9. Nonlinear estimators

- introduction
- extremum estimators
- statistical inference
- maximum likelihood estimation
- nonlinear least-squares

Introduction

a nonlinear estimator is one that is a nonlinear function of the dependent variable

$$\hat{\theta} = f(y), \quad f \ \text{ is nonlinear}$$

e.g., $\hat{\theta}$ is the conditional mean

- statistical results in small samples may be limited for nonlinear estimators
- the asymptotical theory has two major treatments derived from linear model:
  - alternative methods of proof are needed since there is no direct formula for most nonlinear estimators
  - asymptotic distribution is obtained under the weakest distributional assumptions possible

in a **nonlinear regression model** we have

- y (dependent variables)
- x (explanatory variables)
- y is a function of x and they have a joint distribution

fact: the best estimate of y given x is the conditional mean: $\mathbf{E}[y|x]$

objective: we would like to *model* $\mathbf{E}[y|x]$ as a function of x

to this end, we define a **parametric model** for $\mathbf{E}[y|x]$:

$$m(x, \theta)$$

- $x \in \mathbf{R}^n$ is explanatory variable
- $\theta \in \mathbf{R}^p$ is parameter vector (and p can be greater or less than n)

examples of nonlinear regression functions:

- exponential regression function: useful model whenever $y \geq 0$

$$m(x, \theta) = \exp(x^T \theta)$$

- logistic function: when y is restricted in $(0, 1)$

$$m(x, \theta) = \frac{e^{x^T \theta}}{1 + e^{x^T \theta}}$$

these examples are nonlinear functions in θ

if we have a *correctly specified model* for $\mathbf{E}[y|x]$, meaning

$$\exists \theta^\star \quad \text{such that} \quad \mathbf{E}[y|x] = m(x, \theta^\star)$$

then we would like to estimate for θ given we know y

Examples of nonlinear estimators

a Poisson regression model for y having nonnegative integer values $0, 1, \ldots$

aside: Poisson probability mass function:

$$f(y|\lambda) = e^{-\lambda}\lambda^y/y!, \quad y = 0, 1, \ldots, \qquad \mathbf{E}[y] = \lambda, \quad \mathbf{var}(y) = \lambda$$

objective: determine λ from y

- assumption: λ varies across regressors x and parameter vector β
- propose to use the model $\lambda = e^{x^T\beta}$ to guarantee $\lambda > 0$
- based on one sample of y, x, the density of **Poisson regression model** is

$$f(y|x, \beta) = e^{-\exp(x^T\beta)}\exp(x^T\beta)^y/y!$$

suppose we have many indenpendent samples: $(y_i, x_i), i = 1, 2, \ldots, N$

each ith sample obyes the joint density (take the log)

$$\log f(y_i|x_i, \beta) = -\exp(x_i^T \beta) + y_i x_i^T \beta - \log y_i!$$

objective: choose β that maximizes the joint density

$$\log f(y_1, \ldots, y_N | x_1, \ldots, x_N, \beta) = \frac{1}{N} \sum_{i=1}^{N} \left(-\exp(x_i^T \beta) + y_i x_i^T \beta - \log y_i \right)$$

(where we apply that all samples are independent)

- choosing β this way is called *maximum likelihood estimation*
- no explicit solution for $\hat{\beta}$, but requires numerical methods to solve
- once we obtain β, we can determine λ

Estimate model of conditional expectation

a typical model for estimating conditional expectation is

$$y = m(x, \theta) + u, \quad \mathbf{E}[u|x] = 0$$

where u is an additive, unobservable error with a zero conditional mean

- define the error $u = y - m(x, \theta)$
- when y is restricted on some range, u and x cannot be independent, *e.g.*

$$y \geq 0 \quad \Rightarrow \quad u \geq -m(x, \theta)$$

- it is too strong to assume that u_i and x_i are independent

Nonlinear least squares (NLS)

let $\Theta \subset \mathbf{R}^p$ be the **parameter space**

assumptions: for some $\theta^\star \in \Theta$, $\mathbf{E}[y|x] = m(x, \theta^\star)$

we seek for θ that solves the population problem

$$\underset{\theta \in \Theta}{\text{minimize}} \quad \mathbf{E}\{[y - m(x, \theta)]^2\}$$

where the expectation is taken over the joint distribution of (x, y)

we can show that

$$\mathbf{E}\{[y - m(x, \theta)]^2\} \geq \mathbf{E}\{[y - m(x, \theta^\star)]^2\}, \quad \forall \theta \in \Theta$$

conclusion: $\theta^\star$ indexing $\mathbf{E}[y|x]$ in fact minimizes the expected square error the **nonlinear least-squares estimation** is the problem:

$$\underset{\theta \in \Theta}{\text{minimize}} \quad \frac{1}{2N} \sum_{i=1}^{N} [y_i - m(x_i, \theta)]^2$$

- it is the sample analogue problem, when samples of y_i and x_i are drawn from the population
- $\hat{\theta}$ minimizes the **sum of squared residuals**
- the factor $1/2$ simplifies the subsequent analysis
- can be solved by deriving the optimality condition: zero gradient condition
- no explicit solution
- the distribution of the NLS estimator depends on the dgp

m-estimator

more generally, we define an m-estimator $\hat{\theta}$ of θ as

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}} \quad Q_N(\theta) := \frac{1}{N}\sum_{i=1}^{N} q(y_i, x_i, \theta)$$

where

- $q(\cdot)$ is a scalar-valued function (but mapped from vector variables)
- Q_N is a sample average of q where N does not affect the minimization problem
- it is the sample analogue problem, as opposed to the population problem:

$$\underset{\theta\in\Theta}{\text{minimize}} \quad \mathbf{E}[q(y, x, \theta)]$$

examples:

- NLS is a special case of m-estimator where q is the quadratic function:

$$q(y, x, \theta) = (y - m(x, \theta))^2$$

- Poisson maximum likelihood estimation:

$$q(y, x, \beta) = -e^{x^T\beta} + yx^T\beta - \log y!$$

- the term m-estimator stands for **maximum-likelihood estimation** where

$$q(y, x, \theta) = -\log f(y|x, \theta) \qquad \text{called loglikelihood function}$$

(-negative log of joint distribution of y given x and parameter θ)

Properties of m-estimator

- identification
- consistency
- limit normal distribution

details in Cameron 2005, chapter 5.3

Identification of the true value

recall that if for some $\theta^\star \in \Theta$

$$\mathbf{E}[y|x] = m(x, \theta^\star)$$

then we say we have a **correctly specified model** for the conditional mean

and often we say that $\theta^\star$ is called **the true parameter value** of θ

- when the model is correctly specified, $\theta^\star$ is the unique solution to

$$\underset{\theta \in \Theta}{\text{minimize}} \quad \mathbf{E}[q(y, x, \theta)]$$

- identification requires that $\theta^\star$ be the unique solution:

$$\mathbf{E}[q(y, x, \theta^\star)] < \mathbf{E}[q(y, x, \theta)], \quad \forall \theta \in \Theta, \quad \theta \neq \theta^\star$$

Consistency of m-estimator

consistency is established in the following manners

- suppose $Q_N(\theta) \xrightarrow{p} Q^\star(\theta)$ as $N \to \infty$ (or other sense of convergence)
- let $\theta^\star$ be the solution that minimizes $Q^\star(\theta)$
- let $\hat{\theta}$ be the solution that minimizes $Q_N(\theta)$
- a consistency result is established to conclude if $\hat{\theta} \xrightarrow{p} \theta^\star$

formal statements can be further read in Cameron 2005, chapter 5.3

Limit normal distribution

we consider the behaviour of $\sqrt{N}(\hat{\theta} - \theta^\star)$ as $N \to \infty$

under appropriate assumptions this yields the **limit distribution** of an m-estimator

$$\sqrt{N}(\hat{\theta} - \theta^\star) \xrightarrow{d} \mathcal{N}(0, A^{-1}BA^{-1})$$

where

- A is the probability limit of the term involving the Hessian of q
- B is the probability limit of the term involving the gradient of q

Asymptotic Normality of m-estimators

define $z = (x, y)$ (or data samples), so $q(z, \theta)$ denote $q(y, x, \theta)$

notation: all derivatives here are w.r.t. θ

assumptions:

- $\theta^\star$ is in the interior of Θ
- $\nabla q(z, \cdot)$ is continuously differentiable on the interior of Θ
- each element of $\nabla^2 q(z, \theta)$ is bounded in absolute value by $b(z)$ where $\mathbf{E}[b(z)] < \infty$
- $A = \mathbf{E}[\nabla^2 q(z, \theta^\star)]$ is positive definite
- $\mathbf{E}[\nabla q(z, \theta^\star)] = 0$
- each element of $\nabla q(z, \theta^\star)$ has finite second moment

under the given assumptions plus the conditions for consistency and identification, then we have

$$\sqrt{N}(\hat{\theta} - \theta^\star) \xrightarrow{d} \mathcal{N}(0, A^{-1}BA^{-1})$$

where

$$A = \mathbf{E}[\nabla^2 q(z, \theta^\star)], \quad B = \mathbf{E}[\nabla q(z, \theta^\star) \nabla q(z, \theta^\star)^T] \triangleq \mathbf{cov}(\nabla q(z, \theta^\star))$$

thus the asymptotic covariance is given by

$$\mathbf{Avar}(\hat{\theta}) = A^{-1}BA^{-1}/N$$

Maximum Likelihood (ML) Estimation

a special case of m-estimator

- likelihood function
- ML estimator
- examples
- distribution of ML estimator

Likelihood function

let $f(y, x|\theta)$ be the joint probability mass/density function

log-likelihood function is defined as

$$\mathcal{L}_N(\theta) = \log f(y, x|\theta)$$

- because $f(y, x|\theta)$ can be viewed as a function of θ given x, y
- y and x denote the data from N samples, hence $\mathcal{L}$ depends on N

the likelihood principle: choose the value of θ that maximize $\mathcal{L}_N(\theta)$

$$e.g., \mathcal{L}_N(\theta_1) = 0.001, \quad \mathcal{L}_N(\theta_2) = 0.003$$

θ_2 gives a higher probability of the observed data occuring, hence is a better estimator

Conditional likelihood

a likelihood function can be rewritten as

$$f(y, x|\theta) = f(y|x, \theta) f(x|\theta)$$

which requires both conditional density of y given x **and** the marginal of x

- the goal of regression is to model the behavior of y given x
- so estimation is usually based on the **conditional likelihood function**:

$$\mathcal{L}_N(\theta) = \log f(y|x, \theta)$$

  (using that $\log$ is an increasing function)

- we can view x as *nonrandom* vectors that are set ahead of time and appear in the unconditional distribution of y

if the observations (y_i, x_i) are **independent** over i then the joint conditional density is

$$f(y_1, y_2, \ldots, y_N | x_1, x_2, \ldots, x_N, \theta) = \prod_{i=1}^{N} f(y_i | x_i, \theta)$$

this leads to the **conditional log-likelihood function**

$$Q_N(\theta) = (1/N)\mathcal{L}_N(\theta) = \frac{1}{N} \sum_{i=1}^{N} \log f(y_i | x_i, \theta)$$

where we divide by N so that the objective function is an average

example 1 (Bernoulli RVs): let $y_1, \ldots, y_N$ be random samples from a Bernoulli distribution

assume that the probability of success is given by p, a parameter to be estimated

the density function of Bernoulli distribution is

$$f(y_i|p) = p^{y_i}(1-p)^{1-y_i}$$

if we assume y_i's are i.i.d. samples, the joint density function is

$$f(y_1, y_2, \ldots, y_N|p) = \prod_{i=1}^{N} p^{y_i}(1-p)^{1-y_i}$$

the **likelihood function** is

$$Q_N(\theta)(1/N)\log f(y_1, y_2, \ldots, y_N|p) = (1/N)\sum_{i=1}^{N} y_i \log p + (1-y_i)\log(1-p)$$

example 2 (Probit): suppose the observation value of y is binary

$$y = \mathbf{sign}(x\theta + e), \quad e \sim \mathcal{N}(0,1)$$

where $\mathbf{sign}(\cdot)$ is the sign function, *i.e.*, $\mathbf{sign}(y) = 1$ if $y \geq 0$ and 0 otherwise

to derive the conditional density of y, we first compute

$$\begin{aligned} P(y=1|x,\theta) &= P(x\theta + e > 0|x,\theta) = P(e > -x\theta|x,\theta) \\ &= 1 - \Phi(-x\theta) = \Phi(x\theta) \\ P(y=0|x,\theta) &= 1 - \Phi(x\theta) \end{aligned}$$

where $\Phi(\cdot)$ denotes the standard normal CDF

therefore, the dentity of y given x and θ is

$$f(y|x,\theta) = [\Phi(x\theta)]^y[1-\Phi(x\theta)]^{1-y}, \quad y = 0,1$$

and that $f(y|x,\theta) = 0$ when $y \notin \{0,1\}$

suppose i.i.d. N samples of observations are drawn: $y_1, y_2, \ldots, y_N$

the conditional density of y_i given x_i and θ is

$$f(y_i|x_i, \theta) = [\Phi(x_i\theta)]^{y_i}[1 - \Phi(x_i\theta)]^{1-y_i}, \quad y = 0, 1$$

hence, the **joint conditional density** function is

$$f(y_1, \ldots, y_N|x_1, \ldots, x_N, \theta) = \prod_{i=1}^{N}[\Phi(x_i\theta)]^{y_i}[1 - \Phi(x_i\theta)]^{1-y_i}$$

the **conditional loglikelihood function** is

$$Q_N(\theta) = \frac{1}{N}\sum_{i=1}^{N}\{y_i \log(\Phi(x_i\theta)) + (1 - y_i)\log(1 - \Phi(x_i\theta))\}$$

example 3 (Poisson regression): from page 9-4

- determine λ, the mean of the poisson distribution from observations y_i, x_i
- propose to use the model $\lambda = e^{x^T\beta}$ to guarantee $\lambda > 0$
- based on one sample of y, x, the density of **Poisson regression model** is

$$f(y|x,\beta) = e^{-\exp(x^T\beta)}\exp(x^T\beta)^y/y!$$

- when all samples are i.i.d., the conditional loglikelihod function is

$$Q_N(\theta) = \frac{1}{N}\sum_{i=1}^{N}\log f(y_i|x_i,\beta) = (1/N)\sum_{i=1}^{N} -\exp(x_i^T\beta) + y_i x_i^T\beta - \log y_i!$$

example 4 (Gaussian vectors): estimate the mean and covariance matrix of Gaussian RVs

- observe a sequence of *independent* random vectors: $y_1, y_2, \ldots, y_N$
- each y_k is an n-dimensional Gaussian: $y_k \sim \mathcal{N}(\mu, \Sigma)$, but μ, Σ are unknown

the likelihood function of $y_1, \ldots, y_N$ given μ, Σ is

$$f(y_1, \ldots, y_N | \mu, \Sigma) = \frac{1}{(2\pi)^{Nn/2}} \cdot \frac{1}{|\Sigma|^{N/2}} \cdot \textbf{exp} - \frac{1}{2} \sum_{k=1}^{N} (y_k - \mu)^T \Sigma^{-1} (y_k - \mu)$$

the **conditional log-likelihood function** is

$$\begin{aligned} Q_N(\mu, \Sigma) &= (1/N)\mathcal{L}(\mu, \Sigma) \\ &= (n/2)\log(2\pi) + (1/2)\log\det\Sigma^{-1} - (1/2N)\sum_{k=1}^{N}(y_k - \mu)^T\Sigma^{-1}(y_k - \mu) \end{aligned}$$

Maximum likelihood estimator (MLE)

the MLE is the estimator that maximizes the log-likelihood function

$$\hat{\theta} = \operatorname*{argmax}_{\theta} \quad \log f(y, x|\theta)$$

or maximizes the conditional log-likelihood function

$$\hat{\theta} = \operatorname*{argmax}_{\theta} \quad \log f(y|x, \theta)$$

- MLE is a special case of **extremum estimators** since it solves an optimization problem, which typically has no analytical solution
- usually MLE is a local maximum that solves the zero gradient condition:

$$\frac{\partial \mathcal{L}_N(\theta)}{\partial \theta} = 0$$

the **score of the loglikelihood** for observation i is defined as

$$s_i(\theta) = \frac{\partial \log f(y_i|x_i,\theta)}{\partial \theta} = \frac{1}{f(y_i|x_i,\theta)} \nabla_\theta f(y_i|x_i,\theta)$$

- if $\theta \in \mathbf{R}^n$ then s_i is the gradient vector of size $n \times 1$
- the zero gradient condition for solving MLE is then described as

$$\frac{\partial \mathcal{L}_N(\theta)}{\partial \theta} = \sum_{i=1}^{N} s_i(\theta) = \sum_{i=1}^{N} \frac{1}{f(y_i|x_i,\theta)} \nabla_\theta f(y_i|x_i,\theta)$$

  (the sum of the first derivatives of the log density)

- the gradient vector $\frac{\partial \mathcal{L}_N(\theta)}{\partial \theta}$ is called the **score vector**
- when the score is evaluated at $\theta^\star$, it is called the **efficient score**

Some ML estimators have closed-form expression

example 1 (Bernoulli): characterize the score likelihood

$$s_i(p) = y_i \frac{1}{p} - (1 - y_i) \frac{1}{1-p}$$

the zero gradient condition for solving MLE is

$$0 = \sum_{i=1}^{N} s_i(p) = \frac{1}{p} \sum_{i=1}^{N} y_i - \frac{1}{1-p} \sum_{i=1}^{N} (1 - y_i)$$

with some algebra, we can solve that

$$\hat{p} = \frac{1}{N} \sum_{i=1}^{N} y_i$$

MLE of probability of success is in fact the portion of success from N samples

example 4 (Gaussian): rewrite the relevant term in conditional likelihood

$$Q_N(\Sigma, \mu) = \log\det \Sigma^{-1} - (1/N) \sum_{k=1}^{N} (y_k - \mu)^T \Sigma^{-1} (y_k - \mu)$$

two parameters to be estimated, but we can maximize over μ first

the gradient w.r.t. μ is set to zero

$$\frac{\partial Q_N}{\partial \mu} = \sum_{k=1}^{N} \Sigma^{-1}(y_k - \mu) = 0 \quad \Rightarrow \quad \hat{\mu} = (1/N) \sum_{k=1}^{N} y_k$$

the likelihood function evaluated at $\hat{\mu}$ can be expressed as

$$Q_N(\Sigma, \hat{\mu}) = \log\det \Sigma^{-1} - \mathbf{tr}(C\Sigma^{-1}) \quad \triangleq \quad \log\det X - \mathbf{tr}(CX)$$

where $C = (1/N)\sum_{k=1}^{N}(y_k - \hat{\mu})(y_k - \hat{\mu})^T$ is the sample covariance matrix taking the derivative w.r.t. X gives

$$\frac{\partial Q_N}{\partial X} = X^{-1} - C \quad \Rightarrow \quad X = C^{-1}$$

in conclusion, the ML estimators of Σ and μ are

$$\hat{\mu} = (1/N)\sum_{k=1}^{N} y_k,$$

$$\hat{\Sigma} = (1/N)\sum_{k=1}^{N}(y_k - \hat{\mu})(y_k - \hat{\mu})^T$$

the sample mean and sample covariance matrix we already knew

Most ML estimations require numerical algorithms

example 2 (Probit): the zero gradient condition of the likelihood function is

$$\frac{\partial Q_N}{\partial \theta} = \sum_{i=1}^{N} \frac{x_i y_i f(x_i \theta)}{\Phi(x_i \theta)} + \frac{(1 - y_i)(-f_i(x_i \theta)) x_i}{(1 - \Phi(x_i \theta))} = 0$$

(using $\Phi'(x) = f(x)$)

example 3 (Poisson): the zero gradient condition is

$$\frac{\partial Q_N}{\partial \beta} = \sum_{i=1}^{N} (-x_i e^{x_i^T \beta} + y_i x_i) = 0$$

- the zero gradient (or first-order) condition is a nonlinear equation in θ
- numerically solving MLE involves nonlinear optimization such as Newton-Raphson method

Distribution of ML estimators

to derive asymptotic distributin of ML estimators, we discuss

- regularity condition
- Fisher information matrix
- theorem of asymptotic distribution

Regularity conditions

the **ML regularity conditions** are that

1. the score vector has expected value zero:

$$\mathbf{E}\left[\nabla_\theta \log f(y|x,\theta)\right] = \int \nabla_\theta \log f(y|x,\theta) f(y|x,\theta) dy = 0$$

2. the expected Hessian is the expected outer product of the gradient

$$-\mathbf{E}\left[\nabla_\theta^2 \log f(y|x,\theta)\right] = \mathbf{E}\left[(\nabla_\theta \log f(y|x,\theta))(\nabla_\theta \log f(y|x,\theta))^T\right]$$

   when evalued at $\theta = \theta^\star$ it is known as the **unconditional information matrix equality (UIME)**

the regularity conditions **hold** when the expectation is w.r.t $f(y|x,\theta)$

Fisher information matrix

the **Fisher information matrix** for θ contained in y (1 sample) is defined as

$$\mathcal{I}(\theta) = \mathbf{E}\left[(\nabla_\theta \log f(y,|x,\theta))(\nabla_\theta \log f(y|x,\theta))^T\right]$$

the expectation of the **outer product of the score vector**

the Fisher information matrix for θ contained in $y_1, y_2, \ldots, y_N$ is

$$\mathcal{I}_N(\theta) = \mathbf{E}\left[(\nabla_\theta \mathcal{L}_N(\theta))(\nabla_\theta \mathcal{L}_N(\theta))^T\right]$$

since $y_1, y_2, \ldots, y_N$ are identical samples drawn from the same distribution

$$\mathcal{I}_N(\theta) = N\mathcal{I}(\theta)$$

- $\mathcal{I}(\theta$ is a positive semidefinite matrix
- since the score vector has mean zero, $\mathcal{I}_N(\theta)$ is the variance of $\nabla_\theta \mathcal{L}_N(\theta)$
- large $\mathcal{I}_N(\theta)$ means small changes in θ lead to larger change in $\mathcal{L}_N$
- the second regularity condition implies that

$$\mathcal{I}(\theta) = -\mathbf{E}\left[\nabla_\theta^2 \log f(y|x,\theta)\right]$$

  when evaluated at $\theta^\star$ this is called the **information matrix (IM) equality**
- we will see later that $\mathcal{I}$ gives the quality of an estimator

Distribution of ML estimator

assumptions:

1. the dgp is the conditional density $f(y_i|x_i, \theta)$ used to defined the likelihood
2. the density $f(\cdot)$ satisfies $f(y, \theta) = f(y, \alpha)$ iff $\theta = \alpha$
3. the following matrix exists and is finite nonsingular

$$P = -\mathbf{E}\left[\frac{1}{N}\nabla^2 \mathcal{L}_N(\theta^\star)\right]$$

4. the order of differentiation and integration of $\mathcal{L}$ can be reversed

then the ML estimator $\hat{\theta}_{\mathrm{ml}}$ is consistent for $\theta^\star$ and

$$\sqrt{N}(\hat{\theta}_{\mathrm{ml}} - \theta^\star) \xrightarrow{d} \mathcal{N}(0, P^{-1})$$

- condition 1: the conditional density is correctly specified
- condition 1&2: ensure that $\theta^\star$ is identified
- condition 3: analogous to the assumption on $\mathbf{plim}\, N^{-1}X^TX$ for OLS estimator
- condition 4: necessary for the regularity conditions to hold
- if (y_i, x_i) are identical for all i, then

$$\mathbf{E}[\nabla^2 \mathcal{L}_N(\theta^\star)] = \mathbf{E}[\sum_{i=1}^N \nabla^2 \log f(y_i|x_i, \theta^\star)] = N\mathbf{E}[\nabla^2 \log f(y|x, \theta^\star)]$$

  P is replaced by evaluation based on *one* sample of (y, x)

$$P = -\mathbf{E}[\nabla_\theta^2 \log f(y|x, \theta^\star)]$$

- asymptotic normality is obtained from the result on page 9-16 with $A = -B$
- P is essentially the Fisher information matrix, $\mathcal{I}(\theta)$

Estimating the asymptotic covariance

asymptotic normality of ML:

$$\hat{\theta}_{\rm ml} \xrightarrow{d} \mathcal{N}(\theta^\star, P^{-1}/N)$$

where the asymptotic covariance can be also expressed as

$$\mathbf{Avar}(\hat{\theta}_{\rm ml}) = P^{-1}/N = \mathcal{I}(\theta)^{-1}/N = \mathcal{I}_N(\theta)^{-1}$$

at least three possible estimators of $\mathcal{I}$ converges to $-\mathbf{E}[\nabla^2 \log f(y|x,\theta^\star)]$

$$-(1/N)\sum_{i=1}^N \nabla^2 \log f(y_i|\theta), \quad (1/N)\sum_{i=1}^N \nabla \log f(y_i|\theta) \nabla \log f(y_i|\theta)^T$$

$$-(1/N)\sum_{i=1}^N \mathbf{E}_{y|x}[\nabla^2 \log f(y_i|x_i,\theta)]$$

thus $\widehat{\mathbf{Avar}}(\hat{\theta}_{\mathrm{ml}}) = \hat{\mathcal{I}}_N(\theta) = \frac{\hat{\mathcal{I}}(\theta)^{-1}}{N}$ can be taken to be any of the three matrices

$$\left[-\sum_{i=1}^{N} \nabla^2 \log f(y_i|\hat{\theta})\right]^{-1}, \quad \left[\sum_{i=1}^{N} \nabla \log f(y_i|\hat{\theta}) \nabla \log f(y_i|\hat{\theta})^T\right]^{-1}$$

$$\left[-\sum_{i=1}^{N} \mathbf{E}_{y|x}[\nabla^2 \log f(y_i|x_i, \hat{\theta}))]\right]^{-1}$$

example 1 (Bernoulli): the loglikelihood based on one sample is

$$\log f(y|p) = y \log p + (1-y)\log(1-p)$$

the gradient and the Hessian of the loglikelihood (w.r.t. p) is given by

$$\nabla \log(y|p) = \frac{y}{p} - \frac{1-y}{1-p}, \quad \nabla^2 \log(y|p) = -\frac{y}{p^2} + \frac{1-y}{(1-p)^2}$$

the Fisher information matrix (based on 1 sample) is

$$P = \mathcal{I}(\theta) = -\mathbf{E}[\nabla^2 \log(y|p)] = -\left(\frac{p}{p^2} + \frac{1-p}{(1-p)^2}\right) = \frac{1}{p(1-p)} > 0$$

hence, $\mathcal{I}^{-1}(\theta) = p(1-p)$ and the asymptotic distribution is

$$\sqrt{N}(\hat{p}_{\mathrm{ml}} - p^\star) \xrightarrow{d} \mathcal{N}(0, p(1-p))$$

example 2 (Probit): consider the gradient of loglikelihood based on 1 sample

$$\nabla \log f(y|x,\theta) = \frac{xyf(x\theta)}{\Phi(x\theta)} - \frac{(1-y)xf(x\theta)}{1-\Phi(x\theta)} = \frac{xf(x\theta)(y-\Phi(x\theta))}{\Phi(x\theta)(1-\Phi(x\theta))}$$

$$\begin{aligned}\mathcal{I}(\theta) = -\mathbf{E}[\nabla^2 \log f] = \mathbf{E}[\nabla \log f \cdot \nabla \log f^T] &= \mathbf{E}_{y|x}\left[\frac{x^2 f^2(x\theta)(y-\Phi(x\theta))^2}{\Phi^2(x\theta)(1-\Phi(x\theta))^2}\right] \\ &= \frac{x^2 f^2(x\theta)}{\Phi^2(x\theta)(1-\Phi(x\theta))^2}\mathbf{E}_{y|x}[(y-\Phi(x\theta))^2]\end{aligned}$$

note that y is Bernoulli with mean $p = \Phi(x\theta)$ and variance $\Phi(x\theta)(1-\Phi(x\theta))$

$$\mathcal{I}(\theta) = \frac{x^2 f^2(x\theta)\cdot\Phi(x\theta)(1-\Phi(x\theta))}{\Phi^2(x\theta)(1-\Phi(x\theta))^2} = \frac{x^2 f^2(x\theta)}{\Phi(x\theta)(1-\Phi(x\theta))}$$

$$\widehat{\mathbf{Avar}}(\hat{\theta}) = \left(\sum_{i=1}^N \frac{x_i^2 f^2(x_i\theta)}{\Phi(x_i\theta)(1-\Phi(x_i\theta))}\right)^{-1}$$

example 3 (Poisson): the gradient of loglikelihood based on 1 sample is

$$\nabla \log f(y|x,\beta) = -xe^{x^T\beta} + yx$$

it follows that

$$\begin{aligned} \nabla^2 \log f(y|x,\beta) &= -xx^T e^{x^T\beta} \\ \mathcal{I}(\theta) &= -\mathbf{E}_{y|x}[\nabla^2 \log f(y|x,\beta)] = xx^T e^{x^T\beta} \succ 0 \end{aligned}$$

the estimate of asymptotic covariance is

$$\widehat{\mathbf{Avar}}(\hat{\beta}) = \left[\sum_{i=1}^{N} e^{x_i^T\hat{\beta}} x_i x_i^T\right]^{-1}$$

example 4 (scalar Gaussian): here $\theta = (d, \mu)$ where $d = \sigma^2 > 0$

$$\log f(y|\theta) = -(1/2)\log(d) - (1/2)(y-\mu)^2/d$$

$$\nabla \log f = (1/2)\begin{bmatrix} -1/d + (y-\mu)^2/d^2 \\ 2(y-\mu)/d \end{bmatrix}$$

$$\nabla^2 \log f = (1/2)\begin{bmatrix} 1/d^2 - 2(y-\mu)^2/d^3 & -2(y-\mu)/d^2 \\ -2(y-\mu)/d^2 & -2/d \end{bmatrix}$$

$$\mathcal{I}(\theta) = -\mathbf{E}[\nabla^2 \log f] = -(1/2)\begin{bmatrix} 1/d^2 - 2/d^2 & 0 \\ 0 & -2/d \end{bmatrix}$$

$$\mathcal{I}(\theta)^{-1} = \begin{bmatrix} 2d^2 & 0 \\ 0 & d \end{bmatrix} \succ 0$$

$$\widehat{\mathbf{Avar}}(\hat{\sigma}^2) = 2\hat{\sigma}^4/N$$

$$\widehat{\mathbf{Avar}}(\hat{\mu}) = \hat{\sigma}^2/N$$

Cramér-Rao inequality

for any **unbiased** estimator $\hat{\theta}$ with the covariance matrix of the error:

$$\mathbf{cov}(\hat{\theta}) = \mathbf{E}(\theta - \hat{\theta})(\theta - \hat{\theta})^T,$$

we always have a lower bound on $\mathbf{cov}(\hat{\theta})$:

$$\mathbf{cov}(\hat{\theta}) \succeq \mathcal{I}_N(\theta)^{-1}$$

- the RHS is called the **Cramér-Rao** lower bound, and also equal to $\mathcal{I}(\theta)^{-1}/N$
- provide the minimal covariance matrix over all possible estimators $\hat{\theta}$

- a consistent asymptotically normal estimator $\hat{\theta}$ of θ is said to be **asymptotically efficient** if

$$\mathbf{Avar}(\hat{\theta}) = \mathcal{I}(\theta)^{-1}/N$$

- ML estimator has the smallest asymptotic variance among root-N consistent estimators (requiring the correctly specified conditional density)

Example of CR bound

estimating λ in exponential RVs: $f(x) = \lambda e^{-\lambda x}$

$$\log f(x|\lambda) = \log \lambda - \lambda x, \quad \nabla \log f(x|\lambda) = \frac{1}{\lambda} - x, \quad \nabla^2 \log f(x|\lambda) = -\frac{1}{\lambda^2}$$

therefore, $\mathcal{I}(\lambda) = 1/\lambda^2$ and CR bound is $\mathbf{var}(\hat{\lambda}) \geq \lambda^2/N$

estimating θ in Bernoulli RVs: $p(x) = \theta^x (1-\theta)^{1-x}$

$$\begin{aligned} \log p(x|\theta) &= x \log \theta + (1-x)\log(1-\theta), \quad \nabla \log p(x|\theta) = \frac{x}{\theta} - \frac{(1-x)}{(1-\theta)}, \\ \nabla^2 \log p(x|\theta) &= -\frac{x}{\theta^2} - \frac{(1-x)}{(1-\theta)^2}, \quad \mathbf{E}[\nabla^2 \log p(x|\theta)] = -\frac{\theta}{\theta^2} - \frac{1-\theta}{(1-\theta)^2} \end{aligned}$$

therefore, $\mathcal{I}(\theta) = \frac{1}{\theta(1-\theta)}$ and CR bound is $\mathbf{var}(\theta) \geq \theta(1-\theta)/N$

Important proofs

- derivation of regularity conditions
- proof of Cramér-Rao bound

Derivation of regularity conditions

- from $\int f(y|\theta)dy = 1$, differentiate both sides w.r.t θ gives $\nabla_\theta \int f(y|\theta)dy = 0$
- if the range of integration does not depend on θ, by Leibniz integral rule

$$\int \nabla_\theta f(y|\theta)dy = 0$$

- from the derivative of $\log(\cdot)$ function,

$$\nabla_\theta f(y|\theta) = \nabla_\theta \log f(y|\theta) \cdot f(y|\theta)$$

- substitute into the previous equation

$$\int \nabla_\theta \log f(y|\theta) \cdot f(y|\theta)dy = 0 \quad \Rightarrow \quad \mathbf{E}[\nabla_\theta \log f(y|\theta)] = 0$$

this is the regularity condition (1) w.r.t. to the density $f(y|\theta)$

- from $\int \nabla_\theta \log f(y|\theta) \cdot f(y|\theta) dy = 0$, differentiate both sides w.r.t. θ

$$\int \left\{ \nabla_\theta^2 \log f(y|\theta) f(y|\theta) + (\nabla_\theta \log f(y|\theta))(\nabla_\theta f(y|\theta))^T \right\} dy = 0$$

- substitute $\nabla_\theta f(y|\theta) = \nabla_\theta \log f(y|\theta) \cdot f(y|\theta)$ to the previous equation

$$\int \left\{ \nabla_\theta^2 \log f(y|\theta) f(y|\theta) + (\nabla_\theta \log f(y|\theta))(\nabla_\theta \log f(y|\theta))^T f(y|\theta) \right\} dy = 0$$

- this is equivalent to

$$\mathbf{E}[\nabla_\theta^2 \log f(y|\theta)] = -\mathbf{E}[(\nabla_\theta \log f(y|\theta))(\nabla_\theta \log f(y|\theta))^T]$$

  when the expectation is w.r.t. the density $f(y|\theta)$

this is the regularity condition (2)

Proof of the Cramér-Rao inequality

with abuse of notation, we mean $y = (y_1, y_2, \ldots, y_N)$ and $f(y|\theta)$ is a *joint* pdf

- since $\hat{\theta}$ is unbiased, we have $\theta = \int \hat{\theta}(y) f(y|\theta) dy$
- differentiate both sides w.r.t. θ and use $\nabla_\theta \log f(y|\theta) = \nabla f(y|\theta)/f(y|\theta)$

$$I = \int \hat{\theta}(y) \nabla \log f(y|\theta) f(y|\theta) dy = \mathbf{E}[\hat{\theta}(y) \nabla \log f(y|\theta)]$$

- from regularity condition (1), $\mathbf{E}[\nabla \log f(y|\theta)] = 0$ we have

$$\mathbf{E}\left[(\hat{\theta}(y) - \theta) \nabla \log f(y|\theta)\right] = I$$

($\mathbf{E}$ is taken w.r.t y, and θ is fixed) consider a positive semidefinite matrix

$$\mathbf{E} \begin{bmatrix} \hat{\theta}(y) - \theta \\ \nabla_\theta \log f(y|\theta) \end{bmatrix} \begin{bmatrix} \hat{\theta}(y) - \theta \\ \nabla_\theta \log f(y|\theta) \end{bmatrix}^T \succeq 0$$

expand the product into the form

$$\begin{bmatrix} A & I \\ I & D \end{bmatrix}$$

where $A = \mathbf{E}(\hat{\theta}(y) - \theta)(\hat{\theta}(y) - \theta)^T$ and

$$D = \mathbf{E}[\nabla \log f(y|\theta) \cdot (\nabla \log f(y|\theta))^T] = \mathcal{I}_N(\theta)$$

the Schur complement of the $(1,1)$ block must be nonnegative:

$$A - ID^{-1}I \succeq 0$$

which implies the Cramér Rao inequality

Nonlinear Least Squares

- nonlinear least squares (NLS) estimator
- optimality condition
- examples
- distribution of NLS estimator

Nonlinear regression model

define the scalar dependent variable y to have conditional mean

$$\mathbf{E}[y|x] = g(x, \beta)$$

- g is a scalar-valued specified function
- x is a vector of explantory variables
- β is a parameter vector
- for linear case, $g(x, \beta) = x^T \beta$

Exponential regression example

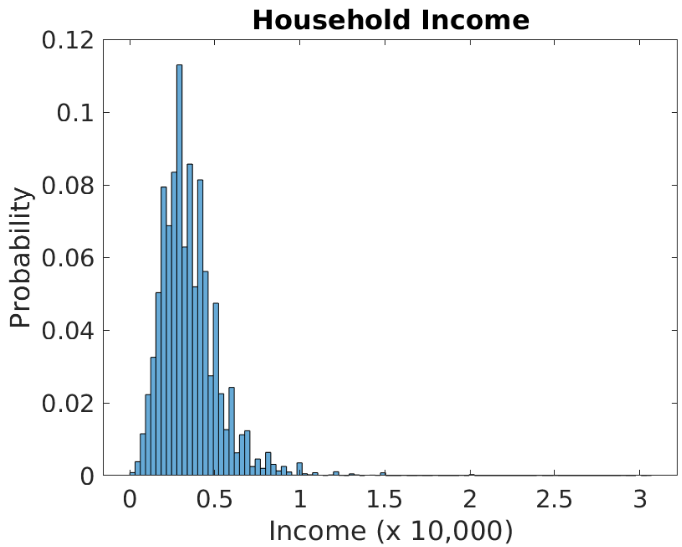
the nonlinear model is

$$y = e^{x^T \beta} + u$$

to study household income with sociodemographic variables

- y: household income

- x: age, age^2, education, female, female $\cdot$ education, age $\cdot$ education



The Box-Cox transformation

the Box-cox transformation for a fixed λ is

$$z^{(\lambda)} = (z^{\lambda} - 1)/\lambda$$

- when $\lambda = 1$ the transformation is linear
- when $\lambda = 0$, it is a log transformation – by L'Hopital)

a regression model can be generalized by using Box-cox transformation

$$y = \beta_0 + \sum_{k=1}^{n} \beta_k x_k^{(\lambda)} + u$$

- if λ is fixed, the regression is linear in β_k's
- if λ is also a parameter, the regression is nonlinear

NLS estimator

the **nonlinear least-squares estimation** is the problem

$$\underset{\beta}{\text{minimize}} \quad Q_N(\beta) := \frac{1}{2N}\sum_{i=1}^{N}(y_i - g(x_i,\beta))^2$$

- given the samples $(y_1, x_1), \ldots, (y_N, x_N)$ are available
- ith is the sample index
- $\hat{\beta}_{\text{nls}}$ minimizes the sum of squared residuals
- the factor $1/2$ is added for simplifying the analysis

Solving NLS

matrix notation: let

$$\mathbf{y} = (y_1, y_2, \ldots, y_N), \quad \mathbf{g}(x, \beta) = (g(x_1, \beta), g(x_2, \beta), \ldots, g(x_N, \beta))$$

the NLS problem can be written in a vector form as

$$\underset{\beta}{\text{minimize}} \;\; (1/2)\|\mathbf{y} - \mathbf{g}(x, \beta)\|_2^2$$

so the **optimality condition** is

$$\nabla_\beta Q_N(\beta) = D\mathbf{g}(x, \beta)^T(\mathbf{y} - \mathbf{g}(x, \beta)) = \sum_{i=1}^{N} \nabla_\beta g(x_i, \beta)(y_i - g(x_i, \beta)) = 0$$

- no explicit solution for $\hat{\beta}_{\text{nls}}$ satisfying the zero gradient condition
- one uses iterative methods (nonlinear optimization techniques) in solving NLS

Exponential regression example

suppose y given x has exponential conditional mean: $\mathbf{E}[y|x] = e^{x^T\beta}$

the model of nonlinear regression is

$$y = e^{x^T\beta} + u$$

- u is the error term
- the conditional mean is nonlinear in β, parameter to be estimated
- the NLS estimator must satisfy the zero gradient condition:

$$\sum_{i=1}^{N} x_i e^{x_i^T\beta}(y_i - e^{x_i^T\beta}) = 0$$

Data-generating process in NLS

the dgp can be written as

$$y_i = g(x_i, \beta^\star) + u_i$$

- u_i is additive error term
- $\beta^\star$ is the true value of parameter
- the conditional mean is correctly specified if

$$\mathbf{E}[y|x] = g(x, \beta^\star)$$

  meaning the error must satisfy $\mathbf{E}[u|x] = 0$

Distribution of NLS estimator

assumptions:

1. the model is $y_i = g(x_i, \beta^\star) + u_i$
2. in the dgp $\mathbf{E}[u_i|x_i] = 0$ and $\mathbf{E}[uu^T|x] = \Lambda$
3. $g(\cdot)$ satisfies $g(x, \beta) = g(x, \alpha)$ iff $\beta = \alpha$
4. the following matrix exists and is finite nonsingular

$$\begin{aligned} F(x, \beta) &= (\nabla g(x_1, \beta)^T, \ldots, \nabla g(x_N, \beta)^T) \in \mathbf{R}^{N \times n} \\ A &= \mathbf{plim}\, \frac{1}{N} F(x, \beta^\star)^T F(x, \beta^\star) \\ &= \mathbf{plim}\, \frac{1}{N} \sum_{i=1}^{N} \nabla g(x_i, \beta^\star) \nabla g(x_i, \beta^\star)^T \end{aligned}$$

5. $(1/\sqrt{N})\sum_{i=1}^{N}\nabla g(x_i,\beta^\star)u_i \xrightarrow{d} \mathcal{N}(0,B)$ where

$$B = \mathbf{plim}\,\frac{1}{N}F^T(x,\beta^\star)\Lambda F(x,\beta^\star)$$
$$= \mathbf{plim}\,\frac{1}{N}\sum_{i=1}^{N}\sigma_i^2\nabla g(x_i,\beta^\star)\nabla g(x_i,\beta^\star)^T$$

then the **NLS estimator** $\hat{\beta}_{\rm nls}$ defined to be a root of

$$\nabla_\beta Q_N(\beta) = 0$$

is consistent for $\beta^\star$ and

$$\sqrt{N}(\hat{\beta}_{\rm nls} - \beta^\star) \xrightarrow{d} \mathcal{N}(0, A^{-1}BA^{-1})$$

- condition 1-3: the regression is correctly specified and the regressors are uncorrelated with the errors and that $\beta^\star$ is specified
- the errors can be heteroskedastic
- condition 4-5: assume the relevant limit results necessary for application of theorem on page 9-16

special case: spherical errors with $\Lambda = \sigma^2 I$

- this implies $B = \sigma^2 A$ and $A^{-1}BA^{-1} = \sigma^2 A^{-1}$
- nonlinear least-squares is then asymptotically efficient among LS estimators

Variance matrix estimation for NLS

from page 9-61, the **asymptotic distribution** of NLS estimators is

$$\hat{\beta}_{\rm nls} \sim \mathcal{N}(\beta^\star, (F^T F)^{-1} F^T \Lambda F (F^T F)^{-1})$$

where $F := F(x, \beta^\star)$ defined on page 9-61

- we consider independent errors with **heteroskedasticity of unknown functional form**
- we provide estimates of A, B and the asymptotic covariance matrix

let $\hat{\beta}$ be a **consistent** estimate of β and define

$$\hat{\mathbf{u}} = \mathbf{y} - \mathbf{g}(x, \hat{\beta})$$

- estimate of A: $\hat{A} = (1/N)F^T(x, \hat{\beta})F(x, \hat{\beta})$
- estimate of Λ: $\hat{\Lambda} = \mathbf{diag}(\hat{\mathbf{u}}^2)$ (squared element-wise)
- estimate of B: $B = (1/N)F^T(x, \hat{\beta})\hat{\Lambda}F(x, \hat{\beta})$

these lead to the **heteroskedastic-consistent** estimate of the asymptotic variance matrix of the NLS estimator:

$$\widehat{\mathbf{Avar}}(\hat{\beta}_{\text{nls}}) = (F^T F)^{-1} F^T \hat{\Lambda} F (F^T F)^{-1}$$

(note that now $F := F(x, \hat{\beta})$; evaluated at $\hat{\beta}$)

Exponential regression example

the model is

$$y = e^{x^T\beta} + u$$

where u has $\mathbf{E}[u|x] = 0$ and u is potentially heteroskedastic

- $g(x,\beta) = e^{x^T\beta}$, and $\nabla g(x,\beta) = xe^{x^T\beta}$
- $F^TF := F^T(x,\hat\beta)F(x,\hat\beta) = \sum_{i=1}^N x_ix_i^Te^{2x_i^T\hat\beta}$
- $\hat\Lambda = \mathbf{diag}(\hat{\mathbf{u}}^2)$ where $\hat u = y - e^{x^T\hat\beta}$
- the heteroskedastic-robust estimate is

$$\widehat{\mathbf{Avar}}(\hat\beta_{\rm nls}) = \left(\sum_{i=1}^N x_ix_i^Te^{2x_i^T\hat\beta}\right)^{-1}\left(\sum_{i=1}^N \hat u_i^2 x_ix_i^Te^{2x_i^T\hat\beta}\right)\left(\sum_{i=1}^N x_ix_i^Te^{2x_i^T\hat\beta}\right)^{-1}$$

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