Lecture 8: Introduction to Unsupervised Learning, K-means, Gaussian Mixture Model (GMM), and EM algorithm

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WESTLAKE UNIVERSITY | SCHOOL OF ENGINEERING

1. Unsupervised Learning
   - Introduction to Unsupervised Learning
   - Unsupervised Representation Learning & Generation
   - Clustering and K-means Methods
   - Gaussian Mixture Model (GMM)
   - Expectation-Maximization Algorithm

Reading materials & Reference

Reading materials:

- Chapter 10, Stanford CS 229 Lecture Notes, `https://cs229.stanford.edu/notes2022fall/main_notes.pdf`
- EPFL, CS-433 Machine Learning, `https://github.com/epfml/ML_course`

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- How to learn a meaningful internal representation for data examples?
  - I.e., to represent them in a way that reflects the semantic structure of the overall collection of input patterns?

This question is the central focus of unsupervised learning.

In unsupervised learning, our data consists only of features (or inputs) $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$, vectors in $\mathbb{R}^D$, and there are **no outputs** y_n available.

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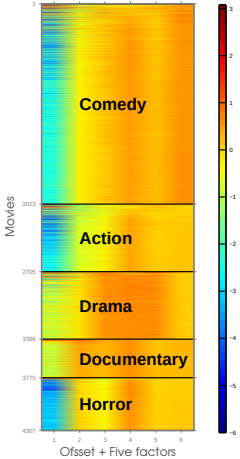
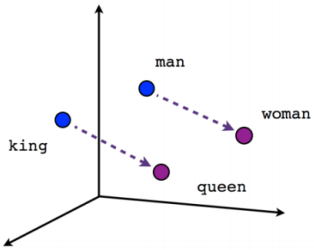
- representation learning and
- density estimation & generative models

Example

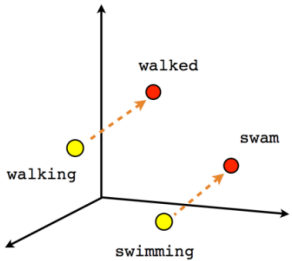
Given ratings of movies and viewers, we use matrix factorization to extract useful features (see e.g. Netflix Prize).



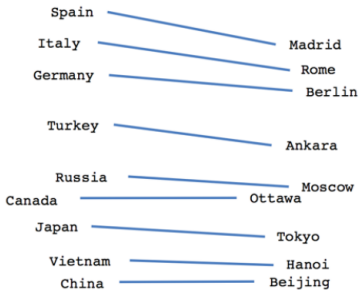
Learning word-representations using matrix-factorizations, `word2vec` (Mikolov et al. 2013).



Male-Female



Verb tense



Country-Capital

Given voting patterns of regions across Switzerland, we use PCA to extract useful features (Etter et al. 2014).

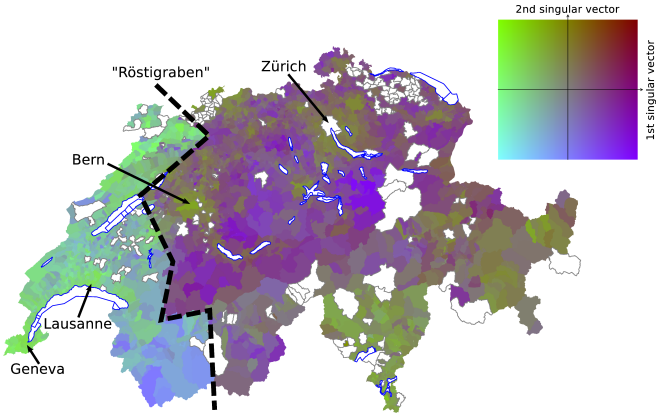
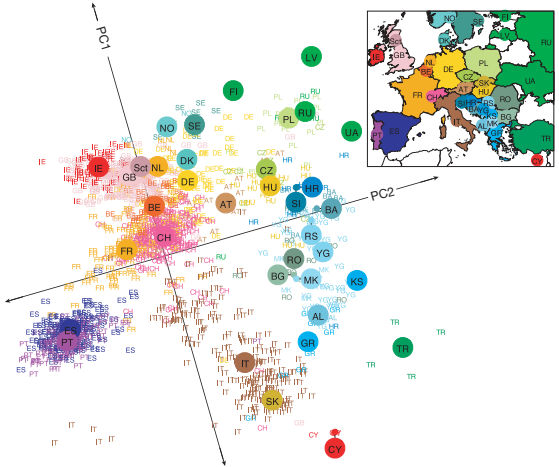


Figure 9: Voting patterns of Swiss municipalities. The color of a municipality is assigned using its location in Figure 8 and the color gradient shown in the upper right corner. Two municipalities with similar colors have similar voting patterns. The *Röstigraben*, corresponding to the cultural difference between French-speaking municipalities and German-speaking ones, is clearly visible from the difference in voting patterns. Regions shown in white are lakes or municipalities for which some vote results are missing (due to a merging of municipalities, for example). A more detailed map can be found online [2].

PCA Example 2: Genes mirror geography



Nature 2008, `http://dx.doi.org/10.1038/nature07331`

Examples for Clustering

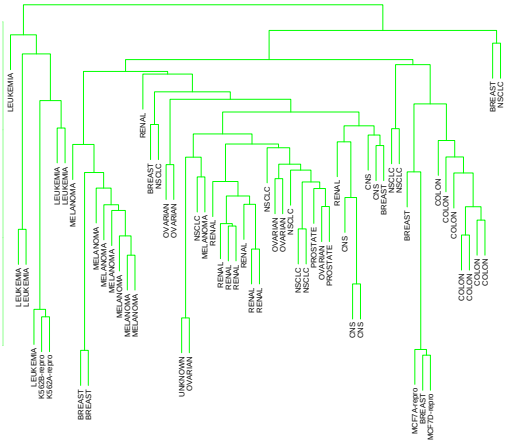


FIGURE 14.12. *Dendrogram from agglomerative hierarchical clustering with average linkage to the human tumor microarray data.*

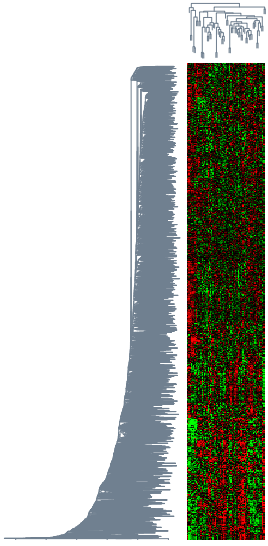
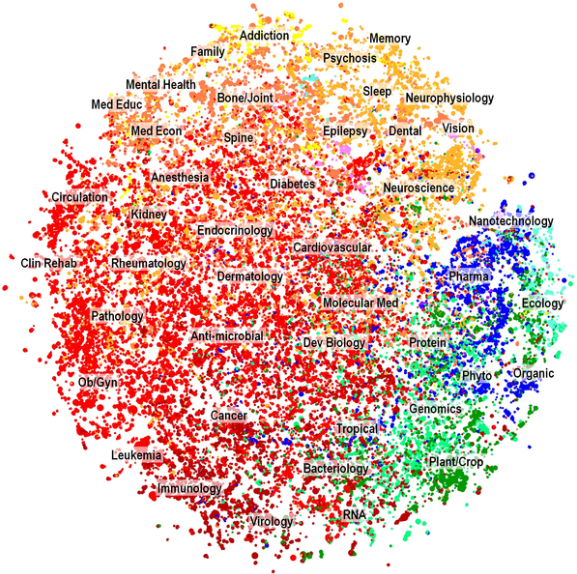


FIGURE 14.14. *DNA microarray data: average linkage hierarchical clustering has been applied independently to the rows (genes) and columns (samples), de-*

Clustering more than two million biomedical publications (Kevin Boyack et.al. 2011)



Clustering articles published in Science (Blei & Lafferty 2007)

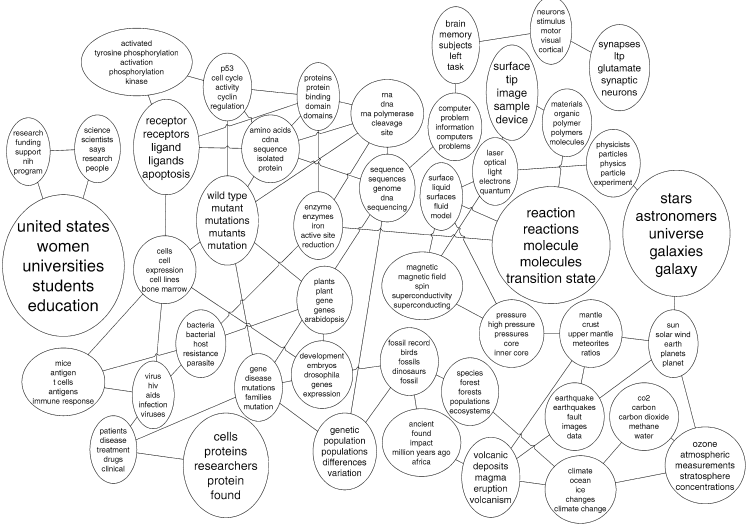


FIG. 2. *A portion of the topic graph learned from* 16,351 *OCR articles from Science* (1990–1999). *Each topic node is labeled with its five most probable phrases and has font proportional to its popularity in the corpus.* (*Phrases are found by permutation test.*) *The full model can be found in* http://www.cs.cmu.edu/~lemur/science/ *and on STATLIB.*

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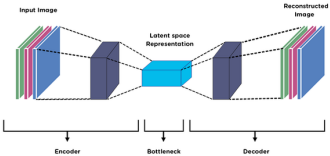

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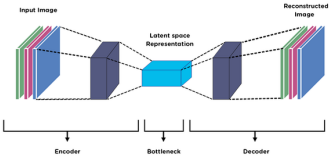

image: Deepak Birla

- Consistency & Contrastive Learning (e.g. Noise-contrastive estimation)

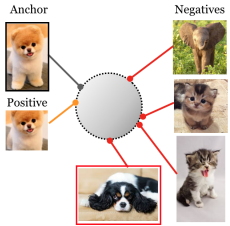

image: arxiv.org/pdf/2004.11362

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  Combining unsupervised representation learning (pre-training) with supervised learning
- Language Models & Sequence Models (G)
  text generation, or sequence continuation, BERT video, audio & timeseries (auto-regressive, contrastive, ...)

- Generative Adversarial Networks (GAN) (G)
  see also *predictability minimization*

"A Style-Based Generator Architecture for Generative Adversarial Networks", CVPR 2019

- Contrastive image-language pretraining (CLIP)
  learns a joint representation space for images and text using contrastive learning

- Diffusion models (G)
  new state-of-the-art in image generation; these models can be adapted to generate images from text prompts (e.g., DALL-E 2, Stable Diffusion, Midjourney)

Source: Stable Diffusion model, https://stability.ai/blog/stable-diffusion-public-releas

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The goal of clustering is to

- find "prototype" points $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K$ and cluster assignments $z_n \in \{1, 2, \ldots, K\}$ for all $n = 1, 2, \ldots, N$ data vectors $\mathbf{x}_n \in \mathbb{R}^D$ of $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$.

K-means clustering

Assume the number of clusters K is known.

$$\min_{\mathbf{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z},\boldsymbol{\mu}) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2 \quad \text{s.t.} \quad \boldsymbol{\mu}_k \in \mathbb{R}^D,\ z_{nk} \in \{0,1\},\ \sum_{k=1}^{K} z_{nk} = 1, \tag{1}$$

$$\text{where } \mathbf{z}_n = [z_{n1}, z_{n2}, \ldots, z_{nK}]^\top \tag{2}$$

$$\mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_N]^\top \tag{3}$$

$$\boldsymbol{\mu} = [\boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \ldots, \boldsymbol{\mu}_K]^\top \tag{4}$$

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Is this optimization problem easy?

K-means Methods

Algorithm: Initialize $\boldsymbol{\mu}_k \, \forall k$, then iterate:

1. **Step 1:** For all n, compute $\mathbf{z}_n$ given $\boldsymbol{\mu}$.
2. **Step 2:** For all k, compute $\boldsymbol{\mu}_k$ given $\mathbf{z}$.

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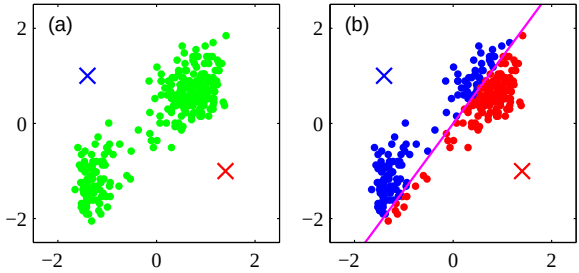
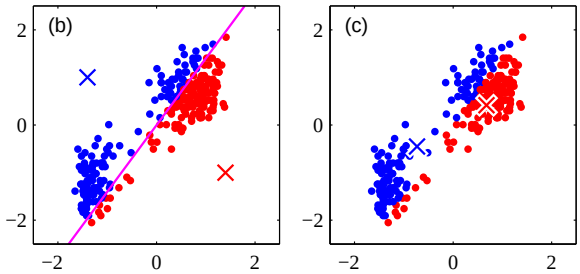


$$z_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_{j=1,2,\ldots,K} \left\| \mathbf{x}_n - \boldsymbol{\mu}_j \right\|_2^2 \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

Step 2: For all k, compute $\boldsymbol{\mu}_k$ given $\mathbf{z}$.



Take derivative w.r.t. $\boldsymbol{\mu}_k$ to get:

$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk}\mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}} \tag{6}$$

Hence, the name 'K-means'.

Summary of K-means

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$$\boldsymbol{\mu}_k = \frac{\sum_{n=1}^{N} z_{nk} \mathbf{x}_n}{\sum_{n=1}^{N} z_{nk}} \tag{8}$$

Convergence to a local optimum is assured since each step decreases the cost.

Coordinate Descent view of K-means method

K-means is a coordinate descent algorithm, where, to find $\min_{\mathbf{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z}, \boldsymbol{\mu})$, we start with some $\boldsymbol{\mu}^{(0)}$ and repeat the following:

$$\mathbf{z}^{(t+1)} := \arg\min_{\mathbf{z}} \; \mathcal{L}(\mathbf{z}, \boldsymbol{\mu}^{(t)}) \tag{9}$$

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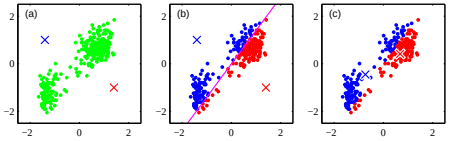
- $\mathcal{L}$ is a convex function?
  NO! So coordinate descent on $\mathcal{L}$ is not guaranteed to converge to the global minimum.

K-means for the “old-faithful” dataset (Bishop’s Figure 9.1)

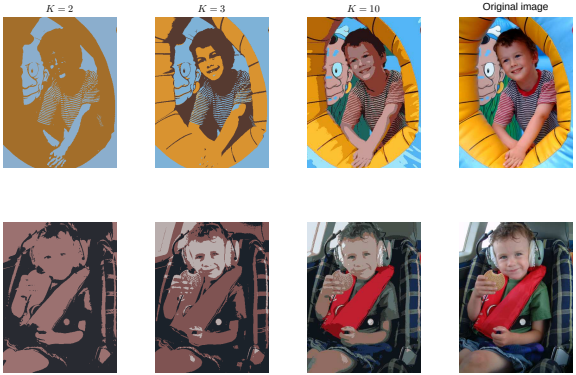


(a) Iteration 0 (b) Iteration 1 (c) Iteration 1

(d) Iteration 2 (e) Iteration 2 (f) Iteration 3

(g) Iteration 3 (h) Iteration 4 (i) Iteration 4

Data compression for images (this is also known as vector quantization).



Probabilistic model for K-means

Recall the objective

$$\min_{\mathbf{z},\boldsymbol{\mu}} \mathcal{L}(\mathbf{z},\boldsymbol{\mu}) = \sum_{n=1}^{N}\sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|_2^2 \tag{11}$$

$$= \left\|\mathbf{X}^\top - \mathbf{M}\mathbf{Z}^\top\right\|_{\text{Frob}}^2 \tag{12}$$

$$\text{s.t. } \boldsymbol{\mu}_k \in \mathbb{R}^D, \tag{13}$$

$$z_{nk} \in \{0,1\}, \sum_{k=1}^{K} z_{nk} = 1. \tag{14}$$

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2. Clusters are forced to be spherical (e.g. cannot be elliptical).
3. Each example can belong to only one cluster (“hard” cluster assignments).

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- GMMs assume data points are generated from a mixture of a finite number of Gaussian distributions with unknown parameters
- Each data point $\mathbf{x}_n$ belongs to one of K clusters with some probability
- The model is defined by the parameters $\boldsymbol{\theta} = \{\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \ldots, \boldsymbol{\Sigma}_K, \boldsymbol{\pi}\}$
  - $\boldsymbol{\mu}_k$ - Means of each Gaussian component
  - $\boldsymbol{\Sigma}_k$ - Covariance matrices
  - $\boldsymbol{\pi}$ - Mixture weights (probabilities of each component)

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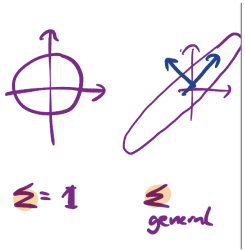

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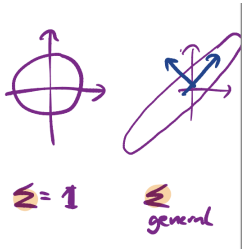

2. Each example in K-means can only belong to one cluster, but this may not always be a good choice, e.g. for data points that are near the “border".

Both of these problems are solved by using Gaussian Mixture Models.

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where $\boldsymbol{\mu} \in \mathbb{R}^{D \times K}$, $\mathbf{\Sigma} \in \mathbb{R}^{D \times D \times K}$, and $\boldsymbol{\pi} \in \mathbb{R}^{K}$.

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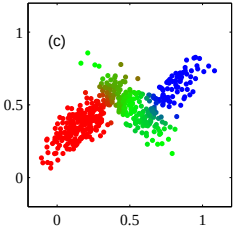
- This leads to soft-clustering as opposed to having “hard" assignments.



Gaussian mixture model

Together, the likelihood and the prior define the joint distribution of Gaussian mixture model (GMM):

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Here,

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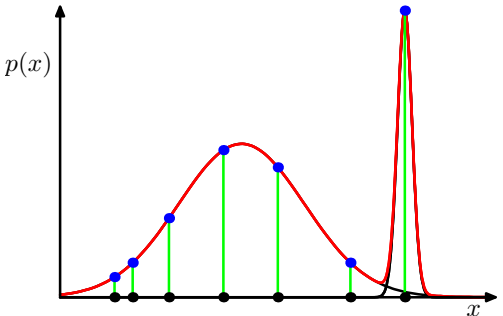

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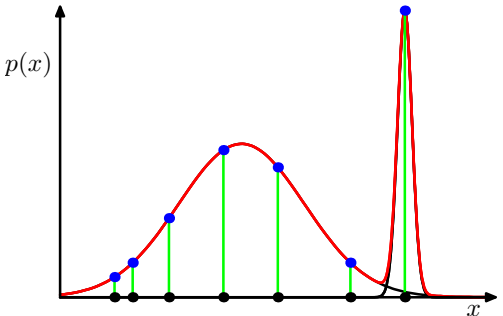

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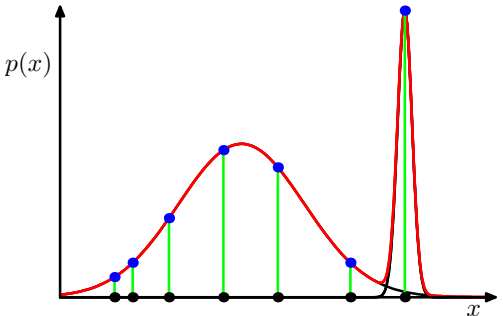
Exercise: non-convex, non-unique optima, unbounded.



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- Introduction to Unsupervised Learning
- Unsupervised Representation Learning & Generation
- Clustering and K-means Methods
- Gaussian Mixture Model (GMM)
- Expectation-Maximization Algorithm

Motivation of Expectation-Maximization (EM)

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- It uses an iterative two-step procedure, where individual steps usually involve problems that are easy to optimize.

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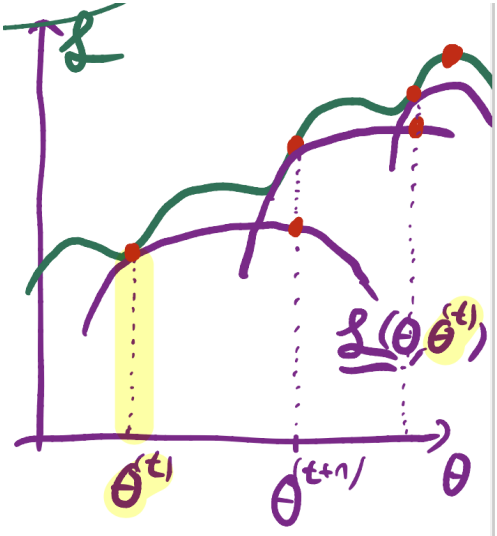

Figure: Visualization of EM iterations: Each bound is tight at the previous parameter value

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- ELBO is tight when $q(\mathbf{z}) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})$ (the posterior distribution)

The Evidence Lower Bound (ELBO)

- The procedure we just derived can be formalized as maximizing the Evidence Lower Bound (ELBO)
- The log-likelihood (evidence) can be decomposed as:

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta}) + \mathsf{KL}(q(\mathbf{z}) \parallel p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \tag{27}$$

  where $\mathcal{L}(q, \boldsymbol{\theta})$ is the ELBO:

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ELBO: Intuition and Properties

- The ELBO can be rewritten in two equivalent forms:

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- ELBO maximization balances:
  - Finding a good fit to the data through $\boldsymbol{\theta}$
  - Finding a good approximation to the posterior through q

The Maximization step (M-step)

Maximizing the lower bound w.r.t. $\boldsymbol{\theta}$ results in

$$\max_{\boldsymbol{\theta}} \sum_{n=1}^{N} \sum_{k=1}^{K} q_{kn}^{(t)} \left[\log \pi_k + \log \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)\right] \quad \text{(exercise. why?)} \tag{31}$$

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$$\boldsymbol{\mu}_k^{(t+1)} := \frac{\sum_{n=1}^{N} q_{kn}^{(t)} \mathbf{x}_n}{\sum_{n=1}^{N} q_{kn}^{(t)}} \tag{32}$$

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For π_k, we use the fact that they sum to 1. Therefore, we add a Lagrangian term, differentiate w.r.t. π_k and set to 0, to get the following update:

$$\pi_k^{(t+1)} := \frac{1}{N} \sum_{n=1}^{N} q_{kn}^{(t)} \tag{34}$$

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Initialize $\boldsymbol{\mu}^{(1)}, \boldsymbol{\Sigma}^{(1)}, \boldsymbol{\pi}^{(1)}$ and iterate between the E and M step, until $\mathcal{L}(\boldsymbol{\theta})$ stabilizes.

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If we let the covariance be diagonal i.e. $\boldsymbol{\Sigma}_k := \sigma^2 \mathbf{I}$, EM algorithm is same as K-means as $\sigma^2 \to 0$.

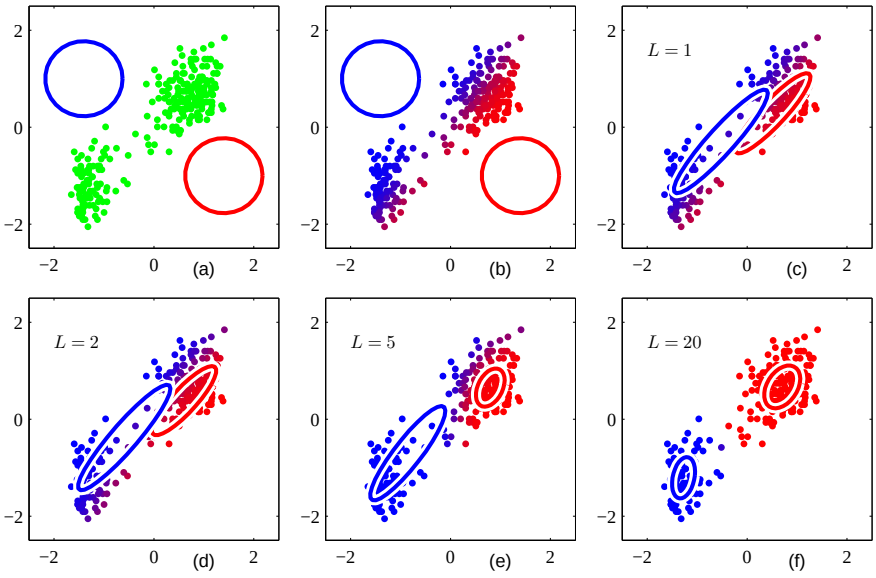
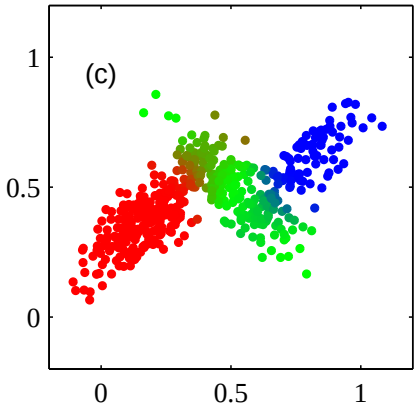


Figure: EM algorithm for GMM: Visualization of the iterative fitting process

Posterior distribution

We now show that $q_{kn}^{(t)}$ is the posterior distribution of the latent variable, i.e. $q_{kn}^{(t)} = p(\mathbf{z}_n = k \mid \mathbf{x}_n, \boldsymbol{\theta}^{(t)})$

$$\underbrace{p(\mathbf{x}_n, \mathbf{z}_n|\boldsymbol{\theta})}_{\text{joint}} = \underbrace{p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\theta})}_{\text{likelihood}} \underbrace{p(\mathbf{z}_n|\boldsymbol{\theta})}_{\text{prior}} = \underbrace{p(\mathbf{z}_n|\mathbf{x}_n, \boldsymbol{\theta})}_{\text{posterior}} \underbrace{p(\mathbf{x}_n|\boldsymbol{\theta})}_{\text{marginal likelihood}} \tag{40}$$



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- "Hard" assignments take values in $\{0, 1\}$ or $\{1, \ldots, K\}$
- Like K-means, EM is also susceptible to local optima, so initializing at several different parameter values may be a good strategy.

EM Convergence Properties

- The EM algorithm is guaranteed to increase the likelihood at each iteration:

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- However, like K-means, it may not find the global maximum.
- The rate of convergence depends on the fraction of information about the parameters contained in the latent variables.
- In practice, we monitor the change in log-likelihood and stop when it falls below a threshold.

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- This connection has led to powerful techniques like variational autoencoders (VAEs)

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  - Bayesian networks with hidden variables
- The same principles apply: identify latent variables, compute their expected values, and maximize parameters.

EM for Gaussian Mixture Models: Derivation

- The log-likelihood for GMM with unknown latent variables $\mathbf{z}_n$ is:

$$\mathcal{L}(\boldsymbol{\theta}) = \sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \tag{43}$$

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This approach gives us the two-step iterative EM algorithm

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  - Using criteria like BIC (Bayesian Information Criterion) or AIC (Akaike Information Criterion)