Computational Data Analysis

Machine Learning

Yao Xie, Ph.D.

Associate Professor

Harold R. and Mary Anne Nash Early Career Professor

H. Milton Stewart School of Industrial and Systems Engineering

Gaussian Mixture Model and EM Algorithm

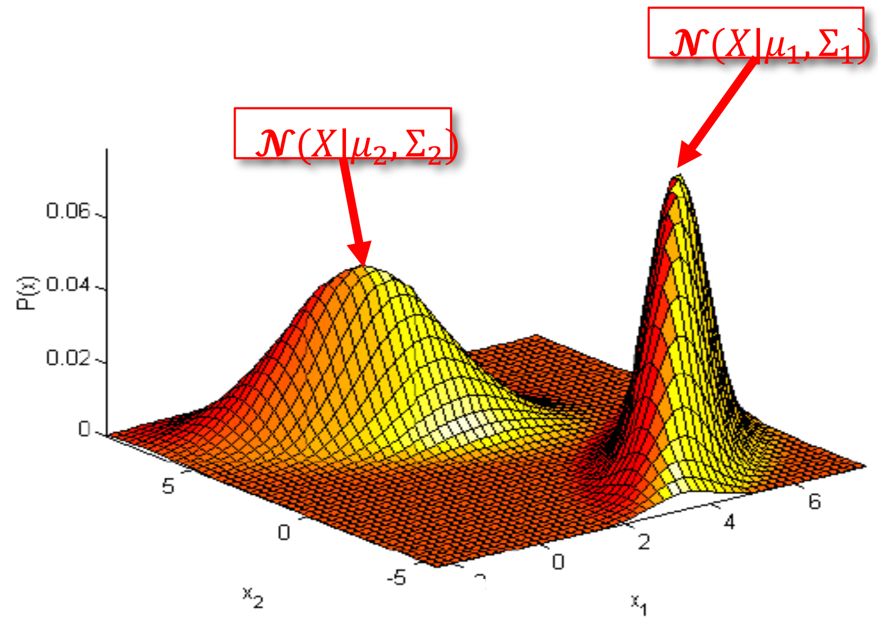
Gaussian mixture model

A density model $p(X)$ may be multi-modal: model it as a mixture of uni-modal distributions (e.g. Gaussians) for n-dimensional observations

$$\mathcal{N}(X|\mu,\Sigma) := \frac{1}{|\Sigma|^{\frac{1}{2}}(2\pi)^{\frac{n}{2}}} exp\left(-\frac{1}{2}(X-\mu)^{\top}\Sigma^{-1}(X-\mu)\right)$$

Consider a mixture of K Gaussians

$$p(X) = \sum_{k=1}^{K} \pi_k \mathcal{N}(X|\mu_k,\Sigma_k)$$



Parametric or nonparametric?

Learn $\pi_k \in (0,1), \mu_k, \Sigma_k$;

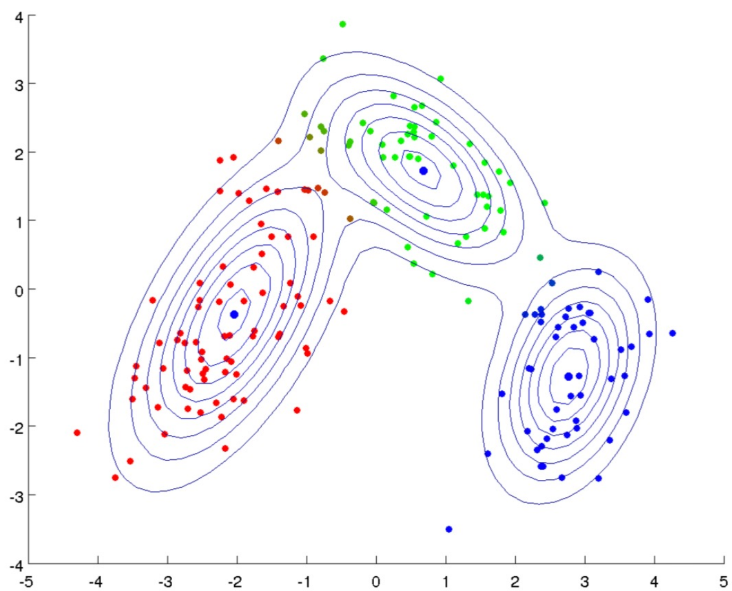
Constraint $\sum_{k=1}^{K} \pi_k = 1$

Motivation: Wine data

- The wine data set was introduced by Forina et al. (1986).
- It originally included the results of 27 chemical measurements on 178 wines made in the same region in Italy but derived from three different cultivars: Barolo, Grignolino and Barbera.
- We extract the first two principle components of the data, and aim to fit a density distribution

Mixture of 3 Gaussians

- First run PCA to reduce the dimension to 2
- $k = 1\ or\ 2\ or\ 3$
- Use τ_1^i as the proportion of red, τ_2^i proportion of green, and τ_3^i proportion of green

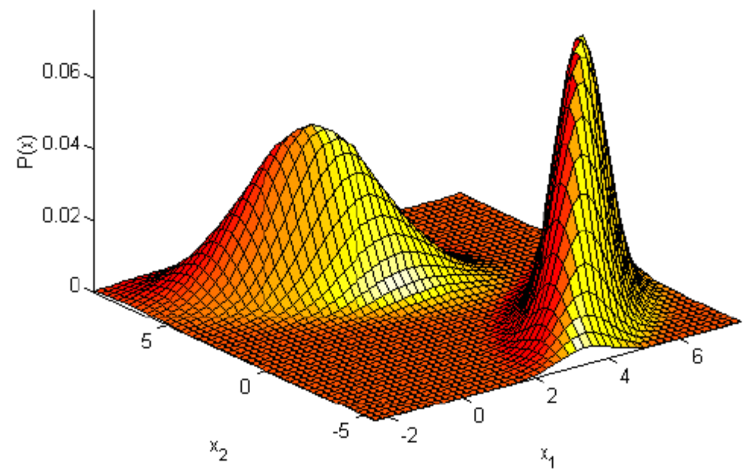


Understanding GMM

- For each data point x^i:
  - Randomly choose a mixture component, $z^i = \{1,2, \dots K\}$, with probability π_{z^i}
  - Then sample the actual value of x^i from a Gaussian distribution $\boldsymbol{\mathcal{N}}\left(x \middle| \mu_{z^i}, \Sigma_{z^i}\right)$

- Joint distribution over $p(x, z)$
- $p(x, z) = \pi_z \boldsymbol{\mathcal{N}}(x|\mu_z, \Sigma_z)$

- Marginal distribution $p(x)$
- $p(x) = \sum_{z=1}^{K} p(x, z) = \sum_{z=1}^{K} p(x|z)p(z)$



Learning Parameters

- How to learn?
- Maximum likelihood learning (let $\theta = (\pi_k, \mu_k, \Sigma_k)$, $k = 1 \ldots K$)
- $\theta^* = \text{argmax } l(\theta; D) = \log \prod_{i=1}^{m} p(x^i)$
- Write down the log-likelihood function

$$l(\theta; D) = \log \prod_{i=1}^{m} \left(\sum_{k=1}^{K} p\left(x^i, z^i = k \middle| \theta\right) \right)$$

- However, we do not know latent factors z^i thus cannot evaluate $l(\theta; D)$ directly
- Idea: imputing missing information: taking "expectation" with respect to unknown latent factors

Details of EM

- We intend to learn the parameters that maximizes the log−likelihood function

$$l(\theta; D) = \log \prod_{i=1}^{m} \left(\sum_{z^i=1}^{K} p\left(x^i, z^i \middle| \theta\right) \right)$$

- Expectation step (E-step): take expectation over posterior distribution conditioning on data: it can be shown this forms a lower bound (in the t-th iteration)

$$l(\theta; D) \geq f(\theta) = E_{q(z^1, z^2, .., z^m | \theta^t)} [\log \prod_{i=1}^{m} \left(p\left(x^i, z^i \middle| \theta\right) \right) \ ]$$

- Maximization step (M-step): how to maximize?

$$\theta^{t+1} = argmax_{\theta} \ f(\theta)$$

Bayes rule

likelihood　　　Prior

$$P(z|x) = \frac{P(x|z)P(z)}{P(x)} = \frac{P(x,z)}{\sum_{z'} P(x,z')}$$

posterior　　　normalization constant

Prior: $p(z) = \pi_z$

Likelihood: $p(x|z) = \mathcal{N}(x|\mu_z, \Sigma_z)$

Posterior: $p(z|x) = \frac{\pi_z \mathcal{N}(x|\mu_z, \Sigma_z)}{\sum_{z'} \pi_{z'} \mathcal{N}(x|\mu_{z'}, \Sigma_{z'})}$

E-step: find the posterior distribution

$q(z^1, z^2, .., z^m)$: posterior distribution of the latent variables in t-th iteration

$$q(z^1, z^2, .., z^m) = \prod_{i=1}^{m} p(z^i | x^i, \theta^t)$$

For each data point x^i, compute $p(z^i = k | x^i)$ for each k

$$\tau_k^i = p\left(z^i = k \middle| x^i, \theta^t\right) = \frac{p\left(x^i \middle| z^i = k\right) p(z^i = k)}{\sum_{k'=1..K} p(z^i = k', x^i)}$$

$$= \frac{\pi_k \mathcal{N}\left(x^i \middle| \mu_k, \Sigma_k\right)}{\sum_{k'=1..K} \pi_{k'} \mathcal{N}\left(x^i \middle| \mu_{k'}, \Sigma_{k'}\right)}$$

E-step: compute the expectation

$$f(\theta) := E_{q(z^1,z^2,\ldots,z^m)}\left[\log \prod_{i=1}^{m} p(x^i, z^i|\theta)\right] = \sum_{i=1}^{m} E_{p(z^i|x^i,\theta^t)}[\log p(x^i, z^i|\theta)]$$

$$= \sum_{i=1}^{m} E_{p(z^i|x^i,\theta^t)}[\log \pi_{z^i} \mathcal{N}(x^i|\mu_{z^i}, \Sigma_{z^i})]$$

Expand log of Gaussian density $\log\mathcal{N}(x^i|\mu_{z^i}, \Sigma_{z^i})$

$$f(\theta) = \sum_{i=1}^{m} E_{p(z^i|x^i,\theta^t)}\left[\log \pi_{z^i} - \frac{1}{2}(x^i - \mu_{z^i})^\top \Sigma_{z^i}^{-1}(x^i - \mu_{z^i}) - \frac{1}{2}\log|\Sigma_{z^i}| - \frac{n}{2}\log(2\pi)\right]$$

$$= \sum_{i=1}^{m}\sum_{k=1}^{K} \tau_k^i \left[\log \pi_k - \frac{1}{2}(x^i - \mu_k)^\top \Sigma_k^{-1}(x^i - \mu_k) - \frac{1}{2}\log|\Sigma_k| - \frac{n}{2}\log(2\pi)\right]$$

M-step: maximize $f(\theta)$

- $f(\theta) = \sum_{i=1}^{m} \sum_{k=1}^{K} \ \tau_k^i \left[\log \pi_k - \frac{1}{2}\left(x^i - \mu_k\right)^\top \Sigma_k^{-1}\left(x^i - \mu_k\right) - \frac{1}{2}\log|\Sigma_k| - \frac{n}{2}\log(2\pi)\right]$

For instance, we want to find π_k, and $\sum_{k=1}^{K} \pi_k = 1$

– Form Lagrangian

$$L = \sum_{i=1}^{m} \sum_{k=1}^{K} \ \tau_k^i [\log \pi_k + \text{other terms}] \ + \lambda(1 - \sum_{i=1}^{K} \pi_k)$$

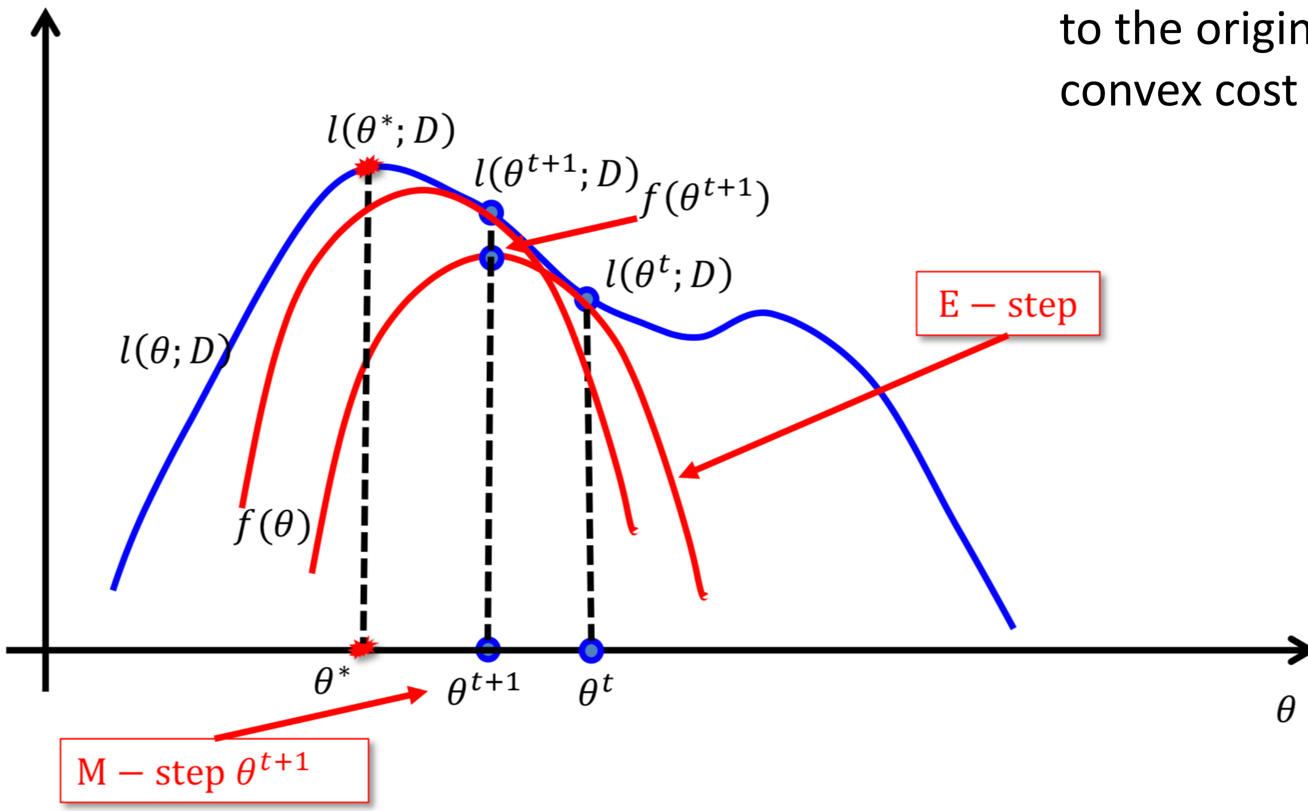
- Take partial derivative and set to 0

$$\frac{\partial L}{\partial \pi_k} = \sum_{i=1}^{m} \frac{\tau_k^i}{\pi_k} - \lambda = 0$$

$$\Rightarrow \pi_k = \frac{1}{\lambda} \sum_{i=1}^{m} \tau_k^i$$

Since $\sum_{k=1}^{K} \pi_k = 1$, $\quad \frac{1}{\lambda} \sum_{k=1}^{K} \sum_{i=1}^{m} \tau_k^i = 1 \Rightarrow \lambda = m \Rightarrow \pi_k = \frac{1}{m} \sum_{i=1}^{m} \tau_k^i$

EM graphically



Maximizing a sequence of quadratic lower bound to the original non-convex cost function.

EM algorithm

Associate the ith data and each component with a τ_k^i

Initialize (π_k, μ_k, Σ_k), $k = 1 \dots K$

Iterate the following two steps till convergence:

- Expectation step (E-step): update τ_k^i given current (π_k, μ_k, Σ_k)

$$\tau_k^i = p(z_k^i = 1 | D, \mu, \Sigma) = \frac{\pi_k \boldsymbol{\mathcal{N}}(x^i | \mu_k, \Sigma_k)}{\sum_{k'=1}^{K} \pi_{k'} \boldsymbol{\mathcal{N}}(x^i | \mu_{k'}, \Sigma_{k'})}$$

$$(k = 1 \dots K, i = 1 \dots m)$$

- Maximization step (M-step): update (π_k, μ_k, Σ_k) given τ_k^i

$$\pi_k = \frac{\sum_i \tau_k^i}{m}, \qquad \mu_k = \frac{\sum_i \tau_k^i x^i}{\sum_i \tau_k^i}$$

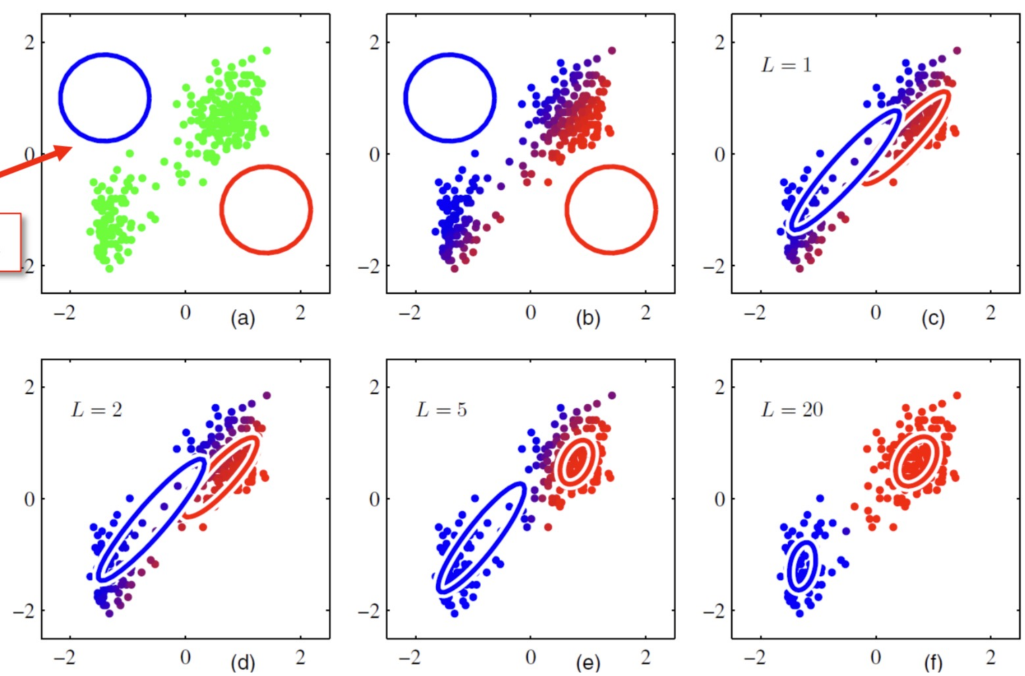
$$\Sigma_k = \frac{\sum_i \tau_k^i (x^i - \mu_k)(x^i - \mu_k)^T}{\sum_i \tau_k^i}$$

$$(k = 1 \dots K, i = 1, \dots, m)$$

Expectation-Maximization Iterations

- $k = 1 \; or \; 2$
- Use τ_1^i as the proportion of red, and τ_2^i proportion of blue
- Draw only one contour for each Gaussian component

Intialization



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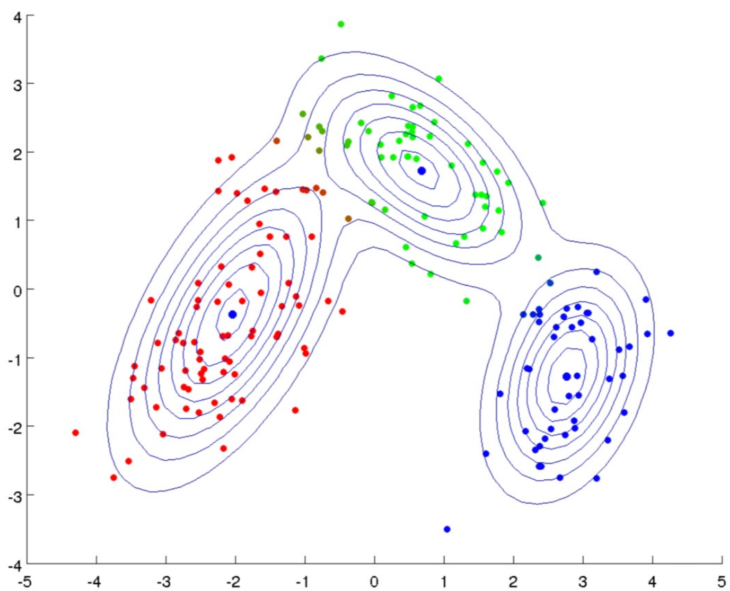
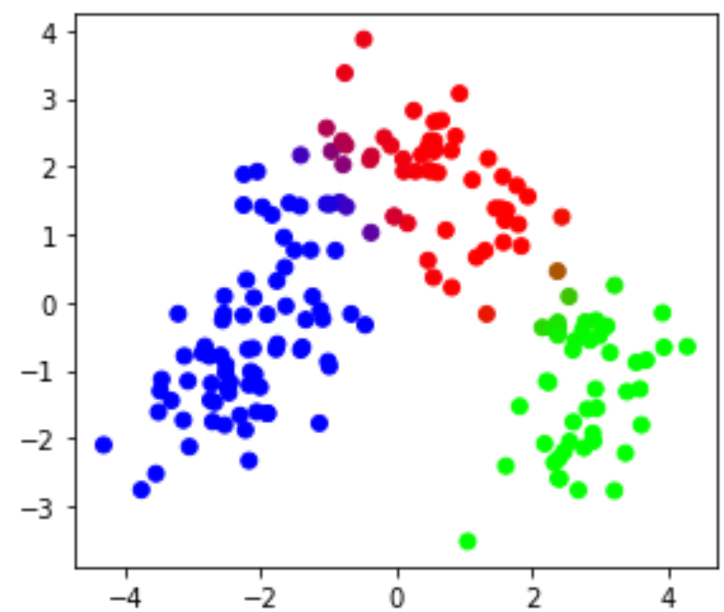
Demo: Wine data

- First run PCA to reduce the dimension to 2
- $k = 1 \; or \; 2 \; or \; 3$
- Use τ_1^i as the proportion of red, τ_2^i proportion of green, and τ_3^i proportion of green



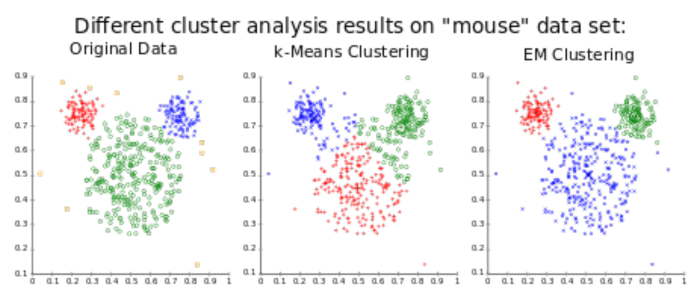


EM vs. K-means

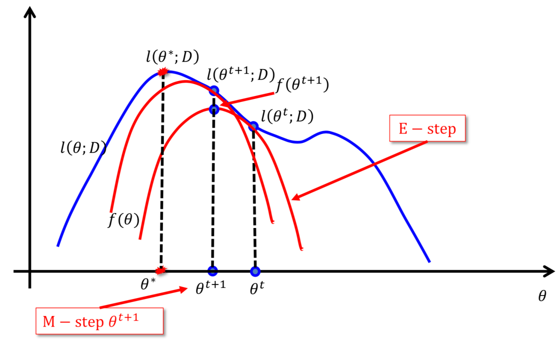
- EM algorithm for GMM can be viewed as a "soft" clustering algorithm

Assignment is in probability sense $\{\tau_k^i, k = 1, \dots, K\}$ for each data point i

- K-means:
  - "E-step": hard assignment:
    - $z^i = argmax_k (x^i - \mu_k)\, \Sigma_k^{-1} (x^i - \mu_k)$
  - "M-step", we update the means and covariance of cluster using maximum likelihood estimate:
    - $\mu_k = \frac{\sum_i \delta(z^i, k) x^i}{\sum_i \delta(z^i, k)}$
    - $\Sigma_k = \frac{\sum_i \delta(z^i, k)(x^i - \mu_k)\,(x^i - \mu_k)^T}{\sum_i \delta(z^i, k)}$



History and Theory of EM



- Dempster, Laird, Rubin 1977
- Convergence (to local solution) proof: Jeff Wu 1983
- Useful for finding **local** maximum likelihood parameters of statistical models when the equation **cannot** be solved directly (involving latent factors, missing data, mixture model)
- No guarantee to converge to true maximum likelihood estimator

Maximum Likelihood from Incomplete Data via the *EM* Algorithm

By A. P. Dempster, N. M. Laird and D. B. Rubin

Harvard University and Educational Testing Service

[Read before the Royal Statistical Society at a meeting organized by the Research Section on Wednesday, December 8th, 1976, Professor S. D. Silvey in the Chair]

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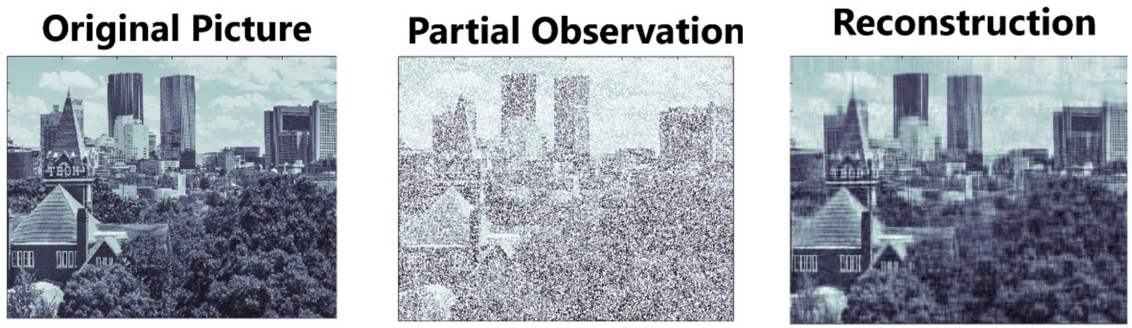
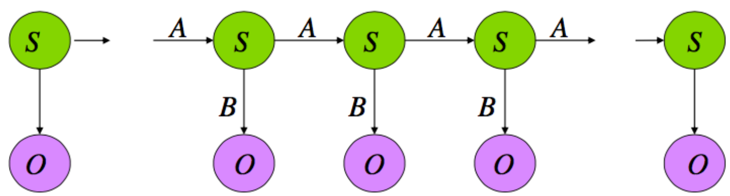
Applications



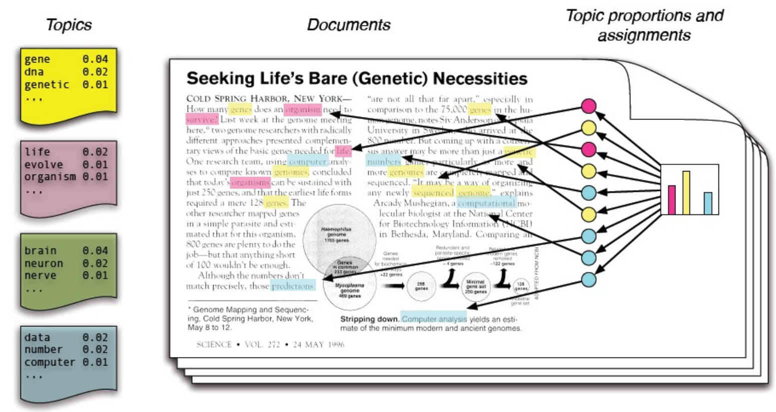
- Data clustering
- Missing data
- Estimating hidden Markov models (for dependent sequence data)
- Estimating latent factor models (in psychometrics, genetics, medical imaging)

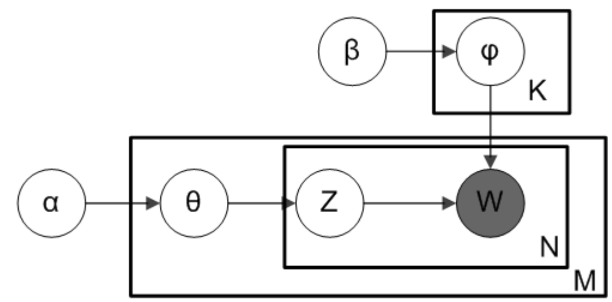


- General types of mixture model: Topic modeling

Topic models

- Mixture models over words provide an alternative to latent semantic indexing
- Instead of finding the principal components of the bag-of-words vectors, assume there are a certain number of topics which documents in the corpus can be about; each topic corresponds to a distribution over words.
- Hofmann (1999) estimated everything by EM
- Latent Dirichlet allocation (Blei *et al.*, 2003): a type of probabilistic graphical model / Bayesian model
- Estimation: finding posterior can be hard, using MCMC





(a) Choose a topic $z_{i,j} \sim \mathrm{Multinomial}(\theta_i)$.

(b) Choose a word $w_{i,j} \sim \mathrm{Multinomial}(\varphi_{z_{i,j}})$.

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SUMMARY