Gov 2001 Section 5: Theory of Maximum Likelihood Estimation

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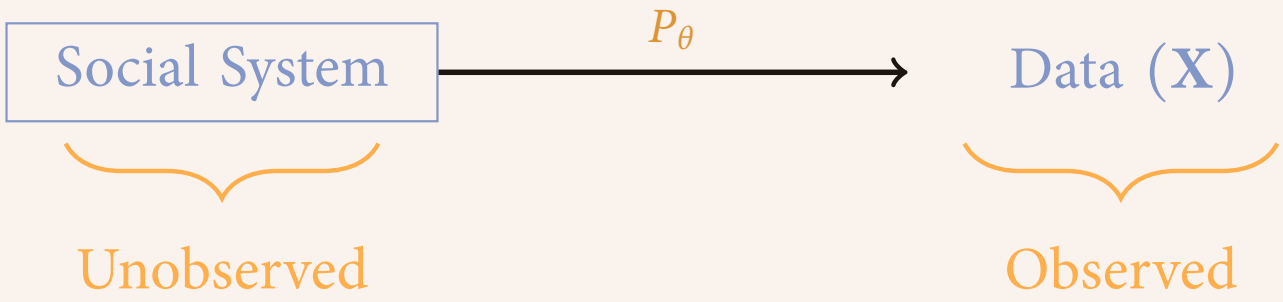
February 28, 2013

Outline

What is Statistical Inference?



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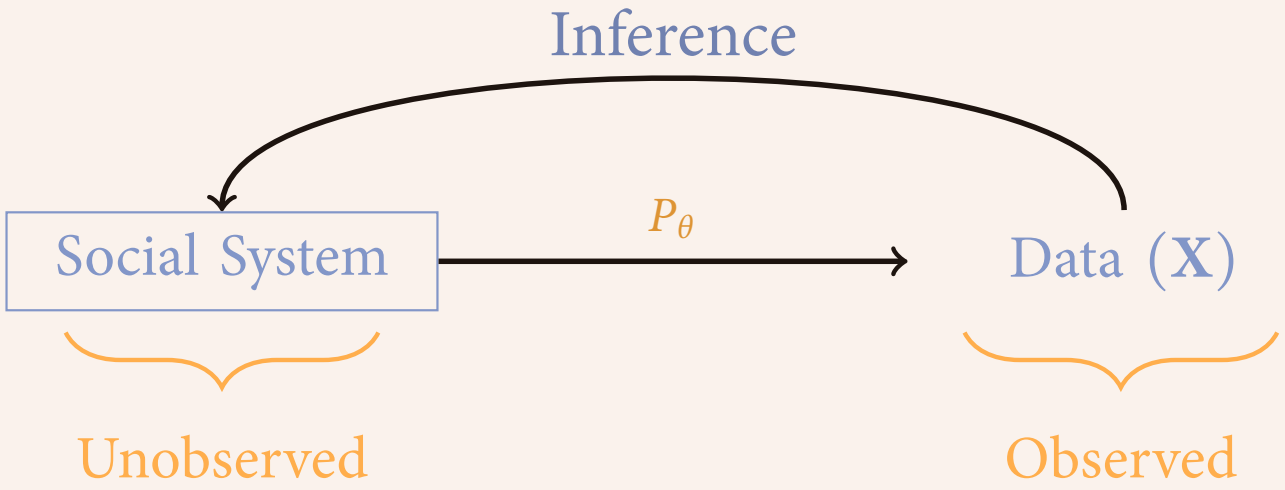

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There are two main theories of doing this:
Frequentist (likelihood) and Bayesian

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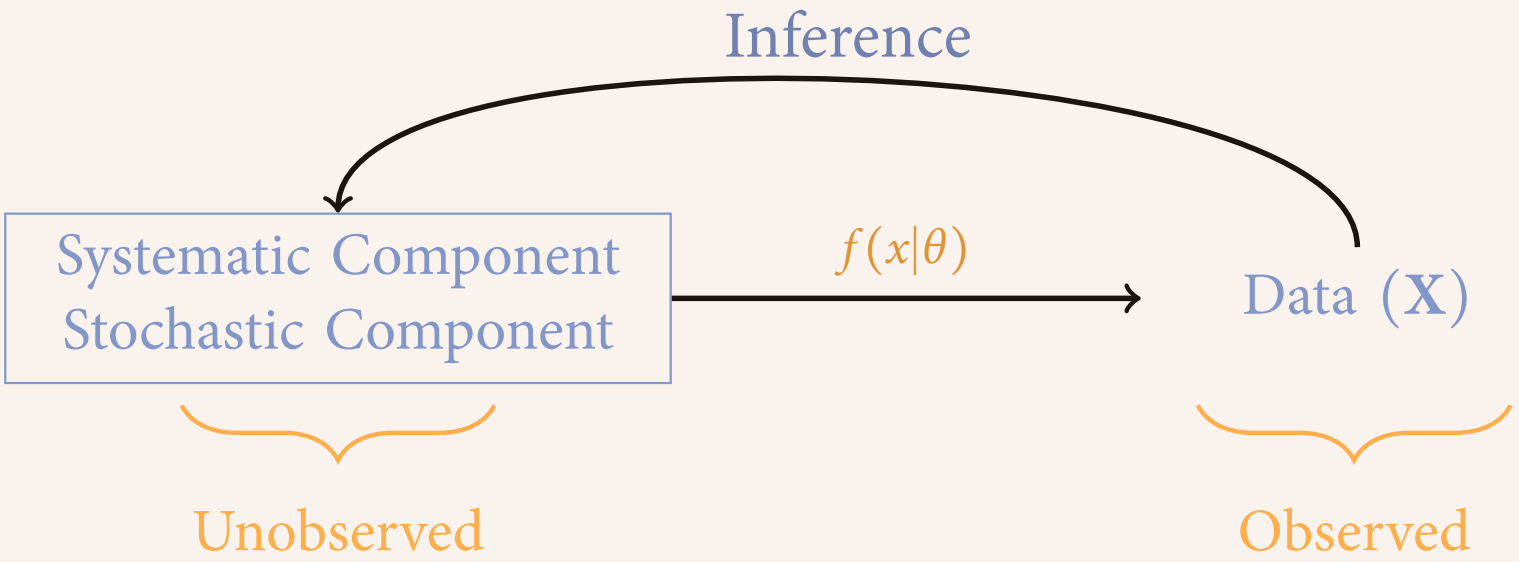

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By Bayes' Rule, we can write this probability as:

$$\xi(\theta|\mathbf{x}) = \frac{f(\mathbf{x}|\theta)\xi(\theta)}{g_n(\mathbf{x})} = \frac{f_n(\mathbf{x}|\theta)\xi(\theta)}{\int_\Omega f_n(\mathbf{x}|\theta)\xi(\theta)}, \text{ for } \theta \in \Omega$$

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- Point summary: maximum a posteriori (MAP) or posterior mean (PM)

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Likelihood

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For a variety of reasons, we work with the log-likelihood:

$$\ell(\theta|\mathbf{x}) = \log L(\theta|\mathbf{x}) = \sum_{i=1}^{n} \log f(x_i|\theta)$$

MLE

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Alternatively, we define the MLE in terms of maximizing the log-likelihood:

$$\hat{\theta}_{MLE} = \max_{\theta \in \Omega} \log L(\theta|\mathbf{x}) = \max_{\theta \in \Omega} \ell(\theta|\mathbf{x}) = \max_{\theta \in \Omega} \sum_{i=1}^{n} \log(f(x_i|\theta))$$

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- **Numeric**: `optim()` in R

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$$J(\boldsymbol{\theta}) = -\nabla \nabla^T \ell(\boldsymbol{\theta}|\boldsymbol{x}) = -\begin{pmatrix} \frac{\partial^2}{\partial \theta_1^2} & \frac{\partial^2}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2}{\partial \theta_1 \partial \theta_k} \\ \frac{\partial^2}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2}{\partial \theta_2^2} & \cdots & \frac{\partial^2}{\partial \theta_2 \partial \theta_k} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial \theta_k \partial \theta_1} & \frac{\partial^2}{\partial \theta_k \partial \theta_2} & \cdots & \frac{\partial^2}{\partial \theta_k^2} \end{pmatrix} \ell(\boldsymbol{\theta}|\boldsymbol{x})$$

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A Geometric MLE

$X_1 \ldots X_n$ form a random sample from a geometric distribution with unknown parameter $0 \leq p \leq 1$. A geometric distribution describes the number of failures before we observe a success in a series of independent Bernoulli trials, each with probability p of a success. We need to find the MLE estimator for p.

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Thus, the likelihood for n i.i.d. draws is:

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Taking the log:

$$\ell(p|\mathbf{x}) = n \log(p) + \sum_{i=1}^{n} x_i \log(1-p) = n \log(p) + (1-p) \sum_{i=1}^{n} x_i$$

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The score, which is the first derivative of the log-likelihood, is:

$$S(p) = \ell'(p|\mathbf{x}) = \frac{n}{p} - \frac{1}{1-p}\sum_{i=1}^{n} x_i$$

A Geometric MLE

To find the MLE, we set the score equal to 0 and solve for p:

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$$\hat{p}_{MLE} = \frac{1}{1+\bar{x}}$$

Observed Fisher Information

First, let's find the second derivative of the log-likelihood function:

$$\ell''(p|\mathbf{x}) = -\frac{n}{p^2} - \frac{1}{(1-p)^2}\sum_{i=1}^{n} x_i$$

Note that the second derivative captures the steepness of the curvature around the point p. A more negative second derivative implies that the function is more steeply concave down around the point p.
The observed Fisher information is just the negation of the second derivative:

$$J_n(p) = -\ell''(p|\mathbf{x}) = \frac{n}{p^2} + \frac{1}{(1-p)^2}\sum_{i=1}^{n} x_i$$

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Conceptually, what is this quantity? We want to understand it conceptually before we can talk about calculating it!

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	Samples from Pop.				
	1	**2**	**3**	$\cdots$	∞
X_1	$x_{1,1}$	$x_{1,2}$	$x_{1,3}$	$\cdots$	$x_{1,\infty}$
X_2	$x_{2,1}$	$x_{2,2}$	$x_{2,3}$	$\cdots$	$x_{2,\infty}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
X_n	$x_{n,1}$	$x_{n,2}$	$x_{n,3}$	$\cdots$	$x_{n,\infty}$
$\hat{\theta}_{MLE}$	$\hat{\theta}_{MLE,1}$	$\hat{\theta}_{MLE,2}$	$\hat{\theta}_{MLE,3}$	$\cdots$	$\hat{\theta}_{MLE,\infty}$
$J_n(\hat{\theta}_{MLE})$	$J_{n,1}(\hat{\theta}_{MLE})$	$J_{n,2}(\hat{\theta}_{MLE})$	$J_{n,3}(\hat{\theta}_{MLE})$	$\cdots$	$J_{n,\infty}(\hat{\theta}_{MLE})$

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We see that $\hat{\theta}_{MLE}$ and $J_n(\hat{\theta}_{MLE})$ are random variables! Thus, they have some theoretical distributions.

$Var(\hat{\theta}_{MLE})$ is just the variance of this theoretical distribution!

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- Score evaluated at the MLE (or any θ): $S(\hat{\theta}_{MLE}) = \ell'(\hat{\theta}_{MLE}|\mathbf{x})$
- Observed Fisher information evaluated at MLE (or any θ): $J_n(\hat{\theta}_{MLE}) = -\ell''(\hat{\theta}_{MLE}|\mathbf{x})$

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- Log-likelihood evaluated at MLE (or any θ): $\ell(\hat{\theta}_{MLE}|\mathbf{x})$
- Score evaluated at the MLE (or any θ): $S(\hat{\theta}_{MLE}) = \ell'(\hat{\theta}_{MLE}|\mathbf{x})$
- Observed Fisher information evaluated at MLE (or any θ): $J_n(\hat{\theta}_{MLE}) = -\ell''(\hat{\theta}_{MLE}|\mathbf{x})$
- Inverse observed Fisher information: $J_n(\hat{\theta}_{MLE})^{-1}$

Expectations of Random Variables

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We thus often talk about the expectation of these random quantities across infinite samples. We can denote this, for the example of the MLE, as:

$$E[\hat{\theta}_{MLE}]$$

or

$$E_{\theta_0}[\hat{\theta}_{MLE}]$$

Variance of the MLE

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Now that we understand it conceptually, how do we estimate it?

Asymptotic Distribution of the MLEs

It can be shown that under certain regularity conditions, the MLE is distributed normally with a mean equal to the true parameter (θ_o) and the variance equal to the inverse of the expected sample Fisher information at the true parameter (denoted as $I_n(\theta_o)$):

$$\hat{\theta}_{MLE} \sim N\left(\theta_o, \left(\underbrace{-E\left[\frac{\partial^2 \ell(\theta|\mathbf{x})}{\partial \theta^2}\Big|_{\theta=\theta_o}\right]}_{I_n(\theta_o)}\right)^{-1}\right)$$

Let's focus on understanding the variance for now...

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In practice, we use the inverse of the observed Fisher information evaluated at the MLE to approximate the true variance of the MLE!

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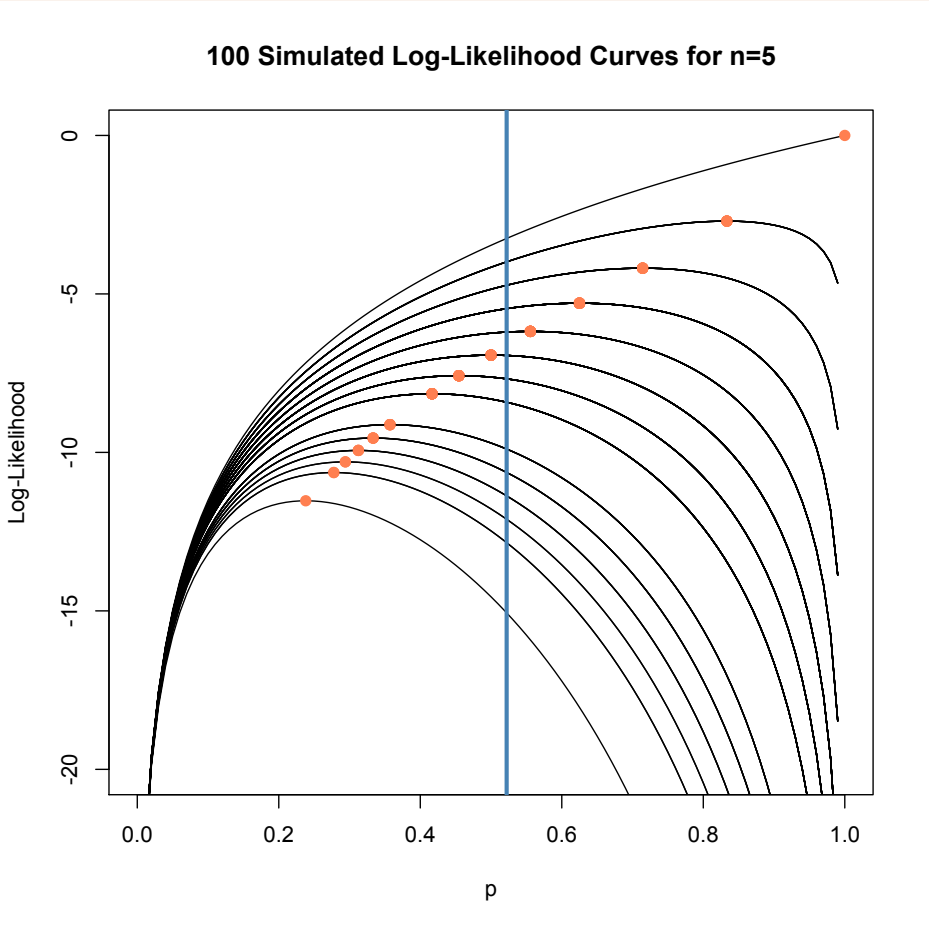
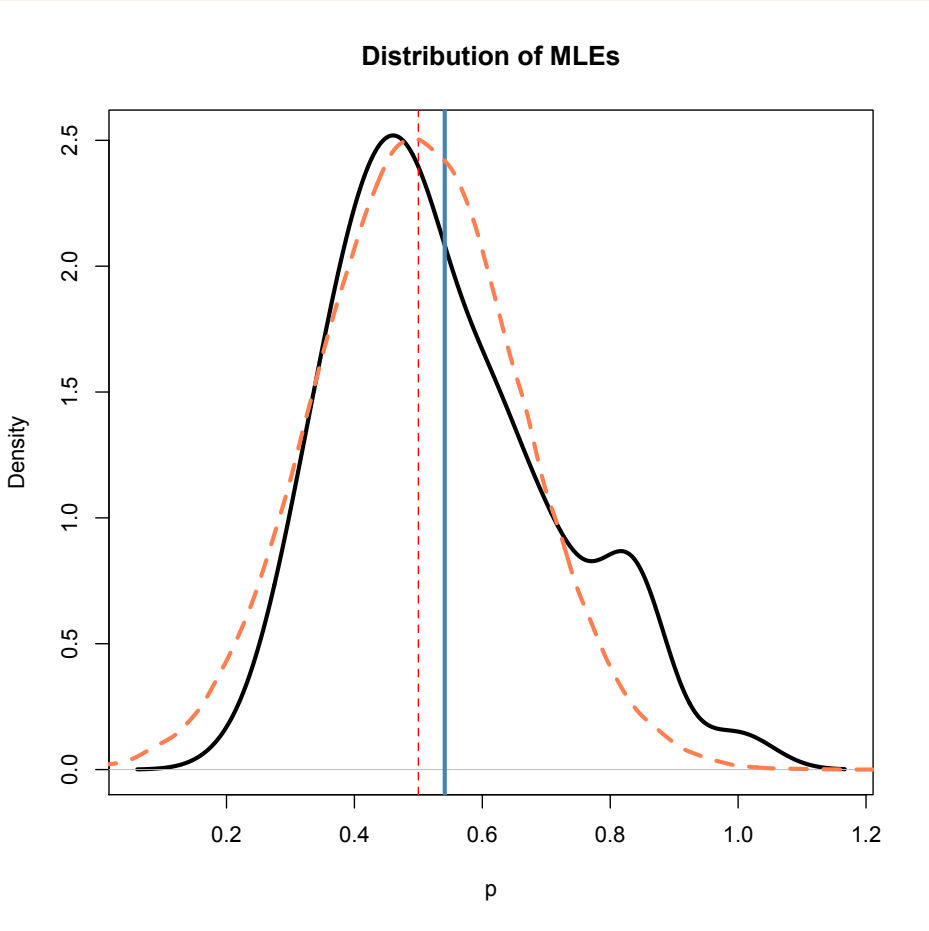
We shall see how as sample size (n) gets larger, $\hat{p}_{MLE} \approx p_0$ and $\left[-\ell''(\hat{p}_{MLE}|\mathbf{x})\right]^{-1} \approx Var(\hat{p}_{MLE})$

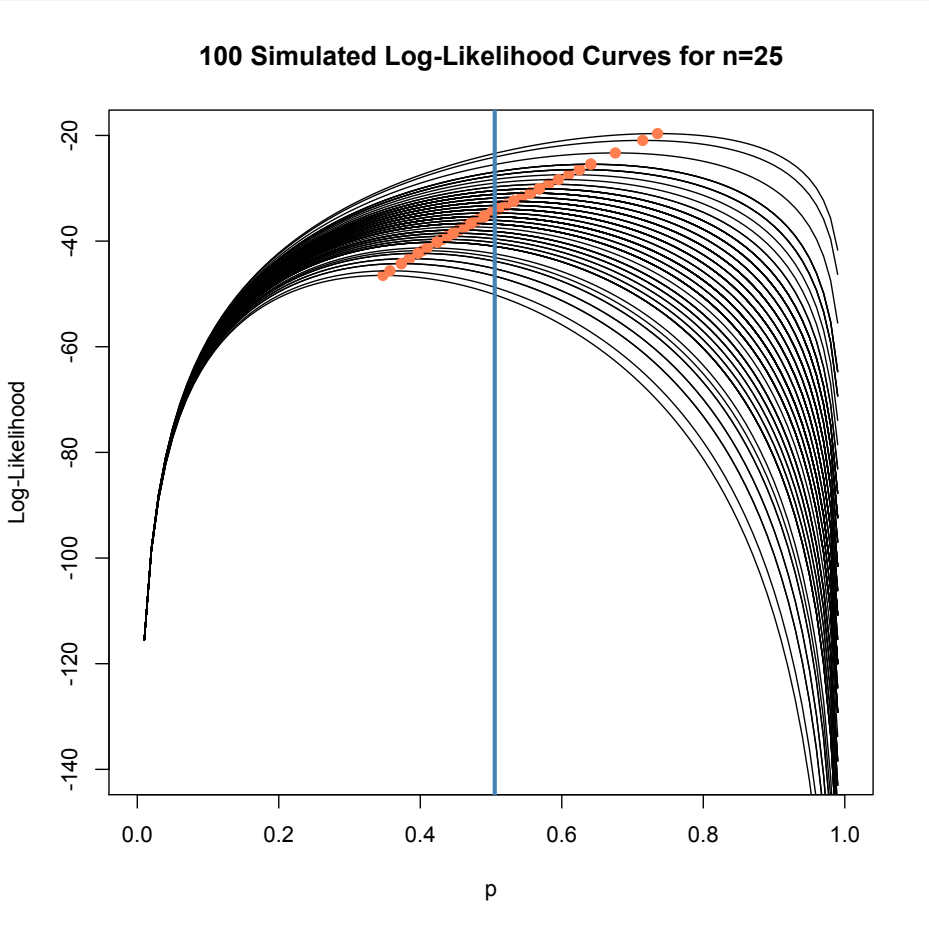
Log-Likelihoods for $n = 5$



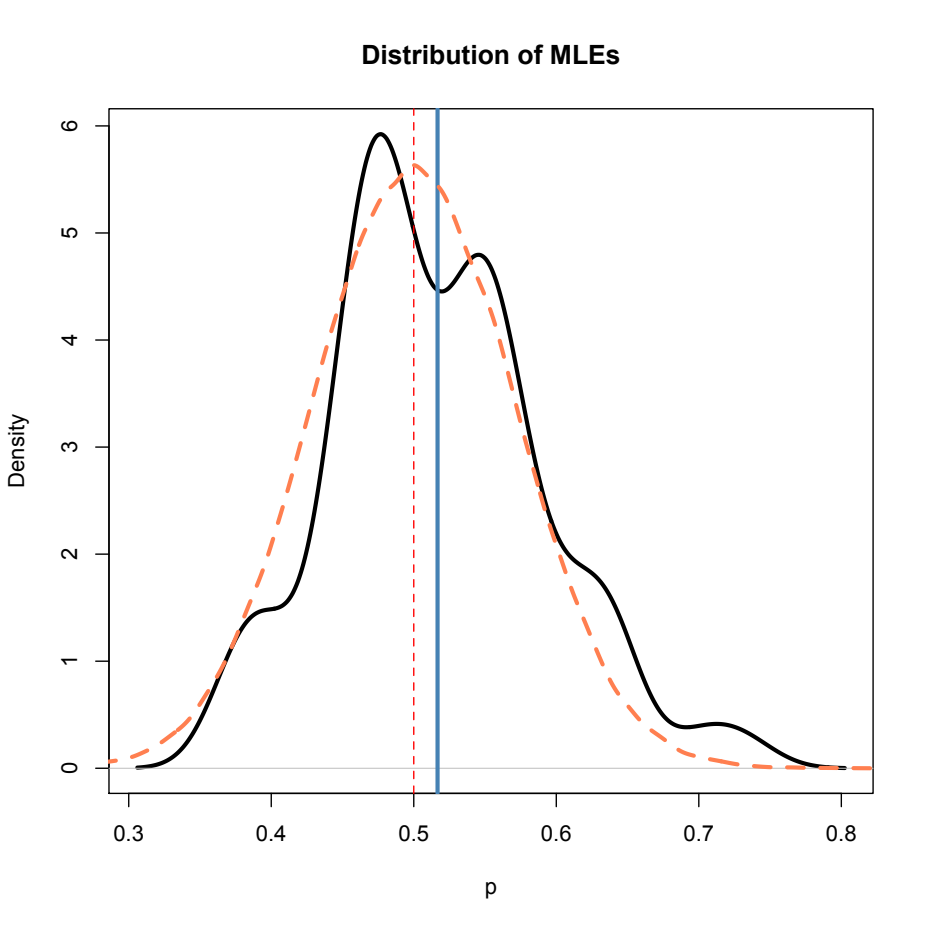
Distribution of MLEs for $n = 5$



Log-Likelihoods for $n = 25$



Distribution of MLEs for $n = 25$

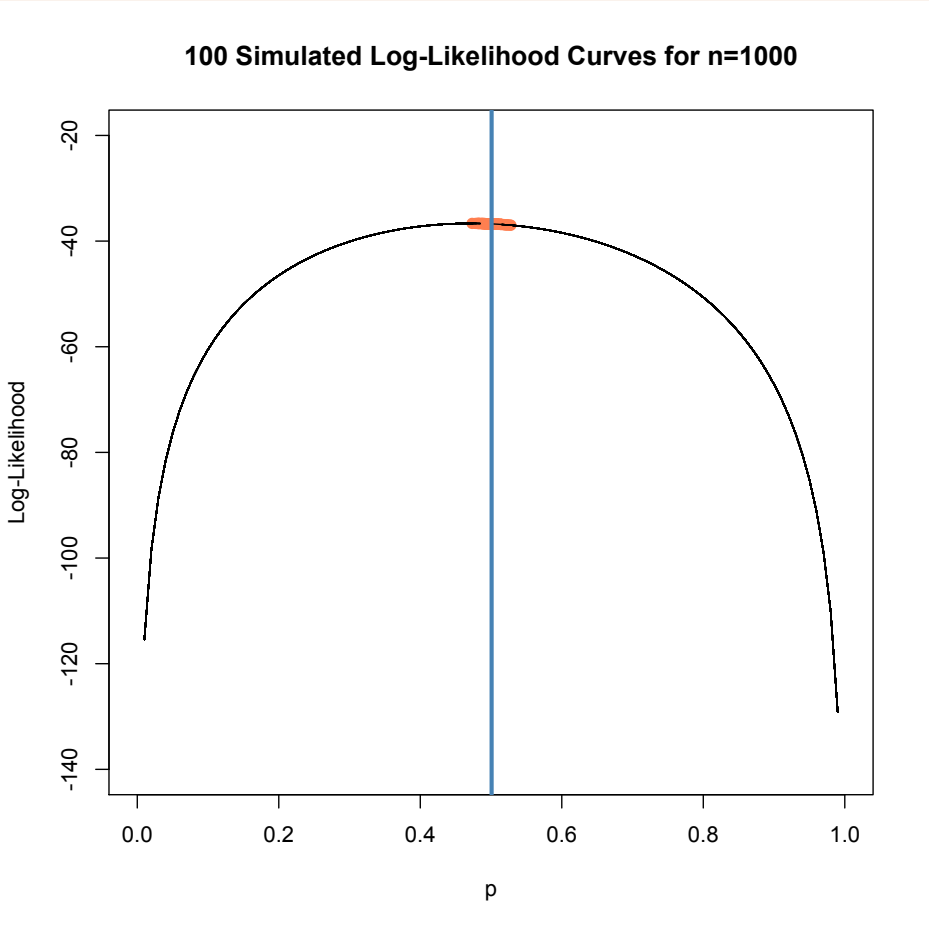


$$Var_{1000}(\hat{\theta}_{MLE}) = 0.005532$$

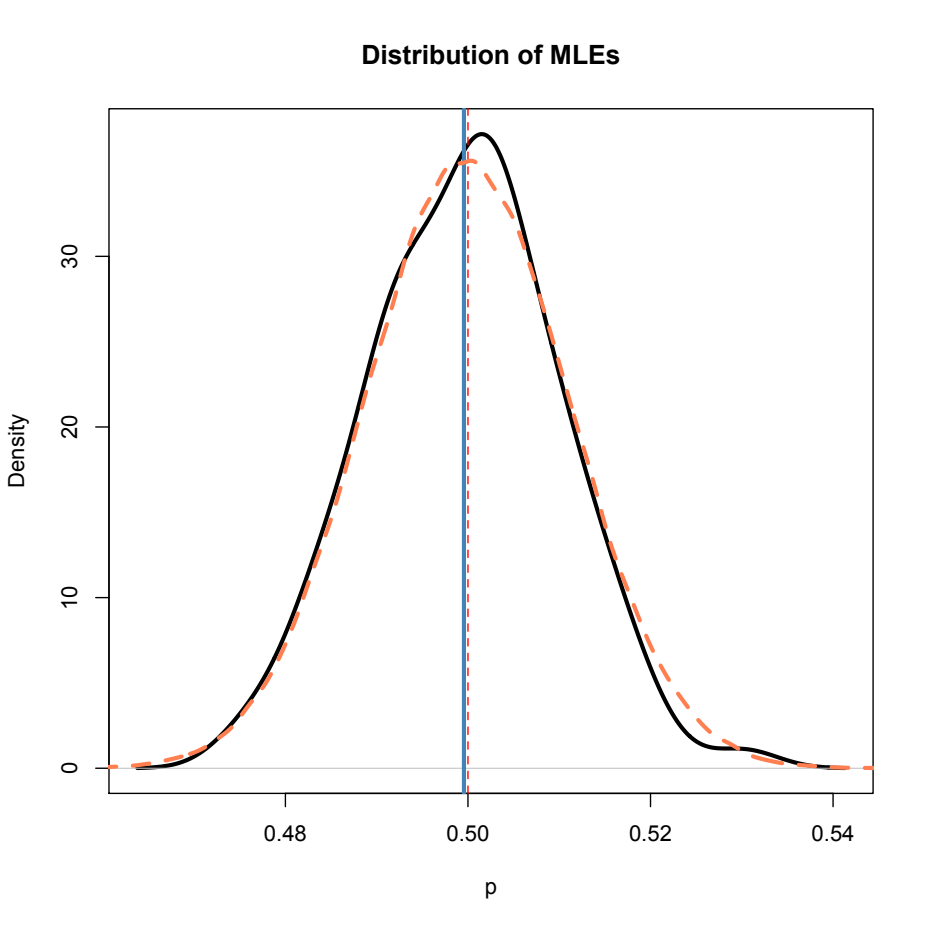
$$J(\hat{\theta}_{MLE})^{-1} = 0.00503$$

$$I(\theta_0)^{-1} = 0.005$$

Log-Likelihoods for $n = 1000$



Distribution of MLEs for $n = 1000$



$$Var_{1000}(\hat{\theta}_{MLE}) = 0.000106$$

$$\overline{J(\hat{\theta}_{MLE})^{-1}} = 0.000124$$

$$I(\theta_0)^{-1} = 0.000125$$

Outline

Summary of Asymptotic Properties

- **Consistency:**

$$\hat{\theta}_{MLE} \xrightarrow{p} \theta_0$$

- **Normality:**

$$\hat{\theta}_{MLE} \sim N\left(\theta_0, \left(\underbrace{-E\left[\frac{\partial^2 \ell(\theta|\mathbf{x})}{\partial \theta^2}\Big|_{\theta=\theta_0}\right]}_{I_n(\theta_0)}\right)^{-1}\right)$$

- **Efficiency:** lowest mean square error amongst asymptotically unbiased estimators

Consistency

As sample size (n) increases, the MLE ($\hat{\theta}_{MLE}$) converges to the true parameter, θ_0:

$$\hat{\theta}_{MLE} \xrightarrow{p} \theta_0$$

Proof relies upon the uniform law of large numbers.

Regularity Conditions for Consistency

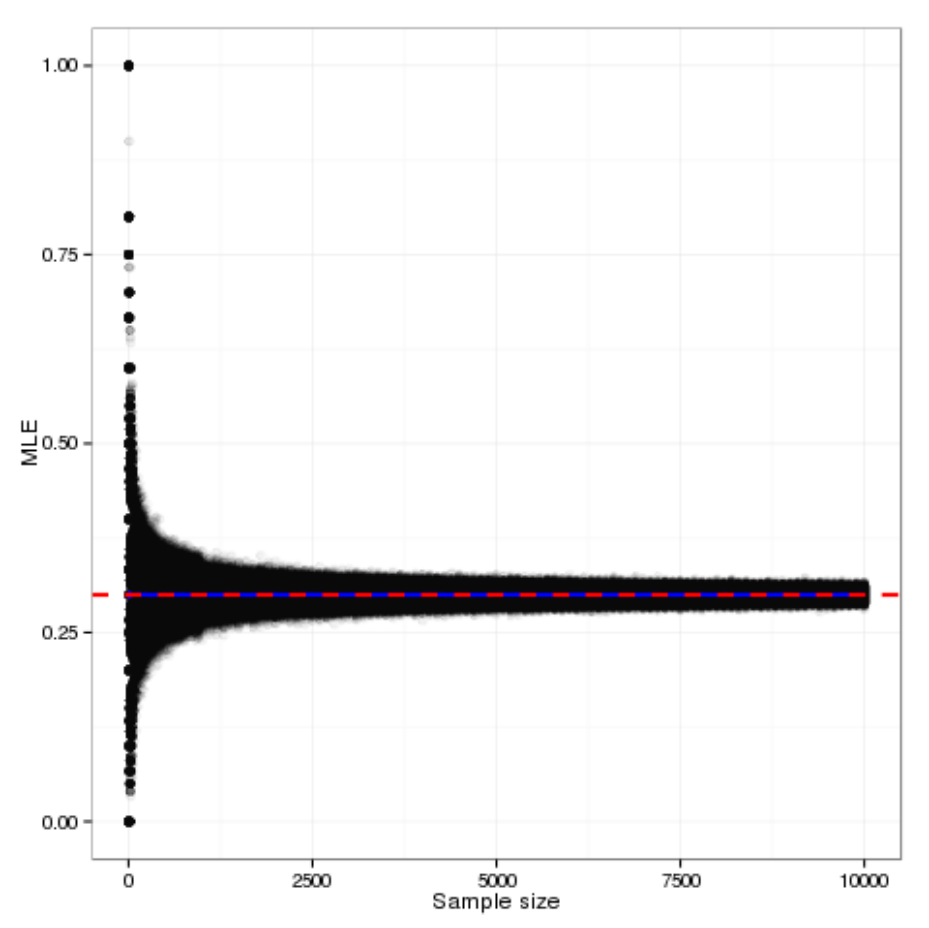
- Model identification: the true parameter θ_o is the unique global maximizer of $E_{\theta_o}[\ell(\theta|\mathbf{x})]$
- Compactness: the parameter space Ω must be a bounded and closed set. That is, Ω must be a *compact subset*.
- The log-likelihood function $\ell(\theta|\mathbf{x})$ is continuous in θ
- Note that compactness condition is sufficient but not necessary: it can be replaced with other conditions for non-compact and infinite parameter spaces

Visualizing Consistency of the MLE

Simple simulation study to look at properties of MLE:

- $X \sim Bern(0.3)$
- Vary sample size n
- For each n, simulate 10,000 datasets of size n and calculate MLE and observed Fisher information
- Take mean across MLEs for each n and compare to true value of the parameter

Visualizing Consistency of the MLE



For each n, 10,000 MLEs are plotted with black dots. The dotted red line denotes the true parameter ($p = 0.3$), while the dotted blue line represents the mean MLE across the 10,000 samples at each value of n.

Normality

The standardized MLE is distributed normally with a mean of 0 and a variance equal to the expected unit Fisher information:

$$\sqrt{n}(\hat{\theta}_{MLE} - \theta_0) \sim N\left(0, \left(\underbrace{-E\left[\frac{\partial^2 \ell(\theta|x)}{\partial \theta^2}\Big|_{\theta=\theta_0}\right]}_{I_1(\theta_0)} \right)^{-1}\right)$$

Proof relies upon the Central Limit Theorem.

Regularity Conditions for Normality

We need all conditions needed for consistency as well as:

- The true value of the parameter, θ_0, must be an interior point of the parameter set: $\theta_0 \in int(\Omega)$. Phrased differently, θ_0 cannot be on the boundary of the set.
  - This is equivalent to saying that Ω doesn't depend on θ
  - A violation of this is the uniform distribution $Unif[0, \theta]$ which has a biased MLE that is not asymptotically normally distributed (see Lehamnn and Casella 1998)
- The likelihood function (or probability distribution $f(x|\theta)$) is continuously twice-differentiable in the neighborhood of θ_0
- Fisher information matrix exists, is non-singular, and finitely bounded
-

$$\left| \frac{d^j \ln f(x|\theta)}{d\theta^j} \leq h_j(x) \right|, \text{ for } j = 1, 2, 3$$

$$E[h_j(y)] < \infty, \; j = 1, 2$$

$$E[h_3(x)] \text{ does not depend on } \theta$$

Normality

Another way to phrase asymptotic normality is:
As sample size (n) increases, the MLE is normally distributed with a mean equal to the true parameter (θ_0) and the variance equal to the inverse of the expected sample Fisher information at the true parameter (denoted as $I_n(\theta_0)$):

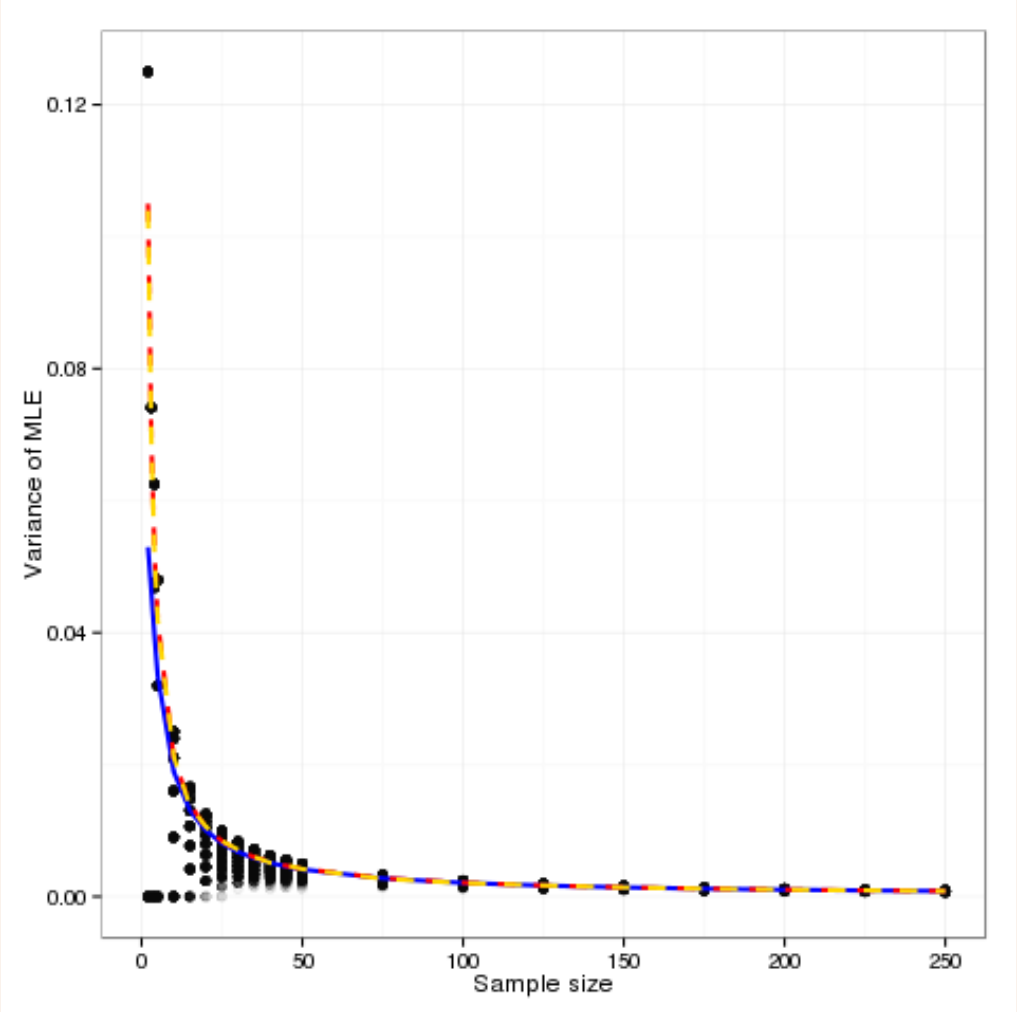
$$\hat{\theta}_{MLE} \sim N\left(\theta_0, \left(\underbrace{-E\left[\frac{\partial^2 \ell(\theta|\mathbf{x})}{\partial \theta^2}\Big|_{\theta=\theta_0}\right]}_{I_n(\theta_0)}\right)^{-1}\right)$$

Normality

However, using the consistency property of the MLE and observed sample Fisher information, we can use the inverse of the observed sample Fisher information evaluated at the MLE, denoted as $J_n(\hat{\theta}_{MLE})$ to approximate the variance:

$$\hat{\theta}_{MLE} \sim N\left(\theta_0, \left(\underbrace{-\left[\frac{\partial^2 \ell(\theta|\mathbf{x})}{\partial \theta^2}\Big|_{\theta=\hat{\theta}_{MLE}}\right]}_{J_n(\hat{\theta}_{MLE})}\right)^{-1}\right)$$

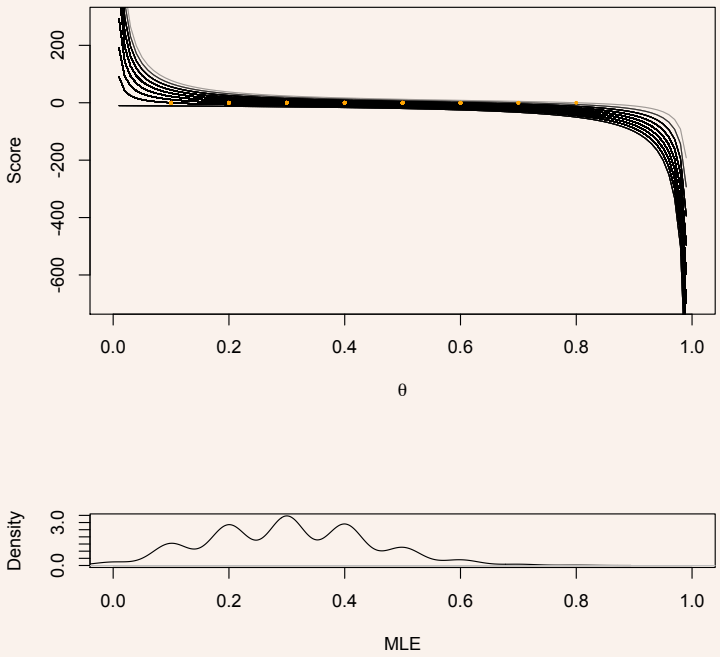
Consistency of the Observed Fisher Information

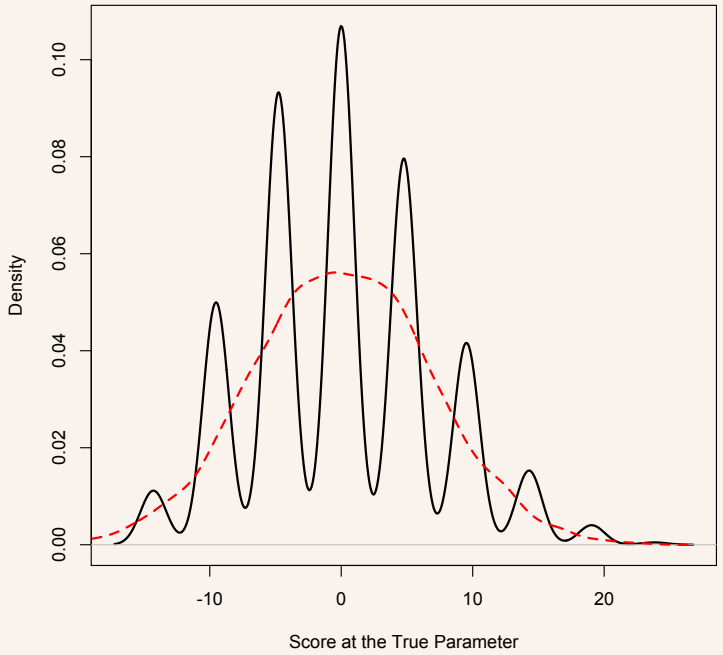


Average observed Fisher information in blue, expected Fisher information in red, and simulated variance across the 10,000 MLEs at each n in gold.

Visualizing Score Functions and Normality of MLE

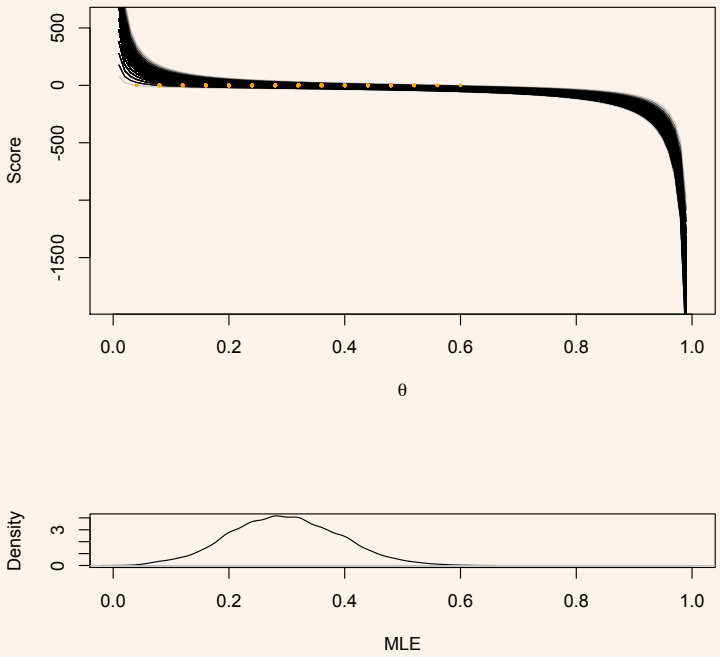
For a sample size of $n = 10$:

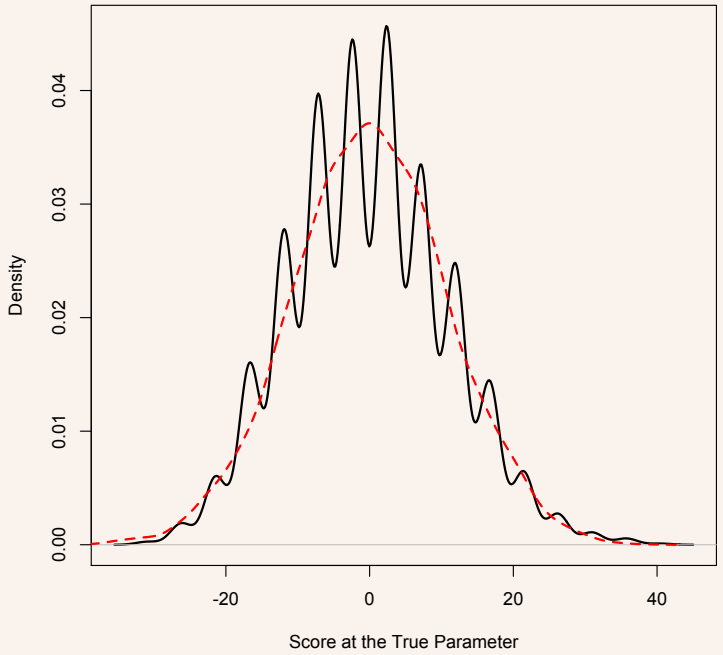




Visualizing Score Functions and Normality of MLE

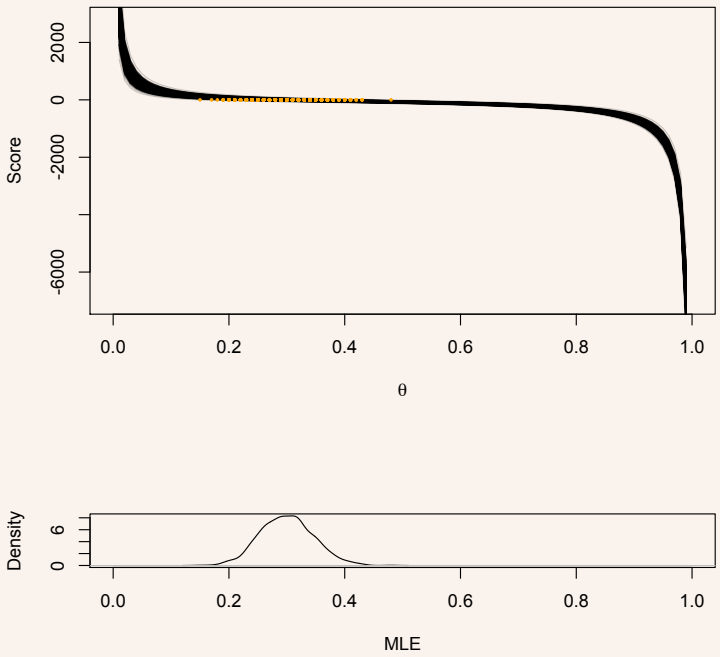
For a sample size of $n = 25$:

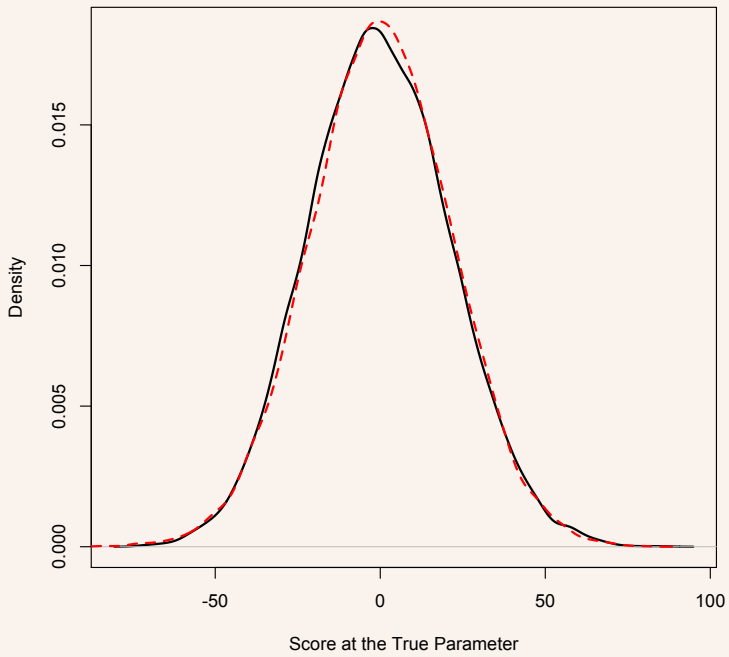




Visualizing Score Functions and Normality of MLE

For a sample size of $n = 100$:





Efficiency

- As sample size (n) increases, MLE is the estimation procedure that generally provides the lowest variance (in the class of other consistent and asymptotically normal estimators)
- ML estimator has a variance equal to Cramer-Rao lower bound