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Advanced Quantitative Methods:
Maximum Likelihood

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1 Likelihoods

2 Linear model

3 Score and Hessian matrices

4 Asymptotics

5 Standard tests

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2. Linear model

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Preliminaries

Ordinary least squares and its variations (GLS, WLS, 2SLS, etc.) is very flexible and applicable in many circumstances, but for some models (e.g. limited dependent variable models) we need more flexible estimation procedures.

The most prominent alternative estimators are **maximum likelihood** (ML) and **Bayesian** estimators. This lecture is about the former.

Likelihood: intuition

Dice example.

Imagine a dice is thrown with unknown number of sides k. We know after throwing the dice that the outcome is 5. How likely is this outcome if $k = 0$? And $k = 1$? Continue until $k = 10$. Plot of this is the likelihood function.

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Likelihood

"Likelihood is the hypothetical probability that an event that has already occurred would yield a specific outcome. The concept differs from that of a probability in that a probability refers to the occurrence of future events, while a likelihood refers to past events with known outcomes."

(Wolfram Mathworld)

Preliminaries

Looking first at just univariate models, we can express the
model as the **probability density function** (PDF) $f(\mathbf{y}, \boldsymbol{\theta})$,
where $\mathbf{y}$ is the dependent variable, $\boldsymbol{\theta}$ the set of parameters, and
$f(\cdot)$ expresses the model specification.

ML is purely **parametric** - we need to make strong
assumptions about the shape of $f(\cdot)$ before we can estimate $\boldsymbol{\theta}$.

Likelihood

Given $\boldsymbol{\theta}$, $f(\cdot, \boldsymbol{\theta})$ is the PDF of $\mathbf{y}$.

Given $\mathbf{y}$, $f(\mathbf{y}, \cdot)$ cannot be interpreted as a PDF and is instead called the **likelihood function**.

$\hat{\boldsymbol{\theta}}^{ML}$ is the $\boldsymbol{\theta}$ that maximizes this likelihood function.

(Davidson and MacKinnon, 2004, 393–396)

(Log)likelihood function

Generally, observations are assumed to be **independent**, in which case the joint density of the entire sample is the product of the densities of the individual observations.

$$f(\mathbf{y}, \boldsymbol{\theta}) = \prod_{i=1}^{n} f(y_i, \boldsymbol{\theta})$$

It is easier to work with the log of this function, because sums are easier to deal with than products and the logarithmic transformation is **monotonic**:
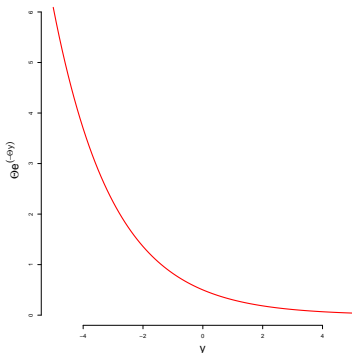
$$\ell(\mathbf{y}, \boldsymbol{\theta}) \equiv \log f(\mathbf{y}, \boldsymbol{\theta}) = \sum_{i=1}^{n} \log f_i(y_i, \boldsymbol{\theta}) = \sum_{i=1}^{n} \ell_i(y_i, \boldsymbol{\theta})$$

(Davidson and MacKinnon, 2004, 393–396)

Example: exponential distribution

For example, take the PDF of **y** to be

$$f(y_i, \theta) = \theta e^{-\theta y_i} \qquad y_i > 0, \quad \theta > 0$$

This distribution is useful
when modeling something
which is by definition positive.

(Davidson and MacKinnon, 2004, 393–396)

Example: exponential distribution

Deriving the loglikelihood function:

$$f(\mathbf{y}, \theta) = \prod_{i=1}^{n} f(y_i, \theta) = \prod_{i=1}^{n} \theta e^{-\theta y_i}$$

$$\ell(\mathbf{y}, \theta) = \sum_{i=1}^{n} \log f(y_i, \theta) = \sum_{i=1}^{n} \log(\theta e^{-\theta y_i})$$

$$= \sum_{i=1}^{n} (\log \theta - \theta y_i) = n \log \theta - \theta \sum_{i=1}^{n} y_i$$

(Davidson and MacKinnon, 2004, 393–396)

Example: exponential distribution

To find the maximum, we take the derivative and set this equal to zero:

$$\ell(\mathbf{y}, \theta) = n \log \theta - \theta \sum_{i=1}^{n} y_i$$

$$\frac{d(n \log \theta - \theta \sum_{i=1}^{n} y_i)}{d\theta} = \frac{n}{\theta} - \sum_{i=1}^{n} y_i$$

$$\frac{n}{\hat{\theta}^{ML}} - \sum_{i=1}^{n} y_i = 0$$

$$\hat{\theta}^{ML} = \frac{n}{\sum_{i=1}^{n} y_i}$$

(Davidson and MacKinnon, 2004, 393–396)

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Model:

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

We assume $\boldsymbol{\varepsilon}$ to be independently distributed and therefore, conditional on $\mathbf{X}$, $\mathbf{y}$ is assumed to be.

$$f_i(y_i, \boldsymbol{\beta}, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{x}_i\boldsymbol{\beta})^2}{2\sigma^2}}$$

(Davidson and MacKinnon, 2004, 396–398)

Linear model: loglikelihood function

$$f(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^{n} f_i(y_i, \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{x}_i\boldsymbol{\beta})^2}{2\sigma^2}}$$

$$\ell(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = \sum_{i=1}^{n} \log f_i(y_i, \boldsymbol{\beta}, \sigma^2) = \sum_{i=1}^{n} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{x}_i\boldsymbol{\beta})^2}{2\sigma^2}} \right)$$

(Davidson and MacKinnon, 2004, 396–398)

Linear model: loglikelihoodfunction

To "zoom in" on one part of this function:

$$\log \frac{1}{\sqrt{2\pi\sigma^2}} = \log \frac{1}{\sigma\sqrt{2\pi}}$$
$$= \log 1 - \log(\sigma\sqrt{2\pi})$$
$$= 0 - (\log \sigma + \log \sqrt{2\pi})$$
$$= -\frac{1}{2}\log \sigma^2 - \frac{1}{2}\log 2\pi, \text{ using}$$
$$\log \sigma = \frac{1}{2}\log \sigma^2$$

Linear model: loglikelihood function

$$f(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^{n} f_i(y_i, \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{x}_i \boldsymbol{\beta})^2}{2\sigma^2}}$$

$$\ell(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = \sum_{i=1}^{n} \log f_i(y_i, \boldsymbol{\beta}, \sigma^2) = \sum_{i=1}^{n} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{x}_i \boldsymbol{\beta})^2}{2\sigma^2}} \right)$$

(Davidson and MacKinnon, 2004, 396–398)

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Linear model: loglikelihood function

$$f(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^{n} f_i(y_i, \boldsymbol{\beta}, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{x}_i\boldsymbol{\beta})^2}{2\sigma^2}}$$

$$\ell(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = \sum_{i=1}^{n} \log f_i(y_i, \boldsymbol{\beta}, \sigma^2) = \sum_{i=1}^{n} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \mathbf{x}_i\boldsymbol{\beta})^2}{2\sigma^2}} \right)$$

$$= \sum_{i=1}^{n} (-\frac{1}{2} \log \sigma^2 - \frac{1}{2} \log 2\pi - \frac{1}{2\sigma^2}(y_i - \mathbf{X}_i\boldsymbol{\beta})^2)$$

$$= -\frac{n}{2} \log \sigma^2 - \frac{n}{2} \log 2\pi - \frac{1}{2\sigma^2} \sum_{i=1}^{n}(y_i - \mathbf{X}_i\boldsymbol{\beta})^2$$

$$= -\frac{n}{2} \log \sigma^2 - \frac{n}{2} \log 2\pi - \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

(Davidson and MacKinnon, 2004, 396–398)

Linear model: estimating σ^2

$$\frac{\partial \ell(\mathbf{y}, \boldsymbol{\beta}, \sigma^2)}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$0 = -\frac{n}{2\hat{\sigma}^2} + \frac{1}{2\hat{\sigma}^4}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$\frac{n}{2\hat{\sigma}^2} = \frac{1}{2\hat{\sigma}^4}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$n = \frac{1}{\hat{\sigma}^2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$\hat{\sigma}^2 = \frac{1}{n}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Thus $\hat{\sigma}^2$ is a function of $\boldsymbol{\beta}$.

(Davidson and MacKinnon, 2004, 396–398)

Linear model: estimating σ^2

$$\hat{\sigma}^2 = \frac{1}{n}(\mathbf{y} - \mathbf{X}\beta)'(\mathbf{y} - \mathbf{X}\beta) = \frac{\mathbf{e}'\mathbf{e}}{n}$$

Note that this is almost the equivalent of the variance estimator of OLS ($\frac{\mathbf{e}'\mathbf{e}}{n-k}$). This estimator is a **biased**, but **consistent**, estimator of $\hat{\sigma}^2$.

Linear model: estimating β

$$\ell(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = -\frac{n}{2}\log \sigma^2 - \frac{n}{2}\log 2\pi - \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$\ell(\mathbf{y}, \boldsymbol{\beta}) = -\frac{n}{2}\log(\frac{1}{n}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})) - \frac{n}{2}\log 2\pi$$

$$- \frac{1}{2(\frac{1}{n}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta}))}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

$$= -\frac{n}{2}\log(\frac{1}{n}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})) - \frac{n}{2}\log 2\pi - \frac{n}{2}$$

Because the middle term is equivalent to minus $n/2$ times the log of SSR, maximizing $\ell(\mathbf{y}, \boldsymbol{\beta})$ with respect to $\boldsymbol{\beta}$ is the equivalent to minimizing SSR: $\hat{\boldsymbol{\beta}}^{ML} = \hat{\boldsymbol{\beta}}^{OLS}$.

(Davidson and MacKinnon, 2004, 396–398)

Maximum Likelihood Estimates

The maximum likelihood estimate of $\boldsymbol{\theta}$ is the value of $\boldsymbol{\theta}$ which maximizes the (log)likelihood function $\ell(\mathbf{y}, \boldsymbol{\theta})$.

In some cases, such as the above exponential distribution or the linear model, we can find this value analytically, but taking the derivative, and setting equal to zero.

In many other cases, there is no such analytical solution, and we use numerical search algorithms to find the value.

Linear model

$$\ell(\mathbf{y}, \boldsymbol{\beta}, \sigma^2) = -\frac{n}{2} \log \sigma^2 - \frac{n}{2} \log 2\pi - \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

```
ll <- function(par, X, y) {
  s2 <- exp(par[1])
  beta <- par[-1]
  n <- length(y)
  r <- y - X %*% beta
  - n/2 * log(s2) - n/2 * log(2*pi) -
          1/(2*s2) * sum(r^2)
}

mlest <- optim(c(1,0,0,0), ll, NULL, X, y,
  control = list(fnscale = -1), hessian = TRUE)
```

Linear model

Some practical tricks:

- By default, optim() minimizes rather than maximizes, hence the need for fnscale = -1.
- To get $\hat{\sigma}^2$, we need to take the exponent of the first parameter—this is done to make sure σ^2 is always assumed positive.

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Gradient vector

The **gradient vector** or **score vector** is a vector with typical element:

$$g_j(\mathbf{y}, \boldsymbol{\theta}) \equiv \frac{\partial \ell(\mathbf{y}, \boldsymbol{\theta})}{\partial \theta_j},$$

i.e. the vector of partial derivatives of the loglikelihood function towards each parameter in $\boldsymbol{\theta}$.

(Davidson and MacKinnon, 2004, 400)

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Hessian matrix

$H(\boldsymbol{\theta})$ is a $k \times k$ matrix with typical element

$$\boldsymbol{h}_{ij} = \frac{\partial^2 \ell(\boldsymbol{\theta})}{\partial \theta_i \theta_j},$$

i.e. the matrix of second derivatives of the loglikelihood function.

Asymptotic equivalent: $\mathcal{H}(\boldsymbol{\theta}) \equiv \text{plim}_{n \to \infty} \frac{1}{n} \mathbf{H}(\mathbf{y}, \boldsymbol{\theta})$.

(Davidson and MacKinnon, 2004, 401, 407)

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Information matrix

$$\mathbf{I}(\boldsymbol{\theta}) = \sum_{i=1}^{n} E_{\boldsymbol{\theta}}((\mathbf{G}_i(\mathbf{y}, \boldsymbol{\theta}))' \mathbf{G}_i(\mathbf{y}, \boldsymbol{\theta}))$$

$\mathbf{I}(\boldsymbol{\theta})$ is the **information matrix**, or the covariance matrix of the score vector.

There is also an asymptotic equivalent, $\mathcal{I}(\boldsymbol{\theta}) \equiv \text{plim}_{n \to \infty} \frac{1}{n} \mathbf{I}(\boldsymbol{\theta})$.

$\mathcal{I}(\boldsymbol{\theta}) = -\mathcal{H}(\boldsymbol{\theta})$ - they both measure the **amount of curvature** in the loglikelihood function.

(Davidson and MacKinnon, 2004, 406–407)

Newton's Method

One numerical optimization algorithm is Newton's Method, which updates each iteration the estimate for the parameters based on the Hessian matrix and the gradient, i.e. based on the amount of curvature of the log-likelihood function at a particular point.

$$\boldsymbol{\theta}_{(m+1)} = \boldsymbol{\theta}_{(m)} - \boldsymbol{H}_{(m)}^{-1}\boldsymbol{g}_{(m)}$$

(Davidson and MacKinnon, 2004, 401)

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Asymptotics

Under some weak conditions, ML estimators are **consistent**, **asymptotically efficient** and **asymptotically normally distributed**.

New ML estimators thus do not require extensive proof of this - once it is shown it is an ML estimator, it "inherits" those properties.

(Davidson and MacKinnon, 2004, 402–403)

Variance-covariance matrix of $\hat{\beta}^{ML}$

$$V\left(plim_{n\to\infty}\sqrt{n}(\hat{\beta}^{ML} - \boldsymbol{\theta})\right) = H^{-1}(\boldsymbol{\theta})I(\boldsymbol{\theta})H^{-1}(\boldsymbol{\theta}) = I^{-1}(\boldsymbol{\theta}),$$

the latter being true iff $\mathcal{I}(\boldsymbol{\theta}) = -\mathcal{H}(\boldsymbol{\theta})$ is true.

One estimator for the variance is: $V(\hat{\beta}^{ML}) = -\mathbf{H}^{-1}(\hat{\beta}^{ML})$. For alternative estimators see reference below.

(Davidson and MacKinnon, 2004, 409–411)

```
mlest <- optim(..., hessian = TRUE)
V <- solve(-mlest$hessian)
sqrt(diag(V))
```

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Example

Imagine, we take a random sample of N colored balls from a vase, with replacement. In the vase, a fraction p of the balls are yellow and the other ones blue. In our sample, there are q yellow balls. Assuming that $y_i = 1$ if the ball is yellow and $y_i = 0$ for blue, the probability of obtaining our sample is:

$$P(q) = p^q (1 - p)^{N-q},$$

which is the likelihood function with unknown parameter p. Write down the loglikelihood function.

$$\ell(p) = \log(p^q (1 - p)^{N-q}) = q \log p + (N - q) \log(1 - p)$$

(Verbeek, 2008, 172–173)

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Example

$$\ell(p) = q \log p + (N - q) \log(1 - p)$$

Take derivative towards p.

$$\frac{d\ell(p)}{dp} = \frac{q}{p} + \frac{N - q}{1 - p}$$

Set equal to zero and find $\hat{p}^{ML}$.

$$\frac{q}{\hat{p}} + \frac{N - q}{1 - \hat{p}} = 0 \qquad \implies \qquad \hat{p} = \frac{q}{N}$$

(Verbeek, 2008, 172–173)

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Example

$$\ell(p) = q \log p + (N - q) \log(1 - p)$$

Using the loglikelihood function and optim(), find p for $N = 100$ and $q = 30$. ML estimates are "invariant under reparametrization", so we will use the logit transform of p instead of p, to avoid probabilities outside $[0, 1]$:
$p^* = (1 + e^{-p})^{-1}$.

```
ll <- function(p, N, q) {
 pstar <- 1 / (1 + exp(-p))
 q * log(pstar) + (N - q) * log(1 - pstar)
}
mlest <- optim(0, ll, NULL, N=100, q=30,
  hessian = TRUE, control = list(fnscale = -1))
phat <- 1 / (1 + exp(-mlest$par))
```

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Example

Using the previous estimate, including the Hessian, calculate a
95% confidence interval around this $\hat{p}$.

```
se <- sqrt(-1/mlest$hessian)
ci <- c(mlest$par - 1.96 * se, mlest$par + 1.96 * se)
ci <- 1 / (1 + exp(-ci))
```

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Standard tests

Within the ML framework, there are three common tests:

- Likelihood ratio test (LR)
- Wald test (W)
- Lagrange multiplier test (LM)

These are asymptotically equivalent. Given r restrictions, all have asymptotically a $\chi^2(r)$ distribution.

In the following, $\tilde{\boldsymbol{\theta}}^{ML}$ will denote the restricted estimate and $\hat{\boldsymbol{\theta}}^{ML}$ the unrestricted one.

(Davidson and MacKinnon, 2004, 414)

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Likelihood ratio test

$$LR = 2(\ell(\hat{\boldsymbol{\theta}}^{ML}) - \ell(\tilde{\boldsymbol{\theta}}^{ML})) = 2\log\frac{L(\hat{\boldsymbol{\theta}}^{ML})}{L(\tilde{\boldsymbol{\theta}}^{ML})},$$

thus twice the log of the ratio of likelihood functions.

If we have two separate estimates, this is thus very easy to compute or even "eye-ball".

(Davidson and MacKinnon, 2004, 414–416)

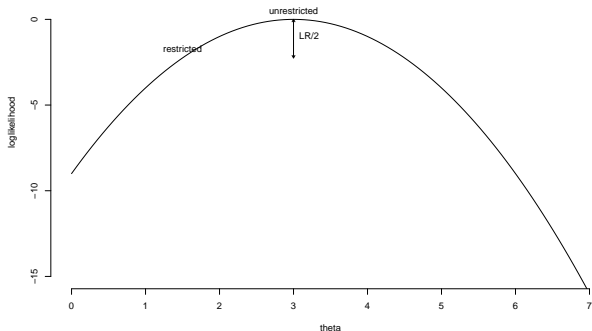# Likelihood ratio test

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Wald test

The basic intuition is that the Wald test is quite comparable to an F-test on a set of restrictions. For a single regression parameter the formule would be:

$$W = -\frac{d^2L(\beta)}{d\beta^2}(\hat{\beta} - \beta_0)^2$$

This test does not require an estimate of $\tilde{\theta}^{ML}$. The test is somewhat sensitive to the formulation of **r**, so that as long as estimating $\tilde{\theta}^{ML}$ is not too costly, it is better to use an LR or LM test.

Intuition: If the second derivative is higher, the slope of $\ell(\cdot)$ changes faster, thus the difference between the likelihoods at the restricted and unrestricted positions will be larger.

(Davidson and MacKinnon, 2004, 416–418)

Wald test
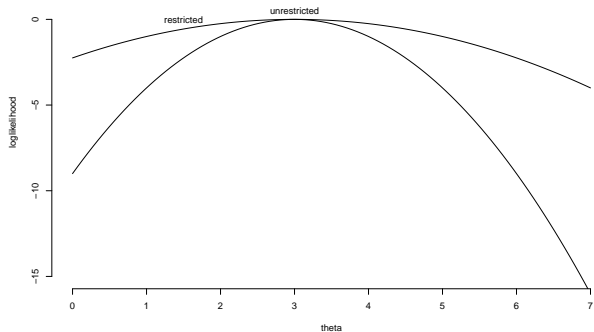
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Lagrange multiplier test

For a single parameter:

$$LM = \frac{\left(\frac{dL(\tilde{\beta})}{d\tilde{\beta}}\right)^2}{\frac{d^2L(\tilde{\beta})}{d\tilde{\beta}^2}}$$

Thus the steeper the slope of the loglikelihood function at the point of the restricted estimate, the more likely it is significantly different from the unrestricted estimate, unless this slope changes very quickly (the second derivative is high).

Lagrange multiplier test
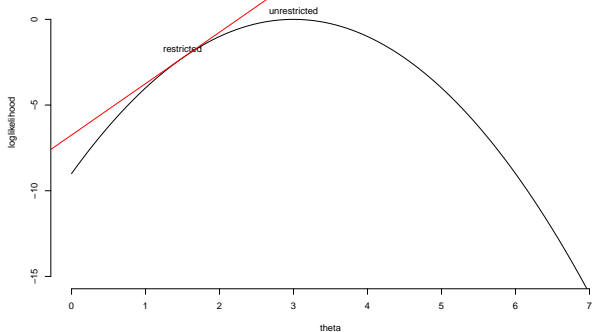
Davidson, Russell and James G. MacKinnon. 2004. *Econometric theory and methods*. Oxford: Oxford University Press.

Verbeek, Marno. 2008. *A guide to modern econometrics*. Chichester: John Wiley & Sons.