Bayesian statistics – Nanjing Forestry University

Lecture 5

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Design Matrices and Experimental Data

Experimental designs expressed as joint distributions

$$
\begin{aligned}
[\alpha, \beta, \sigma \mid \mathbf{y}] \quad &\propto \quad \prod_{i=1}^{N} \prod_{j=1}^{M} \text{normal}\left(y_{i,j} \mid g\left(\alpha, \beta, x_{i,j}, w_{i,j}\right), \sigma^2\right) \times \\
&\qquad \text{normal}\left(\alpha \mid 0, 1000\right) \text{normal}\left(\beta_1 \mid 0, 1000\right) \times \\
&\qquad \text{normal}\left(\beta_2 \mid 0, 1000\right) \text{uniform}\left(\sigma \mid 0, 100\right) \\
g\left(\alpha, \beta, x_{i,j}, w_{i,j}\right) \quad &= \quad \alpha + \beta_1 x_{i,j} + \beta_2 w_{i,j}
\end{aligned}
$$

Photo c/o of the Minnesota Agricultural Experiment Station at http://www.maes.umn.edu.

Design matrix: What is this?

E[y] Design Matrix

$$\begin{bmatrix} \widehat{y_1} \\ \widehat{y_2} \\ \widehat{y_3} \\ \widehat{y_4} \\ \vdots \\ \widehat{y_N} \end{bmatrix} = \begin{bmatrix} 1 & 1.2 \\ 1 & 3.4 \\ 1 & 1.7 \\ 1 & 7.9 \\ & \vdots \\ 1 & 4.3 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \alpha + \beta \times 1.2 \\ \alpha + \beta \times 3.4 \\ \alpha + \beta \times 1.7 \\ \alpha + \beta \times 7.9 \\ \vdots \\ \alpha + \beta \times 4.3 \end{bmatrix}$$

Great! But how do we handle categorical experimental treatments?

Parameterize a model with categorical predictors

unique solution

cell means model

$$g(\boldsymbol{\alpha}, \mathbf{x}) = \alpha_j x_{i,j}^{(j)}$$

over-parameterized

effects model

$$g(\mu, \boldsymbol{\alpha}, \mathbf{x}) = \mu + \sum_{j=1}^{M} \alpha_j x_{i,j}^{(j)}$$

impose constraint

multilevel model

$$\alpha_j \sim N\left(0, \sigma^2\right)$$

set to zero

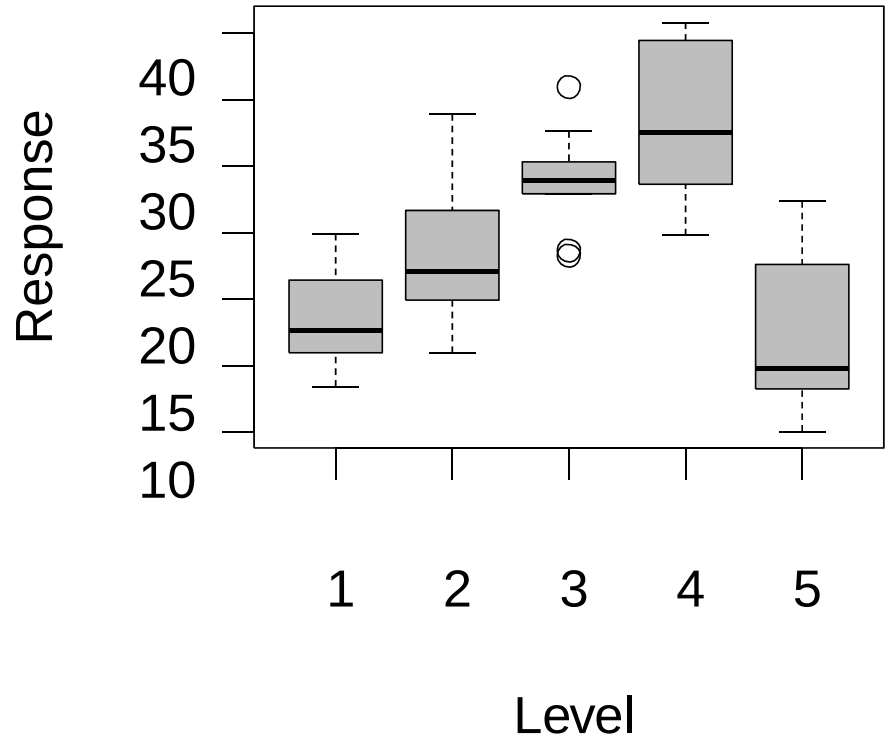
$$\alpha_M = 0$$

sum to zero

$$\alpha_M = -(\alpha_1 + \alpha_2 + \cdots + \alpha_{M-1})$$

Simulate data for CRD Design

Completely randomized design (CRD) with 1 factor and 5 levels
Simulate data for a factor with 5 levels
10 replicates per level, 50 replicates overall



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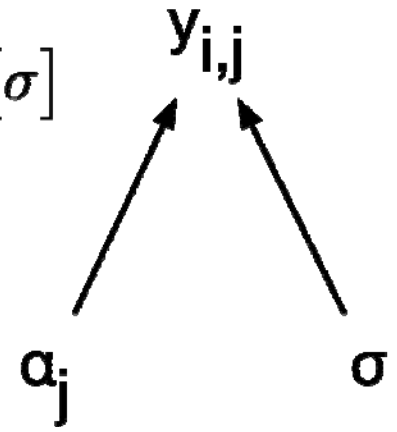
sum to zero

$$\alpha_M = -(\alpha_1 + \alpha_2 + \cdots + \alpha_{M-1})$$

Cell Means Model: Joint and DAG

$$[\boldsymbol{\alpha}, \sigma \mid \mathbf{y}] \propto \prod_{i=1}^{N} \prod_{j=1}^{M} \left[y_{i,j} \mid g(\boldsymbol{\alpha}, \mathbf{x}), \sigma^2 \right] [\alpha_j] [\sigma]$$

$$g(\boldsymbol{\alpha}, \mathbf{x}) = \alpha_j x_{i,j}^{(j)}$$



Interest in group means and not effects
Have prior information for group means
Lack prior information for group means - use vague priors
Recover effects or grand mean as derived quantities

Cell Means Model: Design Matrix

E[y] Design Matrix Parameters

$$\begin{bmatrix} \widehat{y_{n,1}} \\ \widehat{y_{n,2}} \\ \widehat{y_{n,3}} \\ \widehat{y_{n,4}} \\ \widehat{y_{n,5}} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{bmatrix} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{bmatrix}$$

Cell Means Model: JAGS

```
#priors
for (i in 1:5) {
  alpha[i] ~ dnorm(0, 0.001)
}
sigma ~ dunif(0, 100)
tau <- 1 / ( sigma * sigma)

# Likelihood
for (i in 1:50) {
  y[i] ~ dnorm(alpha[x[i]], tau)
}

# Derived quantities
effect.2.1 <- mu[2] - mu[1]
effect.3.1 <- mu[3] - mu[1]
grandMean <- mean(mu[])
```

Compute effects and grand mean as derived quantities.

mu = alpha

Parameterize a model with categorical predictors

unique solution

cell means model

$$g(\boldsymbol{\alpha}, \mathbf{x}) = \alpha_j x_{i,j}^{(j)}$$

over-parameterized

effects model

$$g(\mu, \boldsymbol{\alpha}, \mathbf{x}) = \mu + \sum_{j=1}^{M} \alpha_j x_{i,j}^{(j)}$$

impose constraint

multilevel model

$$\alpha_j \sim N\left(0, \sigma^2\right)$$

set to zero

$$\alpha_M = 0$$

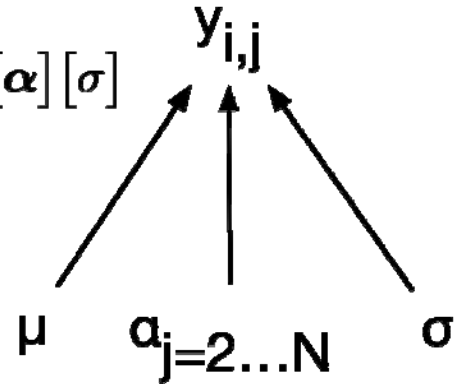
sum to zero

$$\alpha_M = -(\alpha_1 + \alpha_2 + \cdots + \alpha_{M-1})$$

Effects Models - Set to Zero: Joint and DAG

$$[\mu, \boldsymbol{\alpha}, \sigma \mid \mathbf{y}] \propto \prod_{i=1}^{N} \prod_{j=1}^{M} \left[y_{i,j} \mid g(\mu, \boldsymbol{\alpha}, \mathbf{x}), \sigma^2 \right] [\mu] [\boldsymbol{\alpha}] [\sigma]$$

$$g(\mu, \boldsymbol{\alpha}, \mathbf{x}) = \mu + \sum_{j=2}^{M} \alpha_j x_{i,j}^{(j)}$$



Interest in effects and not means
Have prior information for effect sizes
Lack prior information for effect sizes - can estimate conservatively
Recover group means as derived quantities

Effects Model- Set to Zero: Design Matrix

$$\underbrace{\begin{bmatrix} \widehat{y_{n,5}} \\ \widehat{y_{n,1}} \\ \widehat{y_{n,2}} \\ \widehat{y_{n,3}} \\ \widehat{y_{n,4}} \end{bmatrix}}_{\text{E[y]}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 \end{bmatrix}}_{\text{Design Matrix}} \underbrace{\begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix}}_{\text{Parameters}} = \begin{bmatrix} \mu \\ \mu + \alpha_1 \\ \mu + \alpha_2 \\ \mu + \alpha_3 \\ \mu + \alpha_4 \end{bmatrix}$$

CRD with 1 factor and 5 levels

Remove parameter by setting $\alpha_5 = 0$

Group 5 is now represented by intercept μ

α_j represent deviations from this baseline/control group

Effects Models - Set to Zero: JAGS

```
# Priors
for (i in 1:4){
  alpha[i] ~ dnorm(0, 0.001)
}
mu ~ dnorm(0, 0.001)
sigma ~ dunif(0, 100)
tau <- 1 / ( sigma * sigma)

# Likelihood
for (i in 1:50) {
  y[i] ~ dnorm(yhat[i], tau)
  yhat[i] <- mu + alpha[1]*treatment1[i] + alpha[2]*treatment2[i] + alpha[3]*treatment3[i] +
    alpha[4]*treatment4[i]
}

# Derived quantities
cell[5] <- mu
for (i in 1:4){
  cell[i] <- mu + alpha[i]
}
grandMean <- mean(cell[])
```

Compute cell and grand means as derived quantities

Parameterize a model with categorical predictors

unique solution

cell means model

$$g(\boldsymbol{\alpha}, \mathbf{x}) = \alpha_j x_{i,j}^{(j)}$$

over-parameterized

effects model

$$g(\mu, \boldsymbol{\alpha}, \mathbf{x}) = \mu + \sum_{j=1}^{M} \alpha_j x_{i,j}^{(j)}$$

impose constraint

multilevel model

$$\alpha_j \sim N\left(0, \sigma^2\right)$$

set to zero

$$\alpha_M = 0$$

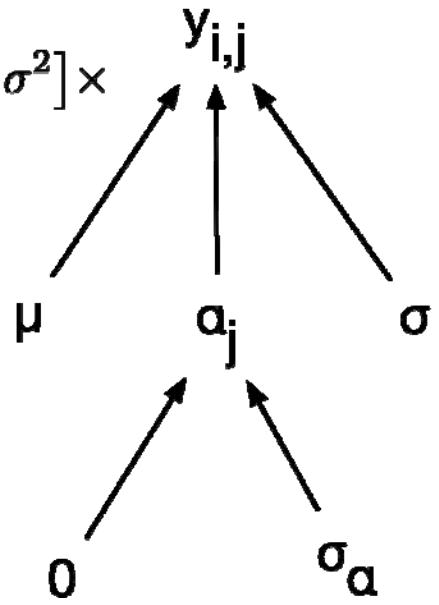
sum to zero

$$\alpha_M = -(\alpha_1 + \alpha_2 + \cdots + \alpha_{M-1})$$

Effects Model - Multi-level: Joint and DAG

$$\left[\mu, \boldsymbol{\alpha}, \sigma, \sigma_{\alpha} \mid \mathbf{y}\right] \propto \prod_{i=1}^{N} \prod_{j=1}^{M} \left[y_{i,j} \mid g\left(\mu, \boldsymbol{\alpha}, \mathbf{x}\right), \sigma^2\right] \times \left[\alpha_j \mid 0, \sigma_{\alpha}\right] \left[\mu\right] \left[\sigma\right] \left[\sigma_{\alpha}\right]$$

$$g\left(\mu, \boldsymbol{\alpha}, \mathbf{x}\right) = \mu + \sum_{j=1}^{M} \alpha_j x_{i,j}^{(j)}$$



Interest in effects and not means

Have prior information for effect sizes

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Recover group means as derived quantities

Effects Model - Multi-Level: Design Matrix

E[y] Design Matrix Parameters

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CRD with 1 factor and 5 levels

Intercept, μ, is the grand mean

α_j represent deviations from the grand mean

α_j are partially pooled allowing us to estimate all of them directly

Effects Models - Multi-level: JAGS

```
# Priors
mu ~ dnorm(0, 0.001)
for (i in 1:2){
  sigma[i] ~ dunif(0, 100)
  tau[i] <- 1 / ( sigma[i] * sigma[i])
}

# Likelihood
for (i in 1:5){
  alpha[i] ~ dnorm (0, tau[2])
}
for (i in 1:50) {
  y[i] ~ dnorm(y.hat[i], tau[1])
  y.hat[i] <- mu + alpha[x[i]]
}

# Derived quantities
for (i in 1:5){
  cell[i] <- mu + mean(alpha[i])
}
```

Compute cell means as derived quantities

Bayesian Approach to Experimental Analysis

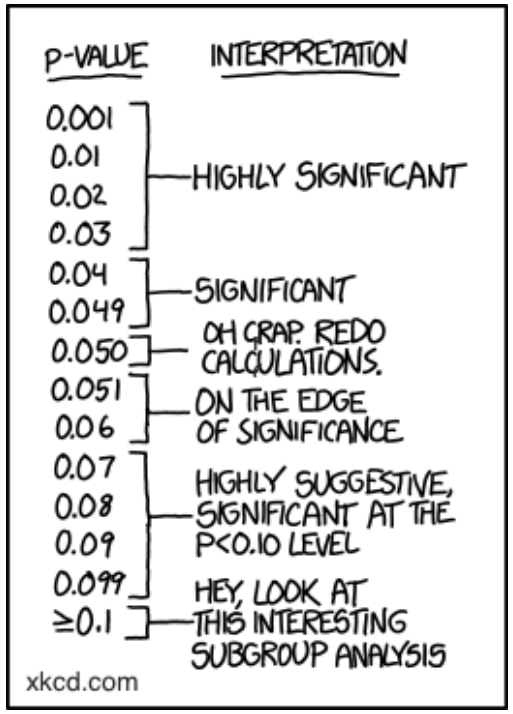
Flexible framework

Ease of interpreting effects

Make statements like:

Pr(Browsed > Unbrowsed) = .8

CI95: effect of browse = -4.0



Bayesian ANOVA

A way to summarize the “relative importance of different sources of variation in a dataset.” (Gelman and Hill, 2007)

- Uses the finite-population SD and not the superpopulation SD
- Can show variation decomposition across multiple levels
- Unbalanced data and complex or incomplete designs easily handled
- Can still be done with “fixed” effects

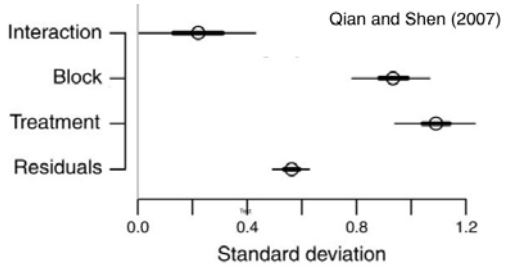


FIG. 1. Seaweed example, with ANOVA display of the estimated standard deviation of the estimated variance components showing a general pattern similar to that of the conventional ANOVA. Circles are estimated posterior means, short thick lines are the 50% posterior credible intervals, and the long thin lines are the 95% posterior credible intervals.

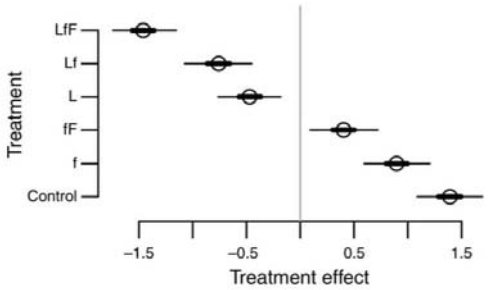


FIG. 2. Estimated treatment main effect of the seaweed grazer example shows that the regeneration rate decreases as grazing pressure increases. The six treatments are: C, control, no grazers allowed; L, only limpets allowed; f, only small fish allowed; Lf, large fish excluded; fF, limpets excluded; and LfF, all grazers allowed. The largest difference between treatments is

Hector et al. 2011, Qian and Shen 2007, Gelman 2005

Bayesian ANOVA: JAGS

Compute finite-population SDs computation as derived quantities

```
# Priors
mu ~ dnorm(0, 0.001)
for (i in 1:2){
  sigma[i] ~ dunif(0, 100)
  tau[i] <- 1 / ( sigma[i] * sigma[i])
}

# Likelihood
for (i in 1:5){
  alpha[i] ~ dnorm (0, tau[2])
}
for (i in 1:50) {
  y[i] ~ dnorm(y.hat[i], tau[1])
  y.hat[i] <- mu + alpha[x[i]]
  s.yerr[i] <- y[i] - y.hat[i]
}

# Derived quantities
for (i in 1:5){
  cell[i] <- mu + mean(alpha[i])
}
s.alpha <- sd(alpha[])
s.y <- sd(y.err[])
```

Mutiple Mean Comparison

Fundamentally different approach to mean comparisons
Shrinkage and/or informed priors

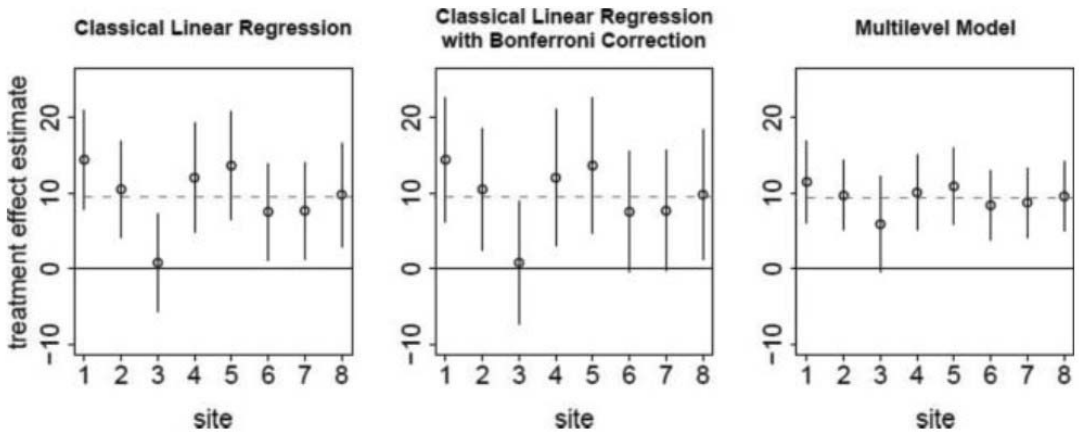


Figure 1. Treatment effect point estimates and 95% intervals across the eight Infant Health and Development Program sites. *Note.* The left panel display classical estimates from a linear regression. The middle panel displays the same point estimates as in the left panel but with confidence intervals adjusted to account for a Bonferroni correction. The right panel displays posterior means and 95% intervals for each of the eight site-specific treatment effects from a fitted multilevel model.

Gelman et al. 2012

Gelman 2013, Gelman et al. 2012

References

[1] A. Gelman. Analysis of variance – why it is more important than ever. Annals of Statistics, 33(1):1–31, 2005.

[2] A. Gelman and J. Hill. Data analysis using regression and multilevel/hierarchical models. Cambridge University Press, Boston, MA, USA, 2007.

[3] A. Gelman, J. Hill, and M. Yajima. Why we (usually) don't have to worry about multiple comparisons. Journal of Research on Educational Effectiveness, 5(2):189–211, 2012.

[4] A. Hector, T. Bell, Y. Hautier, F. Isbell, M. Kéry, P. B. Reich, J. van Ruijven, and B. Schmid. BUGS in the analysis of biodiversity experiments: Species richness and composition are of similar importance for grassland productivity. PLoS ONE, 6(3):e17434, 2011.

[5] S. S. Qian and Z. Shen. Ecological applications of multilevel analysis of variance. Ecology, 88(10):2489– 2495, 2007.

[6] A. Gelman and E. Loken. The garden of forking paths: Why multiple comparisons can be a problem, even when there is no "fishing expedition" or "p-hacking" and the research hypothesis was posited ahead of time. Department of Statistics, Columbia University, 2013.

Bayesian Multi-level Regression

Bayesian, multilevel models for grouped data

- group level intercepts
- group level intercepts with group level covariate
- group level slopes and intercepts

The simple, Bayesian set-up

Deterministic model:

$$g(\boldsymbol{\theta}, x_i)$$

Stochastic model:

$$\underbrace{[\boldsymbol{\theta}, \sigma^2 | y_i]}_{\text{posterior}} \propto \overbrace{\underbrace{[y_i | g(\boldsymbol{\theta}, x_i), \sigma^2]}_{\text{likelihood}} \underbrace{[\boldsymbol{\theta}]}_{\text{priors}}}^{\text{joint}}$$

Draw the DAG.

Recall that

$$\underbrace{[\boldsymbol{\theta}, \sigma^2 | y_i]}_{\text{posterior}} \propto \overbrace{[y_i, \boldsymbol{\theta}, \sigma^2]}^{\text{joint}}$$

Hierarchical models: “ modeling parameters”

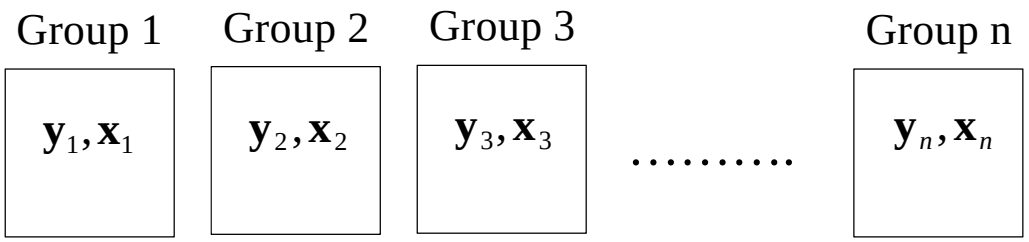
$$
\begin{aligned}
[\theta_1, \boldsymbol{\theta}_2, \boldsymbol{\alpha}, y_i, \sigma^2] \quad &\propto \quad [y_{ij} | g(\theta_1, \theta_{2,j}, x_{ij}), \sigma_1^2] \\
&\times \quad [\theta_{2,j} | h(\alpha_1, \alpha_2, u_j), \sigma_2^2] \\
&\times \quad [\theta_1, \boldsymbol{\theta}_2, \boldsymbol{\alpha}, \boldsymbol{\sigma}^2]
\end{aligned}
$$

Draw the DAG.

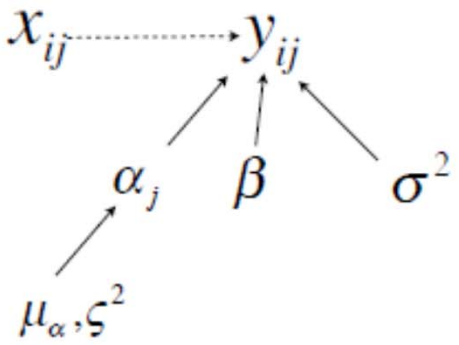
Steps in Bayesian analysis

1. Compose joint distribution of observed and unobserved quantities.
2. Factor joint distribution into sensible parts.
3. Use factored joint distribution to write:
    1. JAGS code *or*
    2. Own MCMC sampler
        1. Write full-conditional distributions
        2. Choose sampling method for each full-conditional
4. Check model
5. Make inference

The problem

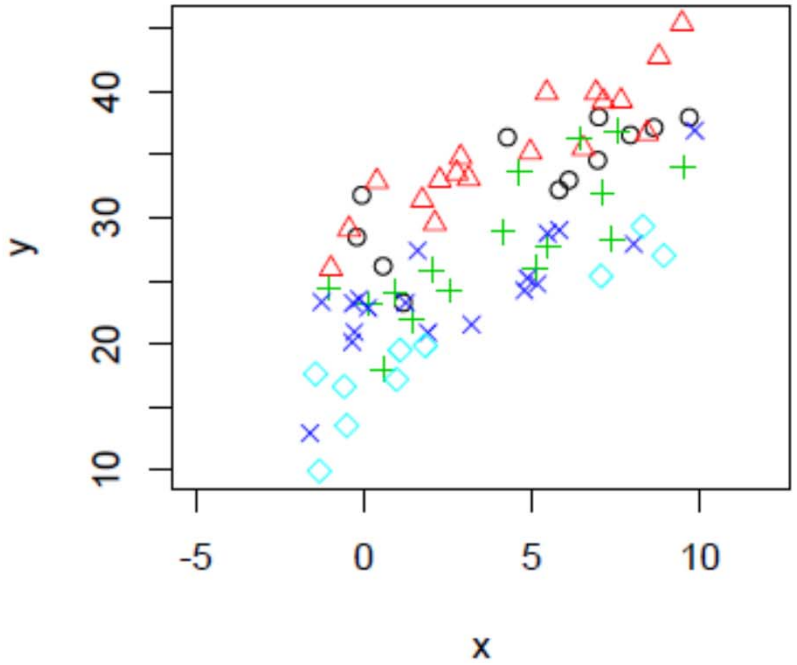

Group 1
Group 2
Group 3
Group n
$\mathbf{y}_1, \mathbf{x}_1$
$\mathbf{y}_2, \mathbf{x}_2$
$\mathbf{y}_3, \mathbf{x}_3$
.....
$\mathbf{y}_n, \mathbf{x}_n$

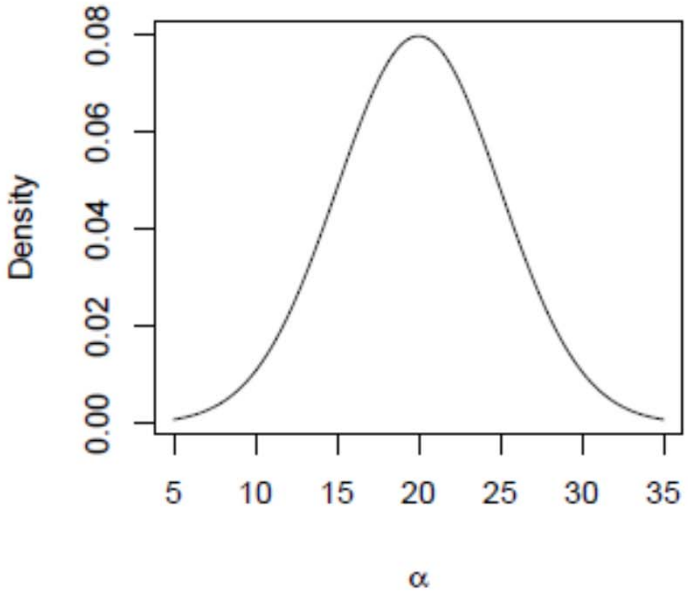
We can model the intercept:



$$[\beta, \boldsymbol{\alpha}, \sigma^2, \mu_\alpha, \varsigma^2, |\mathbf{y}] \propto \prod_{i=1}^{n_j} \prod_{j=1}^{J} \text{normal}\left(y_{ij} | \alpha_j + \beta x_{ij}, \sigma^2\right)$$
$$\times \text{normal}\left(\alpha_j | \mu_\alpha, \varsigma^2\right)$$
$$\times \text{normal}\left(\beta | 0, 10000\right) \text{normal}\left(\mu_\alpha | 0, 1000\right)$$
$$\times \text{inverse gamma}\left(\sigma^2 | .001, .001\right) \text{inverse gamma}\left(\varsigma^2 | .001, .001\right)$$

We seek to understand the distribution of intercepts.





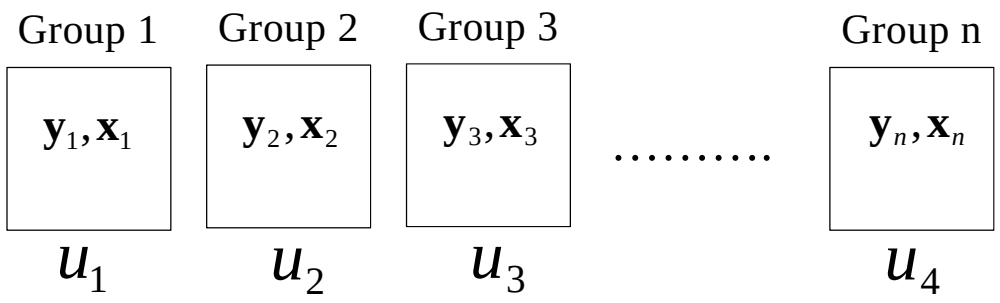
Some notation

$$\mu_{ij} = \beta_0 + \beta_1 x_{ij} + \alpha_j$$
$$y_{ij} \sim \text{normal}(\mu_{ij}, \sigma^2)$$
$$\alpha_j \sim \text{normal}(0, \varsigma^2)$$

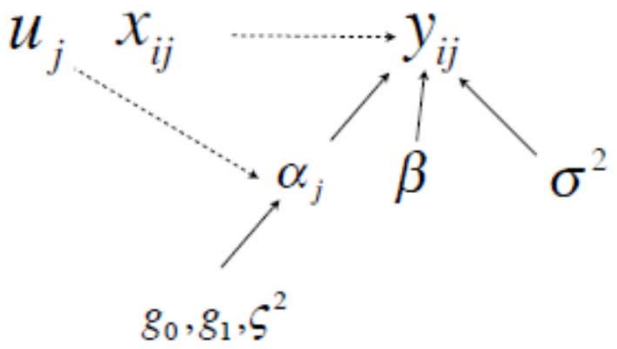
is identical to:

$$\mu_{ij} = \alpha_j + \beta_1 x_{ij}$$
$$y_{ij} \sim \text{normal}(\mu_{ij}, \sigma^2)$$
$$\alpha_j \sim (\mu_\alpha, \varsigma^2)$$

Include data on groups.



We can model the intercept as a function of group level data:

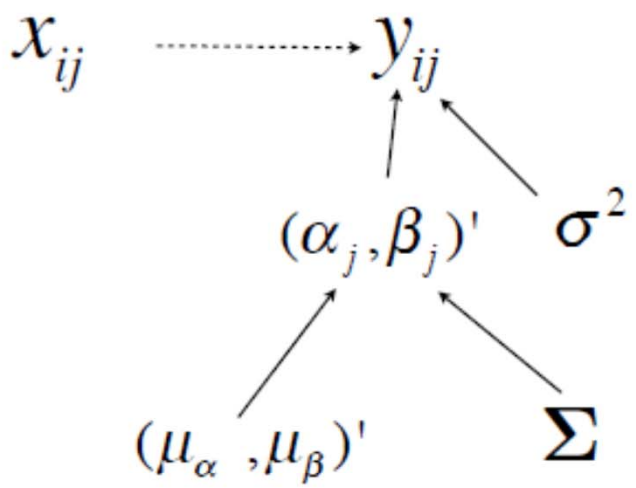


$$[\boldsymbol{\alpha}, \beta, \sigma^2, \mathrm{g}, \varsigma^2, |\mathrm{y}] \propto \prod_{i=1}^{n_j} \prod_{j=1}^{J} \mathrm{normal}\left(y_{ij} | \alpha_j + \beta x_{ij}, \sigma^2\right)$$
$$\times \mathrm{normal}\left(\alpha_j | g_0 + g_1 u_j, \varsigma^2\right)$$
$$\times \mathrm{normal}\left(\beta | 0, .001\right) \mathrm{normal}\left(g_0 | 0, 1000\right) \mathrm{normal}\left(g_1 | 0, 1000\right)$$
$$\times \mathrm{inverse\,gamma}\left(\sigma^2 | .001, .001\right) \mathrm{inverse\,gamma}\left(\varsigma^2 | .001, .001\right)$$

Indexing groups

```
model{
beta ~ dnorm(0,.0001)
sigma ~ dunif(0,50)
tau.p <- 1/sigma^2
g0 ~ dnorm(0,.0001)
g1 ~ dnorm(0,.0001)
varsigma ~ dunif(0,50)
tau.g <- 1/varsigma^2
 for (i in 1:length(y)){
  mu[i] <- alpha[group[i]]+ beta*x[i]
  y[i] ~ dnorm(mu[i],tau.p)
  }
  for(j in 1:n.group){
  mu.g[j] <- g0 + g1*u[j]
  alpha[j]~dnorm(mu.g[j],tau.g)
    }
```

Modeling intercepts *and* slopes



$$\begin{pmatrix} \alpha_j \\ \beta_j \end{pmatrix} \sim \text{multivariate normal}\left(\begin{pmatrix} \mu_\alpha \\ \mu_\beta \end{pmatrix}, \boldsymbol{\Sigma}\right)$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \varsigma_\alpha^2 & \text{Cov}(\boldsymbol{\alpha}, \boldsymbol{\beta}) \\ \text{Cov}(\boldsymbol{\alpha}, \boldsymbol{\beta}) & \varsigma_\beta^2 \end{pmatrix}, \text{Cov}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \rho \varsigma_\alpha \varsigma_\beta$$

Modeling intercepts *and* slopes

$$
\begin{aligned}
[\boldsymbol{\alpha}, \boldsymbol{\beta}, \mu_\alpha, \mu_\beta, \sigma^2, \varsigma_\alpha, \varsigma_\beta, \rho | \mathbf{y}] \quad &\propto \quad \prod_{j=1}^{J} \prod_{i=1}^{n_j} \text{normal}(y_{ij} | \alpha_j + \beta_j x_{ij}, \sigma^2) \\
&\times \quad \text{MVN}\left(\begin{pmatrix} \alpha_j \\ \beta_j \end{pmatrix} \middle| \begin{pmatrix} \mu_\alpha \\ \mu_\beta \end{pmatrix}, \boldsymbol{\Sigma} \right) \\
&\times \quad \text{priors on } \mu_\alpha, \mu_\beta, \sigma^2, \varsigma_\alpha, \varsigma_\beta, \rho
\end{aligned}
$$