Missing Data

EM Algorithm and Multiple Imputation

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Overview

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- x includes data and parameters

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- Stop the algorithm when change of estimated parameter reaches a preset threshold.

A Multinomial Example

Consider data from Rao(1965) with 197 animals multinomially distributed in four categories:

$$\mathbf{y} = (y_1, y_2, y_3, y_4) = (125, 18, 20, 34)$$

A genetic model specifies cell probabilities:

$$(\tfrac{1}{2} + \tfrac{1}{4}\pi, \tfrac{1}{4}(1-\pi), \tfrac{1}{4}(1-\pi), \tfrac{1}{4}\pi)$$

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A Multinomial Example: continued

Complete data: a multinomial population

$$\mathbf{x} = (x_1, x_2, x_3, x_4, x_5)$$

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Next we will show how EM algorithm works in this example.

A Multinomial Example: E-step

- Let $\pi^{(p)}$ be the value of π after p iterations.
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- $x_1 + x_2 = y_1 = 125$ and $\pi = \pi^{(p)}$ gives

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$$x_1^{(p)} = 125 \cdot \frac{\frac{1}{2}}{\frac{1}{2} + \frac{1}{4}\pi^{(p)}}, \qquad x_2^{(p)} = 125 \cdot \frac{\frac{1}{4}\pi^{(p)}}{\frac{1}{2} + \frac{1}{4}\pi^{(p)}}$$

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- The next step will use the complete data estimated in this step.

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And we go back to the E-step to complete the $(p+1)$-th iteration.

We start with $\pi^{(0)} = 0.5$, and the algorithm converges in eight steps:

p	$\pi^{(p)}$	$\pi^{(p)} - \pi^*$	$(\pi^{(p+1)} - \pi^*) \div (\pi^{(p)} - \pi^*)$
0	0·500000000	0·126821498	0·1465
1	0·608247423	0·018574075	0·1346
2	0·624321051	0·002500447	0·1330
3	0·626488879	0·000332619	0·1328
4	0·626777323	0·000044176	0·1328
5	0·626815632	0·000005866	0·1328
6	0·626820719	0·000000779	—
7	0·626821395	0·000000104	—
8	0·626821484	0·000000014	—

At each step we use $\pi^{(p)} = \pi^*$ and $\pi^{(p+1)} = \pi^*$ to solve for π^* as the maximum-likelihood estimate of π .

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  - Normal linear model
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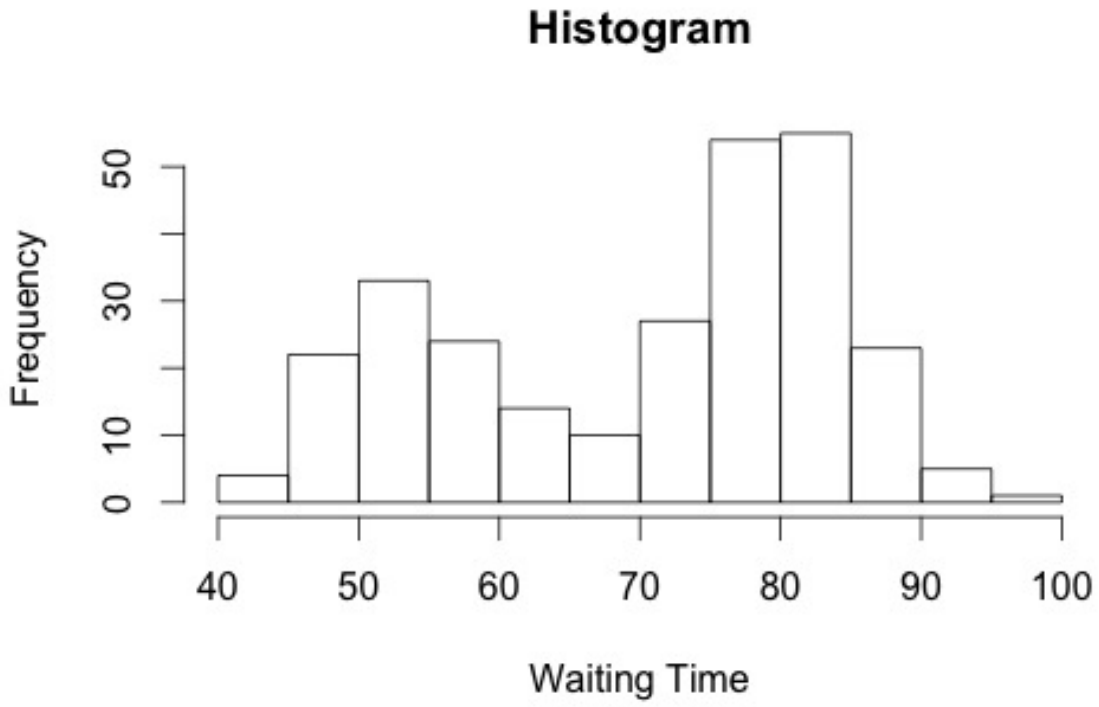
Example: Old Faithful

Waiting time between eruptions and the duration of the eruption for the Old Faithful geyser in Yellowstone National Park, Wyoming.



Old Faithful: EM Setup

$X =$ Waiting time between eruptions.
$p =$ Probability that eruption is of a shorter waiting time
$\theta = (p, \mu_1, \mu_2, \sigma_1, \sigma_2)$

$$f_X(x|\theta) = p\mathrm{N}(\mu_1, \sigma_1) + (1-p)\mathrm{N}(\mu_2, \sigma_2)$$

Define:

$$Y_i = \begin{cases} 1 & X_i \text{ has shorter waiting time} \\ 0 & X_i \text{ has longer waiting time} \end{cases}$$

$Y_i \sim \mathrm{Bern}(p)$ and Y_i is missing data

Old Faithful: E step

$$Y_i | X_i, \theta^{(k)} \sim \text{Bin}(1, p_i^{(k)})$$

where

$$p_i^{(k)} = \frac{p^{(k)} \text{N}(\mu_1^{(k)}, \sigma_1^{(k)})}{p^{(k)} \text{N}(\mu_1^{(k)}, \sigma_1^{(k)}) + (1 - p^{(k)}) \text{N}(\mu_2^{(k)}, \sigma_2^{(k)})} \text{ at } X_i$$

Thus,

$$\text{E}(Y_i | X_i, \theta^{(k)}) = p_i^{(k)}$$

Old Faithful: M step

$$L(\theta|X,Y) = \prod_{i=1}^{n} p^{Y_i} \left[\mathrm{N}(\mu_1,\sigma_1)\right]^{Y_i} (1-p)^{1-Y_i} \left[\mathrm{N}(\mu_2,\sigma_2)\right]^{1-Y_i}$$

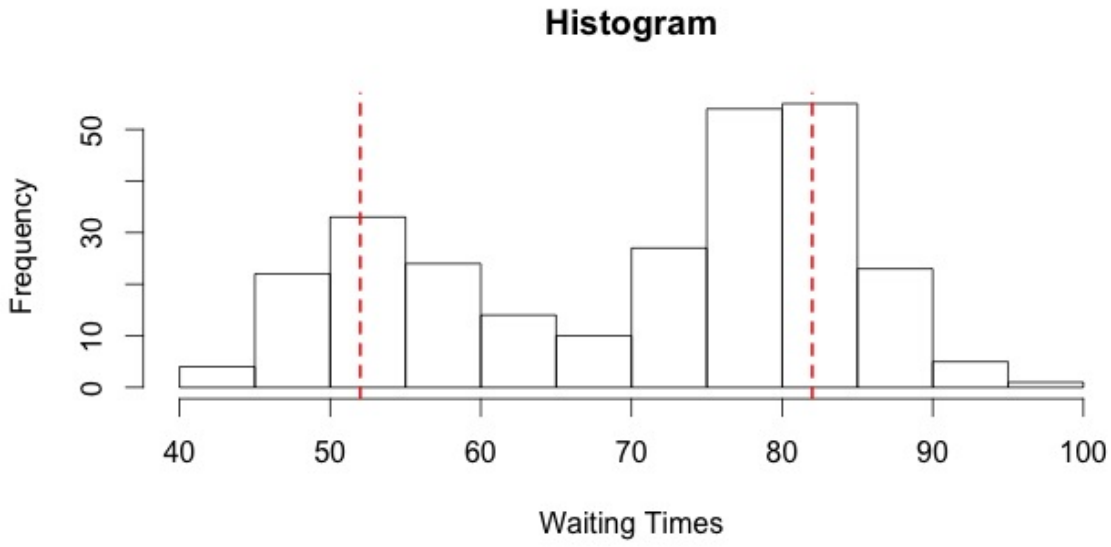
Take log and replace Y_i with $p_i^{(k)}$, then maximize for θ.

$$p^{(k+1)} = \frac{1}{n}\sum_{i=1}^{n} p_i^{(k)}$$

$$\mu_1^{(k+1)} = \frac{\sum_{i=1}^{n} p_i^{(k)} X_i}{\sum_{i=1}^{n} p_i^{(k)}} \qquad \sigma_1^{(k+1)^2} = \frac{\sum_{i=1}^{n} p_i^{(k)} (X_i - \mu_1^{(k+1)})^2}{\sum_{i=1}^{n} p_i^{(k)}}$$

$$\mu_2^{(k+1)} = \frac{\sum_{i=1}^{n} (1-p_i^{(k)}) X_i}{\sum_{i=1}^{n} (1-p_i^{(k)})} \qquad \sigma_2^{(k+1)^2} = \frac{\sum_{i=1}^{n} (1-p_i^{(k)}) (X_i - \mu_1^{(k+1)})^2}{\sum_{i=1}^{n} (1-p_i^{(k)})}$$

Old Faithful: Starting Values



$$p^{(0)} = 0.5, \mu_1^{(0)} = 52, \mu_2^{(0)} = 82, \sigma_1^{(0)} = 4, \sigma_2^{(0)} = 4$$

Estimates

```
em <- function(W,s){

Ep <- s[1]*dnorm(W, s[2], sqrt(s[4]))/
   (s[1]*dnorm(W, s[2], sqrt(s[4]))+
   (1-s[1])*dnorm(W, s[3], sqrt(s[5])))

 s[1] <- mean(Ep)
 s[2] <- sum(Ep*W) / sum(Ep)
 s[3] <- sum((1-Ep)*W) / sum(1-Ep)
 s[4] <- sum(Ep*(W-s[2])^2) / sum(Ep)
 s[5] <- sum((1-Ep)*(W-s[3])^2) / sum(1-Ep)
 s
}
```

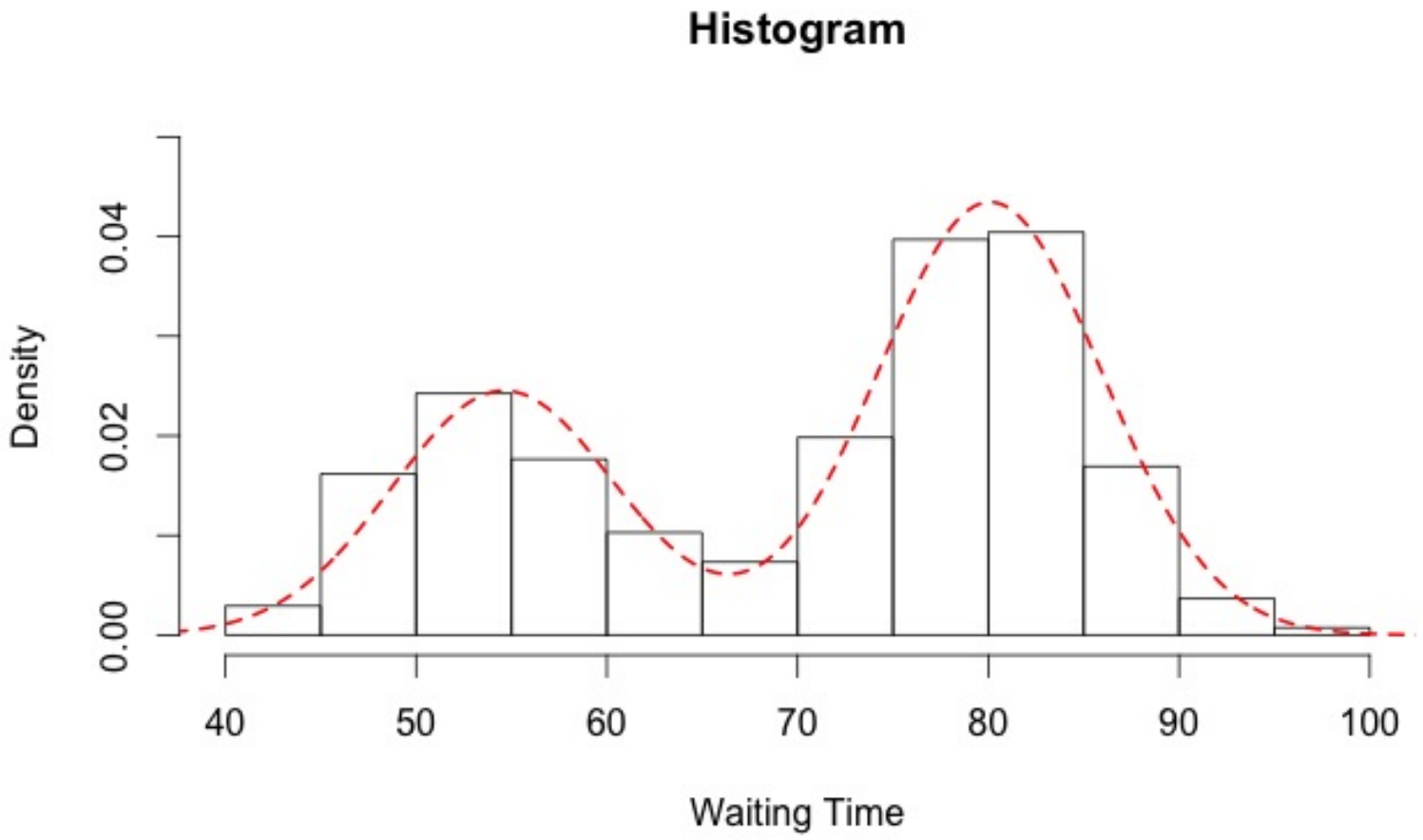
Iterations

```
iter <- function(W, s){
 s1 <- em(W,s)
 cutoff <- rep(.0001,5)
  if(sum(s-s1>cutoff) > 0){
    s = s1
    iter(W,s)
  }
 else s1
 }
```

Implementation

```
> W <- faithful$waiting
> s <- c(0.5, 52, 82, 16, 16)
> iter(W,s)
[1]  0.3608866 54.6148747 80.0910812 34.4714038 34.4301694
```

Estimated Distribution



Multiple Imputation Overview

- Imputation is 'filling in' missing data with plausible values
- Rubin (1987) conceived a method, known as multiple imputation, for valid inferences using the imputed data
  - Multiple Imputation is a Monte Carlo method where missing values are imputed $m > 1$ separate times (typically $3 \leq m \leq 10$)
- Multiple Imputation is a three step procedure:
  - **Imputation**: Impute the missing entries in the data m seperate times
  - **Analysis**: Analyze each of the m complete data sets seperately
  - **Pooling**: Combine the m analysis results into a final result

Theory

- Q is some statistic of scientific interest in the population
  - Could be population means, regression coefficients, population variances, etc.
  - Q cannot depend on the particular sample
- We estimate Q by $\hat{Q}$ or $\bar{Q}$ along with a valid estimate of its uncertainty
  - $\hat{Q}$ is the estimate from complete data
  - $\hat{Q}$ accounts from sampling uncertainty
  - $\bar{Q}$ is a pooled estimate
  - $\bar{Q}$ accounts for sampling and missing data uncertainty

$\hat{Q}$ and $\bar{Q}$

- $\hat{Q}_i$ is our estimate from the i-th imputation
  - $\hat{Q}_i$ has k parameters
  - $\hat{Q}_i$ $k \times 1$ column vector

- To compute $\bar{Q}$ we simply average over all m imputations

$$\bar{Q} = \frac{1}{m} \sum_{i=1}^{m} \hat{Q}_i$$

Within/Between Imputation Variance

- Let U be the squared standard error of Q
- We estimate U by $\bar{U}$
  - $\hat{U}_i$ is the covariance matrix of $\hat{Q}_i$, our estimate from the i-th imputation

$$\bar{U} = \frac{1}{m} \sum_{i=1}^{m} \hat{U}_i$$

  - Notice: $\hat{U}_i$ is the variance **within** the estimate $\hat{Q}_i$
- Let B be the variance **between** the m complete-data estimates:

$$B = \frac{1}{m-1} \sum_{i=1}^{m} (\hat{Q}_i - \bar{Q})(\hat{Q}_i - \bar{Q})^\intercal$$

Total Variance

- Let T denote the total variance of $\bar{Q}$
  - $T \neq \bar{U} + B$
- T is computed by:

$$T = \bar{U} + B + \frac{B}{m}$$
$$= \bar{U} + (1 + \frac{1}{m})B$$

where $\frac{B}{m}$ is simulation error.

Summary

- $T = \bar{U} + (1 + \frac{1}{m})B$
- The intuition for T is as follows:
  - $\bar{U}$ is the variance in $\bar{Q}$ caused by the fact that we are using a sample.
  - B is the variance caused by the fact that there were missing values in our sample
  - $\frac{B}{m}$ is the simulation variance from the fact that $\bar{Q}$ is based on a finite m.

Tests and Confidence Intervals

- For multiple imputation to be valid, we must first assume, that with complete data

$$(\hat{Q} - Q)/\sqrt{U} \sim \mathcal{N}(0, 1)$$

would be appropriate

- Then, after our multiple imputation steps, tests and confidence intervals are based on a Student's t-approximation

$$(\bar{Q} - Q)/\sqrt{T} \sim t_v$$

$$v = (m-1)\left[1 + \frac{\bar{U}}{(1+\frac{1}{m})B}\right]^2$$

Imputation Step

- The validity of inference relies on how imputations are generated.
- Rubin proposed three conditions under which multiple imputation inference is "randomization-valid"

$$E(\bar{Q}|Y) = \hat{Q} \tag{1}$$
$$E(\bar{U}|Y) = U \tag{2}$$
$$(1 + \frac{1}{m})E(B|Y) \geq V(\bar{Q}) \tag{3}$$

- **Result**: If the complete-data inference is randomization valid and the our imputation procedure satisfies the proceeding conditions, then our finite m multiple imputation inference is also randomization-valid.
  - Not always easy to get these conditions, often requires Bayesian approach

Simple Example in R

- The mice package does multiple imputation in R

```
> library(mice)
> head(nhanes)
  age  bmi hyp chl
1   1   NA  NA  NA
2   2 22.7   1 187
3   1   NA   1 187
4   3   NA  NA  NA
5   1 20.4   1 113
6   3   NA  NA 184
```

- We're interested in the simple linear regression of BMI on Age
  - Q $= \beta_1$ from $E(BMI|Age) = \beta_0 + Age^{\intercal}\beta_1$

Simple Example in R

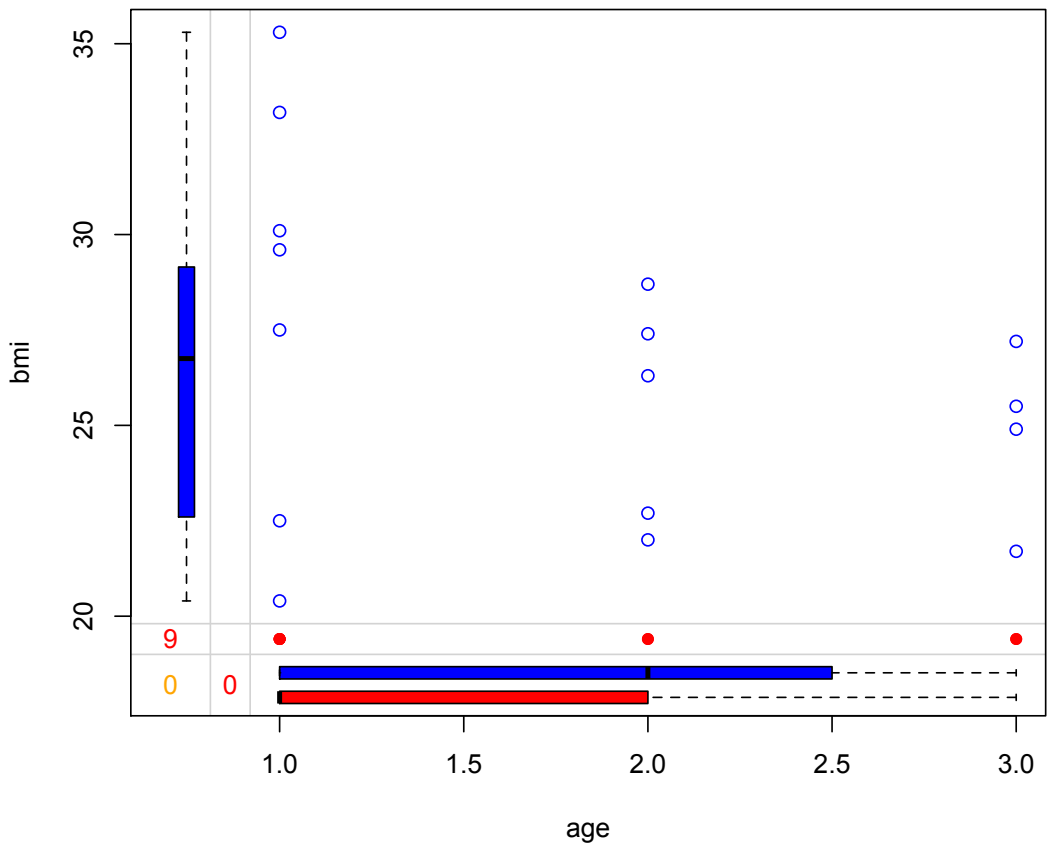
- The *mice* package has some nice functions that summarize our missing data

```
> md.pattern(nhanes)
   age hyp bmi chl
13   1   1   1   1  0
 1   1   1   0   1  1
 3   1   1   1   0  1
 1   1   0   0   1  2
 7   1   0   0   0  3
     0   8   9  10 27
```

- Above, the output shows we have 13 complete rows, 1 missing only BMI, 3 missing Cholesterol, 1 missing Hypertension and BMI, and 7 missing Hypertension, BMI, and Cholesterol.

Simple Example in R

```
> library(VIM)
> marginplot(nhanes[c(1,2)], col = c("blue", "red",
 "orange"))
```



Imputation Methods in *mice*

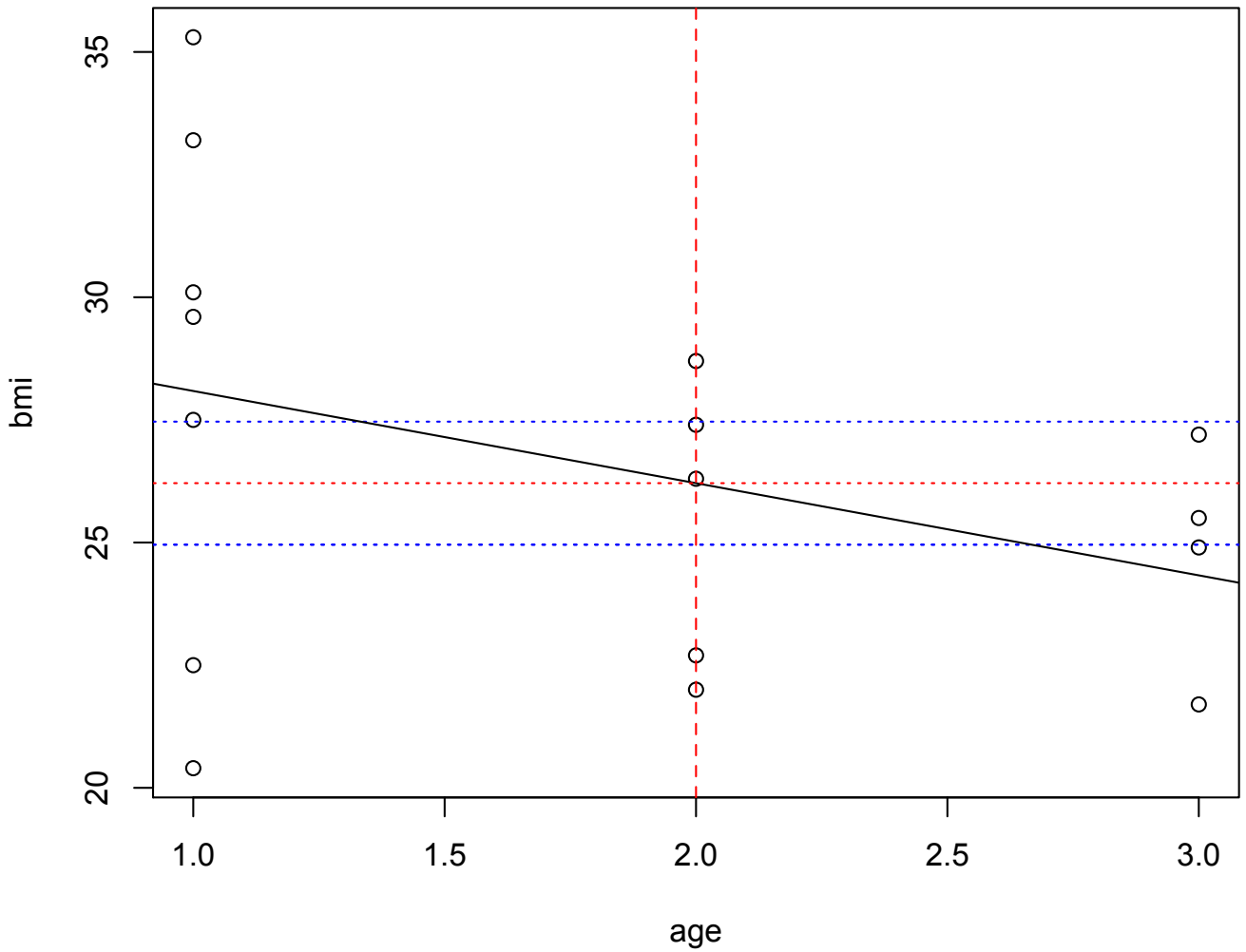
Method	Description	Scale type
pmm	Predictive mean matching	numeric
norm	Bayesian linear regression	numeric
norm.nob	Linear regression, non-Bayesian	numeric
norm.boot	Linear regression with bootstrap	numeric
mean	Unconditional mean imputation	numeric
2L.norm	Two-level linear model	numeric
logreg	Logistic regression	factor, 2 levels
logreg.boot	Logistic regression with bootstrap	factor, 2 level
polyreg	Multinomial logit model	factor $>$ 2 levels
polr	Ordered logit model	ordered, $>$ 2 levels
lda	Linear discriminant analysis	factor
sample	Simple random sample	any

Imputation Approaches

- Except in trivial settings, the probability distributions that we draw from to give 'proper' multiple imputation tend to be complicated
  - Often requires MCMC

- In our example, we will use an approach called Predictive Mean Matching
  - Calculate $\hat{Y}_{observed} = \{\hat{y}_i = x_i^\intercal \beta : i \in Observed\}$
  - For $y_{missing}$, calculate $\hat{Y}_{missing} = \{\hat{y}_j = x_i^\intercal \beta : j \in Missing, i \in Observed\}$
  - Among our $\hat{Y}_{observed}$, locate the observation whose predicted value is closet to $\hat{y}_j$ for all $j \in Missing$ and impute that value
  - For $m = n$, impute random draws the from the n observations whose predicted value is closest to $\hat{y}_m$

Predictive Mean Matching



mice() for Multiple Imputation

- We use the *mice*() function to run multiple imputation using predictive mean modeling

```
> imp.nhanes<-mice(nhanes,m=5,method="pmm",print=FALSE,seed=8053)
```

- We can look at our imputed values for BMI and notice these are sampled observed values

```
> imp.nhanes$imp$bmi
      1    2    3    4    5
1  22.5 25.5 27.2 22.0 33.2
3  26.3 30.1 30.1 35.3 33.2
16 22.5 25.5 29.6 30.1 28.7
21 25.5 35.3 27.5 30.1 35.3

> na.omit(nhanes$bmi)
 [1] 22.7 20.4 22.5 30.1 22.0 21.7 28.7 29.6 27.2 26.3
[11] 35.3 25.5 33.2 27.5 24.9 27.4
```

$\bar{Q}$

- We fit five separate linear regression models

```
> fit<-with(imp.nhanes, lm(bmi~age))
```

- We average our estimates using *pool*() from the *mice* package

```
> est<-pool(fit)
> est$qbar
(Intercept)         age
      30.24       -2.06
```

Inference

- Using the *mice*() package, we can make valid inferences

```
> summary(est)
                   est       se          t       df
(Intercept) 30.242705 2.944000 10.272659 4.719653
age         -2.060628 1.288428 -1.599336 7.255069
                Pr(>|t|)     lo 95      hi 95 nmis
(Intercept) 0.0002086732 22.537686 37.9477244   NA
age         0.1522742652 -5.085695  0.9644395    0
                  fmi    lambda
(Intercept) 0.7087166 0.6068631
age         0.5605660 0.4541020
```

- $p \approx .15 \implies$ no age effect

Simple Example in R

Questions?