Lecture 10
Gaussian Mixture Models

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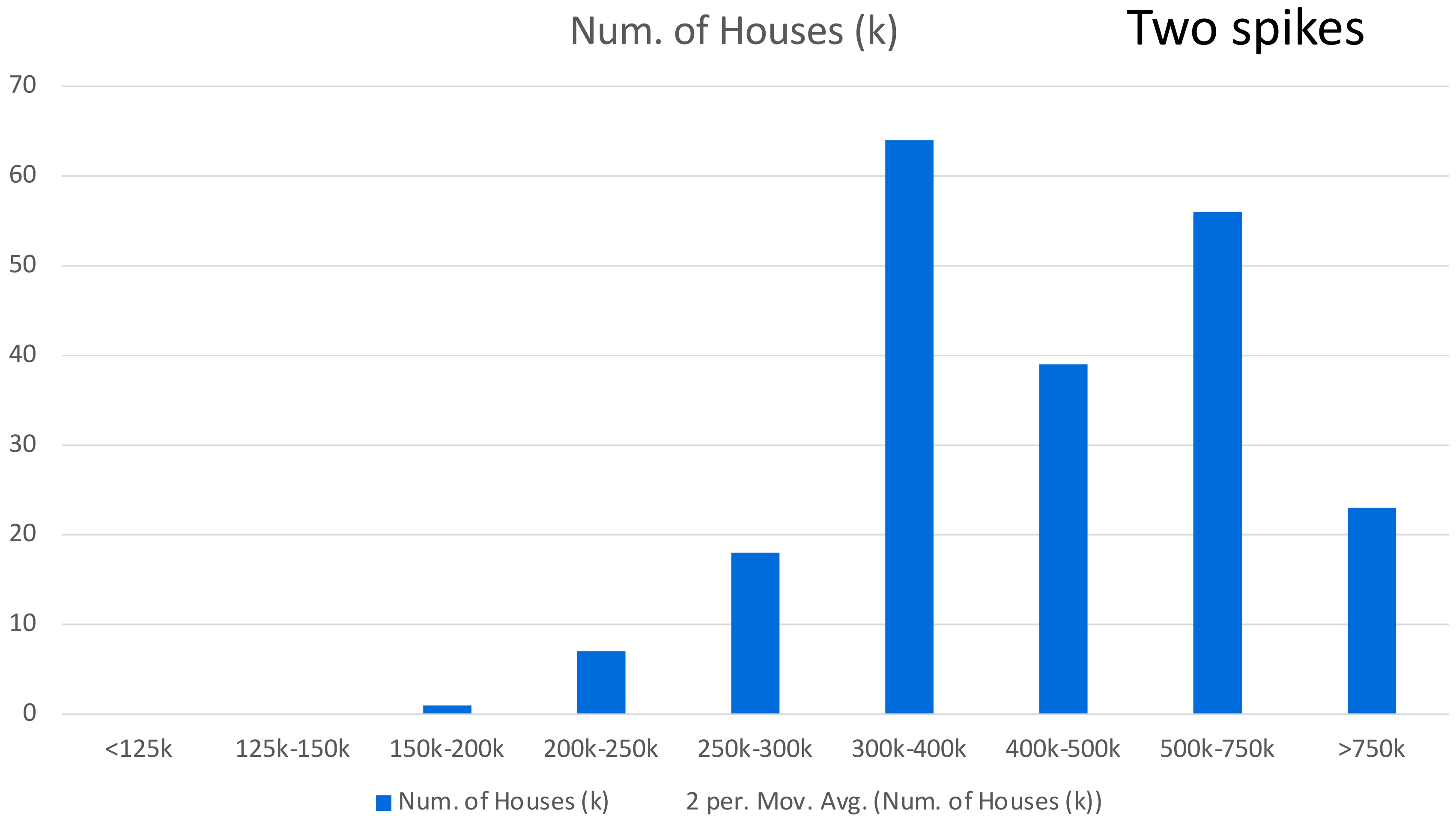
Recap

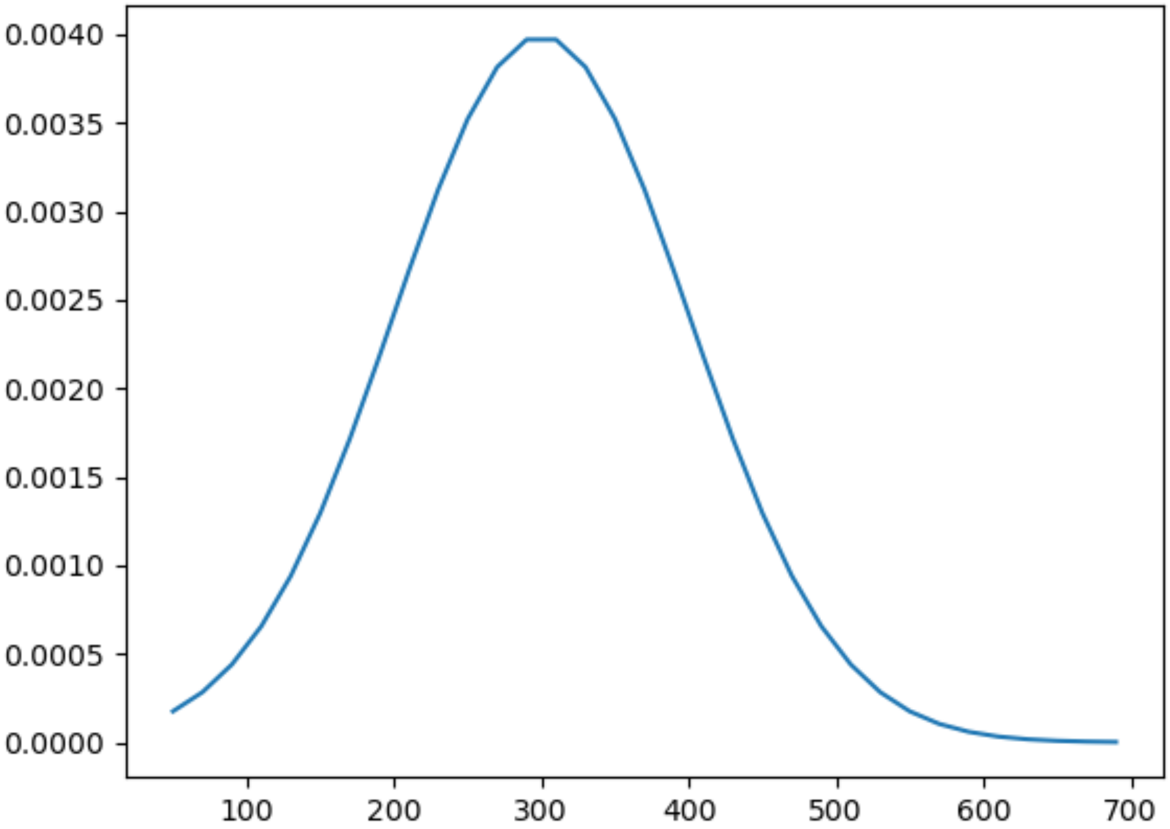
- Bayesian networks:
  - Directed acyclic graph
  - Nodes are random variables
  - arcs are probabilistic dependencies
- Examine dependence of two variables given observation: d-separation

Housing Price Pattern



Gaussian Distribution

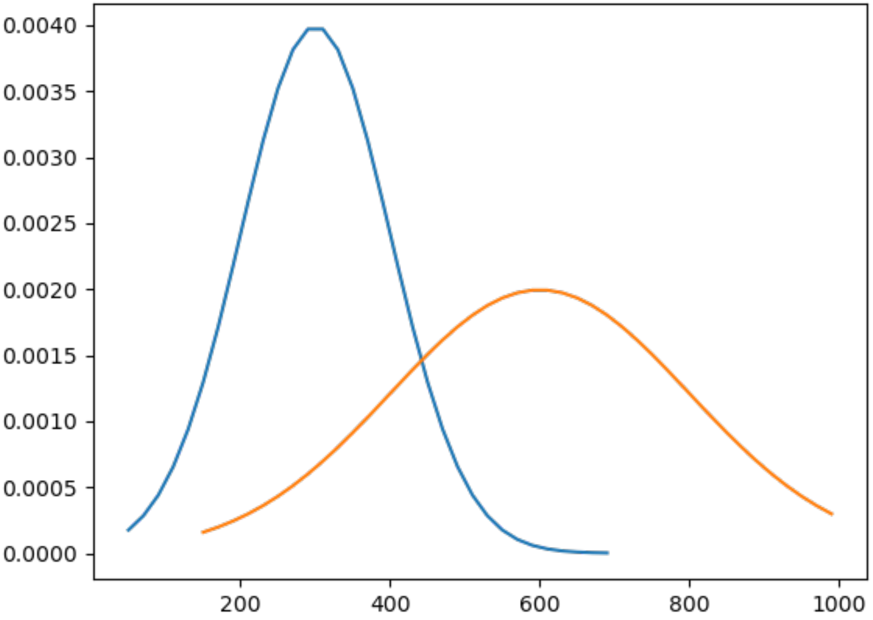
Only single spike



$$p(x) = \frac{1}{\sqrt{(2\pi)^k \det(\Sigma)}} \exp[-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)]$$

Two Underlying Patterns

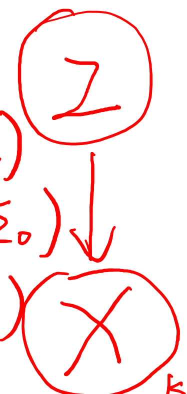
- It might be multiple underlying patterns of Gaussian distribution
  - Los Angeles and Pittsburgh have different median housing price



Gaussian Mixture Model

Generative process:

- z ~ Categorical(K)
- $x|z \sim \text{Gaussian}(\mu_z, \Sigma_z)$
- Density:

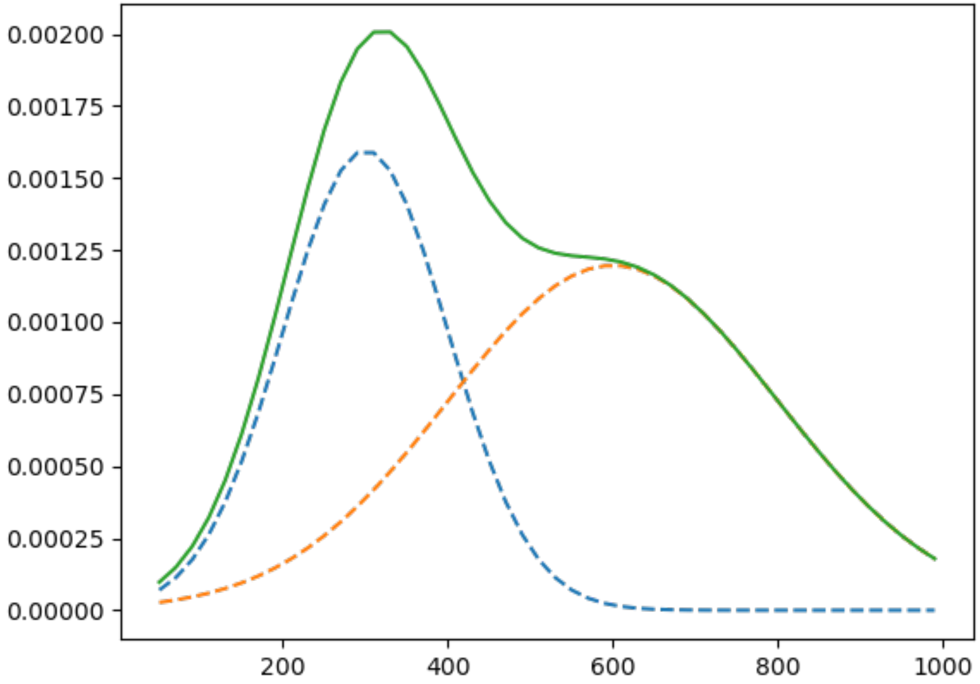


$$p(z,x) = p(z)\cdot p(x|z) = \begin{cases} w_0 \cdot \mathcal{N}(x|\mu_0,\Sigma_0) \\ w_1 \cdot \mathcal{N}(x|\mu_1,\Sigma_1) \end{cases}$$

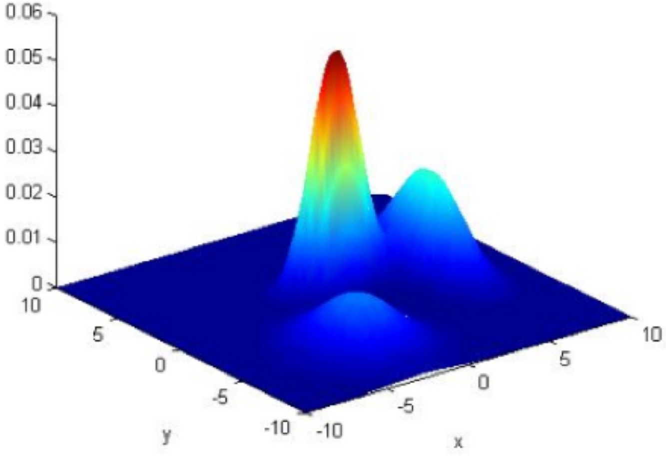
$$p(x) = \sum_{i=1}^{K} p(z=i, x) = \sum_{i=1}^{K} p(z=i)\, p(x|z=i)$$

$$= w_0 \mathcal{N}(x|\mu_0,\Sigma_0) + w_1 \mathcal{N}(x|\mu_1,\Sigma_1)$$

Gaussian Mixture

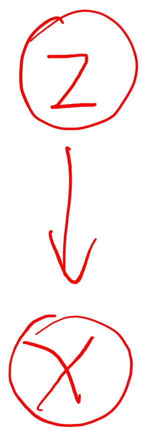


d=2:



Mixture Distribution

- Z: latent variable
- x|z can be any distribution in parametric form (e.g. exponential distribution)



Learning Parameters for GMM

- Observation: $x_{1..N}$
- $\theta = \{w_{1..k}, \mu_{1..k}, \Sigma_{1..k}\}$
- MLE (with latent variable z)
- Log-likelihood:
- Expectation-maximization algorithm

$$p(z,x) = p(z)\cdot p(x|z) = \begin{cases} w_0 \cdot \mathcal{N}(x|\mu_0,\Sigma_0) \\ w_1 \cdot \mathcal{N}(x|\mu_1,\Sigma_1) \end{cases}$$

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

$$= w_0 \mathcal{N}(x|\mu_0,\Sigma_0) + w_1 \mathcal{N}(x|\mu_1,\Sigma_1)$$

$$\mathcal{L}(\theta) = \log \prod_{n=1}^{N} p(x_n|\theta)$$

$$= \sum_{n=1}^{N} \log \sum_{i=1}^{K} p(z_n=i)\cdot p(x_n; \mu_i, \Sigma_i)$$

Optimality condition

taking $\dfrac{\partial \mathcal{L}(\theta)}{\partial \theta} = 0$ no closed form solution

Expected log-likelihood

- $L(\theta) = E_{p(z_n|x_n)} \log p(x_n, z_n)$

$$\ell(\theta) = \sum_{n=1}^{N} \log \sum_{i=1}^{K} p(z_n=i) \cdot p(x_n | z_n=i)$$

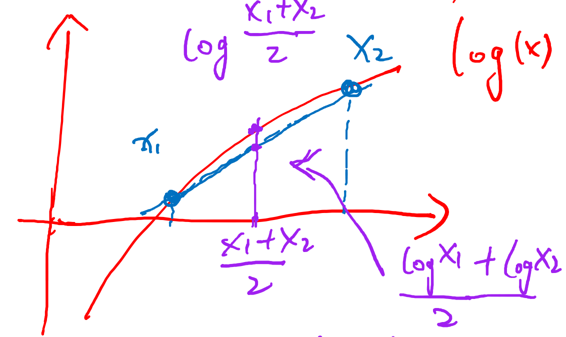
$$= \sum_{n=1}^{N} \log \sum_{i=1}^{K} p(z_n=i|x_n) \cdot \frac{p(z_n=i) \cdot p(x_n|z_n=i)}{p(z_n=i|x_n)}$$

Jensen

$$\geq \sum_{n=1}^{N} \sum_{i=1}^{K} p(z_n=i|x_n) \cdot \log \frac{p(z_n=i) \cdot p(x_n|z_n=i)}{p(z_n=i|x_n)}$$

$$= \sum_{n=1}^{N} E_{z_n|x_n}\left[\log p(z_n=i) \cdot p(x_n|z_n=i) - \log p(z_n=i|x_n)\right]$$

Jensen's Inequality



$$\log \frac{x_1+x_2}{2} \geq \frac{\log x_1 + \log x_2}{2}$$

General case:

$$\log E[X] \geq E[\log X]$$

Posterior

- $p(z_n|x_n) = \dfrac{p(z_n, x_n)}{p(x_n)} = \dfrac{p(z_n) \cdot p(x_n|z_n)}{\sum_{j=1}^{K} p(z_n=j) \cdot p(x_n|z_n=j)}$

$$\hat{z}_{n,i} = p(z_n=i|x_n) = \frac{p(z_n=i) \cdot p(x_n|\mu_i, \Sigma_i)}{\sum_{j=1}^{K} p(z_n=j) \cdot p(x_n|\mu_j, \Sigma_j)}$$

$$= \frac{\omega_i \cdot \mathcal{N}(x_n, \mu_i, \Sigma_i)}{\sum_{j=1}^{K} \omega_j \cdot \mathcal{N}(x_n, \mu_j, \Sigma_j)}$$

Update mixture weights

$$\mathcal{L}(\theta) = \sum_{n=1}^{N} \sum_{i=1}^{K} p(z_n = i \mid x_n) \cdot \log \frac{p(z_n = i) \cdot p(x_n \mid z_n = i)}{p(z_n = i \mid x_n)}$$

$$= \sum_{n=1}^{N} \sum_{i=1}^{K} \hat{z}_{n,i} \log \frac{w_i \cdot \mathcal{N}(x_n, \mu_i, \Sigma_i)}{\hat{z}_{n,i}}$$

$$= \sum_{n=1}^{N} \sum_{i=1}^{K} \hat{z}_{n,i} \left(\log w_i + \log \mathcal{N}(x_n, \mu_i, \Sigma_i) - \log \hat{z}_{n,i} \right)$$

max $f(x)$

s.t. $g(x) = 0$

Lagrangian $Lag(x) = f(x) - \lambda g(x)$

$$\text{s.t. } \sum_{j=1}^{K} w_j = 1$$

$$Lag(\theta) = \mathcal{L}(\theta) - \lambda \left(\sum_{j=1}^{K} w_j - 1 \right)$$

Optimality for w:

$$\frac{\partial Lag(\theta)}{\partial w_i} = 0$$

$$\hookrightarrow = \sum_{n=1}^{N} \hat{z}_{n,i} \cdot \frac{1}{w_i} - \lambda = 0$$

$$w_i = \frac{\sum_{n=1}^{N} \hat{z}_{n,i}}{\lambda}$$

$$\lambda = \sum_{j=1}^{K} \sum_{n=1}^{N} \hat{z}_{n,j}$$

$$w_i = \frac{\sum_{n=1}^{N} \hat{z}_{n,i}}{\sum_{j=1}^{K} \sum_{n=1}^{N} \hat{z}_{n,j}}$$

Update mean and covariance

$$\log \mathcal{N}(x_n, \mu_i, \Sigma_i) = -\frac{d}{2}\log 2\pi - \frac{1}{2}\log|\Sigma_i| - \frac{1}{2}(x_n-\mu_i)^T\Sigma_i^{-1}(x_n-\mu_i)$$

$$L(\theta) = \sum_{n=1}^{N}\sum_{i=1}^{K}\hat{z}_{n,i}\left[-\frac{1}{2}\log|\Sigma_i| - \frac{1}{2}(x_n-\mu_i)^T\Sigma_i^{-1}(x_n-\mu_i)\right] + \ldots$$

Optimality Condition

$$\frac{\partial L(\theta)}{\partial \mu_i} = \sum_{n=1}^{N}\hat{z}_{n,i}\cdot\left(-\frac{1}{2}\cdot 2\cdot\Sigma_i^{-1}\cdot(x_n-\mu_i)\right) = 0$$

$$\mu_i = \frac{\sum_{n=1}^{N}\hat{z}_{n,i}\cdot x_n}{\sum_{n=1}^{N}\hat{z}_{n,i}}$$

$$\frac{\partial L(\theta)}{\partial \Sigma_i} = -\frac{1}{2}\sum_{n=1}^{N}\hat{z}_{n,i}\left(\Sigma_i^{-1} - \Sigma_i^{-1}(x_n-\mu_i)\cdot(x_n-\mu_i)^T\Sigma_i^{-1}\right) = 0$$

$$\Sigma_i = \frac{\sum_{n=1}^{N}(x_n-\mu_i)(x_n-\mu_i)^T\cdot\hat{z}_{n,i}}{\sum_{n=1}^{N}\hat{z}_{n,i}}$$

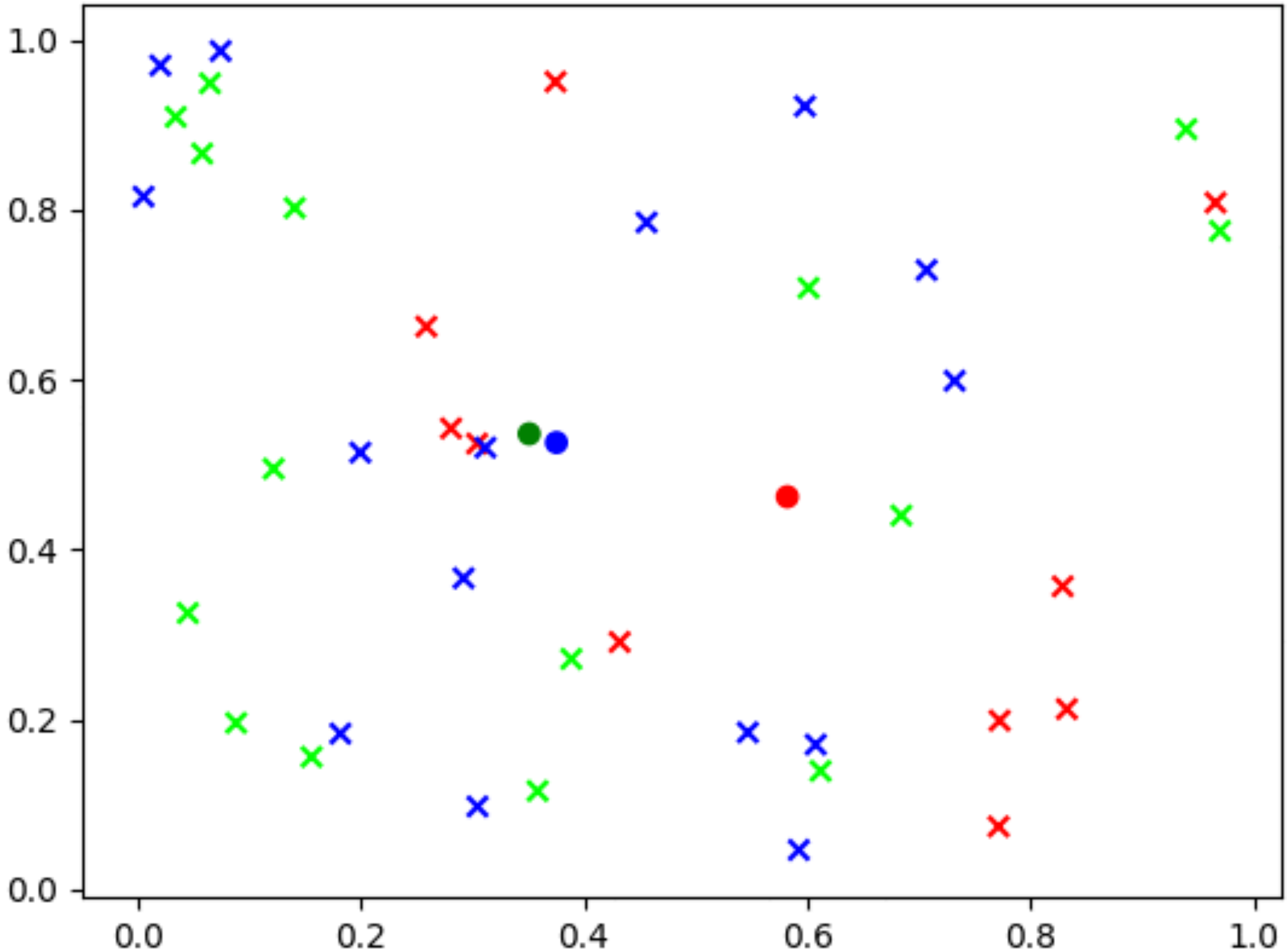
Summary of EM algorithm

- Observation: $x_{1..N}$
- $\theta = \{w_{1..k}, \mu_{1..k}, \Sigma_{1..k}\}$
- Iterate until convergence
  1. E step: use X and current θ to calculate $p(z_{1..N}|x_{1..N};\theta)$
  2. M step:

$$\theta \leftarrow \arg\max_{\theta} E_{p(z_{1..N}|x_{1..N};\theta_{old})} \log p(x_n, z_n|\theta)$$

- Guaranteed to find local maximum
- Works for general mixture model

Illustration of GMM



Property of GMM

- Interpretable:
  - Participation weight of each data point from every component
- Generative:
  - Able to generate new data
- Handles missing values
- Efficient: O(TKN)
- Local optimal:
  - Can be viewed as coordinate descent (why?)
- Need to specify K

K-Means vs GMM

1. Decide on a value for *K*, the number of clusters.
2. Initialize the *K* cluster centers / parameters (randomly).

K-Means

3. Decide the class memberships of the *N* objects by assigning them to the nearest cluster center.

4. Re-estimate the *K* cluster centers using the memberships found above

GMM

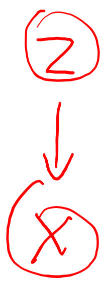
3. E-step: assign *probabilistic* membership

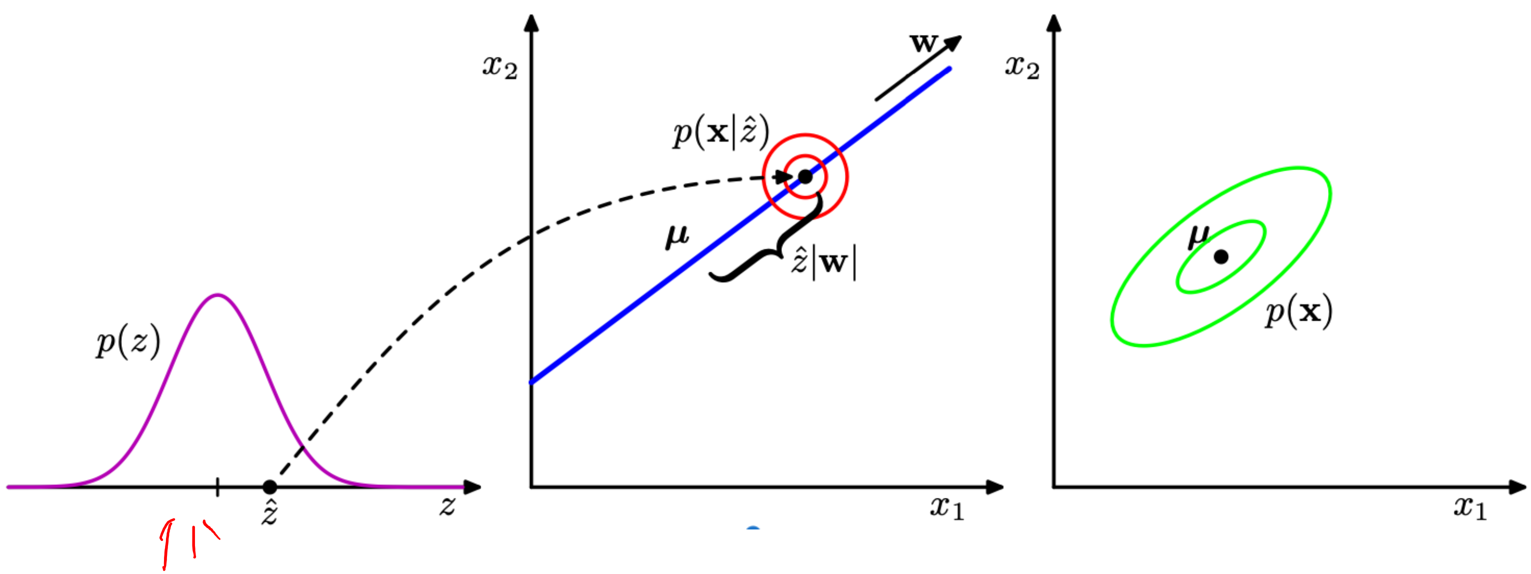
4. M-step: re-estimate parameters based on *probabilistic* membership

5. Repeat 3 and 4 until parameters do not change.

Probabilistic PCA

- Continuous latent variable $z \sim N(0, I)$
- Observation data $x|z \sim N(W \cdot z + \mu, \sigma^2 I)$





Learning Parameters for PPCA

- Again EM algorithm
- $\arg\max_{\theta} E_{p(z_{1..N}|x_{1..N};\theta_{old})} \log p(x_{1..N}, z_{1..N}|\theta)$

A Variational View of EM

- $L(\theta) = \log p(X; \theta)$
- Introduce a variational distribution ~~$q(X; \phi)$~~ $q(z; \phi)$
- Variational bound for this data likelihood

$$= \log \int p(X, z; \theta)\, dz$$

$$= \log \int q(z; \phi) \cdot \frac{p(X, z; \theta)}{q(z; \phi)}\, dz$$

Jensen's

$$\geq \int q(z; \phi) \cdot \log \frac{p(X, z; \theta)}{q(z; \phi)}\, dz \quad \text{(ELBO)}$$

$$= \int q(z; \phi) \cdot \log \frac{p(X|z; \theta) \cdot p(z; \theta)}{q(z; \phi)}\, dz$$

$$= E_{q(z)} \log p(X|z; \theta) - KL(q(z; \phi) \| p(z; \theta))$$

M-step: fix q, ϕ, estimate θ

E-step:

$$= \int q(z; \phi) \cdot \log \frac{p(z|X)\, p(X)}{q(z; \phi)}\, dz$$

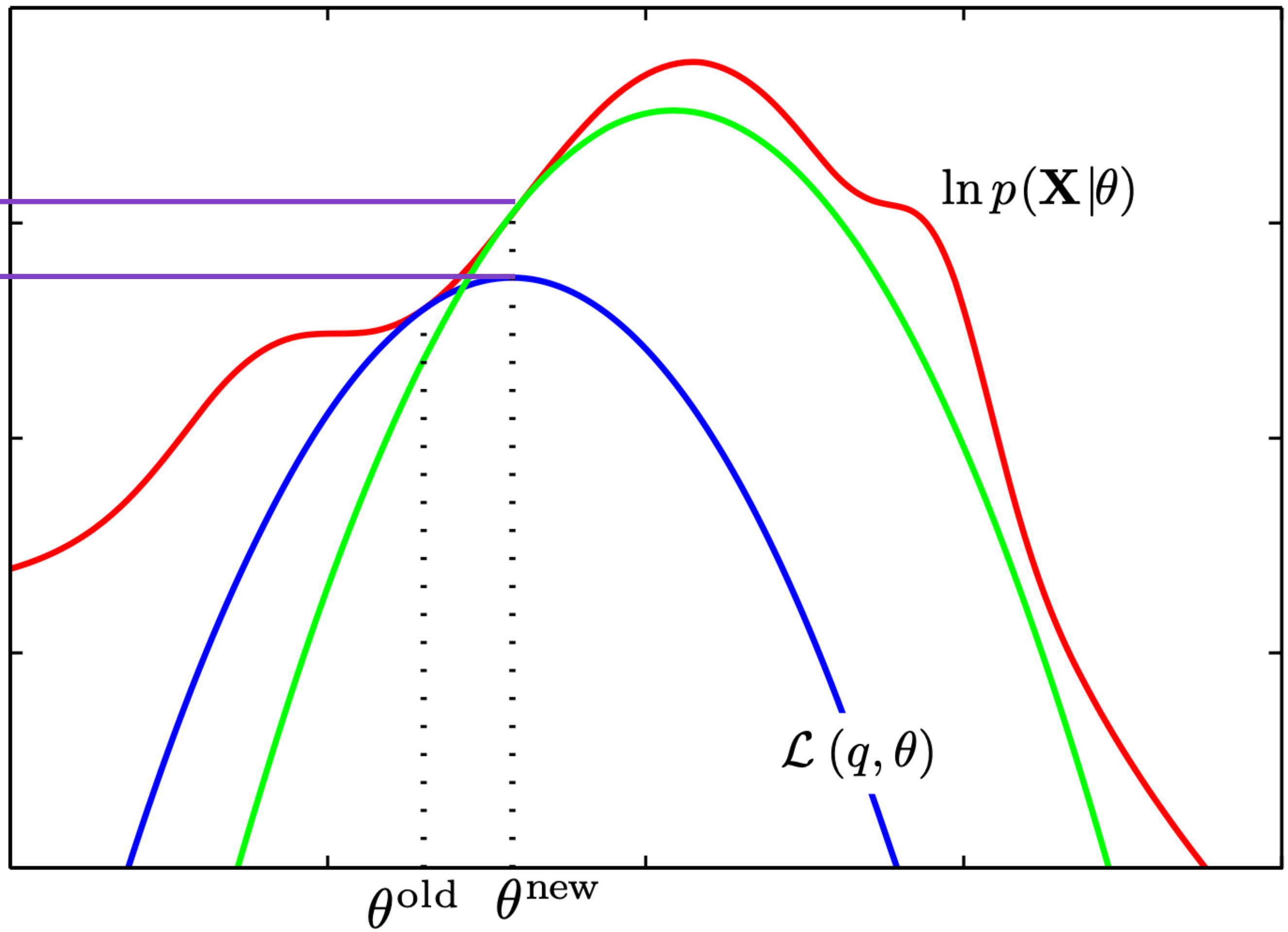
$$= -KL(q(z; \phi) \| p(z|X; \theta)) + \int q(z; \phi) \cdot \log p(X; \theta)\, dz$$

$$\log p(X; \theta)$$

What does EM actually do?

EM is coordinate-descent

$KL(q(z)||p(z|x))$



Summary

- Mixture Distribution: to build more complex distribution from simple ones
- Gaussian Mixture Model: k Gaussian components
- Expectation-Maximization: general for graphical models with latent variables
  - E-step: fix parameter, estimate posterior mean/variance
  - M-step: update parameter
- Probabilistic PCA: latent is continuous

Recommended Reading

- PRML Chapter 9, 12.2

Next up

- Dynamic Bayesian Network
- Linear Dynamical System