Modern Statistical Modeling

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1 Review of Linear Algebra

- Rank of $A \in \mathbb{R}^{m \times n}$: max # of linearly independent row/columns. Facts: (i) $0 \le \operatorname{rank}(A) \le \min(m, n)$; (ii) $\operatorname{rank}(A) = \operatorname{rank}(A^T) = \operatorname{rank}(AA^T) = \operatorname{rank}(A^TA)$; (iii) $\operatorname{rank}(BAC) = \operatorname{rank}(A)$ for nonsingular compatible B, C.
- Range(column space): $\mathcal{C}(A) = \{Ax : x \in \mathbb{R}^n\} \subset \mathbb{R}^m$. Null space: $\mathcal{N}(A) = \{x \in \mathbb{R}^n : Ax = 0\}$. Facts: (i) $\operatorname{rank}(A) = \dim \mathcal{C}(A)$; (ii) $\dim \mathcal{C}(A) + \dim \mathcal{N}(A) = n$; (iii) $\mathcal{N}(A) = \mathcal{C}(A^T)^{\perp}$; (iv) $\mathcal{C}(AA^T) = \mathcal{C}(A)$.
- Trace of $A \in \mathbb{R}^{m \times n}$: $\operatorname{tr}(A) = \sum_{i=1}^{n} a_{ii}$. Facts: (i) linearity: $\operatorname{tr}(A+B) = \operatorname{tr}(A) + \operatorname{tr}(B)$, $\operatorname{tr}(cA) = c\operatorname{tr}(A)$; (ii) cyclic property: $\operatorname{tr}(AB) = \operatorname{tr}(BA)$, $\operatorname{tr}(ABC) = \operatorname{tr}(BCA) = \operatorname{tr}(CAB)$; (iii) $\operatorname{tr}(A) = \sum_{i=1}^{n} \lambda_i a_{ij} b_{ij}$.
- Trace product: $\langle A, B \rangle = \operatorname{tr}(A^T B) = \operatorname{tr}(A B^T) = \sum_i \sum_j a_{ij} b_{ij}$. It induces Frobenius norm: $||A||_F = \sqrt{\langle A, A \rangle} = (\sum_{i,j} a_{ij})^{1/2}$.
- Determinant: $\det(A)$ or |A|. Facts: (i) $\det(cA) = c^n \det(A)$; (ii) $\det(AB) = \det A \det B$; (iii) $\det(A^{-1}) = \det(A)^{-1}$; (iv) $\det(A) = \prod_{i=1}^n \lambda_i$.
- Three decomposition. (1) For symmetric A, spectrum(eigen) decomposition: $A = V\Lambda V^T = \sum_{i=1}^r \lambda_i v_i v_i^T$ where V is orthogonal $(V^TV = VV^T = I)$ and $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$. (2) SVD for $A \in \mathbb{R}^{n \times p}$ of rank r: $A = U\Sigma V^T = \sum_{i=1}^r \sigma_i u_i v_i^T$ where $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0), \sigma_1 \geq \dots \geq \sigma_r \geq 0$ and $\{u_i\}, \{v_i\}$ orthonormal. arg $\min_{Y \in \mathbb{R}^{n \times p}, \operatorname{rank}(Y) \leq r} ||X Y||_F = \sum_{i=1}^r \sigma_i u_i v_i^T$ (low rank-r approximation). (3) QR decomposition: A = QR where Q is orthonormal and R is upper-triangular. It corresponds to Garm-Schmidt orthogonalization process.
- Idempotent: $P^T = P$. Facts: (i) If P is symmetric, then P is idempotent of rank r iff it has r eignevalues 1 and n r 0; (ii) If P is a projection matrix, then tr(P) = rank(P).
- Generalized inverses: For $A \in \mathbb{R}^{m \times n}$, $A^- \in \mathbb{R}^{n \times m}$ is called a generalized inverse of A if $AA^-A = A$. Moore-Penrose inverse A^+ if (i) $AA^+A = A$; (ii) $A^+AA^+ = A$; (iii) $(A^+A)^T = A^+A$; (iv) $(AA^+)^T = AA^+$. Such A^+ is unique, and $A^+ = V\Sigma^+U^T = \sum_{i=1}^r \sigma_i^{-1}v_iu_i^T$.
- Theorem 1.1 $P_X = X(X^TX)^-X^T$ is the orthogonal projection onto C(X). $[P_X$ does not depend on the choice of $(X^TX)^-$]

Proof $\forall v \in \mathbb{R}^n$, write v = x + w where $x \in \mathcal{C}(X), w \in \mathcal{C}(X)^T$. By definition, $P_X v = P_X x + P_X w = P_X x + X(X^T X)^- X^T w = P_X x$. We need to show $u^T X(X^T X)^- X^T X = u^T X, \forall u \in \mathbb{R}^n$.

Lemma 1.1 $C(X^T) = C(X^TX)$.

Proof Use
$$C(X^TX) \subset C(X^T)$$
 and rank $(X^TX) = \text{rank}(X)$.

By the lemma,
$$u^T X(X^T X)^- X^T X = z^T X^T X(X^T X)^- X^T X = z^T X^T X = u^T X$$
.

2 Review of Probability Theory

- Distribution related to multivariate normal: $X \sim \mathcal{N}_p(\mu, \Sigma)$. Moment generating function: $M_X(t) = \mathbb{E}e^{t^TX} = \exp(t^T\mu + \frac{1}{2}t^T\Sigma t)$. Characteristic function: $\phi_X(t) = \mathbb{E}e^{it^TX} = \exp(it^T\mu \frac{1}{2}t^T\Sigma t)$. Facts: (i) $A_{g\times p}X + b_{g\times 1} \sim \mathcal{N}_g(A\mu + b, A\Sigma A^T)$; (ii) $X \sim \mathcal{N}_p(\mu, \Sigma) \Leftrightarrow a^TX \sim \mathcal{N}(a^T\mu, a^T\Sigma a), \forall a \in \mathbb{R}^p$; (iii) $Y_1 = A_1X + b_1 \perp \perp Y_2 = A_2 + b_2 \Leftrightarrow \operatorname{Cov}(Y_1, Y_2) = A_1\Sigma A_2^T = 0$.
- Noncentral χ^2 : $X \sim \mathcal{N}_p(\mu, I_p)$. Then $X^T X \sim \chi_p^2(\lambda)$ with noncenteral parameter $\lambda = \mu^T \mu$. Pdf of $\chi_p^2(\lambda)$: $f(x; p, \lambda) = \sum_{k=0}^{\infty} \frac{e^{-\lambda/2}(\lambda/2)^k}{k!} f(x; p+2k, 0)$ where $f_q(x) = f(x; q, 0) = \frac{x^{q/2}e^{-x/2}}{2^{q/2}\Gamma(q/2)} I(x>0)$, a Poisson $(\frac{\lambda}{2})$ -weighted mixture of χ_{p+2k}^2 . M.g.f.: $M_X(t; p, \lambda) = \frac{1}{(1-2t)^p/2} \exp(\frac{\lambda t}{1-2t})$. Ch.f.: $\Phi_X(t; p, \lambda) = \frac{1}{(1-2it)^{p/2}} \exp(\frac{i\lambda t}{1-2it})$. Facts: (i)

PREDICTION AND NEAREST NEIGHBOR

If $X \sim \mathcal{N}(\mu, \Sigma)$ then $(X - \mu)^T \Sigma^{-1}(X - \mu) \sim \chi_p^2$ and $X^T \Sigma^{-1} X \sim \chi_p^2(\mu^T \Sigma^{-1} \mu)$; (ii) Additivity: If $X \sim \chi_{p_i}^2(\lambda_i)$ independent for $i = 1, \dots, k$, then $\sum_{i=1}^n X_i \sim \chi_{\sum_i p_i}^2(\sum_i \lambda_i)$; (iii) Rank deficient: If $X \sim \mathcal{N}_p(\mu, I_p)$, $A \in \mathbb{R}^{p \times p}$ symmetric, then $X^T A X \sim \chi_p^2(\lambda)$ with $\lambda = \mu^T A \mu \Leftrightarrow A$ is idempotent of rank r; (iv) If $X \sim \mathcal{N}_p(\mu, \Sigma)$, $A \in \mathbb{R}^{p \times p}$ symmetric, $B \in \mathbb{R}^{q \times p}$, then $X^T A X \perp \!\!\!\perp B X \Leftrightarrow B \Sigma A = 0_{q \times p}$; (v) $X^T A X \perp \!\!\!\perp X^T B X \Leftrightarrow A \Sigma B = 0_{p \times p}$.

• Theorem 2.1 (Cochran) $X \sim \mathcal{N}_p(\mu, I_p), X^T X = X^T A_1 X + \dots + X^T A_k X \equiv Q_1 + \dots + Q_k, A_i \in \mathbb{R}^{p \times p}$ symmetric of rank r_i . Then $Q_i \sim \chi^2_{r_i}(\lambda_i)$ independent for $i = 1, \dots, k \Leftrightarrow p = r_1 + \dots + r_k$. In this case, $\lambda_i = \mu^T A_i \mu$ and $\lambda_1 + \dots + \lambda_k = \mu^T \mu$.

Proof " \Leftarrow ": Note that $\forall i, \exists c_{ij} \in \mathbb{R}^p, j = 1, \dots, r_i$ s.t. $Q_i = X^T A_i X = \pm (c_{i1}^T X)^2 \pm \dots \pm (c_{ir_i}^T X)^2$. Let $C_i = (c_{i1}, \dots, c_{ir_i})$ and $C_{p \times r} = (C_1, \dots, C_k)^T$, then $X^T X = X^T C \triangle C X$, where \triangle is $p \times p$ diagnal with diagnol entries $\pm 1 \Rightarrow C^T \triangle C = I_p$. Thus C is of full rank and hence $\triangle = (C^T)^{-1} C^{-1} = (C^{-1})^T C^{-1} = (C^{-1})^T C^{-1}$ is positive definite $\Rightarrow \triangle = I_p$ and $C^T C = I_p$.

"\Rightarrow":
$$X^TA_i \sim \chi^2_{r_i}(\lambda_i)$$
 independent $\Rightarrow X^TX = \sum_i X^TA_iX \sim \chi^2_{\sum_i r_i}(\sum_i \lambda_i) \Rightarrow \sum_i r_i = p$.

- Noncentral F: If $Q_1 \sim \chi_p^2(\lambda)$ and $Q_2 \sim \chi_q^2$ are independent, then $\frac{Q_1/p}{Q_2/q} \sim F_{p,q}(\lambda)$.
- Noncentral t: If $U_1 \sim \mathcal{N}(\lambda, 1)$ and $U_2 \sim \chi_q^2$ are independent, then $T = \frac{U_1}{\sqrt{U_2/q}} \sim t_q(\lambda)$.

3 Prediction and Nearest Neighbor

- Goal: (1) predict y from x ("black box"); (2) which variable(s) in x contributes to the prediction of y (" $x^T\beta$ "), estimation, testing, variable selection.
- Why are prediction and estimation different: (1) model parameters; (2) identifiability $(f_{\theta_1} \neq f_{\theta_2} \Rightarrow \theta_1 \neq \theta_2)$.
- Find prediction function $f: \mathcal{X} \to \mathcal{Y}$ that minimizes $\mathbb{E}_{X,Y} \mathcal{L}(f(X),Y) = \mathbb{E}\{\mathbb{E}(\mathcal{L}(f(X),Y)|X)\}$ where loss function $\mathcal{L}: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$.
- Optimal predictor conditioned on x: $f^*(x) = \arg\min_{f(x) \in \mathcal{Y}} \mathbb{E}\{\mathcal{L}(f(X), Y) | X = x\}$.
- Regression: y numerical, squared error $(L_2$ -loss) $\mathcal{L}(\hat{y}, y) = (\hat{y} y)^2$, $\mathbb{E}\{(Y f(X))^2 | X\} = \{\mathbb{E}(Y|X) f(X)\}^2 + \mathbb{E}\{(Y \mathbb{E}(Y|X))^2 | X\} = \text{bias}^2 + \text{variance. Optimal } f^*(X) = \mathbb{E}(Y|X).$
- To model f^* , $\begin{cases} \text{parametric: linear, } f*(x) = x^T\beta, \beta \in \mathbb{R}^2 \\ \text{nonparametric: infinite dimension, } f^*(x) = m(x), m \text{ satisfying certain smoothness} \end{cases}$.
- Classification: 0-1 loss $\mathcal{L}(\hat{y}, y) = I(\hat{y} = y)$, $\mathbb{E}\{\mathcal{L}(h(X), Y) | X = x\} = \sum_{j \neq h(x)} P(Y = j | X = x) = 1 P(Y = h(X) | X = x)$. Optimal classification (Bayes classifier): $h^*(x) = \arg \max_{h(x) \in \mathcal{Y}} P(Y = h(X) | X = x)$.
- A fully nonparametric approach: k nearest neighbor (k-NN). Given training data $\{(x_i, y_i)\}_{i=1}^m$, use data "around" x to estimate $m(x) = \mathbb{E}(Y|X=x)$. Rationale: "Things that look alike must be alike". Classification: $h_{k\text{-NN}}(x) = \max_{i=1}^m \sum_{i \in N_k(x)} y_i$. k controls size of neighbor set. $k \uparrow$: effective sample size \uparrow , variance \downarrow , heterogeneity \uparrow , bias \uparrow .
- Theory for 1-NN: Consider binary classification: $\mathcal{Y} = \{0,1\}$, $\mathcal{L}(h(x),y) = I(h(x) \neq y)$. Assume $\mathcal{X} \subset [0,1]^d$, ρ Euclidean distance, $S = \{(x_i,y_i)\}_{i=1}^n$. $\forall x \in \mathcal{X}$, let $\pi_1(x), \dots, \pi_n(x)$ be an ordering of $\{1,\dots,n\}$ with increasing distance to x. $\eta(x) = \mathbb{E}(Y = 1|X = x)$. Bayes classifier: $h^*(x) = I(\eta(x) > \frac{1}{2})$. Assumption on η : η is c-Lipschitz for some c > 0. Goal: Derive an upper bound on $\mathbb{E}_{S \sim \mathcal{D}^n} \mathcal{L}(\hat{h}_S) = \mathbb{E}_{S \sim \mathcal{D}^n} \mathbb{E}_{(x,y) \sim \mathcal{D}} I(\hat{h}_S(x) \neq y)$.
- Lemma 3.1 The 1-NN rule \hat{h}_S satisfies $\mathbb{E}_{S \sim \mathcal{D}^n} \mathcal{L}(\hat{h}_S) \leq 2\mathcal{L}(h^*) + c\mathbb{E}_{S \sim \mathcal{D}^n, x \sim \mathcal{D}} ||x x_{\pi_1}(x)||$.

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Proof $\mathbb{E}_{S}\mathcal{L}(\hat{h}_{S}) = \mathbb{E}_{S_{x} \sim \mathcal{D}_{x}^{n}, x \sim \mathcal{D}_{x}, y \sim \eta(x), y' \sim \eta(\pi_{1}(x))} P(y \neq y')$. Note that $P(y \neq y') = \eta(x')(1 - \eta(x)) + (1 - \eta(x'))\eta(x) = (\eta - \eta + \eta')(1 - \eta) + (1 - \eta + \eta - \eta')\eta = 2\eta(1 - \eta) + (\eta - \eta')(2\eta - 1)$. Since η is c-Lipschitz and $|2\eta - 1| \leq 1$, $P(y \neq y') \leq 2\eta(1 - \eta) + c||x - x'||$. Substituting back, $\mathbb{E}_{S}\mathcal{L}(\hat{h}_{S}) \leq 2\mathbb{E}_{x}\eta(x)(1 - \eta(x)) + c\mathbb{E}_{S,x}||x - x_{\pi_{1}(x)}||$. The Bayes error $\mathcal{L}(h^{*}) = \mathbb{E}_{x}\{\eta(x) \wedge (1 - \eta(x))\} \geq \mathbb{E}_{x}(\eta(x)(1 - \eta(x)))$.

• Lemma 3.2 Let C_1, \dots, C_r be a collection of subsets of \mathcal{X} . Then $\mathbb{E}_{S \sim \mathcal{D}^n} \{ \sum_{i:C_i \cap S = \emptyset} \} P(C_i) \leq \frac{r}{ne}$ ("probability of subsets that not hit by S").

Proof By linearity, $\mathbb{E}_S\{\sum_{i:C_i\cap S=\emptyset}P(C_i)\}=\sum_{i=1}^rP(C_i)\mathbb{E}_SI(C_i\cap S=\emptyset)=\sum_{i=1}^rP(C_i)P(C_i\cap S=\emptyset)$. Note that $P(C_i\cap S=\emptyset)=(1-P(C_i))^n\leq e^{-nP(C_i)}$. Thus, LHS $\leq \sum_{i=1}^rP(C_i)e^{-nP(C_i)}\leq r\max P(C_i)e^{-nP(C_i)}\leq \frac{r}{ne}$. \square

• Theorem 3.1 (Generalization upper bound for 1-NN) $\mathbb{E}_S \mathcal{L}(\hat{h}_S) \leq 2\mathcal{L}(h^*) + 2c\sqrt{d}n^{-\frac{1}{d+1}}$.

Proof Take C_i of the form $\{x: x_j \in [(\alpha_j - 1)/T, \alpha_j/T], \forall j\}$, where $\alpha_1, \dots, \alpha_d \in \{1, \dots, T\}^d$.

Case 1: If $x, x' \in C_i$ for some i, then $||x - x'|| \le \sqrt{d\epsilon}$.

Case 2: Otherwise, $||x - x'|| \le \sqrt{d}$.

Hence, $\mathbb{E}_{S,x}||x-x_{\pi_1(x)}|| \leq \mathbb{E}_S\{P(\cup_{i:C_i\cap S\neq\emptyset}C_i)\sqrt{d}\epsilon + P(\cup_{i:C_i\cap S=\emptyset})\sqrt{d}\} \leq \sqrt{d}(\epsilon + \frac{r}{ne})$. Since $r=(\frac{1}{\epsilon})^d$, $\cdots \leq \sqrt{d}(\epsilon + \frac{1}{\epsilon^d ne})$. Matching the two terms gives $\epsilon = (\frac{1}{ne})^{\frac{1}{d+1}}$ and the optimal bound $2\sqrt{d}(ne)^{-\frac{1}{d+1}} \leq 2\sqrt{d}n^{-\frac{1}{d+1}}$. \square

• Theorem 3.2 (Generalization upper bound for k-NN) $\mathbb{E}_S \mathcal{L}(\hat{h}_S) \leq (1 + \sqrt{\frac{8}{k}}) \mathcal{L}(h^*) + (6c\sqrt{d} + k)n^{-\frac{1}{d+1}}$.

Remark 3.1 k is called regularization parameter/hyperparameter and the optimal $k \sim n^d$.

Remark 3.2 Exponential dependence on d: "curse of dimensionality".

• Theorem 3.3 (Lower bound) $\forall c > 1$ and any learning rule h, \exists a distribution over $[0,1]^d \times \{0,1\}$ s.t. $\eta(x)$ is cLipschitz, the Bayes error is 0, but for $n < (c+1)^d/2$, $\mathbb{E}\mathcal{L}(h) > \frac{1}{4}$ (i.e. minimax bound $\inf_h \sup_y \mathbb{E}\mathcal{L}(h) \ge Cn^{-\frac{1}{d+1}}$).

Hint Let G_c^d be the regular grid on $[0,1]^d$ with distance 1/c between points. Then any $\eta: G_c^d \to \{0,1\}$ is c-Lipschitz. Then use the following theorem.

• Theorem 3.4 (No free-lunch theorem) Let A be any learning rule for binary classification with 0-1 loss over \mathcal{X}^d and $n < |\mathcal{X}|/2$. Then \exists distribution D over $\mathcal{X} \times \{0,1\}$ s.t. $\mathbb{E}\mathcal{L}(A) \geq \frac{1}{4}$. Furthermore, with prob $\geq \frac{1}{7}$, $\mathcal{L}(A_S) \geq \frac{1}{8}$.

4 Linear Regression

- $Y_{n\times 1} = X_{n\times p}\beta_{p\times 1} + \epsilon_{n\times 1}$, $\mathbb{E}(\epsilon|X) = 0$, $Var(\epsilon) = \sigma^2 I_n$ and X fixed.
- Least squares estimator (LSE) solves the normal equation $X^T X \hat{\beta} = X^T Y, \hat{\beta} = (X^T X)^- X^T Y.$
- ANOVA: $y_{ij} = \mu + \alpha_j + \epsilon_{ij}, i = 1, \dots, n_j, j = 1, \dots, J. \sum_j n_j = n, \sum_j \alpha_j = 0.$
- **Definition** 4.1 θ is estimable if \exists an unbiased estimator of θ . $c^T\beta$ is linearly estimable if $\exists l \in \mathbb{R}^n$ s.t. $\mathbb{E}(l^TY) = c^T\beta, \forall \beta \in \mathbb{R}^p \Leftrightarrow c = X^Tl \in \mathcal{C}(X^T)$.
- Theorem 4.1 (1) If $c^T\hat{\beta}$ is unique, then $c \in \mathcal{C}(X^TX) = \mathcal{C}(X^T)$.
 - (2) If $c \in \mathcal{C}(X^T)$, then $c^T \hat{\beta}$ is unique and unbiased for $c^T \beta$.
 - (3) If $c^T \beta$ is estimable and $\epsilon \sim \mathcal{N}_n(0, \sigma^2 I_n)$, then $c \in \mathcal{C}(X^T)$.

Proof (1) Let $b \in \mathcal{C}(X^TX)^{\perp}$ be arbitrary, then $X^TY = X^TX\hat{\beta} = X^TX(\hat{\beta} + b) \Rightarrow c^T\hat{\beta} = c^T(\hat{\beta} + b) \Rightarrow c^Tb = 0$. (2) $c = X^Tl$ for some $l \in \mathbb{R}^n$, then $c^T\hat{\beta} = lX^T\hat{\beta} = lX^T(X^TX)^-X^TY = lP_XY$ is unique. $\mathbb{E}(c^T\hat{\beta}) = l^TP_x\mathbb{E}Y = l^TP_XX\beta = l^TX\beta = c^T\beta$.

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(3) If \exists an estimator T(X,Y) unbiased for $c^T\beta$, then $c^T\beta = \int T(X,y) \frac{1}{(2\pi\sigma^2)^{\frac{n}{2}}} \exp\{-\frac{1}{2\sigma^2}||y-X\beta||^2\}dy$. Differentiate with β , $c = X^T \int \frac{y-X\beta}{(2\pi\sigma^2)^{\frac{n}{2}}\sigma^2} T(X,y) \exp\{-\frac{1}{2\sigma^2}||y-X\beta||^2\}dy$.

Remark 4.1 $A\beta$ with $A \in \mathbb{R}^{q \times p}$ is estimable iff $\mathcal{C}(A^T) \subset \mathcal{C}(X^T) \Leftrightarrow A = A_*X$ for some $A_* \in \mathbb{R}^{q \times n}$. In particular, β is estimable iff X has full column.

- Ordinary least squares: $\hat{\beta} = (X^T X)^- X^T Y$.
- Proposition 4.1 For any estimable $A\beta$ and $B\beta$, $Cov(A\hat{\beta}, B\hat{\beta}) = \sigma^2 A(X^T X)^- B^T$, $Var(A\hat{\beta}) = \sigma^2 A(X^T X)^- A^T$.

Proof $\exists A_*$ and B_* s.t. $A = A_*X$, $B = B_*X$. Since $\hat{Y} = X\hat{\beta} = X(X^TX)^-X^TY = P_XY$, we have $\text{Var}(\hat{Y}) = P_X \text{Var}(Y)P_X^T = \sigma^2 P_X$. Hence $\text{Cov}(A\hat{\beta}, B\hat{\beta}) = \text{Cov}(A_*\hat{Y}, B_*\hat{Y}) = A_*\text{Var}(\hat{Y})B_*^T = \sigma^2 A_*P_XB_*^T = A(X^TX)^-B^T$. \square

• Theorem 4.2 (Gauss-Markov) If $c^T\beta$ is estimable, then $c^T\hat{\beta}$ has the minimum variance among all linear unbiased estimates. (Best Linear Unbiased Estimator, BLUE)

Proof Let l^TY be an unbiased estimator of $c^T\beta$. Hence, $c = X^Tl$, so that $c^T\hat{\beta} = l^TX\hat{\beta} = l^T\hat{Y}$. Thus, $\operatorname{Var}(l^TY) - \operatorname{Var}(c^T\hat{\beta}) = l^T[\operatorname{Var}(Y) - \operatorname{Var}(\hat{Y})]l = \sigma^2 l^T(I - P_X)l \ge 0$.

- Residual $\hat{\epsilon} = Y \hat{Y} = (I P_X)Y \in \mathcal{C}(X)^{\perp}$, $\mathbb{E}\hat{\epsilon}(I P_X)\mathbb{E}Y = (I P_X)X\beta = 0$, $\operatorname{Var}(\hat{\epsilon}) = \sigma^2(I P_X)^2 = \sigma^2(I P_X)$, $\operatorname{Cov}(\hat{\epsilon}, \hat{Y}) = \operatorname{Cov}((I P_X)Y, P_XY) = (I P_X)(\sigma^2I)P_X = 0$.
- Residual sum of squares (RSS): $||\hat{\epsilon}||^2 = \hat{\epsilon}^T \hat{\epsilon} = Y^T (I P_X) Y$. $\mathbb{E}(RSS) = \mathbb{E} \operatorname{tr}(\hat{\epsilon} \hat{\epsilon}^T) = \operatorname{tr}(\mathbb{E}(\hat{\epsilon} \hat{\epsilon}^T)) = \operatorname{tr}\{(I P_X)\sigma^2\} = \sigma^2 (n \operatorname{rank}(X))$. $\hat{\sigma}^2 = \frac{RSS}{n-r}$ is an unbiased estimator of σ^2 .
- Restricted LSE: $Y = X\beta + \epsilon$, $\mathbb{E}\epsilon = 0$, $\operatorname{Var}(\epsilon) = \sigma^2 I$, $\operatorname{rank}(X) = r$, $X = (X_1, X_2)$, $\beta = (\beta_1^T, \beta_2^T)^T$. $H_0 : \beta_2 = \beta_2^* \text{ vs } \beta_2 \neq \beta_2^*$. $\beta_2 \text{ is estimable} \Rightarrow \operatorname{rank}(X_2) = s$, $\operatorname{rank}(X_1) = r s$ and $C(X_1) \cap C(X_2) = \{0\}$.

Proof $\exists C \in \mathbb{R}^{q \times n}$ s.t. $(0_{s \times (p-s)}, I_s) = CX = (CX_1, CX_2)$. Hence $\operatorname{rank}(X_2) = s$ and $\operatorname{rank}(X_1) = r - s$. If $X_1b_1 = X_2b_2$ then $b_2 = CX_1b_1 = 0$.

- Under $H_0: \beta_2 = \beta_2^*, \ Y = X_1\beta_1 + X_2\beta_2 + \epsilon$ becomes $Y X_2\beta_2^* = X_1\beta_1 + \epsilon$. Restricted normal equation: $X_1^T X_1 \tilde{\beta}_1 = X_1^T (Y X_2\beta_2^*). \ \mathcal{C}(X_1) \subset \mathcal{C}(X) \Rightarrow P_{X_1} P_X = P_{X_1}. \ \text{Since} \ P_X Y = \hat{Y} = X \hat{\beta} = X_1 \hat{\beta}_1 + X_2 \hat{\beta}_2, \ \text{we}$ have $X_1 \tilde{\beta}_1 = P_{X_1} (Y X_2\beta_2^*) = P_{X_1} (P_X Y X_2\beta_2^*) = P_{X_1} (X_1 \hat{\beta}_1 + X_2 (\hat{\beta}_2 \beta_2^*)) = X_1 \hat{\beta}_1 + P_{X_1} X_2 (\hat{\beta}_2 \beta_2^*).$ Let $\tilde{Y} = X_1 \tilde{\beta}_1 + X_2 \beta_2^*$ the fitted valued of the restricted model. $\hat{Y} \tilde{Y} = X_1 \hat{\beta}_1 + X_2 \hat{\beta}_2 [X_1 \hat{\beta}_1 + P_{X_1} X_2 (\hat{\beta}_2 \beta_2^*)] X_2 \beta_2^* = (I P_{X_1}) X_2 (\hat{\beta}_2 \beta_2^*).$
- Theorem 4.3 $C(Z_2) = C(X_1)^{\perp} \cap C(X)$, where $Z_2 = (I P_{X_1})X_2 = X_2 P_{X_1}X_2$.

Proof $\mathcal{C}(Z_2) \subset \mathcal{C}(I - P_{X_1}) = \mathcal{C}(X_1)^{\perp}$. Since $\mathcal{C}(P_{X_1}X_2) \subset \mathcal{C}(X_1)$, $\mathcal{C}(Z_2) = \mathcal{C}(X_2 - P_{X_1}X_2) \subset \mathcal{C}(X)$. Conversely, if $X = X_1b_1 + X_2b_2 \in \mathcal{C}(X)$ and $X \perp \mathcal{C}(X_1)$, then $X = (I - P_{X_1})X = (I - P_{X_1})X_2b_2 \in \mathcal{C}(Z_2)$.

Corollary 4.1 $P_{Z_2} = P_X - P_{X_1}$.

- Now $\hat{Y} \tilde{Y} = (I P_{X_1})[X_2(\hat{\beta}_2 \beta_2^*) + X_1\hat{\beta}_1] = (I P_{X_1})(P_XY X_2\beta_2^*) = (I P_{X_1})P_X(Y X_2\beta_2^*) = P_{Z_2}(Y X_2\beta_2^*).$ In view of $\mathbb{R}^n = \mathcal{C}(X)^\perp \oplus \mathcal{C}(X)$, $Y - \tilde{Y} = (Y - \hat{Y}) + (\hat{Y} - \tilde{Y})$. $RSS_{H_0} = ||Y - \tilde{Y}||^2 = ||Y - \hat{Y}||^2 + ||\hat{Y} - \tilde{Y}||^2$, $RSS = ||Y - \hat{Y}||^2 = ||(I - P_X)Y||^2 = ||(I - P_X)(Y - X_2\beta_2^*)||^2$. $RSS_{H_0} - RSS = ||\hat{Y} - \tilde{Y}||^2 = ||Z_2(\hat{\beta}_2 - \beta_2^*)||^2 = ||P_{Z_2}(Y - X_2\beta_2^*)||^2$. By Cochran's theorem, $RSS_{H_0} - RSS \sim \chi_s^2(\lambda)$ with $\lambda = ||P_{Z_2}(X\beta - X_2\beta_2^*)||^2$.
- Wald's statistics: $(\hat{\theta} \theta_0) \operatorname{Var}(\hat{\theta})^{-1} (\hat{\theta} \theta_0)$. Since β_2 is estimable, $\exists C \in \mathbb{R}^{s \times n}$, $(0_{s \times p s}, I_s) = CX = (CX_1, CX_2) \Rightarrow CP_{X_1} = CX_1(X_1^TX_1)^- X_1^T = 0$, $CZ_2 = C(I_n P_{X_1})X_2 = CX_2 CP_{X_1}X_2 = I_s \Rightarrow Z_2$ has full column rank. $\hat{\beta}_2 = (0, I)\hat{\beta} = CX\hat{\beta} = CP_XY = C(P_{X_1} + P_{Z_2})Y = CP_{Z_2}Y$. Thus, $\operatorname{Var}(\hat{\beta}_2) = \operatorname{Var}(CP_{Z_2}Y) = CP_{Z_2}\sigma^2 I_n P_{Z_2}C^T = \sigma^2 CZ_2(Z_2^TZ_2)^- Z_2^T C^T = \sigma^2 (Z_2^TZ_2)^{-1}$. $(\hat{\beta}_2 \beta_2^*) \operatorname{Var}(\hat{\beta}_2)^{-1} (\hat{\beta}_2 \beta_2^*) = ||Z_2(\hat{\beta}_2 \beta_2^*)||^2/\sigma^2 = \frac{\operatorname{RSS}_{H_0} \operatorname{RSS}}{\sigma^2}$.

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- Inference: $H = (h_1, \dots, h_s) \in \mathbb{R}^{p \times s}, \xi = \mathbb{R}^s$. General linear hypothesis: $H_0 : H^T \beta = \xi$ (s constraints). Assume (1) $\mathcal{C}(H) \subset \mathcal{C}(X^T)$, so that $H^T \beta$ is estimable; (2) H has full column rank, $s = \operatorname{rank}(H) \leq \operatorname{rank}(X) = r \leq p$.
- Reparameterization: Choose $A \in \mathbb{R}^{p \times (p-s)}$ s.t. $\mathcal{C}(A) = \mathcal{C}(H)^{\perp}$. Let $\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} = \begin{pmatrix} A^T \beta \\ H^T \beta \end{pmatrix}$ and $\tilde{X} = X \begin{pmatrix} A^T \\ H^T \end{pmatrix}^{-1} = (\tilde{X}_1, \tilde{X}_2)$. The reparameterized model $Y = \tilde{X}\theta + \epsilon$. Since $\mathcal{C}(\tilde{X}^T) = \mathcal{C}((A, H)^{-1}X^T) \supset \mathcal{C}((A, H)^{-1}H) = \mathcal{C}(\begin{pmatrix} 0 \\ I_s \end{pmatrix})$, θ_2 is estimable. $\hat{\theta}$ solves the normal equation $\tilde{X}^T \tilde{X} \hat{\theta} = \tilde{X}^T Y$. Under $H_0, \tilde{Y} = \tilde{X}_1 \tilde{\theta}_1 + \tilde{X}_2 \xi = \tilde{X}_1 \hat{\theta}_1 + P_{\tilde{X}_1} \tilde{X}_2 (\hat{\theta}_2 \xi) + \tilde{X}_2 \xi$, $\text{RSS}_{H_0} \text{RSS} = ||Y \tilde{Y}||^2 ||Y \hat{Y}||^2 = ||\hat{Y} \tilde{Y}||^2 = \sigma^2 (\hat{\theta}_2 \xi) \text{Var}(\hat{\theta}_2)^{-1} (\hat{\theta}_2 \xi)$. Substituting into the original model, $\hat{\theta}_2 = H^T \hat{\beta}$, $\text{Var}(\hat{\theta}_2) = \sigma^2 H^T (X^T X)^- H$. Since $\mathbb{E}(X^T A X) = \text{tr}(A \Sigma) + \mu^T A \mu$ where $\mu = \mathbb{E}X, \Sigma = \text{Var}(X)$, $\mathbb{E}||\hat{Y} \tilde{Y}||^2 / \sigma^2 = \text{tr}(\text{Var}(\hat{\theta}_2)^{-1} \text{Var}(\hat{\theta}_2)) + (H^T \beta \xi)^T \text{Var}(H^T \beta)^{-1} (H^T \beta \xi)$. $Y \hat{Y} = (I_n P_{\tilde{X}})(Y \tilde{X}_2 \xi), \hat{Y} \tilde{Y} = \tilde{Z}_2(H^T \hat{\beta} \xi) = P_{\tilde{Z}_2}(Y \tilde{X}_2 \xi)$. By Cochran's thm, $\frac{||Y \hat{Y}||^2}{\sigma^2} \sim \chi_{n-r}^2$ and $\frac{||\hat{Y} \tilde{Y}||^2}{\sigma^2} \sim \chi_s^2(\lambda)$ are independent with $\lambda = (H^T \beta \xi)^T \text{Var}(H^T \beta)^{-1} (H^T \beta \xi)$. Hence, $\frac{(\text{RSS}_{H_0} \text{RSS})/s}{\text{RSS}/(n-r)} \sim F_{s,n-r}(\lambda)$.
- Let $\gamma = H^T \beta$ and $\gamma_0 = \xi$. Test $H_0: \gamma = \gamma_0$ can been regarded as a weighted distance between $\hat{\gamma}$ and γ_0 . To see this, let $\hat{\gamma} = H^T \hat{\beta} \sim \mathcal{N}_s(\gamma, \sigma^2 D)$ where $D = H^T(X^T X)^- H$ and $\hat{\sigma}^2 = \frac{\mathrm{RSS}}{n-r}$. Under H_0 , (1) s = 1: $Z = \frac{\hat{\gamma} \gamma_0}{\sigma \sqrt{D}} \sim \mathcal{N}(0, 1)$ if σ^2 is known; $T = \frac{\hat{\gamma} \gamma_0}{\hat{\sigma}/\sqrt{D}} \sim t_{n-r}$ if σ^2 is unknown. Confidence interval: $\hat{\gamma} \pm t_{n-r,\alpha/2} \hat{\sigma} \sqrt{D}$. (2) $s \geq 1$: Mahalanobis distance $||\hat{\gamma} \gamma_0||_{(\sigma^2 D)^{-1}} = \sqrt{(\hat{\gamma} \gamma_0)^T (\sigma^2 D)^{-1} (\hat{\gamma} \gamma_0)}, ||\hat{\gamma} \gamma_0||_{(\sigma^2 D)^{-1}} = (\hat{\gamma} \gamma_0)^T (\sigma^2 D)^{-1} (\hat{\gamma} \gamma_0) \sim \chi_s^2(\lambda)$ where $\lambda = (\gamma \gamma_0)^T D^{-1} (\gamma \gamma_0)/\sigma^2$. Thus $\mathbb{E}(\hat{\gamma} \gamma_0)^T D^{-1} (\hat{\gamma} \gamma_0)/s = (s + \lambda)\sigma^2/s = (1 + \lambda/s)\sigma^2 \geq \sigma^2$ with equality holding just when $\gamma = \gamma_0$. One may reject H_0 if $(\hat{\gamma} \gamma_0)^T D^{-1} (\hat{\gamma} \gamma_0)/(s\sigma^2)$ is large. If σ^2 is unknown, replacing σ^2 with $\hat{\sigma}^2$ yields $\frac{(\hat{\gamma} \gamma_0)^T D^{-1} (\hat{\gamma} \gamma_0)}{s\hat{\sigma}^2} = \frac{||\hat{Y} \hat{Y}||^2/s}{||Y \hat{Y}||^2/(n-r)} \sim F_{s,n-r}(\lambda)$, where $\lambda = 0$ iff H_0 is true.
- Multiple testing: Simultaneous confidence intervals of level 1α .
- Bonferroni: Replace α by α/m : $P(E_j) = 1 \alpha_j, j = 1, \dots, m$, then $P(\cap_j E_j) = 1 P(\cup_j E_j^c) \ge 1 \sum_j P(E_j) = 1 \sum_j \alpha_j = 1 \alpha$.
- Scheffé's method: Consider $Y = X\beta + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2 I_n)$, $\operatorname{rank}(X) = r$ and test for $u^T \gamma, \forall u \in \mathbb{R}^s$, where $\gamma = H^T \beta$ is estimable and H is of full column rank. $\hat{\gamma} = H\hat{\beta} \sim \mathcal{N}_s(\gamma, \sigma^2 D)$ where $D = H^T(X^TX)^-H$, $\hat{\sigma}^2 = \frac{\operatorname{RSS}}{n-r} \sim \sigma^2 \chi_{n-r}^2$. For any fixed $u \in \mathbb{R}^s$, an (1α) CI for $u^T \gamma : u^T \hat{\gamma} \pm t_{n-r,\frac{\alpha}{2}} \hat{\sigma} \sqrt{u^T D u}$. Now allow $u \in \mathbb{R}^s$ to vary arbitrarily. Since $\sup_{u \neq 0} \frac{|u^T \hat{\gamma} u^T \gamma|^2}{u^T D u} \stackrel{v = D^{\frac{1}{2}} u}{=} \sup_{v \neq 0} \frac{|v^T D^{-\frac{1}{2}}(\hat{\gamma} \gamma)|^2}{v^T v} \stackrel{\text{Cauchy-Schwarz}}{=} (\hat{\gamma} \gamma) D^{-1}(\hat{\gamma} \gamma), P(\sup_{u \neq 0} \frac{|u^T \hat{\gamma} u^T \gamma|^2}{s \hat{\sigma}^2 u^T D u} \le F_{s,n-r,\alpha}) = 1 \alpha$. Simultaneous CIs for $u^T \gamma, \forall u \in \mathbb{R}^s : u^T \hat{\gamma} \pm \hat{\sigma} \sqrt{s F_{s,n-r,\alpha} u^T D u}$. (Bonferrnoi: $t_{n-r,\alpha/(2m)}$)
- Tukey's method: Consider $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$, $\epsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$ i.i.d., $j = 1, \dots, m, i = 1, \dots, k$ and test for $\alpha_i \alpha_{i'}$, $\forall i, i' = 1, \dots, k$. If $Z_1, \dots, Z_n \sim \mathcal{N}(0, 1)$, $R^2 \sim \chi_v^2$, then $\frac{Z_{(n)} Z_{(1)}}{\sqrt{R^2/v}} \sim q_{n,v}$ (studentized range distribution). Thus $\frac{\sqrt{m}}{\hat{\sigma}} \max_{i,i'} \{\bar{y}_i \bar{y}_{i'} (\alpha_i \alpha_{i'})\} = \frac{\left\{\max_i \frac{\sqrt{m}(\bar{y}_i \mu \alpha_i)}{\sigma} \min_i \frac{\sqrt{m}(\bar{y}_i \mu \alpha_i)}{\sigma}\right\}}{\sqrt{\frac{RSS/\sigma^2}{n-k}}} \sim q_{k,n-k}$. Simultaneous CIs: $\bar{y}_i \bar{y}_{i'} \pm \frac{\hat{\sigma}}{\sqrt{m}} q_{k,n-k,\alpha}$. (Bonferrnoi: $t_{n-k,\alpha/[k(k-1)]}$, Scheffé: $\sqrt{kF_{k,n-k,\alpha}}$, Tukey: $q_{k,n-k,\alpha}/\sqrt{2}$ (the best/shortest length))

5 Exponential Families

- One parameter exponential families: $\mathscr{G} = \{g_{\eta}(y) = e^{\eta y \psi(\eta)}g_0(y)d\nu(y), \eta \in A, y \in \mathcal{Y}\}$, or $\log g_{\theta}(x) = A(\theta)B(x) + C(\theta) + D(x)$. η : natural parameter; y: sufficient statistics; $\psi(\eta)$: normalizing function s.t. $\frac{\int e^{\eta y}g_0(y)d\nu(y)}{e^{\psi(\eta)}} = 1$; A: natural parameter space s.t. $\int e^{\eta y}g_0(y)d\nu(y) < \infty$. $e^{\eta y \psi(\eta)}$: exponential tilting, a method of generating an additive distribution family.
- Mean and variance: $e^{\psi(\eta)} = \int_Y e^{\eta y} g_0(y) d\nu(y)$, differentiating w.r.t. y, $\psi'(y) e^{\psi(\eta)} = \int_Y y e^{\eta y} g_0(y) d\nu(y)$, $[\psi''(y) + \psi'(y)^2] e^{\psi(y)} = \int_Y y^2 e^{\eta y} g_0(y) d\nu(y) \Rightarrow \psi'(y) = \mathbb{E}_{\eta} Y = \mu_{\eta}, \psi''(y) = \mathbb{E}_{\eta} Y^2 \mu_{\eta}^2 = \operatorname{Var}_{\eta}(Y) = V_{\eta}$.

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- Cumulants: Let κ_j , $j = 1, 2, \cdots$ satisfy $\psi(\eta) \psi(\eta_0) = \kappa_1(\eta \eta_0) + \frac{\kappa_2}{2}(\eta \eta_0)^2 + \frac{\kappa_3}{3!}(\eta \eta_0)^3 + \cdots$. $\psi'''(\eta_0) = \kappa_3 = \mathbb{E}_0(Y \mu_0)^3$, $\psi''''(\eta_0) = \kappa_4 = \mathbb{E}_0(Y \mu_0)^4 3\kappa_2^2$. They correspond to central/noncentral moments. Skewness($\hat{\beta}$): $\gamma = \frac{\kappa_3}{\kappa_2^{3/2}} = \frac{\mathbb{E}(Y \mathbb{E}Y)^3}{(\operatorname{Var}(Y))^{3/2}}$. Kurtosis($\hat{\beta}$): $\delta = \frac{\kappa_4}{\kappa_2^2} = \frac{\mathbb{E}(Y \mathbb{E}Y)^4}{(\operatorname{Var}(Y))^2} 3$.
- If $y \sim g_{\eta}(\cdot)$ in an exponential family, then $y \sim [\psi', \psi'''^{1/2}, \psi''''/\psi''^{3/2}, \psi''''/\psi''^{2}]$ (expectation, SD, skewness, kurtosis). e.g. Poisson: $\psi = e^{\eta} = \mu, \phi' = \cdots = \phi'''' = \mu, y \sim [\mu, \sqrt{\mu}, 1/\sqrt{\mu}, 1/\mu]$.
- Theorem 5.1 $P(Y \leq \text{median}(Y)) \approx 0.5 + \frac{1}{6\sqrt{2\pi}} \text{skewness}(Y)$.
- Lemma 5.1 $Y = [y_0, y_1]$, then $\mathbb{E}_{\eta}[-l_0'(y)] = \eta (g_{\eta}(y_1) g_{\eta}(y_0))$ where $l_0(y) = \log g_0(y)$ and $l_0'(y) = \frac{dl_0(y)}{dy}$.

Proof Integration by parts.

• MLEs in exponential family: $Y_i \sim g_{\eta}$ i.i.d. for $i = 1, \dots, n$. $g_{\eta}^{(n)}(y) = e^{n(\eta \bar{y} - \psi(\eta))} \prod_{i=1}^n g_0(y_i), \eta^{(n)} = n\eta, \psi^{(n)}(y) = n\psi(\eta^{(n)}/n)$. log-likelihood: $l_{\eta}(y) = \log g_{\eta}^{(n)}(y) = n(\eta \bar{y} - \psi(\eta)) + C$, score: $l'_{\eta}(y) = n(\bar{y} - \mu_{\eta})$, score equation: $l'_{\hat{\eta}}(y) = 0 \Rightarrow \mu_{\hat{\eta}} = \bar{y}$. Since $\frac{d\mu}{d\eta} = \psi''(\eta) = V_{\eta} > 0$, we can solve $\hat{\eta}$ by $\hat{\eta} = \psi'^{-1}(\hat{\mu})$. e.g. (1) Poisson: $\hat{\eta} = \log(\bar{y})$; (2) Binomial: $\hat{\eta} = \log(\frac{\bar{y}}{1 - \bar{y}})$.

- Fisher information: $I_{\eta}^{(n)} = nI_{\eta} = nV_{\eta}, I_{\mu}^{(n)} = nI_{\mu} = \frac{n}{V_{\eta}}$. C-R lower bound: $\xi = h(\eta)$, any unbiased estimator $\bar{\xi}$ of ξ , $\operatorname{Var}(\bar{\xi}) \geq \frac{1}{I_{\mu}^{(n)}(\xi)} = \frac{(h'(\eta))^2}{nV_{\eta}}$. In particular, $\xi = \mu$, then $\operatorname{Var}(\hat{\mu}) \geq \frac{V_{\eta}}{n}$.
- Important distributions: (1) Normal: $\mathcal{N}(\eta, 1), \psi(\eta) = \frac{1}{2}\eta^2, g_0(y) = \frac{1}{\sqrt{2\pi}}e^{-y^2/2};$ (2) Binomial: $g_{\eta}(y) = C_N^y \pi^y (1-\pi)^{N-y} = C_N^y e^{y \log \pi + (N-y) \log(1-\pi)}, y = 0, 1, \cdots, N, \eta = \log \frac{\pi}{1-\pi}, \pi = \frac{1}{1+e^{-\eta}} = \frac{e^{\eta}}{1+e^{\eta}}, \psi(\eta) = N \log(1+e^{\eta});$ (3) Gamma (k, θ) (shape, scale), $\chi_k^2 = \text{Gamma}(k/2, 2);$ (4) Negative Binomial: NB $(k, \theta) = \#$ tails until kth head. $g_{\eta}(y) = C_{y+k-1}^{k-1}(1-\theta)\theta^k = C_{y+k-1}^{k-1}e^{y \log(1-\theta)+k \log \theta}, y = 0, 1, 2, \cdots, \theta \in (0, 1), \eta = \log(1-\theta), \psi(\eta) = k \log(1-\theta), \mu = k \frac{1-\theta}{\theta}, V = \frac{\mu}{\theta} \text{ (property: } k \to \infty, \mu \text{ fixed, } Y \to \text{Poisson}(\mu)).$
- Inverse Gaussian: W(t): Wiener process with drift $1/\mu$. $W(t) = \frac{1}{\mu}t + B(t)$ and $W(t) \sim \mathcal{N}(t/\mu, t)$, Cov(W(t), W(t+s)) = t. Y = 1st passage time to W(t) = 1. Density of $IG(\mu)$: $g(y) = \frac{1}{\sqrt{2\pi y^3}} \exp\{-\frac{(y-\mu)^2}{2\mu^2 y}\} = \frac{1}{\sqrt{2\pi y^3}} \exp(-\frac{y}{2\mu^2} + \frac{1}{\mu} \frac{1}{2\eta})$ with $\eta = -\frac{1}{2\mu^2}$, $\psi(\eta) = -\sqrt{2\eta}$ belongs to the exponential family.
- Tilted hypergeometric: Consider 2×2 talk (Table 1). Counts $X=(x_1,x_2,x_3,x_4)\sim \text{Multinomial}(N,(\pi_1,\pi_2,\pi_3,\pi_4))$. Test: $H_0:\theta=\log(\frac{\pi_1/\pi_2}{\pi_3/\pi_4})=0$. Under H_0 , conditional distribution of x_1 given (r_1,r_2,c_1,c_2) is $g_0(x_1|r_1,r_2,c_1,c_2)=\frac{C_{r_1}^{x_1}C_{r_2}^{c_1-x_1}}{C_N^{c_1}}\sim \text{hypergeometric with max}(0,c_1-r_2)\leq x_1\leq \min(c_1,r_1)$. When H_0 is not true, $g_\theta(x_1|r_1,r_2,c_1,c_2)=\frac{g_0(x_1|r_1,r_2,c_1,c_2)e^{\theta x_1}C_N^{c_1}}{C(\theta)}$ belongs to the exponential family with $C(\theta)=\sum_{x_1}C_{r_1}^{x_1}C_{r_2}^{c_1-x_1}e^{\theta x_1}$.

Table 1: 2×2 talk

	Yes	No	
Male	x_1	x_2	r_1
Female	x_3	x_4	r_2
	c_1	c_2	\overline{N}

- Deviance (Kullback-Leibler divergence): Generating Euclidean distance to exponential families, $2\text{KL}(\eta_1, \eta_2) = D(\eta_1, \eta_2) := 2 \int \eta_1(y) \log \frac{\eta_1(y)}{\eta_2(y)} d\nu(y) = 2\mathbb{E}_{\eta_1}[(\eta_1 \eta_2)y (\psi(\eta_1) \psi(\eta_2))] = 2[(\eta_1 \eta_2)\mu_1 (\psi(\eta_1) \psi(\eta_2))].$ Multual information: D(f(x, y), f(x)f(y))/2. Example: (1) $\mathcal{N}(\mu, 1) : D(\mu_1, \mu_2) = (\mu_1 \mu_2)^2$; (2) Poisson(μ): $D(\mu_1, \mu_2) = 2\mu_1[\log(\frac{\mu_1}{\mu_2}) (1 \frac{\mu_2}{\mu_1})]$; (3) Binomial(N, π): $D(\pi_1, \pi_2) = 2N[\pi_1\log(\frac{\pi_1}{\pi_2}) + (1 \pi_1)\log(\frac{1 \pi_1}{1 \pi_2})]$.
- Theorem 5.2 (Hoeffding's formula) For $g_{\eta}(y) = e^{\eta y \psi(\eta)} g_0(y)$, let $\hat{\eta}$ be the MLE of η and $\hat{\mu}$ be the MLE of μ . Then $g_{\eta}(y) = g_{\hat{\eta}}(y)e^{-D(\hat{\eta},\eta)/2}$, $g_{\mu}(y) = g_{\hat{\mu}}(y)e^{-D(\hat{\mu},\mu)/2}$.

Proof
$$\frac{g_{\eta}(y)}{g_{\hat{\eta}}(y)} = e^{(\eta - \hat{\eta})y - (\psi(\eta) - \psi(\hat{\eta}))} \stackrel{y=\hat{\mu}}{=} e^{-D(\hat{\eta}, \eta)/2}.$$

• Proposition 5.1 $D(\eta_1, \eta_2) = I_{\eta_1} \times (\eta_2 - \eta_1)^2 + O((\eta_2 - \eta_1)^3)$.

Proof
$$\frac{\partial}{\partial \eta_2} D(\eta_1, \eta_2) = \frac{\partial}{\partial \eta_2} 2[(\eta_1 - \eta_2)\mu_1 - (\psi(\eta_1) - \psi(\eta_2))] = 2(-\mu_1 + \mu_2) \Rightarrow \frac{\partial}{\partial \eta_2} D(\eta_1, \eta_2)|_{\eta_2 = \eta_1} = 0. \quad \frac{\partial^2}{\partial \eta_2^2} D(\eta_1, \eta_2) = 2\frac{\partial^2}{\partial \eta_2^2} \Rightarrow \frac{\partial^2}{\partial \eta_2^2} D(\eta_1, \eta_2)|_{\eta_2 = \eta_1} = 2V_{\eta_1}. \text{ Taylor expansion: } D(\eta_1, \eta_2) = 2V_{\eta_1} \frac{(\eta_2 - \eta_1)^2}{2} + O((\eta_2 - \eta_1)^3) = I_{\eta_1} (\eta_2 - \eta_1)^2 + O((\eta_2 - \eta_1)^3).$$

- Deviance residuals: Exponential family analogue of normal residuals $y \mu$: $\operatorname{sgn}(y \mu) \sqrt{D(y, \mu)}$. Let $y_i \sim g_{\mu}(\cdot)$ i.i.d. for $i = 1, \dots, n$. Define the deviance residual $R = \operatorname{sgn}(\bar{y} \mu) \sqrt{nD(\bar{y}, \mu)} = \operatorname{sgn}(\bar{y} \mu) \sqrt{D^{(n)}(\bar{y}, \mu)}$. The hope is that R will be nearly $\mathcal{N}(0, 1)$, at least closer to normal than the more obvious "Pearson residual" $R_p = \frac{\bar{y} \mu}{\sqrt{V_{\mu}/n}}$.
- Theorem 5.3 $R \sim \mathcal{N}(-a_n, (1+b_n)^2)$ where $a_n = \frac{\gamma_\mu/6}{\sqrt{n}}$ and $b_n = \frac{\frac{7}{36}\gamma_\mu^2 \delta_\mu}{n}$ (recall γ_μ, δ_μ is skewness and kurtosis of g_μ). The constants a_n and b_n are called "Bartlett corrections". More precisely, $P(\frac{R+a_n}{1+b_n} > z_\alpha) = \alpha + O(n^{-3/2})$.

Corollary 5.1
$$D^{(n)}(\bar{y},\mu) = R^2 \sim (1 + \frac{5\gamma_{\mu}^2 - 3\delta_{\mu}}{12n})\chi_1^2$$

- We wish to approximate the density under $g_{\mu}^{(n)}$ of the sufficient statistic $\hat{\mu} = \bar{y}$. Normal approximation: $g_{\mu}^{(n)}(\hat{\mu}) = \sqrt{\frac{n}{2\pi V_{\mu}}} e^{-\frac{n(\hat{\mu}-\mu)^2}{2V_{\mu}}}$. Saddlepoint approximation: $g_{\mu}^{(n)}(\hat{\mu}) = \sqrt{\frac{n}{2\pi \hat{V}}} e^{-nD(\hat{\mu},\mu)/2}$.
- Lugananni-Rice Formula: Observing $\bar{y} = \hat{\mu}$, p-value $\alpha(\mu) = \int_{\hat{\mu}}^{\infty} g_{\mu}^{(n)}(t) d\nu(t) \approx 1 \Phi(R) \phi(R) (\frac{1}{R} \frac{1}{Q}) + O(n^{-3/2})$ where Φ and ϕ are cdf/pdf of $\mathcal{N}(0,1)$, $R = \operatorname{sgn}(\hat{\mu} \mu) \sqrt{nD(\hat{\mu}, \mu)}$ is the deviance residual, and $Q = \sqrt{n\hat{V}}(\hat{\eta} \eta)$ is the crude form of the Pearson residual based on the canonical parameter.
- Transformation: $\zeta = H(\mu), \hat{\zeta} = H(\hat{\mu}), \hat{\mu}$ the MLE of $\mu, H'(\mu) = V_{\mu}^{\delta-1}, 0 \le \delta \le 1$.

$\delta =$	0	$\frac{1}{3}$	$\frac{1}{2}$	$\frac{2}{3}$	1
$\zeta =$	Canonical parameter η	Normal likelihood	Stabilized variance	Normal density	Expectation parameter μ

Example (when $\delta = \frac{1}{2}$): (1) Poisson (μ) , $H'(\mu) = \mu^{-1/2}$, $H(\mu) = 2\sqrt{\mu}$, $2\sqrt{y} \sim \mathcal{N}(2\sqrt{\mu}, 1)$; (2) Binomial (N, π) , $\hat{\zeta} = 2\sqrt{N}\sin^{-1}\sqrt{\frac{Np+3/8}{N+3/4}}$.

- Multiparameter exponential families: A *p*-parameter exponential family $\mathscr{G} = \{g_{\eta}(y) : \eta \in A \subset \mathbb{R}^p, y \in \mathcal{Y} \subset \mathbb{R}^p\}$ with $g_{\eta}(y) = e^{\eta^T y \psi(\eta)} g_0(y) d\nu(y), \mu = \mathbb{E}_{\eta} Y = \psi'(\eta), V = \operatorname{Var}_{\eta}(Y) = \psi''(\eta), d\mu = V d\eta, d\eta = V^{-1} d\mu$. Assume V will be positive definite for all η in $A = \{\eta : \int_{\mathcal{Y}} e^{\eta^T y} g_0(y) d\nu < \infty\}$. Let $B = \{\mu = \mathbb{E}_{\eta} Y, \eta \in A\}$.
- Facts: (1) A is convex; (2) $B \subset \text{convex hull of } \mathcal{Y};$ (3) $\text{Angle}(d\eta, d\mu) < \frac{\pi}{2} \ (d\eta^T d\mu = d\eta^T V d\eta > 0).$
- Transformation: $\zeta = h(\eta) = H(\mu) \in \mathbb{R}, \eta, \mu \in \mathbb{R}^p, D = \frac{d\eta}{d\mu} = V^{-1}$. Then $H'(\mu) = Dh'(\eta), H''(\mu) = Dh''(\eta)D^T + D_2h'(\eta)$ where $D_2 = (\frac{\partial^2 \eta_k}{\partial \mu_i \partial \mu_j})_{i,j,k}$.
- One-parameter subfamilies: $\eta_{\theta} = a + b\theta$, $\theta \in \Theta \subset \mathbb{R}$, $a, b \in \mathbb{R}^p$, $\mathscr{F} = \{f_{\theta}(y) = g_{\eta_{\theta}}(y) = e^{(a + b\theta)^T y \psi(a + b\theta)} g_0(y) d\nu$, $\theta \in \Theta$ }. Still a one-parameter exponential family, natural parameter θ , sufficient statistics $x = b^T y$. MLE of θ (score equation): $l'_{\theta}(\bar{y}) = 0 \Rightarrow b^T(\bar{y} \mu_{\theta}) = 0$.



EXPONENTIAL FAMILIES

• Stein's least favorable subfamily: $\zeta = s(\eta) = t(\mu), \zeta_0 = s(\eta_0) = t(\mu_0), s'_0 = \frac{\partial s(\eta)}{\partial \eta}|_{\eta_0}, t'_0 = \frac{\partial t(\mu)}{\partial \mu}|_{\mu_0}$. Define the LFF: $\eta_\theta = \eta_0 + t'_0 \theta, \theta \in \text{neighborhood of } 0$.



• Theorem 5.4 The 1-parameter CRLB for estimating ζ in LFF evaluated at $\theta = 0$ is the same as the *p*-parameter CRLB for estimating ζ in \mathscr{G} at $\eta = \eta_0$, which equals $t'_0V_0t_0$, where V_0 is the variance evaluated at η_0 or μ_0 .

Remark 5.1 In other words, the reduction to the LFF does not make it any easier to estimate ζ . It can be shown that any choice other than $b = t'_0$ for the family $\eta_{\theta} = \eta_0 + b\theta$ makes the one-parameter CRLB smaller than the *p*-parameter CRLB. Stein's construction is useful when some statistical property is easily calculated only in the one-parameter case.

- Examples: (1) $\mathcal{N}(\lambda,\Gamma): g(x) = \frac{1}{\sqrt{2\pi\Gamma}} \exp(-\frac{x^2}{2\Gamma} + \frac{\lambda}{\Gamma}x \frac{\lambda^2}{2\Gamma}), \eta = (\lambda/\Gamma, -\frac{1}{2\Gamma})^T, y = (x, x^2)^T, \mu = (\lambda, \lambda^2 + \Gamma)^T;$ (2) Beta $(\alpha, \beta): g(x) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha, \beta)} = \exp\{\alpha \log x + \beta \log(1-x) \log B(\alpha, \beta)\} \frac{1}{x(1-x)}, \eta = (\alpha, \beta)^T, y = (\log x, \log(1-x))^T;$ (3) Dirichlet $(\alpha_1, \dots, \alpha_p), g_{\alpha}(x) = \frac{1}{B(\alpha)} \prod_{i=1}^p x_i^{\alpha_i-1}, B(\alpha) = \frac{\prod_{i=1}^p \Gamma(\alpha_i)}{\Gamma(\sum_{i=1}^p \alpha_i)}, x \in \mathbb{S}^{p-1};$ (4) Graph/Degree model: $Y_{ij} = I(i-j), \pi_{ij} = P(Y_{ij} = 1) = \frac{e^{\theta_i + \theta_j}}{1+e^{\theta_i + \theta_j}}, \theta_i = \beta^T x_i \text{ where } x_i \text{'s are optional predictors. Sufficient statistics is degree of node } i.$ (5) Bradley-Terry model: $\pi_{ij} = \frac{e^{\theta_i}}{e^{\theta_i} + e^{\theta_j}} = \frac{e^{\theta_i} \theta_j}{1+e^{\theta_i \theta_j}}, w_{ij} \sim \text{Binomial}(n_{ij}, \pi_{ij}), g_{\theta} \propto \exp(\sum_{i,j}(\theta_i \theta_j)w_{ij}) = \exp(\sum_i \theta_i \sum_j w_{ij} \sum_j \theta_j \sum_i w_{ij}) = \exp\{\sum_i \theta_i [\# win(i) \# lose(i)]\}.$
- Truncated data: $y \sim g_{\eta}(y) = e^{\eta^T y \psi(\eta)} g_0(y)$, observed only if y falls in $\mathcal{Y}_0 \subset \mathcal{Y}$. Conditional density: $g_{\eta}(y|\mathcal{Y}_0) = e^{\eta^T y \psi(\eta)} \frac{g_0(y)}{G_{\eta}(\mathcal{Y}_0)}$, where $G_{\eta}(\mathcal{Y}_0) = \int_{\mathcal{Y}_0} g_{\eta}(y) dy$.
- Lemma 5.2 Partition $\eta = (\eta_1, \eta_2), y = (y_1, y_2).y_1|y_2 \sim g_{\eta_1}(y_1|y_2) = e^{\eta_1^T y_1 \psi(\eta_1|\eta_2)} dG_0(y_1|y_2), y_2 \sim g_{\eta_1,\eta_2}(y_2) = e^{\eta_2^T y_2 \psi_{\eta_1}(\eta_2)} dG_{\eta_1,0}(y_2).$

$$\begin{aligned} \mathbf{Proof} \quad g_{\eta}(y_2) &= \int_{\mathcal{Y}_1} e^{\eta_1^T y_1 + \eta_2^T y_2 - \psi(\eta)} g_0(y_1 | y_2) g_0(y_2) dy_1 = e^{\eta_2^T y_2 - \psi(\eta)} (\int_{\mathcal{Y}_1} e^{\eta_1^T y_1} g_0(y_1 | y_2) dy_1) g_0(y_2) \Rightarrow g_{\eta}(y_1 | y_2) = \\ \frac{g_{\eta}(y)}{g_{\eta}(y_2)} &= \frac{e^{\eta_1^T y_1 + \eta_2^T y_2 - \psi(\eta)} g_0(y_2)}{e^{\eta_2^T y_2 - \psi(\eta) + \psi(\eta_1 | \eta_2)} g_0(y_2)} = e^{\eta_1^T y_1 - \psi(\eta_1 | \eta_2)} dG_0(y_1 | y_2). \end{aligned}$$

Remark 5.2 Usually after a transformation $M \in \mathbb{R}^{p \times p}$ nonsingular, $\tilde{\eta} = (M^{-1})^T \eta, \tilde{y} = My$.

• Examples: (1) Fisher's exact test for 2×2 talk (Recall Table 1), $H_0: \theta = \log(\frac{\pi_1/\pi_2}{\pi_3/\pi_4}) = 0$. The natural parameter

 $x_3+x_4)=x_1-\frac{r_1}{2}-\frac{c_1}{2}+\frac{N}{4}$. (2) Wishart statistics: $x_1,\cdots,x_n\sim\mathcal{N}_d(\lambda,\Gamma)$ independent, $y_1=\bar{x},y_2=\frac{1}{n}\sum_{i=1}^nx_ix_i^T$. Wishart statistics $W=\frac{1}{n}\sum_{i=1}^n(x_i-\bar{x})(x_i-\bar{x})^T=y_2-y_1y_1^T$. $y_2|y_1$ is in a $\frac{d(d+1)}{2}$ -dim exponential family. (3) Poisson trick: $s=(s_1,\cdots,s_L),s_l\sim \mathrm{Poisson}(\mu_L)$ independent $\Rightarrow s|n=\sum_{l=1}^Ls_l\sim \mathrm{Multinomial}_L(n,\pi)$ where $\pi_l=\frac{\mu_l}{\sum_j\mu_j}$. Conversely, if $s|n\sim \mathrm{Multinomial}(n,\pi)$ and $n\sim \mathrm{Poisson}(\mu_+)$, then $s_l\sim \mathrm{Poisson}(\mu_+\pi_l)$ i.i.d.

• Rotational speeds of stars: Bimodal: $f(x) = w \frac{\phi(x/c_1)}{c_1} + (1-w) \frac{\phi(x/c_2)}{c_2}$. Two competing candidates candidates for $\phi(x)$: $\phi_1(x) = 2xe^{-x^2}$, $\phi_2(x) = 4x^2e^{-x^2}\pi^{-1/2}$. We take the bin partitions and set y_l to be the count and π_l be the probability of bin l. $y_l \sim \text{Poisson}(\mu_l)$, $\mu_l = n\pi_l$. Any choice of (w, c_1, c_2) produces estimates of π_l and μ_l .

6 Generalized Linear Models

• Data types for response y: $\begin{cases} \text{numerical:} & \text{continuous: Box-Cox transformation:} \begin{cases} \frac{x^{\lambda}-1}{\lambda}, & \lambda \neq 0 \\ \log x, & \lambda = 0 \end{cases} \\ \text{discrete: count} \\ \text{nominal:} & \text{binary} \\ \text{multinomial} \\ \text{ordinal} \end{cases}$

- Three components of GLMs: (1) Random: distribution of Y with $\mathbb{E}Y = \mu$; (2) Systematic: $\eta = \sum_{j=1}^{p} x_j \beta_j$; (3) Link: $g(\mu) = \eta$.
- Example 1 (Dilution assays): density ρ_0 , at the x-th dilation $\rho_x = \rho_0 2^{-x}$, $x = 0, 1, 2, \cdots$, proportion of infected plates $y_x = \frac{r_x}{m_x}$, Y = I(infected), $\mathbb{E}(Y|x) = P(Y = 1|x) = \pi_x$, # organism on a plate: $N_x \sim \text{Poisson}(\rho_x v)$, $\pi_x = P(N_x \ge 1) = 1 e^{-\rho_x v} = 1 e^{-\rho_0 v 2^{-x}}$, link function $g(\pi_x) = \log(-\log(1 \pi_x)) = \log v + \log \rho_0 x \log 2$.
- Example 2 (Dose response): dose level x, survival rate π_x , cell j, dose level x_j , y_j survive out of m_j animals. (1) Probit model: $\pi_x = \Phi(\alpha + \beta x)$, where Φ is the c.d.f. of $\mathcal{N}(0,1)$, link function $g = \Phi^{-1}$. (2) Logisitic/Logit model: $\pi_x = \text{expit}(\alpha + \beta x) = \frac{1}{1+e^{-(\alpha+\beta x)}}$, link function $g(\pi_x) = \text{logit}(\pi_x) = \log \frac{\pi_x}{1-\pi_x}$.
- Random component: Y has a distribution in an exponential family: $f(y;\theta,\phi) = \exp\{\frac{y\theta-b(\theta)}{a(\phi)} + c(y,\phi)\}$ where ϕ is dispersion parameter. Usually $a(\phi) = \phi/w_i$. log-likelihood: $l(\theta;y) = \frac{y\theta-b(\theta)}{a(\phi)} + c(y,\phi)$. $\frac{\partial l}{\partial \theta} = \frac{y-b'(\theta)}{a(\phi)}$, $\frac{\partial^2 l}{\partial \theta^2} = -\frac{b''(\theta)}{a(\phi)}$. $\mathbb{E}\frac{\partial l}{\partial \theta} = 0$, $\mathbb{E}(\frac{\partial l}{\partial \theta})^2 = -\mathbb{E}\frac{\partial^2 l}{\partial \theta^2}$, $\mathbb{E}Y = \mu = b'(\theta)$, $\operatorname{Var}(Y) = a(\phi)b''(\theta)$.
- Systematic component: predictors $(x_1, \dots, x_p), \eta = x^T \beta$.
- Canonical link function: $g = b'^{-1}(\mu)$ so that $\eta = g(\mu) = b'^{-1}(b'(\theta)) = \theta$.
- Goodness of fit: Null model: one parameter, μ common mean. Full model: n parameters, one per oberservation. Idea: Measure discrepancy between an intermediate model and the full model.
- Assume $l(y, \phi; y), l(\hat{\mu}, \phi; y)$ maximize log-likelihood over β with fixed ϕ , g_1/g_2 is full/current model respectively, $\tilde{\theta}/\hat{\theta} = \theta(y)/\theta(\hat{\mu})$ and $a_i(\phi) = \phi/w_i$. $2\mathbb{E}_{P_n} \log \frac{l(y, \phi; y)}{l(\hat{\mu}, \phi; y)} = 2\sum_{i=1}^n \frac{w_i}{\phi} [(\tilde{\theta}_i \hat{\theta}_i)y_i b(\tilde{\theta}_i) + b(\hat{\theta}_i)] := \frac{D(y, \hat{\mu})}{\phi}$. Under suitable regularity conditions, if the fitted model is correct, $D(y, \hat{\mu})/\phi \sim \chi_{n-p}^2$ where p is the dimension of β .
- Pearson's χ^2 -statistic: $\chi^2 = \sum_{i=1}^n \frac{(y_i \hat{\mu}_i)^2}{V(\hat{\mu}_i)/w_i}$ where $V(\mu) = b''(b'^{-1}(\mu))$. Under suitable regularity conditions, if the model is correct, $\chi^2/\phi \sim \chi^2_{n-n}$.
- Residuals: (1) Deviance residual: $r_D = \operatorname{sgn}(y \hat{\mu})\sqrt{d_i}$ where $d_i = 2w_i[(\tilde{\theta}_i \hat{\theta}_i)y_i b(\tilde{\theta}_i) + b(\hat{\theta}_i)]$; (2) Pearson residual: $r_p = \frac{y \hat{\mu}}{\sqrt{V(\hat{\mu})/w_i}}$; (3) Anscombe residual: $\delta = \frac{2}{3}, H'(\mu) = V_{\mu}^{-\frac{1}{3}}, A = \int \frac{d\mu}{V^{1/3}(\mu)}$. For Poisson distribution, $A = \frac{3}{2}\mu^{2/3}$, and we must scale by dividing by the SD of A(Y), i.e. $A'(\mu)\sqrt{V(\mu)} \Rightarrow r_A = \frac{\frac{3}{2}(y^{2/3} \mu^{2/3})}{\mu^{1/6}}$.
- Algorithms for fitting GLMs: $l(\beta)$ log-likelihood, $u(\beta) = \frac{\partial}{\partial \beta} l(\beta), H(\beta) = \frac{\partial^2}{\partial \beta \partial \beta^T} l(\beta)$. The MLE of $\hat{\beta}$ solves the estimating equation. $0 = u(\hat{\beta}) \approx u(\beta^{(0)}) + H(\beta^{(0)})(\hat{\beta} \beta^{(0)})$ giving the update $\beta^{(t+1)} = \beta^{(t)} H(\beta^{(t)})^{-1} u(\beta^{(t)})$. Fisher scoring: $\beta^{(t+1)} = \beta^{(t)} + I(\beta^{(t)})^{-1} u(\beta^{(t)})$ (since $I(\beta) = -\mathbb{E}H(\beta)$). In a GLM, $l = \sum_{i=1}^n l_i, l_i = \frac{y_i \theta_i b(\theta_i)}{a_i(\phi)} + c_i(y_i, \phi), u_{ir} = \frac{\partial l_i}{\partial \theta_i} \frac{\partial \theta_i}{\partial \mu_i} \frac{\partial \mu_i}{\partial \eta_i} \frac{\partial \mu_i}{\partial \eta_i} \frac{\partial \mu_i}{\partial \theta_r} = \frac{y_i \mu_i}{a_i(\phi)} \frac{1}{V(\mu_i)} \frac{1}{g'(\mu_i)} x_{ir} = \frac{(y_i \mu_i)x_{ir}}{a_i(\phi)V(\mu_i)g'(\mu_i)} = (y \mu)^T W \frac{d\eta}{d\mu} x_{(r)}$ where $W = \text{diag}(\frac{1}{a_i(\phi)V(\mu_i)g'(\mu_i)^2})$. Since $\text{Cov}(u_r, u_s) = \sum_{i=1}^n \frac{\text{Var}(y_i)x_{ir}x_{is}}{a_i(\phi)^2V(\mu_i)^2g'(\mu_i)^2} = \sum_{i=1}^n \frac{x_i x_{is}}{a_i(\phi)V(\mu_i)g'(\mu_i)^2} \Rightarrow I(\beta) = \text{Var}(u(\beta)) = X^T W X, u(\beta) = X^T W \frac{d\eta}{d\mu} (y \mu)$ where $X = (x_{ir})_{n \times p}$. $H(\beta) = -X^T W X + X^T \{\frac{\partial}{\partial \beta^T} (W \frac{d\eta}{d\mu})\}(y \mu)$.
- Under what conditions $-H(\beta) = I(\beta)$? Take canonical link $\eta_i = b^{-1}(\mu_i) = \theta_i$, $V(\mu_i) = b''(\theta_i) = \frac{\partial \mu_i}{\partial \theta_i} = \frac{\partial \mu_i}{\partial \eta_i}$, $w_{ii} = \frac{1}{a_i(\phi)V(\mu_i)g'(\mu_i)^2} = \frac{1}{a_i(\phi)\frac{\partial \eta_i}{\partial \mu_i}} \Rightarrow W\frac{d\eta}{d\mu} = \operatorname{diag}(\frac{1}{a_i(\phi)}) \Rightarrow \frac{\partial}{\partial \beta^T}(W\frac{d\eta}{d\mu}) = 0$.

GENERALIZED LINEAR MODELS

• Substituting back, $\beta^{(t+1)} = \beta^{(t)} + (X^T W^{(t)} X)^{-1} X^T W^{(t)} \frac{d\eta}{d\mu} (y - \mu) = (X^T W^{(t)} X)^{-1} X^T W^{(t)} [X \beta^{(t)} + \frac{d\eta}{d\mu} (y - \mu)] = (X^T W^{(t)} X)^{-1} X^T W^{(t)} [\eta^{(t)} + \frac{d\eta}{d\mu} |_{\mu^{(t)}} (y - \mu^{(t)})]$ (iteratively reweighted least squares).