



UiO : Matematisk institutt

Det matematisk-naturvitenskapelige fakultet

STK-4051/9051 Computational Statistics Spring 2022 Chaper 4 (part 1)

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Missing data

- Data often (partly) missing
- Censored data (ex 2.3): Time to event not completely known
- Classification of images: Classes to some pixels known, unknown for most of the pixels
- Clustering: Data to be allocated to groups, group membership unknown
- If complete data, Likelihood “often easy”
- Likelihood becomes complicated when data are missing
- Notation:
 - $Y = (X, Z)$ are complete data
 - X observed,
 - Z missing
 - $X = M(Y)$ is observed part
 - Have $f_Y(y|\theta)$
 - Want $\max_{\theta} f_X(x|\theta)$

$$f_X(x|\theta) = \int_{y:M(y)=x} f_Y(y|\theta) dy = \int_Z f_Y(x, z|\theta) dz$$

$$f_X(x|\theta) = \frac{f_Y(y|\theta)}{f_{Z|x}(z|x, \theta)}$$

EM algorithm

- Main idea: Iterate between
 - Estimate Z given X, θ (E-step)
 - Estimate θ given (X, Z) (M-step)
- Formally a bit more complicated
 - If complete data, we want to maximize $\log L(\theta|Y)$
 - $\log L(\theta|Y)$ unknown, but given a current value $\theta^{(t)}$ we can estimate it by

$$\begin{aligned} Q(\theta|\theta^{(t)}) &= E[\log L(\theta|Y) \mid x, \theta^{(t)}] \\ &= E[\log f_Y(y|\theta) \mid x, \theta^{(t)}] \\ &= \int_Z \log f_Y(y|\theta) f_{Z|x}(z|x, \theta^{(t)}) dz \end{aligned}$$

- Algorithm:
 1. E-step: Compute $Q(\theta|\theta^{(t)})$
 2. M-step: Maximize $Q(\theta|\theta^{(t)})$ wrt θ to obtain $\theta^{(t+1)}$.
 3. Return to E-step unless a stopping criterion has been met

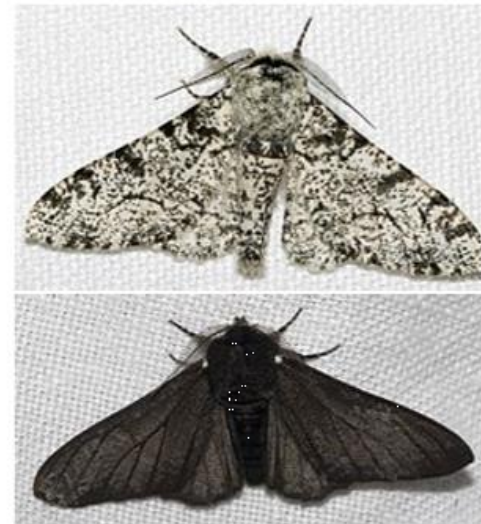
The Q function

- $$\begin{aligned} Q(\boldsymbol{\theta} | \boldsymbol{\theta}^{(t)}) &= E[\log L(\boldsymbol{\theta} | Y) \mid \boldsymbol{x}, \boldsymbol{\theta}^{(t)}] \\ &= E[\log f_Y(\boldsymbol{y} | \boldsymbol{\theta}) | \boldsymbol{x}, \boldsymbol{\theta}^{(t)}] \\ &= \int_{\boldsymbol{z}} \log f_Y(\boldsymbol{y} | \boldsymbol{\theta}) f_{\boldsymbol{z} | \boldsymbol{x}}(\boldsymbol{z} | \boldsymbol{x}, \boldsymbol{\theta}^{(t)}) d\boldsymbol{z} \end{aligned}$$

The expected value of the complete log likelihood (contains $\boldsymbol{\theta}$)
given the observed data and the current estimate of parameter ($\boldsymbol{\theta}^{(t)}$)

Peppered Moths - Example

- Color based on one single gene
- Three different alleles (C,I,T)
- C is dominant to I, and I is dominant to T
 - TT Light-colored
 - II,IT Intermediate
 - CC,CI,CT Black coloring
- Observing color, interest in frequency of C, I, T



- Assume frequencies $p_C, p_I, p_T, p_C + p_I + p_T = 1$

Color	Probability
White	p_T^2
Intermediate	$p_I^2 + 2p_I p_T$
Black	$p_C^2 + 2p_C p_I + 2p_C p_T$

- Observed $(n_T, n_I, n_C) = (341, 196, 85)$
- Complete $(n_{CC}, n_{CI}, n_{CT}, n_{II}, n_{IT}, n_{TT})$

Options	Count
CC	1
CI (IC)	2
CT (TC)	2
II	1
IT (TI)	2
TT	1

Peppered Moths - Likelihood

- Complete data ($n_{CC}, n_{CI}, n_{CT}, n_{II}, n_{IT}, n_{TT}$)
- Complete likelihood (multinomial distribution)

$$\begin{aligned}
 f_Y(\mathbf{y}|\mathbf{p}) &= \frac{n!}{n_{CC}!n_{CI}!n_{CT}!n_{II}!n_{IT}!n_{TT}!} p_C^{2n_{CC}} (2p_C p_I)^{n_{CI}} (2p_C p_T)^{n_{CT}} p_I^{2n_{II}} (2p_I p_T)^{n_{IT}} p_T^{2n_{TT}} \\
 &= \frac{n!}{n_{CC}!n_{CI}!n_{CT}!n_{II}!n_{IT}!n_{TT}!} 2^{n_{CI}+n_{CT}+n_{IT}} \times \\
 &\quad p_C^{2n_{CC}+n_{CI}+n_{CT}} p_I^{2n_{II}+n_{CI}+n_{IT}} p_T^{2n_{TT}+n_{CT}+n_{IT}}
 \end{aligned}$$

- Complete log-likelihood

$$\begin{aligned}
 \log\{f_Y(\mathbf{y}|\mathbf{p})\} &= \log\left(\frac{n!}{n_{CC}!n_{CI}!n_{CT}!n_{II}!n_{IT}!n_{TT}!}\right) + \\
 &\quad [n_{CI} + n_{CT} + n_{IT}] \log(2) + [2n_{CC} + n_{CI} + n_{CT}] \log(p_C) + \\
 &\quad [2n_{II} + n_{CI} + n_{IT}] \log(p_I) + [2n_{TT} + n_{CT} + n_{IT}] \log(p_T)
 \end{aligned}$$

- $Q(\mathbf{p}|\mathbf{p}^{(t)}) = E[\log\{f_Y(\mathbf{y}|\mathbf{p})\} | n_C, n_I, n_T, \mathbf{p}^{(t)}]$
- Note: First term do not depend on $\mathbf{p} = (p_C, p_I, p_T)$, not needed in the optimization step!

Peppered Moths – updating E & M

- Complete log-likelihood

$$\begin{aligned}
 Q(\mathbf{p}|\mathbf{p}^{(t)}) = & \text{Const} + E[n_{CI} + n_{CT} + n_{IT}|\mathbf{p}^{(t)}] \log(2) + \\
 & E[2n_{CC} + n_{CI} + n_{CT}|\mathbf{p}^{(t)}] \log(p_C) + \\
 & E[2n_{II} + n_{CI} + n_{IT}|\mathbf{p}^{(t)}] \log(p_I) + \\
 & E[2n_{TT} + n_{CT} + n_{IT}|\mathbf{p}^{(t)}] \log(p_T)
 \end{aligned}$$

$$E[N_{CC}|n_C, n_I, n_T, \mathbf{p}^{(t)}] = n_{CC}^{(t)} = \frac{n_C(p_C^{(t)})^2}{(p_C^{(t)})^2 + 2p_C^{(t)}p_I^{(t)} + 2p_C^{(t)}p_T^{(t)}}$$

Expectation

- Updating:

$$p_C^{(t+1)} = \frac{2n_{CC}^{(t)} + n_{CI}^{(t)} + n_{CT}^{(t)}}{2n}$$

$$p_I^{(t+1)} = \frac{2n_{II}^{(t)} + n_{IT}^{(t)} + n_{CI}^{(t)}}{2n}$$

Maximization

$$p_T^{(t+1)} = \frac{2n_{TT}^{(t)} + n_{CT}^{(t)} + n_{IT}^{(t)}}{2n},$$

- MoTh_EM.R

$$E[N_{CC}|n_C, n_I, n_T, \mathbf{p}^{(t)}] = n_{CC}^{(t)} = \frac{n_C(p_C^{(t)})^2}{(p_C^{(t)})^2 + 2p_C^{(t)}p_I^{(t)} + 2p_C^{(t)}p_T^{(t)}}$$

X could be either C, T, or I

$$E(N_{CC}|n_C, n_I, n_T, \mathbf{p}^{(t)}) = n_C \cdot P(CC|CX, \mathbf{p}^{(t)})$$

$$= n_C \cdot \frac{P(CC \& CX|\mathbf{p}^{(t)})}{P(CX|\mathbf{p}^{(t)})}$$

$$= n_C \frac{P(CC|\mathbf{p}^{(t)})}{P(CC|\mathbf{p}^{(t)}) + P(CI|\mathbf{p}^{(t)}) + P(CT|\mathbf{p}^{(t)})}$$

$$P(CC) = p_C^2$$

$$P(CI) = 2p_C p_I$$

$$P(CT) = 2p_C p_T$$

Insert to get result

Moths in R

Data = (85, 196, 341)

```

> show(c(p.old, l.old, NA))
[1] 0.3333333 0.3333333 0.3333333 0.0000000      NA
> more = TRUE
> while(more) {
+   n = allele.e(x, p)
+   p = allele.m(x, n)
+   l = loglik(p, n)
+   more = abs(l-l.old) > eps
+   R = sum((p-p.old)^2)/sum(p.old^2)
+   more = R > eps
+   show(c(p, l, R))
+   l.old = l
+   p.old = p
+ }
[1] 0.08199357 0.23740622 0.68060021 -90.55303903 0.57890393
[1] 0.071248952 0.197869614 0.730881433 -68.467059735 0.007993122
[1] 7.085204e-02 1.903604e-01 7.387876e-01 -6.526257e+01 2.058264e-04
[1] 7.083746e-02 1.890227e-01 7.401398e-01 -6.474409e+01 6.163093e-06
[1] 7.083693e-02 1.887869e-01 7.403762e-01 -6.465487e+01 1.894317e-07
[1] 7.083691e-02 1.887454e-01 7.404177e-01 -6.463926e+01 5.851928e-09
>
> ## OUTPUT
> p      # FINAL ESTIMATE FOR ALLELE PROBABILITIES (p.c, p.i, p.t)
[1] 0.07083691 0.18874537 0.74041772

```

Convergence EM

- Iterations increases log likelihood

- Jensen's inequality

$$\ell(\boldsymbol{\theta}|\mathbf{x}) = \log f_X(\mathbf{x}|\boldsymbol{\theta})$$

- For convex $f(x)$, we have:

$$f(E(X)) \leq E(f(X))$$

- Convergence order $\beta > 0$:

How fast
iteration $x^{(t)}$
approaches
the true
solution x^*

$$\epsilon^{(t)} = x^{(t)} - x^*$$

$$\lim_{t \rightarrow \infty} |\epsilon^{(t)}| \rightarrow 0$$

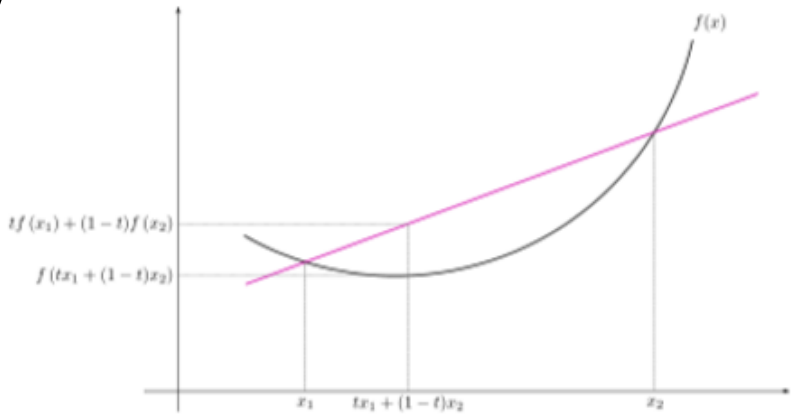
$$\lim_{t \rightarrow \infty} \frac{|\epsilon^{(t+1)}|}{|\epsilon^{(t)}|^\beta} = c$$

Jensen's inequality

- Convex functions

$$f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$$

for $t \in [0, 1]$



- Finite form

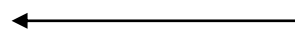
$$f\left(\sum t_i x_i\right) \leq \sum t_i f(x_i), \quad t_i \text{ positive, } \sum t_i = 1$$

- Infinite form ($g(\cdot)$ non-negative, integrable):

$$f\left(\frac{1}{b-a} \int_a^b g(x) dx\right) \leq \frac{1}{b-a} \int_a^b f(g(x)) dx$$

- Probabilistic form ($g(\cdot)$ density):

$$f(E^g[X]) \leq E^g[f(X)]$$



I'll prove this next week in exercise

Iterations increase the value of, $\ell(\theta|\mathbf{x}) = \log(f_X(\mathbf{x}|\theta))$

$$f_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}, \theta) = \frac{f_Y(\mathbf{y}|\theta)}{f_X(\mathbf{x}|\theta)}$$

$$\Downarrow$$

$$\log f_X(\mathbf{x}|\theta) = \log f_Y(\mathbf{y}|\theta) - \log f_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}, \theta)$$

$$\Downarrow$$

$$E[\log f_X(\mathbf{x}|\theta)] = E[\log f_Y(\mathbf{y}|\theta)] - E[\log f_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}, \theta)]$$

Any expectation

- If expectation with respect to $\mathbf{Z}|\mathbf{x}, \theta^{(t)}$,

$$\begin{aligned} \log f_X(\mathbf{x}|\theta) &= Q(\theta|\theta^{(t)}) - E[\log f_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}, \theta)|\mathbf{x}, \theta^{(t)}] \\ &= Q(\theta|\theta^{(t)}) - H(\theta|\theta^{(t)}) \end{aligned}$$

$$Q(\theta|\theta^{(t)}) = E[\log f_Y(\mathbf{y}|\theta)|\mathbf{x}, \theta^{(t)}]$$

$$H(\theta|\theta^{(t)}) = E[\log f_{\mathbf{z}|\mathbf{x}}(\mathbf{z}|\mathbf{x}, \theta)|\mathbf{x}, \theta^{(t)}]$$

Select :
Expectation with respect to the distribution the missing data have under the current estimate of the parameter

Proof: $H(\theta^{(t)}|\theta^{(t)}) \geq H(\theta|\theta^{(t)})$ for any θ

$$H(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = E[\log f_{z|x}(\mathbf{z}|x, \boldsymbol{\theta}) | x, \boldsymbol{\theta}^{(t)}]$$

$$H(\theta^{(t)}|\theta^{(t)}) - H(\theta|\theta^{(t)}) = E\{\log f_{z|x}(z|x, \theta^{(t)}) - \log f_{z|x}(z|x, \theta)\}$$

$$= E\left\{-\log \frac{f_{z|x}(z|x, \theta)}{f_{z|x}(z|x, \theta^{(t)})}\right\} \geq -\log E\left\{\frac{f_{z|x}(z|x, \theta)}{f_{z|x}(z|x, \theta^{(t)})}\right\}$$

Jensen's

$$= -\log \int \frac{f_{z|x}(z|x, \theta)}{f_{z|x}(z|x, \theta^{(t)})} f_{z|x}(z|x, \theta^{(t)}) dz$$

$$= -\log \int f_{z|x}(z|x, \theta) dz = -\log E\{1\} = 0$$

Proof of increasing likelihood

$$\log f_x(\mathbf{x}|\theta^{(t+1)}) - \log f_x(\mathbf{x}|\theta^{(t)})$$

$$= \underbrace{Q(\theta^{(t+1)}, \theta^{(t)}) - Q(\theta^{(t)}, \theta^{(t)})}_{> 0} - \underbrace{[H(\theta^{(t+1)}, \theta^{(t)}) - H(\theta^{(t)}, \theta^{(t)})]}_{\geq 0}$$

In maximization step choose the $\theta^{(t+1)}$ such that it improves the old $\theta^{(t)}$
 > 0 .

If you are not able to improve Q, you have converged

Select $\theta = \theta^{(t+1)}$ and apply result from previous page.
 Result holds for any θ in particular for $\theta = \theta^{(t+1)}$
 ≥ 0

$$H(\theta^{(t)}|\theta^{(t)}) \geq H(\theta^{(t+1)}|\theta^{(t)})$$

$$\Updownarrow$$

$$-H(\theta^{(t+1)}|\theta^{(t)}) + H(\theta^{(t)}|\theta^{(t)}) \geq 0$$

$$\log f_x(x|\theta^{(t+1)}) > \log f_x(x|\theta^{(t)})$$

Convergence order (good to know, but need not derive)

- The EM algorithm defines a mapping $\theta^{(t+1)} = \Psi(\theta^{(t)})$
- When the EM algorithm converges, $\hat{\theta} = \Psi(\hat{\theta})$
- Taylor expansion:

$$\begin{aligned}
 \epsilon^{(t+1)} &\equiv \theta^{(t+1)} - \hat{\theta} \\
 &= \Psi(\theta^{(t)}) - \Psi(\hat{\theta}) \\
 &\approx \Psi(\theta^{(t)}) - [\Psi(\theta^{(t)}) + \Psi'(\theta^{(t)})(\hat{\theta} - \theta^{(t)})] \\
 &= \Psi'(\theta^{(t)})(\theta^{(t)} - \hat{\theta}) \\
 &= \Psi'(\theta^{(t)})\epsilon^{(t)}
 \end{aligned}$$

- Convergence order β if $\lim_{t \rightarrow \infty} \frac{|\epsilon^{(t+1)}|}{|\epsilon^{(t)}|^\beta} = \rho$

- $p = 1$: $\lim_{t \rightarrow \infty} \frac{|\epsilon^{(t+1)}|}{|\epsilon^{(t)}|} = \Psi'(\hat{\theta})$, **linear convergence**

- $p > 1$: Still linear if $-\ell''(\hat{\theta}|\mathbf{x})$ is positive definite
- (Newton's method has convergence order $\beta = 2$)

Example: Mixture Gaussian clustering

- Assume $\mathbf{Y}_i = (X_i, C_i)$ are distributed according to

$$\Pr(C_i = k) = \pi_k, \quad k = 1, \dots, K$$

$$X_i | C_i = k \sim N(\mu_k, \sigma_k)$$

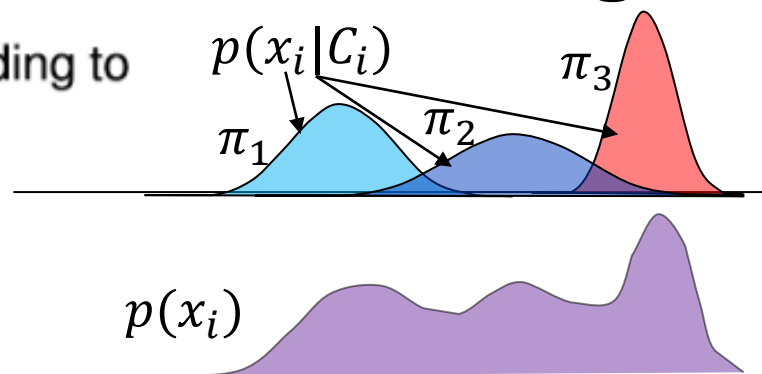
- The C_i 's are **missing**
- Complete log-density:

$$\log f(\mathbf{y}_i) = \log(\pi_{c_i}) + \log[\phi(x_i; \mu_{c_i}, \sigma_{c_i})]$$

$$= \sum_{k=1}^K I(C_i = k) [\log(\pi_k) + \log[\phi(x_i; \mu_k, \sigma_k)]]$$

- Complete log-likelihood:

$$\log f_Y(\mathbf{y}|\theta) = \sum_{i=1}^n \sum_{k=1}^K I(C_i = k) [\log(\pi_k) + \log[\phi(x_i; \mu_k, \sigma_k^2)]]$$



E-step- Mixture Gaussian

- Complete log-likelihood:

$$\log f_Y(\mathbf{y}|\boldsymbol{\theta}) = \sum_{i=1}^n \sum_{k=1}^K I(C_i = k) [\log(\pi_k) + \log[\phi(x_i; \mu_k, \sigma_k^2)]]$$

- E-step** (the C_i 's the only stochastic part)

$$Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = E \left[\sum_{i=1}^n \sum_{k=1}^K I(C_i = k) [\log(\pi_k) + \log[\phi(x_i; \mu_k, \sigma_k^2)]] | \mathbf{x}, \boldsymbol{\theta}^{(t)} \right]$$

$$= \sum_{i=1}^n \sum_{k=1}^K E[I(C_i = k | \mathbf{x}, \boldsymbol{\theta}^{(t)})] [\log(\pi_k) + \log[\phi(x_i; \mu_k, \sigma_k)]]$$

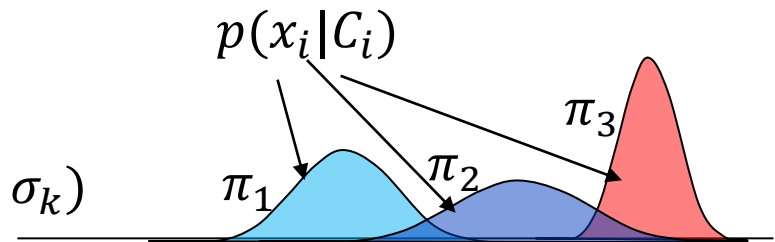
$$= \sum_{i=1}^n \sum_{k=1}^K \Pr(C_i = k | \mathbf{x}, \boldsymbol{\theta}^{(t)}) [\log(\pi_k) + \log[\phi(x_i; \mu_k, \sigma_k)]]$$

$$\Pr(C_i = k | \mathbf{x}, \boldsymbol{\theta}^{(t)}) = \frac{\pi_k^{(t)} \phi(x_i, \mu_k^{(t)}, \sigma_k^{(t)})}{\sum_l \pi_l^{(t)} \phi(x_i, \mu_l^{(t)}, \sigma_l^{(t)})}$$

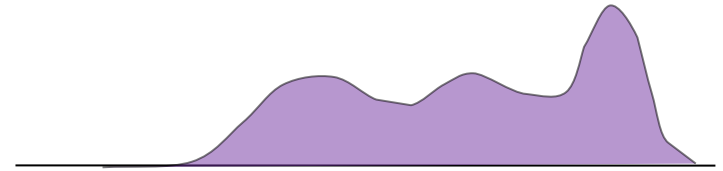
$$\Pr(C_i = k | \mathbf{x}, \boldsymbol{\theta}^{(t)}) = \frac{\pi_k^{(t)} \phi(x_i, \mu_k^{(t)}, \sigma_k^{(t)})}{\sum_l \pi_l^{(t)} \phi(x_i, \mu_l^{(t)}, \sigma_l^{(t)})}$$

$$P(C_i = k) = \pi_k$$

$$p(x_i | C_i = k) = \phi(x_i; \mu_k, \sigma_k)$$



$$p(x_i) = \sum_l \pi_l \phi(x_i; \mu_l, \sigma_l)$$



$$P(C_i = k | X_i = x_i) = \frac{p(C_i = k \& X_i = x_i)}{p(X_i = x_i)} = \frac{P(C_i = k) p(x_i | C_i = k)}{p(x_i)}$$

M-step- Mixture Gaussian

- **M-step:** Taking into account $\sum_{k=1}^K \pi_k = 1$:

$$Q_{\text{lagr}}(\theta|\theta^{(t)}) = \sum_{i=1}^n \sum_{k=1}^K \Pr(C_i = k|\mathbf{x}, \theta^{(t)}) [\log(\pi_k) + \log[\phi(x_i; \mu_k, \sigma_k^2)]] + \lambda(1 - \sum_{k=1}^K \pi_k)$$

$$\frac{\partial}{\partial \pi_k} Q_{\text{lagr}}(\theta|\theta^{(t)}) = \sum_{i=1}^n \Pr(C_i = k|\mathbf{x}, \theta^{(t)}) \pi_k^{-1} - \lambda$$

\Downarrow

$$\begin{aligned} \pi_k^{(t+1)} &= \frac{\sum_{i=1}^n \Pr(C_i = k|\mathbf{x}, \theta^{(t)})}{\lambda} \\ &= \frac{1}{n} \sum_{i=1}^n \Pr(C_i = k|\mathbf{x}, \theta^{(t)}) \end{aligned}$$

$$\sum_{k=1}^K \sum_{i=1}^n \frac{\Pr(C_i = k|x, \theta^{(t)})}{\lambda} = 1$$

$$\frac{1}{\lambda} \sum_{i=1}^n \sum_{k=1}^K \Pr(C_i = k|x, \theta^{(t)}) = 1$$

$\underbrace{\hspace{10em}}_{= 1}$

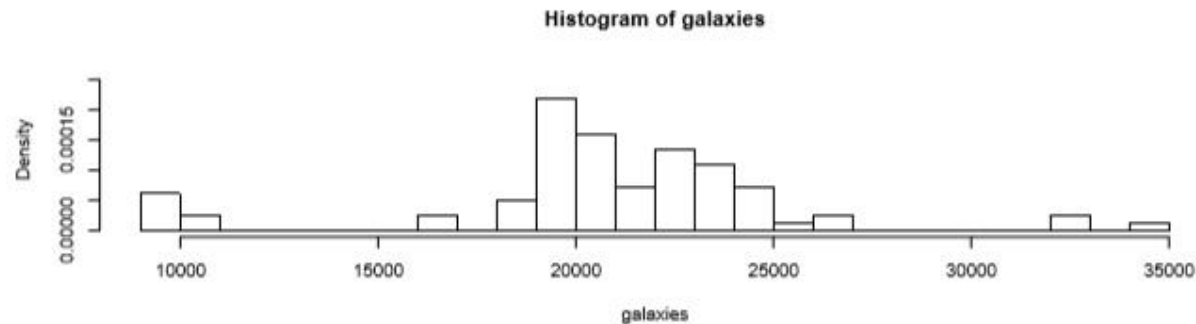
Similarly

$$\mu_k^{(t+1)} = \frac{1}{n\pi_k^{(t+1)}} \sum_{i=1}^n \Pr(C_i = k|\mathbf{x}, \theta^{(t)}) x_i$$

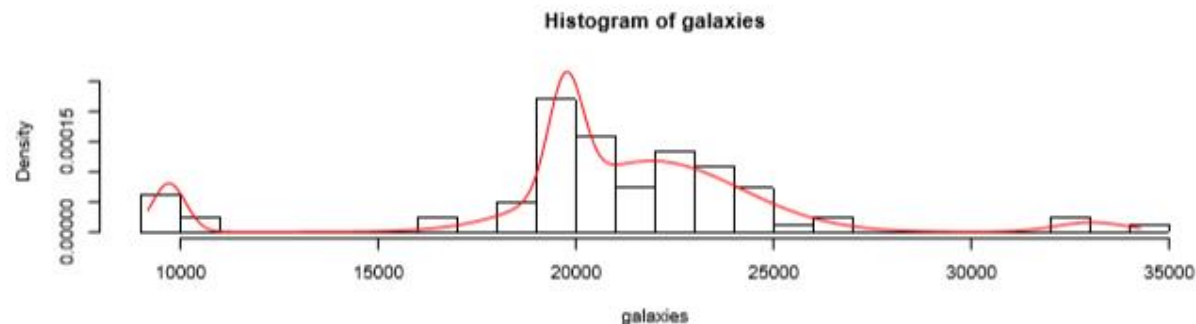
$$(\sigma_k^2)^{(t+1)} = \frac{1}{n\pi_k^{(t+1)}} \sum_{i=1}^n \Pr(C_i = k|\mathbf{x}, \theta^{(t)}) (x_i - \mu_k^{(t+1)})^2$$

Examples galaxy

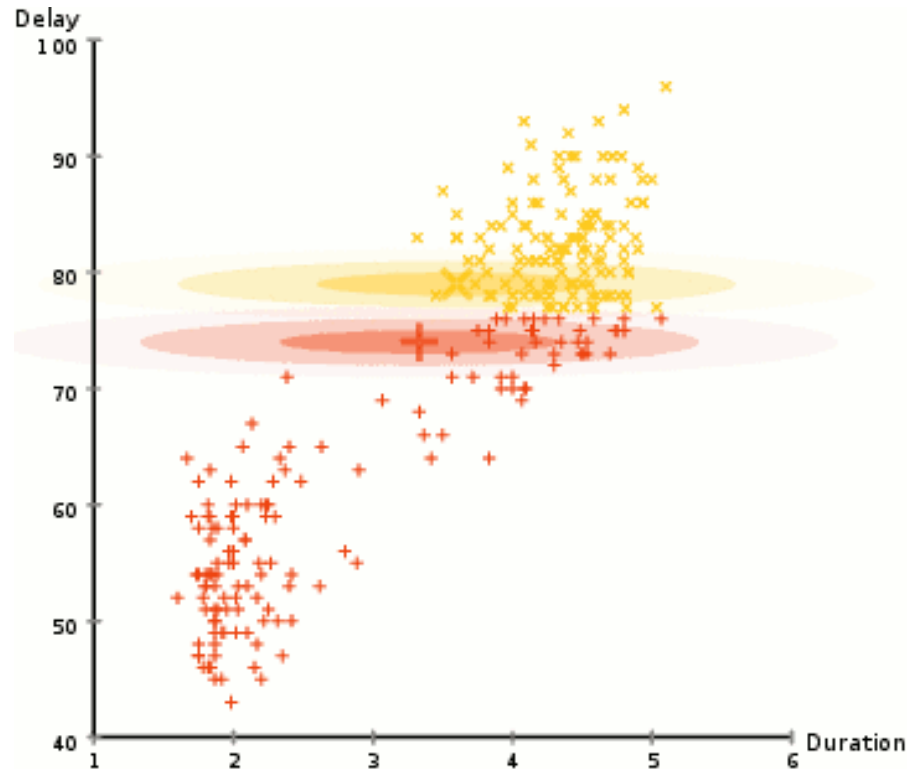
- A numeric vector of velocities in km/sec of 82 galaxies from 6 well-separated conic sections of an unfilled survey of the Corona Borealis region. Multimodality in such surveys is evidence for voids and superclusters in the far universe.



- `galaxies_EM.R`



EM clustering of Old Faithful eruption data.



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