STAT406- Methods of Statistical Learning Lecture 22

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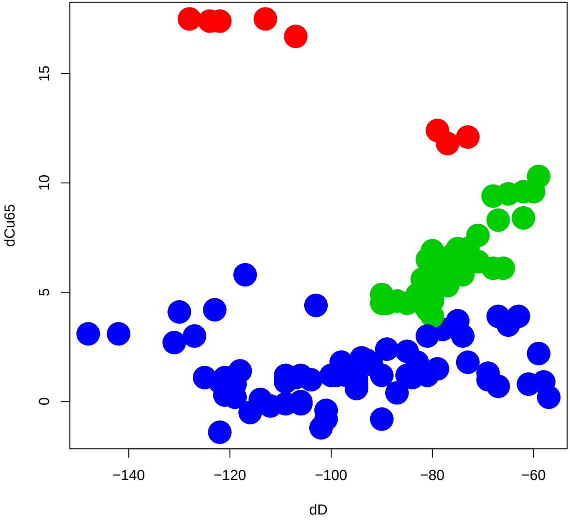
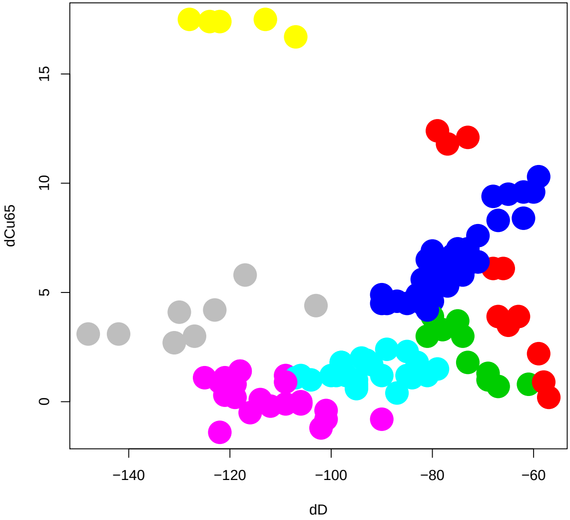
`mclust` initialization issues

```
> a <- dget('mclust-fail-dump.txt')
> # n = 130, p = 3 (one is labels, so effectively p = 2)
>
> library(mclust)
>
> # run model-based clustering with features (dCu65, dD)
> m1 <- Mclust(a[,2:3])
> # no. of clusters found (based on BIC)
> m1$G
[1] 3
>
> # run model-based clustering with features (dD, dCu65)
> m2 <- Mclust(a[,3:2])
> # no. of clusters found (based on BIC)
> m2$G
[1] 7
```

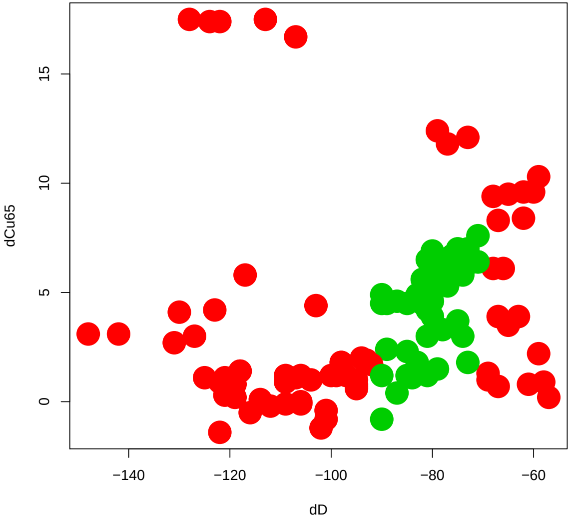

(dCu65, dD)



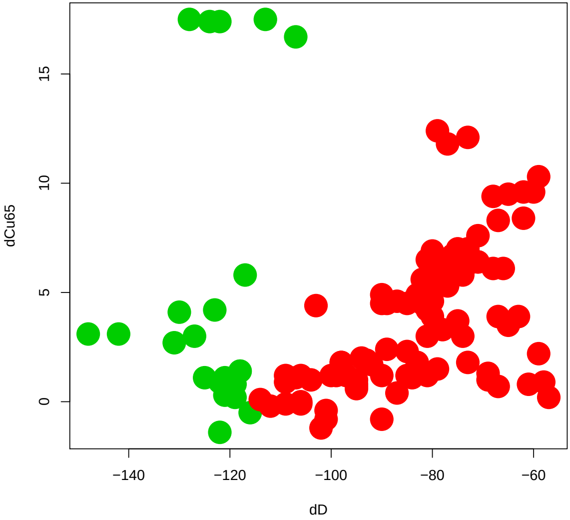
(dD, dCu65)



Initial (dCu65, dD)



Initial (dD, dCu65)



EM algorithm

- Let $\mathbf{X}$ the observed data, $\mathbf{X}^m$ the missing data
- Let $\ell\left(\mathbf{X}, \mathbf{X}^m; \boldsymbol{\theta}\right)$ the log-likelihood of the complete data

1. Initiate with $\hat{\boldsymbol{\theta}}^{(0)}$
2. Compute $H\left(\boldsymbol{\theta}\right) = E\left(\ell\left(\mathbf{X}, \mathbf{X}^m; \boldsymbol{\theta}\right) \middle| \mathbf{X}, \hat{\boldsymbol{\theta}}^{(j)}\right)$
3. Find $\hat{\boldsymbol{\theta}}^{(j+1)} = \arg\max_{\boldsymbol{\theta}} H\left(\boldsymbol{\theta}\right)$
4. $j \leftarrow j + 1$ and repeat from step 2.

EM algorithm

Bottlenecks:

- Computing

$$H(\boldsymbol{\theta}) = E\left(\ell(\mathbf{X}, \mathbf{X}^m; \boldsymbol{\theta}) \Big| \mathbf{X}, \hat{\boldsymbol{\theta}}^{(j)}\right)$$

- Maximizing $H(\boldsymbol{\theta})$

Why does EM work?

- Data: $(\mathbf{X}, \mathbf{X}^m)$
- Full log-likelihood $\ell_0(\mathbf{X}, \mathbf{X}^m; \boldsymbol{\theta})$

$$P\left(\mathbf{X}^m \middle| \mathbf{X}; \boldsymbol{\theta}\right) = \frac{P\left((\mathbf{X}, \mathbf{X}^m); \boldsymbol{\theta}\right)}{P(\mathbf{X}; \boldsymbol{\theta})}$$

and then

$$\ell(\mathbf{X}; \boldsymbol{\theta}) = \ell_0(\mathbf{X}, \mathbf{X}^m; \boldsymbol{\theta}) - \ell_1\left(\mathbf{X}^m \middle| \mathbf{X}; \boldsymbol{\theta}\right)$$

Why does EM work?

- Hence, for any $\tilde{\boldsymbol{\theta}}$

$$\ell\left(\mathbf{X};\boldsymbol{\theta}\right) = E\left[\ell_0\left(\mathbf{X},\mathbf{X}^m;\boldsymbol{\theta}\right)\Big|\mathbf{X},\tilde{\boldsymbol{\theta}}\right] -$$

$$E\left[\ell_1\left(\mathbf{X}^m\middle|\mathbf{X};\boldsymbol{\theta}\right)\Big|\mathbf{X},\tilde{\boldsymbol{\theta}}\right]$$

- The M-step increases the first term by finding the max over $\boldsymbol{\theta}$
- The second term can only decrease when $\boldsymbol{\theta}$ moves away from $\tilde{\boldsymbol{\theta}}$

Missing data & EM

- In general, Gaussian distributions yield closed forms for the maximizers of the expected likelihood
- The method is more general, but requires “specialized software”
- Probably the second most common use of the EM algorithm is **imputation**.

Missing data & EM

	Bahamas	Bangladesh	Belarus	Belgium	Bolivia	Botswana
3249	1	NA	1	2	1	1
3254	1	1	3	1	1	1
3347	1	1	1	2	NA	1
3357	1	3	NA	1	NA	1
3372	2	1	1	2	1	1
3379	NA	1	1	1	1	1

Missing data & EM

- Just using the complete observations might waste a lot of information

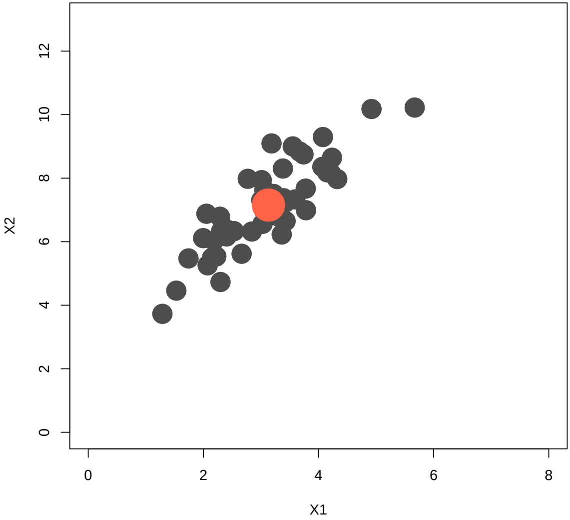
```
> sum(complete.cases(X))
[1] 145

> dim(X)
[1] 368  77
```

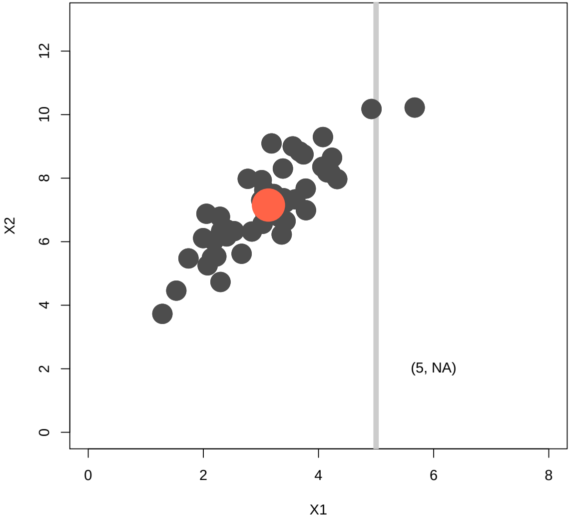
Missing data & EM

- Using only complete records is "sub-optimal"
- Imputation is the process by which one "fills in" missing entries
- Simplest one is to replace `NA`'s with the average of the observed values

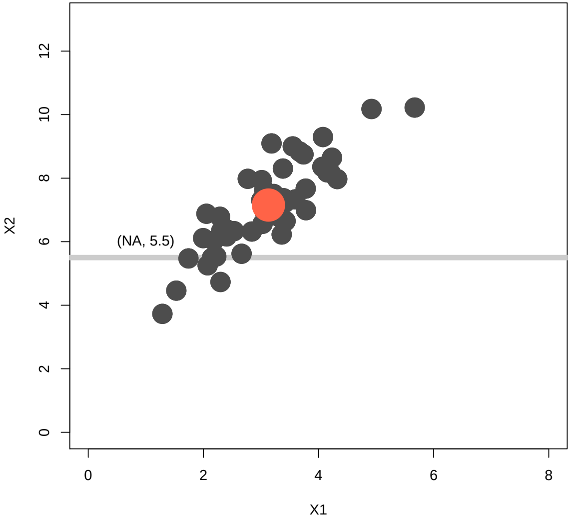
Imputation + EM



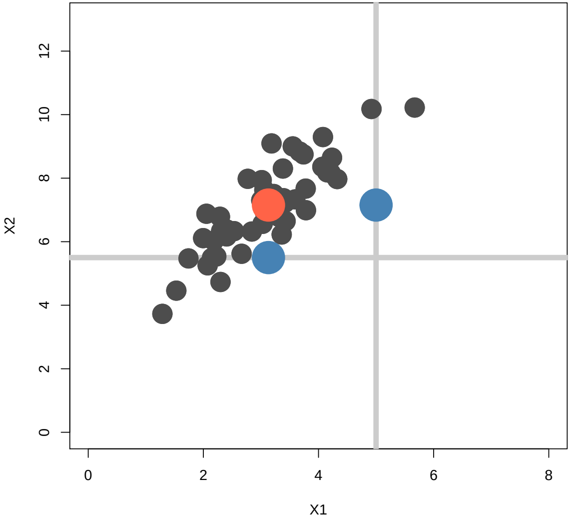
Imputation + EM



Imputation + EM



“Marginal imputation”



Imputation + EM

- If we assume that $\mathbf{X}$ is Gaussian

$$\log f\left(\mathbf{X};\theta\right) = -\frac{1}{2}\log\left(|\mathbf{\Sigma}|\right) - \frac{1}{2}\left(\mathbf{X}-\boldsymbol{\mu}\right)^\top \mathbf{\Sigma}^{-1}\left(\mathbf{X}-\boldsymbol{\mu}\right)$$

$$\ell\left(\mathbf{X}_1,\ldots,\mathbf{X}_n;\boldsymbol{\theta}\right) = \sum_{i=1}^{n}\log f\left(\mathbf{X}_i;\boldsymbol{\theta}\right)$$

Imputation + EM

- Suppose that

$$\mathbf{X}_i = (X_1, X_2)^\top = (\texttt{NA}, X)^\top$$

- We need to compute

$$E\left[\log f\left((X_1, X_2)^\top ; \boldsymbol{\theta}\right) \middle| X_2, \boldsymbol{\theta}^{(k)}\right]$$

which is not easy, but possible

Imputation + EM

- One can show that

$$E\left[\log f\left((X_1, X_2)^\top ; \boldsymbol{\theta}\right) \Big| X_2, \boldsymbol{\theta}^{(k)}\right] =$$

$$C\left(\boldsymbol{\theta}^{(k)}\right) + \log f\left(\left(\tilde{X}_1, X_2\right)^\top ; \boldsymbol{\theta}\right)$$

where

$$\tilde{X}_1 = \mu_1^{(k)} + \sigma_{12}^{(k)} \left[\sigma_{22}^{(k)}\right]^{-1} \left(X_2 - \mu_2^{(k)}\right)$$

Imputation + EM

- where

$$\boldsymbol{\theta}^{(k)} = \left(\boldsymbol{\mu}^{(k)}, \boldsymbol{\Sigma}^{(k)} \right)$$

and

$$\boldsymbol{\mu}^{(k)} = \begin{pmatrix} \mu_1^{(k)} \\ \\ \mu_2^{(k)} \end{pmatrix} \quad \boldsymbol{\Sigma}^{(k)} = \begin{pmatrix} \sigma_{11}^{(k)} & \sigma_{12}^{(k)} \\ \\ \sigma_{21}^{(k)} & \sigma_{22}^{(k)} \end{pmatrix}$$

Imputation + EM

- Hence, maximizing

$$H(\boldsymbol{\theta}) = E\left(\ell(\mathbf{X}, \mathbf{X}^m; \boldsymbol{\theta}) \middle| \mathbf{X}, \hat{\boldsymbol{\theta}}^{(j)}\right)$$

is the same as maximizing

$$\ell\left(\mathbf{X}, \tilde{\mathbf{X}}; \boldsymbol{\theta}\right)$$

which is the usual Gaussian MLE for $\boldsymbol{\theta}$, but using $\mathbf{X}$ and $\tilde{\mathbf{X}}$.

Imputation + EM

- Hence, we get

$$\mu^{(k+1)} = \frac{1}{n}\sum_{i=1}^{n} \tilde{\mathbf{X}}_i$$

and

$$\boldsymbol{\Sigma}^{(k+1)} = \frac{1}{n}\sum_{i=1}^{n} \left(\tilde{\mathbf{X}}_i - \mu^{(k+1)}\right)\left(\tilde{\mathbf{X}}_i - \mu^{(k+1)}\right)^\top$$

Imputation + EM