

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) $0 \leq \text{rank}(A) \leq \min(m, n)$; (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: $P^T = P$. 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 $x \in \mathcal{C}(X), w \in \mathcal{C}(X)^T$. 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 $\mathcal{C}(X^T) = \mathcal{C}(X^T X)$.

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 $c^T \hat{\beta} = l^T X^T \hat{\beta} = l^T X^T (X^T X)^{-1} X^T Y = l^T P_X Y$ 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, $\text{RSS}_{H_0} - \text{RSS} \sim \chi_s^2(\lambda)$ 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 $\mathcal{C}(\tilde{X}^T) = \mathcal{C}((A, H)^{-1}X^T) \supset \mathcal{C}((A, H)^{-1}H) = \mathcal{C}\begin{pmatrix} 0 \\ I_s \end{pmatrix}$, θ_2 is estimable. $\hat{\theta}$ solves the normal equation $\tilde{X}^T \tilde{X} \hat{\theta} = \tilde{X}^T Y$. Under H_0 , $\tilde{Y} = \tilde{X}_1 \tilde{\theta}_1 + \tilde{X}_2 \xi = \tilde{X}_1 \hat{\theta}_1 + P_{\tilde{X}_1} \tilde{X}_2 (\hat{\theta}_2 - \xi) + \tilde{X}_2 \xi$, $\text{RSS}_{H_0} - \text{RSS} = \|Y - \tilde{Y}\|^2 - \|Y - \hat{Y}\|^2 = \|\hat{Y} - \tilde{Y}\|^2 = \sigma^2 (\hat{\theta}_2 - \xi)^T \text{Var}(\hat{\theta}_2)^{-1} (\hat{\theta}_2 - \xi)$. 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 $u^T \gamma : u^T \hat{\gamma} \pm t_{n-r, \alpha/2} \hat{\sigma} \sqrt{u^T D u}$. Now allow $u \in \mathbb{R}^s$ to vary arbitrarily. Since $\sup_{u \neq 0} \frac{|u^T \hat{\gamma} - u^T \gamma|^2}{u^T D u} \stackrel{v=D^{-1/2}u}{=} \sup_{v \neq 0} \frac{|v^T D^{-1/2}(\hat{\gamma} - \gamma)|^2}{v^T v} \stackrel{\text{Cauchy-Schwarz}}{=} (\hat{\gamma} - \gamma)^T D^{-1} (\hat{\gamma} - \gamma)$, $P(\sup_{u \neq 0} \frac{|u^T \hat{\gamma} - u^T \gamma|^2}{s \hat{\sigma}^2 u^T D u} \leq F_{s, n-r, \alpha}) = 1 - \alpha$. 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 $\frac{\sqrt{m}}{\hat{\sigma}} \max_{i, i'} \{\bar{y}_i - \bar{y}_{i'} - (\alpha_i - \alpha_{i'})\} = \frac{\{\max_i \frac{\sqrt{m}(\bar{y}_i - \mu - \alpha_i)}{\hat{\sigma}} - \min_i \frac{\sqrt{m}(\bar{y}_i - \mu - \alpha_i)}{\hat{\sigma}}\}}{\sqrt{\text{RSS}/\sigma^2}} \sim q_{k, n-k}$. 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 Generalized Linear Models

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

- 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) Logisitic/Logit model: $\pi_x = \text{expit}(\alpha + \beta x) = \frac{1}{1 + e^{-(\alpha + \beta x)}}$, link function $g(\pi_x) = \text{logit}(\pi_x) = \log \frac{\pi_x}{1 - \pi_x}$.