Linear mixed models Standard assumptions:

$$y = X\beta + Z\alpha + \epsilon$$

where $\alpha \sim N(0, G)$ independent of $\epsilon \sim N(0, R)$.

Marginal model $y \sim N(X\beta, V)$ where V = R + ZGZ'.

Restricted maximum likelihood (REML) uses a linear transformation Ay to remove the fixed effects, and then estimates the variance. We have $\operatorname{rank}(A) = n - p$ where $p = \operatorname{rank}(X)$ and A'X = 0. Then $z = A'y \sim N(0, A'VA)$ and we can maximize the restricted log likelihood to estimate the variance parameters. Let $P = A(A'VA)^{-1}A'$ and solve

$$0 = \frac{\partial l_R}{\partial \theta_i} = \frac{1}{2} \left(y' P \frac{\partial V}{\partial \theta_i} P y - tr(P \frac{\partial V}{\partial \theta_i}) \right)$$

Predictions Let $\xi = b'\beta + a'\alpha$ be a mixed effect. These are what we're interested in estimating. We call them predictions rather than estimations because we're predicting a random component.

BLUE - Best linear unbiased estimator, $\tilde{\beta} = (X'V^{-1}X)^{-1}X'V^{-1}y$. This is the MLE of β .

BLUP - Best linear predictor, which plugs in $\tilde{\beta}$ into BP.

BP - Best predictor, $E(\xi|y) = b'\beta + a'GZ'V^{-1}(y - X\beta)$ a theoretical ideal that's usually difficult or impossible to derive.

EBLUP - Empirical best linear predictor, plugs in estimates for both fixed and variance components into the BP. This is typically the one we compute and use.

library(lme4)

library(HLMdiag)

fit1 = lmer(y ~ X1 + X2 + (1 | V), data=somedata)
s1 = summary(fit1)

2 ways to extract variance estimates:

s1\$sigma^2

s1\$varcar\$V

HLMdiag::varcomp.mer(fit1)

getME(fit1, ...) # Extract various components
predict(fit1, data=newdata) # EBLUPs

2 ways to get standard errors for variance estimates are parametric bootstrap and asymptotic covariance matrix of the estimates.

232A

Linear Models

Least Squares Principle

$$\operatorname{arg\,min}_{\beta} \|Y - X\beta\|^2$$

Normal Model

$$Y = X\beta + \epsilon, \qquad \epsilon \sim N(0, \sigma^2 I)$$

Normal Equations - Any b satisffying this solves the least squares

$$X^T X b = X^T y$$

Gauss Markov Theorem - $\hat{\beta}$ is Best Linear Unbiased Estimator (BLUE) of β .

$$\hat{\beta} = (X^T X)^{-1} X^T y \sim N(\beta, \sigma^2 (X^T X)^{-1})$$

Estimating the variance: $\frac{\left\|y - X\hat{\beta}\right\|^2}{\sigma^2} \sim \chi_{n-p}^2$.

$$\hat{\sigma}^2 = \frac{\left\| y - X \hat{\beta} \right\|^2}{n - p}$$

Use t test for hypothesis testing and confidence intervals for the value of a particular β_j coefficient. Let w_{ii} be the *i*th diagonal entry of $(X^TX)^{-1}$.

$$\frac{\beta_j - \beta_j^*}{\hat{\sigma}\sqrt{w_{ii}}} \sim t_{n-p}$$

 $1 - \alpha$ Confidence intervals for new observation Y_h at x_h and $E[Y_h]$:

$$E[y_h] \approx \hat{y_h} \pm t(n-p, 1-\frac{\alpha}{2})\hat{\sigma}\sqrt{x_h^T(X^TX)^{-1}x_h}$$

$$y_h \approx \hat{y_h} \pm t(n-p, 1-\frac{\alpha}{2})\hat{\sigma}\sqrt{1+x_h^T(X^TX)^{-1}x_h}$$

Simultaneous (Working-Hotelling) confidence interval for $E(y_h)$:

$$\hat{y}_h \pm \sqrt{pF_{p,n-p,1-\alpha}} se\{\hat{y}_h\}$$
$$\frac{(\hat{\beta} - \beta)^T X^T X (\hat{\beta} - \beta)/p}{\hat{\sigma}^2} \sim F_{p,n-p}$$

General linear tests. Partition $\beta = (\beta_1, \beta_2)$ where β_1 is an r vector and β_2 is p-r. Null hypothesis $H_0: \beta_2 = \beta_2^*$ (often 0), and $H_a: \beta_2 \neq \beta_2^*$. Then $SSE_r = \left\|y - X_2\beta_2^* - X_1\tilde{\beta}_1\right\|^2$ is the sum of squared error for the reduced model and $SSE_f = \left\|y - X\hat{\beta}\right\|^2$ is the squared sum of error for the full model. Under H_0 :

$$\frac{\frac{SSE_r - SSE_f}{p - r}}{\frac{SSE_f}{n - p}} \sim F_{p - r, n - p}$$

Alternate forms of linear test, and testing a linear combination if $R\beta = r$, for R full rank $s \times p$ matrix.

$$\frac{(R\hat{\beta} - r)^T (R(X^T X)^{-1} R^T)^{-1} (R\beta - r)/s}{\hat{\sigma}^2} \sim F_{s,n-p}$$

Model selection and diagnostics

$$SSTO = \sum_{i=1}^{n} (y_i - \bar{y}) = \|y - \bar{y}1_n\|^2 = \|(I - J)y\|^2$$

$$SSR = \sum_{i=1}^{n} (\hat{y}_i - \bar{y}) = \|\hat{y} - \bar{y}1_n\|^2 = \|(H - P)y\|^2$$

$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i) = \|y - \hat{y}\|^2 = \|(I - H)y\|^2$$

If the model contains the intercept in the column space of X then SSTO = SSR + SSE.

$$R^2 = 1 - \frac{SSE}{SSTO}$$

Adjusted
$$R_a^2 = 1 - \frac{SSE/(n-p)}{SSTO/(n-1)}$$

$$AIC = n\log SSE + 2p$$

$$BIC = n \log SSE + p \log n$$

$$Cp = \frac{SSE}{MSE} - (n - 2p)$$

Residuals:
$$\hat{\epsilon}_i = y_i - \hat{y}_i$$

Studentized residuals (rstandard in R):

$$\gamma_i = \frac{\hat{\epsilon}_i}{s\{\hat{\epsilon}_i\}} = \frac{\hat{\epsilon}_i}{\hat{\sigma}\sqrt{1 - h_{ii}}}$$

Prediction sum of squares (PRESS) is the same as leave one out cross validation (LOOCV). Prediction error on ith observation is called deleted residuals:

$$y_i - \hat{y}_{i(-i)} = \frac{y_i - \hat{y}_i}{1 - H_{ii}}$$

Works for ridge regression also, letting $H = X(X^TX + \lambda I)^{-1}X^T$.

Studentized deleted residuals:

$$t_i = \frac{\hat{\epsilon}_i}{\sqrt{MSE_{(-i)}(1 - h_{ii})}} \sim t_{n-p-1}$$

Where $MSE_{(-i)}=SSE_{(-i)}/(n-1-p)$ and $SSE_{(-i)}=SSE-\frac{\hat{\epsilon}_i}{1-h_{i:i}}$ can be used to calculate without refitting model.

ANOVA

Three principles of experimental design: 1) Replication 2) Randomization 3) Blocking

One way ANOVA with n total observations, K groups:

$$\begin{array}{cccc} \text{SS} & & \text{DF} \\ \text{SSTR} & \sum_{j=1}^{K} n_{j} (\bar{y_{j}}. - \bar{y_{\cdot \cdot}})^{2} & \text{K - 1} \\ \text{SSE} & \sum_{i=1}^{n} (y_{ij} - \bar{y_{j \cdot}})^{2} & \text{n - K} \\ \text{SSTO} & \sum_{i=1}^{n} (y_{ij} - \bar{y_{\cdot \cdot}})^{2} & \text{n - 1} \end{array}$$

Contrasts are sums of the form $\Phi = \sum_{i=1}^{K} c_i \mu_i$ with $\sum_{i=1}^{K} c_i = 0$. Tukey's works for all pairwise contrasts. Scheffe's and extended Tukey works for all contrasts. Bonferroni's is for a limited number of pre specified contrasts.

Ridge Regression for $\lambda > 0$ solves

$$\min_{\beta} ||Y - X\beta||^2 + \lambda ||\beta||^2$$

Multivariate Normal

log likelihood for k vector $x \sim N(\mu, \Sigma)$

$$l_x = -\frac{k}{2}\log 2\pi - \frac{1}{2}\{\log \det \Sigma + (x-\mu)^T \Sigma^{-1}(x-\mu)\}$$

Stein's formula: $X \sim N(\mu, \sigma)$

$$E(g(X)(X - \mu)) = \sigma^2 E(g'(X))$$

assuming these expectations are finite.

 $X \sim N(\mu, \Sigma)$, A an $m \times n$ matrix, then

$$AX \sim N(A\mu, A\Sigma A^t)$$

For Σ full rank it's possible to transform between $Z \sim N(0,I)$ and X:

$$X = \Sigma^{1/2}Z + \mu$$
 $Z = \Sigma^{-1/2}(X - \mu)$

In block matrix form:

$$X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \sim N \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right)$$

Assuming Σ_{11} is positive definite then the conditional distribution

$$X_2|X_1 \sim N(\mu_2 + \Sigma_{21}\Sigma_{11}^{-1}(X_1 - \mu_1), \Sigma_{22} - \Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12})$$

Conditional Distributions

Conditional pdf:

$$f_{X|Y}(x|y) \equiv \frac{f_{X,Y}(x,y)}{f_{Y}(y)}$$

Iterated expectation:

$$E(Y) = E(E(Y|X))$$

Conditional variance formula:

$$Var(Y) = Var(E(Y|X)) + E(Var(Y|X))$$

General Techniques

Singular Value Decompostion (SVD) Any matrix X can be written

$$X = UDV^T$$

with U, V orthogonal, and D diagonal.

Moore Penrose Psuedoinverse A^+ exists uniquely for every matrix A.

Projection matrix P are symmetric and idempotent. They have eigenvalues either 0 or 1.

$$P = P^T$$
 $P^2 = P$

Covariance of linear transformations

$$Cov(Ay, Bx) = ACov(y, x)B^T$$

Invert 2×2 matrix: $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$

$$A^{-1} = \frac{1}{\det(A)} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

Block matrix: $\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} =$

$$\begin{bmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix}$$

Sum identities:

$$\sum_{k=0}^{\infty} p^k = \frac{p}{1-p} \qquad \sum_{k=0}^{\infty} kp^k = \frac{p}{(1-p)^2} \qquad |p| < 1$$

Integration by parts:

$$\int uv' = uv - \int u'v$$

Matrix / Vector differentiation

$$\frac{\partial A^T \beta}{\partial \beta} = A$$
, $\frac{\partial \beta^T A \beta}{\partial \beta} = (A + A^t)\beta = 2A\beta$ for A symmetric.

$$\frac{\partial}{\partial \theta_i} \log(|A|) = tr(A^{-1} \frac{\partial A}{\partial \theta_i})$$

Binomial $X \sim B(n, p)$

$$p(k) = \binom{n}{k} p^k (1-p)^{n-k}$$
 $k = 0, 1, ..., n$

EX = np, Var X = np(1-p)

 $mgf: M_X(t) = (pe^t + 1 - p)^n$

Beta is conjugate prior, Fisher info $I(p) = \frac{1}{p(1-p)}$

Poisson $X \sim P(\lambda)$

$$p(k) = \frac{e^{-\lambda} \lambda^k}{k!} \qquad k = 0, 1, \dots$$

 $E X = \lambda, \quad Var X = \lambda$

mgf: $M_X(t) = e^{\lambda(e^t - 1)}$ Use recursive relation to compute $\mathrm{E}(X_i)$.

Gamma is conjugate prior, Fisher info $I(\lambda) = \frac{1}{\lambda}$

Normal $X \sim N(\mu, \Sigma)$, Σ positive definite

$$f(x) = \frac{\exp\{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)\}}{(2\pi)^{\frac{k}{2}} \sqrt{\det(\Sigma)}} = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

mgf: $M_X(t) = \exp(\mu' t + \frac{1}{2} t' \Sigma t)$

Normal is conj. prior, Fisher info $I(\mu, \sigma^2) = \begin{bmatrix} 1/\sigma^2 & 0 \\ 0 & 1/2\sigma^4 \end{bmatrix}$

Beta $X \sim \text{Beta}(\alpha, \beta)$

$$f(x) = \frac{x^{\alpha - 1}(1 - x)^{\beta - 1}}{B(\alpha, \beta)} \qquad 0 \le x \le 1$$

$$E X = \frac{\alpha}{\alpha + \beta}, \quad Var X = \frac{\alpha \beta}{(\alpha + \beta)^2 (\alpha + \beta + 1)}$$

using the beta function:

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)} = \int_0^1 t^{\alpha - 1} (1 - t)^{\beta - 1} dt$$

Gamma $X \sim \text{Gamma}(\alpha, \beta)$

$$f(x) = \frac{\beta^{\alpha} x^{\alpha - 1} e^{-\beta x}}{\Gamma(\alpha)}$$
 $x > 0$

 $EX = \frac{\alpha}{\beta}, \quad Var X = \frac{\alpha}{\beta^2}$

mgf: $M_X(t) = (1 - \frac{t}{\beta})^{-\alpha}, t < \beta$

 $X \sim \text{Gamma}(\alpha, \beta) \iff \beta X \sim \text{Gamma}(\alpha, 1)$

 X_i iid Gamma (α_i, β) , then

$$\sum X_i \sim \text{Gamma}(\sum \alpha_i, \beta)$$

Gamma function: $\Gamma(\alpha) = \int_0^\infty t^{\alpha-1} e^{-t} dt$.

$$\Gamma(\frac{1}{2}) = \sqrt{\pi}.$$

$$\Gamma(\alpha + 1) = \alpha \Gamma(\alpha)$$

 $\Gamma(k) = (k-1)!$ for k positive integer.

Exponential Special case: $X \sim \text{Exp}(\lambda) \equiv \text{Gamma}(1, \lambda)$

$$f(x) = \lambda e^{-\lambda x}, \quad x > 0 \qquad \to X = \frac{1}{\lambda}, \quad \text{Var} \, X = \frac{1}{\lambda^2}$$
 CDF $F(x) = 1 - e^{-\lambda x}$

Chi square Special case: $X \sim \chi_n^2 \equiv \operatorname{Gamma}(\frac{n}{2}, \frac{1}{2})$

$$f(x) \propto x^{\frac{n}{2}-1}e^{\frac{-x}{2}}, \quad x > 0$$
 E $X = n$, Var $X = 2n$
Let Z_i be iid $N(0,1)$.

$$\sum_{i=1}^{n} Z_i^2 \sim \chi_n^2$$

Noncentral χ^2 . Let $Y \sim N(\mu, I)$ be an *n* vector. Then

$$||Y||^2 \sim \chi_n^2(||\mu||^2)$$

 \mathbf{F}

$$F(m,n) \equiv \frac{\frac{\chi_m^2}{m}}{\frac{\chi_n^2}{n}}$$

Where numerator and denominator are independent χ^2 .

 \mathbf{T}

$$t(n) = \frac{N(0,1)}{\sqrt{\frac{\chi_n^2}{n}}}$$

Where numerator and denominator are independent.

Transformations If g 1:1 with continuous derivatives and nonzero Jacobian, and Y = g(X), then the density

$$f_Y(y) = f_X(g^{-1}(y))|J_{g^{-1}}(y)|$$

For affine transformation Y = AX + c then

$$f_Y(y) = f_X(A^{-1}(y-c))|\det A|^{-1}$$

Moment generating functions determine distribution

$$M_X(t) \equiv \mathcal{E}(e^{tX}), \quad M_X'(0) = \mathcal{E}(X)$$

 X_i independently distributed \iff

$$M_{\sum X_i}(t) = \prod M_{X_i}(t)$$

Characteristic function

$$\phi(t) = \mathcal{E}(e^{it^T X)} = \mathcal{E}(\cos(t^T X)) + i \mathcal{E}(\sin(t^T X))$$

Order statistics for sorted sample $X_{(1)}, \ldots, X_{(n)}$ has pdf:

$$n! \prod_{i=1}^{n} f(X_{(i)}) \quad I(X_{(1)} < \dots < X_{(n)})$$

TODO - add measure theory

Jensen's Inequality if $S \subset R^k$ convex and closed, g convex on S, $P[X \in S] = 1$, and $\to X$ is finite, then $\to X \in S$, $\to X \in S$, and

$$E g(X) \ge g(E X)$$

Holder's Inequality if r, s > 1 and $\frac{1}{r} + \frac{1}{s} = 1$ then

$$E|XY| \le (E|X|^r)^{\frac{1}{r}} (E|X|^s)^{\frac{1}{s}}$$

T(X) Sufficient means the distribution of X|T(X) does not depend on θ .

Factorization theorem: T(x) is sufficient \iff

$$f_{\theta}(x) = h(x)g(\theta, T(x))$$

 $L_x(\theta) = p_{\theta}(x) = p(x, \theta)$ likelihood is function of θ , density is function of x.

The likelihood ratio

$$\lambda_x(\theta) = \frac{L_x(\theta)}{L_x(\theta_0)}$$

is minimal sufficient. To show T(x) is minimal sufficient show that it is sufficient and a function of the likelihood $\lambda_x(\theta)$.

Fisher information

$$I(\theta) = \mathcal{E}_{\theta} \left[\frac{\partial}{\partial \theta} \log L_X(\theta) \right]^2 = \mathcal{E}_{\theta} \left[-\frac{\partial^2}{\partial \theta^2} \log L_X(\theta) \right]$$

bias $\hat{v} \equiv E(\hat{v}) - v$

$$MSE(\hat{v}) \equiv E(\hat{v} - v)^2 = Var(\hat{v}) + (bias \hat{v})^2$$

Rao-Blackwell Let S(X) be an unbiased point estimator for $g(\theta)$. Conditioning on a sufficient statistic T(X) reduces variance.

$$\operatorname{Var}_{\theta}(S(X)) \geq \operatorname{Var}_{\theta}(\operatorname{E}(S(X)|T(X)))$$

Also holds for more general convex loss function L:

$$R(\theta, S) \equiv E_{\theta} L(\theta, S(X)) \ge E_{\theta} L(\theta, E(S(X)|T(X)))$$

Completeness T(X) is complete if E g(T(X)) = 0 implies g = 0 almost surely for all θ .

Cramer Rao Inequality Let $g: \Theta \to R$. Suppose there exists an unbiased estimator U(X), $\to U(X) = g(\theta)$. Then

$$\operatorname{Var}_{\theta} U(X) \ge \left(\frac{\partial g(\theta)}{\partial \theta}\right)^T I(\theta)^{-1} \left(\frac{\partial g(\theta)}{\partial \theta}\right)$$

Basu's Theorem - If T(X) complete sufficient statistic and A(X) is ancillary then A(X) and T(X) are independent.

Lehmann - Scheffe Suppose T(X) is complete sufficient. Then there exists unique unbiased estimator $\operatorname{E} h(T(x))$ of $g(\theta) \in R$ with smallest variance (MVUE).

Exponential Families T(x) is natural sufficient statistic and is complete sufficient if the k parameter exponential family is full rank.

$$p(x, \theta) = h(x) \exp\{\eta(\theta)^T T(x) - B(\theta)\}\$$

Canonical form model indexed by η .

$$q(x,\eta) = h(x) \exp\{\eta^T T(x) - A(\eta)\}\$$

$$\dot{A}(\eta) = \mathcal{E}_{\eta}(T(X)) \quad \ddot{A}(\eta) = I(\eta) = \operatorname{Var}_{\eta}(T(X))$$

Then moment generating function for T(X) is

$$M_{T(X)}(t) = \exp\{A(t+\eta) - A(\eta)\}\$$

Equivalent statements useful for GLM's such as $Y \sim N(X\beta, \sigma_0^2 I)$, where Z is $n \times p$:

1. $I(\beta) = \frac{1}{\sigma_0^2} X^T X$ positive definite 2. $\operatorname{rank}(X) = p$ 3. model is identifiable. More generally another equivalent statement is $\operatorname{Var}(T(X)) = \ddot{A}(\eta)$ is positive definite.

Decision Theory

Decision rule $\delta : \mathcal{X} \to \mathcal{A}$, where $\delta \in \mathcal{D}$, the space of possible decision rules and \mathcal{A} is the action space.

Loss function $l: \Theta \times \mathcal{A} \to \mathbb{R}^+$ Posterior mean minimizes square error loss; median minimizes absolute loss.

Risk function $R:\Theta\times\mathcal{D}\to\mathbb{R}^+$ expected loss for a particular value of θ

$$R(\theta, \delta) = \mathcal{E}_{\theta} l(\theta, \delta(X)) = \int l(\theta, \delta(x)) \cdot p_{\theta}(x) dx$$

Bayes setup:

$$\pi(\theta|x) = \frac{p_{\theta}(x)\pi(\theta)}{m(x)}$$

Bayes decision rule If there exists $\delta_{\pi} \in \mathcal{D}$ w.r.t prior π such that

$$r(\pi, \delta_{\pi}) = \inf_{\delta \in \mathcal{D}} r(\pi, \delta)$$

To find Bayes rule minimize the posterior risk:

$$\delta_{\pi}(x) = \min_{a \in \mathcal{A}} r_{\pi}(a|x)$$

Bayes risk $r_{\pi}: \mathcal{D} \to \mathbb{R}^+$ expected loss for fixed prior π

$$r_{\pi}(\delta) = \mathcal{E}_{\pi} R(\theta, \delta) = \int_{\Theta} R(\theta, \delta) \pi(d\theta) = \int_{\mathcal{X}} r_{\pi}(\delta(x)|x) m(x) dx$$

To find Bayes risk: 1) find the Bayes rule 2) compute the risk function 3) take the expectation of the risk wrt prior π .

Minimax decision rule δ^* minimizes the worst case scenario, satisfies

$$\sup_{\theta} R(\theta, \delta^*) = \inf_{\delta} \sup_{\theta} R(\theta, \delta)$$

To show δ^* is minimax, first check for constant risk $R(\theta, \delta^* = c \text{ for all } \theta$, then find a prior π such that δ^* is the Bayes rule. This π is least favorable. More generally can find a sequence of priors (π_k) such that the Bayes risk $r_{\pi_k}(\delta_{\pi_k}) \to c$.

Asymptotics

Almost Sure convergence

$$X_n \xrightarrow{a.s.} X$$
 means $P(X_n \to X) = 1$

Theorem: $\iff P(\sup_{m>n} |X_m - X| > \epsilon) \to 0 \quad \forall \epsilon > 0.$

Convergence in Probability

$$X_n \xrightarrow{p} X$$

means that $P(|X_n - X| > \epsilon) \to 0$ for all $\epsilon > 0$.

Generalized Chebychev Inequality Let X be a r.v. and g be a nonnegative function increasing on the range of X. Then

$$P(X \ge a) \le \frac{\operatorname{E} g(X)}{g(a)}$$

Borel Cantelli Lemma

Hoeffding Inequality Let X_1, \ldots, X_n be independent (not necessarily iid) with $a_i \leq X_i \leq b_i$ and $E[X_i] = 0$. Then

$$P\left(\sum_{i=1}^{n} X_i \ge \eta\right) \le \exp\left\{-\frac{2\eta^2}{\sum_{i=1}^{n} (b_i - a_i)^2}\right\}$$