Methods of Estimation I

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MIT 18.655

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Minimum Contrast Estimates Least Squares and Weighted Least Squares Gauss-Markov Theorem Generalized Least Squares (GLS) Maximum Likelihood



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• Minimum Contrast Estimates

- Least Squares and Weighted Least Squares
- Gauss-Markov Theorem
- Generalized Least Squares (GLS)
- Maximum Likelihood

Minimum Contrast Estimates

 $X \in \mathcal{X}, X \sim P \in \mathcal{P} = \{P_{\theta}, \theta \in \Theta\}.$ Problem: Finding a function $\hat{\theta}(X)$ which is "close" to θ .

Consider

 $\rho: \mathcal{X} \times \Theta \to R.$

and define $\mathcal{D}(\theta_0, \theta)$ to measure the *discrepancy* between θ and the true value θ_0 .

 $\mathcal{D}(\theta_0, \theta) = E_{\theta_0} \rho(X, \theta).$

As a discrepancy measure, \mathcal{D} makes sense if the value of θ minimizing the function is $\theta = \theta_0$.

If P_{θ_0} were true, and we knew $D(\theta_0, \theta)$, we could obtain θ_0 as the minimizer.

Instead of observing $D(\theta_0, \theta)$, we observe $\rho(X, \theta)$.

- $\rho(\cdot, \cdot)$ is a contrast function
- $\hat{\theta}(X)$ is a minimum-contrast estimate.

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The definition extends to

- Euclidean $\Theta \subset R^d$.
- θ_0 an interior point of Θ .
- Smooth mapping: $\theta \to D(\theta_0, \theta)$.

•
$$\theta = \theta_0$$
 solves
 $\nabla_{\theta} D(\theta_0, \theta) = 0.$
where $\nabla_{\theta} = (\frac{\partial}{\partial \theta_1}, \dots, \frac{\partial}{\partial \theta_d})^T$
• Substitute $\rho(X, \theta)$ for $D(\theta_0, \theta)$ and solve
 $\nabla_{\theta} \rho(X, \theta) = 0$ at $\theta = \hat{\theta}.$

Estimating Equations:

- $\Psi : \mathcal{X} \times R^d \to R^d$, where $\Psi = (\psi_1, \dots, \psi_d)^T$.
- For every $\theta_0 \in \Theta$, the expectation of Ψ given P_{θ_0} has a unique solution

$$V(heta_0, heta)=E_{ heta_0}[\Psi(X, heta)]=0$$
 at $heta= heta_0.$

Example 2.1.1 Least Squares.

•
$$\mu(z) = g(\beta, z), \beta \in \mathbb{R}^d.$$

- $x = \{(z_i, Y_i) : 1 \le i \le n\}$, where Y_1, \ldots, Y_n are independent.
- Define $\rho(X,\beta) = |Y \mu|^2 = \sum_{i=1}^{n} [Y_i g(\beta, z_i)]^2$.
- Consider $Y_i = \mu(z_i) + \epsilon_i$, where $\mu(z_i) = g(\beta, z_i)$ and the ϵ_i are iid $N(0, \sigma_0^2)$.

Then, β parametrizes the model and we can write:

 $\begin{array}{rcl} D(\beta_0,\beta) &=& E_{\beta_0}\rho(X,\beta) \\ &=& n\sigma_0^2 + \sum_{i=1}^n [g(\beta_0,z_i) - g(\beta,z_i)]^2]. \end{array}$ This is minimized by $\beta = \beta_0$ and uniquely so iff β identifiable.

- The *least-squares estimate* β̂ minimizes ρ(X, β).
 Conditions to guarantee existence of β̂:
 - Continuity of $g(\cdot, z_i)$.
 - Minimum of $\rho(X, \cdot)$ existing on compact set $\{\beta\}$ e.g., $\lim_{|\beta| \to \infty} |g(\beta, z_i)| = \infty.$
 - If $g(\beta, z_i)$ is differentiable in β , then $\hat{\beta}$ satisfies the Normal Equations obtained by taking partial derivatives of $\rho(X, \beta) = |Y \mu|^2 = \sum_{i=1}^{n} [Y_i g(\beta, z_i)]^2$ and solving:

$$rac{\partial
ho(X,eta)}{\partial eta_j} = 0$$

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$$ho(X, eta) = |Y - \mu|^2 = \sum_{i=1}^{n} [Y_i - g(\beta, z_i)]^2$$

Solve:



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• Linear case: $g(\beta, z_i) = \sum_{i=1}^d z_{ij}\beta_i = \mathbf{z}_i^T \boldsymbol{\beta}$ $\frac{\partial \rho(X,\beta)}{\partial \beta_i} = 0$ $\sum_{i=1}^{\cdots} \frac{\partial g(\beta, z_i)}{\partial \beta_j} Y_i - \sum_{i=1}^{''} \frac{\partial g(\beta, z_i)}{\partial \beta_j} g(\beta, z_i) =$ $\sum_{i=1}^{n} z_{ij} Y_i - \sum_{i=1}^{n} z_{i,j} (\mathbf{z}_i^{\mathsf{T}} \boldsymbol{\beta}) = 0$ $\sum_{i=1}^{n} z_{ij} Y_i - \sum_{\substack{k=1 \ D \ D}}^{d} \sum_{\substack{i=1 \ D \ D}}^{n} z_{i,j} z_{i,k} \beta_k = 0, \quad j = 1, \dots, d$ $\mathbf{Z}_D^T \mathbf{Y} - \mathbf{Z}_D^T \mathbf{Z}_D \beta = 0$

where \mathbf{Z}_D is the $(n \times d)$ design matrix with (i, j) element $z_{i,j}$

Note:

- Least Squares exemplifies *minimum contrast* and *estimating equation* methodology.
- Distribution assumptions are not necessary to motivate the estimate as a mathematical approximation.

Method of Moments

Method of Moments

•
$$X_1, \ldots, X_n$$
 iid $X \sim P_{\theta}, \theta \in \mathbb{R}^d$.
• $\mu_1(\theta), \mu_2(\theta), \ldots, \mu_d(\theta)$:
 $\mu_j(\theta) = \mu_j = E[X^j \mid \theta]$ the *j*th moment of *X*.

• Sample moments:

$$\hat{\mu}_j = \prod_{i=1}^n X_i^j$$
, $j = 1, \dots, d$.

• Method of Moments: Solve for θ in the system of equations

$$\begin{array}{rcl} \mu_1(\theta) &=& \hat{\mu}_1 \\ \mu_2(\theta) &=& \hat{\mu}_2 \\ \vdots && \vdots \\ \mu_d(\theta) &=& \hat{\mu}_d \end{array}$$

Note: .

- θ must be identifiable
- Existence of μ_j : $\lim_{n \to \infty} \hat{\mu}_j = \mu_j$ with $|\mu_j| < \infty$.
- If $q(\theta) = h(\mu_1, \dots, \mu_d)$, then the Method-of-Moments Estimate of $q(\theta)$ is $\hat{q}(\theta) = h(\hat{\mu}_1, \dots, \hat{\mu}_d)$.
- The MOM estimate of θ may not be unique! (See Problem 2.1.11)

Plug-In and Extension Principles

Frequency Plug-In

- Multinomial Sample: X_1, \ldots, X_n with K values v_1, \ldots, v_K $P(X_i = v_j) = p_j \ j = 1, \ldots, K$
- Plug in estimates: $\hat{p}_j = N_j/n$ where $N_j = count(\{i : X_i = v_j\})$
- Apply to any function $q(p_1, \ldots, p_K)$: $\hat{q} = q(\hat{p}_1, \ldots, \hat{p}_K)$
- Equivalent to substituting the true distribution function $P_{\theta}(t) = P(X \leq t \mid \theta)$

underlying an iid sample with the empirical distribution function:

$$\hat{P}(t) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\{x_i \le t\}$$

 \hat{P} is an estimate of P, and $\nu(\hat{P})$ is an estimate of $\nu(P)$.

• Example: α th population quantile $\nu_{\alpha}(P) = \frac{1}{2}[F^{-1}(\alpha) + F_U^{-1}(\alpha)], \text{ with } 0 < \alpha < 1:$

where

$$F^{-1}(\alpha) = \inf \{ x : F(x) \ge \alpha \}$$

$$F^{-1}_{U}(\alpha) = \sup \{ x : F(x) \le \alpha \}$$

The plug-in estimate is

$$\hat{\nu}_{\alpha}(P) = \nu_{\alpha}(\hat{P}) = \frac{1}{2}[\hat{F}^{-1}(\alpha) + \hat{F}_{U}^{-1}(\alpha)].$$

• Example: Method of Moments Estimates of *j*th Moment

$$\nu(P) = \mu_j = E(X^j)$$
$$\hat{\nu}(P) = \hat{\mu}_j = \nu(\hat{P}) = \frac{1}{n} \sum_{i=1}^n x_i^j$$

Extension Principle

- Objective: estimate $q(\theta)$, a function of θ .
- Assume $q(\theta) = h(p_1(\theta), \dots, p_K(\theta))$, where h() is continuous.
- The extension principle estimates $q(\theta)$ with

$$\hat{q}(\theta) = h(\hat{p}_1, \ldots, \hat{p}_K)$$

● h() may not be unique: what h() is optimal? ♂ + = + + = + = - ? <

Notes on Method-of-Moments/Frequency Plug-In Estimates

- Easy to compute
- Valuable as initial estimates in iterative algorithms.
- Consistent estimates (close to true parameter in large samples).
- Best Frequency Plug-In Estimates are Maximum-Likelihood Estimates.
- In some cases, MOM estimators are foolish (See Example 2.1.7).

Least Squares and Weighted Least Squares





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Least Squares

General Model: Only Y Random

•
$$X = \{(z_i, Y_i) : 1 \le i \le n\}$$
, where
 Y_1, \ldots, Y_n are independent.
 $z_1, \ldots, z_n \in R^d$ are fixed, non-random.

• For cases i = 1, ..., n $Y_i = \mu(z_i) + \epsilon_i$, where $\mu(z) = g(\beta, z), \beta \in \mathbb{R}^d$. ϵ_i are independent with $E[\epsilon_i] = 0$.

- The Least-Squares Contrast function is $\rho(X,\beta) = |Y - \mu|^2 = \sum_{i=1}^{n} [Y_i - g(\beta, z_i)]^2.$
- β parametrizes the model and we can write the discrepancy function

$$D(\beta_0,\beta) = E_{\beta_0}\rho(X,\beta)$$

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Least Squares: Only Y Random

Contrast Function:

 $\rho(X,\beta) = |Y - \mu|^2 = \sum_{i=1}^{n} [Y_i - g(\beta, z_i)]^2.$

Discrepancy Function:

$$\begin{array}{rcl} \mathcal{D}(\beta_0,\beta) &=& E_{\beta_0}\rho(X,\beta) \\ &=& \sum_{i=1}^n Var(\epsilon_i) + \sum_{i=1}^n [g(\beta_0,z_i) - g(\beta,z_i)]^2]. \end{array}$$

 The model is semiparametric with unknown parameter β and unknown (joint) distribution P_ε of ε = (ε₁,..., ε_n).

Gauss-Markov Assumptions

• Assume that the distribution of ϵ satisfy:

$$E(\epsilon_i) = 0$$

$$Var(\epsilon_i) = \sigma^2$$

$$Cov(\epsilon_i, \epsilon_j) = 0 \text{ for } i \neq j$$

General Model: (Y,Z) Both Random

- $(Y_1, Z_1), \ldots, (Y_n, Z_n)$ are i.i.d. as $X = (Y, Z) \sim P$
- Define $\mu(z) = E[Y | Z = z] = g(\beta, z)$, where $g(\cdot, \cdot)$ is a known function and $\beta \in R^d$ is unknown parameter
- Given $Z_i = z_i$, define $\epsilon_i = Y_i \mu(z_i)$ for i = 1, ..., n

• Conditioning on the *z_i* we can write:

 $Y_i = g(\beta, z_i) + \epsilon_i, i = 1, 2, ..., n$ where $\epsilon = (\epsilon_1, ..., \epsilon_n)$ has (joint) distribution P_{ϵ}

- The Least-Squares Estimate of β̂ is the plug-in estimate β(P̂), where P̂ is the empirical distribution for the sample {(Z_i, Y_i), i = 1,..., n}
- The function $g(\beta, z)$ can be linear in β and z or nonlinear.
- Closed-form solutions exist for $\hat{\beta}$ when g is linear in β .

Gauss-Markov Theorem

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Gauss-Markov Theorem: Assumptions

Data
$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$
 and $\mathbf{X} = \begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,p} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1} & x_{n,2} & \cdots & x_{p,n} \end{bmatrix}$

follow a linear model satisfying the **Gauss-Markov Assumptions** if **y** is an observation of random vector $\mathbf{Y} = (Y_1, Y_2, \dots, Y_N)^T$ and

- $E(\mathbf{Y} | \mathbf{X}, \beta) = \mathbf{X}\beta$, where $\beta = (\beta_1, \beta_2, \dots, \beta_p)^T$ is the *p*-vector of regression parameters.
- Cov(Y | X, β) = σ²I_n, for some σ² > 0.
 I.e., the random variables generating the observations are uncorrelated and have constant variance σ² (conditional on X, and β).

Gauss-Markov Theorem

For known constants $c_1, c_2, \ldots, c_p, c_{p+1}$, consider the problem of estimating

 $\theta = c_1\beta_1 + c_2\beta_2 + \cdots + c_p\beta_p + c_{p+1}.$

Under the Gauss-Markov assumptions, the estimator

$$\hat{\theta} = c_1 \hat{\beta}_1 + c_2 \hat{\beta}_2 + \cdots + c_p \hat{\beta}_p + c_{p+1},$$

where $\hat{\beta}_1, \hat{\beta}_2, \dots \hat{\beta}_p$ are the least squares estimates is

1) An **Unbiased Estimator** of θ

2) A Linear Estimator of θ , that is

 $\tilde{\theta} = \sum_{i=1}^{n} b_i y_i$, for some known (given **X**) constants b_i .

Theorem: Under the Gauss-Markov Assumptions, the estimator $\hat{\theta}$ has the smallest (*Best*) variance among all *Linear Unbiased Estimators* of θ , i.e., $\hat{\theta}$ is *BLUE*.

Gauss-Markov Theorem: Proof

Proof: Without loss of generality, assume $c_{p+1} = 0$ and define $\mathbf{c} = (c_1, c_2, \dots, c_n)^T$. The Least Squares Estimate of $\theta = \mathbf{c}^T \boldsymbol{\beta}$ is: $\hat{\theta} = \mathbf{c}^T \hat{\boldsymbol{\beta}} = \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \equiv \mathbf{d}^T \mathbf{y}$ a linear estimate in **y** given by coefficients $\mathbf{d} = (d_1, d_2, \dots, d_n)^T$. Consider an alternative linear estimate of θ : $\tilde{\theta} = \mathbf{b}^T \mathbf{v}$ with fixed coefficients given by $\mathbf{b} = (b_1, \dots, b_n)^T$. Define $\mathbf{f} = \mathbf{b} - \mathbf{d}$ and note that $\tilde{\theta} = \mathbf{b}^T \mathbf{v} = (\mathbf{d} + \mathbf{f})^T \mathbf{v} = \hat{\theta} + \mathbf{f}^T \mathbf{v}$ • If $\hat{\theta}$ is unbiased then because $\hat{\theta}$ is unbiased $0 = E(\mathbf{f}^T \mathbf{y}) = \mathbf{f}^T E(\mathbf{y}) = \mathbf{f}^T (\mathbf{X} \boldsymbol{\beta})$ for all $\boldsymbol{\beta} \in R^p$ \implies **f** is orthogonal to column space of **X** \implies **f** is orthogonal to **d** = **X**(**X**^T**X**)⁻¹**c**

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If $\tilde{\theta}$ is unbiased then

 $\bullet\,$ The orthogonality of f to d implies

$$Var(\tilde{\theta}) = Var(\mathbf{b}^{\mathsf{T}}\mathbf{y}) = Var(\mathbf{d}^{\mathsf{T}}\mathbf{y} + \mathbf{f}^{\mathsf{T}}\mathbf{y})$$

$$= Var(\mathbf{d}^{\mathsf{T}}\mathbf{y}) + Var(\mathbf{f}^{\mathsf{T}}\mathbf{y}) + 2Cov(\mathbf{d}^{\mathsf{T}}\mathbf{y}, \mathbf{f}^{\mathsf{T}}\mathbf{y})$$

$$= Var(\hat{\theta}) + Var(\mathbf{f}^{\mathsf{T}}\mathbf{y}) + 2\mathbf{d}^{\mathsf{T}}Cov(\mathbf{y})\mathbf{f}$$

$$= Var(\hat{\theta}) + Var(\mathbf{f}^{\mathsf{T}}\mathbf{y}) + 2\mathbf{d}^{\mathsf{T}}(\sigma^{2}\mathbf{l}_{n})\mathbf{f}$$

$$= Var(\hat{\theta}) + Var(\mathbf{f}^{\mathsf{T}}\mathbf{y}) + 2\sigma^{2}\mathbf{d}^{\mathsf{T}}\mathbf{f}$$

$$= Var(\hat{\theta}) + Var(\mathbf{f}^{\mathsf{T}}\mathbf{y}) + 2\sigma^{2} \times 0$$

$$\geq Var(\hat{\theta})$$

Generalized Least Squares (GLS)

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Generalized Least Squares (GLS) Estimates

Consider generalizing the Gauss-Markov assumptions for the linear regression model to

 $\mathbf{Y} = \mathbf{X} \boldsymbol{eta} + \boldsymbol{\epsilon}$

where the random *n*-vector $\boldsymbol{\epsilon}$: $E[\boldsymbol{\epsilon}] = \mathbf{0}_n$ and $E[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^T] = \sigma^2 \Sigma$.

- $\bullet \ \sigma^2$ is an unknown scale parameter
- Σ is a known (n × n) positive definite matrix specifying the relative variances and correlations of the component observations.

Transform the data (\mathbf{Y}, \mathbf{X}) to $\mathbf{Y}^* = \Sigma^{-\frac{1}{2}} \mathbf{Y}$ and $\mathbf{X}^* = \Sigma^{-\frac{1}{2}} \mathbf{X}$ and the model becomes

 $\mathbf{Y}^* = \mathbf{X}^* \boldsymbol{\beta} + \boldsymbol{\epsilon}^*, \text{ where } E[\boldsymbol{\epsilon}^*] = \mathbf{0}_n \text{ and } E[\boldsymbol{\epsilon}^*(\boldsymbol{\epsilon}^*)^T] = \sigma^2 \mathbf{I}_n$ By the Gauss-Markov Theorem, the BLUE ('GLS') of $\boldsymbol{\beta}$ is $\hat{\boldsymbol{\beta}} = [(\mathbf{X}^*)^T (\mathbf{X}^*)]^{-1} (\mathbf{X}^*)^T (\mathbf{Y}^*) = [\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{X}]^{-1} (\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{Y})$

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Maximum Likelihood Estimation

- $X \sim P_{\theta}, \theta \in \Theta$ with density or pmf function $p(x \mid \theta)$.
- Given an observation X = x, define the likelihood function $L_x(\theta) = p(x \mid \theta)$:
 - a mapping: $\Theta \rightarrow R$.
- $\hat{\theta}_{ML} = \hat{\theta}_{ML}(x)$: the Maximum-Likelihood Estimate of θ is the value making $L_x(\cdot)$ a maximum

$$heta$$
 is the MLE if $L_x(\hat{ heta}) = \max_{ heta \in \Theta} L_x(heta).$

- The MLE $\hat{\theta}_{ML}(x)$ identifies the distribution making x "most likely"
- The MLE coincides with the mode of the Posterior Distribution if the Prior Distribution on Θ is uniform:

Maximum Likelihood

Examples

- Example 2.2.4: Normal Distribution with Known Variance
- Example 2.2.5: Size of a Population X_1, \ldots, X_n are iid $U\{1, 2, \ldots, \theta\}$, with $\theta \in \{1, 2, \ldots\}$. For $x = (x_1, \ldots, x_n)$, $L_x(\theta) = \prod_{i=1}^n \theta^{-1} \mathbf{1} (1 \le x_i \le \theta)$ $= \theta^{-n} \times \mathbf{1} (\max(x_1, \ldots, x_n)) \le \theta)$ $= \begin{cases} 0 & \text{, if } \theta = 0, 1, \ldots, \max(x_i) - 1 \\ \theta^{-n} & \text{if } \theta \ge \max(x_i) \end{cases}$

Maximum Likelihood As a Minimum Contrast Method

- Define $l_x(\theta) = \log L_x(\theta) = \log p(x \mid \theta)$
- Because $-log(\cdot)$ is monotone decreasing, $\hat{\theta}_{ML}(x)$ minimizes $-l_x(\theta)$
- For an iid sample $X = (X_1, ..., X_n)$ with densities $p(x_i | \theta)$, $I_X(\theta) = \log p(x_1, ..., x_n | theta)$ $= \log [\prod_{i=1}^n p(x_i | \theta)]$ $= \sum_{i=1}^n \log p(x_i | \theta)$
- As a minimum contrast function ,

$$\label{eq:rho} \begin{split} \rho(X,\theta) = & -l_X(\theta) \\ \text{yields the MLE } \hat{\theta}_{ML}(x) \end{split}$$

• The discrepancy function corresonding to the contrast function $\rho(X, \theta)$ is $D(\theta_0, \theta) = E[\rho(X, \theta) \mid \theta_0] = -E[\log p(x \mid \theta) \mid \theta_0]$ • Suppose that $\theta = \theta_0$ uniquely minimizes $D(\theta_0, \cdot)$. Then

$$D(\theta_0, \theta) - D(\theta_0, \theta_0) = -E[\log p(x \mid \theta) \mid \theta_0] - (-E[\log p(x \mid \theta_0) \mid \theta_0]]$$

= $-E[\log \frac{p(x \mid \theta)}{p(x \mid \theta_0)} \mid \theta_0]$
> 0, unless $\theta = \theta_0$.

This difference is the Kullback-Leibler Information Divergence between distribution P_{θ_0} and P_{θ} :

$$K(P_{\theta_0}, P_{\theta}) = -E[log(\frac{p(x|\theta)}{p(x|\theta_0)}) | \theta_0]$$

Lemma 2.2.1 (Shannon, 1948) The mutual entropy $K(P_{\theta_0}, P_{\theta})$
is always well defined and

- $K(P_{\theta_0}, P_{\theta}) \geq 0$
- Equality holds if and only if {x : p(x | θ) = p(x | θ₀)} has probability 1 under both P_{θ0} and P_θ.

Proof Apply Jensen's Inequality (B.9.3)

Likelihood Equations

Suppose:

- $X \sim P_{ heta}$, with $heta \in \Theta$, an open parameter space
- the likelihood function $I_X(\theta)$ is differentiable in θ
- $\hat{\theta}_{ML}(x)$ exists

Then: $\hat{\theta}_{ML}(x)$ must satisfy the **Likelihood Equation(s)** $\nabla_{\theta} l_X(\theta) = 0.$

Important Cases

For independent X_i with densities/pmfs $p_i(x_i | \theta)$, $\bigtriangledown_{\theta} l_X(\theta) = \sum_{i=1}^n \bigtriangledown_{\theta} \log p_i(x_i | \theta) = 0$ NOTE: $p_i(\cdot | \theta)$ may vary with *i*.

Examples

- Hardy-Weinberg Proportions (Example 2.2.6)
- Queues: Poisson Process Models (Exponential Arrival Times and Poisson Counts) (Example 2.2.7)
- Multinomial Trials (Example 2.2.8)
- Normal Regression Models (Example 2.2.9).

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