Improved estimation based on sufficiency

### Theorem 6 (Rao-Blackwell theorem)

Let  $\theta_*$  satisfy  $E_{\theta}(\theta_*) = \theta$  and let  $\gamma_n$  be sufficient for  $\theta$ . Define the estimator

 $\theta_n = E(\theta_*|\gamma_n)$ 

(which is a function of the data through  $\gamma_n$  only). Then  $\theta_n$  is unbiased and

 $\operatorname{var}_{\theta}(\theta_n) \leq \operatorname{var}_{\theta}(\theta_*)$ 

holds.

#### **Proof.**

Unbiasedness of  $\theta_n$  follows from iterating expectations on  $\theta_*$ .

Next, by the law of total variance,

 $\operatorname{var}_{\theta}(\theta_*) = \operatorname{var}(E(\theta_*|\gamma_n)) + E_{\theta}(\operatorname{var}(\theta_*|\gamma_n)) = \operatorname{var}_{\theta}(\theta_n) + \text{non-negative term},$ 

and so  $\operatorname{var}_{\theta}(\theta_*) \geq \operatorname{var}_{\theta}(\theta_n)$ .

Finally,  $\theta_n$  is a statistic (and so computable from data) by sufficiency.

### **Rao-Blackwellization for Bernoulli**

A simple unbiased estimator of  $\theta$  is  $\theta_* = x_1$ ; its variance is  $\theta(1 - \theta)$ . Define

$$\theta_n = E\left(x_1 \left| \sum_{i=1}^n x_i \right. \right) = P_{\theta}(x_1 = 1 | \sum_{i=1}^n x_i).$$

Note that

$$P_{\theta}(x_{1} = 1 | \sum_{i=1}^{n} x_{i} = x) = \frac{P_{\theta}(\sum_{i=1}^{n} x_{i} = x | x_{1} = 1) P_{\theta}(x_{1} = 1)}{P_{\theta}(\sum_{i=1}^{n} x_{i} = x)}$$
$$= \frac{P_{\theta}(\sum_{j \neq i}^{n} x_{j} = (x - 1) | x_{1} = 1) P_{\theta}(x_{1} = 1)}{P_{\theta}(\sum_{i=1}^{n} x_{i} = x)}$$
$$= \frac{P_{\theta}(\sum_{j \neq i}^{n} x_{j} = (x - 1))}{P_{\theta}(\sum_{i=1}^{n} x_{i} = x)} P_{\theta}(x_{1} = 1)$$
$$= \frac{\binom{n-1}{x-1} \theta^{x-1} (1 - \theta)^{n-x}}{\binom{n}{x} \theta^{s} (1 - \theta)^{n-x}} \theta = \frac{\frac{(n-1)!}{(n-x)!x!}}{\frac{n!}{(n-x)!x!}}$$
$$= \frac{(n-1)!}{n!} \frac{x!}{(x-1)!} = \frac{x}{n}.$$

Thus,  $\theta_n = n^{-1} \sum_{i=1}^n x_i = \overline{x}_n$ , which has variance  $\theta(1-\theta)/n$  (and is, in fact, best unbiased).

A statistic  $\gamma_n$  is complete (for  $f_{\theta}$ ) if it holds that

if 
$$E_{\theta}(\varphi(\gamma_n)) = 0$$
 for all  $\theta$ , then  $P_{\theta}(\varphi(\gamma_n) = 0) = 1$  for all  $\theta$ ,

for all  $\varphi$  for which the expectation exists.

To clarify take  $x_i \sim N(\theta, \sigma^2)$ . Consider the statistic  $x_2 - x_1$ . We have

$$E_{\theta}(x_2 - x_1) = \theta - \theta = 0,$$
 for all  $\theta$ .

However,  $x_2 - x_1 \sim N(0, 2\sigma^2)$ , and so

$$P_{\theta}(x_2 - x_1 = 0) = 0 \quad \text{for all } \theta.$$

So, this statistic is not complete.

### Completeness in the normal problem

A complete statistic here is  $\overline{x}_n = n^{-1} \sum_{i=1}^n x_i$ .

We look for a function  $\varphi$  such that  $E_{\theta}(\varphi(\overline{x}_n)) = 0$  for all  $\theta$ .

We have

$$\begin{split} E_{\theta}(\varphi(\overline{x}_{n})) &= \int_{-\infty}^{+\infty} \varphi(x) \, \frac{1}{\sigma/\sqrt{n}} \phi\left(\frac{\overline{x}_{n}-\theta}{\sigma/\sqrt{n}}\right) \, dx \\ &= \frac{1}{\sqrt{2\pi\sigma^{2}/n}} e^{-\frac{n}{2}(\theta/\sigma)^{2}} \int_{-\infty}^{+\infty} \varphi(x) \, e^{-\frac{n}{2}(x/\sigma)^{2}} \, e^{n(\theta/\sigma^{2})x} \, dx \\ &= \frac{1}{\sqrt{2\pi\sigma^{2}/n}} e^{-\frac{n}{2}(\theta/\sigma)^{2}} \mathcal{L}\left(\varphi(x) \, e^{-\frac{n}{2}(x/\sigma)^{2}}\right), \end{split}$$

for  $\mathcal{L}(g(x))$  the (two-sided) Laplace transform of g(x).

The Laplace transform  $\mathcal{L}(g(x))$  cannot be zero unless g(x) is zero (almost everywhere). As the exponential function is non-zero it must be that  $\varphi(x) = 0$  (almost everywhere), as claimed.

### Completeness in the Bernoulli problem

Remember that, if  $P_{\theta}(x_i = 1) = \theta$  for  $\theta \in (0, 1)$ , then  $\gamma_n = \sum_{i=1}^n x_i$  is Binomial with parameters  $(n, \theta)$ .

So, if

$$E_{\theta}(\varphi(\gamma_n)) = \sum_{\gamma=0}^n \gamma \binom{n}{\gamma} \theta^{\gamma} (1-\theta)^{n-\gamma} = (1-\theta)^n \sum_{\gamma=0}^n \varphi(\gamma) \binom{n}{\gamma} \left(\frac{\theta}{1-\theta}\right)^{\gamma} = 0$$

for all  $\theta \in (0,1)$  then the following polynomial in  $\lambda = \theta/(1-\theta)$ 

$$\sum_{\gamma=0}^{n} c_{\gamma} \, \lambda^{\gamma} = 0, \qquad c_{\gamma} = \varphi(\gamma) rac{n!}{\gamma(n-\gamma)!},$$

must be zero for all  $\theta \in (0, 1)$ .

But the latter can only hold if  $c_{\gamma} = 0$  for all  $\gamma$ , and so  $\varphi(\gamma) = 0$  must hold for all  $\gamma \in \{0, 1, \ldots, n\}$ .

Hence,

$$P_{\theta}(\varphi(\gamma_n)=0)=1$$

follows.

### Theorem 7 (Lehmann-Scheffé theorem)

Let  $\gamma_n$  be a complete sufficient statistic for  $\theta$  and consider  $\theta_n = \varphi(\gamma_n)$  for some function  $\varphi$ . If  $E_{\theta}(\theta_n) = \theta$  then

 $\operatorname{var}_{\theta}(\theta_n) \leq \operatorname{var}(\theta_*)$ 

where  $\theta_*$  is any unbiased estimator; i.e.,  $\theta_n$  is the best unbiased estimator.

#### Proof.

By the Rao-Blackwell result, under sufficiency, any efficient estimator must be a function of  $\gamma_n$  only; so,  $\theta_n = \varphi(\gamma_n)$ . Then, by assumption,  $E_{\theta}(\theta_n) = \theta$ .

It is enough to show that  $\varphi$  is unique. Suppose there exist another  $\psi$  such that  $E_{\theta}(\psi(\gamma_n)) = \theta$ . Then, by unbiasedness of both estimators,

$$E_{\theta}(\varphi(\gamma_n) - \psi(\gamma_n)) = 0.$$

But, by completeness, this implies that  $P_{\theta}(\varphi(\gamma_n) = \psi(\gamma_n)) = 1$  (a.e.).

We have shown above that

$$\gamma_n = \sum_{i=1}^n x_i$$

is both a complete and sufficient statistic for  $\theta$ .

An unbiased estimator based on it is the sample mean

$$\overline{x}_n = n^{-1} \sum_{i=1}^n x_i = \gamma_n / n.$$

This confirms the Cramér-Rao result for Bernoulli that  $\overline{x}_n$  is best unbiased.

# Estimating the maximum of a uniform distribution

Recall

$$f_{\theta}(x) = \frac{\{0 \le x \le \theta\}}{\theta}$$

Easy to see that the maximum-likelihood estimator here is  $\max_i(x_i)$ . This estimator is biased.

For all  $x \in [0, \theta]$ ,

$$P_{\theta}\left(\max_{i}(x_{i}) \leq x\right) = P_{\theta}(x_{1} \leq x, x_{2} \leq x, \dots, x_{n} \leq x) = (x/\theta)^{n}.$$

Further,

$$E_{\theta}(\max_{i}(x_{i})) = \int_{0}^{\theta} 1 - (x/\theta)^{n} dx = \frac{n}{n+1}\theta.$$

(The first step holds for any non-negative random variable  $z \in [0, b]$ , say; integrate by parts to see that

$$\int_{0}^{b} (1 - F(z)) \, dz = (1 - F(z)) \, z \big|_{0}^{b} + \int_{0}^{b} z \, f(z) \, dz = E(z),$$

as claimed.)

It follows that

$$\theta_n = \frac{n+1}{n} \max_i (x_i).$$

is unbiased.

Remains to show that  $\gamma_n = \max_i(x_i)$  is a complete sufficient statistic for  $\theta$ . We already know that  $P_{\theta}(\gamma_n \leq \gamma) = (\gamma/\theta)^n$  and so its density is

$$n \, \frac{\gamma^{n-1}}{\theta^n}$$

for  $\gamma \in [0, \theta]$  (and zero elsewhere).

Hence,

$$E_{\theta}(\varphi(\gamma_n)) = \int_0^{\theta} \varphi(\gamma) \, n \, \frac{\gamma^{n-1}}{\theta^n} \, d\gamma = (n/\theta^n) \, \left( \int_0^{\theta} \varphi(\gamma) \gamma^{n-1} \, d\gamma \right) =: (n/\theta^n) \, Q(\theta).$$

Note that, by Leibniz' rule,

$$\frac{\partial Q(\theta)}{\partial \theta} = \varphi(\theta) \, \theta^{n-1}.$$

So, if  $E_{\theta}(\varphi(\gamma_n)) = 0$  for all  $\theta$  then  $Q(\theta) = 0$  must hold for all  $\theta$ , but then its derivative must be zero and so  $\varphi(\theta) = 0$  must hold. So,  $\gamma_n$  is indeed complete.

To see sufficiency we look at the ratio of the density of the data,

$$\prod_{i=1}^{n} \frac{\{x_i \le \theta\}}{\theta} = \frac{\{\gamma_n \le \theta\}}{\theta^n},$$

and the density of the sample maximum,

$$n\gamma_n^{n-1} \, \frac{\{\gamma_n \le \theta\}}{\theta^n}$$

(from above).

As this ratio is

 $\gamma_n^{1-n}/n$ 

it is free from  $\theta$  and so  $\gamma_n$  is indeed sufficient.

Working out the first two moments of  $\gamma_n$  using its density from above gives

$$\frac{1}{n(n+2)}\theta^2$$

as the variance of the unbiased estimator  $\theta_n$ .

Note that this variance shrinks like  $n^{-2}$ , which is faster than the parametric rate of  $n^{-1}$ .

In many cases an (best) unbiased estimator will not exist. So we need to widen our search to allow for bias.

First generalize Cramér-Rao bound to case where  $\theta_n$  is biased, i.e.,

$$E_{\theta}(\theta_n) = \theta + b_n(\theta).$$

Following the same steps as before gives the efficiency bound

$$\operatorname{var}_{\theta}(\theta_n) \ge I_{\theta}^{-1} (1 + b'_n(\theta))^2 / n.$$

Quite generally,  $b'_n(\theta) = O(n^{-1})$ , and so

$$\operatorname{var}_{\theta}(\theta_n) \ge I_{\theta}^{-1}/n + O(n^{-2});$$

the bias vanishes faster than the standard deviation.

From an asymptotic perspective, this paves the way for best asymptotically unbiased estimators.

# Asymptotics (for the univariate sample mean)

Asymptotic analysis is an approximation to the finite-sample behavior of an estimator based on what happens when n becomes large.

While exact small-sample results are few and ad hoc. Large-sample analysis is well established and widely applicable.

The behavior of the sample mean as  $n \to \infty$  brings us a long way.

This is so because almost all estimators you will ever look at behave, as  $n \to \infty$ , like a sample mean.

Such estimators are called asymptotically linear; we can always represent them as

$$(\theta_n - \theta) = n^{-1} \sum_i \varphi_\theta(x_i) + o_p(n^{-1/2})$$

for some function  $\varphi_{\theta}$  for which  $E_{\theta}(\varphi_{\theta}(x_i)) = 0$  and  $\operatorname{var}_{\theta}(\varphi_{\theta}(x_i)) < \infty$ . We will see many examples.

Slide 25 gives the influence function for the best unbiased estimator (when it exists).

# Orders of magnitude (deterministic sequences)

Let h and g be two functions (and h(x) > 0 for large x).

We say that g(x) = O(h(x)) if and only if there exists a positive number b and a real number <u>x</u> such that

$$|g(x)| \le b h(x)$$
 for all  $x \ge \underline{x}$ .

That is,

$$\lim \sup_{x \to \infty} \left| \frac{g(x)}{h(x)} \right| < \infty;$$

h(x) grows at least as fast as g(x).

We say that g(x) = o(h(x)) if and only if for every positive number b there exists a real number  $\underline{x}$  such that

$$|g(x)| \le b h(x)$$
 for all  $x \ge \underline{x}$ .

That is,

$$\lim_{x \to \infty} \left| \frac{g(x)}{h(x)} \right| = 0;$$

h(x) grows faster than g(x).

# Orders of magnitude (random sequences)

Let  $\{x_n\}$  be a sequence of random variables and let  $\{a_n\}$  be a deterministic sequence of numbers.

Consider the limit behavior as  $n \to \infty$ .

We say that  $x_n = O_p(a_n)$  if and only if for every  $\delta$  there exists a finite number  $\epsilon$  and an <u>n</u> such that

$$P\left(\left|\frac{x_n}{a_n}\right| > \epsilon\right) < \delta \text{ for all } n \ge \underline{n}.$$

That is,  $|x_n/a_n|$  is stochastically bounded.

We say that  $x_n = o_p(a_n)$  if and only if for every  $\delta$  and finite number  $\epsilon$  there exists an <u>n</u> such that

$$P\left(\left|\frac{x_n}{a_n}\right| > \epsilon\right) < \delta \text{ for all } n \ge \underline{n}.$$

That is,

$$\lim_{n \to \infty} P\left( \left| \frac{x_n}{a_n} \right| > \epsilon \right) = 0$$

for every  $\epsilon > 0$ .

We say that  $x_n$  converges in probability to x if, for every  $\epsilon > 0$ ,

$$\lim_{n \to \infty} P\left(|x_n - x| > \epsilon\right) = 0,$$

i.e., if  $x_n - x = o_p(1)$ .

We write  $x_n \xrightarrow{p} x$  and call x the probability limit of the sequence  $\{x_n\}$ .

#### Theorem 8 ((weak) law of large numbers)

Suppose that  $\mu = E(x_i)$  exists. For any  $\epsilon > 0$  and  $\delta > 0$ , there exists an  $\underline{n}$  such that

$$P(|\overline{x}_n - \mu| > \epsilon) < \delta, \quad for \ all \quad n > \underline{n}.$$

That is,  $\overline{x}_n \xrightarrow{p} \mu$  as  $n \to \infty$ . Equivalently,  $\overline{x}_n - \mu = o_p(1)$ .

#### Proof.

Suppose that  $\sigma^2$  exists. Then (by Chebychev's inequality)

$$P(|\overline{x}_n - \mu| > \epsilon) = P((\overline{x}_n - \mu)^2 > \epsilon^2) \le \frac{E((\overline{x}_n - \mu)^2)}{\epsilon^2} = n^{-1} \frac{\sigma^2}{\epsilon^2}.$$

Taking limits gives the result.

Note that we immediately get the same result for any transformation  $\varphi(x_i)$  provided that  $E(|\varphi(x_i)|) < \infty$ . That is,

$$n^{-1}\sum_i \varphi(x_i) \xrightarrow{p} E(\varphi(x_i))$$

as  $n \to \infty$ .

normal (a2 exists) Student (µ exists but o<sup>2</sup> does not) Cauchy (µ does not exist) 0.4 ዞ 0.8 0.3 0.6 0.2 0.4 0.1 0.2 o deciles -0.2 -0.2 -0.4 -0.3 -0.6 -0.4 -0.8 -0.5 L 500 2500 500 2500 1000 1500 2000 0 1000 1500 2000 500 1000 1500 2000 2500 n n n

The below plots give deciles of  $\overline{x}_n$  as a function of n.

An estimator  $\theta_n$  is consistent for an estimand  $\theta$  if  $\theta_n \xrightarrow{p} \theta$ .

The mean squared error of is

$$E_{\theta}((\theta_n - \theta)^2) = (E_{\theta}(\theta_n - \theta))^2 + \operatorname{var}_{\theta}(\theta_n) = b_n(\theta)^2 + \operatorname{var}_{\theta}(\theta_n);$$

so a sufficient condition for consistency is that both bias and variance vanish as  $n \to \infty$ .

# Uniform convergence

A more general situation has  $\varphi_{\theta}(x_i)$  indexed by  $\theta \in \Theta$  (continuous on  $\Theta$  compact).

A pointwise convergence result (i.e., for any fixed  $\theta \in \Theta$ ) follows from above:

$$P\left(\left|n^{-1}\sum_{i}\varphi_{\theta}(x_{i})-E(\varphi_{\theta}(x_{i}))\right|>\epsilon\right)<\delta, \quad \text{for all} \quad n>\underline{n}_{\theta},$$

A uniform result is as follows.

Theorem 9 (Uniform law of large numbers) Suppose that  $\varphi_{\theta}(x) \leq \gamma(x)$  and  $E(|\gamma(x_i)|) < \infty$ . Then, for all  $\theta \in \Theta$ ,  $P\left(\left|n^{-1}\sum_{i}\varphi_{\theta}(x_i) - E(\varphi_{\theta}(x_i))\right| > \epsilon\right) < \delta$ , for all  $n > \underline{n}$ ,

with  $\underline{n}$  independent of  $\theta$ .

We write

$$\sup_{\theta \in \Theta} \left| n^{-1} \sum_{i} \varphi_{\theta}(x_{i}) - E(\varphi_{\theta}(x_{i})) \right| \stackrel{p}{\to} 0$$

as  $n \to \infty$ .

To appreciate the difference between pointwise and uniform convergence take a simple non-stochastic example:

$$\varphi_{\theta}(x_i) = n\theta e^{-n\theta}$$

for  $\theta \in \Theta = [0, 1]$ . This function is continuous in  $\theta$ .

For any fixed  $\theta$ ,

$$n\theta e^{-n\theta} \to 0$$

as  $n \to \infty$ . (because the exponential term vanishes more quickly than the linear term grows.)

However, at  $\theta = n^{-1}$  the function equals  $e^{-1}$  for any *n*. Hence,

$$\sup_{\theta \in \Theta} |n\theta e^{-n\theta}| \nrightarrow 0$$

as  $n \to \infty$ .

Note that (in general), uniform convergence implies pointwise convergence.

### Theorem 10 (Continuous-mapping theorem)

Suppose that  $x_n \xrightarrow{p} x$ .

Then

$$\varphi(x_n) \xrightarrow{p} \varphi(x)$$

for (non-stochastic) continuous functions  $\varphi$ .

Let  $\{x_n\}$  be a sequence of random variables with distribution  $\{F_n\}$  and let  $x \sim F$ 

We say that  $x_n \xrightarrow{d} x$  if

$$F_n(a) \to F(a) \text{ as } n \to \infty$$

at all continuity points a of F.

We call F the limit distribution of  $\{x_n\}$ .

If  $x_n \stackrel{d}{\to} x$  it is stochastically bounded, i.e.,  $x_n = O_p(1)$ .
### Theorem 11 (Lindeberg-Lévy central limit theorem)

Suppose that  $x_i \sim \text{i.i.d.} (\mu, \sigma^2)$ . Then

$$\frac{\overline{x}_n - \mu}{\sigma/\sqrt{n}} \stackrel{d}{\to} N(0, 1)$$

as  $n \to \infty$ .

This means that the sample distribution of the standardized sample mean approaches the standard-normal distribution.

In practice, this means that

$$\overline{x}_n \stackrel{a}{\sim} N(\mu, \sigma^2/n),$$

where the a can be interpreted as either 'asymptotically' or 'approximately'.

Observe that this result holds for any distribution, as long as  $\mu, \sigma^2$  exist.

The plots below concern the standardized sample mean of samples of Bernoulli random variables.

Observe how the histogram approaches the standard-normal density as  $\boldsymbol{n}$  grows.



#### Proof.

Let  $\varphi_x(t) = E(e^{\iota tx})$  be the characteristic function of x.

Then

$$z = \frac{\overline{x}_n - \mu}{\sigma/\sqrt{n}} = \sum_{i=1}^n \frac{1}{\sqrt{n}} \frac{x_i - \mu}{\sigma} = \sum_{i=1}^n \frac{z_i}{\sqrt{n}} \text{ (say)},$$

has characteristic function

$$\varphi_z(t) = E(e^{\iota t \sum_i z_i/\sqrt{n}}) = \prod_i E(e^{\iota(t/\sqrt{n})z_i}) = \varphi_{z_i}(t/\sqrt{n})^n,$$

where we used random sampling.

Now, as  $\varphi_{z_i}(0) = 1$ ,  $\varphi_{z_i}'(0) = 0$ , and  $\varphi_{z_i}''(0) = -1$  we have

$$\varphi_{z_i}(t/\sqrt{n}) = \varphi_{z_i}(0) + \varphi'_{z_i}(0) \frac{t}{\sqrt{n}} + \varphi''_{z_i}(0) \frac{t^2}{2n} + o\left(\frac{t^2}{n}\right) = 1 - \frac{t^2}{2n} + o\left(\frac{t^2}{n}\right)$$

as  $n \to \infty$ , and so

$$\lim_{n \to \infty} \varphi_z(t) = \lim_{n \to \infty} \left( 1 + \frac{-t^2/2}{n} \right)^n = e^{-t^2/2} (= \varphi \text{ of the standard normal})$$

by definition of the exponential function.

### Theorem 12 (Slutzky's theorem)

Suppose that  $x_n \xrightarrow{p} c$  (a constant) and  $y_n \xrightarrow{d} y$  (a random variable). Then (i)  $x_n + y_n \xrightarrow{d} c + y$ ; and (ii)  $x_n y_n \xrightarrow{d} c y$ . Take  $x_i \sim N(\mu, \sigma^2)$ . Best 'estimator' of  $\sigma^2$  is  $n^{-1} \sum_i (x_i - \mu)^2$ .

As an example of (i),

$$\hat{\sigma}^2 = n^{-1} \sum_i (x_i - \overline{x}_n)^2 = n^{-1} \sum_i (x_i - \mu)^2 - (\overline{x}_n - \mu)^2.$$

As  $(\overline{x}_n - \mu) \xrightarrow{p} 0$  and  $(a - \mu)^2$  is continuous in a we have  $(\overline{x}_n - \mu)^2 \xrightarrow{p} 0$ . Hence,

$$\hat{\sigma}^2 = n^{-1} \sum_i (x_i - \mu)^2 + o_p(1).$$

In fact,

$$(\overline{x}_n - \mu)^2 = (O_p(1/\sqrt{n}))^2 = O_p(1/n) = o_p(1/\sqrt{n}),$$

and so

$$\sqrt{n}(\hat{\sigma}^2 - \sigma^2) = \frac{1}{\sqrt{n}} \sum_i ((x_i - \mu)^2 - \sigma^2) + o_p(1).$$

Hence,  $\hat{\sigma}^2$  and  $n^{-1} \sum_i (x_i - \mu)^2$  are asymptotically equivalent; their limit distribution is  $\sqrt{n}(\hat{\sigma}^2 - \sigma^2) \xrightarrow{d} N(0, 2\sigma^4)$ . This is the same limit distribution as that of (the unbiased)  $\tilde{\sigma}^2$ .

As an example of (ii),

$$\frac{\overline{x}_n - \mu}{\hat{\sigma}/\sqrt{n}} = \frac{\sigma}{\hat{\sigma}} \frac{\overline{x}_n - \mu}{\sigma/\sqrt{n}} = (1 + o_p(1)) \frac{\overline{x}_n - \mu}{\sigma/\sqrt{n}} = \frac{\overline{x}_n - \mu}{\sigma/\sqrt{n}} + o_p(1) \stackrel{d}{\to} N(0, 1).$$

Now given an asymptotically-linear estimator,

$$(\theta_n - \theta) = n^{-1} \sum_i \varphi_\theta(x_i) + o_p(n^{-1/2})$$

where  $E_{\theta}(\varphi_{\theta}(x_i)) = 0$  and  $\operatorname{var}_{\theta}(\varphi_{\theta}(x_i)) < \infty$  our results immediately yield that

(a)  $\theta_n - \theta = O_p(n^{-1/2})$ ; and (b)  $\sqrt{n}(\theta_n - \theta) \stackrel{a}{\sim} N(0, \operatorname{var}_{\theta}(\varphi_{\theta}(x_i))).$ 

We call  $\operatorname{var}_{\theta}(\varphi_{\theta}(x_i))$  the asymptotic variance.

## Mean-value theorem

Let  $\varphi$  be a differentiable function on an interval  $[\underline{x}, \overline{x}_n]$ . Then, for any  $(x_1, x_2) \in [\underline{x}, \overline{x}_n]^2$  there always exists a  $x_* \in [\underline{x}, \overline{x}_n]$  (not necessarily unique) so that

$$\varphi(x_2) - \varphi(x_1) = \frac{\partial \varphi(x_*)}{\partial x} (x_2 - x_1).$$



# Asymptotics for smooth transformations

### Theorem 13 (Delta method)

If  $\sqrt{n}(\theta_n - \theta) \stackrel{d}{\rightarrow} N(0, \sigma^2)$ , then

$$\sqrt{n}(\varphi(\theta_n) - \varphi(\theta)) \stackrel{d}{\to} N\left(0, \left(\partial\varphi(\theta)/\partial\theta\right)^2 \sigma^2\right)$$

for continuously-differentiable  $\varphi$ .

#### Proof.

A mean-value expansion gives

$$\varphi(\theta_n) - \varphi(\theta) = \frac{\partial \varphi(\theta_*)}{\partial \theta} (\theta_n - \theta).$$

The continuous-mapping theorem yields

$$\frac{\partial \varphi(\theta_*)}{\partial \theta} \xrightarrow{p} \frac{\partial \varphi(\theta)}{\partial \theta}.$$

Slutzky's theorem gives

$$\sqrt{n}(\varphi(\theta_n) - \varphi(\theta)) = \frac{\partial \varphi(\theta)}{\partial \theta} \sqrt{n} \left(\theta_n - \theta\right) + o_p(1) \stackrel{d}{\to} N\left(0, \left(\frac{\partial \varphi(\theta)}{\partial \theta}\right)^2 \sigma^2\right).$$

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Now suppose that  $x_i$  is a vector with mean  $\mu$  and variance  $\Sigma$ .

The multivariate central limit theorem reads

$$\sqrt{n} \Sigma^{-1/2} (\overline{x}_n - \mu) \stackrel{d}{\to} N(0, I),$$

where I is the identity matrix of conformable dimension. Here, the limit distribution is a multivariate standard normal.

The Delta method extends as follows. Suppose  $\sqrt{n}(\theta_n - \theta) \xrightarrow{d} N(0, \Sigma)$ . Then

$$\sqrt{n}(\varphi(\theta_n) - \varphi(\theta)) \stackrel{d}{\to} N(0, \Gamma \Sigma \Gamma')$$

for

$$\Gamma = \frac{\partial \varphi(\theta)}{\partial \theta'}$$

the Jacobian matrix.

A nonsingular matrix A has eigendecomposition

$$A = VDV^{-1}$$

where D is a diagonal matrix of eigenvalues and V is the matrix of associated eigenvectors.

The inverse is

$$A^{-1} = V D^{-1} V^{-1}.$$

A matrix square root is

$$A^{1/2} = V D^{1/2} V^{-1}.$$

Note that

$$A^{-1/2}AA^{-1/2} = (VD^{-1/2}V^{-1})(VDV^{-1})(VD^{-1/2}V^{-1}) = I.$$

So, for example, if  $\sqrt{n}(\theta_n - \theta) \xrightarrow{d} N(0, \Sigma)$  for an  $m \times m$  nonsingular variance  $\Sigma$ , then

(i) 
$$\sqrt{n} \Sigma^{-1/2}(\theta_n - \theta) \stackrel{d}{\to} N(0, I_m)$$
; and  
(ii)  $n(\theta_n - \theta)' \Sigma^{-1}(\theta_n - \theta) \stackrel{d}{\to} \chi_m^2$ .

If  $x \sim N(\mu, \Sigma)$  its density is

$$\frac{1}{\sqrt{(2\pi)^{\dim x}\det(\Sigma)}}e^{-\frac{(x-\mu)'\Sigma^{-1}(x-\mu)}{2}}.$$

Any subset of x is again normal. All conditional distributions are again normal.

Partition  $x = (x'_1, x'_2)'$  and write

$$\left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) \sim N \left(\begin{array}{c} \left(\begin{array}{c} \mu_1 \\ \mu_2 \end{array}\right) & \left(\begin{array}{c} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{array}\right) \end{array}\right).$$

The marginal distribution of  $x_1$  is normal,  $x_1 \sim N(\mu_1, \Sigma_{11})$ .

The conditional distribution of  $x_1$  given  $x_2$  is

$$N\left(\mu_1 + \Sigma_{12}\Sigma_{22}^{-1}(x_2 - \mu_2), \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21}\right).$$

The above is particularly tractable in the bivariate case, where  $x_1$  and  $x_2$  are both scalars.

Write

$$\left(\begin{array}{c} x_1 \\ x_2 \end{array}\right) \sim N \left(\begin{array}{c} \left(\begin{array}{c} \mu_1 \\ \mu_2 \end{array}\right) & \left(\begin{array}{c} \sigma_1^2 & \rho \, \sigma_1 \sigma_2 \\ \rho \, \sigma_1 \sigma_2 & \sigma_2^2 \end{array}\right) \end{array}\right)$$

for  $\rho$  the correlation between  $x_1$  and  $x_2$ .

Here,

$$x_1|x_2 \sim N\left(\mu_1 + \rho \frac{\sigma_1}{\sigma_2} (x_2 - \mu_2), (1 - \rho^2) \sigma_1^2\right).$$

Note that

$$E(x_1|x_2) = \mu_1 + \rho \frac{\sigma_1}{\sigma_2} (x_2 - \mu_2) = \left(\mu_1 - \rho \frac{\sigma_1}{\sigma_2} \mu_2\right) + \rho \frac{\sigma_1}{\sigma_2} x_2$$

is linear in  $x_2$ .

Also,  $var(x_1|x_2)$  is a constant (i.e., not a function of  $x_2$ ).

We say that  $\theta_n$  is best asymptotically unbiased for  $\theta$  if

$$\sqrt{n}(\theta_n - \theta) \stackrel{d}{\to} N(0, I_{\theta}^{-1}),$$

so it achieves the Cramér-Rao bound in large samples.

It exists under weak regularity conditions.

A coherent way of finding it is through the method of maximum likelihood.

The maximum-likelihood estimator is

$$\hat{\theta} = \arg \max_{\theta \in \Theta} \prod_{i=1}^{n} f_{\theta}(x_i) = \arg \max_{\theta \in \Theta} \sum_{i=1}^{n} \log f_{\theta}(x_i).$$

The likelihood function,  $\prod_{i=1}^{n} f_{\theta}(x_i)$ , represents the density of the sample when sampling from  $f_{\theta}$ .

In the discrete case, it is the probability of observing the actual sample, when sampling from  $f_{\theta}.$ 

Maximize this probability as a function of  $\theta$ .

Intuitively attractive. Pretty much what anyone without any prior statistical knowledge would do.

# Maximization program

Let

$$L_n(\theta) = \sum_i \log f_{\theta}(x_i)$$

be the log-likelihood function.

The first-order condition is that

$$\frac{\partial L_n(\theta)}{\partial \theta} = \sum_i \frac{\partial \log f_\theta(x_i)}{\partial \theta} = 0;$$

this is the score equation.

The second-order condition for a maximum is that

$$\frac{\partial^2 L_n(\theta)}{\partial \theta \partial \theta'} = \sum_i \frac{\partial^2 \log f_\theta(x_i)}{\partial \theta \partial \theta'} < 0;$$

the Hessian matrix is negative definite.

Note how these derivatives relate to the Cramér-Rao bound.

## Numerical maximization: Newton-Raphson

Often we need to tackle the maximization problem numerically.

Newton-Raphson is a popular algorithm for finding the roots of the score equation.

Want to solve  $\varphi(x) = 0$ . Let  $x_0$  be an initial guess. For a new guess  $x_1$  we have

$$\frac{\varphi(x_1) - \varphi(x_0)}{x_1 - x_0} \approx \left. \frac{\partial \varphi(x)}{\partial x} \right|_{x = x_0} = \varphi'(x_0).$$

So,

$$\varphi(x_0) + (x_1 - x_0) \,\varphi'(x_0) \approx \varphi(x_1).$$

We want that  $\varphi(x_1) = 0$ . Solving for  $x_1$  yields

$$x_1 = x_0 - \varphi(x_0) / \varphi'(x_0)$$

as our new guess.

In practice, when maximizing a function whose derivative is  $\varphi$ , we start at  $x_0$  and then evaluate  $\varphi$  in  $x_1$ . If the function would not improve at  $x_1$  we re-evaluate in  $x'_1 = x_0 - h(x_0 - x_1)$  for  $h \in (0, 1)$  a step size and re-evaluate. We then iterate this procedure untill no further improvement (up to some specified tolerance level) is found.

### Bernoulli

When  $x_i \in \{0, 1\}$  with probability  $\theta \in (0, 1)$  we have

$$L_n(\theta) = \log\left(\prod_{i=1}^n \theta^{x_i} (1-\theta)^{1-x_i}\right) = \sum_{i=1}^n x_i \log \theta + (1-x_i) \log(1-\theta).$$

So, solving

$$\frac{\partial L_n(\theta)}{\partial \theta} = \sum_{i=1}^n \frac{x_i - \theta}{\theta(1 - \theta)} = n \frac{\overline{x}_n - \theta}{\theta(1 - \theta)} = 0$$

for  $\theta$  yields  $\hat{\theta} = \overline{x}_n$  as the unique solution. This is a global maximum as

$$\frac{\partial^2 L_n(\theta)}{\partial \theta^2} = -\sum_{i=1}^n \frac{(x_i - \theta)^2}{\theta^2 (1 - \theta)^2} < 0$$

for all  $\theta \in (0, 1)$ .

This estimator is best unbiased and so also best asymptotically unbiased.

Maximum likelihood is invariant to one-to-one parametrizations,  $\beta = \beta(\theta)$ .

If  $L_n(\theta)$  is the log-likelihood and  $L_n^*(\beta)$  is the reparametrized log-likelihood, then

$$\hat{\beta} = \arg\max_{\beta} L_n^*(\beta) = \beta(\arg\max_{\theta} L_n(\theta)) = \beta(\hat{\theta}).$$

This is an interesting property.

A consequence of invariance is that maximum likelihood will not be unbiased, in general.

If  $\hat{\theta}$  is unbiased and the transformation  $\beta(\theta)$  is nonlinear, then  $\hat{\beta} = \beta(\hat{\theta})$  will be biased, in general, by Jensen's inequality.

# Jensen's inequality

A univariate function  $\varphi$  is concave if

$$\varphi(\lambda x + (1 - \lambda)x') \ge \lambda \varphi(x) + (1 - \lambda)\varphi(x')$$

and convex if

$$\varphi(\lambda x + (1 - \lambda)x') \le \lambda \varphi(x) + (1 - \lambda)\varphi(x')$$

for all  $\lambda \in [0, 1]$ .

#### Theorem 14 (Jensen's inequality)

If  $\varphi$  is concave,  $E(\varphi(x_i)) \leq \varphi(E(x_i))$ . If  $\varphi$  is convex,  $E(\varphi(x_i)) \geq \varphi(E(x_i))$ .

#### Proof.

Take  $\varphi$  concave. Let  $\psi$  be the tangent line at  $E(x_i)$ ; i.e.,  $\psi(x) = a + bx$  for constants a, b such that  $\varphi(E(x_i)) = \psi(E(x_i))$ .

By concavity  $\varphi(x) \leq \psi(x)$  for any x. Hence, using linearity of the tangent,

$$E(\varphi(x_i)) \le E(\psi(x_i)) = \psi(E(x_i)) = \varphi(E(x_i)).$$

## Probit

The simplest probit model from above had

$$P_{\theta}(x_i = 1) = \Phi(\theta).$$

The score equation is

$$\sum_{i=1}^{n} (x_i - \Phi(\theta)) \frac{\phi(\theta)}{\Phi(\theta)(1 - \Phi(\theta))} = 0$$

and the efficiency bound was

$$\frac{1}{n} \frac{\Phi(\theta)(1 - \Phi(\theta))}{\phi(\theta)^2}.$$

Finding  $\hat{\theta}$  by solving the score equation requires numerical optimization.

Notice that the success probability  $\beta = \Phi(\theta)$  is a one-to-one transformation of  $\theta$ . The likelihood for  $\beta$  is the ordinary Bernoulli likelihood, with maximizer  $\hat{\beta} = \overline{x}_n$ .

It follows that  $\hat{\theta} = \Phi^{-1}(\overline{x}_n)$ .

Further, as

$$\sqrt{n}(\hat{\beta} - \beta) \stackrel{d}{\to} N(0, \beta(1 - \beta))$$

by the central limit theorem,

$$\frac{\partial \Phi^{-1}(\beta)}{\partial \beta} = \frac{1}{\phi(\theta)},$$

and  $\beta = \Phi(\theta)$ , the Delta method gives

$$\sqrt{n}(\hat{\theta} - \theta) \xrightarrow{d} N\left(0, \frac{\Phi(\theta)(1 - \Phi(\theta))}{\phi(\theta)^2}\right).$$

The asymptotic variance is indeed the Cramér-Rao bound.

The maximum-likelihood estimator may fail to exist in small samples.

In the probit model this happens when complete separation is possible. In essence, this means we can classify outcomes exactly.

In our model, where

$$P_{\theta}(x_i = 1) = \beta = \Phi(\theta),$$

a data set consisting of only successes (ones) will have  $\hat{\beta} = 1$ , and so  $\hat{\theta} = +\infty$ . If  $\beta \in (0, 1)$  this problem will not occur in large samples.

In an extended model with explanatory variables perfect separation would happen, for example, when all successes can be assigned to one covariate and all failures to another.

This problem may, in principle, persist in large samples.

# Why does maximizing the likelihood work: Identification

Note that the expected log-likelihood

$$L(\theta_*) = E_{\theta}(L_n(\theta_*)) = \sum_{i=1}^n E_{\theta}(\log f_{\theta_*}(x_i)) = n E_{\theta}(\log f_{\theta_*}(x_i))$$

is maximized at  $\theta$ .

Indeed,

$$E_{\theta}(L_n(\theta_*) - L_n(\theta)) = n E_{\theta}\left(\log\left(\frac{f_{\theta_*}(x_i)}{f_{\theta}(x_i)}\right)\right) \le n \log E_{\theta}\left(\frac{f_{\theta_*}(x_i)}{f_{\theta}(x_i)}\right) = 0,$$

using Jensen's inequality and the fact that  $E_{\theta}(f_{\theta_*}(x_i)/f_{\theta}(x_i)) = \int f_{\theta_*}(x) dx = 1.$ 

Crudely put,  $L(\theta)$  is the log-likelihood function we would use if we would have an infinitely-large sample.

(Point) identification means that, in that case, we would be able to learn  $\theta$ ; so

$$\theta = \arg \max_{\theta_* \in \Theta} L(\theta_*),$$

and is unique.

Identification may fail (we will give an example below).

Global identification:  $\theta$  is the unique maximizer of L on  $\Theta$ .

Local identification:  $\theta$  is the unique maximizer of L in some neighborhood around  $\theta$ .

Local identification is

$$\frac{\partial^2 L(\theta)}{\partial \theta \partial \theta'} < 0.$$

Note that, as

$$\frac{\partial^2 L(\theta)}{\partial \theta \partial \theta'} = n \, E_{\theta} \left( \frac{\partial^2 \log f_{\theta}(x_i)}{\partial \theta \partial \theta'} \right) = -n I_{\theta}$$

this is equivalent to the information matrix being positive definite and, hence, of full rank.

Local identification can be tested.

By a uniform law of large numbers,

$$\sup_{\theta \in \Theta} |n^{-1}L_n(\theta) - n^{-1}L(\theta)| \xrightarrow{p} 0, \text{ as } n \to \infty,$$

provided  $f_{\theta}$  is continuous,  $|\log f_{\theta}(x)| < b(x)$  so that  $E(b(x_i)) < \infty$ , and  $\Theta$  is closed and bounded (compact).

Then, if  $\theta$  is identified as the unique global maximizer of  $L(\theta)$ , we will have that

$$\arg\max_{\theta\in\Theta} L_n(\theta) \xrightarrow{p} \arg\max_{\theta\in\Theta} L(\theta),$$

but this is just

$$\hat{\theta} \stackrel{p}{\to} \theta$$
, as  $n \to \infty$ ,

which is consistency.

A uniform  $\varepsilon$ -band around  $L(\theta)$  and the corresponding interval  $[\theta_{\min}, \theta_{\max}]$  in which  $\hat{\theta}$  must lie.



As  $n \to \infty$ , the  $\varepsilon$ -band tightens and so the interval  $[\theta_{\min}, \theta_{\max}]$  shrinks to a point. By identification this point must be  $\theta$ . As  $\hat{\theta} \in [\theta_{\min}, \theta_{\max}]$  it must be that  $\hat{\theta}$  converges to  $\theta$ .

Regarding uniform convergence, consider the probit model as an example. There,

$$\log f_{\theta}(y|x) = y \, \log \Phi(x'\theta) + (1-y) \log \Phi(-x\theta).$$

We have, by a mean-value expansion, that

$$\log \Phi(x\theta) = \log \Phi(0) + \frac{\phi(x\theta_*)}{\Phi(x\theta_*)} x\theta$$

and  $0 < \frac{\phi(u)}{\Phi(u)} \le c |1+u|$  for some finite c (visual inspection will help to see this). Consequently,

$$\begin{aligned} |\log \Phi(x\theta)| &\le |\log \Phi(0)| + \frac{\phi(x\theta_*)}{\Phi(x\theta_*)} |x\theta| \le |\log(2)| + c |1 + x\theta_*| |x||\theta| \\ &\le |\log(2)| + c |x||\theta_*| + c |x|^2 |\theta|^2 \end{aligned}$$

so an integrable upper bound on log  $f_{\theta}(x_i)$  exists provided  $E(x_i^2) < \infty$ .

By definition

$$\sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right|_{\hat{\theta}} = 0.$$

A mean-value expansion around the true  $\theta$  gives

$$\sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \right|_{\hat{\theta}} = \sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \right|_{\theta} + \sum_{i=1}^{n} \left. \frac{\partial^{2} \log f_{\theta}(x_{i})}{\partial \theta \partial \theta'} \right|_{\theta_{*}} (\hat{\theta} - \theta) = 0,$$

where  $\theta_*$  is some vector that (elementwise) lies between  $\hat{\theta}$  and  $\theta$ . Inversion of this equation gives the sampling-error representation

$$(\hat{\theta} - \theta) = -\left(\sum_{i=1}^{n} \left. \frac{\partial^2 \log f_{\theta}(x_i)}{\partial \theta \partial \theta'} \right|_{\theta_*} \right)^{-1} \left. \sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right|_{\theta}$$

Now, by invoking a uniform law of large numbers together with consistency,

$$\frac{1}{n}\sum_{i=1}^{n}\left.\frac{\partial^{2}\log f_{\theta}(x_{i})}{\partial\theta\partial\theta'}\right|_{\theta_{*}} \xrightarrow{p} E_{\theta}\left(\left.\frac{\partial^{2}\log f_{\theta}(x_{i})}{\partial\theta\partial\theta'}\right|_{\theta}\right) = -I_{\theta}.$$

Also, by the central limit theorem,

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right|_{\theta} \stackrel{d}{\to} N(0, I_{\theta}).$$

Then, by the continuous-mapping theorem and Slutzky's theorem, we get the influence-function representation

$$\sqrt{n}(\hat{\theta} - \theta) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} I_{\theta}^{-1} \left. \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right|_{\theta} + o_p(1)$$

and we have the following result (note we use the information equality here).

### Theorem 15 (Optimality of maximum likelihood)

Under regularity conditions,

$$\sqrt{n}(\hat{\theta} - \theta) \stackrel{d}{\to} N(0, I_{\theta}^{-1}).$$

## Variance estimation

The information matrix—and, hence, the asymptotic variance of maximum likelihood—can be estimated.

There are two obvious choices.

The first follows from its definition as the variance of the score:

$$\frac{1}{n}\sum_{i=1}^{n}\left.\left(\frac{\partial\log f_{\theta}(x_{i})}{\partial\theta}\frac{\partial\log f_{\theta}(x_{i})}{\partial\theta'}\right)\right|_{\hat{\theta}}.$$

The second follows from the information equality:

$$-\frac{1}{n}\sum_{i=1}^{n}\left.\frac{\partial^{2}\log f_{\theta}(x_{i})}{\partial\theta\partial\theta'}\right|_{\hat{\theta}}$$

In both cases, a uniform law of large numbers can be used to show consistency.

The square root of the diagonal entries (of the inverse) give (estimated) standard errors on the maximum-likelihood estimator (after dividing through by  $\sqrt{n}$ ) and so can serve to assess its precision. They will equally serve us in testing later on.

## Labor-force participation

Consider the decision of married women to participate to labor market,  $y_i$ .

Individuals make decisions based on their own situation/characteristics,  $x_i$ . PSID has data on a variety of characteristics (age, education, number of children, and so on).

Standard Bernoulli is too simple to capture this dependence on observable characteristics.

A (possible) specification for a conditional model would be

$$p_i = P(y_i = 1 | x_i) = \Phi(x'_i \beta).$$

Here, choice probabilities are heterogenous in characteristics.

We can derive an econometric model from a specification of an economic model for the women's decision problem:

$$y_i = 1 \Leftrightarrow u(x_i, \varepsilon_i) \ge 0;$$

 $u(x_i, \varepsilon_i)$  is *i*'s utility from working;  $\varepsilon_i$  is not observed to the econometrician. Our specification has  $u(x_i, \varepsilon_i) = x'_i\beta + \varepsilon_i$  for  $\varepsilon_i \sim N(0, 1)$  independent of  $x_i$ . , probit inlf educ exper expersq age kidslt6 kidsge6

Iteration 0: log likelihood = -514.8732 Iteration 1: log likelihood = -405.33752 Iteration 2: log likelihood = -404.44693 Iteration 3: log likelihood = -404.4461 Iteration 4: log likelihood = -404.4461

Probit regression

Number of obs	=	753
LR chi2(6)	=	220.85
Prob > chi2	=	0.0000
Pseudo R2	=	0.2145

.og likelihood = -404.4461

inlf	Coef.	Std. Err.	z	P> z	[95% Conf.	Interval]
educ exper expersq age kidslt6	.1098675 .1259602 001843 05629 8597359	.0236192 .0186456 .0005967 .0083529 .1174379	4.65 6.76 -3.09 -6.74 -7.32	0.000 0.000 0.002 0.000 0.000	.0635747 .0894154 0030125 0726614 -1.08991	.1561603 .1625049 0006736 0399186 6295618
_cons	.4007683	.50461	0.70	0.482	5882492	1.389786

What are the parameters of interest in the probit model?

Take  $x_i$  scalar continuous for a moment.

The average marginal effect is

$$\frac{\partial E(y_i|x_i)}{\partial x_i} = \frac{\partial \Phi(x_i\beta)}{\partial x_i} = \beta \, \phi(x_i\beta).$$

This is nonlinear and heterogenous.

Can look at the distribution of this marginal effect (in  $x_i$ ), and its functionals. For example, the mean

$$\theta = E\left(\frac{\partial E(y_i|x_i)}{\partial x_i}\right) = \beta E(\phi(x_i\beta)).$$

The maximum-likelihood estimator is

$$\hat{\theta} = n^{-1} \sum_{i=1}^{n} \hat{\beta} \, \phi(x_i \hat{\beta}).$$

To obtain a standard error, use the Delta method.

We can also look at other functionals of the distribution of the marginal effects.

. margins, dydx(educ exper expersq age kidslt6 kidsge6)

Average marginal effects Model VCE : OIM Number of obs = 753

Expression : Pr(inlf), predict() dy/dx w.r.t. : educ exper expersq age kidslt6 kidsge6

	dy/dx	Delta-method Std. Err.	z	P> z	[95% Conf.	Interval]
educ	.0332836	.0068685	4.85	0.000	.0198215	.0467456
exper	.0381587	.0051453	7.42	0.000	.0280742	.0482433
expersq	0005583	.0001775	-3.15	0.002	0009062	0002104
age	0170527	.0023099	-7.38	0.000	0215799	0125254
kidslt6	2604509	.0317991	-8.19	0.000	322776	1981259

The classical linear regression model is an extension of the location/scale model from above in that it adds regressors.

Data on outcome  $y_i$  and a (column) vector of regressors (or covariates or explanatory variables)  $x_i$ .

The model is

$$y_i | x_i \sim N(x_i'\beta, \sigma^2),$$

and  $\theta = (\beta', \sigma^2)'$ . Equivalently (and more commonly) we can write the model as

$$y_i = x'_i \beta + \varepsilon_i, \qquad \varepsilon_i | x_i \sim N(0, \sigma^2).$$

Unless explicitely stated otherwise the first covariate is taken to be a constant term.

This is a simple model for analyzing how the distribution of  $y_i$  changes with  $x_i$ . Here, only impact is through the mean:

$$E(y_i|x_i) = x_i'\beta.$$

Often convenient to look at this model in matrix form.

We have a set of n equations with k regressors, as in

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,k} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{n,k} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix},$$

which we write as

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \qquad \boldsymbol{\varepsilon} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I}).$$

The log-likelihood (conditional on the regressors) then is

$$-\frac{n}{2}\log\sigma^2 - \frac{1}{2}\sum_i \frac{(y_i - x_i'\beta)^2}{\sigma^2} = -\frac{n}{2}\log\sigma^2 - \frac{(\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta)}{2\sigma^2}$$
The score equation for  $\beta$  is

$$\frac{\mathbf{X}'(\mathbf{y} - \mathbf{X}\beta)}{\sigma^2} = 0.$$

It has the unique solution

$$\hat{\beta} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$$

(independent of  $\sigma^2$ ) provided that the inverse of the matrix X'X exists. This is known as the ordinary least-squares estimator.

So,  $\hat{\beta}$  is uniquely defined if X has maximal rank. This is the well-known 'no-multicolinearity condition'. No column of X can be written as a linear combination of the other columns.

A simple counter-example is the dummy-variable trap, where the regressors would be a constant and a collection of dummies for events whose union happens with probability one. Say,  $x_i = (1, d_i, 1 - d_i)'$  where  $d_i$  is a binary indicator.

Then  $x_{i,1} = x_{i,2} + x_{i,3}$  for all *i* and the rank condition fails.

The model

$$y_i = \beta_1 + d_i\beta_2 + (1 - d_i)\beta_3 + \varepsilon_i$$

is observationally-equivalent to the three-parameter/two-regressor model

$$y_i = (\beta_1 + \beta_3) + d_i(\beta_2 - \beta_3) + \varepsilon_i = \alpha_1 + d_i\alpha_2 + \varepsilon_i.$$

We can only learn the reduced-form parameters  $(\alpha_1, \alpha_2)$ . The identified set for  $\beta$  is

$$\{\beta \in \mathbb{R} : \beta_1 + \beta_3 = \alpha_1, \beta_2 - \beta_3 = \alpha_2\}.$$

For example, given  $\beta_3$ , we can back out  $(\beta_1, \beta_2)$  but, without this knowledge, we can only say things such as  $\beta_1 - \beta_2 = \alpha_1 - \alpha_2$ .

As another example of identification failure, suppose that we do not observe  $y_i$  in the data but, instead, observe variables  $\underline{y}_i \leq \overline{y}_i$  for which we know that

$$\underline{y}_i \le y_i \le \overline{y}_i$$

(income data in social security records, for example, is often bracketed in this way). Here we cannot even compute the value of the likelihood.

Then the conditional mean is only restricted by

$$E(\underline{y}_i|x_i) \le x_i'\beta \le E(\overline{y}_i|x_i)$$

(where we use  $E(y_i|x_i) = x'_i\beta$ ).

An implication is that

$$E(x_i\underline{y}_i) \le E(x_ix'_i)\beta \le E(x_i\overline{y}_i).$$

We can estimate all  $\beta$  compatible with this moment inequality by the set  $[\hat{\beta}, \overline{\hat{\beta}}]$ , with

$$\underline{\hat{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\underline{\mathbf{y}}, \qquad \overline{\hat{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\overline{\mathbf{y}}$$

in obvious notation.

We will write

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}}, \qquad \hat{\boldsymbol{\varepsilon}} = \boldsymbol{y} - \boldsymbol{X}\hat{\boldsymbol{\beta}},$$

for fitted values and residuals, respectively.

We have the decomposition

$$\boldsymbol{y} = \hat{\boldsymbol{y}} + \hat{\boldsymbol{\varepsilon}},$$

where the fitted values and residuals are uncorrelated, i.e.,  $\hat{y}' \hat{\varepsilon} = 0$ . Indeed, the score equation at  $\hat{\beta}$  equals

$$\frac{X'\hat{\varepsilon}}{\sigma^2} = 0$$

so we can say that  $\hat{\beta}$  gives us that linear combination of the regressors for which residuals and regressors are exactly uncorrelated.

An implication is that

$$oldsymbol{y}'oldsymbol{y} = (\hat{oldsymbol{y}}+\hat{oldsymbol{arepsilon}})'(\hat{oldsymbol{y}}+\hat{oldsymbol{arepsilon}}) = \hat{oldsymbol{y}}'\hat{oldsymbol{y}}+\hat{oldsymbol{arepsilon}}'\hat{oldsymbol{arepsilon}},$$

and so the uncentered  $\mathbb{R}^2$ 

$$R_u^2 = \frac{\hat{\boldsymbol{y}}'\hat{\boldsymbol{y}}}{\boldsymbol{y}'\boldsymbol{y}} = 1 - \frac{\hat{\boldsymbol{\varepsilon}}'\hat{\boldsymbol{\varepsilon}}}{\boldsymbol{y}'\boldsymbol{y}} \in [0,1]$$

gives a relative contribution of the variation in fitted values to the variation in observed outcomes. More popular to report is the (centered)  $\mathbb{R}^2$ , which looks at deviations from the mean, as

$$R^2 = \frac{ESS}{TSS} = 1 - \frac{SSR}{TSS}$$

where the total sum of squares decomposes as

$$TSS = \sum_{i=1}^{n} (y_i - \bar{y})^2 = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2 + \sum_{i=1}^{n} \hat{\varepsilon}_i^2 = ESS + SSR,$$

into the explained sum of squares and sum of squared residuals (note that  $\overline{\hat{y}} = \overline{y}$  because  $\sum_i \hat{\varepsilon}_i = 0$ ).

The intuition is that we want to compare the improvement in fit of a model with regressors to a model without regressors.

Such a desire for fit comes from the use of the regression model to form linear predictions.

The vector  $\boldsymbol{y}$  is a point in  $\mathbb{R}^n$ . The column space of the  $n \times k$  matrix  $\boldsymbol{X}$  is the subspace of linear combinations

$$\mathcal{X} = \{ \boldsymbol{a} \in \mathbb{R}^n : \boldsymbol{a} = \boldsymbol{X}\boldsymbol{b} \text{ for some vector } \boldsymbol{b} \}.$$

That is,  $\mathcal{X}$  is the vector space spanned by the columns of  $\mathbf{X}$ . If rank  $\mathbf{X} = k$  the columns of  $\mathbf{X}$  are basis vectors for  $\mathcal{X}$ .

The orthogonal projection of  $\boldsymbol{y}$  onto  $\boldsymbol{\mathcal{X}}$  is the solution to

$$\min_{\boldsymbol{a}\in\mathcal{X}} \|\boldsymbol{y}-\boldsymbol{a}\| = \min_{\boldsymbol{b}\in\mathbb{R}^k} \|\boldsymbol{y}-\boldsymbol{X}\boldsymbol{b}\| = \min_{\boldsymbol{b}\in\mathbb{R}^k} \sqrt{(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{b})'(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{b})}$$

and equals

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y} = \boldsymbol{P}_{\boldsymbol{X}}\boldsymbol{y}.$$

The deviation of  $\boldsymbol{y}$  from its projection is

$$\hat{\boldsymbol{\varepsilon}} = \boldsymbol{y} - \hat{\boldsymbol{y}} = \boldsymbol{y} - \boldsymbol{P}_{\boldsymbol{X}} \boldsymbol{y} = (\boldsymbol{I} - \boldsymbol{P}_{\boldsymbol{X}}) \boldsymbol{y} = \boldsymbol{M}_{\boldsymbol{X}} \boldsymbol{y},$$

and lives in the orthogonal complement  $\mathcal{X}^{\perp}$ , so  $\hat{y}'\hat{\varepsilon} = 0$ . The projection matrices

$$P_X = X(X'X)^{-1}X', \qquad M_X = I - P_X = I - X(X'X)^{-1}X',$$

will prove convenient. Note that  $P_X = P'_X$  and  $P^2_X = P_X$  (and the same for  $M_X$ ) and that  $P_X M_X = 0$ .

Least squares projection in a three-dimensional space:



Partition  $\boldsymbol{X} = (\boldsymbol{X}_1, \boldsymbol{X}_2)$  so that

$$\boldsymbol{y} = \boldsymbol{X}_1 \beta_1 + \boldsymbol{X}_2 \beta_2 + \boldsymbol{\varepsilon}$$

and, hence,

$$\left(\begin{array}{c}\hat{\beta}_1\\\hat{\beta}_2\end{array}\right) = \left(\begin{array}{c} \boldsymbol{X}_1'\boldsymbol{X}_1 & \boldsymbol{X}_1'\boldsymbol{X}_2\\ \boldsymbol{X}_2'\boldsymbol{X}_1 & \boldsymbol{X}_2'\boldsymbol{X}_2\end{array}\right)^{-1} \left(\begin{array}{c} \boldsymbol{X}_1'\boldsymbol{y}\\ \boldsymbol{X}_2'\boldsymbol{y}\end{array}\right)$$

Some algebra using formulae for partitioned matrix inversion shows that

$$\hat{\beta}_1 = (X'_1 M_{X_2} X_1)^{-1} (X'_1 M_{X_2} y)$$

(and likewise for  $\hat{\beta}_2$ ).

 $M_{X_2}y$  is the residual vector of a regression of y on  $X_2$ .

 $M_{X_2}X_1$  is the residual matrix of a regression of the columns of  $X_1$  on  $X_2$ .

These residuals are uncorrelated with  $X_2$ . Moreover,  $M_{X_2}y$  is y, and  $M_{X_2}X_1$  is  $X_1$ , respectively, after their linear dependence on  $X_2$  has been filtered out.  $\hat{\beta}_1$  is the slope coefficient in a regression of these residuals on each other.

This gives (multiple) least squares its partialling-out interpretation. The results is known as the Frisch-Waugh-Lovell theorem.

The estimator  $\hat{\beta}$  is (conditionally) unbiased,

$$E(\hat{\beta}|\boldsymbol{X}) = E((\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}|\boldsymbol{X}) = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'E(\boldsymbol{y}|\boldsymbol{X}) = \beta$$

(because  $E(\boldsymbol{y}|\boldsymbol{X}) = \boldsymbol{X}\beta$ ). Its variance is

$$\begin{aligned} \operatorname{var}(\hat{\beta}|\boldsymbol{X}) &= E((\hat{\beta} - \beta)(\hat{\beta} - \beta)'|\boldsymbol{X}) \\ &= E((\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}'\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}|\boldsymbol{X}) \\ &= (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'E(\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}'|\boldsymbol{X})\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1} \\ &= (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\sigma^{2}\boldsymbol{I}_{n}\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1} \\ &= \sigma^{2}(\boldsymbol{X}'\boldsymbol{X})^{-1}. \end{aligned}$$

In fact, its exact (conditional) distribution is normal,

$$\hat{\beta} \sim N(\beta, \sigma^2 (\boldsymbol{X}' \boldsymbol{X})^{-1}),$$

because, for any conformable non-stochastic matrix A,  $A\varepsilon \sim N(\mathbf{0}, \sigma^2 A A')$ , and thus also for  $A = (X'X)^{-1}X'$ .

It is also **best unbiased**, as  $\hat{\beta} - \beta = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\varepsilon}$  is proportional to the score equation at the truth  $(\mathbf{X}'\boldsymbol{\varepsilon}/\sigma^2)$ , with factor of proportionality equal to  $\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ .

The score equation for  $\sigma^2$  is

$$-\frac{n}{\sigma^2} + \frac{(\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta)}{\sigma^4} = 0.$$

which, given  $\hat{\beta}$ , has solution

$$\hat{\sigma}^2 = \frac{\hat{\varepsilon}'\hat{\varepsilon}}{n}.$$

We already know that this estimator is biased; an unbiased version would be

$$ilde{\sigma}^2 = rac{\hat{oldsymbol{arepsilon}}'\hat{oldsymbol{arepsilon}}}{n-k}.$$

Indeed,

$$E\left(\left.\frac{\hat{\varepsilon}'\hat{\varepsilon}}{n}\right|\mathbf{X}\right) = \frac{E\left(\mathbf{y}'\mathbf{M}_{\mathbf{X}}\mathbf{y}|\mathbf{X}\right)}{n} = \frac{E\left(\varepsilon'\mathbf{M}_{\mathbf{X}}\varepsilon|\mathbf{X}\right)}{n} = \sigma^{2}\frac{\operatorname{tr}(\mathbf{M}_{\mathbf{X}})}{n} = \sigma^{2}\frac{n-k}{n}$$

because

$$\operatorname{tr}(\boldsymbol{M}_{\boldsymbol{X}}) = \operatorname{tr}(\boldsymbol{I}_n - \boldsymbol{P}_{\boldsymbol{X}}) = \operatorname{tr}(\boldsymbol{I}_n) - \operatorname{tr}(\boldsymbol{P}_{\boldsymbol{X}}) = n - k;$$

using that  $\operatorname{tr}(\boldsymbol{P}_{\boldsymbol{X}}) = \operatorname{tr}(\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}') = \operatorname{tr}(\boldsymbol{X}'\boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}) = \operatorname{tr}(I_k) = k.$ Finally,

$$(n-k)\,\tilde{\sigma}^2/\sigma^2 \sim \chi^2_{n-k}.$$

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Now consider the behavior of the estimators as  $n \to \infty$ . We let  $\Sigma = E(x_i x_i')$ . First,

$$\hat{\beta} - \beta = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\varepsilon},$$

and

$$\frac{\boldsymbol{X}'\boldsymbol{X}}{n} \xrightarrow{p} \Sigma, \qquad \frac{\boldsymbol{X}'\boldsymbol{\varepsilon}}{n} \xrightarrow{p} 0,$$

so that  $\hat{\beta} \xrightarrow{p} \beta$  by the continuous-mapping theorem. Next, we have

$$\sqrt{n}(\hat{\beta}-\beta) = \sqrt{n}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\varepsilon} = \left(\frac{\mathbf{X}'\mathbf{X}}{n}\right)^{-1}\frac{\mathbf{X}'\boldsymbol{\varepsilon}}{\sqrt{n}},$$

and

$$\frac{\boldsymbol{X}'\boldsymbol{\varepsilon}}{\sqrt{n}} \stackrel{d}{\to} N(0,\sigma^2 \Sigma).$$

So,

$$\sqrt{n}(\hat{\beta} - \beta) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \Sigma^{-1} x_i \varepsilon_i + o_p(1) \xrightarrow{d} N(0, \sigma^2 \Sigma^{-1}).$$

The influence function here is  $\Sigma^{-1} x_i \varepsilon_i$ .

For the variance estimator,

$$\begin{split} \hat{\sigma}^2 &= \frac{\hat{\varepsilon}'\hat{\varepsilon}}{n} \\ &= \frac{(\boldsymbol{y} - \boldsymbol{X}\hat{\beta})'(\boldsymbol{y} - \boldsymbol{X}\hat{\beta})}{n} \\ &= \frac{(\boldsymbol{X}(\beta - \hat{\beta}) + \varepsilon)'(\boldsymbol{X}(\beta - \hat{\beta}) + \varepsilon)}{n} \\ &= \frac{\varepsilon'\varepsilon}{n} + \frac{(\hat{\beta} - \beta)'(\boldsymbol{X}'\boldsymbol{X})(\hat{\beta} - \beta)}{n} + 2(\hat{\beta} - \beta)'\frac{\boldsymbol{X}'\varepsilon}{n} \\ &= \frac{\varepsilon'\varepsilon}{n} + o_p(n^{-1/2}), \end{split}$$

because  $\|\hat{\beta} - \beta\| = O_p(n^{-1/2}), \mathbf{X}'\mathbf{X} = O_p(n)$  and  $\mathbf{X}'\boldsymbol{\varepsilon} = o_p(n)$ .

Therefore,

$$\sqrt{n}(\hat{\sigma}^2 - \sigma^2) = \frac{\varepsilon'\varepsilon - E(\varepsilon'\varepsilon)}{\sqrt{n}} + o_p(1) = \sum_{i=1}^n \frac{\varepsilon_i^2 - E(\varepsilon_i^2)}{\sqrt{n}} + o_p(1) \xrightarrow{d} N(0, 2\sigma^4)$$

(recall that, under normality,  $E(\varepsilon_i^4) = 3\sigma^4$ .)

This estimator is best asymptotically unbiased (and so is  $\tilde{\sigma}^2$ ).

Suppose a firm creates output according to Cobb-Douglas technology. The associated cost function is linear in logs. The regressors are a constant term, (the log of) total output, and the log of the price of inputs (labor, capital, and so on).

Source	SS	df		MS		Number of obs	=	145
Model Residual	269.514813 21.5520098	4 140	67.3 .153	3787034 3942927		Prob > F R-squared	=	437.09 0.0000 0.9260
Total	291.066823	144	2.02	2129738		Root MSE	-	.39236
log_cost	Coef.	Std.	Err.	t	P>ItI	[95% Conf.	In	terval]
log_output log_wage log_capital log_fuel _cons	.7203941 .4363412 2198882 .4265169 -3.526503	.0174 .2910 .3394 .1003 1.774	1664 1476 1286 1692 1366	41.24 1.50 -0.65 4.25 -1.99	0.000 0.136 0.518 0.000 0.049	.685862 1390756 8909567 .2280817 -7.034521	1 	7549262 .011758 4511803 6249521 0184857

. regress log\_cost log\_output log\_wage log\_capital log\_fuel

The coefficients on the input prices are elasticities.

The linear regression model will typically be inappropriate when data are not continuous.

An example is  $y_i \in \mathbb{N}$ , i.e., count data.

Patent-application data fits this framework.

A Poisson regression model has (conditional) mass function

$$\frac{\mu_i^{y_i} e^{-\mu_i}}{y_i!}, \qquad \mu_i = e^{x_i'\beta}.$$

Remember that  $\mu_i = e^{x'_i\beta}$  is the conditional mean of the outcome variable.

The log-likelihood (up to a constant) is

$$\sum_{i=1}^{n} (y_i x_i' \beta - e^{x_i' \beta}) + \text{constant.}$$

The score equation is

$$\sum_{i=1}^{n} x_i (y_i - e^{x'_i \beta}) = 0,$$

and the Hessian matrix is

$$-\sum_{i=1}^{n} (x_i x_i') e^{x_i'\beta} < 0.$$

The maximum-likelihood estimator of  $\beta$  is not unbiased.

It is best asymptotically unbiased, however, with limit distribution

$$\sqrt{n}(\hat{\beta}-\beta) \stackrel{d}{\to} N(0, E(x_i x_i' \mu_i)^{-1}).$$

# Patent applications (innovation) and R&D spending

The # of patents applied for on R&D spending, stratified by sector.

Poisson regression	Number of obs	=	181
	Wald chi2( <b>10</b> )	=	250144.38
Log likelihood = -28112.312	Prob > chi2	=	0.0000

p90	Coef.	Std. Err.	z	P> z	[95% Conf.	Interval]
aerosp	-2.384742	.5506521	-4.33	0.000	-3.464001	-1.305484
chemist	4147255	.1063933	-3.90	0.000	6232525	2061985
computer	-2.176611	.1299919	-16.74	0.000	-2.43139	-1.921832
machines	-3.423707	.1746431	-19.60	0.000	-3.766001	-3.081413
vehicles	1.47125	.2608972	5.64	0.000	.959901	1.982599
c.lr90#c.aerosp	.9357491	.0908713	10.30	0.000	.7576445	1.113854
c.lr90#c.chemist	.9115045	.0164141	55.53	0.000	.8793336	.9436755
c.lr90#c.computer	1.087077	.0177896	61.11	0.000	1.05221	1.121944
c.lr90#c.machines	1.381847	.0282344	48.94	0.000	1.326509	1.437186
c.lr90#c.vehicles	.3479149	.0356582	9.76	0.000	.2780262	.4178037

We can test whether the impact of R&D spending on innovation is different across sectors.

```
. test c.lr90#c.aerosp =c.lr90#c.chemist=c.lr90#c.computer=c.lr90#c.machines=c.lr90#c.vehicles
```

```
( 1) [p90]c.lr90#c.aerosp - [p90]c.lr90#c.chemist = 0
```

- ( 2) [p90]c.lr90#c.aerosp [p90]c.lr90#c.computer = 0
- ( 3) [p90]c.lr90#c.aerosp [p90]c.lr90#c.machines = 0
- ( 4) [p90]c.lr90#c.aerosp [p90]c.lr90#c.vehicles = 0

chi2( 4) = 569.85 Prob > chi2 = 0.0000 Arellano, M. and C. Meghir (1992). Female labour supply and on-the-job search: An empirical model estimated using complementary data sets. *Review of Economic Studies* 59, 537–557.

Blundell, R., P.-A. Chiappori, T. Magnac, and C. Meghir (2007). Collective labour supply: Heterogeneity and non-participation. *Review of Economic Studies* 74, 417–445.

Heckman, J. J. (1974). Shadow prices, market wages, and labor supply. *Econometrica* 42, 679–694.

Magnac, T. (1991). Segmented or competitive labor markets. Econometrica 59, 165-187.

Rust, J. (1987). Optimal replacement of GMC bus engines: An empirical model of Harold Zurcher. *Econometrica* 55, 999–1033.

Tobin, J. (1958). Estimation of relationships from limited dependent variables. *Econometrica* 26, 24–36.

#### Skip the remainder of this section

Before seeing the data you have beliefs about  $\theta$ . Suppose we can summarize those beliefs into a distribution function  $\pi(\theta)$  on  $\Theta$ , the prior.

Upon seeing the data we can evaluate the distribution of the sample,  $\prod_{i=1}^{n} f_{\theta}(x_i)$ , at any  $\theta \in \Theta$ .

When confronted with the data we may alter our beliefs about  $\theta$ . Bayes rule gives the posterior as

$$\pi(\theta|x_1,\ldots,x_n) = \frac{\prod_{i=1}^n f_\theta(x_i) \pi(\theta)}{\int_{\Theta} \prod_{i=1}^n f_u(x_i) \pi(u) \, du}.$$

When prior is a proper distribution, so is the posterior.

The updated beliefs summarized in the posterior distribution can be used to construct a point estimator if desired. An example is

$$\int_{\Theta} \theta \, \pi(\theta | x_1, \dots, x_n) \, d\theta,$$

the posterior mean.

Other natural choices would be the posterior median and mode.

Take

$$x_i \sim N(\theta, \sigma^2)$$

(with  $\sigma^2$  known for simplicity), so that

$$f_{\theta}(x_1, \dots, x_n) = \prod_{i=1}^n \frac{1}{\sigma} \phi\left(\frac{x_i - \theta}{\sigma}\right) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2}\left(\frac{\sum_{i=1}^n (x_i - \overline{x}_n)^2}{\sigma^2} + \frac{n(\theta - \overline{x}_n)^2}{\sigma^2}\right)}.$$

Suppose that

$$\pi(\theta) = \frac{1}{\tau} \phi\left(\frac{\theta - \mu}{\tau}\right) = \frac{1}{(2\pi\tau^2)^{1/2}} e^{-\frac{1}{2}\left(\frac{(\theta - \mu)^2}{\tau^2}\right)},$$

i.e., our prior belief is that  $\theta \sim N(\mu, \tau^2)$ .

A calculation gives the posterior as normal, i.e.,

$$\theta|(x_1,\ldots,x_n) \sim N\left(\frac{\tau^2}{\tau^2 + \sigma^2/n}\overline{x}_n + \frac{\sigma^2/n}{\tau^2 + \sigma^2/n}\mu, \frac{\tau^2\sigma^2/n}{\tau^2 + \sigma^2/n}\right)$$

The posterior mean is the point estimator

$$\frac{\tau^2}{\tau^2 + \sigma^2/n}\overline{x}_n + \frac{\sigma^2/n}{\tau^2 + \sigma^2/n}\mu,$$

which is a weighted average of the sample mean  $\overline{x}_n$  (the Frequentist estimator) and the prior mean  $\mu$ .

Note that this estimator is not unbiased.

In fact, Bayesian posterior means are never unbiased.

As  $n \to \infty$ , the relative contribution of the prior vanishes and

$$\theta|(x_1,\ldots,x_n) \stackrel{a}{\sim} N\left(\overline{x}_n,\sigma^2/n\right),$$

which is the Frequentist asymptotic approximation.

The similarity between the Bayesian posterior and the Frequentist asymptotic-distribution approximation in the above example holds much more generally.

This is the Bernstein-von Mises result.

It states that, in an appropriate metric (known as the total-variation norm), the difference between  $\pi(\theta|x_1,\ldots,x_n)$  and

$$N(\hat{\theta}, I_{\theta}^{-1}/n)$$

converges to zero in probability as  $n \to \infty$ .

One implication is that both procedures are asymptotically equivalent.

Remember the posterior mean in our example was

$$\frac{\tau^2}{\tau^2 + \sigma^2/n} \overline{x}_n + \frac{\sigma^2/n}{\tau^2 + \sigma^2/n} \mu = \left(1 - \frac{(\sigma^2/\tau^2)/n}{1 + (\sigma^2/\tau^2)/n}\right) \overline{x}_n + \left(\frac{(\sigma^2/\tau^2)/n}{1 + (\sigma^2/\tau^2)/n}\right) \mu.$$

For example, when  $\mu = 0$  (for notational simplicity) we have

$$\left(1 - \frac{(\sigma^2/\tau^2)/n}{1 + (\sigma^2/\tau^2)/n}\right)\overline{x}_n = \left(1 - \frac{\sigma^2/n}{\tau^2 + \sigma^2/n}\right)\overline{x}_n$$

The term in brackets lies in (0, 1). So, this estimator is downward biased. The bias is introduced by the shrinkage of  $\overline{x}_n$  towards the prior mean of zero.

A multivariate version would have  $\overline{\boldsymbol{x}} \sim N(\boldsymbol{\theta}, (\sigma^2/n) \boldsymbol{I}_m)$  and  $\boldsymbol{\theta} \sim N(\boldsymbol{0}, \tau^2 \boldsymbol{I}_m)$ with shrinkage estimator

$$\left(1 - \frac{(\sigma^2/\tau^2)/n}{1 + (\sigma^2/\tau^2)/n}\right) \overline{\boldsymbol{x}}.$$

The James-Stein estimator (assuming that  $\sigma^2$  is known and that  $m \ge 2$ ) is

$$\left(1-\sigma^2 \, \frac{m-2}{\|\overline{\boldsymbol{x}}\|^2}\right) \, \overline{\boldsymbol{x}}.$$

While this estimator is biased, we have

$$E(\|\overline{\boldsymbol{x}} - \boldsymbol{0}\|^2) > E\left(\left\|\left(1 - \sigma^2 \frac{m-2}{\|\overline{\boldsymbol{x}}\|^2}\right) \overline{\boldsymbol{x}} - \boldsymbol{0}\right\|^2\right).$$

as soon as m > 2.

So, in terms of estimation risk (as measured by expected squared loss), the James-Stein estimator dominates the Frequentist sample mean estimator  $\overline{x}$ .

The key is that shrinkage reduces variance. Indeed, taking the infeasible estimator for simplicity

$$\operatorname{var}\left(\left(1 - \frac{(\sigma^2/\tau^2)/n}{1 + (\sigma^2/\tau^2)/n}\right) \overline{\boldsymbol{x}}\right) = \left(1 - \frac{(\sigma^2/\tau^2)/n}{1 + (\sigma^2/\tau^2)/n}\right) \tau^2 \boldsymbol{I}_m$$
$$= \left(\tau^2 - \frac{\sigma^2/\tau^2}{n}\right) \boldsymbol{I}_m + o(n^{-1}).$$

## TESTING IN PARAMETRIC PROBLEMS

General discussion:

Casella and Berger, Chapter 8 Hansen I, Chapter 13 and 14

Testing in the likelihood framework:

Davidson and MacKinnon, Chapter 13

Hansen II, Chapter 9

Classical linear regression model:

Goldberger, Chapters 19-21

Suppose we wish to test the simple null  $H_0$ :  $\theta = \theta_0$  against the simple alternative  $H_1: \theta = \theta_1$ .

The data distribution is completely specified under both null and alternative. Write

$$\ell_n(\theta) = e^{L_n(\theta)} = \prod_{i=1}^n f_\theta(x_i)$$

for the likelihood and define the likelihood ratio as

$$\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)}.$$

If  $H_0$  is false we would expect  $\ell_n(\theta_0)/\ell_n(\theta_1)$  to be small.



A decision rule based on the likelihood ratio is to

Reject the null in favor of the alternative when

$$\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)} < c,$$

Accept the null when

$$\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)} \ge c,$$

for a chosen value c.

We might wrongfully reject the null. This is called a type-I error. The significance level or size of the test is

$$P_{\theta_0}\left(\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)} < c\right).$$

We might wrongfully accept the null. This is called a type-II error. The power of the test is

$$P_{\theta_1}\left(\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)} < c\right).$$

# Normal

Suppose that

$$x_i \sim N(\theta, \sigma^2)$$

for known  $\sigma^2$ .

(From before; see Slide 49) the density of the data is

$$\frac{1}{(2\pi\sigma^2)^{n/2}}e^{-\frac{1}{2}\left(\frac{\sum_{i=1}^{n}(x_i-\overline{x}_n)^2}{\sigma^2}\right)}e^{-\frac{1}{2}\left(\frac{n(\theta-\overline{x}_n)^2}{\sigma^2}\right)}$$

The likelihood ratio thus is

$$\frac{e^{-\frac{1}{2}\left(\frac{n(\theta_0 - \overline{x}_n)^2}{\sigma^2}\right)}}{e^{-\frac{1}{2}\left(\frac{n(\theta_1 - \overline{x}_n)^2}{\sigma^2}\right)}} = e^{-\frac{1}{2}\frac{n}{\sigma^2}\left((\overline{x}_n - \theta_0)^2 - (\overline{x}_n - \theta_1)^2\right)} = e^{\frac{\theta_0 - \theta_1}{\sigma/\sqrt{n}}\left(\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} + \frac{1}{2}\frac{\theta_0 - \theta_1}{\sigma/\sqrt{n}}\right)}.$$

If  $\theta_0 < \theta_1$  the likelihood ratio is no greater than c when

$$\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \ge c^*,$$

for some  $c^*$ .

So a level  $\alpha$  test is obtained on choosing  $c^*$  so that

$$P_{\theta_0}\left(\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)} < c\right) = P_{\theta_0}\left(\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \ge c^*\right) = 1 - \Phi(c^*) = \alpha,$$

which requires that

$$c^* = \Phi^{-1}(1 - \alpha) \equiv z_\alpha,$$

the  $(1 - \alpha)$ th quantile of the standard-normal distribution. These values are tabulated.

Then the decision rule we obtain is that, if,

$$\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \ge z_\alpha,$$

we reject the null in favor of the alternative.

#### The c.d.f. of the standard normal distribution



.2	0.00	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09
0.0	0.50000	0.50399	0.50798	0.51197	0.51595	0.51994	0.52392	0.52790	0.53188	0.53586
0.1	0.53983	0.54380	0.54776	0.55172	0.55567	0.55962	0.56356	0.56749	0.57142	0.57535
0.2	0.57926	0.58317	0.58706	0.59095	0.59483	0.59871	0.60257	0.60642	0.61026	0.61409
0.3	0.61791	0.62172	0.62552	0.62930	0.63307	0.63683	0.64058	0.64431	0.64803	0.65173
0.4	0.65542	0.65910	0.66276	0.66640	0.67003	0.67364	0.67724	0.68082	0.68439	0.68793
0.5	0.69146	0.69497	0.69847	0.70194	0.70540	0.70884	0.71226	0.71566	0.71904	0.72240
0.6	0.72575	0.72907	0.73237	0.73565	0.73891	0.74215	0.74537	0.74857	0.75175	0.75490
0.7	0.75804	0.76115	0.76424	0.76730	0.77035	0.77337	0.77637	0.77935	0.78230	0.78524
0.8	0.78814	0.79103	0.79389	0.79673	0.79955	0.80234	0.80511	0.80785	0.81057	0.81327
0.9	0.81594	0.81859	0.82121	0.82381	0.82639	0.82894	0.83147	0.83398	0.83646	0.83891
1										

The power of the test is

$$P_{\theta_1}\left(\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \ge z_\alpha\right) = P_{\theta_1}\left(\frac{\overline{x}_n - \theta_1}{\sigma/\sqrt{n}} + \frac{\theta_1 - \theta_0}{\sigma/\sqrt{n}} \ge z_\alpha\right) = 1 - \Phi\left(z_\alpha - \frac{\theta_1 - \theta_0}{\sigma/\sqrt{n}}\right)$$

Note that the power increases when

- the difference  $\theta_1 \theta_0$  (> 0 here) increases; and
- the samples size n increases.

The latter observation implies that

$$P_{\theta_1}\left(\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \ge z_\alpha\right) \stackrel{n \to \infty}{\to} 1,$$

i.e., if the null is false this will be spotted with probability approaching one. This is called **consistency** of a test.

Note that if, in stead,  $\theta_0 > \theta_1$ , the decision rule becomes that, if,

$$\frac{\overline{x}_n - \theta_0}{\sigma / \sqrt{n}} \le -z_\alpha,$$

we reject the null in favor of the alternative.

Now take the reverse situation where

$$x_i \sim N(\mu, \theta)$$

and  $\mu$  is known.

Wish to test  $H_0: \theta = \theta_0$  against  $H_1: \theta = \theta_1$ .

The likelihood ratio is

$$(\theta_1/\theta_0)^{n/2} e^{-\frac{1}{2}\frac{\theta_1-\theta_0}{\theta_1}\sum_{i=1}^n \frac{(x_i-\mu)^2}{\theta_0}}.$$

If  $\theta_0 < \theta_1$  this is small when

$$\sum_{i=1}^{n} \frac{(x_i - \mu)^2}{\theta_0}$$

is large (and vice versa). Now, under the null, this statistic is  $\chi^2_n$  and so

$$P_{\theta_0}\left(\sum_{i=1}^n \frac{(x_i - \mu)^2}{\theta_0} \ge \chi^2_{n,\alpha}\right) = \alpha,$$

where  $\chi^2_{n,\alpha}$  is the  $(1-\alpha)$ th quantile of the  $\chi^2_n$  distribution. The power is the probability that a  $\chi^2_n$  is greater than  $\chi^2_{n,\alpha}(\theta_0/\theta_1)$ .

The quantile function of the  $\chi^{\scriptscriptstyle 2}$  distribution



							α						
	0.500	0.600	0.700	0.800	0.850	0.900	0.925	0.950	0.975	0.990	0.995	0.999	0.995
$\nu$													
1	0.455	0.708	1.074	1.642	2.072	2.706	3.170	3.841	5.024	6.635	7.879	10.83	12.12
2	1.386	1.833	2.408	3.219	3.794	4.605	5.181	5.991	7.378	9.210	10.60	13.82	15.20
3	2.366	2.946	3.665	4.642	5.317	6.251	6.905	7.815	9.348	11.34	12.84	16.27	17.73
4	3.357	4.045	4.878	5.989	6.745	7.779	8.496	9.488	11.14	13.28	14.86	18.47	20.00
5	4.351	5.132	6.064	7.289	8.115	9.236	10.01	11.07	12.83	15.09	16.75	20.52	22.11
6	5.348	6.211	7.231	8.558	9.446	10.64	11.47	12.59	14.45	16.81	18.55	22.46	24.10
7	6.346	7.283	8.383	9.803	10.75	12.02	12.88	14.07	16.01	18.4 8	20.28	24.32	26.02
8	7.344	8.351	9.524	11.03	12.03	13.36	14.27	15.51	17.53	20.09	21.95	26.12	27.87
9	8.343	9.414	10.66	12.24	13.29	14.68	15.63	16.92	19.02	21.67	23.59	27.88	29.67
10	9.342	10.47	11.78	13.44	14.53	15.99	16.97	18.31	20.48	23.21	25.19	29.59	31.42

### Exponential

Take  $x_i$  to be exponentially distribution, i.e.,

$$f_{\theta}(x) = \frac{e^{-x/\theta}}{\theta}, \qquad x \ge 0, \quad \theta > 0.$$

Note that the likelihood is

$$\frac{1}{\theta^n} \prod_{i=1}^n e^{-x_i/\theta} = \frac{1}{\theta^n} e^{-n\overline{x}_n/\theta},$$

and so the likelihood-ratio statistic for simple null and alternative equals

$$\frac{\frac{1}{\theta_0^n}e^{-n\overline{x}_n/\theta_0}}{\frac{1}{\theta_1^n}e^{-n\overline{x}_n/\theta_1}} = \left(\frac{\theta_1}{\theta_0}\right)^n e^{-n\overline{x}_n\frac{\theta_1-\theta_0}{\theta_0\theta_1}}.$$

If  $\theta_1 > \theta_0$  this statistic is small when  $n\overline{x}_n$  is large. Now,

$$n\overline{x}_n = \sum_{i=1}^n x_i \sim \text{Gamma}(n, \theta)$$

(or  $\operatorname{Erlang}(n, 1/\theta)$  as n is an integer) so size is easily controlled for any n.
### Theorem 16 (Neyman-Pearson lemma)

When both the null and alternative hypothesis are simple, the likelihood ratio test that rejects the null when

$$\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)} < \epsilon$$

for a constant c such that

$$P_{\theta_0}\left(\frac{\ell_n(\theta_0)}{\ell_n(\theta_1)} < c\right) = \alpha$$

is the most powerful test among all level- $\alpha$  tests.

Now test the simple null  $H_0: \theta = \theta_0$  against a composite alternative  $H_1: \theta \in \Theta_1$ , where  $\Theta_1 \subset \Theta$ .

We can generalize the likelihood ratio to

$$\frac{\ell_n(\theta_0)}{\sup_{\theta_1\in\Theta_1}\ell_n(\theta_1)}$$

The data distribution is no longer fully specified under the alternative; there are many possible alternatives.

A test is uniformly most powerful if it is most powerful against all  $\theta_1 \in \Theta_1$ .

Power is now a function; i.e.,

$$\beta(\theta) = P_{\theta} \left( \frac{\ell_n(\theta_0)}{\sup_{\theta_1 \in \Theta_1} \ell_n(\theta_1)} < c \right)$$

### A level- $\alpha$ test is unbiased if

 $\beta(\theta) \geq \alpha$ 

for all  $\theta \in \Theta_1$ .

The null is more likely to be rejected when it is false than when it is true.

Unbiasedness is clearly desirable.

We could consider looking for the uniformly most powerful unbiased test.

## Normal (One-sided)

Again take  $x_i \sim N(\theta, \sigma^2)$  for known  $\sigma^2$ .

Now test  $H_0: \theta = \theta_0$  against  $H_1: \theta > \theta_0$ .

The set of alternatives is thus  $\Theta_1 = \{\theta \in \Theta : \theta > \theta_0\}$ . This is a one-sided alternative.

Clearly,

$$\hat{\theta}_1 = \arg \max_{\theta_1 \in \Theta_1} \ell_n(\theta_1) = \overline{x}_n \{ \overline{x}_n > \theta_0 \} + \theta_0 \{ \overline{x}_n \le \theta_0 \}.$$

Then,

$$\begin{split} \ell_n(\theta_0) &= \frac{e^{-\frac{1}{2}\frac{n(\overline{x}_n - \theta_0)^2}{\sigma^2}}}{e^{-\frac{1}{2}\frac{n(\overline{x}_n - \theta_1)^2}{\sigma^2}}} \\ &= e^{-\frac{n}{2}\frac{(\overline{x}_n - \theta_0)^2 - (\overline{x}_n - \theta_0)^2 \, \{\overline{x}_n \le \theta_0\} - (\overline{x}_n - \overline{x}_n)^2 \, \{\overline{x}_n > \theta_0\}}}{\sigma^2} \\ &= e^{-\frac{1}{2}\frac{(\overline{x}_n - \theta_0)^2}{\sigma^2/n} \left\{\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} > 0\right\}} \end{split}$$

which is no greater than some constant c if

$$\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \left\{ \frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} > 0 \right\} \ge c^*.$$
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The random variable

$$\overline{z} \{\overline{z} > 0\}, \qquad \overline{z} \sim N(0,1)$$

is truncated standard normal with cumulative distribution function

$$P(\overline{z} < c^* | \overline{z} > 0) = 2\left(\Phi(c^*) - \frac{1}{2}\right).$$

So, noting that only positive values for  $c^*$  make sense,

$$P(\overline{z} \{\overline{z} > 0\} \le c^*) = P(\overline{z} \le c^* | \overline{z} > 0) P(\overline{z} > 0) + P(\overline{z} \le 0)$$
$$= \frac{1}{2} \left( 2 \left( \Phi(c^*) - \frac{1}{2} \right) \right) + \frac{1}{2}$$
$$= \Phi(c^*),$$

and, therefore, the size of our test can be set to  $\alpha \in (0,1)$  by setting

$$c^* = \Phi^{-1}(1 - \alpha) = z_\alpha.$$

We get the decision rule

Reject  $H_0: \theta = \theta_0$  in favor of  $H_1: \theta > \theta_0$  if

$$\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \left\{ \frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} > 0 \right\} \ge z_{\alpha};$$

Accept  $H_0: \theta = \theta_0$  if

$$\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \left\{ \frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} > 0 \right\} < z_\alpha.$$

With  $z_{\alpha} > 0$  we can just look at

Reject  $H_0: \theta = \theta_0$  in favor of  $H_1: \theta > \theta_0$  if

$$\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \ge z_\alpha;$$

Accept  $H_0: \theta = \theta_0$  if

$$\frac{\overline{x}_n - \theta_0}{\sigma / \sqrt{n}} < z_\alpha.$$

This test is uniformly the most powerful.

This conclusion follows from the fact that the decision rule is the same as for the simple alternative  $\theta = \theta_1$  from above, and that test was the most powerful for any  $\theta_1 > \theta_0$ .

We have

$$P_{\theta}\left(\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \ge z_{\alpha}\right) = P_{\theta}\left(\frac{\overline{x}_n - \theta}{\sigma/\sqrt{n}} \ge z_{\alpha} + \frac{\theta_0 - \theta}{\sigma/\sqrt{n}}\right)$$

so the power function is

$$1 - \Phi\left(z_{\alpha} + \frac{\theta_0 - \theta}{\sigma/\sqrt{n}}\right).$$

This test is consistent.

 $\beta(\theta)$  is presented graphically below for a setting where  $\theta_0 = 0$  and  $\sigma = 1$ , with  $\alpha = .05$ .



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Continue to work with  $x_i \sim N(\theta, \sigma^2)$  for known  $\sigma^2$ .

Now test  $H_0: \theta = \theta_0$  against  $H_1: \theta \neq \theta_0$ .

The set of alternatives is thus  $\Theta_1 = \{\theta \in \Theta : \theta \neq \theta_0\} = \Theta \setminus \{\theta_0\}$ . This is a two-sided alternative.

The likelihood-ratio is simply

$$e^{-\frac{1}{2}\left(\frac{\overline{x}_n-\theta_0}{\sigma/\sqrt{n}}\right)^2},$$

which is no greater than some constant c if

$$\left|\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}}\right| \ge c^*.$$

So,

$$P_{\theta_0}\left(\left|\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}}\right| \ge c^*\right) = 1 - P_{\theta_0}\left(-c^* < \frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} \le c^*\right)$$

which is simply

$$1 - (\Phi(c^*) - \Phi(-c^*)) = 1 - (1 - \Phi(-c^*) - \Phi(-c^*)) = 2\Phi(-c^*) = 2(1 - \Phi(c^*)).$$

Equalizing this probability to  $\alpha$  and inverting toward  $c^*$  yields

$$c^* = \Phi^{-1}(1 - \alpha/2) = z_{\alpha/2},$$

giving the decision rule:

Reject  $H_0: \theta = \theta_0$  in favor of  $H_1: \theta \neq \theta_0$  if

$$\left|\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}}\right| \ge z_{\alpha/2},$$

and accept the null if not.

Note that we reject if either

$$\frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} < -z_{\alpha/2} \quad \text{or} \quad \frac{\overline{x}_n - \theta_0}{\sigma/\sqrt{n}} > z_{\alpha/2};$$

each of these events has probability  $\alpha/2$  under the null.

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This test is not uniformly most powerful. In fact, for two-sided alternatives, such tests cannot exist.

The one-sided tests with size  $\alpha$  are better on their respective sides of the null:



The two-sided test is unbiased and consistent.

Below are the power functions for two sample sizes.



## Normal (Two-sided; variance unknown)

Again

$$x_i \sim N(\mu, \sigma^2)$$

but now with both  $\mu, \sigma^2$  unknown.

Consider the hypothesis

$$H_0: \mu = \mu_0, \qquad H_1: \mu \neq \mu_0.$$

The likelihood is

$$\frac{1}{(2\pi\sigma^2)^{n/2}}e^{-\frac{1}{2}\frac{\sum_{i=1}^n(x_i-\mu)^2}{\sigma^2}}.$$

The unconstrained maximizers are

$$\hat{\mu} = \overline{x}_n, \qquad \hat{\sigma}^2 = n^{-1} \sum_{i=1}^n (x_i - \overline{x}_n)^2,$$

while, when  $\mu = \mu_0$ , maximizing with respect to  $\sigma^2$  only yields

$$\check{\sigma}^2 = n^{-1} \sum_{i=1}^n (x_i - \mu_0)^2.$$

The likelihood ratio is simply

$$\left(\frac{\hat{\sigma}^2}{\check{\sigma}^2}\right)^{n/2} = \left(1 + \frac{(\bar{x}_n - \mu_0)^2}{\hat{\sigma}^2}\right)^{-n/2}$$

This statistic is smaller than some critical value if and only if

$$\left(\frac{\overline{x}_n - \mu_0}{\hat{\sigma}/\sqrt{n}}\right)^2 = \left(\frac{n}{n-1}\right) \left(\frac{\overline{x}_n - \mu_0}{\tilde{\sigma}/\sqrt{n}}\right)^2$$

exceeds some other critical value; where, recall,  $\tilde{\sigma}^2 = \hat{\sigma}^2 n/(n-1)$ . But,

$$\frac{\overline{x}_n - \mu_0}{\tilde{\sigma}/\sqrt{n}} = \frac{\sigma}{\tilde{\sigma}} \frac{\overline{x}_n - \mu_0}{\sigma/\sqrt{n}} = \frac{\overline{x}_n - \mu_0}{\sigma/\sqrt{n}} \bigg/ \sqrt{\frac{\tilde{\sigma}^2}{\sigma^2}} = \frac{\overline{x}_n - \mu_0}{\sigma/\sqrt{n}} \bigg/ \frac{\sqrt{(n-1)(\tilde{\sigma}^2/\sigma^2)}}{\sqrt{n-1}}.$$

We know that

$$\frac{\overline{x}_n - \mu_0}{\sigma/\sqrt{n}} \sim N(0, 1), \qquad (n-1)\frac{\tilde{\sigma}^2}{\sigma^2} \sim \chi_{n-1}^2;$$

and so the ratio follows a t distribution with n-1 degrees of freedom.

The statistic

$$\frac{\overline{x}_n - \mu_0}{\tilde{\sigma}/\sqrt{n}} \sim t_{n-1}.$$

is commonly called the t-statistic.

Exact inference is thus possible on choosing critical values from Student's t distribution with n-1 degrees of freedom.

As n grows,  $t_{n-1}$  approaches the standard normal. So large-sample theory justifies the use of  $z_{\alpha/2}$  as a critical value.

The quantile function of the Student's t distribution



								α						
		0.600	0.700	0.750	0.800	0.850	0.900	0.925	0.950	0.975	0.990	0.995	0.999	0.9995
	ν													
I	1	0.325	0.727	1.000	1.376	1.963	3.078	4.165	6.314	12.71	31.82	63.66	318.3	636.6
	2	0.289	0.617	0.816	1.061	1.386	1.886	2.282	2.920	4.303	6.965	9.925	22.33	31.60
	3	0.277	0.584	0.765	0.978	1.250	1.638	1.924	2.353	3.182	4.541	5.841	10.21	12.92
	4	0.271	0.569	0.741	0.941	1.190	1.533	1.778	2.132	2.776	3.747	4.604	7.173	8.610
l	5	0.267	0.559	0.727	0.920	1.156	1.476	1.699	2.015	2.571	3.365	4.032	5.893	6.869
	6	0.265	0.553	0.718	0.906	1.134	1.440	1.650	1.943	2.447	3.143	3.707	5.208	5.959
	7	0.263	0.549	0.711	0.896	1.119	1.415	1.617	1.895	2.365	2.998	3.499	4.785	5.408
I	8	0.262	0.546	0.706	0.889	1.108	1.397	1.592	1.860	2.306	2.896	3.355	4.501	5.041
	9	0.261	0.543	0.703	0.883	1.100	1.383	1.574	1.833	2.262	2.821	3.250	4.297	4.781
	10	0.260	0.542	0.700	0.879	1.093	1.372	1.559	1.812	2.228	2.764	3.169	4.144	4.587
I	11	0.260	0.540	0.697	0.876	1.088	1.363	1.548	1.796	2.201	2.718	3.106	4.025	4.437
I	12	0.259	0.539	0.695	0.873	1.083	1.356	1.538	1.782	2.179	2.681	3.055	3.930	4.318
	13	0.259	0.538	0.694	0.870	1.079	1.350	1.530	1.771	2.160	2.650	3.012	3.852	4.221
	14	0.258	0.537	0.692	0.868	1.076	1.345	1.523	1.761	2.145	2.624	2.977	3.787	4.140
I	15	0.258	0.536	0.691	0.866	1.074	1.341	1.517	1.753	2.131	2.602	2.947	3.733	4.073
	16	0.258	0.535	0.690	0.865	1.071	1.337	1.512	1.746	2.120	2.583	2.921	3.686	4.015
	17	0.257	0.534	0.689	0.863	1.069	1.333	1.508	1.740	2.110	2.567	2.898	3.646	3.965
l	18	0.257	0.534	0.688	0.862	1.067	1.330	1.504	1.734	2 101	2 552	2.878	3 610	3 922

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The more general case has both composite null and alternative, as in

$$H_0: \theta \in \Theta_0, \qquad H_1: \theta \in \Theta_1,$$

where  $\Theta_0$  and  $\Theta_1$  are subsets of the parameter space  $\Theta$ .

An obvious generalization of the likelihood ratio would be

$$\frac{\sup_{\theta_0\in\Theta_0}\ell_n(\theta_0)}{\sup_{\theta_1\in\Theta_1}\ell_n(\theta_1)}.$$

The statistic used above for only the alternative composite is a special case. Much more common is to work with a likelihood ratio statistic defined as

$$\frac{\sup_{\theta_0\in\Theta_0}\ell_n(\theta_0)}{\sup_{\theta\in\Theta}\ell_n(\theta)};$$

note that the denominator features the full parameter space. This is often much easier to work with.

By definition

$$\sup_{\theta \in \Theta} \ell_n(\theta) = \ell_n(\hat{\theta}),$$

where  $\hat{\theta}$  is the (unconstrained) maximum-likelihood estimator. Likewise, we can think of

$$\check{\theta} = \arg\max_{\theta\in\Theta_0} \ell_n(\theta)$$

as the constrained maximum-likelihood estimator obtained on enforcing the null.

The likelihood ratio is then simply

$$\frac{\ell_n(\check{\theta})}{\ell_n(\hat{\theta})}.$$

# Normal (Composite)

 $x_i \sim N(\theta, \sigma^2)$  for known  $\sigma^2$ .

Now test  $H_0: \theta \leq 0$  against  $H_1: \theta > 0$ .

Here,

$$\arg\max_{\theta_0\in\Theta_0}\ell_n(\theta)=\overline{x}_n\,\{\overline{x}_n\leq 0\},\qquad\arg\max_{\theta_1\in\Theta_1}\ell_n(\theta)=\overline{x}_n\,\{\overline{x}_n>0\},$$

and, also,

$$\arg\max_{\theta\in\Theta}\ell_n(\theta)=\overline{x}_n.$$

So,

$$\frac{\sup_{\theta_0\in\Theta_0}\ell_n(\theta_0)}{\sup_{\theta_1\in\Theta_1}\ell_n(\theta_1)} = e^{-\frac{1}{2}\left(\frac{\overline{x}_n}{\sigma/\sqrt{n}}\right)^2\operatorname{sign}(\overline{x}_n)} = e^{-\frac{1}{2}\left(\frac{\overline{x}_n}{\sigma/\sqrt{n}}\right)\left|\frac{\overline{x}_n}{\sigma/\sqrt{n}}\right|}$$

for sign $(x) = \{x > 0\} - \{x \le 0\}$ , while

$$\frac{\sup_{\theta_0\in\Theta_0}\ell_n(\theta_0)}{\sup_{\theta\in\Theta}\ell_n(\theta)} = e^{-\frac{1}{2}\left(\frac{\overline{x}_n}{\sigma/\sqrt{n}}\right)^2\left\{\overline{x}_n>0\right\}} = e^{-\frac{1}{2}\left(\frac{\overline{x}_n}{\sigma/\sqrt{n}}\right)^2\left\{\frac{\overline{x}_n}{\sigma/\sqrt{n}}>0\right\}}.$$

The latter likelihood ratio is smaller then c when

$$\frac{\overline{x}_n}{\sigma/\sqrt{n}} \left\{ \frac{\overline{x}_n}{\sigma/\sqrt{n}} > 0 \right\} > c^*$$

for some  $c^*$ . Note that only positive  $c^*$  make sense, otherwise we will never reject.

For any fixed  $\theta$ , let

$$\overline{z}_{\theta} = \frac{\overline{x}_n - \theta}{\sigma/\sqrt{n}}.$$

Then

$$P_{\theta}\left(\frac{\overline{x}_{n}}{\sigma/\sqrt{n}}\left\{\frac{\overline{x}_{n}}{\sigma/\sqrt{n}}>0\right\}>c^{*}\right)=P_{\theta}\left(\overline{z}_{\theta}>c^{*}-\frac{\theta}{\sigma/\sqrt{n}}\right)=1-\Phi\left(c^{*}-\frac{\theta}{\sigma/\sqrt{n}}\right)$$

This function is monotone increasing on  $\Theta_0 = (-\infty, 0]$ . The size of the test is

$$\sup_{\theta \in \Theta_0} P_{\theta} \left( \frac{\overline{x}_n}{\sigma/\sqrt{n}} \left\{ \frac{\overline{x}_n}{\sigma/\sqrt{n}} > 0 \right\} > c^* \right) = 1 - \Phi(c^*) = \alpha$$

so that size control yields the critical value  $c^* = \Phi^{-1}(1-\alpha) = z_{\alpha}$ .

The former likelihood ratio is small when either

$$0 < \frac{\overline{x}_n}{\sigma/\sqrt{n}}$$
 and  $c^* < \frac{\overline{x}_n}{\sigma/\sqrt{n}}$ 

or when

$$\frac{\overline{x}_n}{\sigma/\sqrt{n}} < 0 \text{ and } c^* < \frac{\overline{x}_n}{\sigma/\sqrt{n}}$$

For any  $\theta \in \Theta_0$  the probability of this happening is

$$P_{\theta}\left(\overline{z}_{\theta} > c^{*} - \frac{\theta}{\sigma/\sqrt{n}}, \, \overline{z}_{\theta} > -\frac{\theta}{\sigma/\sqrt{n}}\right) + P_{\theta}\left(\overline{z}_{\theta} > c^{*} - \frac{\theta}{\sigma/\sqrt{n}}, \, \overline{z}_{\theta} < -\frac{\theta}{\sigma/\sqrt{n}}\right).$$

For  $c^* > 0$  this equals

$$P_{\theta}\left(\overline{z}_{\theta} > c^* - \frac{\theta}{\sigma/\sqrt{n}}\right) = 1 - \Phi\left(c^* - \frac{\theta}{\sigma/\sqrt{n}}\right)$$

while for  $c^* \leq 0$  this equals

$$P_{\theta}\left(\overline{z}_{\theta} > -\frac{\theta}{\sigma/\sqrt{n}}\right) + P_{\theta}\left(c^* - \frac{\theta}{\sigma/\sqrt{n}} < \overline{z}_{\theta} \le -\frac{\theta}{\sigma/\sqrt{n}}\right) = 1 - \Phi\left(c^* - \frac{\theta}{\sigma/\sqrt{n}}\right).$$

In either case the supremum over  $\Theta_0$  is achieved at  $\theta = 0$  for which we find that  $c^* = z_{\alpha}$  yields size control. Again, for any reasonable size the critical value is positive.

### Likelihood-ratio test

Now consider a general setting where  $\theta$  is a k-dimensional vector and

$$H_0: r(\theta) = 0, \qquad H_1: r(\theta) \neq 0,$$

for a continuously-differentiable m-dimensional function r.

We will denote the  $m \times k$  Jacobian matrix by  $R(\theta)$ .

Exact size control is difficult in general.

A general approach that is asymptotically valid is the decision rule Reject the null if

$$-2\log\left(\frac{\ell_n(\check{\theta})}{\ell_n(\hat{\theta})}\right) > \chi^2_{m,\alpha};$$

Accept the null if

$$-2\log\left(\frac{\ell_n(\check{\theta})}{\ell_n(\hat{\theta})}\right) \le \chi^2_{m,\alpha}.$$

Note that

$$-2\log\left(\ell_n(\check{\theta})/\ell_n(\hat{\theta})\right) = 2(L_n(\hat{\theta}) - L_n(\check{\theta})).$$

The validity of the test procedure comes from the following theorem.

Theorem 17 (Limit distribution of the Likelihood-ratio statistic) Under the null,  $2(L_n(\hat{\theta}) - L_n(\check{\theta})) \xrightarrow{d} \chi_m^2$ as  $n \to \infty$ .

#### Proof.

We work under the null. A Taylor expansion gives

$$L_n(\check{\theta}) - L_n(\hat{\theta}) = -\frac{n}{2}(\check{\theta} - \hat{\theta})' I_{\theta}(\check{\theta} - \hat{\theta}) + o_p(1).$$

It can be shown that (under the null)

$$\sqrt{n}(\hat{\theta} - \check{\theta}) = I_{\theta}^{-1} R' (RI_{\theta}^{-1} R')^{-1} RI_{\theta}^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right|_{\theta} + o_p(1),$$

where  $R = R(\theta)$ . Plugging this into the expansion gives  $2(L_n(\hat{\theta}) - L_n(\check{\theta}))$  as

$$\left(RI_{\theta}^{-1}\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\left.\frac{\partial\log f_{\theta}(x_{i})}{\partial\theta}\right|_{\theta}\right)'(RI_{\theta}^{-1}R')^{-1}\left(RI_{\theta}^{-1}\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\left.\frac{\partial\log f_{\theta}(x_{i})}{\partial\theta}\right|_{\theta}\right)$$

(up to  $o_p(1)$  terms). But, as

$$RI_{\theta}^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}}{\partial \theta} \right|_{\theta} \xrightarrow{d} N(0, RI_{\theta}^{-1}R'),$$

this quadratric form is asymptotically  $\chi_m^2$ .

### Analysis of the constrained estimator

Completing the proof requires finding the asymptotic distribution of

$$\check{\theta} = \arg \max_{\theta: r(\theta) = 0} L_n(\theta).$$

This estimator maximizes the Lagrangian problem

$$L_n(\theta) + \lambda' r(\theta).$$

The first-order conditions are

$$\frac{\partial L_n(\theta)}{\partial \theta}\Big|_{\check{\theta}} + \check{\lambda}' R(\check{\theta}) = 0, \qquad r(\check{\theta}) = 0.$$

We can Taylor expand

$$\frac{\partial L_n(\theta)}{\partial \theta}\Big|_{\check{\theta}} = \frac{\partial L_n(\theta)}{\partial \theta}\Big|_{\theta} + \frac{\partial^2 L_n(\theta)}{\partial \theta \partial \theta'}\Big|_{\theta} (\check{\theta} - \theta) + o_p(1)$$
$$= \sum_{i=1}^n \frac{\partial \log f_\theta(x_i)}{\partial \theta}\Big|_{\theta} - nI_\theta (\check{\theta} - \theta) + o_p(1),$$

and  $r(\check{\theta}) = r(\theta) + R(\check{\theta} - \theta) + o_p(1) = R(\check{\theta} - \theta) + o_p(1)$  (enforcing the null  $r(\theta) = 0$ ).

Plugging the expansions into the first-order conditions and re-arranging yields the system of equations

$$n^{-1/2} \begin{pmatrix} -nI_{\theta} & R' \\ R & 0 \end{pmatrix} \begin{pmatrix} \check{\theta} - \theta \\ \check{\lambda} \end{pmatrix} = -n^{-1/2} \begin{pmatrix} \sum_{i=1}^{n} \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \Big|_{\theta} \\ 0 \end{pmatrix}$$

(up to  $o_p(1)$  terms).

A block-inversion formula shows that

$$\left(\begin{array}{cc} -nI_{\theta} & R \\ R' & 0 \end{array}\right)^{-1}$$

equals

$$\begin{pmatrix} -n^{-1}I_{\theta}^{-1} + n^{-1}I_{\theta}^{-1}R'(RI_{\theta}^{-1}R')^{-1}RI_{\theta}^{-1} & I_{\theta}^{-1}R'(RI_{\theta}^{-1}R')^{-1} \\ (RI_{\theta}^{-1}R')^{-1}RI_{\theta}^{-1} & n(RI_{\theta}^{-1}R')^{-1} \end{pmatrix}.$$

Then we obtain

$$\sqrt{n}(\check{\theta} - \theta) = (I_{\theta}^{-1} - I_{\theta}^{-1}R'(RI_{\theta}^{-1}R')^{-1}RI_{\theta}^{-1}) \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \right|_{\theta} + o_{p}(1),$$

which implies that

$$\sqrt{n}(\hat{\theta} - \check{\theta}) = I_{\theta}^{-1} R' (RI_{\theta}^{-1} R')^{-1} RI_{\theta}^{-1}) \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left. \frac{\partial \log f_{\theta}(x_i)}{\partial \theta} \right|_{\theta} + o_p(1)$$

under the null.

For future reference we also note that

$$\frac{\check{\lambda}}{\sqrt{n}} = -(RI_{\theta}^{-1}R')^{-1}RI_{\theta}^{-1}\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\left.\frac{\partial\log f_{\theta}(x_{i})}{\partial\theta}\right|_{\theta} + o_{p}(1) \xrightarrow{d} N(0, (RI_{\theta}^{-1}R')^{-1}).$$

$$\chi^2$$
-statistic

The derivation of the limit distribution of the likelihood-ratio statistic shows that

$$n \, (\check{\theta} - \hat{\theta})' I_{\theta} (\check{\theta} - \hat{\theta}) \stackrel{d}{\to} \chi_m^2$$

under the null.

Let  $I_{\theta}$  be a consistent estimator of the information under the null. Obvious choices are

$$-\frac{1}{n} \left. \frac{\partial^2 L_n(\theta)}{\partial \theta \partial \theta'} \right|_{\check{\theta}} = -\frac{1}{n} \sum_{i=1}^n \left. \frac{\partial^2 \log f_\theta(x_i)}{\partial \theta \partial \theta'} \right|_{\check{\theta}}$$

and

$$\frac{1}{n}\sum_{i=1}^{n} \left( \left. \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \right|_{\check{\theta}} \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \right|_{\check{\theta}}' \right) - \left( \frac{1}{n}\sum_{i=1}^{n} \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \right|_{\check{\theta}} \right) \left( \frac{1}{n}\sum_{i=1}^{n} \frac{\partial \log f_{\theta}(x_{i})}{\partial \theta} \right|_{\check{\theta}} \right)'$$

note that recentering of the score is needed here as  $\check{\theta}$  does not maximize the unconstrained likelihood problem, in general.

Slutzky's theorem gives us the following result.

Theorem 18 (Limit distribution of the $\chi^2$ -statistic)									
Under the null,									
$n  (\check{ heta} - \hat{ heta})' \check{I}_{ heta} (\check{ heta} - \hat{ heta}) \stackrel{d}{ ightarrow} \chi_m^2$									

as  $n \to \infty$ .

This result gives us an alternative, but asymptotically equivalent, testing procedure.

The intuition behind a test based on this result is to look at a distance between the constrained and the unconstrained estimators which, under the null, should be small. The analysis of the constrained estimator implies the following result.

Theorem 19 (Limit distribution of the Score statistic)

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Under the null,

$$\frac{\partial L_n(\theta)}{\partial \theta}\Big|_{\tilde{\theta}}' \left(\frac{\check{I}_{\theta}^{-1}}{n}\right) \left.\frac{\partial L_n(\theta)}{\partial \theta}\right|_{\tilde{\theta}} \stackrel{d}{\to} \chi_m^2,$$

as  $n \to \infty$ .

This statistic is also known as the Lagrange-multiplier statistic as it can be written as

$$\check{\lambda}'\left(\frac{R(\check{\theta})\check{I}_{\theta}^{-1}R(\check{\theta})'}{n}\right)\check{\lambda},$$

where  $\lambda$  is the Lagrangian multiplier for the constraint  $r(\theta) = 0$ .

One interpretation for this is that, if the null is true, the constraint should be ineffective, aside from sampling error, so  $\tilde{\lambda}$  should be small.

Another interpretation is that, under the null, the unconstrained score should be close to zero at  $\check{\theta}$ .

Rather than evaluating some distance between  $\check{\theta}$  and  $\hat{\theta}$  as in the  $\chi^2$ -statistic

$$n\,(\check{\theta}-\hat{\theta})'\check{I}_{\theta}(\check{\theta}-\hat{\theta}),$$

we may look at a distance of  $r(\hat{\theta})$  from zero (the null). Because we have that

$$r(\hat{\theta}) = r(\hat{\theta}) - r(\check{\theta}) = R\left(\hat{\theta} - \check{\theta}\right) + o_p(1)$$

under the null, we equally have the following.

Theorem 20 (Limit distribution of the Wald statistic)

Under the null,

$$n r(\hat{\theta})'(R(\check{\theta})\check{I}_{\theta}^{-1}R(\check{\theta})')^{-1} r(\hat{\theta}) \stackrel{d}{\to} \chi_m^2,$$

as  $n \to \infty$ .

The Wald statistic can equally be derived without reference to a constrained estimation problem.

Because

$$\sqrt{n}(\hat{\theta} - \theta) \stackrel{d}{\rightarrow} N(0, I_{\theta}^{-1}) \text{ and } r(\hat{\theta}) = R(\hat{\theta} - \theta) + o_p(1),$$

under the null, the Delta method gives

$$\sqrt{n}\,r(\hat{\theta})\stackrel{d}{\rightarrow} N(0,RI_{\theta}^{-1}R'),$$

and so also

Theorem 21 (Limit distribution of the Wald statistic (cont'd)) Under the null, $n r(\hat{\theta})' (R(\hat{\theta}) \hat{I}_a^{-1} R(\hat{\theta})')^{-1} r(\hat{\theta}) \xrightarrow{d} \chi_m^2,$ 

as  $n \to \infty$ .

Here it makes sense to use an unconstrained estimator of the information.

All test statistics can be used in the same way to perform (asymptotically) valid inference.

In small samples they can lead to different test conclusions.

The likelihood-ratio statistic is attractive because

- It does not require an estimator of  $I_{\theta}$ ;
- It is invariant with respect to one-to one transformations.

The second point is important as it implies that the test conclusion is the same no matter how the null is formulated.

The score statistic is attractive because it requires estimation only under the null, which is often easier.

In the likelihood context there is no strong argument in favor of the Wald statistic. In fact it is not likelihood based. Its power lies in that it can be applied more generally.

The exponential distribution is

$$f_{\theta}(x) = \frac{e^{-x/\theta}}{\theta}.$$

Its mean is  $\theta$ .

We set up several tests for the null  $H_0: \theta = \theta_0$  against  $\theta \neq \theta_0$ . First note that

$$L_n(\theta) = -\sum_{i=1}^n (x_i/\theta + \log \theta) = -n\overline{x}_n/\theta - n\log \theta.$$

Hence,

$$\frac{\partial L_n(\theta)}{\partial \theta} = (n/\theta)(\overline{x}_n/\theta - 1), \qquad \frac{\partial^2 L_n(\theta)}{\partial \theta^2} = -(n/\theta^2)(2\overline{x}_n/\theta - 1).$$

Therefore,  $\hat{\theta} = \overline{x}_n$  and  $I_{\theta}^{-1}/n = \theta^2/n$ .

The likelihood-ratio statistic is

$$-2(L_n(\theta_0) - L_n(\hat{\theta})) = 2n\left(\left(\frac{\overline{x}_n}{\theta_0} - 1\right) - \log\frac{\overline{x}_n}{\theta_0}\right).$$

The score statistic is

$$n(\overline{x}_n/\theta_0 - 1)^2 = \frac{(\overline{x}_n - \theta_0)^2}{\theta_0^2/n}$$

The  $\chi^2\mbox{-statistic}$  and the Wald statistic are

$$rac{(\overline{x}_n- heta_0)^2}{ heta_0^2/n}, \qquad rac{(\overline{x}_n- heta_0)^2}{\overline{x}_n^2/n},$$

respectively. The latter is again the usual t-statistic, which should not be surprising here.

Recall the setup

$$y_i | x_i \sim N(x_i'\beta, \sigma^2)$$

or, in matrix notation,

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \qquad \boldsymbol{\varepsilon} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I}).$$

The log-likelihood (up to a constant) is

$$L_n(\beta, \sigma^2) = -\frac{n}{2}\log\sigma^2 - \frac{(\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta)}{2\sigma^2}.$$

Let  $SSR_{\beta} = (\boldsymbol{y} - \boldsymbol{X}\beta)'(\boldsymbol{y} - \boldsymbol{X}\beta)$ . Then the profiled log-likelihood for  $\beta$  is

$$L_n(\beta) = -\frac{n}{2}\log\left(SSR_\beta\right) = \log(SSR_\beta^{-n/2})$$

(again up to a constant), and

$$\ell_n(\beta) \propto SSR_{\beta}^{-n/2}.$$
We consider a set of m linear restrictions on  $\beta.$  We express the null hypothesis as

$$R\beta = r,$$

where R is an  $m \times k$  matrix and r and is an m-vector.

The *m* restrictions are non-redundant, so rank R = m.

The unconstrained estimator solves

$$\min_eta SSR_eta = \min_eta (oldsymbol{y} - oldsymbol{X}eta)'(oldsymbol{y} - oldsymbol{X}eta)$$

and equals

$$\hat{\beta} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}\boldsymbol{y},$$

as before.

The constrained estimator solves the Lagrangian problem

$$\min_{\beta} \frac{1}{2} SSR_{\beta} - \lambda' (R\beta - r).$$

The first-order conditions are

$$\mathbf{X}'(\mathbf{y} - \mathbf{X}\beta) - R'\lambda = 0, \qquad R\beta - r = 0.$$

Re-arranging the first condition gives

$$(\boldsymbol{X}'\boldsymbol{X})\beta = \boldsymbol{X}'\boldsymbol{y} - R'\lambda$$

and so

$$\check{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y} - (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{R}'\boldsymbol{\lambda} = \hat{\boldsymbol{\beta}} - (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{R}'\boldsymbol{\lambda}.$$

Further, pre-multiplying by R and enforcing that  $R\check{\beta}=r$  gives

$$R\check{\beta} = R\hat{\beta} - R(\boldsymbol{X}'\boldsymbol{X})^{-1}R'\lambda = r,$$

which we solve for  $\lambda$  to obtain

$$\check{\lambda} = (R(\boldsymbol{X}'\boldsymbol{X})^{-1}R')^{-1}(R\hat{\beta} - r).$$

We then find that

$$\check{\beta} = \hat{\beta} - (\boldsymbol{X}'\boldsymbol{X})^{-1}R'(R(\boldsymbol{X}'\boldsymbol{X})^{-1}R')^{-1}(R\hat{\beta} - r).$$

The likelihood ratio statistic is

$$\left(rac{SSR_{\check{eta}}}{SSR_{\hat{eta}}}
ight)^{-n/2},$$

which is small when the ratio in brackets is large. Now,

$$\frac{SSR_{\hat{\beta}}}{SSR_{\hat{\beta}}} - 1 = \frac{SSR_{\hat{\beta}} - SSR_{\hat{\beta}}}{SSR_{\hat{\beta}}}$$

where

$$SSR_{\hat{\beta}} = \hat{\varepsilon}'\hat{\varepsilon} = \varepsilon' M_{X}\varepsilon$$

and, using that  $\boldsymbol{y} = \boldsymbol{X}\hat{\beta} + \hat{\boldsymbol{\varepsilon}}$  to simplify  $SSR_{\check{\beta}} = (\boldsymbol{y} - \boldsymbol{X}\check{\beta})'(\boldsymbol{y} - \boldsymbol{X}\check{\beta})$  to

$$SSR_{\check{\beta}} = \boldsymbol{\varepsilon}' \boldsymbol{M}_{\boldsymbol{X}} \boldsymbol{\varepsilon} + (\hat{\beta} - \check{\beta})' (\boldsymbol{X}' \boldsymbol{X}) (\hat{\beta} - \check{\beta}).$$

Hence,

$$\frac{SSR_{\hat{\beta}} - SSR_{\hat{\beta}}}{SSR_{\hat{\beta}}} = \frac{(\hat{\beta} - \check{\beta})'(\mathbf{X}'\mathbf{X})(\hat{\beta} - \check{\beta})}{\boldsymbol{\varepsilon}'\mathbf{M}_{\mathbf{X}}\boldsymbol{\varepsilon}} = \frac{(R\hat{\beta} - r)'(R(\mathbf{X}'\mathbf{X})^{-1}R')^{-1}(R\hat{\beta} - r)}{\boldsymbol{\varepsilon}'\mathbf{M}_{\mathbf{X}}\boldsymbol{\varepsilon}}.$$

Note that, under the null,

$$R\hat{\beta} - r \sim N(0, \sigma^2 R(\boldsymbol{X}'\boldsymbol{X})^{-1}R')$$

such that

$$\frac{SSR_{\check{\beta}} - SSR_{\hat{\beta}}}{\sigma^2} \sim \chi_m^2.$$

We also know that

$$\frac{SSR_{\hat{\beta}}}{\sigma^2} = (n-k)\frac{\tilde{\sigma}^2}{\sigma^2} \sim \chi^2_{n-k}.$$

Lastly, both terms are independent because they are functions of  $\hat{\beta}$  and  $\hat{\varepsilon}$ , respectively. These variables are jointly normal and independent, as the covariance is

$$E((\hat{\beta}-\beta)\hat{\varepsilon}'|\mathbf{X}) = E\left((\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\varepsilon\varepsilon'\mathbf{M}_{\mathbf{X}}|\mathbf{X}\right) = \sigma^{2}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{M}_{\mathbf{X}} = 0$$

(using that  $\boldsymbol{M}_{\boldsymbol{X}}\boldsymbol{X}=0$ )

Therefore,

$$\frac{n-k}{m}\frac{SSR_{\hat{\beta}}-SSR_{\hat{\beta}}}{SSR_{\hat{\beta}}}\sim F_{m,n-k},$$

where F is Snedecor's F distribution.

# Snedecor's F distribution

The quantile function of the F distribution



$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$									$\alpha = 0.9$	)							
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$		$\nu_1$															
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		1	2	3	4	5	6	7	8	9	10	12	15	20	30	50	$\infty$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\nu_2$																
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	1	39.9	49.5	53.6	55.8	57.2	58.2	58.9	59.4	59.9	60.2	60.7	61.2	61.7	62.3	62.7	63.3
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	2	8.53	9.00	9.16	9.24	9.29	9.33	9.35	9.37	9.38	9.39	9.41	9.42	9.44	9.46	9.47	9.49
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3	5.54	5.46	5.39	5.34	5.31	5.28	5.27	5.25	5.24	5.23	5. 22	5.20	5.18	5.17	5.15	5.13
5         4.06         3.78         3.62         3.52         3.45         3.40         3.37         3.34         3.32         3.30         3.27         3.24         3.21         3.17         3.15         3.10           6         3.78         3.46         3.29         3.18         3.11         3.05         3.01         2.98         2.94         2.90         2.87         2.84         2.80         2.77         2.72           7         3.59         3.26         3.07         2.96         2.88         2.83         2.78         2.75         2.72         2.70         2.67         2.63         2.59         2.56         2.54         2.42         2.88         2.35         2.242         2.88         2.35         2.242         2.88         2.35         2.25         2.61         2.50         2.64         2.40         2.42         2.88         2.35         2.242         2.38         2.34         2.30         2.25         2.24         2.42         2.88         2.35         2.262         2.44         2.48         2.39         2.34         2.30         2.25         2.24         2.20         2.16         2.15         2.16         2.16         2.16         2.16         2.16	4	4.54	4.32	4.19	4.11	4.05	4.01	3.98	3.95	3.94	3.92	3.90	3.87	3.84	3.82	3.80	3.76
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	5	4.06	3.78	3.62	3.52	3.45	3.40	3.37	3.34	3.32	3.30	3. 27	3.24	3.21	3.17	3.15	3.10
7         3.59         3.26         3.07         2.96         2.88         2.83         2.75         2.75         2.70         2.67         2.63         2.59         2.56         2.52         2.44           8         3.46         3.11         2.92         2.81         2.73         2.67         2.62         2.59         2.56         2.54         2.50         2.46         2.42         2.38         2.35         2.29         9         3.66         3.01         2.81         2.69         2.61         2.55         2.51         2.44         2.42         2.38         2.30         2.25         2.22         2.16         2.12         2.06         2.44         2.42         2.38         2.30         2.52         2.22         2.16         2.12         2.06           10         3.29         2.92         2.73         2.61         2.45         2.39         2.34         2.30         2.25         2.21         2.17         2.12         2.06         2.04         1.97           12         3.18         2.81         2.61         2.45         2.39         2.33         2.28         2.24         2.19         2.15         2.10         2.06         2.01         1.97 <td< td=""><td>6</td><td>3.78</td><td>3.46</td><td>3.29</td><td>3.18</td><td>3.11</td><td>3.05</td><td>3.01</td><td>2.98</td><td>2.96</td><td>2.94</td><td>2.90</td><td>2.87</td><td>2.84</td><td>2.80</td><td>2.77</td><td>2.72</td></td<>	6	3.78	3.46	3.29	3.18	3.11	3.05	3.01	2.98	2.96	2.94	2.90	2.87	2.84	2.80	2.77	2.72
8         3.46         3.11         2.92         2.81         2.73         2.67         2.62         2.59         2.56         2.54         2.50         2.46         2.42         2.38         2.35         2.29         9         3.36         3.01         2.81         2.73         2.67         2.52         2.51         2.54         2.50         2.46         2.42         2.38         2.35         2.22         2.10           10         3.29         2.92         2.73         2.61         2.55         2.51         2.47         2.44         2.42         2.38         2.34         2.30         2.25         2.22         2.16         2.12         2.06           10         3.29         2.92         2.73         2.61         2.55         2.31         2.37         2.28         2.24         2.38         2.35         2.22         2.16         2.12         2.06           11         3.32         2.86         2.66         2.54         2.45         2.30         2.27         2.25         2.21         2.17         2.12         2.08         2.04         1.97           12         3.18         2.81         2.61         2.43         2.35         2.28         2.2	7	3.59	3.26	3.07	2.96	2.88	2.83	2.78	2.75	2.72	2.70	2.67	2.63	2.59	2.56	2.52	2.47
9         3.36         3.01         2.81         2.69         2.61         2.55         2.51         2.47         2.44         2.42         2.38         2.34         2.30         2.25         2.22         2.16           10         3.29         2.92         2.73         2.61         2.55         2.51         2.47         2.44         2.42         2.38         2.34         2.30         2.25         2.22         2.16         2.12         2.06           11         3.29         2.92         2.73         2.61         2.55         2.34         2.30         2.27         2.20         2.16         2.12         2.06           12         3.18         2.81         2.61         2.45         2.39         2.34         2.30         2.27         2.21         2.17         2.12         2.08         2.04         1.97           12         3.18         2.81         2.61         2.45         2.39         2.33         2.28         2.24         2.10         2.10         2.06         2.01         1.96         1.92         1.83           13         3.14         2.76         2.56         2.43         2.35         2.28         2.24         2.10         2.10<	8	3.46	3.11	2.92	2.81	2.73	2.67	2.62	2.59	2.56	2.54	2.50	2.46	2.42	2.38	2.35	2.29
10         3.29         2.92         2.73         2.61         2.52         2.46         2.41         2.38         2.35         2.32         2.28         2.24         2.20         2.16         2.12         2.06           11         3.23         2.86         2.66         2.54         2.45         2.39         2.34         2.30         2.27         2.25         2.21         2.17         2.12         2.08         2.04         1.97           12         3.18         2.81         2.61         2.48         2.39         2.34         2.30         2.27         2.25         2.21         2.17         2.12         2.08         2.04         1.97           12         3.18         2.81         2.61         2.48         2.39         2.33         2.28         2.24         2.19         2.15         2.10         2.06         2.01         1.97         1.90           13         3.14         2.76         2.56         2.43         2.35         2.28         2.20         2.16         2.14         2.10         2.05         2.01         1.96         1.92         1.85           14         3.10         2.73         2.70         2.40         2.36         2.02	9	3.36	3.01	2.81	2.69	2.61	2.55	2.51	2.47	2.44	2.42	2.38	2.34	2.30	2.25	2.22	2.16
11         3.23         2.86         2.66         2.54         2.45         2.39         2.34         2.30         2.27         2.25         2.11         2.17         2.12         2.08         2.04         1.97           12         3.18         2.81         2.61         2.48         2.39         2.33         2.28         2.24         2.11         2.15         2.10         2.06         2.01         1.97         1.90           13         3.14         2.76         2.56         2.43         2.35         2.28         2.20         2.16         2.14         2.10         2.05         2.01         1.96         1.92         1.85           14         3.10         2.73         2.72         2.21         2.10         2.01         2.96         1.91         1.87         1.80           15         3.07         2.77         2.70         2.49         2.31         2.24         2.19         2.15         2.12         2.10         2.05         2.01         1.96         1.92         1.87           15         3.07         2.77         2.49         2.36         2.02         2.10         2.05         2.01         1.96         1.91         1.87         1.88	10	3.29	2.92	2.73	2.61	2.52	2.46	2.41	2.38	2.35	2.32	2.28	2.24	2.20	2.16	2.12	2.06
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$																	
12         3.18         2.81         2.61         2.48         2.39         2.33         2.28         2.24         2.11         2.19         2.15         2.10         2.06         2.01         1.97         1.90           13         3.14         2.76         2.56         2.43         2.35         2.28         2.24         2.20         2.16         2.10         2.05         2.01         1.96         1.92         1.85           14         3.10         2.73         2.52         2.39         2.31         2.24         2.19         2.15         2.10         2.05         2.01         1.96         1.92         1.85           14         3.10         2.73         2.52         2.39         2.31         2.24         2.19         2.15         2.10         2.05         2.01         1.96         1.92         1.87         1.80           15         3.07         2.70         2.40         2.36         2.12         2.10         2.05         2.01         1.96         1.91         1.87         1.80           15         3.07         2.70         2.40         2.36         2.02         2.02         2.06         2.06         2.02         1.97         1.92	11	3.23	2.86	2.66	2.54	2.45	2.39	2.34	2.30	2.27	2.25	2.21	2.17	2.12	2.08	2.04	1.97
13         3.14         2.76         2.56         2.43         2.35         2.28         2.20         2.16         2.14         2.10         2.05         2.01         1.96         1.92         1.85           14         3.10         2.73         2.52         2.39         2.31         2.24         2.19         2.15         2.12         2.10         2.05         2.01         1.96         1.92         1.85           15         3.07         2.77         2.40         2.36         2.24         2.19         2.15         2.12         2.10         2.05         2.01         1.96         1.92         1.87           15         3.07         2.70         2.40         2.36         2.24         2.19         2.15         2.12         2.10         2.05         2.01         1.96         1.91         1.87         1.80           15         3.07         2.70         2.40         2.36         2.02         2.02         1.97         1.92         1.87         1.83         1.76	12	3.18	2.81	2.61	2.48	2.39	2.33	2.28	2.24	2.21	2.19	2.15	2.10	2.06	2.01	1.97	1.90
14 3.10 2.73 2.52 2.39 2.31 2.24 2.19 2.15 2.12 2.10 2.05 2.01 1.96 1.91 1.87 1.80 15 3.07 2.70 2.49 2.36 2.27 2.21 2.16 2.12 2.09 2.06 2.02 1.97 1.92 1.87 1.83 1.76	13	3.14	2.76	2.56	2.43	2.35	2.28	2.23	2.20	2.16	2.14	2.10	2.05	2.01	1.96	1.92	1.85
15 3 07 2 70 2 49 2 36 2 27 2 21 2 16 2 12 2 09 2 06 2 02 1 97 1 92 1 87 1 83 1 76	14	3.10	2.73	2.52	2.39	2.31	2.24	2.19	2.15	2.12	2.10	2.05	2.01	1.96	1.91	1.87	1.80
10 0.01 2.10 2.10 2.11 2.21 2.10 2.12 2.00 2.02 1.01 1.02 1.01 1.00 1.19	15	3.07	2.70	2.49	2.36	2.27	2.21	2.16	2.12	2.09	2.06	2.02	1.97	1.92	1.87	1.83	1.76

A popular restriction in a regression model that includes a constant term is that all slopes are zero.

Under the null we only estimate a constant term, i.e.,  $\check{\beta} = \overline{y}_n$ , and so we have

$$SSR_{\tilde{\beta}} = \sum_{i=1}^{n} (y_i - \overline{y}_n)^2 = TSS.$$

It follows that the F-statistic can be written as

$$\frac{n-k}{m} \frac{SSR_{\hat{\beta}} - SSR_{\hat{\beta}}}{SSR_{\hat{\beta}}} = \frac{n-k}{m} \frac{TSS - SSR_{\hat{\beta}}}{SSR_{\hat{\beta}}} = \frac{n-k}{m} \frac{1-R^2}{R^2}$$

with  $R^2 = SSR_{\hat{\beta}}/TSS$  the (centered) coefficient of determination of the unrestricted model.

When we test only the restriction  $\beta_{\kappa} = \beta_{\kappa_0}$  the *F*-statistic is

$$\frac{(\hat{\beta}_{\kappa} - \beta_{\kappa,0})([(\boldsymbol{X}'\boldsymbol{X})^{-1}]_{\kappa,\kappa})^{-1}(\hat{\beta}_{\kappa} - \beta_{\kappa,0})}{\tilde{\sigma}^2} = \left(\frac{\hat{\beta}_{\kappa} - \beta_{\kappa,0}}{\sqrt{\tilde{\sigma}^2[(\boldsymbol{X}'\boldsymbol{X})^{-1}]_{\kappa,\kappa}}}\right)^2.$$

This is the square of the usual *t*-statistic

$$rac{\hat{eta}_\kappa-eta_{\kappa,0}}{\sqrt{ ilde{\sigma}^2[(m{X}'m{X})^{-1}]_{\kappa,\kappa}}}.$$

So the square of a  $t_{n-k}$  random variable is  $F_{1,n-k}$  distributed.

## Joint hypothesis versus multiple single hypotheses

To jointly test the k restrictions  $\beta = \beta_0$  we use the F-statistic

$$rac{1}{k}rac{(\hateta-eta_0)'(oldsymbol{X}'oldsymbol{X})(\hateta-eta_0)}{ ilde{\sigma}^2}.$$

This is not the mean of the *t*-statistics for the *k* individual hypotheses that  $\beta_{\kappa} = \beta_{\kappa,0}$ . The individual *t*-statistics are correlated.

Jointly testing hypothesis gives acceptance regions that are ellipsoids. The union of acceptance regions of multiple individual tests is a hypercube.

Multiple testing problems need size corrections which, in turn, lead to low power.

The family-wise error rate is

$$P\left(\bigcup_{\kappa} \left\{ \left| \frac{\hat{\beta}_{\kappa} - \beta_{\kappa,0}}{\sqrt{\hat{\sigma}^2[(\mathbf{X}'\mathbf{X})^{-1}]_{\kappa,\kappa}}} \right| > t_{n-k,\alpha/2} \right\} \right) \leq \sum_{\kappa} P\left( \left| \frac{\hat{\beta}_{\kappa} - \beta_{\kappa,0}}{\sqrt{\hat{\sigma}^2[(\mathbf{X}'\mathbf{X})^{-1}]_{\kappa,\kappa}}} \right| > t_{n-k,\alpha/2} \right) = k \times \alpha.$$

To keep the family-wise error rate below  $\alpha$  we need to test each of k individual hypothesis at significance level  $\alpha/k$ .

# p-values

If we follow the Neyman-Pearson decision rule we either accept or reject the null.

We may also look at the p-value of a test statistic.

Consider a test procedure where we reject the null when the statistic  $\psi_n$  is large.

If the statistic  $\psi_n$  takes on value  $\psi$  in the data the *p*-value is

 $\sup_{\theta\in\Theta_0} P_{\theta} \left(\psi_n > \psi\right).$ 

This is the probability of observing a value of the test statistic greater than  $\psi$  if the null holds.

Small *p*-values suggest the null is likely to be false.

The  $p\mbox{-}value$  gives a cut-off of significance levels for which a Neyman-Pearson decision rule would accept/reject...

But the *p*-value is informative in its own right and need not lead to a decision about the null. This is Fisher's view.

#### **Inverting test statistics**

As an alternative to a point estimator, testing procedures can give rise to interval estimators.

Suppose we test  $H_0: \theta = \theta_0$  using a decision rule of the form

Accept  $H_0$  if  $\psi_n(\theta_0) \leq c$ 

for some critical value c.

Then the set

$$\hat{\Theta} = \{\theta \in \Theta : \psi_n(\theta) \le c\}$$

constitutes an interval estimator.

If the original test has size  $\alpha$  then

$$P_{\theta_0}(\theta_0 \in \hat{\Theta}) = 1 - \alpha.$$

The interval estimator is also called a  $(1 - \alpha)$  confidence set.

# Normal

Suppose  $x_i \sim N(\theta, \sigma^2)$ .

Consider  $H_0: \theta = \theta_0$  and  $H_1: \theta \neq \theta_0$ .

The likelihood ratio decision rule goes in favor of the null if

$$\left|\frac{\overline{x}_n - \theta_0}{\tilde{\sigma}/\sqrt{n}}\right| \le t_{n-1,\alpha/2}.$$

This means that, for any  $\theta$  in the interval

$$\hat{\Theta} = \left[\overline{x}_n - \frac{\tilde{\sigma}}{\sqrt{n}} t_{n-1,\alpha/2}, \, \overline{x}_n + \frac{\tilde{\sigma}}{\sqrt{n}} t_{n-1,\alpha/2}\right]$$

the null would be accepted.

 $\hat{\Theta}$  is an interval estimator of  $\theta_0$ .

We have

$$P_{\theta_0}\left(\theta_0\in\hat{\Theta}\right)=1-\alpha;$$

and so  $\hat{\Theta}$  is a  $(1 - \alpha)$  confidence interval for  $\theta_0$ .

Now,

 $x_i \sim N(\mu, \theta)$ 

and, say,

$$H_0: \theta = \theta_0, \qquad H_1: \theta > \theta_0.$$

Under the null,

$$\frac{\sum_{i=1}^{n} (x_i - \overline{x}_n)^2}{\theta_0} \sim \chi_{n-1}^2,$$

and we would accept the null if the sample variance

$$\tilde{\theta} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \overline{x}_n)^2$$

satisfies  $\tilde{\theta} \leq (n-1)\theta_0 \chi^2_{n-1,\alpha}$ 

The corresponding interval estimator thus is

$$\left[ (n-1)\,\tilde{\theta}/\chi^2_{n-1,\alpha}, +\infty \right)$$

and has coverage probability  $1 - \alpha$ .

Given a Bayesian posterior  $\pi(\theta|x_1, \ldots, x_n)$  and a region  $\mathcal{R}$  of its support, we may calculate

$$P(\theta \in \mathcal{R} | x_1, \dots, x_n) = \int \{\theta \in \mathcal{R}\} \pi(\theta | x_1, \dots, x_n) \, d\theta.$$

This is a credible probability for the credible set  $\mathcal{R}$ .

Credible regions can be formed in many ways.

For scalar  $\theta$  we could, for example, take the interval  $[q_{\alpha/2}, q_{1-\alpha/2}]$ , where  $q_{\tau}$  is the  $\tau$  quantile of the posterior distribution.

Return to the example where  $x_i \sim N(\theta, \sigma^2)$  (with  $\sigma^2$  known) and we have prior information  $\theta \sim N(\mu, \tau^2)$ .

Here, the posterior was

$$N\left(m,v^2\right)$$

for mean and variance

$$m = \frac{\tau^2}{\tau^2 + \sigma^2/n}\overline{x}_n + \frac{\sigma^2/n}{\tau^2 + \sigma^2/n}\mu, \qquad v^2 = \frac{\tau^2\sigma^2/n}{\tau^2 + \sigma^2/n}$$

So,

$$\frac{\theta - m}{v} \sim N(0, 1)$$

and a  $1 - \alpha$  credible interval is

$$[m-z_{\alpha/2}v; m-z_{\alpha/2}v].$$

We can compute the Frequentist coverage probability of this credible set.

The Frequentist framework has  $\overline{x}_n \sim N(\theta, \sigma^2/n)$  (here  $\theta$  is fixed).

The posterior depends on the data only through its mean,

$$m = \frac{1}{1+\delta}\overline{x}_n + \frac{\delta}{1+\delta}\mu, \qquad \delta = \frac{\sigma^2/n}{\tau^2}.$$

A calculation shows that

$$P_{\theta} \left( m - z_{\alpha/2} v \le \theta \le m + z_{\alpha/2} v \right)$$

equals

$$\Phi\left(\sqrt{1+\delta}\,z_{\alpha/2}+\delta\frac{\theta-\mu}{\sigma/\sqrt{n}}\right)-\Phi\left(-\sqrt{1+\delta}\,z_{\alpha/2}+\delta\frac{\theta-\mu}{\sigma/\sqrt{n}}\right)$$

which is different from  $\Phi(z_{\alpha/2}) - \Phi(-z_{\alpha/2}) = 1 - \alpha$ .

# Stratifying regressions

log wages are (approximately) normal.

Suppose different means but common variance for males and females.

Source	SS	df	MS	Number of	obs =	3,296
Model Residual	8362.48119 1256.29954	2 3,294	4181.240 .38139026	6 Prob > F 8 R-squared	= = =	0.0000
Total	9618.78073	3,296	2.918319	4 Root MSE	=	.61757
lwage	Coef.	Std. Err.	t	P> t  [95	% Conf.	Interval]
male female	1.693011 1.474751	.0148607 .015591	113.93 94.59	0.000 1.6 0.000 1.4	63874 44182	1.722148 1.50532

#### . regress lwage male female, noconstant

Common variance is unrealistic and can be relaxed.

(This will lead us to semiparametric problems; considered below.)

#### . regress lwage male female, noconstant r

Linear regression

Number of obs	=	3,296
F(2, 3294)	=	11042.99
Prob > F	=	0.0000
R-squared	=	0.8694
Root MSE	=	.61757

lwage	Coef.	Robust Std. Err.	t	P> t	[95% Conf.	Interval]
male	1.693011	.0145662	116.23	0.000	1.664452	1.721571
female	1.474751	.0159242	92.61	0.000	1.443529	1.505973

Add homogenous impact of experience.

- . gen exper\_sq = exper\*exper
- . regress lwage male female exper exper\_sq, noconstant

Source	SS	df MS		Numbe	r of obs	=	3,296	
Model Residual	8386.99808 1231.78265	4 3,292	2096.74952 .37417456	Prob R-squa	Prob > F R-squared		0.0000	
Total	9618.78073	3,296	2.9183194	- Adj K Root I	ISE	=	.6117	
lwage	Coef.	Std. Err.	t	P> t	[95% C	Conf.	Interval]	
male female exper exper_sq	.9908539 .7777044 .16438 008899	.0880349 .0876789 .0211123 .0012535	11.26 8.87 7.79 -7.10	0.000 0.000 0.000 0.000	.81824 .60579 .12298 01135	152 137 155 166	1.163462 .9496151 .2057746 0064413	

# Stratify impact of experience by gender.

Source		SS	df	MS	. N	lumber of ob	s =	3,	296
Model Residual	8389 1229	9.4973 .28344	6 3,290	1398.24 .373642	955 F 383 F	Prob > F -squared	=	0.0	000 722
Total	9618	.78073	3,296	2.9183	194 F	Adj K-squared Root MSE		.61	126
	lwage	Coe	ef. St	td. Err.	t	P> t	[95%	Conf.	Interval]
f	male emale	1.2122	294 .1 934 .1	L227945 L320425	9.87 4.15	0.000	.971	5326 1996	1.453055 .8069872
c.male#c.	exper	. 1158	651 .	028354	4.09	0.000	.0602	2719	.1714583
c.male#c.exp	er_sq	0064	624 .0	0016021	-4.03	0.000	009	6036	0033211
c.female#c.	exper	.21952	256.0	345253	6.36	0.000	. 151	8323	.2872189
c.female#c.exp	er_sq	01194	499 .0	0022043	-5.42	0.000	0162	2719	007628

Test the equality of the regression lines.

```
. test (male=female) (c.male#c.exper=c.female#c.exper) (c.male#c.exper_sq=c.female#c.exper_sq)
( 1) male - female = 0
( 2) c.male#c.exper - c.female#c.exper = 0
( 3) c.male#c.exper_sq - c.female#c.exper_sq = 0
F( 3, 3290) = 34.95
Prob > F = 0.0000
```

Test the equality of the intercept and slopes separately.

```
. test (male=female)
( 1) male - female = 0
F( 1, 3290) = 13.57
Prob > F = 0.0002
. test (c.male#c.exper=c.female#c.exper)
( 1) c.male#c.exper - c.female#c.exper = 0
F( 1, 3290) = 5.38
Prob > F = 0.0204
. test (c.male#c.exper_sq=c.female#c.exper_sq)
( 1) c.male#c.exper_sq - c.female#c.exper_sq = 0
F( 1, 3290) = 4.06
Prob > F = 0.0441
```

# $\begin{array}{c} \text{SEMIPARAMETRIC PROBLEMS: (GENERALIZED) METHOD OF} \\ \text{MOMENTS} \end{array}$

# Reading

Asymptotic theory:

Arellano, Appendix A

Hansen II, Chapter 13

Hayashi, Chapter 7

Wooldridge, Chapter 12

Linear instrumental variables:

Hansen II, Chapter 12

Hayashi, Chapter 3

Wooldridge, Chapters 5 and 8

Optimality in conditional moment problems:

Arellano, Appendix B

## Linear model

Recall,

$$y_i = x_i'\theta + \varepsilon_i.$$

Before we had imposed  $\varepsilon_i | x_i \sim N(0, \sigma^2)$ . but suppose that we only require that

$$E(\varepsilon_i|x_i) = 0.$$

We no longer assume that  $y_i | x_i \sim N(x'_i \theta, \sigma^2)$  and so we cannot write down the likelihood.

For example,  $var(\varepsilon_i|x_i)$  is unknown and may depend on  $x_i$ .

All the information we have is contained in conditional moment condition

$$E(\varepsilon_i|x_i) = E_{\theta}(y_i - x'_i\theta|x_i) = 0.$$

This is a semiparametric problem:

The model has a parametric part, the conditional mean, and a nonparametric part, the distribution of  $\varepsilon_i | x_i$ .

Iterating expectations shows that

$$E_{\theta}(x_i(y_i - x'_i\theta)) = 0$$

and the analogy principle suggest estimating  $\theta$  by the solving the empirical moment

$$n^{-1} \sum_{i=1}^{n} x_i (y_i - x'_i \theta) = 0.$$

This gives the ordinary least-squares estimator,

$$\left(n^{-1}\sum_{i=1}^n x_i \, x'_i\right)^{-1} \left(n^{-1}\sum_{i=1}^n x_i \, y_i\right),\,$$

as unique solution provided  $\sum_i x_i x'_i$  has maximal rank.

So, for learning  $\theta$  here, normality of the errors (and knowledge thereof) is not needed.

The errors can be heteroskedastic, skewed, and so on.

But is ordinary least squares still the best estimator of  $\theta$ ? Aside from

$$E_{\theta}(x_i(y_i - x'_i\theta)) = 0$$

we equally have that

$$E_{ heta}((x_i\otimes x_i)(y_i-x_i' heta))=0, \ E_{ heta}((x_i\otimes x_i\otimes x_i)(y_i-x_i' heta))=0, \ .$$

:

$$E_{\theta}((x_i \otimes x_i \otimes \cdots \otimes x_i)(y_i - x'_i \theta)) = 0,$$

and, indeed, that

$$E_{\theta}(\psi(x_i)(y_i - x'_i\theta)) = 0$$

for any vector function  $\psi$ .

How do we optimally exploit all this information?

In a semiparametric model the distribution of the data is no longer known up to a small number of parameters.

The model has parametric part  $(\theta)$ ; and a nonparametric part (say F).

Often (i.e., in these slides), the primary interest lies in the parametric part,  $\theta$  and all available information on  $\theta$  is formulated in terms of (conditional) moment conditions.

A general approach to estimation is GMM.

Can be devised to hit the semiparametric efficiency bound.

Intuitively, this bound is

$$\sup_F I_{\theta,F}^{-1};$$

that is, the largest of the Cramér-Rao bounds in the parametric submodels contained in our semiparametric setting.

In the linear regression model from above this would be the Cramér-Rao bound under the least-favorable distribution for  $\varepsilon_i | x_i$  that satisfies mean independence.

Suppose all we know is that

$$E_{\theta}(\varphi(x_i;\theta)) = 0$$

for some known function  $\varphi$ .

A unique solution will generally not exist when  $\dim \varphi < \dim \theta$ . We say  $\theta$  is underidentified.

Suppose, for now, that  $\dim \varphi = \dim \theta$ . We call this the just-identified case.

A method of moment estimator is a solution to

$$n^{-1}\sum_{i=1}^{n}\varphi(x_i;\theta)=0.$$

The intuition is the analogy principle and similar to the argmax argument.

The argmax result requires that

$$E_{\theta}(\varphi(x_i;\theta_*)) \neq 0$$

for any  $\theta_* \neq \theta$ .

This is **global** identification.

In contrast, local identification means there is a neighborhood around  $\theta$  in which it is the unique solution.

A sufficient condition for this is that the Jacobian matrix

$$E_{\theta}\left(\frac{\partial\varphi(x_i;\theta)}{\partial\theta'}\right)$$

is full rank.

When  $\varphi$  is linear in  $\theta$  local and global identification are the same.

Let  $\hat{\theta}$  satisfy

$$n^{-1}\sum_{i=1}^{n}\varphi(x_i;\hat{\theta}) = 0.$$

We can use a similar argument as used for maximum likelihood to derive its behavior as  $n \to \infty$ .

Under smoothness conditions an expansion gives

$$n^{-1}\sum_{i=1}^{n}\varphi(x_i;\hat{\theta}) = n^{-1}\sum_{i=1}^{n}\varphi(x_i;\theta) + n^{-1}\sum_{i=1}^{n}\left.\frac{\partial\varphi(x_i;\theta)}{\partial\theta'}\right|_{\theta_*}(\hat{\theta} - \theta).$$

Re-arrangement gives

$$\sqrt{n}(\hat{\theta} - \theta) = \left( -\frac{1}{n} \sum_{i=1}^{n} \left. \frac{\partial \varphi(x_i; \theta)}{\partial \theta'} \right|_{\theta_*} \right)^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \varphi(x_i; \theta).$$

Under a dominance condition we have

$$-\frac{1}{n}\sum_{i=1}^{n}\left.\frac{\partial\varphi(x_{i};\theta)}{\partial\theta'}\right|_{\theta_{*}} \xrightarrow{p} -E_{\theta}\left(\frac{\partial\varphi(x_{i};\theta)}{\partial\theta'}\right) = -\Gamma_{\theta} \text{ (say)}.$$

Also,  $\varphi(x_i; \theta)$  is i.i.d. with zero mean. So we have

$$\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\varphi(x_i;\theta) \stackrel{d}{\to} N(0,\Omega_{\theta})$$

provided that the asymptotic variance

$$\Omega_{\theta} = \operatorname{var}_{\theta}(\varphi(x_i;\theta)) = E_{\theta}(\varphi(x_i;\theta)\varphi(x_i;\theta)')$$

exists.

Combined with Slutzky's theorem we get the following result.

Theorem 22 (Limit distribution of MM estimator)

Under regularity conditions,

$$\sqrt{n}(\hat{\theta} - \theta) \stackrel{d}{\to} N(0, \Gamma_{\theta}^{-1}\Omega_{\theta}\Gamma_{\theta}^{-\prime}),$$

as  $n \to \infty$ .

#### Linear model

Our model is

$$y_i = x'_i \theta + \varepsilon_i, \qquad E_\theta(x_i \varepsilon_i) = 0.$$

Here,  $\varphi(x_i; \theta) = x_i(y_i - x_i'\theta)$ , which gives the least-squares estimator. Further,

$$\Omega_{\theta} = E(\varepsilon_i^2 x_i x_i'), \qquad \Gamma_{\theta} = -E(x_i x_i').$$

The asymptotic variance is

$$E(x_i x_i')^{-1} E(\varepsilon_i^2 x_i x_i') E(x_i x_i')^{-1}.$$

The variance would simplify if we additionally have that  $var(\varepsilon_i|x_i) = \sigma^2$ . This is an assumption of homoskedasticity.

Then (by iterating expectations)

$$E(\varepsilon_i^2 x_i x_i') = \sigma^2 E(x_i x_i'),$$

so that the asymptotic variance would be

$$\sigma^2 E(x_i x_i')^{-1}$$

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We estimate the asymptotic variance as

$$\left(\frac{1}{n}\sum_{i=1}^n x_i x_i'\right)^{-1} \left(\frac{1}{n}\sum_{i=1}^n \hat{\varepsilon}_i^2 x_i x_i'\right) \left(\frac{1}{n}\sum_{i=1}^n x_i x_i'\right)^{-1},$$

where  $\hat{\varepsilon}_i = y_i - x'_i \hat{\theta}$  are the residuals from the least-squares regression. Under homosked asticity we can use

$$\left(\frac{1}{n}\sum_{i=1}^{n}\hat{\varepsilon}_{i}^{2}\right)\left(\frac{1}{n}\sum_{i=1}^{n}x_{i}x_{i}'\right)^{-1}$$

(could also apply the usual degrees-of-freedom correction to the first term).

Note that least squares is no longer normally distributed for small n because the errors need no longer be normal.

Consequently, the exact distribution of usual t and F statistics is unknown.

### Exponential regression

Nonlinear conditional-mean models can be handled in the same way. For example,

$$E_{\theta}(y_i|x_i) = e^{x'_i \theta} = \mu_i \text{ (say)}$$

implies the moment condition

$$E_{\theta}(x_i(y_i - \mu_i)) = E_{\theta}(x_i\varepsilon_i) = E_{\theta}(x_i(y_i - e^{x'_i\theta})) = 0$$

(among others) and so the estimator that sets

$$n^{-1} \sum_{i=1}^{n} x_i (y_i - e^{x'_i \theta}) = 0.$$

This equals the score equation for Poisson (see Slides 122–123).

Sometimes called the pseudo Poisson estimator.

However, the maximum-likelihood standard errors do not apply because the information equality does not hold here:

$$\Omega_{\theta} = E(x_i x_i' \varepsilon_i^2) \neq E(x_i x_i' \mu_i) = -\Gamma_{\theta}.$$

#### Pseudo Poisson : gravity equation

Poisson regres	ssion			Number	of obs	= 18,360
				LR chi	2(14)	= 2.10e+10
				Prob >	chi2	= 0.0000
Log likelihood	d = -8.702e+0	В		Pseudo	R2	= 0.9235
trade	Coef.	Std. Err	. z	P> z	[95% Con	f. Interval]
lypex	.7324808	.0000147	5.0e+04	0.000	.732452	.7325095
lypim	.741078	.0000148	5.0e+04	0.000	.7410491	.741107
lyex	.1567117	.0000237	6614.74	0.000	.1566653	.1567581
lyim	.1350185	.0000235	5749.58	0.000	.1349725	.1350645
ldist	7838006	.0000321	-2.4e+04	0.000	7838635	7837376
border	.1929108	.0000616	3130.61	0.000	.19279	.1930316
comlang	.745984	.0000672	1.1e+04	0.000	.7458522	.7461157
colony	.0250065	.0000783	319.50	0.000	.0248531	.0251599
landl_ex	8634737	.0001035	-8346.36	0.000	8636765	8632709
landl_im	6964204	.0000977	-7130.30	0.000	6966119	696229
lremot_ex	.65984	.0000862	7652.08	0.000	.659671	.6600091
lremot_im	.5615002	.000086	6529.56	0.000	.5613317	.5616687
comfrt_wto	.1811072	.0000644	2811.04	0.000	.1809809	.1812334
open_wto	1068187	.0000694	-1538.35	0.000	1069548	1066826
_cons	-32.3261	.0010727	-3.0e+04	0.000	-32.32821	-32.324

		Robust				
trade	Coef.	Std. Err.	z	P> z	[95% Conf.	Interval]
lypex	.7324808	.0267915	27.34	0.000	.6799703	.7849912
lypim	.741078	.0274146	27.03	0.000	.6873463	.7948098
lyex	.1567117	.0533293	2.94	0.003	.0521882	.2612352
lyim	.1350185	.0448872	3.01	0.003	.0470412	.2229957
ldist	7838006	.0546055	-14.35	0.000	8908255	6767757
border	.1929108	.1043179	1.85	0.064	0115486	.3973702
comlang	.745984	.1347222	5.54	0.000	.4819333	1.010035
colony	.0250065	.1498038	0.17	0.867	2686036	.3186166
landl_ex	8634737	.157181	-5.49	0.000	-1.171543	5554047
landl_im	6964204	.1407874	-4.95	0.000	9723586	4204823
lremot_ex	.65984	.1337805	4.93	0.000	.397635	.9220451
lremot_im	.5615002	.1185181	4.74	0.000	.329209	.7937914
comfrt_wto	.1811072	.0885591	2.05	0.041	.0075344	.3546799
open_wto	1068187	.131239	-0.81	0.416	3640425	.1504051
_cons	-32.3261	2.059504	-15.70	0.000	-36.36266	-28.28955

The maximum-likelihood estimator is a method-of-moment estimator. The moment condition is

$$E_{\theta}\left(\frac{\partial \log f_{\theta}(x_i)}{\partial \theta}\right) = 0$$

and is always just identified.

Here,

$$\Omega_{\theta} = -\Gamma_{\theta}$$

holds by the information equality.

When the distribution of the data is misspecified (so the sample is not drawn from  $f_{\theta}$ ) the score equation is biased and maximum likelihood inconsistent, in general.

This makes semiparametric alternatives attractive.
An Extremum (or M-) estimator is generic terminology for estimators that maximize an objective function, i.e,

$$\arg\max_{\theta} Q_n(\theta),$$

where  $Q_n(\theta) = \sum_i q(x_i; \theta)$  need not be a likelihood function. (Nonlinear) least-squares, for example, has

$$Q_n(\theta) = -\sum_{i=1}^n (y_i - \varphi(x_i; \theta))^2,$$

where  $E_{\theta}(y_i|x_i) = \varphi(x_i; \theta)$  (e.g., probit, logit, poisson, etc.).

If  $Q_n$  is differentiable, the extremum estimator is a GMM estimator, with moment conditions

$$E_{\theta}\left(\frac{\partial q(x_i;\theta)}{\partial \theta}\right) = 0.$$

An example of an M-estimator that is not a GMM estimator is the maximizer of

$$\sum_{i=1}^{n}\sum_{i < j}y_i \left\{ x_i'\theta > x_j'\theta \right\} + y_j \left\{ x_i'\theta < x_j'\theta \right\}.$$

The objective function is a U-process of order two.

The intuition is that, if

$$E(y_i|x_i) = G(x_i'\theta)$$

is monotonic, then

$$\begin{split} E(y_i|x_i) &> E(y_j|x_j) \Rightarrow x'_i\theta > x'_j\theta \\ E(y_i|x_i) &< E(y_j|x_j) \Rightarrow x'_i\theta < x'_j\theta \end{split}$$

However, this objective function is not differentiable in  $\theta$ .

In fact, the summands in the objective function are not independent. We need a different argument to establish the limit behavior of this estimator.

# Quantile regression

Another example of an M-estimator that has a non-smooth objective function is linear quantile regression.

Take an unconditional setting where  $x_i$  has continuous (strictly increasing, for simplicity) distribution F. Let

$$\varrho = \operatorname{med}(x_i) = F^{-1}(1/2).$$

We have

$$\varrho = \arg\min_{\rho} E(|x_i - \rho|).$$

Indeed,

$$E(|x_i - \rho|) = \int |x - \rho| \, dF(x) = \int_{-\infty}^{\rho} (\rho - x) \, dF(x) + \int_{\rho}^{+\infty} (x - \rho) \, dF(x).$$

Using Leibniz's rule,

$$\frac{\partial E(|x_i - \rho|)}{\partial \rho} = \int_{-\infty}^{\rho} dF(x) - \int_{\rho}^{+\infty} dF(x) = F(\rho) - (1 - F(\rho)) = 0$$

has unique solution  $\rho = \varrho$ .

The sample analog is  $n^{-1} \sum_{i=1}^{n} |x_i - \rho|$  and is not differentiable.

An alternative representation of the median follows from

$$F(\varrho) = \frac{1}{2},$$

 $\mathbf{as}$ 

$$E\left(\left\{x \le \varrho\right\} - \frac{1}{2}\right) = 0,$$

which is a moment condition.

This suggest as estimator an (approximate) solution to the empirical moment

$$n^{-1} \sum_{i=1}^{n} \{x_i \le \rho\} - \frac{1}{2} = 0.$$

The solution, say  $\hat{\varrho}$ , has 'nice' asymptotic properties,

$$\hat{\varrho} - \varrho \stackrel{a}{\sim} N\left(0, \frac{1}{n} \frac{1/4}{f(\varrho)^2}\right),$$

but showing this requires different machinery than the one discussed here.

You wish to predict  $y_i$  based on  $x_i$ .

The best predictor depends on how you quantify errors, i.e., the loss function. If  $p(x_i)$  is the predictor,

$$E((y_i - p(x_i))^2)$$

is the expected squared loss.

Under this loss specification the best predictor p minimizes

$$E((y_i - p(x_i))^2) = E(((y_i - E(y_i|x_i)) - (p(x_i) - E(y_i|x_i)))^2)$$
  
=  $E((y_i - E(y_i|x_i))^2) + E((p(x_i) - E(y_i|x_i))^2)$   
=  $E(\operatorname{var}(y_i|x_i)) + E((p(x_i) - E(y_i|x_i))^2)$   
 $\ge E(\operatorname{var}(y_i|x_i)).$ 

The unique solution is  $p(x_i) = E(y_i|x_i)$ .

# Linear prediction

A linear predictor is a linear function of  $x_i$ , i.e.,  $x'_i\beta$  for any vector  $\beta$ .

The best linear predictor under expected squared loss uses the coefficients

$$\arg\min_{\beta} E((y_i - x_i'\beta)^2).$$

They solve

$$E(x_i(y_i - x_i'\beta)) = 0.$$

(uniquely if  $E(x_i x'_i)$  has full rank) and equal

$$\beta = E(x_i x_i')^{-1} E(x_i y_i).$$

This is the population ordinary least-squares coefficient. By very definition,  $x_i$  and  $\varepsilon_i = y_i - x'_i \beta$  are uncorrelated.

Consequently, we can always write

$$y_i = x_i'\beta + \varepsilon_i$$

for some vector  $\beta$  such that  $E(x_i \varepsilon_i) = 0$ .

We call this the linear projection of  $y_i$  on  $x_i$  and write it as  $E^*(y_i|x_i) = x'_i\beta$ . This does not mean that  $E(y_i|x_i) = x'_i\beta$ .

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Again consider

$$y_i = x'_i \theta + \varepsilon_i$$
 but now we allow that  $E(x_i \varepsilon) \neq 0$ .

Note that

- $\bullet E^*(y_i|x_i) \neq x_i'\theta,$
- so  $\theta$  is not a regression coefficient;

• 
$$E(y_i|x_i) = x'_i\theta + E(\varepsilon_i|x_i) \neq x'_i\theta$$
,

SO

$$\frac{\partial E(y_i|x_i)}{\partial x_i} \neq \theta.$$

# **Omitted variables**

Say we have

$$y_i = \alpha_i + x'_i \theta + \eta_i, \qquad E(\eta_i | x_i, \alpha_i).$$

Say an agricultural (log-linearized) Cobb-Douglas production function.

- $y_i$  is output;
- $x_i$  are observable inputs ;
- $\alpha_i$  is soil quality;
- $\eta_i$  is rainfall.

Farmer observes  $(\alpha_i, x_i)$ . We only observe  $x_i$ . In general,  $x_i, \alpha_i$  are not independent.

Estimating

$$y_i = x'_i \theta + (\alpha_i + \eta_i) = x'_i \theta + \varepsilon_i$$

via least-squares suffers from endogeneity bias.

The problem is that  $\alpha_i$  is not observed in data. Otherwise, can just include it in  $x_i$ .

Suppose that

$$y_i = w'_i \theta + \epsilon_i, \qquad E(\epsilon_i | w_i) = 0$$

but (together with  $y_i$ ) we only observe a noisy version of  $w_i$ , say

$$x_i = w_i + \eta_i,$$

for measurement error  $\eta_i$ .

Then

$$y_i = w'_i \theta + \epsilon_i = (x_i - \eta_i)' \theta + \epsilon_i = x'_i \theta + (\epsilon_i - \eta'_i \theta) = x'_i \theta + \varepsilon_i.$$

Suppose, for simplicity, that  $E(\eta_i \epsilon_i) = 0$  and  $E(w_i \eta_i) = 0$ . Then

$$E(x_i\varepsilon_i) = E(x_i(\epsilon_i - \eta'_i\theta)) = -E(x_i\eta'_i)\theta = -E(\eta_i\eta'_i)\theta \neq 0.$$

A least-squares regression would estimate the population quantity

$$E(x_i x_i')^{-1} E(x_i y_i) = \theta + E(x_i x_i')^{-1} E(x_i \varepsilon_i) = \theta - E(x_i x_i')^{-1} E(\eta_i \eta_i') \theta.$$

# Simultaneity

Temporary deviation from notational conventions to analyze market model

$$d_i = \alpha_d - \theta_d p_i + u_i$$
$$s_i = \alpha_s + \theta_s p_i + v_i$$

where  $d_i, s_i, p_i$  are demand, supply, and price, respectively.



We do not observe supply and demand for any given price.

Collected data is on quantity traded and transaction price,  $(q_i, p_i)$ .



Data comes from markets in equilibrium.

So, we solve

$$s_i = d_i$$

for the equilibrium price to get

$$p_i = \frac{\alpha_d - \alpha_s}{\theta_d + \theta_s} + \frac{u_i - v_i}{\theta_d + \theta_s}.$$

This gives traded quantity as

$$q_i = \frac{\alpha_d \theta_s + \alpha_s \theta_d}{\theta_d + \theta_s} + \frac{\theta_s u_i + \theta_d v_i}{\theta_d + \theta_s}.$$

(With  $E(u_i v_i) = 0$ ) the population regression slope of  $q_i$  on  $p_i$  equals

$$\frac{\sigma_u^2}{\sigma_u^2 + \sigma_v^2} \,\theta_s - \frac{\sigma_v^2}{\sigma_u^2 + \sigma_v^2} \,\theta_d,$$

for  $\sigma_u^2 = E(u_i^2)$  and  $\sigma_v^2 = E(v_i^2)$ .

Least-squares estimates a weighted average of supply and demand elasticities.



To see the problem in terms of endogeneity, focus on the estimation of the demand curve.

Then, collecting equations from above,

$$d_i = \alpha_d - \theta_d p_i + u_i, \qquad p_i = \frac{\alpha_d - \alpha_s}{\theta_d + \theta_s} + \frac{u_i - v_i}{\theta_d + \theta_s},$$

Clearly,

$$E(p_i u_i) = E\left(u_i \left(\frac{u_i - v_i}{\theta_d + \theta_s}\right)\right) = \frac{\sigma_u^2}{\theta_d + \theta_s} \neq 0,$$

as the errors in both equations are correlated.

The same happens for the supply curve, as

$$s_i = \alpha_s + \theta_s p_i + v_i, \qquad p_i = \frac{\alpha_d - \alpha_s}{\theta_d + \theta_s} + \frac{u_i - v_i}{\theta_d + \theta_s}$$

and

$$E(p_i v_i) = E\left(v_i\left(\frac{u_i - v_i}{\theta_d + \theta_s}\right)\right) = -\frac{\sigma_v^2}{\theta_d + \theta_s} \neq 0.$$

## Linear instrumental-variable problem

Now suppose we have

$$y_i = x_i'\theta + \varepsilon_i, \qquad E(z_i\varepsilon_i) = 0$$

for instrumental variables  $z_i$  (with dim  $z_i = \dim x_i$ ).

This gives us the moment conditions

$$E_{\theta}(z_i \left(y_i - x'_i \theta\right)) = 0.$$

An instrument is

- valid if  $E(z_i \varepsilon_i) = 0$ ; and
- relevant if  $E(z_i x'_i)$  is full rank.

We then obtain the instrumental-variable estimator

$$\hat{\theta} = \left(\frac{1}{n}\sum_{i=1}^{n} z_i x_i'\right)^{-1} \left(\frac{1}{n}\sum_{i=1}^{n} z_i y_i\right).$$

It is useful to proceed in matrix notation:

$$oldsymbol{y} = oldsymbol{X} heta + oldsymbol{arepsilon}$$

and we set to zero the sample covariance of the errors and instruments. The solution is

$$\hat{\theta} = (\boldsymbol{Z}'\boldsymbol{X})^{-1}(\boldsymbol{Z}'\boldsymbol{y}).$$

Note that this gives least squares when regressors instrument for themselves.

We need at least as many instruments as we have covariates.

To motivate the sequel suppose dim  $z_i > \dim x_i$ . Then the dim  $z_i$  equations

$$\boldsymbol{Z}'(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) = 0$$

involve dim  $x_i < \dim z_i$  unknowns. Then (generically) these equations do not have a solution (for finite n).

The method-of-moment idea fails to provide us with an estimator when we have overidentification.

## Resolving simultaneity with instrumental variables

Return to the estimation of a demand curve but now suppose that

$$d_i = \alpha_d - \theta_d p_i + u_i$$
$$s_i = \alpha_s + \theta_s p_i + \pi z_i + v_i$$

where  $E(z_i u_i) = 0$ .

 $z_i$  shifts supply (relevance) but not demand (exclusion).

We now have the triangular system of equations

$$d_i = \alpha_d - \theta_d \, p_i + u_i$$
$$p_i = \frac{\alpha_d - \alpha_s}{\theta_d + \theta_s} - \frac{\pi}{\theta_d + \theta_s} \, z_i + \frac{u_i - v_i}{\theta_d + \theta_s}.$$

Further, by relevance and exclusion,

$$\operatorname{cov}(d_i, z_i) = \operatorname{cov}(\alpha_d - \theta_d \, p_i + u_i, z_i) = -\theta_d \operatorname{cov}(p_i, z_i),$$

and so

$$-\theta_d = \frac{\operatorname{cov}(d_i, z_i)}{\operatorname{cov}(p_i, z_i)}.$$



Suppose again that

$$y_i = w_i\theta + \epsilon_i,$$

but that  $w_i$  is measured with error, say as  $x_i = w_i + \eta_i$ . Then

$$y_i = x_i\theta + (\epsilon_i - \eta_i\theta)$$

and a regression of  $y_i$  on  $x_i$  does not deliver a consistent estimator of  $\theta$ .

Suppose that we have an additional noisy measurement of  $w_i$ ,

$$z_i = w_i + \zeta_i.$$

If  $E(\zeta_i \eta_i) = 0$  and  $E(\zeta_i \epsilon_i) = 0$  we can estimate  $\theta$  by instrumental variables.

We have

$$E(z_i x_i) = E((w_i + \zeta_i) (w_i + \eta_i)) = \sigma_w^2, \qquad E(z_i (\epsilon_i - \eta_i \theta)) = 0,$$

so  $z_i$  is relevant and valid.

In overidentified problems (where we have more equations than unknowns) we cannot satisfy all empirical moment conditions,

$$\hat{g}(\theta) = n^{-1} \sum_{i=1}^{n} \varphi(x_i; \theta) = 0,$$

exactly.

The solution is to minimize the quadratic form

 $\hat{g}(\theta)' A \hat{g}(\theta).$ 

for some (positive semi-definite) weight matrix A.

This is the generalized method of moments

Intuitively, we minimize the distance  $\|\hat{g}(\theta) - 0\|_A$ .

With

$$\hat{G}(\theta) = \frac{\partial \hat{g}(\theta)}{\partial \theta'} = n^{-1} \sum_{i=1}^{n} \frac{\partial \varphi(x_i; \theta)}{\partial \theta'},$$

the first-order condition to the GMM problem is

$$\hat{G}(\theta)' A \,\hat{g}(\theta) = 0.$$

This is a set of dim  $\theta$  linear combinations of the dim  $\varphi$  original moments. Linear combination is determined by weight matrix A (which we may choose). So different A give different estimators.

The optimal weight matrix turns out to be

$$A = \Omega_{\theta}^{-1}$$

(or a consistent estimator thereof).

# Limit distribution

Combine the convergence result  $\hat{G}(\theta_*) \xrightarrow{p} \Gamma_{\theta}$  for any consistent  $\theta_*$  with the expansion

$$n^{-1}\sum_{i=1}^{n}\varphi(x_i;\hat{\theta}) = n^{-1}\sum_{i=1}^{n}\varphi(x_i;\theta) + n^{-1}\sum_{i=1}^{n}\left.\frac{\partial\varphi(x_i;\theta)}{\partial\theta'}\right|_{\theta_*}(\hat{\theta}-\theta)$$

to see that

$$(\hat{\theta} - \theta) = -(\Gamma_{\theta}' A \Gamma_{\theta})^{-1} \Gamma_{\theta}' A \frac{1}{n} \sum_{i} \varphi(x_{i}; \theta) + o_{p}(n^{-1/2})$$

$$h = \frac{1}{n} \sum_{i} \varphi(x_{i}; \theta) \frac{1}{n} \sum_{i} \varphi(x_{i}; \theta)$$

Then, with

$$\frac{1}{\sqrt{n}}\sum_{i}\varphi(x_{i};\theta)\stackrel{d}{\to}N(0,\Omega_{\theta}),$$

we get the result.

### Theorem 23 (Limit distribution of GMM estimator)

Under regularity conditions,

$$\sqrt{n}(\hat{\theta} - \theta) \xrightarrow{d} N(0, (\Gamma_{\theta}' A \Gamma_{\theta})^{-1} (\Gamma_{\theta}' A \Omega_{\theta} A' \Gamma_{\theta}) (\Gamma_{\theta}' A \Gamma_{\theta})^{-1})$$

as  $n \to \infty$ .

# Theorem 24 (Semiparametric efficiency)

The efficiency bound (for a given set of moment conditions) is

 $(\Gamma_{\theta}'\Omega_{\theta}^{-1}\Gamma_{\theta})^{-1}.$ 

We can establish this by showing that the difference

$$(\Gamma_{\theta}' A \Gamma_{\theta})^{-1} (\Gamma_{\theta}' A \Omega_{\theta} A' \Gamma_{\theta}) (\Gamma_{\theta}' A \Gamma_{\theta})^{-1} - (\Gamma_{\theta}' \Omega^{-1} \Gamma_{\theta})^{-1}$$

is a positive semi-definite matrix.

The bound is achieved if

$$A = \Omega_{\theta}^{-1}$$

(up to a scale) or if we use a consistent estimator.

Note that in this case we have a generalized information equality.

### Proof.

Let

$$C = (\Gamma'_{\theta} A \Gamma_{\theta})^{-1} \Gamma'_{\theta} A \Omega_{\theta}^{1/2}, \qquad D = \Omega_{\theta}^{-1/2} \Gamma_{\theta}.$$

Then

$$(\Gamma_{\theta}' A \Gamma_{\theta})^{-1} (\Gamma_{\theta}' A \Omega_{\theta} A' \Gamma_{\theta}) (\Gamma_{\theta}' A \Gamma_{\theta})^{-1} - (\Gamma_{\theta}' \Omega_{\theta}^{-1} \Gamma_{\theta})^{-1}$$

can be written as

$$CC' - CD(D'D)^{-1}D'C'.$$

But this is

$$CM_DC' \ge 0, \qquad M_D = I_m - D(D'D)^{-1}D'.$$

The inequality follows because  $M_D$  is an orthogonal projection matrix, and so all its eigenvalues are zero or one. Hence, it is positive semi-definite.

To see that the eigenvalues of an orthogonal projector P are all zero or one, let  $\lambda \neq 0$  be an eigenvalue of P. Then  $Px = \lambda x$  for some  $x \neq 0$ . Because Pis idempotent we must also have that  $P^2x = Px = \lambda Px = \lambda^2 x$ . Therefore it must hold that

$$\lambda x = \lambda^2 x_1$$

which can only be true if  $\lambda \in \{0, 1\}$ .



To illustrate the efficiency gain of combining moments suppose that  $x_i \sim \chi_{\theta}^2$ . We know that

$$E_{\theta}(x_i - \theta) = 0$$

so we could estimate  $\theta$  by the sample mean.

But  $\operatorname{var}_{\theta}(x_i) = 2\theta$  so also have the moment condition  $E_{\theta}((x_i - \theta)^2 - 2\theta) = 0$ . Let

$$\varphi(x_i; \theta) = \begin{pmatrix} x_i - \theta \\ (x_i - \theta)^2 - 2\theta \end{pmatrix}.$$

Then

$$\Omega_{\theta} = E_{\theta}(\varphi(x_i;\theta) \,\varphi(x_i;\theta)') = 2\theta \left(\begin{array}{cc} 1 & 4 \\ 4 & 6(\theta+4) \end{array}\right).$$

So,

$$\Omega_{\theta}^{-1} = \frac{1}{\theta(3\theta+4)} \left( \begin{array}{cc} \frac{3(\theta+4)}{2} & -1 \\ -1 & \frac{1}{4} \end{array} \right).$$

The Jacobian of the moment conditions is simply -(1, 2)' and so we find that the asymptotic variance equals

$$2\theta \,\frac{\theta + 4/3}{\theta + 2}.$$

If we would just use one of the moments the asymptotic variance would be

$$2\theta$$
, and  $3\theta(\theta+4)$ ,

respectively. Both are larger.

Note that  $\Omega_{\theta}$  depends on  $\theta$ . So the optimal GMM estimator will generally be a two-step estimator (see below).

Estimation of the weight matrix introduces additional sampling noise that leads to bias and affects the coverage of confidence intervals/size and power of tests.

## Poisson

When  $x_i$  is Poisson we similarly have

$$E_{\theta}(x_i - \theta) = 0, \qquad E_{\theta}((x_i - \theta)^2 - \theta) = 0$$

by the mean/variance equality.

Here,

$$\Omega_{\theta} = \theta \begin{pmatrix} 1 & 1 \\ 1 & 1+2\theta \end{pmatrix}, \qquad \Omega_{\theta}^{-1} = \frac{1}{2\theta^2} \begin{pmatrix} 1+2\theta & -1 \\ -1 & 1 \end{pmatrix}$$

But as  $\Gamma'_{\theta} = -(1,1)$  we get

$$\Gamma'_{\theta}\Omega_{\theta}^{-1}\Gamma_{\theta} = \frac{1}{\theta}.$$

So the asymptotic variance is the same as for the simple estimator  $\overline{x}_n$  based on the first moment condition only.

We knew we should have reached this conclusion here because  $\overline{x}_n$  is the maximum-likelihood estimator and is best unbiased.

We can estimate  $\Omega_{\theta} = E_{\theta}(\varphi(x_i; \theta) \varphi(x_i; \theta)')$  by

$$\hat{\Omega}_{\hat{\theta}} = n^{-1} \sum_{i} \varphi(x_i; \hat{\theta}) \, \varphi(x_i; \hat{\theta})',$$

where we use a first-step GMM estimator  $\hat{\theta}$  (constructed using a feasible A). We then re-estimate  $\theta$  by

$$\hat{\hat{\theta}} = \arg\min_{\theta} \hat{g}(\theta)' \hat{\Omega}_{\hat{\theta}}^{-1} \hat{g}(\theta).$$

In principle, this two-step procedure can be iterated.

Could also consider continuously-updated GMM:

$$\arg\min_{\theta} \hat{g}(\theta)' \hat{\Omega}_{\theta}^{-1} \hat{g}(\theta), \qquad \hat{\Omega}_{\theta} = n^{-1} \sum_{i} \varphi(x_{i};\theta) \, \varphi(x_{i};\theta)'.$$

This is computationally more challenging; first-order condition features extra terms (use MCMC).

Avery, R. B., L. P. Hansen, and V. J. Hotz (1983). Multiperiod probit models and orthogonality condition estimation. *International Economic Review* 24, 21–35.

Becker, G. S., M. Grossman, and K. M. Murphy (1994). An empirical analysis of cigarette addiction. *American Economic Review* 84, 396–418.

Berry, S. T. (1994). Estimating discrete-choice models of product differentiation. RAND Journal of Economics 25, 242–262.

Goldberg, P. K. and F. Verboven (2001). The evolution of price dispersion in the European car market. *Review of Economic Studies* 68, 811–848.

Hansen, L. P. and K. J. Singleton (1982). Generalized instrumental variables estimation of nonlinear rational expectations models. *Econometrica* 50, 1269–1286.

Pakes, A. (1986). Patents as options: Some estimates of the value of holding European patent stocks. *Econometrica* 54, 755–784.

In the linear instrumental-variable problem (with more instruments than covariates) we minimize

$$(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})' \boldsymbol{Z}\boldsymbol{A} \, \boldsymbol{Z}'(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}).$$

The first-order condition is  $(\mathbf{X}'\mathbf{Z})A\mathbf{Z}'(\mathbf{y}-\mathbf{X}\theta)=0$  and the solution is thus

$$\hat{\theta} = (\boldsymbol{X}' \boldsymbol{Z} A \boldsymbol{Z}' \boldsymbol{X})^{-1} (\boldsymbol{X}' \boldsymbol{Z} A \boldsymbol{Z}' \boldsymbol{y}).$$

Under homoskedasticity,

$$\Omega_{\theta} = E(\varepsilon_i^2 z_i z_i') = \sigma_{\varepsilon}^2 E(z_i z_i')$$

so that the optimal weight matrix is simply  $\hat{\sigma}_{\varepsilon}^2 (\mathbf{Z}'\mathbf{Z})^{-1}$ .

The efficient estimator is a one-step estimator and takes the form

$$\hat{\theta} = (X'Z(Z'Z)^{-1}Z'X)^{-1}(X'Z(Z'Z)^{-1}Z'y) = (X'P_ZX)^{-1}(X'P_Zy).$$

This is the two-stage least squares estimator.

To understand 2SLS recall the model

$$y_i = x'_i \theta + \varepsilon_i, \qquad E(z_i \varepsilon_i) = 0$$

and note that we can always use  $E^*(x_i|z_i) = z'_i \pi$  to decompose the covariates as

$$x_i = z'_i \pi + \eta_i = \tilde{x}_i + \eta_i \text{ (say)}.$$

By the validity of  $z_i$  as instrument we have  $E(z_i \varepsilon_i) = 0$  and so we know that

$$E(x_i\varepsilon_i) = E(\tilde{x}_i\varepsilon_i) + E(\eta_i\varepsilon_i) = E(\eta_i\varepsilon_i),$$

i.e.,  $\eta_i$  is the endogenous part of  $x_i$ . Also, by virtue of the linear projection,  $E(z_i\eta_i) = 0$  and so

$$E(\tilde{x}_i\eta_i)=0.$$

It follows that, in

$$y_i = x'_i \theta + \varepsilon_i = \tilde{x}'_i \theta + (\varepsilon_i + \eta'_i \theta) = \tilde{x}'_i \theta + \epsilon_i$$
(say).

the covariates  $\tilde{x}_i$  and error  $\epsilon_i$  are uncorrelated.

In practice,  $\tilde{x}_i$  is unknown. Replacing it with an estimator gives 2SLS:

- Estimate  $\tilde{x}_i$  by  $\hat{x}_i$ , the fitted values from a linear regression of  $x_i$  on  $z_i$ ;
- Estimate  $\theta$  by regressing  $y_i$  on  $\hat{x}_i$ .

Replacing population projection with sample projection introduces bias.

We have

$$\hat{\pi} = (\boldsymbol{Z}'\boldsymbol{Z})^{-1}\boldsymbol{Z}'\boldsymbol{X} = \pi + (\boldsymbol{Z}'\boldsymbol{Z})^{-1}\boldsymbol{Z}'\boldsymbol{\eta}$$

and so

$$\hat{X} = \tilde{X} + P_Z \eta$$

The second term correlates with  $\pmb{\varepsilon}$  and so

 $E(\hat{x}_i\varepsilon_i)\neq 0,$ 

which introduces bias.

Which vanishes as  $n \to \infty$ , yielding consistency.

Source	SS	df	MS	Number of obs	=	3,010
Model Residual	9427.23552 12134.8445	3 3,006	3142.41184 4.03687443	Prob > F R-squared	= =	0.0000
Total	21562.0801	3,009	7.16586243	Adj R-squared Root MSE	= =	0.4367 2.0092

. regress ed76 exp76 exp762 nearc4

ed76	Coef.	Std. Err.	t	P> t	[95% Conf.	Interval]
exp76	4225143	.034817	-12.14	0.000	4907818	3542468
exp762	.000235	.0017044	0.14	0.890	0031069	.0035769
nearc4	.6002325	.0788038	7.62	0.000	.4457177	.7547472
_cons	16.57345	.1701704	97.39	0.000	16.23978	16.90711

#### . predict ed76\_hat

(option **xb** assumed; fitted values)

#### . regress lwage76 ed76\_hat exp76 exp762

Source	SS	df	MS	Number of obs	=	3,010
				F(3, 3006)	=	42.94
Model	24.3527183	3	8.11757276	Prob > F	=	0.0000
Residual	568.288928	3,006	.189051539	R-squared	=	0.0411
				Adj R-squared	=	0.0401
Total	592.641646	3,009	.196956346	Root MSE	=	.4348

lwage76	Coef.	Std. Err.	t	P> t	[95% Conf.	. Interval]
ed76_hat	.2587155	.0284116	9.11	0.000	.2030075	.3144236
exp76	.1596791	.0141659	11.27	0.000	.1319033	.1874549
exp762	0024875	.0003688	-6.75	0.000	0032106	0017644
_cons	1.653985	.4842957	3.42	0.001	.7044003	2.603569

# Precision of instrumental variables

Instrumental-variable estimators are always more variable than least squares. Suppose we only have one covariate  $x_i$ , one instrument  $z_i$ , and homoskedastic errors.

The usual first-order approximation to the least-squares estimator is

$$\hat{\theta} - \theta \stackrel{a}{\sim} N\left(0, n^{-1} \frac{\sigma_{\varepsilon}^2}{\sigma_x^2}\right)$$

(under exogeneity).

The same first-order approximation to the instrumental-variable estimator is

$$\hat{\theta} - \theta \stackrel{a}{\sim} N\left(0, \frac{n^{-1}}{\rho_{xz}^2} \frac{\sigma_{\varepsilon}^2}{\sigma_x^2}\right),$$

where  $\rho_{xz}$  is the correlation between  $x_i$  and  $z_i$ .

The intuition is that  $x_i$  is (in terms of relevance/fit) its own best instrument.

The instrument is said to be weak when  $\rho_{xz}$  is small.

In this case the first-order approximation becomes poor.

Take the simple univariate problem, where we only have one covariate  $x_i$  and m instruments  $z_i$  (treat these as fixed), and suppose we have homoskedastic errors.

We can approximate the mean squared error of 2SLS to second order to get

$$\frac{1}{n} \frac{\sigma_{\varepsilon}^2 / \sigma_{\eta}^2}{\tau} + \left(\frac{m}{n}\right)^2 \left(\frac{\rho \sigma_{\varepsilon}}{\tau}\right)^2 + o(n^{-2}),$$
  
VARIANCE SQUARED BIAS

where

$$n \tau = rac{\pi' \mathbf{Z}' \mathbf{Z} \pi}{\sigma_{\eta}^2} = rac{\overline{R}^2}{1 - \overline{R}^2}$$

is the concentration parameter.

 $\overline{R}^2$  is the (uncentered) population  $R^2$  of the first-stage regression. This relates directly to the first-stage *F*-statistic.

When  $\tau$  is small most of the variation on  $x_i$  comes from  $\eta_i$ , and not from  $z_i$ .
Sampling distribution of two-stage least squares as a function of the value of the concentration parameter (simulation details omitted).



Note also how

$$\frac{1}{n} \frac{\sigma_{\varepsilon}^2 / \sigma_{\eta}^2}{\sigma_{VARIANCE}} + \left(\frac{m}{n}\right)^2 \left(\frac{\rho \, \sigma_{\varepsilon}}{\tau}\right)^2 + o(n^{-2})$$

depends on the number of instruments (m).

More instruments decrease the relative contribution of  $\eta_i$  to  $x_i$ .

But the fitted values  $\tilde{x}_i = z'_i \pi$  have to be estimated.

Under regularity conditions,

$$\hat{x}_i - \tilde{x}_i = O_p(\sqrt{m/n})$$

The noise in the fitted values grows with m.

Sampling distribution of two-stage least squares as a function of the number of instruments (simulation details omitted).



Let

$$e = M_Z X$$

be the residuals from the least-squares regression of X on Z (i.e., from the first stage).

Then 2SLS can be written as

$$\hat{\theta} = (\boldsymbol{X}' \boldsymbol{P}_{\boldsymbol{Z}} \boldsymbol{X})^{-1} (\boldsymbol{X}' \boldsymbol{P}_{\boldsymbol{Z}} \boldsymbol{y}) = (\boldsymbol{X}' \boldsymbol{M}_{\boldsymbol{e}} \boldsymbol{X})^{-1} (\boldsymbol{X}' \boldsymbol{M}_{\boldsymbol{e}} \boldsymbol{y}).$$

Indeed,

$$M_e X = M_e (P_Z X + M_Z X) = (I - P_e) P_Z X + M_e e = P_Z X.$$

So 2SLS can equally be performed in the following two steps:

- Estimate  $\eta_i$  by  $e_i$ , the residuals from a linear regression of  $x_i$  on  $z_i$ ;
- Estimate  $\theta$  by regressing  $y_i$  on  $x_i$  and  $e_i$ .

This view on 2SLS gives us a way to test the null of exogeneity.

Work through the simple model with

$$y_i = x_i\theta + \varepsilon_i$$
$$x_i = z_i\pi + \eta_i$$

where the errors are jointly normal.

Let  $e_i$  be the residual from the first stage.

Then 2SLS solves the empirical moments

$$\sum_{i} \begin{pmatrix} x_i \\ e_i \end{pmatrix} (y_i - x_i\theta - e_i\gamma) = 0.$$

for  $\theta, \gamma$ .

As  $e_i = x_i - z_i \hat{\pi} = \eta_i - z_i (\hat{\pi} - \pi)$  we can write this as (evaluating at true parameter values)

$$\sum_{i} \begin{pmatrix} x_i \\ \eta_i \end{pmatrix} u_i + \begin{pmatrix} x_i \\ \eta_i \end{pmatrix} z_i \gamma \left(\hat{\pi} - \pi\right) + \begin{pmatrix} 0 \\ z_i(\hat{\pi} - \pi) \end{pmatrix} \varepsilon_i + \begin{pmatrix} 0 \\ 1 \end{pmatrix} z_i^2 (\hat{\pi} - \pi)^2$$

for  $u_i = y_i - x_i \theta - \eta_i \gamma = \varepsilon_i - \eta_i \gamma$  (which does not correlate with  $x_i$  or  $\eta_i$ ).

Because  $E(z_i\eta_i) = 0$  and  $E(z_i\varepsilon_i) = 0$ , and because  $\|\hat{\pi} - \pi\|^2 = O_p(n^{-1})$ , this behaves like (as  $n \to \infty$  and scaled by  $n^{-1}$ )

$$n^{-1}\sum_{i} \begin{pmatrix} x_i \\ \eta_i \end{pmatrix} u_i + n^{-1}\sum_{i} \begin{pmatrix} \pi\gamma \\ 0 \end{pmatrix} z_i\eta_i,$$

were we have used that  $\hat{\pi} - \pi = n^{-1} \sum_{i=1}^{n} z_i \eta_i / E(z_i^2) + o_p(n^{-1/2})$  The first term is standard, it also showed up when  $\eta_i$  was directly observed. The second term is present because we have replaced  $\eta_i$  by an estimator  $e_i$ ; this introduces additional noise that has to be accounted for.

The variance-covariance matrix of the above random variable is

$$\begin{split} \Omega_{\theta} &= \left( \begin{array}{cc} \sigma_x^2 \sigma_u^2 + \gamma^2 \pi^2 \sigma_z^2 \sigma_\eta^2 & \sigma_\eta^2 \sigma_u^2 \\ \sigma_\eta^2 \sigma_u^2 & \sigma_\eta^2 \sigma_u^2 \end{array} \right) \\ &= \sigma_u^2 \left( \begin{array}{cc} \sigma_x^2 & \sigma_\eta^2 \\ \sigma_\eta^2 & \sigma_\eta^2 \end{array} \right) + \left( \begin{array}{cc} \gamma^2 (\sigma_x^2 - \sigma_\eta^2) \sigma_\eta^2 & 0 \\ 0 & 0 \end{array} \right). \end{split}$$

The limit of the Jacobian of the moment conditions is

$$\Gamma_{\theta} = \begin{pmatrix} \sigma_x^2 & \sigma_\eta^2 \\ \sigma_\eta^2 & \sigma_\eta^2 \end{pmatrix}, \qquad \Gamma_{\theta}^{-1} = \frac{1}{\sigma_\eta^2(\sigma_x^2 - \sigma_\eta^2)} \begin{pmatrix} \sigma_\eta^2 & -\sigma_\eta^2 \\ -\sigma_\eta^2 & \sigma_x^2 \end{pmatrix}.$$

The asymptotic variance of the estimator,

$$\Gamma_{\theta}^{-1}\Omega_{\theta}\Gamma_{\theta}^{-1},$$

then equals

$$\sigma_u^2 \Gamma_\theta^{-1} + \gamma^2 \frac{\sigma_\eta^2}{\sigma_x^2 - \sigma_\eta^2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Under the null of exogeneity ( $\gamma = 0$ ), this is just  $\sigma_u^2 \Gamma_{\theta}^{-1}$  and so the usual least-squares standard error will be consistent.

Hence, the reported *t*-statistic is valid for testing exogeneity.

For our estimator of  $\theta$  we do need a correction to the usual least-squares standard error as we want to allow that  $\gamma \neq 0$ .

#### . ivregress 2sls lwage76 (ed76 = nearc4) exp76 exp762

Instrumental variables (2SLS) regression

Number of obs	=	3,010
Wald chi2(3)	=	89.88
Prob > chi2	=	0.0000
R-squared	=	
Root MSE	=	.52053

lwage76	Coef.	Std. Err.	z	P> z	[95% Conf.	. Interval]
ed76 exp76 exp762 _cons	.2587156 .1596791 0024875 1.653985	.0340135 .016959 .0004415 .579785	7.61 9.42 -5.63 2.85	0.000 0.000 0.000 0.004	.1920503 .1264401 0033528 .5176268	.3253808 .1929181 0016222 2.790342

Instrumented: ed76

Instruments: exp76 exp762 nearc4

Source	SS	df	MS	Number of obs	=	3,010
Model Residual	9427.23552 12134.8445	3 3,006	3142.41184 4.03687443	Prob > F R-squared	= =	0.0000 0.4372
Total	21562.0801	3,009	7.16586243	Adj R-squared Root MSE	= =	0.4367 2.0092

. regress ed76 exp76 exp762 nearc4

ed76	Coef.	Std. Err.	t	P> t	[95% Conf.	Interval]
exp76	4225143	.034817	-12.14	0.000	4907818	3542468
exp762	.000235	.0017044	0.14	0.890	0031069	.0035769
nearc4	.6002325	.0788038	7.62	0.000	.4457177	.7547472
_cons	16.57345	.1701704	97.39	0.000	16.23978	16.90711

. predict u, residual

Source	SS	df	MS	Number of obs	=	3,010
Model Residual	122.591904 470.049742	4 3,005	30.6479761	Prob > F R-squared	= =	0.0000
Total	592.641646	3,009	.196956346	Adj R-squared Root MSE	= =	0.2058 .3955

#### . regress lwage76 ed76 u exp76 exp762

lwage76	Coef.	Std. Err.	t	P> t	[95% Conf.	Interval]
ed76 u exp76 exp762 _cons	.2587156 1687399 .1596791 0024875 1.653984	.0258437 .0260919 .0128855 .0003355 .4405246	10.01 -6.47 12.39 -7.42 3.75	0.000 0.000 0.000 0.000 0.000 0.000	.2080424 2198996 .1344137 0031453 .7902243	.3093887 1175801 .1849445 0018298 2.517745

For a fixed weight matrix A, the bias in the GMM objective function is

$$E_{\theta}(\hat{g}(\theta)'A\hat{g}(\theta)) = \operatorname{tr}(A\Omega_{\theta})/n.$$

The bias shrinks with n but grows (typically linearly) with dim  $\varphi$ .

A bias-corrected GMM estimator minimizes

$$\hat{g}(\theta)'Ag(\theta) - \operatorname{tr}(A\hat{\Omega}_{\theta})/n = \frac{\sum_{i} \sum_{j \neq i} \varphi(x_{i};\theta)'A\varphi(x_{j};\theta)}{n^{2}}$$

The continuously-updated estimator from above has a similar bias-correction interpretation.

For 2SLS we have  $A = (\mathbf{Z}'\mathbf{Z})^{-1}$  and so the bias-corrected objective function equals

$$rac{\sum_i \sum_{j 
eq i} (y_i - x_i' heta) \, p_{ij} \, (y_j - x_j' heta)}{n^2}$$

for  $p_{ij} = (\mathbf{P}_{\mathbf{Z}})_{ij} = z'_i (\mathbf{Z}' \mathbf{Z})^{-1} z_j.$ 

Its minimizer is the jackknife instrumental-variable estimator

$$\left(\sum_{i}\sum_{j\neq i}x_{i}p_{ij}x_{j}'\right)^{-1}\left(\sum_{i}\sum_{j\neq i}x_{i}p_{ij}y_{j}\right) = \left(\sum_{i}\check{x}_{i}x_{i}'\right)^{-1}\left(\sum_{i}\check{x}_{i}y_{i}\right),$$

where

$$\check{x}_i = \sum_{j \neq i} x_j p_{ji} = \sum_{j \neq i} x_j z'_j (\mathbf{Z}' \mathbf{Z})^{-1} z_i = \hat{\Pi}_{-i} z_i.$$

Recall that the first-stage equation is of the form

$$x_i = \Pi z_i + \eta_i.$$

Here,  $\hat{\Pi}_{-i}$  is a leave-one-out estimator of the first-stage coefficient matrix and  $\check{x}_i$  is the associated fitted value.

Recall that bias in (feasible) 2SLS arose from the fact that  $\hat{\Pi}$  is a function of  $\eta_i$  and  $\eta_i$  correlates with  $\varepsilon_i$  (See Slide 248). By construction the leave-one-out fitted values do not depend on  $\eta_i$ .

As an example of nonlinear instrumental-variable estimation, suppose that

$$y_i = \varphi(x_i; \theta) \varepsilon_i, \qquad E(\varepsilon_i | z_i) = 1.$$

We have (conditional) moment condition

$$E_{\theta}\left(\left.\frac{y_i}{\varphi(x_i;\theta)} - 1\right|z_i\right) = 0$$

and so many unconditional moment conditions; for example

$$E_{\theta}\left(z_{i}\left(\frac{y_{i}}{\varphi(x_{i};\theta)}-1\right)\right)=E_{\theta}\left(\frac{z_{i}}{\varphi(x_{i}\theta)}\left(y_{i}-\varphi(x_{i};\theta)\right)\right)=0.$$

An example is an exponential model.

Bekker, P. A. (1994). Alternative approximations to the distributions of instrumental variable estimators. *Econometrica* 62, 657–681.

Bound, J., D. A. Jaeger, and R. M. Baker (1995). Problems with instrumental variables estimation when the correlation between the instruments and the endogeneous explanatory variable is weak. *Journal of the American Statistical Association* 90, 443–450.

Staiger, D. and J. H. Stock (1997). Instrumental variabels regression with weak instruments. *Econometrica* 65, 557–586.

Stock, J. H. and M. Yogo (2005). Testing for weak instruments in linear IV regression. In Andrews, D. W. K. and J. H. Stock (Editors), *Identification and Inference for Econometric Models: Essays in Honor of Thomas Rothenberg*, Chapter 5, 80–108 (Cambridge UP, Cambridge, UK). Now consider testing the *m*-dimensional constraint that  $r(\theta) = 0$ .

Let

$$\check{\check{\theta}} = \arg\min_{\theta: r(\theta) = 0} \hat{g}(\theta)' \hat{\Omega}_{\hat{\theta}}^{-1} \hat{g}(\theta);$$

the efficient GMM estimator under the constraint.

Theorem 25 (Limit distribution of LR-type statistic)

Under the null,

$$n\,\hat{g}(\mathring{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{g}(\mathring{\theta}) - n\,\hat{g}(\hat{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{g}(\hat{\theta}) \stackrel{d}{\to} \chi_m^2$$

as  $n \to \infty$ .

This result requires optimal weighting.

Note that we use the same weight matrix throughout.

Similarly, we can look whether the first-order condition of the unconstrained problem,

$$\hat{G}(\theta)'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{g}(\theta) = 0,$$

when evaluated in the constrained estimator  $\check{\theta}$ , is far from zero.

#### Theorem 26 (Limit distribution of LM-type statistic)

Under the null,

$$n\,\hat{g}(\check{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{G}(\check{\theta})\,(\hat{G}(\check{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{G}(\check{\theta}))^{-1}\,\hat{G}(\check{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{g}(\check{\theta})\stackrel{d}{\to}\chi_m^2$$

as  $n \to \infty$ .

This result requires optimal weighting.

The Wald statistic works without reference to the constrained problem.

Under optimal weighting we would have the following, where R is again the Jacobian matrix of the constraint vector r.

Theorem 27 (Limit distribution of the Wald statistic)

Under the null,

$$n r(\hat{\theta})' (R(\hat{G}(\hat{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{G}(\hat{\theta}))^{-1}R')^{-1}r(\hat{\theta}) \stackrel{d}{\to} \chi_m^2,$$

as  $n \to \infty$ .

More generally, when using estimator  $\hat{\theta}$  computed using weight matrix A it equals

 $n \, r(\hat{\theta})' (R((\hat{G}(\hat{\theta})'A\,\hat{G}(\hat{\theta}))^{-1}(\hat{G}(\hat{\theta})'A\hat{\Omega}_{\hat{\theta}}A'\hat{G}(\hat{\theta}))(\hat{G}(\hat{\theta})'A\,\hat{G}(\hat{\theta}))^{-1})^{-1}R')^{-1}r(\hat{\theta}).$ 

Note that

$$n\,\hat{g}(\hat{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{g}(\hat{\theta}) \stackrel{d}{\to} \chi^2_{\dim\varphi-\dim\theta}$$

if all moments hold.

So we can test the specification.

Only possible when we have overidentification, i.e., when

 $\dim \varphi - \dim \theta > 0$ 

(Otherwise the test statistic is exactly zero).

If the J-statistic is large relative to the quantiles of the  $\chi^2$ -distribution at least some of the moment conditions are likely to be invalid.

This does not tell us which moments are troublesome.

We can test subset of the moments as well.

Partition the moments using  $\varphi(x;\theta) = (\varphi_1(x;\theta)', \varphi_2(x;\theta))'$ .

Also partition

$$\hat{\Omega}_{\theta} = \begin{pmatrix} (\hat{\Omega}_{\theta})_{11} & (\hat{\Omega}_{\theta})_{12} \\ (\hat{\Omega}_{\theta})_{21} & (\hat{\Omega}_{\theta})_{22} \end{pmatrix}.$$

Want to test

$$E_{\theta}(\varphi_2(x_i;\theta)) = 0$$

assuming that  $E_{\theta}(\varphi_1(x_i; \theta)) = 0.$ 

If  $\dim \varphi_1 \ge \dim \theta$  we can compute

1

$$\check{\theta} = \arg\min_{\theta} \hat{g}_1(\theta)' (\hat{\Omega}_{\hat{\theta}})_{11}^{-1} \hat{g}_1(\theta),$$

where  $\hat{g}_1(\theta) = n^{-1} \sum_i \varphi_1(x_i; \theta)$ .

We can also compute the estimator using all moment conditions, i.e., the usual

$$\hat{\theta} = \arg\min_{\theta} \hat{g}(\theta)' \hat{\Omega}_{\hat{\theta}}^{-1} \hat{g}(\theta).$$

We then have the following simple result.

#### Theorem 28 (Testing moment validity)

If all moment conditions hold,

$$n\,\hat{g}(\hat{\theta})'\hat{\Omega}_{\hat{\theta}}^{-1}\hat{g}(\hat{\theta}) - n\,\hat{g}_1(\check{\theta})'(\hat{\Omega}_{\hat{\theta}})_{11}^{-1}\hat{g}_1(\check{\theta}) \stackrel{d}{\to} \chi^2_{\dim\varphi-\dim\varphi_1}$$

as  $n \to \infty$ .

Note that we use the same weight matrix in both terms.

This ensures (in small samples) that the test statistic is non-negative.

In the linear model

 $oldsymbol{y} = oldsymbol{X} heta + oldsymbol{arepsilon}$ 

with homosked astic errors, the optimally-weighted GMM estimator is 2SLS and the objective function (scaled up by n and evaluated at its minimizer) equals

$$\frac{\hat{\boldsymbol{\varepsilon}}' \boldsymbol{P}_{\boldsymbol{Z}} \hat{\boldsymbol{\varepsilon}}}{\hat{\sigma}^2},$$

where  $\hat{\pmb{\varepsilon}}$  are the 2SLS residuals.

This statistic is known as Sargan's statistic.

Note that  $P_Z \hat{\varepsilon}$  are the fitted values of a regression of the 2SLS residuals on the instruments

Moreover, as  $\hat{\sigma}^2 = \hat{\varepsilon}' \hat{\varepsilon}/n$  we can equivalently write

$$n \, \frac{\hat{\boldsymbol{\varepsilon}}' \boldsymbol{P}_{\boldsymbol{Z}} \hat{\boldsymbol{\varepsilon}}}{\hat{\boldsymbol{\varepsilon}}' \hat{\boldsymbol{\varepsilon}}} = n \, \frac{ESS}{TSS} = n \, R^2.$$

Invalid instruments can be detected by looking at correlation between the residuals and the instruments.

# Optimal moment conditions in conditional models

Now suppose that we know

$$E_{\theta}(\varphi(x_i;\theta)|z_i) = 0$$

(a.s.)

This yields an infinite amount of unconditional moments.

We look for the optimal moment conditions, i.e., the function  $\psi$  in

$$E_{\theta}(\psi(z_i)\,\varphi(x_i;\theta)) = 0$$

for which the asymptotic variance of the resulting GMM estimator is minimal.

The optimal instrument turns out to be

$$\psi(z_i) = -E_{\theta} \left( \left. \frac{\partial \varphi(x_i; \theta)}{\partial \theta'} \right| z_i \right)' E_{\theta} \left( \varphi(x_i; \theta) \varphi(x_i; \theta)' \right| z_i \right)^{-1} = -\Gamma_{\theta}(z_i)' \Omega_{\theta}(z_i)^{-1}.$$

Note that  $\dim \psi = \dim \theta$ .

Notice that, now,

$$\Omega_{\theta} = \operatorname{var}_{\theta}(\psi(z_i) \,\varphi(x_i; \theta)) = E_{\theta} \left( \Gamma_{\theta}(z_i)' \,\Omega_{\theta}(z_i)^{-1} \Gamma_{\theta}(z_i) \right),$$

and

$$\Gamma_{\theta} = E_{\theta} \left( \psi(z_i) \frac{\partial \varphi(x_i; \theta)}{\partial \theta'} \right) = -E_{\theta} \left( \Gamma_{\theta}(z_i)' \Omega_{\theta}(z_i)^{-1} \Gamma_{\theta}(z_i) \right),$$

(use iterated expectations) such that

$$\Omega_{\theta} = -\Gamma_{\theta}.$$

Hence, the generic sandwich-form asymptotic variance becomes

$$\operatorname{avar}_{\theta}(\hat{\theta}) = (\Gamma_{\theta}' \Omega_{\theta}^{-1} \Gamma_{\theta})^{-1} = \Omega_{\theta}^{-1};$$

that is,

$$\sqrt{n}(\hat{\theta} - \theta) \stackrel{d}{\to} N(0, \Omega_{\theta}^{-1}).$$

This is the semiparametric efficiency bound.

### Proof.

Let

$$g_i = \psi(z_i) \varphi(x_i; \theta), \qquad h_i = \Gamma'_{\theta} A \phi(z_i) \varphi(x_i; \theta)$$

for arbitrary alternative weight matrix A and instrument vector  $\phi$ .

The asymptotic variances of the associated GMM estimators are

$$E_{\theta}(g_i g'_i)^{-1}, \qquad E_{\theta}(h_i g'_i)^{-1} E_{\theta}(h_i h'_i) E_{\theta}(g_i h'_i)^{-1},$$

respectively.

Rewriting gives

$$E_{\theta}(h_{i}g_{i}')^{-1} E_{\theta}(h_{i}h_{i}') E_{\theta}(g_{i}h_{i}')^{-1} - E_{\theta}(g_{i}g_{i}')^{-1} = E_{\theta}(h_{i}g_{i}')^{-1} E_{\theta}(v_{i}v_{i}') E_{\theta}(g_{i}h_{i}')^{-1} = E_{\theta}(h_{i}g_{i}')^{-1} E_{\theta}(v_{i}v_{i}') E_{\theta}(v_{i}v_{i}')^{-1} = E_{\theta}(h_{i}g_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} = E_{\theta}(h_{i}g_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} = E_{\theta}(h_{i}g_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} = E_{\theta}(h_{i}g_{i}')^{-1} E_{\theta}(v_{i}v_{i}')^{-1} E_{\theta}(v_{i}v_{i}'$$

for

$$v_i = h_i - g'_i \gamma, \qquad \gamma = E_\theta (g_i g'_i)^{-1} E_\theta (g_i h'_i).$$

This difference is positive semi-definite because  $E(v_i v'_i) \ge 0$ .

# Linear model

With

$$y_i = x'_i \theta + \varepsilon_i, \qquad E_\theta(\varepsilon_i | x_i) = 0$$

we have

$$E_{\theta}(y_i - x'_i \theta \,|\, x_i) = 0.$$

Here,

$$\Gamma_{\theta}(x_i) = E_{\theta} \left( \left. \frac{\partial (y_i - x'_i \theta)}{\partial \theta'} \right| x_i \right) = -x'_i, \qquad \Omega_{\theta}(x_i) = E_{\theta}(\varepsilon_i^2 \mid x_i) = \sigma_i^2 \text{ (say).}$$
  
So,

$$\psi(x_i) = -\Gamma_{\theta}(x_i)' \,\Omega_{\theta}(x_i)^{-1} = \frac{x_i}{\sigma_i^2},$$

and the optimal estimator solves the empirical moment condition

$$n^{-1} \sum_{i=1}^{n} \frac{x_i(y_i - x'_i \theta)}{\sigma_i^2} = 0.$$

Observation i gets less weight if  $\sigma_i^2$  is higher. This is weighted least squares.

If we write

$$\boldsymbol{V} = \operatorname{diag}(\sigma_1^2, \ldots, \sigma_n^2).$$

Then the optimal estimator is

$$\hat{\theta} = (X'V^{-1}X)^{-1}(X'V^{-1}y)$$

Under homoskedasticity, i.e., when  $\sigma_i^2 = \sigma^2$  for all *i* this reduces to the simple

$$\hat{\theta} = (\boldsymbol{X}'\boldsymbol{X})^{-1}(\boldsymbol{X}'\boldsymbol{y}),$$

which is ordinary least squares.

This is the Gauss-Markov theorem.

# Exponential model

We have

$$y_i = e^{x_i'\theta} \varepsilon_i, \qquad E_\theta(\varepsilon_i | x_i) = 1,$$

and so

$$E_{\theta}(y_i - e^{x_i'\theta} | x_i) = 0.$$

Here,

$$\Gamma_{\theta}(x_i) = -e^{x'_i \theta} x'_i, \qquad \Omega_{\theta}(x_i) = \sigma_i^2 \text{ (say)}.$$

The optimal empirical moment condition thus is

$$n^{-1} \sum_{i=1}^{n} \frac{x_i e^{x'_i \theta} (y_i - e^{x'_i \theta})}{\sigma_i^2} = 0$$

With Poisson data, for example,  $\sigma_i^2 = e^{x_i'\theta}$  and the estimating equation is

$$n^{-1} \sum_{i=1}^{n} x_i (y_i - e^{x'_i \theta}) = 0.$$

With homosked astic errors  $\sigma_i^2 = \sigma^2 \, (e^{x_i' \theta})^2$  and we solve

$$n^{-1} \sum_{i=1}^{n} \frac{x_i (y_i - e^{x'_i \theta})}{e^{x'_i \theta}} = 0.$$
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Now if

$$E_{\theta}(y_i - x_i'\theta | z_i) = 0$$

we obtain

$$\Gamma_{\theta}(z_i)' = -E(x_i|z_i), \qquad \Omega_{\theta}(z_i) = E(\varepsilon_i^2|z_i) = \sigma_i^2 \text{ (say)}.$$

So, we solve

$$n^{-1} \sum_{i=1}^{n} \frac{E(x_i | z_i) (y_i - x'_i \theta)}{\sigma_i^2} = 0.$$

Here, the reduced form is nonlinear, in general.

This is also true under homoskedasticity. So two-stage least squares is not optimal, in general.

Two-stage least squares approximates  $E(x_i|z_i)$  by the linear projection  $E^*(x_i|z_i)$ .

### Linear model for panel data

Suppose now that we have repeated measurements, as in

$$y_{it} = x'_{it}\theta + \varepsilon_{it}, \qquad t = 1, \dots, T.$$

For each i we have a set of T equations.

This fits our framework on stacking observations for each i and writing

$$y_i = x_i'\theta + \varepsilon_i;$$

here, e.g.,  $y_i = (y_{i1}, \ldots, y_{iT})'$ .

Suppose that

$$\varepsilon_{it} = \alpha_i + u_{it}.$$

We may have that  $\alpha_i$  and  $x_i$  are correlated. Then  $E(\varepsilon_i|x_i) \neq 0$ .

However, with  $\Delta$  the first-differencing operator, we have the T-1 equations

$$\Delta y_{it} = \Delta x'_{it}\theta + \Delta \varepsilon_{it} = \Delta x'_{it}\theta + \Delta u_{it}$$

that are free of  $\alpha_i$ .

A sufficient condition for estimation is  $E(u_{it}|x_i, \alpha_i) = 0$ .

Define the  $(T-1) \times T$  first-differencing matrix D as

$$D = \begin{pmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}.$$

We have the conditional moment conditions

$$E_{\theta}[D(y_i - x'_i \theta) | x_{i1}, \dots, x_{iT}] = 0.$$

The first-differenced least-squares estimator solves

$$\sum_{i=1}^{n} x_i D' D(y_i - x'_i \theta) = 0.$$

This is pooled least-squares on first-differenced data. It is inefficient as the  $\Delta u_{it}$  are correlated.

Suppose that  $u_i \sim (0, \sigma^2 I_T)$ . Then  $Du_i \sim (0, \sigma^2 DD')$ .

The optimal unconditional (empirical) moments are

$$\sum_{i=1}^{n} x_i D' (DD')^{-1} D (y_i - x'_i \theta) = 0.$$

This yields a generalized least-squares estimator. It is a pooled least-squares estimator on demeaned data.

A calculation gives

$$M = D' (DD')^{-1} D = I_T - \frac{\iota_T \iota'_T}{T},$$

where  $\iota_T$  is a vector of ones.

The matrix M transforms data into deviations from within-group means. For example,  $My_i = y_i - \overline{y}_i$ .

## Feedback

The above estimator requires that  $u_{it}$  is uncorrelated with  $x_{i1}, \ldots, x_{iT}$ . This rules out dynamics and, more generally, feedback.

A simple model where the problem arises is the (first-order) autoregression

$$y_{it} = y_{it-1}\theta + \alpha_i + u_{it},$$

where the initial value  $y_{i0}$  is taken as observed.

First-differencing (and, equivalently, demeaning) sweeps out  $\alpha_i$ ,

$$\Delta y_{it} = \Delta y_{it-1}\theta + \Delta u_{it},$$

but (taking  $u_{it}$  to be homoskedastic and serially uncorrelated for simplicity)

$$E(\Delta y_{it-1}\,\Delta u_{it}) = E(\Delta u_{it-1}\,\Delta u_{it}) = -E(u_{t-1}^2) = -\sigma^2 \neq 0,$$

and so introduces a new endogeneity problem.

An assumption of sequential exogeneity, i.e.,  $E(u_{it}|y_{i0}, \ldots, y_{it-1}, \alpha_i) = 0$  is enough to obtain a GMM estimator.

It implies (sequential) conditional moments

$$E_{\theta}(\Delta y_{it} - \Delta y_{it-1}\theta | y_{i0}, \dots, y_{it-2}) = 0.$$

The conventional GMM estimator uses the linear moment conditions

$$E\left(\begin{pmatrix} y_{it-2}\\y_{it-3}\\\vdots\\y_{i0}\end{pmatrix}\left(\Delta y_{it}-\Delta y_{it-1}\theta\right)\right)=0$$

(for all t = 2, ..., T).

# DEALING WITH (WEAK) DEPENDENCE

Hansen II, Chapters 14 and 15

Hayashi, Chapter 6

Random sampling may be too strong a requirement:

- Time series data;
- Interactions and other network data;
- Snowball sampling (and so on).

Consider a scalar sequence  $\{x_i\}$ .

 $\{x_i\}$  is (strictly) stationary if, for any  $h \ge 0$ , the distribution of  $(x_i, \ldots, x_{i+h})$  does not depend on i.

An implication (if the moments exist) is weak stationarity: the mean  $E(x_i)$ and covariance  $E(x_i x_{i+h}) - E(x_i) E(x_{i+h})$  do not depend on *i*.

The techniques discussed so far can be adapted to stationary data provided they are weakly dependent.
Weak dependence is a requirement that the overall behavior of  $\{x_i\}$  is not driven by the realizations of the initial random variables (or any of the other variables later on).

Blocks of data  $(x_i, \ldots, x_{i+j})$  and  $(x_{i+j+h}, \ldots, x_{i+j+h+k})$  separated by h units become independent as h grows.

One way to formalize weak dependence is through mixing.

For  $h \ge 1$  define the mixing coefficients

$$\alpha_h = \sup_{A \in \mathcal{A}, B \in \mathcal{B}} |P(A \cap B) - P(A) P(B)|,$$

where (somewhat crudely stated) the sets  $\mathcal{A}$  and  $\mathcal{B}$  cover all events involving  $x_{-\infty}, \ldots, x_{i-1}, x_i$  and  $x_{i+h}, x_{i+h+1}, \ldots, x_{+\infty}$ , respectively. Note how these sets depend on h.

The process  $\{x_i\}$  is strongly mixing (or alpha mixing) if  $\alpha_h \to 0$  as  $h \to \infty$ . Note that independent data has  $\alpha_h = 0$  for any h.

# Consistency of the sample mean

Now let

$$\overline{x}_n = n^{-1} \sum_{i=1}^n x_i$$

be the sample mean.

### Theorem 29 (Law of large numbers)

Suppose that  $\{x_i\}$  is stationary and mixing, and that  $\mu = E(x_i)$  exists. Then

$$\overline{x}_n \stackrel{p}{\to} \mu$$

as  $n \to \infty$ .

This is a substantial generalization of our earlier law of large numbers for random samples.

Note that this also implies that the continuous-mapping theorem generalizes in the same way.

#### Theorem 30 (Central limit theorem)

Suppose that  $\{x_i\}$  is stationary and mixing with mixing coefficient satisfying

$$\sum_{h=1}^{\infty} \alpha_h^{\delta/(2+\delta)} < +\infty,$$

that  $E(x_i) = \mu$  exists and that  $E(||x_i||^{2+\delta})$  for some  $\delta > 0$ . Then

$$\sqrt{n}\Sigma^{-1/2}(\overline{x}_n-\mu) \stackrel{d}{\to} N(0,I)$$

for

$$\Sigma = \lim_{n \to \infty} \left( \Sigma_0 + \sum_{h=1}^{n-1} \frac{n-h}{n} (\Sigma_h + \Sigma'_h) \right) = \Sigma_0 + \sum_{h=1}^{\infty} (\Sigma_h + \Sigma'_h) = \sum_{h=-\infty}^{+\infty} \Sigma_h < \infty,$$
  
where  $\Sigma_h = E((x_i - \mu)(x_{i+h} - \mu)').$ 

Many special cases of this theorem are available with (complicated) low-level conditions for specific processes.

The summability of the covariances (i.e., the fact that  $\Sigma$  is finite) follows from the restriction on the mixing coefficients. A sufficient condition for summability is that  $\Sigma_h \to 0$  faster than  $1/h \to 0$ .

The variance formula follows from (again for the scalar case)

$$\operatorname{var}\left(\sum_{i=1}^{n} x_{i}\right) = \sum_{i=1}^{n} \sum_{j=1}^{n} \operatorname{cov}(x_{i}, x_{j})$$
$$= \sum_{i=1}^{n} \left(\operatorname{cov}(x_{i}, x_{i}) + \sum_{h=1}^{i-1} \operatorname{cov}(x_{i}, x_{i-h}) + \sum_{h=1}^{n-i} \operatorname{cov}(x_{i}, x_{i+h})\right)$$
$$= \sum_{i=1}^{n} \left(\Sigma_{0} + \sum_{h=1}^{i-1} \Sigma_{-h} + \sum_{h=1}^{n-i} \Sigma_{h}\right)$$
$$= n\Sigma_{0} + (n-1)(\Sigma_{1} + \Sigma_{-1}) + \dots + (\Sigma_{n-1} + \Sigma_{-(n-1)})$$
$$= n \left(\Sigma_{0} + \sum_{h=1}^{n-1} \frac{(n-h)}{n}(\Sigma_{h} + \Sigma_{-h})\right).$$

We have  $\Sigma_{-h} = \Sigma'_h$ .

A (truncated) estimator of the long-run variance  $\Sigma$  can be constructed as

$$\hat{\Sigma} = \hat{\Sigma}_0 + \sum_{h=1}^{\kappa-1} \frac{(\kappa-h)}{\kappa} (\hat{\Sigma}_h + \hat{\Sigma}'_h)$$

for chosen integer  $\kappa \leq n$  and

$$\hat{\Sigma}_h = \frac{1}{n-h} \sum_{i=1}^{n-h} (x_i - \overline{x}_n) (x_{i+h} - \overline{x}_n)'.$$

The resulting estimator is typically referred to as a HAC estimator.

The truncation at  $\kappa$  lags is needed because  $\hat{\Sigma}_h$  becomes increasingly noisy as a function of h (for given n). (Consistency requires that  $\kappa \to \infty$  with n, but not too fast.)

 $\hat{\Sigma}$  is also called the Newey-West variance estimator. It can be interpreted as a 'kernel' estimator with a triangular kernel. Importantly, an unlike most other such 'kernel' estimators, it is ensured to be positive semi-definite.

### Autoregression

#### Suppose that

$$x_i = \alpha + \rho x_{i-1} + \varepsilon_i, \qquad \varepsilon_i \sim \text{i.i.d. } N(0, \sigma^2).$$

We impose that  $|\rho| < 1$ .

We have  $E(x_i) = \alpha + \rho E(x_{i-1})$  and so

$$\mu = E(x_i) = \frac{\alpha}{1-\rho}.$$

Also,  $\operatorname{var}(x_i) = \rho^2 \operatorname{var}(x_{i-1}) + \sigma^2$  and, hence,

$$\Sigma_0 = \frac{\sigma^2}{1 - \rho^2}.$$

The univariate stationary distribution, therefore, is  $x_i \sim N(\mu, \Sigma_0)$ . The covariances are proportional to  $\Sigma_0$ :

$$\Sigma_h = \rho^h \, \Sigma_0;$$

for example,

$$\Sigma_1 = \operatorname{cov}(x_i, x_{i-1}) = \operatorname{cov}(\alpha + \rho x_{i-1} + \varepsilon_i, x_{i-1}) = \rho \operatorname{cov}(x_{i-1}, x_{i-1}) = \rho \Sigma_0.$$

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 $\Sigma_h = \rho^h \, \Sigma_0$  shrinks at a geometric rate. The long-run variance is well-defined and equals

$$\Sigma = \Sigma_0 + 2\sum_{h=1}^{\infty} \rho^h \Sigma_0 = \frac{1+\rho}{1-\rho} \Sigma_0.$$

Here, the particularly simple structure of  $\Sigma$  suggests the simple alternative HAC estimator

$$\frac{1+\hat{\rho}}{1-\hat{\rho}}\hat{\Sigma}_0$$

where

$$\hat{\rho} = \frac{\sum_{i=2}^{n} x_{i-1} \left( x_i - \overline{x}_n \right)}{\sum_{i=2}^{n} (x_i - \overline{x}_n)^2}, \quad \hat{\Sigma}_0 = \frac{\hat{\sigma}^2}{1 - \hat{\rho}^2}.$$

and

$$\hat{\sigma}^{2} = \frac{\sum_{i=2}^{n} ((x_{i} - \overline{x}_{n}) - \hat{\rho} (x_{i-1} - \overline{x}_{n}))^{2}}{n-1}$$

When  $\rho = 0$  { $x_i$ } is i.i.d. and  $\Sigma = \Sigma_0$  but, for example, when  $\rho = .5$  { $x_i$ } is dependent and  $\Sigma = 3\Sigma_0$ .

Ignoring the non-zero covariances can lead to large underestimation of the actual variability of the series.

## Moving average

### Another example has

$$x_i = \mu + \varepsilon_i + \beta \varepsilon_{i-1}, \qquad \varepsilon_i \sim \text{i.i.d. } N(0, \sigma^2).$$

Here,  $E(x_i) = \mu$  is immediate. Further,

$$\Sigma_0 = (1 + \beta^2) \sigma^2$$
 and  $\Sigma_1 = \beta \sigma^2$ .

However,

$$\Sigma_h = 0, \qquad |h| > 1,$$

so the dependence in short-lived and vanishes abruptly beyond the first-order autocovariance.

It follows that

$$\Sigma = \Sigma_0 + \Sigma_{-1} + \Sigma_1 = (1+\beta)^2 \sigma^2.$$

A combination of both examples gives

$$x_i = \alpha + \rho x_{i-1} + \varepsilon_i + \beta \varepsilon_{i-1}, \qquad \varepsilon_i \sim \text{i.i.d. } N(0, \sigma^2).$$

Extensions to higher-order are immediate. This gives a parsimonious way to modelling dependence.

In practice the above is important for getting correct standard errors with serially dependent data.

The two-step GMM estimator solves

$$\min_{\theta} \hat{g}(\theta)' \hat{\Omega}_{\hat{\theta}}^{-1} \hat{g}(\theta).$$

where, now,  $\hat{\Omega}_{\hat{\theta}}$  is a HAC estimator of the long-run covariance matrix of the moment condition

$$\hat{g}(\theta) = n^{-1} \sum_{i=1}^{n} \varphi(x_i; \theta).$$

The same robust estimator needs to be used when constructing test statistics. The remainder of the argument for GMM carries over without modification.

## Linear model with correlated errors

 $\operatorname{Consider}$ 

$$y_i = x_i'\theta + \varepsilon_i$$

with  $E(\varepsilon_i|x_1,\ldots,x_n) = 0$ . Then, as before,

$$\sqrt{n}(\hat{\theta} - \theta) = \left(\frac{1}{n}\sum_{i=1}^{n} x_i x_i'\right)^{-1} \left(\frac{1}{\sqrt{n}}\sum_{i=1}^{n} x_i \varepsilon_i\right).$$

Now,

$$\frac{1}{\sqrt{n}}\sum_{i=1}^{n} x_i\varepsilon_i \stackrel{d}{\to} N(0,\Omega), \qquad \Omega = \sum_{h=-\infty}^{+\infty} E((\varepsilon_i\varepsilon_{i+h})(x_ix'_{i+h})).$$

This covariance allows for both heteroskedasticity and autocorrelation in the errors.

Under homoskedasticity,  $E(\varepsilon_i\varepsilon_{i+h}|x_1,\ldots,x_n) = E(\varepsilon_i\varepsilon_{i+h})$ , and the formula simplifies to

$$\Omega = \sum_{h=-\infty}^{+\infty} E(\varepsilon_i \varepsilon_{i+h}) E(x_i x'_{i+h}).$$

If, in addition, we also have  $E(\varepsilon_i \varepsilon_{i+h}) = 0$  for  $h \neq 0$ , then  $\Omega = \sigma^2 E(x_i x'_i)$ .

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A simple dynamic model is

$$y_i = \rho y_{i-1} + \varepsilon_i, \qquad E(\varepsilon_i | y_1, \dots, y_{i-1}) = 0.$$

Here the regressor (the lagged outcome) is not strictly exogenous but only weakly exogenous.

Nonetheless,

$$E(y_{i-1}\varepsilon_i) = E_{\rho}(y_{i-1}(y_i - \rho y_{i-1})) = 0$$

and so least-squares continues to be consistent and asymptotically normal (under the usual regularity conditions).

As

$$y_i = \sum_{h=0}^{\infty} \rho^h \, \varepsilon_{i-h},$$

weak exogeneity implies that the  $\varepsilon_i$  are uncorrelated.

An extension would be

 $y_i = \rho y_{i-1} + \varepsilon_i, \qquad \varepsilon_i = \eta_i + \theta \eta_{i-1},$ 

where  $\eta_i \sim \text{i.i.d.} (0, \sigma^2)$ .

Now, least-squares is not consistent. Indeed,

$$E(y_{i-1}\varepsilon_i) = \theta \,\sigma^2,$$

so the usual moment condition is no longer valid.

However, lack of higher-order correlation in the error does imply that

$$E(y_{i-h}\varepsilon_i) = 0,$$
 for all  $h \ge 2,$ 

opening the way for an instrumental-variable approach.

The extension to higher-order MA processes is immediate.

Note that this approach does not work for autoregressive errors.

A consumer chooses consumption stream  $\{x_i\}$  to maximize her expected (discounted) utility stream

$$E(\sum_{h=0}^{\infty} \alpha^h u(x_{i+h};\beta)|z_i),$$

where u is a well-behaved utility function and  $z_i$  is the information set at baseline i.

Optimality of the consumption path implies that, for all i, the Euler equation

$$\alpha^{i} u'(x_{i};\beta) \, dx_{i} = \alpha^{i+1} u'(x_{i+1};\beta) \, r \, dx_{i}$$

holds. Here, r is the asset return.

Hence,

$$E(\alpha r u'(x_{i+1};\beta)/u'(x_i;\beta) - 1 | z_i) = 0$$

is a valid conditional moment condition for  $\alpha, \beta$ .

# NONPARAMETRIC PROBLEMS: CONDITIONAL-MEAN FUNCTIONS

Hansen II, Chapters 19 and 20 Li and Racine, Chapters 1 and 2 Horowitz, Appendix

## Nonparametric specification

Let  $y_i$  and  $x_i$  be i.i.d. univariate random variables.

Suppose that

$$y_i = m(x_i) + \varepsilon_i, \qquad E(\varepsilon_i | x_i) = 0.$$

We want to estimate m without imposing a functional form.

If  $x_i$  takes values  $v_1, \ldots, v_k$  for finite k < n this is a parametric problem: Regress  $y_i$  on k dummy variables  $d_{i,\kappa} = \{x_i = v_{\kappa}\}$ , i.e.,

$$y_i = \sum_{\kappa=1}^k d_{i,\kappa} \,\beta_\kappa + \varepsilon_i;$$

then  $\beta_{\kappa} = m(v_{\kappa})$ . Equivalently, for a fixed value  $x \in \{v_1, \ldots, v_k\}$ ,

$$\hat{m}(x) = \sum_{i=1}^{n} \omega_i y_i, \qquad \omega_i = \frac{\{x_i = x\}}{\sum_{j=1}^{n} \{x_j = x\}};$$

this is the slope of a regression of  $y_i$  on  $d_{i,x}$ , or sample mean in the subsample with  $x_i = x$ .

When  $x_i$  is continuous the probability that it takes on any given value is zero.

We could estimate m(x) by the weighted average

$$\hat{m}_h(x) = \sum_{i=1}^n \omega_i y_i, \qquad \omega_i = \frac{\{|x_i - x| \le h\}}{\sum_j \{|x_j - x| \le h\}},$$

where h is some chosen positive number, the bandwidth.

This makes sense if we believe m is smooth, so that m(x) does not change too fast when x changes little.

A small choice for the bandwidth h defines a small neighborhood and so decreases bias. But it also increases variance as there will be less observations 'close' to x.

Binning yields a non-smooth estimator of m(x) (as a function of x). Which may not be attractive.

A (second-order) kernel function is any (symmetric) non-negative and bounded function k for which  $\int k(u) du = 1$ ,  $\int u k(u) du = 0$ , and  $\int u^2 k(u) du < \infty$ .

Note that any probability density function with finite second moments can be made to satisfy these requirements.

Commonly-used examples are

- Uniform :  $\frac{1}{2}\{|u| \leq 1\}$
- Triangular :  $(1 |u|) \{ |u| \le 1 \}$
- Epanechnikov :  $\frac{3}{4}(1-u^2) \{|u| \le 1\}$

Gaussian: 
$$\frac{1}{\sqrt{2\pi}}e^{-u^2/2}$$

# A locally-constant estimator

A kernel estimator of m(x) is

$$\hat{m}_h(x) = \sum_{i=1}^n \omega_i y_i, \qquad \omega_i = \frac{k\left(\frac{x_i - x}{h}\right)}{\sum_j k\left(\frac{x_j - x}{h}\right)}.$$

This is the Nadaraya-Watson estimator.

The binning estimator is the special case that uses the uniform kernel. Smooth choices for the kernel k deliver smooth estimators of m.

In practice the choice of h is far more important to the behavior of  $\hat{m}_h$  than is the choice of k.

Note that  $\hat{m}_h(x)$  solves the weighted least squares problem

$$\min\sum_{i=1}^{n}\omega_i\left(y_i-\alpha\right)^2$$

with respect to  $\alpha$ .

The above optimization problem is equivalent to minimizing

$$\frac{1}{n}\sum_{i=1}^{n}k\left(\frac{x_i-x}{h}\right)\frac{(y_i-\alpha)^2}{h}.$$

As n grows this sample averages converges to its expectation, which equals

$$E\left(k\left(\frac{x_i-x}{h}\right)\frac{(y_i-\alpha)^2}{h}\right) = E\left(k\left(\frac{x_i-x}{h}\right)\frac{E((y_i-\alpha)^2|x_i)}{h}\right)$$

Let f be the density of  $x_i$  and  $g(x_i) = E((y_i - \alpha)^2 | x_i) f(x_i)$ . A change of variable to  $u = (x_i - x)/h$  and a second-order expansion around u = 0 show the expectation to equal

$$\int k\left(\frac{x_i - x}{h}\right) \frac{E((y_i - \alpha)^2 | x_i) f(x_i)}{h} dx_i = \int k(u) g(x + hu) du = \int k(u) \left(g(x) + hu g'(x) + \frac{1}{2}h^2 u^2 g''(u^*)\right) du$$

where  $u^*$  lies between u and zero.

Using the properties of the kernel function and assuming that  $|g''|_{\infty} < \infty$ ,

$$E\left(k\left(\frac{x_i-x}{h}\right)\frac{(y_i-\alpha)^2}{h}\right) = E\left(\left(y_i-\alpha\right)^2\right|x_i=x\right)f(x) + O(h^2).$$

Consistency requires that  $h \stackrel{n\uparrow\infty}{\to} 0$ .

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Can also show that the variance is proportional to  $(nh)^{-1}$ . So, if f is equally well behaved, and f(x) > 0,

$$\sum_{i=1}^{n} \omega_{i} (y_{i} - \alpha)^{2} = \frac{\sum_{i=1}^{n} k \left(\frac{x_{i} - x}{h}\right) (y_{i} - \alpha)^{2}}{\sum_{i=1}^{n} k \left(\frac{x_{i} - x}{h}\right)} \xrightarrow{p} E \left( (y_{i} - \alpha)^{2} \middle| x_{i} = x \right)$$

if  $n \to \infty$  provided  $h \to 0$  and  $nh \to \infty$ .

The solution of this limit problem is, of course,

$$\alpha = m(x),$$

justifying the Nadaraya-Watson estimator.

We have implicitely derived the nonparametric kernel density estimator

$$\hat{f}_h(x) = \frac{1}{nh} \sum_{i=1}^n k\left(\frac{x_i - x}{h}\right)$$

for f(x).

The conditions on h relative to n represent the bias/variance trade-off.

As we need  $h \to 0$  the estimator  $\hat{m}(x)$  will converge at a slower rate than  $n^{-1/2}$  (the parametric rate).

We have

$$\sqrt{nh}\left(\hat{m}_h(x) - m(x) - h^2 b(x) \int u^2 k(u) \, du\right) \xrightarrow{d} N\left(0, \frac{\sigma^2(x)}{f(x)} \int k(u)^2 \, du\right),$$

where we let

$$b(x) = \frac{m''(x)}{2} + \frac{f'(x)m'(x)}{f(x)}, \qquad \sigma^2(x) = \operatorname{var}(y_i|x_i = x) = E(\varepsilon_i^2|x_i = x),$$

be first-order bias and variance, respectively.

The convergence rate can be no faster than  $n^{-2/5}$ , which happens when bias and standard deviation shrink at the same rate.

With the bias being  $O(h^2)$  and the variance  $O((nh)^{-1})$  bias vanishes if we choose h such that  $nh^5 \to 0$ .

This is called undersmoothing; it makes bias small relative to standard error.

Alternatives are bias correction or the use of higher-order kernels. Needed to perform valid inference.

Rather than a (weighted) regression on a constant alone we may equally fit a linear approximation to m at x.

This amounts to estimating m(x) by the intercept in

$$\min_{\alpha,\beta} \sum_{i=1}^{n} \omega_i \left( y_i - \alpha - (x_i - x)\beta \right)^2.$$

Although it has the same asymptotic behavior, such an estimator tends to perform better than the standard kernel estimator.

In principle, there is no reason to stop at linearity.

Local polynomial regressions, where we add powers of  $(x_i - x)$  as regressors, are common practice.

A bandwidth that is 'good' (in an overall sense but not at a point) minimizes

$$\int E((\hat{m}_h(x) - m(x))^2) f(x) \, dx,$$

the integrated (with respect to f) mean squared error.

This measure is unknown but can be estimated (up to a constant) by

$$n^{-1} \sum_{i=1}^{n} (y_i - \check{m}_h(x_i))^2,$$

where  $\check{m}_h(x_i)$  is the leave-one-out estimator; for Nadaraya-Watson it equals

$$\check{m}_h(x_i) = \frac{\sum_{j \neq i} k\left(\frac{x_j - x_i}{h}\right) y_j}{\sum_{j \neq i} k\left(\frac{x_j - x_i}{h}\right)}$$

for example.

(Least-squares) cross-validation selects h by min<sub>h</sub>  $n^{-1} \sum_{i=1}^{n} (y_i - \check{m}_h(x_i))^2$ .

This can also be used to select between different estimators (pick the one with lowest IMSE).

Kernel estimators extend easily to the case where the conditioning variable is the vector  $x_i = (x_{i,1}, \ldots, x_{i,\kappa})'$ .

It suffices to redefine k to be multivariate. A simple choice would be a kernel of the form

$$k\left(\frac{x_{i,1}-x_1}{h_1}\right) \times \cdots \times k\left(\frac{x_{i,\kappa}-x_{\kappa}}{h_{\kappa}}\right);$$

a product kernel.

The main problem with multivariate regressors is that the variance of the estimator now becomes inverse-proportional to  $n(h_1 \times \cdots \times h_{\kappa})$ . This implies that the convergence rate decreases with  $\kappa$ . This is known as the curse of dimensionality.

There is a middle-ground between nonparametric and parametric that aims to tackle this issue.

## Matching estimators

We wish to infer the average effect of a treatment on an outcome.

If treatment is randomly assigned,

$$\theta = E(y_i | d_i = 1) - E(y_i | d_i = 0)$$

is the average treatment effect.

Estimate the effect by a least-squares regression on a constant and treatment indicator.

Now suppose that treatment is only random conditional on a set of control variables  $x_i$ .

Then,

$$\theta = \int \left( E(y_i | d_i = 1, x_i = x) - E(y_i | d_i = 0, x_i = x) \right) f(x) \, dx.$$

Let  $m_1(x) = E(y_i | d_i = 1, x_i = x)$  and  $m_0(x) = E(y_i | d_i = 0, x_i = x)$ . Then

$$n^{-1} \sum_{i=1}^{n} \hat{m}_{1,h}(x_i) - \hat{m}_{0,h}(x_i)$$

is a nonparametric matching estimator of  $\theta$ .

Potential problem is limited overlap.

Well-known result says that matching on propensity score,

$$m(x) = P(d_i = 1 | x_i = x),$$

is equivalent.

(Can estimate m nonparametrically and proceed as before but) a convenient alternative follows from observation that

$$E(y_i d_i | x_i = x) = E(y_i | d_i = 1, x_i = x) m(x),$$
  
$$E(y_i (1 - d_i) | x_i = x) = E(y_i | d_i = 0, x_i = x) (1 - m(x)),$$

so that we can write

$$\theta = E\left(\frac{y_i d_i}{m(x_i)} - \frac{y_i(1-d_i)}{1-m(x_i)}\right).$$

Still important to have the propensity vary over entire (0, 1) for identification.

# **Regression discontinuity**

Now suppose treatment is assigned according to

$$d_i = \begin{cases} 0 & \text{if } x_i < c \\ 1 & \text{if } x_i \ge c \end{cases},$$

where the (continuous) running variable  $x_i$  cannot be manipulated and c is a known cut-off value.

Identifying assumption is that people around the cut-off are comparable. Can then identify the local treatment effect

$$\theta = \lim_{x \downarrow c} E(y_i | d_i = 1, x_i = x) - \lim_{x \uparrow c} E(y_i | d_i = 0, x_i = x)$$

at the cut-off.

Natural is to fit separate nonparametric regressions to the left and right of cut-off. Using a rectangular kernel, for example, we use observations in the regions [c - h, c] and [c, c + h] only.

Locally-linear estimators are preferable here as they have better properties at the boundary.

Consider the binary-choice model

$$y_i = \{x'_i \theta \ge \varepsilon_i\}, \ \varepsilon_i \sim \text{ i.i.d. } F,$$

where, now F, is unknown.

A semiparametric maximum-likelihood estimator is the maximizer of

$$\sum_{i=1}^{n} y_i \log(\check{F}(x'_i\theta)) + (1-y_i) \log(1-\check{F}(x'_i\theta))$$

(where we ignore issues of trimming) for

$$\check{F}(x'_i\theta) = \frac{\sum_{j \neq i} k\left(\frac{x'_j\theta - x'_i\theta}{h}\right) y_j}{\sum_{j \neq i} k\left(\frac{x'_j\theta - x'_i\theta}{h}\right)}.$$

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