Lecture 6a: Maximum Likelihood

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Consider a linear regression with $\varepsilon_i \mid X_i \sim \mathcal{N}(0, \sigma^2)$

$$Y_{it} = X_i \beta + \varepsilon_i$$

We've discussed the least squares estimator:

$$\hat{\beta}_{ols} = \arg\min_{\beta} \sum_{i=1}^{N} (Y_i - X_i \beta)^2$$

$$\hat{\beta}_{ols} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

Review: What is a Likelihood?

Suppose we write down the joint distribution of our data (y_i, x_i) for $i = 1, \ldots, n$.

$$\Pr(y_1, \ldots, y_n, x_1, \ldots, x_n \mid \theta)$$

If (y_i, x_i) are I.I.D then we can write this as:

$$\Pr(y_1, \ldots, y_n, x_1, \ldots, x_n \mid \theta) = \prod_{i=1}^{N} \Pr(y_i, x_i \mid \theta) \propto \prod_{i=1}^{N} \Pr(y_i \mid x_i, \theta) = \mathbb{L}(\mathbf{y} \mid \mathbf{x}, \theta)$$

We call this $\mathbb{L}(\mathbf{y} \mid \mathbf{x}, \theta)$ the likelihood of the observed data.

MLE: Example

If we know the distribution of ε_i we can construct a maximum likelihood estimator

$$(\hat{\beta}_{MLE}, \hat{\sigma}^2_{MLE}) = \arg\min_{\beta,\sigma^2} \mathbb{L}(\beta, \sigma^2)$$

Where

$$\begin{aligned}
\mathbb{L}(\beta, \sigma^2) &= \prod_{i=1}^{N} \Pr(y_i \mid x_i, \beta, \sigma^2) \\
&= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2\sigma^2}(Y_i - X_i\beta)^2\right] \\
\ell(\beta, \sigma^2) &= \sum_{i=1}^{N} -\frac{1}{2}\ln(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{N}(Y_i - X_i\beta)^2
\end{aligned}$$

Take the FOC's of: $\ell(\beta, \sigma^2) = -\frac{N}{2}\,\text{ln}(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{N}(Y_i - X_i\beta)^2$:

$$\frac{\partial \ell(\beta, \sigma^2)}{\partial \beta} = \frac{1}{\sigma^2}\sum_{i=1}^{N} X_i'(Y_i - X_i\beta) = 0 \rightarrow \hat{\beta}_{MLE} = \hat{\beta}_{OLS}$$

$$\frac{\partial \ell(\beta, \sigma^2)}{\partial \sigma^2} = -N\frac{1}{2\sigma^2} - \frac{1}{2\sigma^4}\sum_{i=1}^{N}(Y_i - X_i\beta)^2 = 0$$

$$\sigma^2_{MLE} = \frac{1}{N}\sum_{i=1}^{N}(Y_i - X_i\beta)^2$$

Note: the unbiased estimator uses $\frac{1}{N-K-1}$.

MLE: General Case

1. Start with the joint density of the data $Z_1, \ldots, Z_N$ with density $f_Z(z, \theta)$
2. Construct the likelhood function of the sample $z_1, \ldots, z_n$

$$\mathbb{L}(\mathbf{z} \mid \theta) = \prod_{i=1}^{N} f_Z(z_i, \theta)$$

3. Construct the log likelihood (this has the same arg max)

$$\ell(\mathbf{z} \mid \theta) = \sum_{i=1}^{N} \ln f_Z(z_i, \theta)$$

4. Take the FOC's to find $\hat{\theta}_{MLE}$ that solves

$$\frac{\partial \ell(\theta)}{\partial \theta} = 0 \text{ or } \nabla_\theta \ell(\theta) = 0 \text{ or } \sum_{i=1}^{N} \frac{\partial \ln f_Z(z_i, \theta)}{\partial \theta} = 0.$$

Basic Setup: we know $F(z \mid \theta_0)$ but not θ_0. We know $\theta_0 \in \Theta \subset \mathbb{R}^K$.

- Begin with a sample of z_i from $i = 1, \ldots, N$ which are I.I.D. with CDF $F(z|\theta_0)$.
- The MLE chooses

$$\hat{\theta}_{MLE} = \arg\max_{\theta} \ell(\theta) = \arg\max_{\theta} \sum_{i=1}^{N} \ln f_Z(z_i, \theta)$$

- In practice the computer always minimizes negative log-likelihood so that $\hat{\theta}_{MLE} = \arg\min_{\theta} -\ell(\theta)$.

MLE: Technical Details

1. Consistency. When is it true that for $\epsilon > 0$?

$$\lim_{N\to\infty} \Pr\left(\left\|\widehat{\theta}_{MLE} - \theta_0\right\| > \varepsilon\right) = 0$$

2. Asymptotic Normality. What else do we need to show?

$$\sqrt{N}\left(\widehat{\theta}_{MLE} - \theta_0\right) \xrightarrow{d} \mathcal{N}\left(0, -\mathbb{E}\left[\frac{\partial^2 \log f(Z_i, \theta_0)}{\partial\theta\partial\theta'}\right]^{-1}\right)$$

3. Optimization. How to we obtain $\widehat{\theta}_{MLE}$ anyway?

- $Z_i \sim \mathcal{N}(\theta_0, 1)$ and $\Theta = (-\infty, \infty)$. In this case:

$$\ell(\theta) = -N \cdot \ln(2\pi) - \sum_{i=1}^{N} (z_i - \theta)^2 / 2$$

- MLE is $\widehat{\theta}_{MLE} = \overline{z}$ which is consistent for $\theta_0 = \mathbb{E}[Z_i]$
- Asymptotic distribution is $\sqrt{N}(\overline{z} - \theta_0) \sim \mathcal{N}(0, 1)$.
- Calculating mean is easy!

MLE: Example # 2

- $Z_i = (Y_i, X_i)$ where X_i has finite mean and variance (but arbitrary distribution)
- $(Y_i | X_i = x) \sim \mathcal{N}(x'\beta_0, \sigma_0^2)$

$$\hat{\beta}_{MLE} = (X'X)^{-1}X'Y$$
$$\hat{\sigma}^2_{MLE} = \frac{1}{N}\sum(y_i - x_i\hat{\beta}_{MLE})^2$$

- We already have shown consistency and AN for linear regression with normally distributed errors...

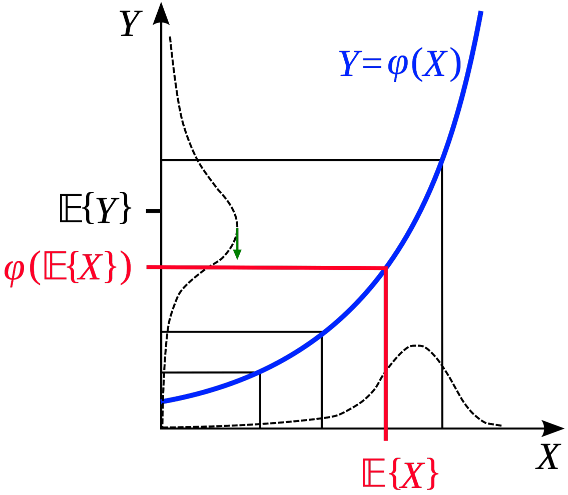
MLE: Example # 3

- $Z_i = (Y_i, X_i)$ where X_i has finite mean and variance (but arbitrary distribution)
- $\Pr(Y_i = 1 | X_i = x) = \frac{e^{x'\theta_0}}{1+e^{x'\theta_0}}$
- Solution is the logit model.
- No simple MLE solution, establishing properties is not obvious...

Jensen's Inequality

Let $\phi(z)$ be a convex function.

Then $\mathbb{E}[\phi(Z)] \geq \phi(\mathbb{E}[Z])$, with equality only in the case of a linear function.



More Technical Details

Define Y as the ratio of the density at θ to the density at the true value θ_0 both evaluated at Z

$$Y = \frac{f_Z(Z;\theta)}{f_Z(Z;\theta_0)}$$

- Let $g(a) = -\ln(a)$ so that $g'(a) = \frac{-1}{a}$ and $g''(a) = \frac{1}{a^2}$.
- Then by Jensen's Inequality $\mathbb{E}[-\ln Y] \geq -\ln \mathbb{E}[Y]$.
- This gives us

$$\mathbb{E}_z\left[-\ln\left(\frac{f_Z(Z;\theta)}{f_Z\left(Z;\theta_0\right)}\right)\right] \geq -\ln\left(\mathbb{E}_z\left[\frac{f_Z(Z;\theta)}{f_Z\left(Z;\theta_0\right)}\right]\right)$$

- The RHS is

$$\mathbb{E}_z\left[\frac{f_Z(Z;\theta)}{f_Z\left(Z;\theta_0\right)}\right] = \int \frac{f_Z(z;\theta)}{f_Z\left(z;\theta_0\right)} \cdot f_Z\left(z;\theta_0\right) dz = \int f_Z(z;\theta) dz = 1$$

More Technical Details

Because $\log(1) = 0$ this implies:

$$\mathbb{E}_z\left[-\ln\left(\frac{f_Z(Z;\theta)}{f_Z\left(Z;\theta_0\right)}\right)\right] \geq 0$$

Therefore

$$-\mathbb{E}\left[\ln f_Z(Z;\theta)\right] + \mathbb{E}\left[\ln f_Z\left(Z;\theta_0\right)\right] \geq 0$$
$$\mathbb{E}\left[\ln f_Z\left(Z;\theta_0\right)\right] \geq \mathbb{E}\left[\ln f_Z(Z;\theta)\right]$$

- We maximize the expected value of the log likelihood at the true value of θ!
- Helpful to work with $\mathbb{E}[\log f(z;\theta)]$ sometimes.

Information Matrix Equality

We can relate the Fisher Information to the Hessian of the log-likelihood

$$\mathcal{J}\left(\theta_0\right) = -\mathbb{E}\left[\frac{\partial^2 \ln f}{\partial\theta\partial\theta}\left(z;\theta_0\right)\right] = \mathbb{E}\left[\frac{\partial \ln f}{\partial\theta}\left(z;\theta_0\right) \times \frac{\partial \ln f}{\partial\theta}\left(z;\theta_0\right)'\right]$$

- This is sometimes known as the outer product of scores.
- This matrix is negative definite
- Recall that $\mathbb{E}\left[\frac{\partial \ln f}{\partial\theta}\left(z;\theta_0\right)\right] \approx 0$ at the maximum

Proof

$$1 = \int_z f_Z(z;\theta)dz \Rightarrow 0 = \frac{\partial}{\partial\theta}\int_z f_Z(z;\theta)dz$$

With some regularity conditions

$$0 = \int_z \frac{\partial f_Z}{\partial\theta}(z;\theta)dz = \underbrace{\int_z \frac{\partial \ln f_Z}{\partial\theta}(z;\theta)\cdot f_Z(z;\theta)dz}_{\mathbb{E}\left[\frac{\partial \ln f_Z}{\partial\theta}(z;\theta_0)\right]}$$

- This gives us the FOC we needed.
- Can get information identity with another set of derivatives.

We can relate the Fisher Information to the Hessian of the log-likelihood

$$\mathcal{I}(\theta) = -\mathbb{E}\left[\frac{\partial^2 \ln f}{\partial\theta\partial\theta'}(Z|\theta)\right]$$

It turns out this provides a bound on the variance

$$\text{Var}(\hat{\theta}(Z)) \geq \mathcal{I}\left(\theta_0\right)^{-1}$$

Because we can't do better than Fisher Information we know that MLE is most efficient estimator!

Tradeoffs

- How does this compare to GM Theorem?
- If MLE is most efficient estimate, why ever use something else?

Examples

We are going to practice writing down the:

- Likelihood $L(\theta) = \text{Pr}(z_1, \ldots, z_n; \theta) = \prod_{i=1}^{N} f(z_i; \theta)$.
- log likelihood $\ell(\theta) = \sum_{i=1}^{N} \ln f(z_i; \theta) = \sum_{i=1}^{N} \ell_i(z_i; \theta)$.
- Scores $\mathcal{S}_i(z_i, \theta) = -\frac{\partial \ln f(z_i;\theta)}{\partial \theta} = \frac{\partial \ell_i(z_i;\theta)}{\partial \theta}$.
- Hessian contribution $\mathcal{H}_i(z_i, \theta) = \frac{\partial^2 \ell_i(z_i;\theta)}{\partial \theta \partial \theta'}$.
- Information Matrix $\mathcal{I}(z_i, \theta) = \mathbb{E}_z[-\mathcal{H}_i(z_i, \theta)] = \mathbb{E}_z[\mathcal{S}_i(z_i, \theta)\mathcal{S}_i(z_i, \theta)^T]$
- Variance $V(\theta) \geq [\mathcal{I}(z_i, \theta)]^{-1}$ (Cramer-Rao Lower Bound).

Exponential Example

- Suppose we have data that are exponentially distributed $Y_i \sim \text{Exp}(\lambda)$. The goal is to estimate the parameter λ via MLE and $f(y_i|\lambda) = \lambda e^{-\lambda y_i}$ so that $\mathbb{E}[y_i] = \frac{1}{\lambda}$.
- Sometimes we want to parameterize the rate $\lambda_i = x_i'\beta$ with covariates.
- Example: Time until next customer arrives varies with time of day, day of week, etc. Time until default might depend on credit score, debt-to-income, market conditions, etc.

Exponential Regression Example (Careful: two parameterizations here!)

$$\text{For } y_i > 0, \quad f_{y|x}(y_i \mid x_i, \beta) = (x_i\,\beta)e^{-(x_i\beta)\,y_i} \qquad \text{so that } \mathbb{E}[y_i] = \frac{1}{x_i\,\beta}$$

With log likelihood

$$\ell(\beta) = \sum_{i=1}^{N} \ln f_{y|x}\,(y_i \mid x_i, \beta) = \sum_{i=1}^{N} \log(x_i'\,\beta) - (x_i'\,\beta)\;y_i$$

And Score, Hessian, and Information Matrix:

$$\frac{\partial\,\ell_i}{\partial\,\theta} = \mathcal{S}_i(y_i, x_i, \beta) = x_i'\left(\frac{1}{x_i\,\beta} - y_i\right)$$

$$\frac{\partial^2\,\ell_i}{\partial\,\theta^2} = \mathcal{H}_i(y_i, x_i, \beta) = -\frac{x_i'\,x_i}{(x_i'\,\beta)^2}$$

$$\mathcal{I}\,(\beta_0) = \sum_i \frac{x_i' x_i}{(x_i\,\beta)^2}$$

Computing Maximum Likelihood Estimators

Newton's Method for Root Finding

Consider the Taylor series for $f(x)$ approximated around $f(x_0)$:

$$f(x) \approx f(x_0) + f'(x_0) \cdot (x - x_0) + f''(x_0) \cdot (x - x_0)^2 + o_p(3)$$

Suppose we wanted to find a root of the equation where $f(x^*) = 0$ and solve for x:

$$0 = f(x_0) + f'(x_0) \cdot (x - x_0)$$
$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

This gives us an iterative scheme to find x^*:

1. Start with some x_k. Calculate $f(x_k), f'(x_k)$
2. Update using $x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$
3. Stop when $|x_{k+1} - x_k| < \epsilon_{tol}$.

Newton-Raphson for Minimization

We can re-write optimization as root finding;

- We want to know $\hat{\theta} = \arg\max_\theta \ell(\theta)$.
- Construct the FOCs $\frac{\partial \ell}{\partial \theta} = 0 \rightarrow$ and find the zeros.
- How? using Newton's method! Set $f(\theta) = \frac{\partial \ell}{\partial \theta}$

$$\theta_{k+1} = \theta_k - \left[\frac{\partial^2 \ell}{\partial \theta^2}(\theta_k)\right]^{-1} \cdot \frac{\partial \ell}{\partial \theta}(\theta_k)$$

The SOC is that $\frac{\partial^2 \ell}{\partial \theta^2} > 0$. Ideally at all θ_k.

This is all for a single variable but the multivariate version is basically the same.

Newton's Method: Multivariate

Start with the objective $Q(\theta) = -\ell(\theta)$:

- Approximate $Q(\theta)$ around some initial guess θ_0 with a quadratic function
- Minimize the quadratic function (because that is easy) call that θ_1
- Update the approximation and repeat.

$$\theta_{k+1} = \theta_k - \left[\frac{\partial^2 Q}{\partial\theta\partial\theta'}\right]^{-1} \frac{\partial Q}{\partial\theta}(\theta_k)$$

- The equivalent SOC is that the Hessian Matrix is positive semi-definite (ideally at all θ).
- In that case the problem is globally convex and has a unique maximum that is easy to find.

We can generalize to Quasi-Newton methods:

$$\theta_{k+1} = \theta_k - \lambda_k \underbrace{\left[\frac{\partial^2 Q}{\partial\theta\partial\theta'}\right]^{-1}}_{A_k} \frac{\partial Q}{\partial\theta}(\theta_k)$$

Two Choices:

- Step length λ_k
- Step direction $d_k = A_k \frac{\partial Q}{\partial \theta}(\theta_k)$
- Often rescale the direction to be unit length $\frac{d_k}{\|d_k\|}$.
- If we use A_k as the true Hessian and $\lambda_k = 1$ this is a full Newton step.

Choices for A_k

- $A_k = I_k$ (Identity) is known as gradient descent or steepest descent
- BHHH. Specific to MLE. Exploits the Fisher Information.

$$\begin{aligned} A_k &= \left[\frac{1}{N} \sum_{i=1}^{N} \frac{\partial \ln f}{\partial \theta} (\theta_k) \frac{\partial \ln f}{\partial \theta'} (\theta_k) \right]^{-1} \\ &= -\mathbb{E} \left[\frac{\partial^2 \ln f}{\partial \theta \partial \theta'} (Z, \theta^*) \right] = \mathbb{E} \left[\frac{\partial \ln f}{\partial \theta} (Z, \theta^*) \frac{\partial \ln f}{\partial \theta'} (Z, \theta^*) \right] \end{aligned}$$

- Alternatives SR1 and DFP rely on an initial estimate of the Hessian matrix and then approximate an update to A_k.
- Usually updating the Hessian is the costly step.
- Non invertible Hessians are bad news.

Thanks!