

Modern Statistical Modeling

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1 Review of Linear Algebra and Probability

- Rank of $A \in \mathbb{R}^{m \times n}$: max # of linearly independent row/columns. Facts: (i) $0 \leq \text{rank}(A) \leq \min(m, n)$; (ii) $\text{rank}(A) = \text{rank}(A^T) = \text{rank}(AA^T) = \text{rank}(A^T A)$; (iii) $\text{rank}(BAC) = \text{rank}(A)$ 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) $\text{rank}(A) = \dim \mathcal{C}(A)$; (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 $A \in \mathbb{R}^{m \times n}$: $\text{tr}(A) = \sum_{i=1}^n a_{ii}$. Facts: (i) linearity: $\text{tr}(A+B) = \text{tr}(A) + \text{tr}(B)$, $\text{tr}(cA) = c\text{tr}(A)$; (ii) cyclic property: $\text{tr}(AB) = \text{tr}(BA)$, $\text{tr}(ABC) = \text{tr}(BCA) = \text{tr}(CAB)$; (iii) $\text{tr}(A) = \sum_{i=1}^n \lambda_i a_{ij} b_{ij}$.
- Trace product: $\langle A, B \rangle = \text{tr}(A^T B) = \text{tr}(AB^T) = \sum_i \sum_j a_{ij} b_{ij}$. It induces Frobenius norm: $\|A\|_F = \sqrt{\langle A, A \rangle} = (\sum_{i,j} a_{ij}^2)^{1/2}$.
- 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 ($V^T V = V V^T = I$) and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$. (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 $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0)$, $\sigma_1 \geq \dots \geq \sigma_r \geq 0$ and $\{u_i\}, \{v_i\}$ orthonormal. $\arg \min_{Y \in \mathbb{R}^{n \times p}, \text{rank}(Y) \leq r} \|X - Y\|_F = \sum_{i=1}^r \sigma_i u_i v_i^T$ (low rank- r approximation). (3) QR decomposition: $A = QR$ where Q is orthonormal and R is upper-triangular. It corresponds to Gram-Schmidt orthogonalization process.
- Idempotent: $P^2 = P$. Facts: (i) If P is symmetric, then P is idempotent of rank r iff it has r eigenvalues 1 and $n - r$ 0; (ii) If P is a projection matrix, then $\text{tr}(P) = \text{rank}(P)$.
- 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 $A^+ = V\Sigma^+U^T = \sum_{i=1}^r \sigma_i^{-1} v_i u_i^T$.
- **Theorem 1.1** $P_X = X(X^T X)^- X^T$ is the orthogonal projection onto $\mathcal{C}(X)$. [P_X does not depend on the choice of $(X^T X)^-$]

Proof $\forall v \in \mathbb{R}^n$, write $v = x + w$ where $x \in \mathcal{C}(X), w \in \mathcal{C}(X)^\perp$. 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 $\mathcal{C}(X^T) = \mathcal{C}(X^T X)$.

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

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: $M_X(t) = \mathbb{E}e^{t^T X} = \exp(t^T \mu + \frac{1}{2} t^T \Sigma t)$. Characteristic function: $\phi_X(t) = \mathbb{E}e^{it^T X} = \exp(it^T \mu - \frac{1}{2} t^T \Sigma t)$. Facts: (i) $A_{g \times p} X + b_{g \times 1} \sim \mathcal{N}_g(A\mu + b, A\Sigma A^T)$; (ii) $X \sim \mathcal{N}_p(\mu, \Sigma) \Leftrightarrow a^T X \sim \mathcal{N}(a^T \mu, a^T \Sigma a), \forall a \in \mathbb{R}^p$; (iii) $Y_1 = A_1 X + b_1 \perp\!\!\!\perp Y_2 = A_2 X + b_2 \Leftrightarrow \text{Cov}(Y_1, Y_2) = A_1 \Sigma A_2^T = 0$.
- Noncentral χ^2 : $X \sim \mathcal{N}_p(\mu, I_p)$. Then $X^T X \sim \chi_p^2(\lambda)$ with noncentral 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 $\text{Poisson}(\frac{\lambda}{2})$ -weighted mixture of χ_{p+2k}^2 . M.g.f.: $M_X(t; p, \lambda) = \frac{1}{(1-2it)^{p/2}} \exp(\frac{\lambda t}{1-2it})$. Ch.f.: $\Phi_X(t; p, \lambda) = \frac{1}{(1-2it)^{p/2}} \exp(\frac{i\lambda t}{1-2it})$. Facts: (i)

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 $Q_i \sim \chi_{r_i}^2(\lambda_i)$ 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 $X^T X = X^T C \Delta C X$, where Δ is $p \times p$ diagonal with diagonal entries $\pm 1 \Rightarrow C^T \Delta C = I_p$. Thus C is of full rank and hence $\Delta = (C^T)^{-1} C^{-1} = (C^{-1})^T C^{-1} = (C^{-1})^T C^{-1}$ is positive definite $\Rightarrow \Delta = I_p$ and $C^T C = I_p$.

“ \Rightarrow ”: $X^T A_i \sim \chi_{r_i}^2(\lambda_i)$ independent $\Rightarrow X^T X = \sum_i X^T A_i X \sim \chi_{\sum_i r_i}^2(\sum_i \lambda_i) \Rightarrow \sum_i r_i = p$. \square

- 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 $f: \mathcal{X} \rightarrow \mathcal{Y}$ that minimizes $\mathbb{E}_{X,Y} \mathcal{L}(f(X), Y) = \mathbb{E}\{\mathbb{E}(\mathcal{L}(f(X), Y) | X)\}$ where loss function $\mathcal{L}: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$.
- 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 $\mathcal{L}(\hat{y}, y) = I(\hat{y} \neq y)$, $\mathbb{E}\{\mathcal{L}(h(X), Y) | X = x\} = \sum_{j \neq h(x)} P(Y = j | X = x) = 1 - P(Y = h(X) | X = x)$. 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: $h_{k\text{-NN}}(x) = \text{majority label among } \{y_i, i \in N_k(x)\}$. Regression: $m_{k\text{-NN}}(x) = \frac{1}{k} \sum_{i \in N_k(x)} y_i$. 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 $\mathbb{E}_{S \sim \mathcal{D}^n} \mathcal{L}(\hat{h}_S) \leq 2\mathcal{L}(h^*) + c \mathbb{E}_{S \sim \mathcal{D}^n, x \sim \mathcal{D}} \|x - x_{\pi_1}(x)\|$.

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 $\mathcal{L}(h^*) = \mathbb{E}_x \{\eta(x) \wedge (1 - \eta(x))\} \geq \mathbb{E}_x (\eta(x)(1 - \eta(x)))$. \square

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

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

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 $\|x - x'\| \leq \sqrt{d}\epsilon$.

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

Hence, $\mathbb{E}_{S,x} \|x - x_{\pi_1(x)}\| \leq \mathbb{E}_S \{P(\cup_{i: C_i \cap S \neq \emptyset} C_i) \sqrt{d}\epsilon + P(\cup_{i: C_i \cap S = \emptyset} C_i) \sqrt{d}\} \leq \sqrt{d}(\epsilon + \frac{r}{ne})$. Since $r = (\frac{1}{\epsilon})^d, \dots \leq \sqrt{d}(\epsilon + \frac{1}{\epsilon^d ne})$. Matching the two terms gives $\epsilon = (\frac{1}{ne})^{\frac{1}{d+1}}$ and the optimal bound $2\sqrt{d}(ne)^{-\frac{1}{d+1}} \leq 2\sqrt{dn}^{-\frac{1}{d+1}}$. \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 c -Lipschitz, the Bayes error is 0, but for $n < (c+1)^d/2$, $\mathbb{E} \mathcal{L}(h) > \frac{1}{4}$ (i.e. minimax bound $\inf_h \sup_y \mathbb{E} \mathcal{L}(h) \geq Cn^{-\frac{1}{d+1}}$).

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

- **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

- $Y_{n \times 1} = X_{n \times p} \beta_{p \times 1} + \epsilon_{n \times 1}$, $\mathbb{E}(\epsilon|X) = 0$, $\text{Var}(\epsilon) = \sigma^2 I_n$ and X fixed.
- Least squares estimator (LSE) solves the normal equation $X^T X \hat{\beta} = X^T Y$, $\hat{\beta} = (X^T X)^{-1} X^T Y$.
- 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. $\mathbb{E}(l^T Y) = c^T \beta$, $\forall \beta \in \mathbb{R}^p \Leftrightarrow c = X^T l \in \mathcal{C}(X^T)$.
- **Theorem 4.1** (1) If $c^T \hat{\beta}$ is unique, then $c \in \mathcal{C}(X^T X) = \mathcal{C}(X^T)$.
 (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 $b \in \mathcal{C}(X^T X)^\perp$ be arbitrary, then $X^T Y = X^T X \hat{\beta} = X^T X(\hat{\beta} + b) \Rightarrow c^T \hat{\beta} = c^T(\hat{\beta} + b) \Rightarrow c^T b = 0$.
 (2) $c = X^T l$ for some $l \in \mathbb{R}^n$, then $c^T \hat{\beta} = l^T X \hat{\beta} = l^T X(X^T X)^{-1} X^T Y = l^T P_X Y$ is unique. $\mathbb{E}(c^T \hat{\beta}) = l^T P_X \mathbb{E} Y = l^T P_X X \beta = l^T X \beta = c^T \beta$.

(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 , $c = X^T \int \frac{y - X\beta}{(2\pi\sigma^2)^{\frac{n}{2}} \sigma^2} T(X, y) \exp\{-\frac{1}{2\sigma^2} \|y - X\beta\|^2\} dy$. \square

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: $\hat{\beta} = (X^T X)^{-1} X^T Y$.
- **Proposition 4.1** For any estimable $A\beta$ and $B\beta$, $\text{Cov}(A\hat{\beta}, B\hat{\beta}) = \sigma^2 A(X^T X)^{-1} B^T$, $\text{Var}(A\hat{\beta}) = \sigma^2 A(X^T X)^{-1} A^T$.

Proof $\exists A_*$ and B_* s.t. $A = A_* X, B = B_* X$. Since $\hat{Y} = X\hat{\beta} = X(X^T X)^{-1} X^T Y = P_X Y$, we have $\text{Var}(\hat{Y}) = P_X \text{Var}(Y) P_X^T = \sigma^2 P_X$. Hence $\text{Cov}(A\hat{\beta}, B\hat{\beta}) = \text{Cov}(A_* \hat{Y}, B_* \hat{Y}) = A_* \text{Var}(\hat{Y}) B_*^T = \sigma^2 A_* P_X B_*^T = A(X^T X)^{-1} B^T$. \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 $l^T Y$ be an unbiased estimator of $c^T \beta$. Hence, $c = X^T l$, so that $c^T \hat{\beta} = l^T X \hat{\beta} = l^T \hat{Y}$. Thus, $\text{Var}(l^T Y) - \text{Var}(c^T \hat{\beta}) = l^T [\text{Var}(Y) - \text{Var}(\hat{Y})] l = \sigma^2 l^T (I - P_X) l \geq 0$. \square

- Residual $\hat{\epsilon} = Y - \hat{Y} = (I - P_X)Y \in \mathcal{C}(X)^\perp$, $\mathbb{E}\hat{\epsilon} = (I - P_X)\mathbb{E}Y = (I - P_X)X\beta = 0$, $\text{Var}(\hat{\epsilon}) = \sigma^2(I - P_X)^2 = \sigma^2(I - P_X)$, $\text{Cov}(\hat{\epsilon}, \hat{Y}) = \text{Cov}((I - P_X)Y, P_X Y) = (I - P_X)(\sigma^2 I)P_X = 0$.
- Residual sum of squares (RSS): $\|\hat{\epsilon}\|^2 = \hat{\epsilon}^T \hat{\epsilon} = Y^T (I - P_X) Y$. $\mathbb{E}(\text{RSS}) = \mathbb{E}\text{tr}(\hat{\epsilon}\hat{\epsilon}^T) = \text{tr}(\mathbb{E}(\hat{\epsilon}\hat{\epsilon}^T)) = \text{tr}\{(I - P_X)\sigma^2\} = \sigma^2(n - \text{rank}(X))$. $\hat{\sigma}^2 = \frac{\text{RSS}}{n-r}$ is an unbiased estimator of σ^2 .
- Restricted LSE: $Y = X\beta + \epsilon$, $\mathbb{E}\epsilon = 0$, $\text{Var}(\epsilon) = \sigma^2 I$, $\text{rank}(X) = r$, $X = \begin{pmatrix} X_1 & X_2 \end{pmatrix}$, $\beta = \begin{pmatrix} \beta_1^T & \beta_2^T \end{pmatrix}^T$. $H_0 : \beta_2 = \beta_2^*$ vs $\beta_2 \neq \beta_2^*$. β_2 is estimable $\Rightarrow \text{rank}(X_2) = s$, $\text{rank}(X_1) = r - s$ and $\mathcal{C}(X_1) \cap \mathcal{C}(X_2) = \{0\}$.

Proof $\exists C \in \mathbb{R}^{q \times n}$ s.t. $(0_{s \times (p-s)}, I_s) = CX = (CX_1, CX_2)$. Hence $\text{rank}(X_2) = s$ and $\text{rank}(X_1) = r - s$. If $X_1 b_1 = X_2 b_2$ then $b_2 = CX_1 b_1 = 0$. \square

- 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: $X_1^T X_1 \tilde{\beta}_1 = X_1^T (Y - X_2 \beta_2^*)$. $\mathcal{C}(X_1) \subset \mathcal{C}(X) \Rightarrow P_{X_1} P_X = P_{X_1}$. Since $P_X Y = \hat{Y} = X \hat{\beta} = X_1 \hat{\beta}_1 + X_2 \hat{\beta}_2$, 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 value 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** $\mathcal{C}(Z_2) = \mathcal{C}(X_1)^\perp \cap \mathcal{C}(X)$, 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 $X = X_1 b_1 + X_2 b_2 \in \mathcal{C}(X)$ and $X \perp \mathcal{C}(X_1)$, then $X = (I - P_{X_1}) X = (I - P_{X_1}) X_2 b_2 \in \mathcal{C}(Z_2)$. \square

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

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

- 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, $s = \text{rank}(H) \leq \text{rank}(X) = r \leq p$.
- 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 $\mathcal{C}(\tilde{X}^T) = \mathcal{C}((A, H)^{-1}X^T) \supset \mathcal{C}((A, H)^{-1}H) = \mathcal{C}\left(\begin{pmatrix} 0 \\ I_s \end{pmatrix}\right)$, θ_2 is estimable. $\hat{\theta}$ solves the normal equation $\tilde{X}^T \tilde{X} \hat{\theta} = \tilde{X}^T Y$. Under H_0 , $\tilde{Y} = \tilde{X}_1 \tilde{\theta}_1 + \tilde{X}_2 \xi = \tilde{X}_1 \hat{\theta}_1 + P_{\tilde{X}_1} \tilde{X}_2 (\hat{\theta}_2 - \xi) + \tilde{X}_2 \xi$, $\text{RSS}_{H_0} - \text{RSS} = \|Y - \tilde{Y}\|^2 - \|Y - \hat{Y}\|^2 = \|\hat{Y} - \tilde{Y}\|^2 = \sigma^2 (\hat{\theta}_2 - \xi)^T \text{Var}(\hat{\theta}_2)^{-1} (\hat{\theta}_2 - \xi)$. Substituting into the original model, $\hat{\theta}_2 = H^T \hat{\beta}$, $\text{Var}(\hat{\theta}_2) = \sigma^2 H^T (X^T X)^{-1} H$. 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 be 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 $D = H^T (X^T X)^{-1} H$ and $\hat{\sigma}^2 = \frac{\text{RSS}}{n-r}$. Under H_0 , (1) $s = 1$: $Z = \frac{\hat{\gamma} - \gamma_0}{\hat{\sigma} \sqrt{D}} \sim \mathcal{N}(0, 1)$ 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 $\|\hat{\gamma} - \gamma_0\|_{(\sigma^2 D)^{-1}} = \sqrt{(\hat{\gamma} - \gamma_0)^T (\sigma^2 D)^{-1} (\hat{\gamma} - \gamma_0)}$, $\|\hat{\gamma} - \gamma_0\|_{(\sigma^2 D)^{-1}}^2 = (\hat{\gamma} - \gamma_0)^T (\sigma^2 D)^{-1} (\hat{\gamma} - \gamma_0) \sim \chi_s^2(\lambda)$ 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 $\frac{(\hat{\gamma} - \gamma_0)^T D^{-1} (\hat{\gamma} - \gamma_0)}{s \hat{\sigma}^2} = \frac{\|\hat{Y} - \tilde{Y}\|^2 / s}{\|Y - \hat{Y}\|^2 / (n-r)} \sim F_{s, n-r}(\lambda)$, where $\lambda = 0$ iff H_0 is true.
- Multiple testing: Simultaneous confidence intervals of level $1 - \alpha$.
- Bonferroni: Replace α by α/m : $P(E_j) = 1 - \alpha_j, j = 1, \dots, m$, then $P(\cap_j E_j) = 1 - P(\cup_j E_j^c) \geq 1 - \sum_j P(E_j) = 1 - \sum_j \alpha_j = 1 - \alpha$.
- Scheffé's method: Consider $Y = X\beta + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2 I_n), \text{rank}(X) = r$ 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. $\hat{\gamma} = H^T \hat{\beta} \sim \mathcal{N}_s(\gamma, \sigma^2 D)$ where $D = H^T (X^T X)^{-1} H$, $\hat{\sigma}^2 = \frac{\text{RSS}}{n-r} \sim \sigma^2 \chi_{n-r}^2$. For any fixed $u \in \mathbb{R}^s$, an $(1 - \alpha)$ 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 $\sup_{u \neq 0} \frac{|u^T \hat{\gamma} - u^T \gamma|^2}{u^T D u} \stackrel{v=D^{-\frac{1}{2}}u}{=} \sup_{v \neq 0} \frac{|v^T D^{-\frac{1}{2}}(\hat{\gamma} - \gamma)|^2}{v^T v} \stackrel{\text{Cauchy-Schwarz}}{=} (\hat{\gamma} - \gamma)^T D^{-1} (\hat{\gamma} - \gamma)$, $P(\sup_{u \neq 0} \frac{|u^T \hat{\gamma} - u^T \gamma|^2}{s \hat{\sigma}^2 u^T D u} \leq F_{s, n-r, \alpha}) = 1 - \alpha$. Simultaneous CIs for $u^T \gamma, \forall u \in \mathbb{R}^s$: $u^T \hat{\gamma} \pm \hat{\sigma} \sqrt{s F_{s, n-r, \alpha} u^T D u}$. (Bonferroni: $t_{n-r, \alpha/(2m)}$)
- 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 $\frac{\sqrt{m}}{\hat{\sigma}} \max_{i, i'} \{\bar{y}_i - \bar{y}_{i'} - (\alpha_i - \alpha_{i'})\} = \frac{\{\max_i \frac{\sqrt{m}(\bar{y}_i - \mu - \alpha_i)}{\hat{\sigma}} - \min_i \frac{\sqrt{m}(\bar{y}_i - \mu - \alpha_i)}{\hat{\sigma}}\}}{\sqrt{\frac{\text{RSS}/\sigma^2}{n-k}}} \sim q_{k, n-k}$. Simultaneous CIs: $\bar{y}_i - \bar{y}_{i'} \pm \frac{\hat{\sigma}}{\sqrt{m}} q_{k, n-k, \alpha}$. (Bonferroni: $t_{n-k, \alpha/[k(k-1)]}$, Scheffé: $\sqrt{k F_{k, n-k, \alpha}}$, Tukey: $q_{k, n-k, \alpha} / \sqrt{2}$ (the best/shortest length))

5 Exponential Families

- One parameter exponential families: $\mathcal{G} = \{g_\eta(y) = e^{\eta y - \psi(\eta)} g_0(y) d\nu(y), \eta \in A, y \in \mathcal{Y}\}$, 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 , $\psi'(\eta) e^{\psi(\eta)} = \int_Y y e^{\eta y} g_0(y) d\nu(y)$, $[\psi''(\eta) + \psi'(\eta)^2] e^{\psi(\eta)} = \int_Y y^2 e^{\eta y} g_0(y) d\nu(y) \Rightarrow \psi'(\eta) = \mathbb{E}_\eta Y = \mu_\eta, \psi''(\eta) = \mathbb{E}_\eta Y^2 - \mu_\eta^2 = \text{Var}_\eta(Y) = V_\eta$.

- Cumulants: Let $\kappa_j, j = 1, 2, \dots$ satisfy $\psi(\eta) - \psi(\eta_0) = \kappa_1(\eta - \eta_0) + \frac{\kappa_2}{2}(\eta - \eta_0)^2 + \frac{\kappa_3}{3!}(\eta - \eta_0)^3 + \dots$. $\psi'''(\eta_0) = \kappa_3 = \mathbb{E}_0(Y - \mu_0)^3$, $\psi''''(\eta_0) = \kappa_4 = \mathbb{E}_0(Y - \mu_0)^4 - 3\kappa_2^2$. They correspond to central/noncentral moments. Skewness(偏度): $\gamma = \frac{\kappa_3}{\kappa_2^{3/2}} = \frac{\mathbb{E}(Y - \mathbb{E}Y)^3}{(\text{Var}(Y))^{3/2}}$. Kurtosis(峰度): $\delta = \frac{\kappa_4}{\kappa_2^2} = \frac{\mathbb{E}(Y - \mathbb{E}Y)^4}{(\text{Var}(Y))^2} - 3$.
- 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: $\psi = e^\eta = \mu, \phi' = \dots = \phi'''' = \mu, y \sim [\mu, \sqrt{\mu}, 1/\sqrt{\mu}, 1/\mu]$.
- **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: $l'_\eta(y) = 0 \Rightarrow \mu_{\hat{\eta}} = \bar{y}$. 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 , $\text{Var}(\bar{\xi}) \geq \frac{1}{I_\mu^{(n)}(\xi)} = \frac{(h'(\eta))^2}{nV_\eta}$. In particular, $\xi = \mu$, then $\text{Var}(\hat{\mu}) \geq \frac{V_\eta}{n}$.
- 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: $g_\eta(y) = C_N^y \pi^y (1-\pi)^{N-y} = C_N^y e^{y \log \pi + (N-y) \log(1-\pi)}, y = 0, 1, \dots, N, \eta = \log \frac{\pi}{1-\pi}, \pi = \frac{1}{1+e^{-\eta}} = \frac{e^\eta}{1+e^\eta}, \psi(\eta) = N \log(1+e^\eta)$; (3) Gamma(k, θ)(shape, scale), $\chi_k^2 = \text{Gamma}(k/2, 2)$; (4) Negative Binomial: $\text{NB}(k, \theta) = \# \text{ tails until } k\text{th head}$. $g_\eta(y) = C_{y+k-1}^{k-1} (1-\theta)^y \theta^k = C_{y+k-1}^{k-1} e^{y \log(1-\theta) + k \log \theta}, y = 0, 1, 2, \dots, \theta \in (0, 1), \eta = \log(1-\theta), \psi(\eta) = k \log(1-e^\eta), \mu = k \frac{1-e^\eta}{\theta}, V = \frac{\mu}{\theta}$ (property: $k \rightarrow \infty, \mu$ fixed, $Y \rightarrow \text{Poisson}(\mu)$).
- Inverse Gaussian: $W(t)$: Wiener process with drift $1/\mu$. $W(t) = \frac{1}{\mu}t + B(t)$ and $W(t) \sim \mathcal{N}(t/\mu, t)$, $\text{Cov}(W(t), W(t+s)) = t$. $Y = 1\text{st passage time to } W(t) = 1$. Density of $\text{IG}(\mu)$: $g(y) = \frac{1}{\sqrt{2\pi y^3}} \exp\{-\frac{(y-\mu)^2}{2\mu^2 y}\} = \frac{1}{\sqrt{2\pi y^3}} \exp(-\frac{y}{2\mu^2} + \frac{1}{\mu} - \frac{1}{2y})$ 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	N

- Deviance (Kullback-Leibler divergence): Generating Euclidean distance to exponential families, $2\text{KL}(\eta_1, \eta_2) = D(\eta_1, \eta_2) := 2 \int \eta_1(y) \log \frac{\eta_1(y)}{\eta_2(y)} d\nu(y) = 2\mathbb{E}_{\eta_1}[(\eta_1 - \eta_2)y - (\psi(\eta_1) - \psi(\eta_2))] = 2[(\eta_1 - \eta_2)\mu_1 - (\psi(\eta_1) - \psi(\eta_2))]$. Mutual 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 $\frac{g_\eta(y)}{g_{\hat{\eta}}(y)} = e^{(\eta - \hat{\eta})y - (\psi(\eta) - \psi(\hat{\eta}))} \stackrel{y \equiv \hat{\mu}}{=} e^{-D(\hat{\eta}, \eta)/2}.$ □

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

Proof $\frac{\partial}{\partial \eta_2} D(\eta_1, \eta_2) = \frac{\partial}{\partial \eta_2} 2[(\eta_1 - \eta_2)\mu_1 - (\psi(\eta_1) - \psi(\eta_2))] = 2(-\mu_1 + \mu_2) \Rightarrow \frac{\partial}{\partial \eta_2} D(\eta_1, \eta_2)|_{\eta_2=\eta_1} = 0.$ $\frac{\partial^2}{\partial \eta_2^2} D(\eta_1, \eta_2) = 2\frac{\partial \mu_2}{\partial \eta_2} \Rightarrow \frac{\partial^2}{\partial \eta_2^2} D(\eta_1, \eta_2)|_{\eta_2=\eta_1} = 2V_{\eta_1}.$ 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 $y - \mu$: $\text{sgn}(y - \mu)\sqrt{D(y, \mu)}$. Let $y_i \sim g_\mu(\cdot)$ i.i.d. for $i = 1, \dots, n$. Define the deviance residual $R = \text{sgn}(\bar{y} - \mu)\sqrt{nD(\bar{y}, \mu)} = \text{sgn}(\bar{y} - \mu)\sqrt{D^{(n)}(\bar{y}, \mu)}$. 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 $b_n = \frac{7/36 \gamma_\mu^2 - \delta_\mu}{n}$ (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, $P(\frac{R + a_n}{1 + b_n} > z_\alpha) = \alpha + O(n^{-3/2})$.

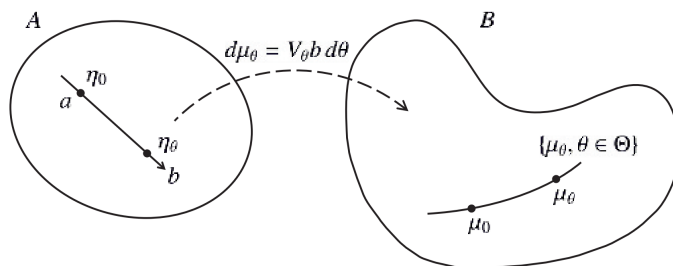
Corollary 5.1 $D^{(n)}(\bar{y}, \mu) = R^2 \sim (1 + \frac{5\gamma_\mu^2 - 3\delta_\mu}{12n})\chi_1^2.$

- 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 $\mathcal{N}(0, 1)$, $R = \text{sgn}(\hat{\mu} - \mu)\sqrt{nD(\hat{\mu}, \mu)}$ 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 $\mu, H'(\mu) = V_\mu^{\delta-1}, 0 \leq \delta \leq 1.$

$\delta =$	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), $H'(\mu) = \mu^{-1/2}, H(\mu) = 2\sqrt{\mu}, 2\sqrt{\bar{y}} \sim \mathcal{N}(2\sqrt{\mu}, 1)$; (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 $\mathcal{G} = \{g_\eta(y) : \eta \in A \subset \mathbb{R}^p, y \in \mathcal{Y} \subset \mathbb{R}^p\}$ with $g_\eta(y) = e^{\eta^T y - \psi(\eta)} g_0(y) d\nu(y), \mu = \mathbb{E}_\eta Y = \psi'(\eta), V = \text{Var}_\eta(Y) = \psi''(\eta), d\mu = V d\eta, d\eta = V^{-1} d\mu.$ 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 $H'(\mu) = Dh'(\eta), H''(\mu) = Dh''(\eta)D^T + D_2 h'(\eta)$ where $D_2 = (\frac{\partial^2 \eta_k}{\partial \mu_i \partial \mu_j})_{i,j,k}.$
- One-parameter subfamilies: $\eta_\theta = a + b\theta, \theta \in \Theta \subset \mathbb{R}, a, b \in \mathbb{R}^p, \mathcal{F} = \{f_\theta(y) = g_{\eta_\theta}(y) = e^{(a+b\theta)^T y - \psi(a+b\theta)} g_0(y) d\nu, \theta \in \Theta\}.$ Still a one-parameter exponential family, natural parameter θ , sufficient statistics $x = b^T y$. MLE of θ (score equation): $l'_\theta(\bar{y}) = 0 \Rightarrow b^T(\bar{y} - \mu_\theta) = 0.$



- 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 \mathcal{G} at $\eta = \eta_0$, which equals $t'_0 V_0 t_0$, 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(α, β) : $g(x) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha, \beta)} = \exp\{\alpha \log x + \beta \log(1-x) - \log B(\alpha, \beta)\}$, $\eta = (\alpha, \beta)^T$, $y = (\log x, \log(1-x))^T$; (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: $Y_{ij} = I(i=j)$, $\pi_{ij} = P(Y_{ij} = 1) = \frac{e^{\theta_i + \theta_j}}{1 + e^{\theta_i + \theta_j}}$, $\theta_i = \beta^T x_i$ where x_i 's are optional predictors. Sufficient statistics is degree of node i . (5) Bradley-Terry model: $\pi_{ij} = \frac{e^{\theta_i}}{e^{\theta_i} + e^{\theta_j}} = \frac{e^{\theta_i - \theta_j}}{1 + e^{\theta_i - \theta_j}}$, $w_{ij} \sim \text{Binomial}(n_{ij}, \pi_{ij})$, $g_\theta \propto \exp(\sum_{i,j} (\theta_i - \theta_j) w_{ij}) = \exp(\sum_i \theta_i \sum_j w_{ij} - \sum_j \theta_j \sum_i w_{ij}) = \exp\{\sum_i \theta_i [\#\text{win}(i) - \#\text{lose}(i)]\}$.
- 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: $g_\eta(y|\mathcal{Y}_0) = \frac{e^{\eta^T y - \psi(\eta)} g_0(y)}{G_\eta(\mathcal{Y}_0)}$, where $G_\eta(\mathcal{Y}_0) = \int_{\mathcal{Y}_0} g_\eta(y) dy$.
- **Lemma 5.2** Partition $\eta = (\eta_1, \eta_2)$, $y = (y_1, y_2)$. $y_1|y_2 \sim g_{\eta_1}(y_1|y_2) = e^{\eta_1^T y_1 - \psi(\eta_1|\eta_2)} dG_0(y_1|y_2)$, $y_2 \sim g_{\eta_1, \eta_2}(y_2) = e^{\eta_2^T y_2 - \psi_{\eta_1}(\eta_2)} dG_{\eta_1, 0}(y_2)$.

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

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

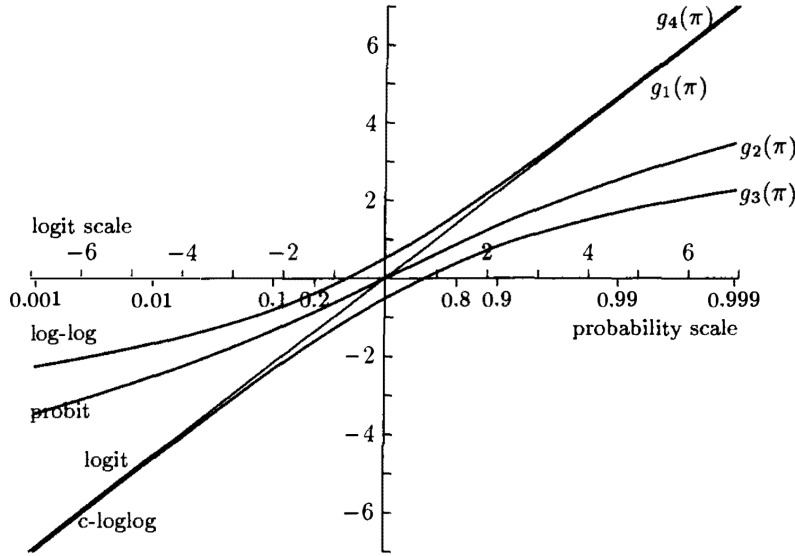
- Examples: (1) Fisher's exact test for 2×2 table (Recall Table 1), $H_0 : \theta = \log(\frac{\pi_1/\pi_2}{\pi_3/\pi_4}) = 0$. The natural parameter is $\eta = (\log \pi_1, \dots, \log \pi_4)$. Let $(M^{-1})^T = \begin{pmatrix} 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$, so that $M = \frac{1}{4}(M^{-1})^T$, $\tilde{y} = Mx$, $\tilde{y}_1 = \frac{1}{4}(x_1 - x_2 - x_3 + x_4) = x_1 - \frac{r_1}{2} - \frac{c_1}{2} + \frac{N}{4}$. (2) Wishart statistics: $x_1, \dots, x_n \sim \mathcal{N}_d(\lambda, \Gamma)$ independent, $y_1 = \bar{x}$, $y_2 = \frac{1}{n} \sum_{i=1}^n x_i x_i^T$. Wishart statistics $W = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(x_i - \bar{x})^T = y_2 - y_1 y_1^T$. $y_2|y_1$ is in a $\frac{d(d+1)}{2}$ -dim exponential family. (3) Poisson trick: $s = (s_1, \dots, s_L)$, $s_l \sim \text{Poisson}(\mu_L)$ independent $\Rightarrow s|n = \sum_{l=1}^L s_l \sim \text{Multinomial}_L(n, \pi)$ where $\pi_l = \frac{\mu_l}{\sum_j \mu_j}$. Conversely, if $s|n \sim \text{Multinomial}(n, \pi)$ and $n \sim \text{Poisson}(\mu_+)$, then $s_l \sim \text{Poisson}(\mu_+ \pi_l)$ 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 for $\phi(x) : \phi_1(x) = 2xe^{-x^2}$, $\phi_2(x) = 4x^2 e^{-x^2} \pi^{-1/2}$. 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

6.1 Basic Concepts

- Data types for response y :
$$\left\{ \begin{array}{l} \text{numerical:} \left\{ \begin{array}{l} \text{continuous: Box-Cox transformation: } \left\{ \begin{array}{ll} \frac{x^\lambda - 1}{\lambda}, & \lambda \neq 0 \\ \log x, & \lambda = 0 \end{array} \right. \\ \text{discrete: count} \end{array} \right. \\ \text{categorical:} \left\{ \begin{array}{l} \text{nominal:} \left\{ \begin{array}{l} \text{binary} \\ \text{multinomial} \end{array} \right. \\ \text{ordinal} \end{array} \right. \end{array} \right.$$
- 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 dilution $\rho_x = \rho_0 2^{-x}$, $x = 0, 1, 2, \dots$, proportion of infected plates $y_x = \frac{r_x}{m_x}$, $Y = I(\text{infected})$, $\mathbb{E}(Y|x) = P(Y = 1|x) = \pi_x$, # organism on a plate: $N_x \sim \text{Poisson}(\rho_x v)$, $\pi_x = P(N_x \geq 1) = 1 - e^{-\rho_x v} = 1 - e^{-\rho_0 v 2^{-x}}$, 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) Logistic/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: $l(\theta; y) = \frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi)$. $\frac{\partial l}{\partial \theta} = \frac{y - b'(\theta)}{a(\phi)}$, $\frac{\partial^2 l}{\partial \theta^2} = -\frac{b''(\theta)}{a(\phi)}$. $\mathbb{E} \frac{\partial l}{\partial \theta} = 0$, $\mathbb{E}(\frac{\partial l}{\partial \theta})^2 = -\mathbb{E} \frac{\partial^2 l}{\partial \theta^2}$, $\mathbb{E}Y = \mu = b'(\theta)$, $\text{Var}(Y) = a(\phi)b''(\theta)$.
- 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 observation. 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, $\chi^2/\phi \sim \chi_{n-p}^2$.
- Residuals: (1) Deviance residual: $r_D = \text{sgn}(y - \hat{\mu})\sqrt{d_i}$ 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, $l = \sum_{i=1}^n l_i$, $l_i = \frac{y_i \theta_i - b(\theta_i)}{a_i(\phi)} + c_i(y_i, \phi)$, and $u_{ir} = \frac{\partial l_i}{\partial \beta_r} = \frac{\partial l_i}{\partial \theta_i} \frac{\partial \theta_i}{\partial \mu_i} \frac{\partial \mu_i}{\partial \beta_r} \frac{\partial \eta_i}{\partial \beta_r} = \frac{y_i - \mu_i}{a_i(\phi)} \frac{1}{V(\mu_i)} \frac{1}{g'(\mu_i)} x_{ir} = \frac{(y_i - \mu_i)x_{ir}}{a_i(\phi)V(\mu_i)g'(\mu_i)} = (y - \mu)^T W \frac{d\eta}{d\mu} x_{(r)}$ where $W = \text{diag}(\frac{1}{a_i(\phi)V(\mu_i)g'(\mu_i)^2})$. Since $\text{Cov}(u_r, u_s) = \sum_{i=1}^n \frac{\text{Var}(y_i)x_{ir}x_{is}}{a_i(\phi)^2 V(\mu_i)^2 g'(\mu_i)^2} = \sum_{i=1}^n \frac{x_{ir}x_{is}}{a_i(\phi)V(\mu_i)g'(\mu_i)^2} \Rightarrow I(\beta) = \text{Var}(u(\beta)) = X^T W X$, $u(\beta) = X^T W \frac{d\eta}{d\mu} (y - \mu)$ 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 $\eta_i = b^{-1}(\mu_i) = \theta_i$, $V(\mu_i) = b''(\theta_i) = \frac{\partial \mu_i}{\partial \theta_i} = \frac{\partial \mu_i}{\partial \eta_i}$, $w_{ii} = \frac{1}{a_i(\phi)V(\mu_i)g'(\mu_i)^2} = \frac{1}{a_i(\phi)\frac{\partial \eta_i}{\partial \mu_i}} \Rightarrow W \frac{d\eta}{d\mu} = \text{diag}(\frac{1}{a_i(\phi)}) \Rightarrow \frac{\partial}{\partial \beta^T} (W \frac{d\eta}{d\mu}) = 0$.
- 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).
- Inference about β : $I(\beta)^{\frac{1}{2}}(\hat{\beta} - \beta) \Rightarrow \mathcal{N}_p(0, I)$, $\widehat{\text{Var}}(\hat{\beta}) = (X^T W(\hat{\beta}) X)^{-1}$, $h(\hat{\beta}) \sim \mathcal{N}(h(\beta), h'(\beta)^T I(\beta)^{-1} h'(\beta))$, $\hat{\eta} = x^T \hat{\beta} \sim \mathcal{N}(x^T \beta, x^T I(\beta)^{-1} x)$.
- CI for x that gives rise to a specified mean response μ_0 : $\{x : \frac{x^T \hat{\beta} - g(\mu_0)}{\sqrt{x^T I(\hat{\beta})^{-1} x}} < z_{\alpha/2}\}$ (Fieller's method).
- Binary responses: $g(\pi_i) = \eta_i = x_i^T \beta$, $g : (0, 1) \rightarrow \mathbb{R}$, link functions: $g_1 = \log(\frac{\pi}{1-\pi})$, $g_2 = \Phi^{-1}(\pi)$, $g_3 = \log(-\log(1-\pi))$ (complementary log-log), $g_4 = \log(-\log \pi)$ (log-log). These g_i 's are from the inverse of the cdfs: $f_1 = \frac{e^x}{(1+e^x)^2}$ (logistic), $f_3 = e^{x-e^x}$, i.e. $\log X, X \sim \text{Exp}(1)$, $f_4 = e^{-x+e^x}$, i.e. $-\log X, X \sim \text{Exp}(1)$ (Gumbel).



- Application: Many epidemiological studies have the goal of comparing distinct groups, e.g., assessing risk factors for some disease. Denote D = disease status, X = exposure status.

	\bar{D}	D	
\bar{X}	π_{00}	π_{01}	$\pi_{0\cdot}$
X	π_{10}	π_{11}	$\pi_{1\cdot}$
	$\pi_{\cdot 0}$	$\pi_{\cdot 1}$	1

Sampling probabilities: $P(D|x) = \frac{e^{\alpha+x^T \beta}}{1+e^{\alpha+x^T \beta}}$, $\pi_0 = P(Z=1|D)$, $\pi_1 = P(Z=1|\bar{D})$ where Z is indicator of being sampled. This is because $|D|$ may be much smaller than $|\bar{D}|$ and we need more data on D (i.e. $\pi_0 \gg \pi_1$). Then $P(D|Z=1, x) = \frac{P(Z=1|D, x)P(D|x)}{P(Z=1|D, x)P(D|x) + P(Z=1|\bar{D}, x)P(\bar{D}|x)} = \frac{\pi_0 e^{\alpha+x^T \beta}}{\pi_0 e^{\alpha+x^T \beta} + \pi_1 (1-e^{\alpha+x^T \beta})} = \frac{e^{\alpha+x^T \beta + \log(\pi_0/\pi_1)}}{1+e^{\alpha+x^T \beta + \log(\pi_0/\pi_1)}} := \frac{e^{\alpha^*+x^T \beta}}{1+e^{\alpha^*+x^T \beta}}$ by Bayes formula. Thus, the “biased” random sampling of D and \bar{D} does not impact the value of β , and only translates α to $\alpha + \log(\pi_0/\pi_1)$. We can conduct logistic regression on the new dataset.

6.2 Binomial Regression

- $Y_i \sim \text{Binomial}(m_i, \pi_i)$, $i = 1, \dots, n$. For simplicity, $m_i = m, \forall i$. The log-likelihood $l(\pi; y) = \sum_{i=1}^n [y_i \log \frac{\pi_i}{1-\pi_i} + m \log(1-\pi_i)] + C(y)$. Under logistic link, $\log \frac{\pi_i}{1-\pi_i} = x_i^T \beta$, or $\pi_i = \frac{e^{x_i^T \beta}}{1+e^{x_i^T \beta}}$, so that $l(\beta; y) = \sum_{i=1}^n [y_i x_i^T \beta - m \log(1+e^{x_i^T \beta})]$. Exponential family has the form $l(\theta; y) = \sum_{i=1}^n [\frac{y_i \theta_i - b(\theta_i)}{a_i(\phi)} + c(y_i, \phi)]$, so $\eta_i = \theta_i = x_i^T \beta$, $b(\theta_i) =$

$m \log(1 + e^{x_i^T \beta})$, $a_i(\phi) \equiv 1$. General likelihood equation $u(\beta) = X^T W \frac{d\eta}{d\mu}(y - \mu) = 0$ where $W \frac{d\eta}{d\mu} = \text{diag}(\frac{1}{a_i(\phi)})$ under canonical link. Now $a_i(\phi) \equiv 1$, so $u(\beta) = X^T(y - \mu) = 0$. The weight matrix $W = \frac{d\mu}{d\eta} = m \frac{d\pi}{d\eta} = \text{diag}\{m\pi_i(1 - \pi_i)\}$. The working response $z_i = \eta_i + \frac{d\eta_i}{d\mu_i}(y_i - \mu_i) = \eta_i + \frac{y_i - m_i\pi_i}{m_i} \frac{d\eta_i}{d\pi_i} = \eta_i + \frac{y_i - m_i\pi_i}{m_i\pi_i(1 - \pi_i)}$. Solve $X^T W X \hat{\beta} = X^T W Z$.

- **Theorem 6.1** (Wedderburn, 1976) If the link function is log concave and $0 < y_i < m_i, \forall i$, then $\hat{\beta}$ is finite and the log-likelihood has a unique maximum at $\hat{\beta}$.
- **Theorem 6.2** (Shao, Ex 4.117) For logistic regression, if $\sum_{i=1}^n x_i x_i^T$ is positive definite, $\forall n \geq n_0$, then the log-likelihood equation has at most one solution when $n \geq n_0$ and a solution exists with probability $\rightarrow 1$.
- Deviance: The fitted log-likelihood $l(\hat{\pi}; y) = \sum_{i=1}^n [y_i \log(\frac{\hat{\pi}_i}{1 - \hat{\pi}_i}) + m_i \log(1 - \hat{\pi}_i)] = \sum_{i=1}^n [y_i \log \hat{\pi}_i + (m_i - y_i) \log(1 - \hat{\pi}_i)]$, maximum achievable log-likelihood $l(\tilde{\pi}; y)$ where $\tilde{\pi}_i = \frac{y_i}{m_i}$, $D(y, \hat{\pi}) = 2l(\tilde{\pi}; y) - 2l(\hat{\pi}; y) = 2 \sum_{i=1}^n [y_i \log(\frac{y_i}{\hat{\pi}_i}) + (m_i - y_i) \log(\frac{m_i - y_i}{m_i - \hat{\pi}_i})]$. Asymptotic properties: $D(y, \hat{\pi}) \sim \chi_{n-p}^2$ (assumptions: no overdispersion; $m_i \rightarrow \infty$ with n fixed). Note that if $n \rightarrow \infty$ while m_i fixed, D is not independent of $\hat{\pi}$ and large $D \nrightarrow$ poor fit.
- Extrapolation: predict x_0 corresponding to π_0 . Using Fieller's method, $|\frac{\hat{\beta}_0 + \hat{\beta}_1 x_0 - g(\pi_0)}{V(x_0)}| \leq Z_{\alpha/2}$ where $V(x_0)^2 = \text{Var}(\hat{\beta}_0) + 2x_0 \text{Cov}(\hat{\beta}_0, \hat{\beta}_1) + x_0^2 \text{Var}(\hat{\beta}_1)$.
- Overdispersion: “nominal” variance: $m\pi(1 - \pi)$. $\text{Var}(y) > / < m\pi(1 - \pi)$: over/under dispersion. Mechanism: clustering is the population. Assume m subjects from m/k clusters, each of size k . $Z_i \sim \text{Binomial}(k, \pi_i)$ and $Y = Z_1 + \dots + Z_{m/k}$. If $\mathbb{E}\pi_i = \pi$ and $\text{Var}(\pi_i) = \tau^2\pi(1 - \pi)$, then $\mathbb{E}Y = \mathbb{E}(\mathbb{E}(Y|\pi)) = \mathbb{E}[k(\pi_1 + \dots + \pi_{m/k})] = m\pi$, $\text{Var}(Y) = \mathbb{E}[\text{Var}(Y|\pi)] + \text{Var}[\mathbb{E}(Y|\pi)] = m\pi(1 - \pi)(1 - \tau^2) + m\tau^2\pi(1 - \pi) = m\pi(1 - \pi)[1 + (k - 1)\tau^2]$. Since $0 \leq \tau^2 \leq 1$ ($\text{Var}(\pi_i) = \mathbb{E}\pi_i^2 - \pi^2 \leq \mathbb{E}\pi_i - \pi^2 = \pi(1 - \pi)$), $1 \leq \sigma^2 := 1 + (k - 1)\tau^2 \leq k \leq m$.
- Estimation of σ^2 with overdispersion: Case 1 (with replication): For the same x -value, observe $(y_1, m_1), \dots, (y_r, m_r)$, $\tilde{\pi} = \frac{\sum_{i=1}^r y_i}{\sum_{i=1}^r m_i}$, $\mathbb{E}[\sum_{j=1}^r \frac{(y_j - m_j \tilde{\pi})^2}{m_j}] = (r - 1)\sigma^2\pi(1 - \pi)$, $\hat{\sigma}^2 = \frac{1}{r - 1} \sum_{j=1}^r \frac{(y_j - m_j \tilde{\pi})^2}{m_j \tilde{\pi}(1 - \tilde{\pi})}$ approximately unbiased for σ^2 . Case 2 (without replication): Using the fitted $\hat{\pi}_i$, $\hat{\sigma}^2 = \frac{1}{n - p} \sum_{i=1}^n \frac{(y_i - m_i \hat{\pi}_i)^2}{m_i \hat{\pi}_i(1 - \hat{\pi}_i)} \sim \chi_{n-p}^2$, $\text{Var}(\hat{\beta}) \approx \hat{\sigma}^2 (X^T W X)^{-1}$.

6.3 Poisson Regression

- $Y \sim$ counts of events that occur over a period of time or a region at a constant rate. log-link: $\log \mu_i = \eta_i = x_i^T \beta$. Nominal variance $\text{Var}(y_i) = \mu_i$. More generally, let $\text{Var}(y_i) = \sigma^2 \mu_i$. Over/Under dispersion: $\sigma^2 > / < 1$.
- Mechanism for overdispersion: clustered Poisson process. $Y = Z_1 + \dots + Z_N$, Z_i i.i.d., $N \sim \text{Poisson}$ independent of Z_i . $\mathbb{E}Y = \mathbb{E}N\mathbb{E}Z$, $\text{Var}(Y) = \mathbb{E}[\text{Var}(Y|N)] + \text{Var}(\mathbb{E}(Y|N)) = \mathbb{E}N\text{Var}(Z) + \text{Var}(N)(\mathbb{E}Z)^2 = \mathbb{E}N\mathbb{E}Z^2 (> \mathbb{E}Y$ if $\mathbb{E}Z^2 > \mathbb{E}Z$). Estimation of σ^2 : $\hat{\sigma}^2 = \frac{1}{n - p} \sum_{i=1}^n \frac{(y_i - \hat{\mu}_i)^2}{\hat{\mu}_i}$.

6.4 Gamma Regression

- Motivation: $\text{Var}(Y) = \text{Const} - \text{linear}$; $\text{Var}(Y) \propto \mathbb{E}Y - \text{Poisson}$; $\text{Var}(Y) \propto (\mathbb{E}Y)^2 - \text{Gamma}$. $\sigma := \frac{\sqrt{\text{Var}(Y)}}{\mathbb{E}Y} = \text{const}$: coefficient of variance.
- Mechanism: (1) Multiplicative error: $Y = \mu(1 + \epsilon)$, $\mathbb{E}\epsilon = 0$, $\text{Var}(\epsilon) = \sigma^2$, $\mathbb{E}Y = \mu$, $\text{Var}(Y) = \mu^2 \sigma^2$. (2) log-transformed additive: $\log Y = \mu + \epsilon$, $\mathbb{E}\epsilon = 0$, $\text{Var}(\epsilon) = \sigma^2$, $Y = e^\mu e^\epsilon$, $\mathbb{E}Y = e^\mu \mathbb{E}(e^\epsilon)$, $\text{Var}(Y) = e^{2\mu} \text{Var}(e^\epsilon)$, $\frac{\text{Var}(Y)}{(\mathbb{E}Y)^2} = \frac{\text{Var}(e^\epsilon)}{(\mathbb{E}e^\epsilon)^2} \approx \frac{\text{Var}(1 + \epsilon)}{(1 + \mathbb{E}\epsilon)^2} = \text{Var}(\epsilon) = \sigma^2$.
- Parameterization of gamma: Gamma(k, θ) pdf $\frac{1}{\Gamma(k)\theta^k} y^{k-1} e^{-y/\theta} dy I(y > 0)$, $\mathbb{E}Y = k\theta$, $\text{Var}(Y) = k\theta^2$, $\sigma^2 = \frac{1}{k}$; Gamma(μ, ν) pdf $\frac{1}{\Gamma(\nu)} (\frac{\nu y}{\mu})^\nu e^{-\nu y/\mu} d(\log y) I(y > 0)$.
- Choice of link function: (1) Canonical link $g(\mu) = \frac{1}{\mu}$. Example: Plants density experiments: x density, yield per plant $\propto \frac{1}{\beta_0 x + \beta_1}$, yield per unit area $\propto \frac{x}{\beta_0 x + \beta_1}$, $\mu = \eta^{-1} = \frac{x}{\beta_0 + \beta_1}$ or $\eta = \beta_0 + \frac{\beta_1}{x}$. (2) log link: $\eta = \log \mu = x^T \beta$. (3) identity link: $\eta = \mu = x^T \beta$.

- Estimation of σ^2 : $\nu = \frac{1}{\sigma^2}$, $D(y, \hat{\mu}) = 2n[\log \hat{\nu} - \frac{\Gamma'(\hat{\nu})}{\Gamma(\hat{\nu})}]$.
- Example (Rainfall data): Daily rainfall skewed to the right with a spike around 0. Two stages: (1) wet/dry day: Markov chain and logistic; (2) rainfall on wet days: gamma/log-normal. Stage 1: $\pi_0(t) = P(\text{day } t \text{ is wet} | \text{day } t-1 \text{ is wet})$, $\pi_1(t) = P(\text{day } t \text{ is wet} | \text{day } t-1 \text{ is dry})$. logistic model: $\text{logit}(\pi_i(t)) = \alpha_i + \alpha_{i,1} \sin(\frac{2\pi t}{365}) + \beta_{i,1} \cos(\frac{2\pi t}{365})$. Stage 2: $\log(\mu(t)) = \text{const} + \text{harmonic terms}$ where $\mu(t)$ is mean rainfall on day t | wet day.

6.5 Categorical Data and Multinomial Regression

- Types of measurement scales: $\begin{cases} \text{nominal: exchangeable} \\ \text{ordinal: ordered but no measure of distance} \\ \text{interval: numerical scores} \\ \text{cardinal: counts} \end{cases}$
- Ordinal: Response probabilities: π_1, \dots, π_k ; cumulative probabilities: $\gamma_j = \sum_{i=1}^j \pi_i, j = 1, 2, \dots, k-1, \gamma_k \equiv 1$. Principle: Inferences should not essentially change by combining adjacent categories. Proportional odds model: $\log(\frac{\gamma_j(x)}{1-\gamma_j(x)}) = \theta_j - \beta^T x, j = 1, 2, \dots, k-1$ (parallel regressions), $\frac{\text{odds}(Y \leq j | x_1)}{\text{odds}(Y \leq j | x_2)} = e^{-\beta^T(x_1 - x_2)}$. Why “-”? Latent variable interpretation: $Z \sim \text{logistic}(\beta^T x, 1), Z - \beta^T x \sim \text{logistic}(0, 1)$. Let $Y = j$ whenever $\theta_{j-1} < Z \leq \theta_j$. Then $P(Y \leq j) = P(Z \leq \theta_j) = P(Z - \beta^T x \leq \theta_j - \beta^T x) = \frac{e^{\theta_j - \beta^T x}}{1 + e^{\theta_j - \beta^T x}}$. Extensions: (1) Nonparallel: $\text{logit}(\gamma_j(x)) = \theta_j - \beta_j^T x$; (2) Scale modeling: $\text{logit}(\gamma_j(x)) = \frac{\theta_j - \beta^T x}{e^{\tau^T x}}$.
- Interval: Features: (1) The categories are of interest in themselves and are not chosen arbitrarily; (2) It does not normally make sense to form a new category by amalgamating adjacent categories; (3) difference between scores s_j is a measure of distance. Modeling strategies: (1) Extend proportional odds model: $\theta_j = \xi_0 + \xi_1(\frac{s_j + s_{j+1}}{2})$ and replace $\beta^T x$ by $\beta^T x + \xi^T x(c_j - \bar{c}), c_j = \frac{s_j + s_{j+1}}{2}$ or $\text{logit}(\frac{s_j + s_{j+1}}{2})$; (2) Model log-probabilities: $\eta_{ij} = \log \pi_j(x_i), \pi_j(x_i) = \frac{e^{\eta_{ij}}}{\sum_j e^{\eta_{ij}}}, \eta_j(x_i) = \eta_j + \alpha_i$ or $\eta_j(x_i) = \eta_j + (\beta^T x_i)s_j + \alpha_i, \frac{\pi_j}{\pi_{j'}} \nearrow$ by a factor $e^{s_j - s_{j'}}$ with a unit change in $\beta^T x$; (3) Model the scores $\mathbb{E}(S | x_i) = \sum_{j=1}^k \pi_j(x_i)s_j = \beta^T x_i$.
- Nominal: model π_j or η_j : e.g. $\eta_j(x_i) = \eta_j(x_0) + \beta_j^T(x_i - x_0) + \alpha_i$.
- Multinomial: Data $(y_1, \dots, y_n), y_i = (y_{i1}, \dots, y_{ik}), \sum_j y_{ij} = m_i$ fixed, parameters $\pi_i, i = 1, \dots, n, \pi_i = (\pi_{i1}, \dots, \pi_{ik})$ s.t. $\sum_j \pi_{ij} = 1$. Log-likelihood: $l(\pi, y) = \sum_{i,j} y_{ij} \log \pi_{ij}$. Use the method of Lagrange multipliers $\Rightarrow \mathcal{L}_\lambda(\pi, y) = \sum_{i,j} y_{ij} \log \pi_{ij} - \sum_i \lambda_i (\sum_j \pi_{ij} - 1), \frac{\partial \mathcal{L}}{\partial \pi_{ij}} = \frac{y_{ij}}{\pi_{ij}} - \lambda_i = 0 \Rightarrow m_i = \lambda_i \Rightarrow \pi_{ij} = \frac{y_{ij}}{m_i}$. Let $\Sigma_i = m \{\text{diag}(\pi_i) - \pi_i \pi_i^T\}$ (rank $k-1$) and $\Sigma_i^- = \text{diag}(\frac{1}{m \pi_{ij}})$. In matrix form, $\frac{\partial \mathcal{L}}{\partial \pi} = M \Sigma^- (y - \mu) = 0$ where $\Sigma = \text{diag}(\Sigma_1, \dots, \Sigma_n)$ of rank $n(k-1)$ and $M = \text{diag}(\underbrace{m_1, \dots, m_1}_{k \text{ times}}, \dots, \underbrace{m_n, \dots, m_n}_{k \text{ times}})$. Full score equation w.r.t. β_r : $\frac{\partial l}{\partial \pi_{ij}} \frac{\partial \pi_{ij}}{\partial \beta_r} = 0$. GLMs: (1) log-linear: $\log \pi_{ij} = x_{ij}^T \beta^*$; (2) prop odds: $\text{logit}(\gamma_{ij}) = x_{ij}^T \beta^*$ (γ_{ij} : cumulative probability). Overdispersion: $\mathbb{E}Y = m\pi, \text{Var}(Y) = \sigma^2 \Sigma, \hat{\sigma}^2 = \frac{X^2}{\text{residual d.f.} = n(k-1) - p}$ where X^2 is Pearson's statistic.

6.6 Quasi-Likelihood Estimation

- For a GLM, the inference depends on the assumed distribution for y_i only through the mean μ_i and the variance function $V(\cdot)$. In addition, a GLM specifies the independence of observations, which is not indispensable.
- More generally, suppose $\text{Var}(y) = \sigma^2 V(\mu)$. Independent: $V(\mu) = \text{diag}\{V_1(\mu), \dots, V_n(\mu)\} = \{V_1(\mu_1), \dots, V_n(\mu_n)\}$. Dependent: $V(\mu)$ nondiagonal. Quasi-score function: $u(\beta) = D^T V^{-1}(y - \mu) / \sigma^2$ where $D = \frac{\partial \mu}{\partial \beta^T} = (\frac{\partial \mu_i}{\partial \beta_r})_{n \times p}$. Facts: $\mathbb{E}u(\beta) = 0, \text{Var}(\beta) = D^T V^{-1} D / \sigma^2, \frac{\partial}{\partial \beta^T} u(\beta) = \frac{1}{\sigma^2} [\frac{\partial}{\partial \beta^T} (D^T V^{-1})(y - \mu) - D^T V^{-1} D], \mathbb{E}[\frac{\partial}{\partial \beta^T} u(\beta)] = -D^T V^{-1} D / \sigma^2$. Quasi-information matrix: $I(\beta) = \text{Var}(u(\beta)) = -\mathbb{E} \frac{\partial}{\partial \beta^T} u(\beta) = D^T V^{-1} D / \sigma^2$.

- Independent: $\frac{\partial u(\beta)}{\partial \beta^T}$ diagonal. Dependent: $\frac{\partial u_r(\beta)}{\partial \beta_s} \neq \frac{\partial u_s(\beta)}{\partial \beta_r}$ in general. Thm: symmetric $\frac{\partial u(\beta)}{\partial \beta^T} \Leftrightarrow$ the line integral (quasi-log-likelihood) $Q(\mu; \gamma, \gamma(s)) = \frac{1}{\sigma^2} \int_{s_0}^{s_1} (y - \gamma)^T V(\gamma)^{-1} d\vec{\gamma}(s)$ along a path $\gamma : [s_0, s_1] \rightarrow \mathbb{R}^n$ from $\gamma(s_0) = y$ to $\gamma(s_1) = \mu$ is path-independent. Independent: $Q(\mu, y) = \sum_{i=1}^n Q_i(\mu_i, y_i) = \sum_{i=1}^n \int_{y_i}^{\mu_i} \frac{y_i - t}{\sigma^2 V_i(t)} dt$, quasi-deviance: $D(y, \mu) = 2[Q(y, y) - Q(\mu, y)]\sigma^2 = 2 \sum_{i=1}^n \int_{\mu_i}^{y_i} \frac{y_i - t}{V_i(t)} dt$. Dependent: Solve $\sigma^2 u(\beta) = D^T V^{-1}(y - \mu) = 0$ (GEE).
- Fisher-scoring: $\beta^{(t+1)} = \beta^{(t)} + I(\beta^{(t)})^{-1} u(\beta^{(t)}) = \beta^{(t)} + [D(\beta^{(t)}) V(\beta^{(t)})^{-1} D(\beta^{(t)})]^{-1} D(\beta^{(t)})^T V(\beta^{(t)})^{-1} (y - \mu(\beta^{(t)})) = (X^T W^{(t)} X)^{-1} X^T W^{(t)} Z^{(t)}$ where $Z^{(t)} = X \beta^{(t)} + \frac{d\eta}{d\mu}|_{\mu(\beta^{(t)})} (y - \mu(\beta^{(t)}))$ and $W^{(t)} = (\frac{d\eta}{d\mu}|_{\mu(\beta^{(t)})})^{-1} V(\beta^{(t)})^{-1} (\frac{d\eta}{d\mu}|_{\mu(\beta^{(t)})})^{-1}$.
- Asymptotics: Under regularity conditions, $\hat{\beta}$ is consistent and asymptotic normal with variance $\text{Var}(\hat{\beta}) = I(\beta)^{-1} = \sigma^2 (D^T V^{-1} D)^{-1}$.
- Optimality: Estimating function $G(\beta; y)$ if $\mathbb{E}G(\beta; y) = 0, \forall \beta$. Linear estimating function $h(\beta) = H^T (y - \mu(\beta))$. Let $\tilde{\beta}$ solve $h(\beta) = 0$. Taylor expansion $\Rightarrow 0 = h(\tilde{\beta}) = h(\beta) + [\frac{\partial H^T}{\partial \beta} (y - \mu(\beta)) - H^T D](\tilde{\beta} - \beta)$. Take expectations $\Rightarrow 0 = h(\beta) - H^T D(\tilde{\beta} - \beta) \Rightarrow \tilde{\beta} \approx \beta + (H^T D)^{-1} h(\beta)$. Thus, $\mathbb{E}\tilde{\beta} \approx \beta$, $\text{Var}(\tilde{\beta}) \approx (H^T D)^{-1} H^T V H (D^T H)^{-1}$. Since $\text{Var}(\hat{\beta}) = \sigma^2 (D^T V^{-1} D)^{-1}$, $\text{Var}(\hat{\beta})^{-1} - \text{Var}(\tilde{\beta})^{-1} \approx \sigma^{-2} D^T V^{-1} D - \sigma^{-2} D^T H (H^T V H)^{-1} H^T D = \sigma^{-2} D^T V^{-1/2} (I - P_{V^{1/2} H}) V^{-1/2} D \succeq 0 \Rightarrow \text{Var}(\hat{\beta})$ is minimal.

6.7 Longitudinal Data and GLMMs

- Longitudinal study: individuals (subjects) are measured repeatedly over time.
- Questions: (1) average time course of response change; (2) degree of heterogeneity across individuals; (3) factors that predict response change.
- Two perspectives: (1) Marginal/population-averaged: linear, normal, $\mathbb{E}Y_{ij} = \beta_0 + \beta_1 t_{ij}$; (2) Subject-specific: $Y_{ij} = \beta_{0i} + \beta_{1i} t_{ij} + \epsilon_{ij}$, $\beta_i = \beta + b_i$, $\mathbb{E}b_i = 0 \Rightarrow \mathbb{E}(Y_{ij}|b_i) = \beta_0 + b_{0i} + (\beta_1 + b_{1i}) t_{ij}$, $\mathbb{E}Y_{ij} = \beta_0 + \beta_1 t_{ij}$.
- GLMMs: $Y_{ij}|b_i = f_{y_{ij}|b_i}(y_{ij}|b_i) = \exp\{\frac{y_{ij}\theta_{ij} - \psi(\theta_{ij})}{\phi} + c(y_{ij}, \phi)\}$ i.i.d., $\mathbb{E}(Y_{ij}|b_i) = \mu_i = \psi'(\theta_{ij})$, $\text{Var}(Y_{ij}|b_i) = \phi\psi''(\theta_{ij})$, $g(\mu_{ij}) = \eta_{ij} = x_{ij}^T \beta + z_{ij}^T b_i$. Typically $b_i \sim \mathcal{N}(0, D)$.
- Mean of Y_{ij} : $\mathbb{E}Y_{ij} = \mathbb{E}[\mathbb{E}(Y_{ij}|b_i)] = \mathbb{E}\mu_{ij} = \mathbb{E}[g^{-1}(x_{ij}^T \beta + z_{ij}^T b_i)]$. Example: $g(\mu) = \log \mu$, $h(\mu) = g^{-1}(\mu) = e^\mu$, $z_{ij} \equiv 1$, $b_i \sim \mathcal{N}(0, \sigma_b^2)$. Then $\mathbb{E}Y_{ij} = e^{x_{ij}^T \beta} e^{\sigma_b^2/2}$.
- Variance of Y_{ij} : $\text{Var}(Y_{ij}) = \text{Var}[\mathbb{E}(Y_{ij}|b_i)] + \mathbb{E}[\text{Var}(Y_{ij}|b_i)] = \text{Var}(\mu_{ij}) + \mathbb{E}[\phi V(\mu_{ij})] = \text{Var}[g^{-1}(x_{ij}^T \beta + z_{ij}^T b_i)] + \mathbb{E}[\phi V(g^{-1}(x_{ij}^T \beta + z_{ij}^T b_i))]$. Example (cont'd): $Y_{ij}|b_i \sim \text{Poisson}(\mu_{ij})$, so that $\mathbb{E}(Y_{ij}|b_i) = \text{Var}(Y_{ij}|b_i) = \mu_{ij}$. Then $\text{Var}(Y_{ij}) = \text{Var}(\mu_{ij}) + \mathbb{E}\mu_{ij}$. Still assume $b_i \sim \mathcal{N}(0, \sigma_b^2)$. Then $\text{Var}(Y_{ij}) = \text{Var}(e^{x_{ij}^T \beta + b_i}) + \mathbb{E}(e^{x_{ij}^T \beta + b_i}) = e^{2x_{ij}^T \beta} (e^{2\sigma_b^2} - e^{\sigma_b^2}) + e^{x_{ij}^T \beta} e^{\sigma_b^2/2} = e^{x_{ij}^T \beta + \sigma_b^2/2} [e^{x_{ij}^T \beta} e^{\sigma_b^2/2} (e^{\sigma_b^2} - 1) + 1] > \mathbb{E}Y_{ij}$ (overdispersed).
- Estimation of GLMMs: (1) Maximum likelihood: log-likelihood $l(\beta, D) = \log \prod_{i=1}^N \int \varphi(b_i; 0, D) \prod_{j=1}^{n_i} f(y_{ij}|b_i) db_i$, or more generally, $\log \int \prod_{i,j} f_{y_{ij}|b_i}(y_{ij}|b_i) f_{b_i}(b_i) db_i$. Let $b_i = Qv_i$, where $v_i \sim \mathcal{N}_q(0, I_q)$ and $D = QQ^T$ (Cholesky decomposition), then $l(\beta, D) = \log \prod_i \int_{\mathbb{R}} \phi(v_{i1}) \cdots \int_{\mathbb{R}} \phi(v_{i1}) \prod_j f(y_{ij}|v_i) dv_i$. Approximate 1-D integral by Gauss-Hermite quadrature: $\int_{\mathbb{R}} e^{-u^2} f(u) du \approx \sum_{k=1}^K w_k f(u_k)$ where u_k are roots of Hermite polynomials $H_k(u)$ and $w_k = \frac{2^{k-1} k! \sqrt{\pi}}{k^2 (H_{k-1}(u_k))^2}$. Back to our integral, $\int_{\mathbb{R}} \phi(v_{i1}) \prod_j f(y_{ij}|v_i) dv_{i1} \approx \sum_k \frac{w_k}{\sqrt{\pi}} \prod_j f(y_{ij}|(\sqrt{2}u_k, v_{i2}, \dots, v_{iq}))$. Adaptive GH: For simplicity, $\int_{\mathbb{R}} \phi(v_i) \prod_j f(y_{ij}|v_i) dv_i \propto$ posterior density of $v_i|y_{ij}$. Approximate $f(v_i|y_{ij})$ by $\phi(v_i; \mu_i, \tau_i^2)$ and write $\int_{\mathbb{R}} \varphi(v_i; \mu_i, \tau_i^2) [\frac{\phi(v_i) \prod_j f(y_{ij}|v_i)}{\varphi(v_i; \mu_i, \tau_i^2)}] dv_i \approx w_{ik} \prod_j f(y_{ij}|u_{ik})$. u_{ik} and w_{ik} are subject-specific, $u_{ik} = \mu_i + \tau_i u_k$, $w_{ik} = \sqrt{2\pi} \tau_i e^{u_k^2/2} \phi(\mu_i + \tau_i u_k) w_k$. (2) Quasi-likelihood: Similar to IRLS, use current estimates $(\beta^k, D^k, V^k, b_i^k)$ to linearize the model for y_{ij} : $y_{ij} \approx h(\eta_{ij}^k) + x_{ij}^T (\beta - \beta^k) h'(\eta_{ij}^k) + z_{ij}^T (b_i - b_i^k) h'(\eta_{ij}^k) + \epsilon_{ij}$ where $\text{Var}(\epsilon_{ij}) = \phi V(\mu_{ij}^k)$. Let the offset $o_{ij} = h(\eta_{ij}^k) - h'(\eta_{ij}^k) x_{ij}^T \beta^k - h'(\eta_{ij}^k) z_{ij}^T b_i^k$, total residual $\xi_{ij} = h'(\eta_{ij}^k) z_{ij}^T b_i + \epsilon_{ij} \Rightarrow y_{ij} = o_{ij} + h'(\eta_{ij}^k) x_{ij}^T \beta + \xi_{ij}$ (just an OLS).
- Prediction of random effects $b_i \sim \mathcal{N}(0, D)$: posterior $f(b_i|y_i, \beta, D, \phi) = \frac{f(y_i|\beta, D, \phi) f(b_i|D)}{\int f(y_i|\beta, D, \phi) f(b_i|D) db_i}$, estimate b_i by MAP.

- Marginal/Population-average models: Idea: specify only the mean and variance structure of Y_{ij} rather than the full likelihood.
- Generalized Estimating Eqs (GEE): (1) Mean response: $\mu_{ij} = \mathbb{E}Y_{ij} = h(x_{ij}^T\beta)$; (2) Variance: $\text{Var}(Y_{ij}) = \phi V(\mu_{ij})$; (3) Within subject correlation structure, $\Gamma_i \in \mathbb{R}^{n_i \times n_i}$ correlation matrix for subject i , $\Sigma_i = \text{Var}(Y_{ij}) = \phi T_i^{1/2} \Gamma_i T_i^{1/2}$ where $T_i = \text{diag}(V(\mu_{i1}), \dots, V(\mu_{in_i}))$. “Working correlation structure”: $G_i = G_i(\alpha)$ so that working covariance $S_i = \phi T_i^{1/2} G_i T_i^{1/2}$. Choice of G_i may effect efficiency but not consistency. Solve $u(\beta) = \sum_{i=1}^N D_i^T \Sigma_i^{-1} (y_i - \mu_i(\beta)) = 0$ where $D = \frac{\partial \mu_i}{\partial \beta^T} \in \mathbb{R}^{n_i \times p}$. Possible choices of G_i : (1) Unsturctured: $G_i = (\rho_{ik})$,

parameters $\frac{n_i(n_i-1)}{2}$; (2) Independence: $G_i = I_{n_i}$; (3) Exchangeable: $G_i = \begin{pmatrix} 1 & \rho & \cdots & \rho \\ \rho & 1 & \cdots & \rho \\ \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \cdots & 1 \end{pmatrix}$; (4) AR(1):

$$G_i = \begin{pmatrix} 1 & \rho & \cdots & \rho^{n_i-1} \\ \rho & 1 & \cdots & \vdots \\ \vdots & \vdots & \ddots & \rho \\ \rho^{n_i-1} & \cdots & \rho & 1 \end{pmatrix}; \text{ (5) Continuous AR(1) (spatial): } G_i = \begin{pmatrix} 1 & \cdots & \rho^{|t_j-t_k|} \\ & \ddots & \vdots \\ & & 1 \end{pmatrix}.$$

- Estimation of $\beta, \text{Var}(\hat{\beta}), \phi, \alpha, \Sigma_i$: Find $\hat{\phi}$ and $\hat{\alpha}$: Let $r_{ij} = \frac{y_{ij} - \mu_{ij}(\hat{\beta})}{V(\mu_{ij}(\hat{\beta}))^{1/2}}$, then $\hat{\phi} = \frac{1}{n-p} \sum_{i=1}^N \sum_{j=1}^{n_i} r_{ij}^2$ and $\hat{\rho}_{jk} = \frac{\frac{1}{N\hat{\phi}} \sum_{i=1}^N r_{ij} r_{ik}}{\frac{1}{N\hat{\phi}} \sum_{i=1}^N \frac{1}{n_i-1} \sum_{j=1}^{n_i-1} r_{ij} r_{i,j+1}}$ (corresponds to G_i 's in the above (1) and (3)).
- Iterative procedure: Step 1: Initialize β_0 (acquired by assuming complete independence). Repeat until convergence: Step 2: Given β , estimate ϕ and α for the working correlation structure; Step 3: Use current estimates of β, ϕ and $\hat{\alpha}$ to form $\hat{\Sigma}_i$ and solve GEE for a new $\hat{\beta}$.
- Inference: $\hat{\beta} \sim \mathcal{N}_p(\beta, V(\hat{\beta}))$ for n large where $V(\hat{\beta}) = \phi(\sum_{i=1}^n D_i^T S_i^{-1} D_i)$.
- Robust covariance estimation: In general, G_i are misspecified, then

$$\hat{V}_{\hat{\beta}}^{\text{robust}} = \hat{\phi} \left(\sum_{i=1}^N \hat{D}_i^T \hat{S}_i^{-1} \hat{D}_i \right)^{-1} \left(\sum_{i=1}^N \hat{D}_i^T \hat{S}_i^{-1} \hat{C}_i \hat{S}_i \hat{D}_i \right) \left(\sum_{i=1}^N \hat{D}_i^T \hat{S}_i^{-1} \hat{D}_i \right)^{-1}$$

where $\hat{C}_i = (y_i - \mu_i(\hat{\beta}))(y_i - \mu_i(\hat{\beta}))^T$. (“sandwich estimator”)

7 Nonparametric Statistics

- Nonparametric models: (1) Kernel smoothing (local polynomial regression); (2) Splines (e.g. B-splines): smoothing splines (+penalty), # knots = n ; regression splines, # knots $\ll n$; (3) Orthogonal series expansion; (4) Wavelets; (5) Sharp-constrained: isotonic, log-concavity.
- Model: $Y = r(X) + \epsilon_i, r(x) = \mathbb{E}(Y|X = x)$. Linear smoothers: $\hat{r}_n(x) = \sum_{i=1}^n l_i(x) y_i, (\hat{r}_n(x_1), \dots, \hat{r}_n(x_n))^T := \hat{r} = LY, L = (l_j(x_i))_{ij}$, effective d.f. $v = \text{rank}(L), \sum_{i=1}^n l_i(x) = 1$. Example: (1) Histogram regression: $\hat{r}_n(x) = \frac{1}{k_j} \sum_{i: x_i \in B_j} y_i = \sum_{i=1}^n l_i(x) y_i$, where $l(x) = (0, \dots, 0, 1/k_j, \dots, 1/k_j, 0, \dots, 0)^T$; (2) Local average: Let $B_x = \{i : |x_i - x| \leq h\}, \hat{r}_n(x) = \frac{1}{n} \sum_{i \in B_x} y_i$.
- Leave-one-out CV: $\hat{R}(h) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{r}^{(-i)}(x_i))^2, R(h) = \mathbb{E}[\frac{1}{n} \sum_{i=1}^n (\hat{r}_n(x_i) - r(x_i))^2]$. Linear smoother: $R = \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \hat{r}_n(x_i)}{1 - l_{ii}} \right)^2$. Generalized CV: Replace l_{ii} by v/n .
- Kernel Smoothing: N-W estimator: $\hat{r}_n(x) = \sum_{i=1}^n l_i(x) y_i$ where $l_i(x) = \frac{K(\frac{x-x_i}{h})}{\sum_{j=1}^n K(\frac{x-x_j}{h})}$. $f(x)$ is pdf of x , and MSE $R(\hat{r}_n, r) = \frac{h_n^4}{4} \left(\int x^2 K(x) dx \right)^2 \int \left(r''(x) + 2r'(x) \frac{f'(x)}{f(x)} \right)^2 dx + \frac{\sigma^2 \int K^2(x) dx}{nh_n} \int \frac{1}{f(x)} dx + \dots$ as $h_n \rightarrow 0$ and $nh_n \rightarrow \infty$, optimal $h^* \sim n^{-1/5}, R(\hat{r}_n, r) \sim n^{-4/5}$.

- Local Polynomial/Linear Regression: $\min_c \sum_{i=1}^n w_i(x)(y_i - c)^2$ or $\min \sum_{i=1}^n w_i(x)(y_i - P_x(x_i; c))^2$. N-W boundary bias: $O(h_n)$; LLR: $O(h_n^2)$.
- Smoothing Splines: $\min M(\lambda) = \sum_{i=1}^n (y_i - \hat{r}_n(x_i))^2 + \lambda J(r)$ where $J(r) = \int r''(x)^2 dx$ or $\min \|Y - B\beta\|^2 + \lambda \beta^T \Omega \beta$ where $B_{ij} = B_j(x_i)$, $\Omega_{jk} = \int B_j''(x) B_k''(x) dx$.
- Equivalence between kernel and spline estimators: spline estimator can be expressed by $\hat{r}_n(x) = \sum_{i=1}^n l_i(x) y_i$ with $l_i(x) \approx \frac{1}{f(x_i)h(x_i)} K(\frac{x-x_i}{h(x_i)})$ (e.g. $K(t) = \frac{1}{2} e^{-|t|/2} \sin(\frac{|t|}{\sqrt{2}} + \frac{\pi}{4})$).
- Regression splines: Regress Y_i directly (w/o penalty) on B : $\hat{r} = LY$, $L = B(B^T B)^{-1} B^T$. Tuning parameter: # knots of B .
- Variance estimation: $\hat{\sigma}^2 = \frac{1}{n-2v+\tilde{v}} \sum_{i=1}^n (y_i - \hat{r}(x_i))^2$ with $v = \text{tr}(L)$ and $\tilde{v} = \text{tr}(L^T L) = \sum_{i=1}^n \|l(x_i)\|^2$ (quadratic form: $\hat{\sigma}^2 = \frac{Y^T \Lambda Y}{\text{tr}(\Lambda)}$ and $\Lambda = (I - L)^T (I - L) = I - L - L^T + L^T L$). $\mathbb{E} \hat{\sigma}^2 = \frac{\sigma^2 \text{tr}(\Lambda) + r^T \Lambda r}{\text{tr}(\Lambda)} = \sigma^2 + \frac{r^T \Lambda r}{\text{tr}(\Lambda)}$. If r is sufficiently smooth, $v = o(n)$ and $\tilde{v} = o(n)$, $\hat{\sigma}^2$ is consistent for σ^2 . Another estimator: $\tilde{\sigma}^2 = \frac{1}{2(n-1)} \sum_{i=1}^{n-1} (y_{i+1} - y_i)^2$.
- Heteroscedastic case: $y_i = r(x_i) + \sigma(x_i) \epsilon_i \Rightarrow (y_i - r(x_i))^2 = \sigma^2(x_i) \epsilon_i^2 \Rightarrow Z_i := \log(y_i - r(x_i))^2 = \log \sigma^2(x_i) + \log \epsilon_i^2$. Regress Z_i on x_i using a nonparametric method, denoted as $\hat{q}(x_i)$. Then $\hat{\sigma}^2(x) = e^{\hat{q}(x)}$.
- Confidence bands: $\hat{r}_n(x) \pm c s_n(x)$. $\bar{r}_n(x) = \mathbb{E} \hat{r}_n(x)$, $\frac{\hat{r}_n(x) - r(x)}{s_n(x)} = \frac{\hat{r}_n(x) - \bar{r}_n(x)}{s_n(x)} + \frac{\bar{r}_n(x) - r(x)}{s_n(x)} = \underbrace{Z_n(x)}_{\sim \mathcal{N}(0,1)} + \underbrace{\frac{\text{bias}(\hat{r}_n(x))}{\sqrt{\text{Var}(\hat{r}_n(x))}}}_{\text{smoothing bias}}$.

Remedy: (1) CB for $\bar{r}_n(x)$ rather than $r(x)$; (2) undersmooth. To find c , consider $I(x) = (\hat{r}_n(x) - c\sigma \|l(x)\|, \hat{r}_n(x) + c\sigma \|l(x)\|)$, $x \in [a, b]$. Assume σ is known, then $P(\bar{r}_n(x) \notin I(x) \text{ for some } x \in [a, b]) = P(\sup_x \frac{|\hat{r}_n(x) - \bar{r}_n(x)|}{\sigma \|l(x)\|} > c) = P(\sup_x |\sum_{i=1}^n \frac{l_i(x)}{\|l(x)\|} \frac{\epsilon_i}{\sigma}| > c) := P(\sup_x |W_n(x)| > c)$.

Lemma 7.1 $P(\sup_x |W_n(x)| > c) = 2(1 - \Phi(c)) + \frac{\kappa_0}{\pi} e^{-c^2/2}$ where $\kappa_0 = \int_a^b \|T'(x)\| dx$ and $T_i(x) = \frac{l_i(x)}{\sigma \|l(x)\|}$.

Choose c to solve $2(1 - \Phi(c)) + \frac{\kappa_0}{\pi} e^{-c^2/2} = \alpha$. If σ is unknown, then $P(\sup_x |W_n(x)| > c) \approx P(|T_m| > c) + \frac{\kappa_0}{\pi} (1 + \frac{c^2}{m})^{-m/2}$, $T_m \sim t_m$, $m = n - \text{tr}(L)$. Average coverage: $C = \frac{1}{b-a} \int_a^b P(\bar{r}_n(x) \in I(x)) dx$.

- Local likelihood for nonparametric EM regression: Data (x_i, y_i) , $i = 1, \dots, n$, $y_i \in \{0, 1\}$. $Y_i \sim \text{Bernolli}(r(x_i))$. log-likelihood: $l(r) = \sum_{i=1}^n \log\{r(x_i)^{y_i} (1 - r(x_i))^{1-y_i}\} = \sum_{i=1}^n \{y_i \log \frac{r(x_i)}{1-r(x_i)} + \log(1 - r(x_i))\} := \sum_{i=1}^n l(y_i, \xi(x_i))$ where $\xi(x_i) = \log \frac{r(x_i)}{1-r(x_i)}$. Local linear regression: approximate $\xi(x)$ around x_0 by $a_0 + a_1(x - x_0)$. Local loglik $l_x(a) = \sum_{i=1}^n K(\frac{x-x_i}{h}) l(y_i, a_0 + a_1(x - x_0))$. MLE: $\hat{a}(x) = (\hat{a}_0(x), \hat{a}_1(x)) \Rightarrow \hat{r}_n(x) = \frac{e^{\hat{a}_0(x)}}{1 + e^{\hat{a}_0(x)}}$. Leave-one-out CV: $\text{CV} = \sum_{i=1}^n l(y_i, \hat{\xi}_{(-i)}(x_i))$.
- Multiple nonparametric regression: $y_i = r(x_i) + \epsilon_i$, $x_i = (x_{i1}, \dots, x_{id})^T$. Optimal rate of convergence: $n^{-\frac{2\beta}{2\beta+d}}$.
- Method 1: Local regression: multivariate kernel $K_H(x) = \frac{1}{\det(H)^{1/2}} K(H^{-1/2} X)$ where H is $d \times d$ bandwidth metrix. Univariate kernel: $h^{-d} K(\frac{\|x\|}{h})$. Minimise $\sum_{i=1}^n K(\frac{\|x_i - x\|}{h}) (y_i - a_0 - \sum_{j=1}^d a_j (x_{ij} - \bar{x}_j))^2$ at $x = (x_1, \dots, x_d)^T$. $\hat{a} = (X_x^T W_x X_x)^{-1} X_x^T W_x Y$.
- Method 2: Splines: $d = 2$ thin-plate: $\min_r \sum_{i=1}^n (y_i - r(x_i))^2 + \lambda J(r)$, $J(r) = \iint_{\mathbb{R}^2} (\frac{\partial^2 r(x)}{\partial x_1^2} + 2 \frac{\partial^2 r(x)}{\partial x_1 \partial x_2} + \frac{\partial^2 r(x)}{\partial x_2^2}) dx_1 dx_2$.
- Method 3: Additive model: $y_i = \alpha + \sum_{j=1}^d r_j(x_{ij}) + \epsilon_i$, with $\sum_{i=1}^n r_j(x_{ij}) = 0$. Backfitting algorithm: Set $\hat{\alpha} = \bar{y}$ and initialize $\hat{r}_1, \dots, \hat{r}_d$; Repeat for $j = 1, \dots, d, 1, \dots, d, \dots$ until convergence: $\tilde{y}_i = y_i - \hat{\alpha} - \sum_{k \neq j} r_k(x_{ik})$, $\forall i$; Regress \tilde{y}_i on x_j by a 1-d smoother to set \hat{r}_j ; $\hat{r}_j(x) \leftarrow \hat{r}_j(x) - \frac{1}{n} \sum_i \hat{r}_j(x_i)$.

8 Survival Analysis

- Survival data: Survival/failure time/time-to-event, binary data subject to censoring.

- Examples: (1) Heart transplant. Response: survival time from date of admission. Covariates (might be time-varying): surgery, age, donor/receipient variable. Censoring: drop-out (e.g. withdrawal, loss to follow up, death due to irrelevant reasons). Goal: effect of heart transplant (prediction) on survival. (2) Accelerated life test:

Temp	Hours to Failure
150°C	0 until 8064h
170°C	7 failures + 3 successes
190°C	5 + 5
220°C	5

Question: Failure time distribution at 130°C?

- Censoring type: (1) predetermined time; (2) # failures reached; (3) right/left/interval censoring.
- Survival function for continuous T : $S(t) = P(T > t) = 1 - F(t)$. Hazard function: $\lambda(t) = \lim_{h \rightarrow 0+} \frac{P(t \leq T < t+h | T \geq t)}{h} = \lim_{h \rightarrow 0+} \frac{P(t \leq T < t+h)}{hP(T \geq t)} = \frac{f(t)}{S(t)} = -\frac{d}{dt} \log S(t) \Rightarrow S(t) = \exp(-\int_0^t \lambda(s) ds) := e^{-\Lambda(t)}$ where $\Lambda(t)$ is defined as cumulative hazard function. $f(t) = \lambda(t)e^{-\Lambda(t)}$. Assumption: $\exists t = \int_0^t \lambda(s) ds < \infty$ and $\int_0^\infty \lambda(s) ds = \infty$.

- Independent censoring: censoring time C , at-risk indicator $y(t) = \begin{cases} 1, & \text{at risk} \\ 0, & \text{failed or censored} \end{cases}$, covariates x . Then $\lambda(t) = \lim_{h \rightarrow 0+} \frac{P(T \in [t, t+h] | x, T \geq t)}{h} = \lim_{h \rightarrow 0+} \frac{P(T \in [t, t+h] | x, T \geq t, y(t)=1)}{h} = \lim_{h \rightarrow 0+} \frac{P(T \in [t, t+h] | x, T \geq t, C \geq t)}{h}$.

- Nonparametric estimation of survival function: w/o censoring: $F_n(t) = \frac{\#\{i: T_i \leq t\}}{n}$. How to deal with censoring? At-risk set $R(t) = \{i : y_i(t) = 1\}$. $t_0 = 0, t_{k+1} = \infty, t_1 < \dots < t_k$ from $n = n_0$ subjects. d_j failed at t_j , m_j censored in $[t_j, t_{j+1})$, $n_j = \#$ at risk just prior to t_j and $n_j = \sum_{l=j}^k (d_l + m_l)$. $P(T = t_j) = S(t_{j-}) - S(t_j)$, $P(T > t_{jl}) = S(t_{jl})$. Assume independent censoring, the likelihood $L = \prod_{j=0}^k \{S(t_{j-}) - S(t_j)\}^{d_j} \prod_{l=1}^{m_j} S(t_{jl})$. NPMLE: $\hat{S} = \arg \max_S L(S)$. Facts: (1) discontinuous at all t_j ; (2) $S(t_{jl}) = S(t_j), \forall j, l$. $\hat{S}(t)$ with hazard components $\hat{\lambda}_1, \dots, \hat{\lambda}_k$ at t_1, \dots, t_k , respectively: $\hat{S}(t_j) = \prod_{l=1}^j (1 - \hat{\lambda}_l)$, $\hat{S}(t_{j-}) = \prod_{l=1}^{j-1} (1 - \hat{\lambda}_l)$. To determine the values of λ_j , maximize $L(\lambda) = \prod_{j=1}^k \lambda_j^{d_j} \prod_{l=1}^{j-1} (1 - \lambda_l)^{d_j} \prod_{l=1}^{j-1} (1 - \lambda_l)^{m_j} = \prod_{j=1}^k \lambda_j^{d_j} (1 - \lambda_j)^{n_j - d_j}$. $\frac{\partial}{\partial \lambda_j} \log L(\lambda) = 0 \Rightarrow \hat{\lambda}_j = \frac{d_j}{n_j}$. NPMLE of $S(t) : \hat{S}(t) = \prod_{j:t_j \leq t} \frac{n_j - d_j}{n_j}$ (Kplan-Meier product limit estimator).

- Inference: $\widehat{\text{Var}}(\hat{\lambda}_j) = \frac{\hat{\lambda}_j(1 - \hat{\lambda}_j)}{n_j} = \frac{d_j(n_j - d_j)}{n_j^3}$. For $\log \hat{S}(t) = \sum_{j:t_j \leq t} \log(1 - \hat{\lambda}_j)$, by the delta method, $\widehat{\text{Var}}(\log \hat{S}(t)) = \sum_{j:t_j \leq t} \frac{1}{(1 - \hat{\lambda}_j)^2} \widehat{\text{Var}}(\hat{\lambda}_j) = \sum_{j:t_j \leq t} \frac{d_j}{n_j(n_j - d_j)}$ and $\widehat{\text{Var}}(\hat{S}(t)) = (\hat{S}(t))^2 \sum_{j:t_j \leq t} \frac{d_j}{n_j(n_j - d_j)}$. Hence $\hat{\Lambda}(t) = \int_0^t \hat{\lambda}(s) ds = \sum_{j:t_j \leq t} \hat{\lambda}_j$ (Nelson-Aalen estimator).

- Counting process: $N_i(t) = \#$ failures in $[0, t]$, $y_i(t)$ is at-risk process, and $N(t) = \sum_{i=1}^n N_i(t)$, $y(t) = \sum_{i=1}^n y_i(t)$. Nelson-Aalen: $\hat{\Lambda}(t) = \int_0^t \frac{I(y(u) > 0)}{y(u)} dN(u)$.

- Cox's proportional hazards model: Conditional hazard function $\lambda(t|z) = \lim_{h \rightarrow 0+} \frac{P(t \leq T < t+h | T > t, z)}{h} = \lambda_0(t) e^{z(t)^T \beta} = \lambda_0(t) r(t, z)$. Other forms: (1) additive hazards $\lambda(t|z) = \lambda_0(t) + z(t)^T \beta$; (2) NP/SP Cox: $r(t, z) = \sum_{j=1}^d g_j(z_j(t))$.

- Estimation of β : Partial likelihood: Suppose the information of y is constrained in $A_1, B_1, \dots, A_m, B_m$. The joint density $\prod_{j=1}^m f(b_j | b^{(j-1)}, a^{(j-1)}; \theta, \beta) \prod_{j=1}^m f(a_j | b^{(j)}, a^{(j-1)}; \beta)$. In our case, B_j = censoring information in $[t_{j-1}, t_j]$ + information that 1 individual fails in $[t_j, t_j + dt_j)$ and A_j = individual j fails in $[t_j, t_j + dt_j)$. The j -th failure contributes $L_j(\beta) = f(a_j | b^{(j)}, a^{(j-1)}; \beta) = \frac{\lambda(t_j | z_j) dt_j}{\sum_{l \in R(t_j)} \lambda(t_j | z_l) dt_j} \stackrel{\text{Cox model}}{=} \frac{e^{z_j(t_j)^T \beta}}{\sum_{l \in R(t_j)} e^{z_l(t_j)^T \beta}} \Rightarrow L(\beta) = \prod_{j=1}^n \frac{e^{z_j(t_j)^T \beta}}{\sum_{l \in R(t_j)} e^{z_l(t_j)^T \beta}}, \hat{\beta} = \arg \max_{\beta} L(\beta)$. Partial score equation:

$$0 = u(\beta) = \frac{\partial \log L}{\partial \beta} = \sum_{j=1}^m \left\{ z_j(t_j) - \sum_{l \in R(t_j)} z_l(t_j) \frac{e^{z_l(t_j)^T \beta}}{\sum_{k \in R(t_j)} e^{z_k(t_j)^T \beta}} \right\} := \sum_{j=1}^m \{z_j(t_j) - \bar{z}(\beta, t_j)\}$$

Furthermore, the observed information matrix

$$I_n(\beta) = -\frac{\partial^2 \log L}{\partial \beta \partial \beta^T} = \sum_{j=1}^k \sum_{l \in R(t_j)} z_l(t_j) \{z_l(t_j) - \bar{z}(\beta, t_j)\}^T p_l(\beta, t_j) = \sum_{j=1}^k \sum_{l \in R(t_j)} \{z_l(t_j) - \bar{z}(\beta, t_j)\}^{\otimes 2} p_l(\beta, t_j)$$

where $p_l(\beta, t_j) = \frac{\lambda(t_j|z_l)dt_j}{\sum_{k \in R(t_j)} \lambda(t_j|z_k)dt_j}$ and $b^{\otimes 2} = bb^T$. Asymptotics: $\sqrt{n}(\hat{\beta} - \beta_0) \rightarrow_d \mathcal{N}_d(0, I(\beta_0)^{-1})$. Using counting process notation,

$$\begin{aligned} l(\beta) &= \sum_{i=1}^n \int_0^\infty \left[z_i(t) - \log \left(\sum_{i=1}^n y_i(t) e^{z_i(t)^T \beta} \right) \right] dN_i(t) \\ u(\beta) &= \sum_{i=1}^n \int_0^\infty [z_i(t) - \bar{z}(\beta, t)] dN_i(t) \\ I_n(\beta) &= \sum_{i=1}^n \int_0^\infty [z_i(t) - \bar{z}(\beta, t)]^{\otimes 2} e^{z_i(t)^T \beta} dN_i(t) \end{aligned}$$

- Breaking the ties: average partial likelihood over all possible permutations:

$$\prod_{j=1}^k e^{s_j(t_j)} \sum_{P \in Q_j} \prod_{r=1}^{d_j} \left\{ \sum_{l \in R(t_j, P, r)} e^{z_l(t_j)^T \beta} \right\}^{-1}$$

where Q_j is the set of $d_j!$ permutations and $s_j = \sum_{i=1}^{d_j} z_{j_i}(t_j)$.

- Approximations: (1) Breslow's:

$$L = \prod_{j=1}^k \frac{e^{s_j(t_j)^T \beta}}{(\sum_{l \in R(t_j)} e^{z_l(t_j)^T \beta})^{d_j}}$$

(2) Efron's:

$$L = \prod_{j=1}^k \frac{e^{s_j(t_j)^T \beta}}{\prod_{r=0}^{d_j-1} \left(\sum_{k \in R(t_j)} e^{z_k(t_j)^T \beta} - r \bar{A}(\beta, t_j) \right)}$$

where $\bar{A}(\beta, t_j) = \frac{1}{d_j} \sum_{l \in D(t_j)} e^{z_l(t_j)^T \beta}$ and D_j is the set of failures at t_j .

- Estimation of $\Lambda_0(\cdot)$: NPMLE: $L = \prod_{j=1}^k \prod_{l \in D_j} \{S(t_j - |z_l) - S(t_j | z_l)\} \prod_{l \in C_j} S(t_j | z_l)$ where C_j is the set of censoring at t_j . Let $\Lambda_0(t) = \sum_{j: t_j \leq t} (1 - \alpha_j)$, maximise $\prod_{j=1}^k \prod_{l \in D_j} (1 - \alpha_j^{e^{z_l(t_j)^T \beta}}) \prod_{l \in C_j} \alpha_j^{e^{z_l(t_j)^T \beta}}$ over $\alpha = (\alpha_1, \dots, \alpha_k)^T$.
 $\hat{\alpha}_j = \left\{ 1 - \frac{e^{z_j(t_j)^T \beta}}{\sum_{l \in R(t_j)} e^{z_l(t_j)^T \beta}} \right\} e^{-z_j(t_j)^T \beta}, \hat{\Lambda}_0(t) = \sum_{j: t_j \leq t} (1 - \hat{\alpha}_j).$