Machine Learning

- Gradient Descent Algorithm
- Linear Regression
- Non-Linear Regression
- Logistic Regression
- Decision Trees
  - Regression Trees
  - Classification Trees
  - Model complexity and ensemble models
- Clustering Algorithms
  - K-Means
  - Hierarchical clustering
  - DB-Scan
  - Mean Shift
  - GMM
- Support Vector Machine

Deep Learning

- MLP
- CNN

Datasets

- Breast Cancer Wisconsin
- MIMIC-III
- Framingham Heart Study
- Alzheimer’s Disease Neuroimaging Initiative
- Drug discovery
- Microbiome

C8 - GMM

Probability basics (sum and product rule)

Discrete:
Suppose 2 random variables X, Y

$$p(X) = \sum_{Y} p(X, Y)$$

$$p(X, Y) = p(Y|X)p(X)$$

$$p(X) = \sum_{Y} p(X|Y)p(Y).$$

Probability overview (Bayes’ rule)

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

$$\underbrace{\boxed{P(A|B)}}_{\text{posterior}} = \underbrace{\boxed{P(A)}}_{\text{prior}} \times \frac{\boxed{P(B|A)}\ \text{likelihood}}{\boxed{P(B)}\ \text{marginal}}$$

$$\overset{\text{Posterior}}{P(A|B)} = \frac{\overset{\text{Likelihood}}{P(B|A)} * \overset{\text{Prior}}{P(A)}}{\underset{\text{Evidence}}{P(B)}}$$

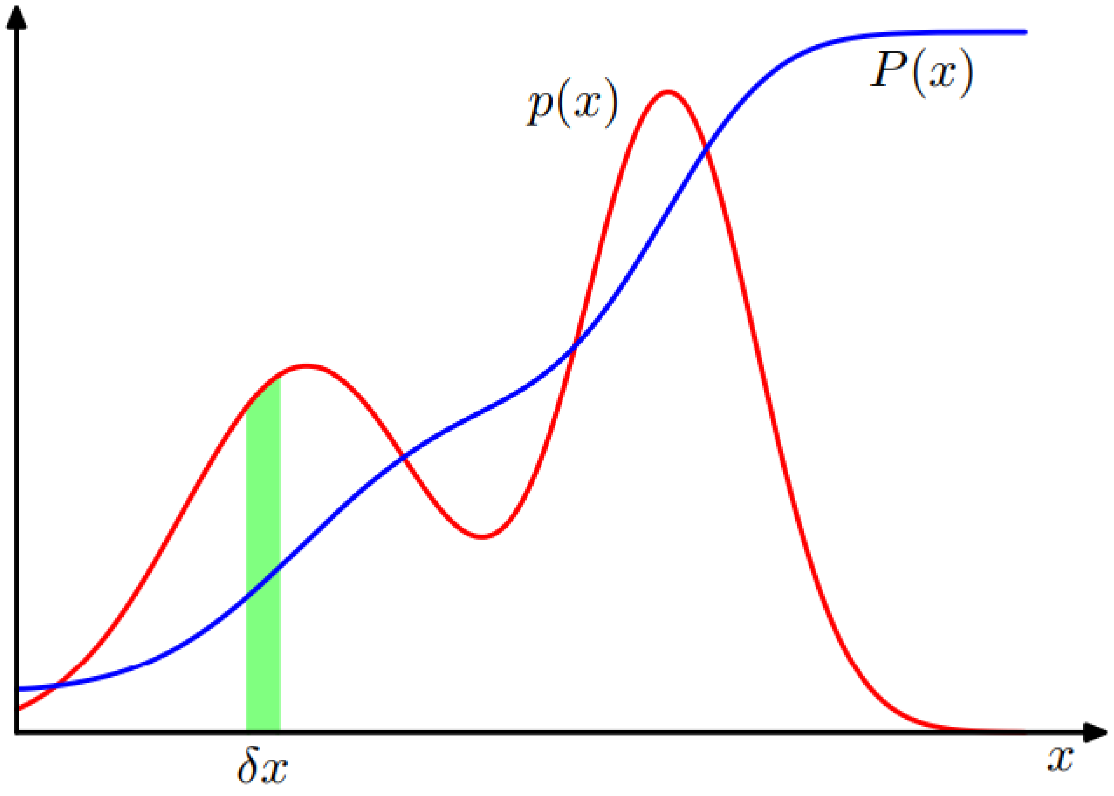
Probability densities

Continuous space

$$p(x \in (a,b)) = \int_a^b p(x)\,\mathrm{d}x.$$

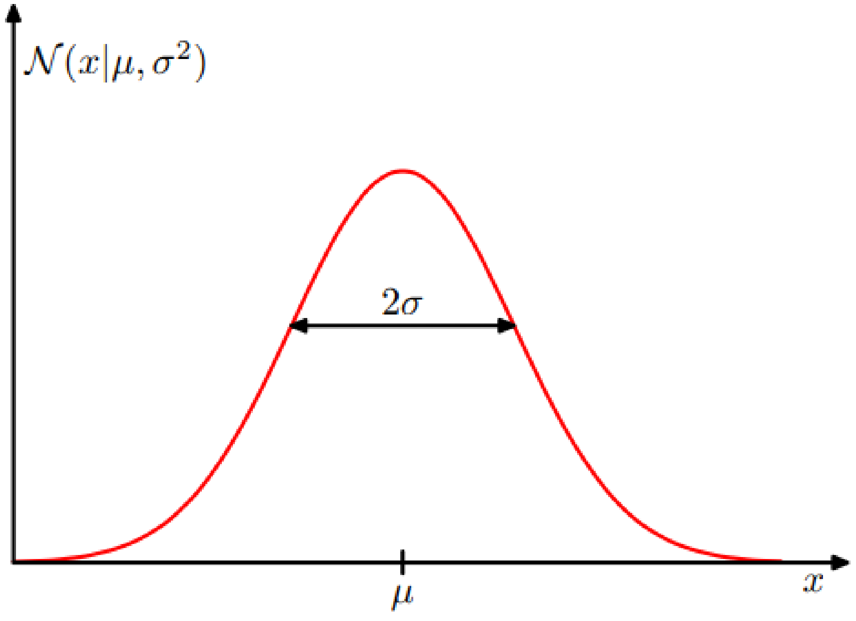
$$\begin{aligned} p(x) &\geqslant 0 \\ \int_{-\infty}^{\infty} p(x)\,\mathrm{d}x &= 1. \end{aligned}$$

$$\begin{aligned} p(x) &= \int p(x,y)\,\mathrm{d}y \\ p(x,y) &= p(y|x)p(x). \end{aligned}$$

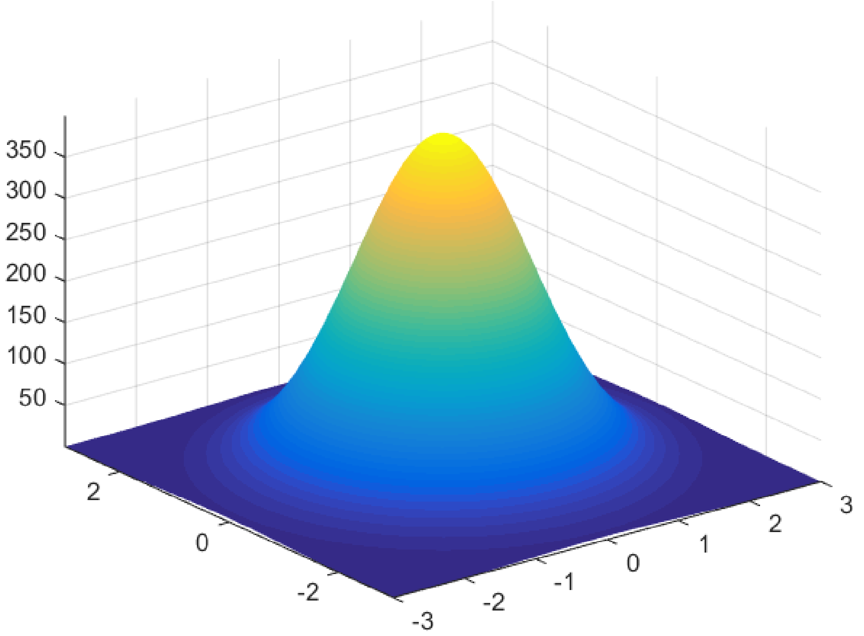


Gaussian distribution

$$\mathcal{N}\left(x|\mu,\sigma^2\right) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$

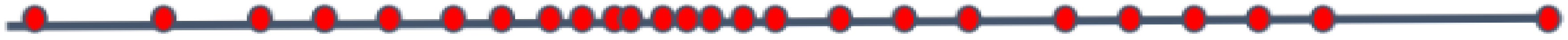


$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$



Likelihood

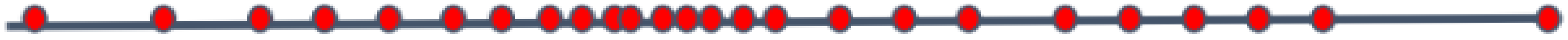
GOAL: Find the correct distribution of the data.



Likelihood

The likelihood function (often simply called the likelihood) is the joint probability (or probability density) of observed data viewed as a function of the parameters of a statistical model.

$$p(\mathbf{x}|\mu, \sigma^2) = \prod_{n=1}^{N} \mathcal{N}\left(x_n|\mu, \sigma^2\right).$$



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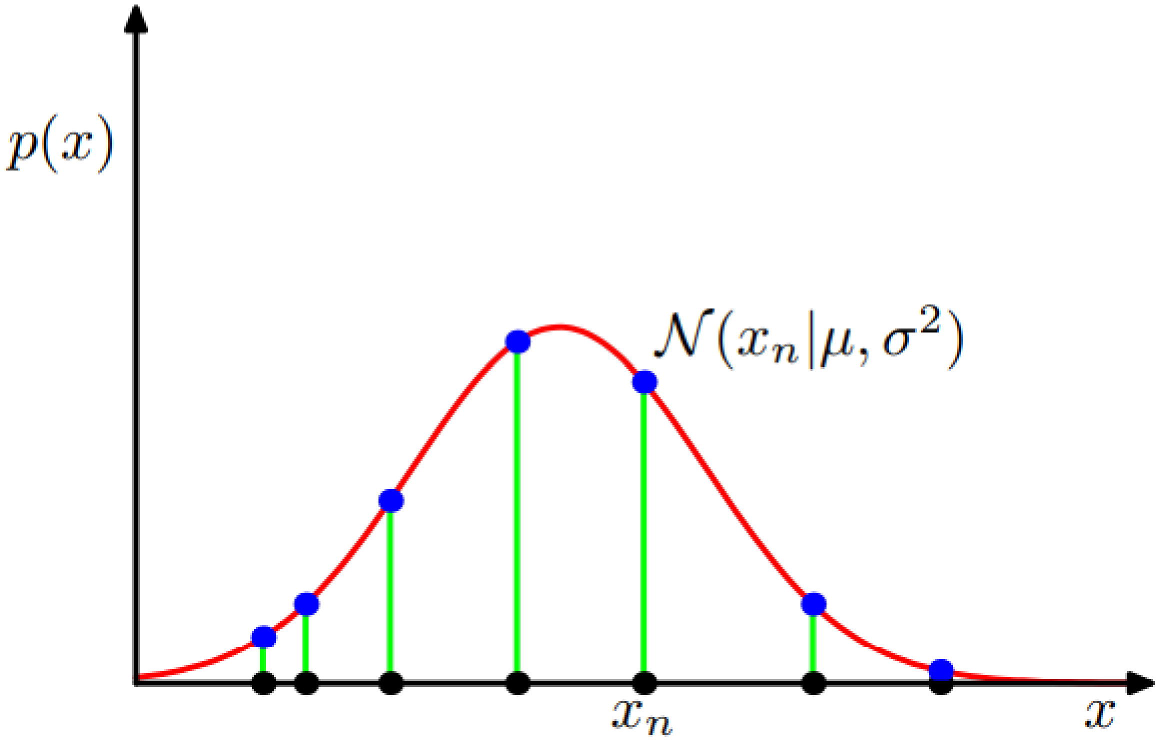

Log-likelihood

We shall determine values for the unknown parameters μ and σ2 in the Gaussian by maximizing the likelihood function.
In practice, it is more convenient to maximize the log of the likelihood function.

$$\ln p\left(\mathbf{x}|\mu,\sigma^2\right) = -\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu)^2 - \frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi).$$

$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N} x_n$$

$$\sigma^2_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}(x_n-\mu_{\mathrm{ML}})^2$$

Mixture of Gaussians

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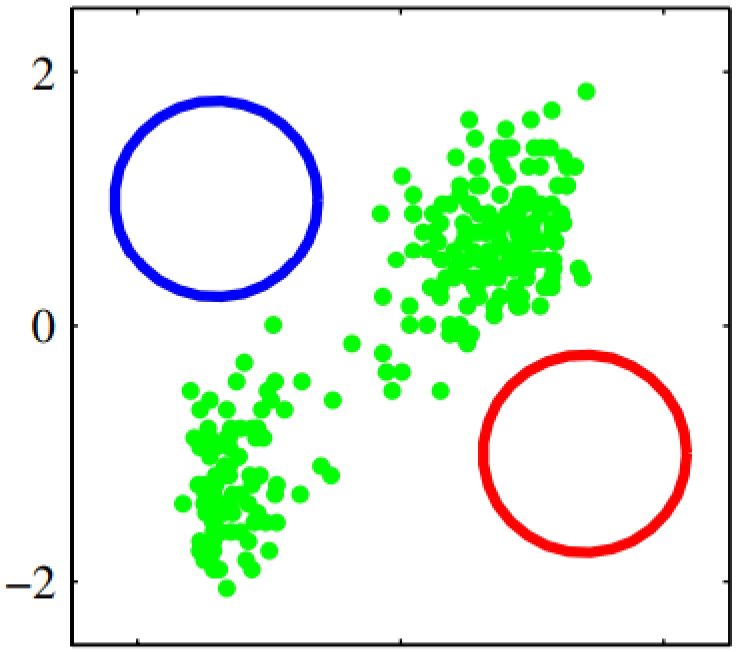
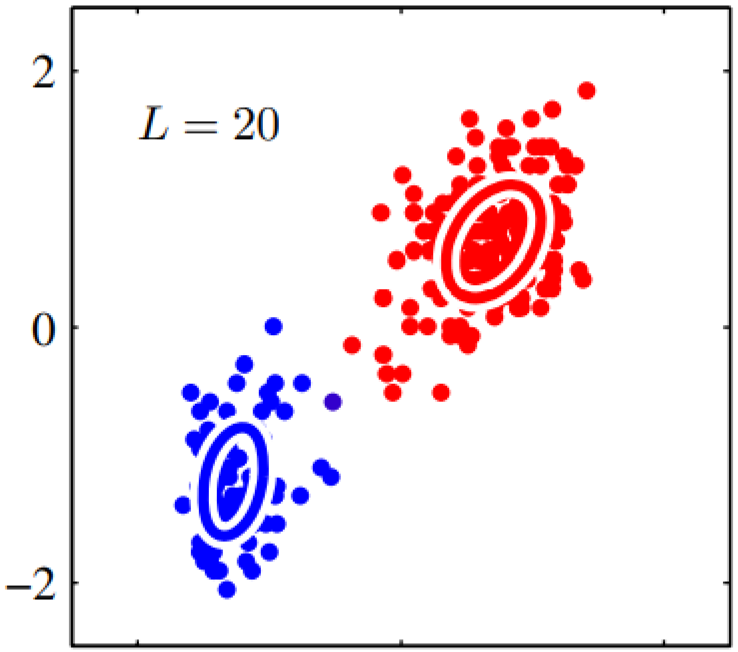


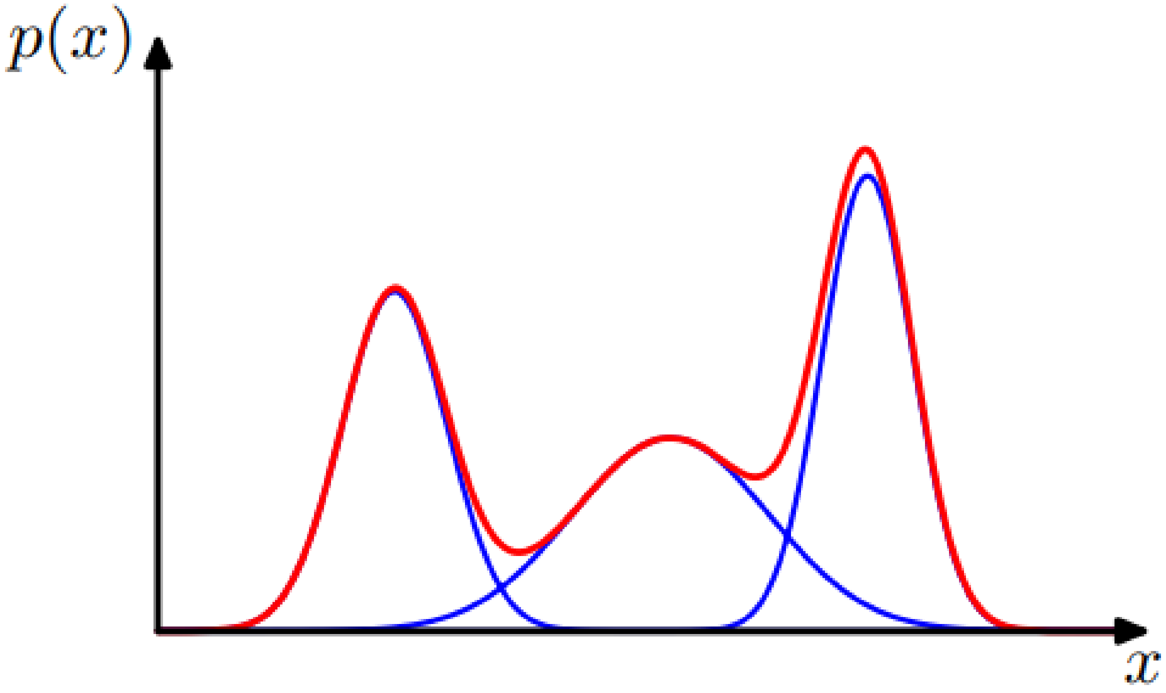
(a)



(f)

Mixture of Gaussians

A simple Gaussian distribution is unable to capture this structure, whereas a linear superposition of 2 Gaussians gives a better characterization of the data set.



$$p(\mathbf{x}) = \sum_{k=1}^{K} p(k)p(\mathbf{x}|k)$$

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

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

$$0 \leqslant \pi_k \leqslant 1.$$

Mixture of Gaussians

MODEL:

$$p(\mathbf{x}) = \sum_{k=1}^{K} p(k)p(\mathbf{x}|k) \qquad p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

"LOSS FUNCTION ": log-likelihood

CONSTRAINTS:

$$\sum_{k=1}^{K} \pi_k = 1. \qquad 0 \leqslant \pi_k \leqslant 1.$$

RESPONSIBILITIES:

$$\begin{aligned} \gamma_k(\mathbf{x}) &\equiv p(k|\mathbf{x}) \\ &= \frac{p(k)p(\mathbf{x}|k)}{\sum_l p(l)p(\mathbf{x}|l)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_l \pi_l \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_l, \boldsymbol{\Sigma}_l)}. \end{aligned}$$

Log-likelihood of GMM

GOAL: Maximize

LOSS FUNCTION:

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

CONSTRAINTS:

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

$$0 \leqslant \pi_k \leqslant 1.$$

GMM in terms of discrete latent variables

z is a one-hot encode state vector, there are K possible states.

$$z_n \qquad z_{1\times K} = \begin{bmatrix} 0 & 0 & \dots & 1 & \dots & 0 \end{bmatrix}$$

$$z_{nk}$$

$$p(z_k = 1) = \pi_k$$

z_n is associated with the n-th data point.
π_k is the proportion of elements belongs to the cluster K.

GMM in terms of discrete latent variables

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$$z_{1\times K} = \begin{bmatrix} 0 & 0 & \ldots & 1 & \ldots & 0 \end{bmatrix}$$

$$\begin{aligned}\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) &= \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}.\end{aligned}$$

Derivative framework (= 0)

GOAL: Maximize

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

with respect to the mean

$$0 = -\sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}_{\gamma(z_{nk})} \boldsymbol{\Sigma}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}).$$

Derivative framework (= 0)

GOAL: Maximize

$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

with respect to the covariance matrix

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

with more math we obtain

$$\pi_k = \frac{N_k}{N}$$

Expectation–Maximization

When we know the probabilities $\rightarrow$ **estimate means and proportions**

When we know the means and proportions $\rightarrow$ **estimate the probabilities**

Estimate probabilities

$$\begin{aligned}\gamma_k(\mathbf{x}) &\equiv p(k|\mathbf{x}) \\ &= \frac{p(k)p(\mathbf{x}|k)}{\sum_l p(l)p(\mathbf{x}|l)} \\ &= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_l \pi_l \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_l, \boldsymbol{\Sigma}_l)}.\end{aligned}$$

Estimate parameters

$$\boldsymbol{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n$$

$$\boldsymbol{\Sigma}_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^{\mathrm{T}}$$

$$\pi_k = \frac{N_k}{N}$$

EM algorithm for GMM

EM for Gaussian Mixtures

Given a Gaussian mixture model, the goal is to maximize the likelihood function with respect to the parameters (comprising the means and covariances of the components and the mixing coefficients).

1. Initialize the means $\boldsymbol{\mu}_k$, covariances $\boldsymbol{\Sigma}_k$ and mixing coefficients π_k, and evaluate the initial value of the log likelihood.
2. **E step**. Evaluate the responsibilities using the current parameter values

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}. \tag{9.23}$$

3. **M step**. Re-estimate the parameters using the current responsibilities

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n \tag{9.24}$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}} \tag{9.25}$$

$$\pi_k^{\text{new}} = \frac{N_k}{N} \tag{9.26}$$

where

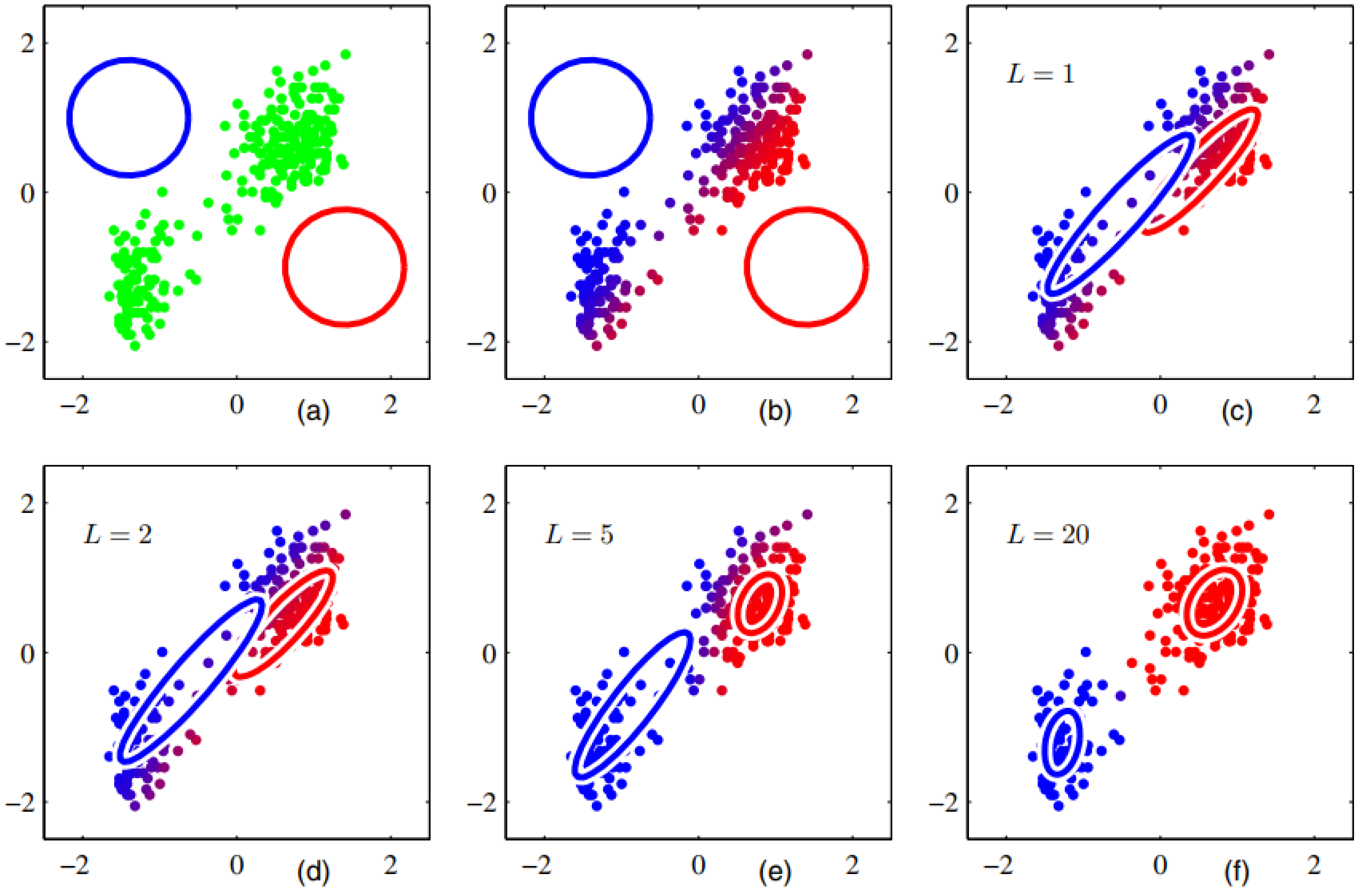
$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}). \tag{9.27}$$

4. Evaluate the log likelihood

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\} \tag{9.28}$$

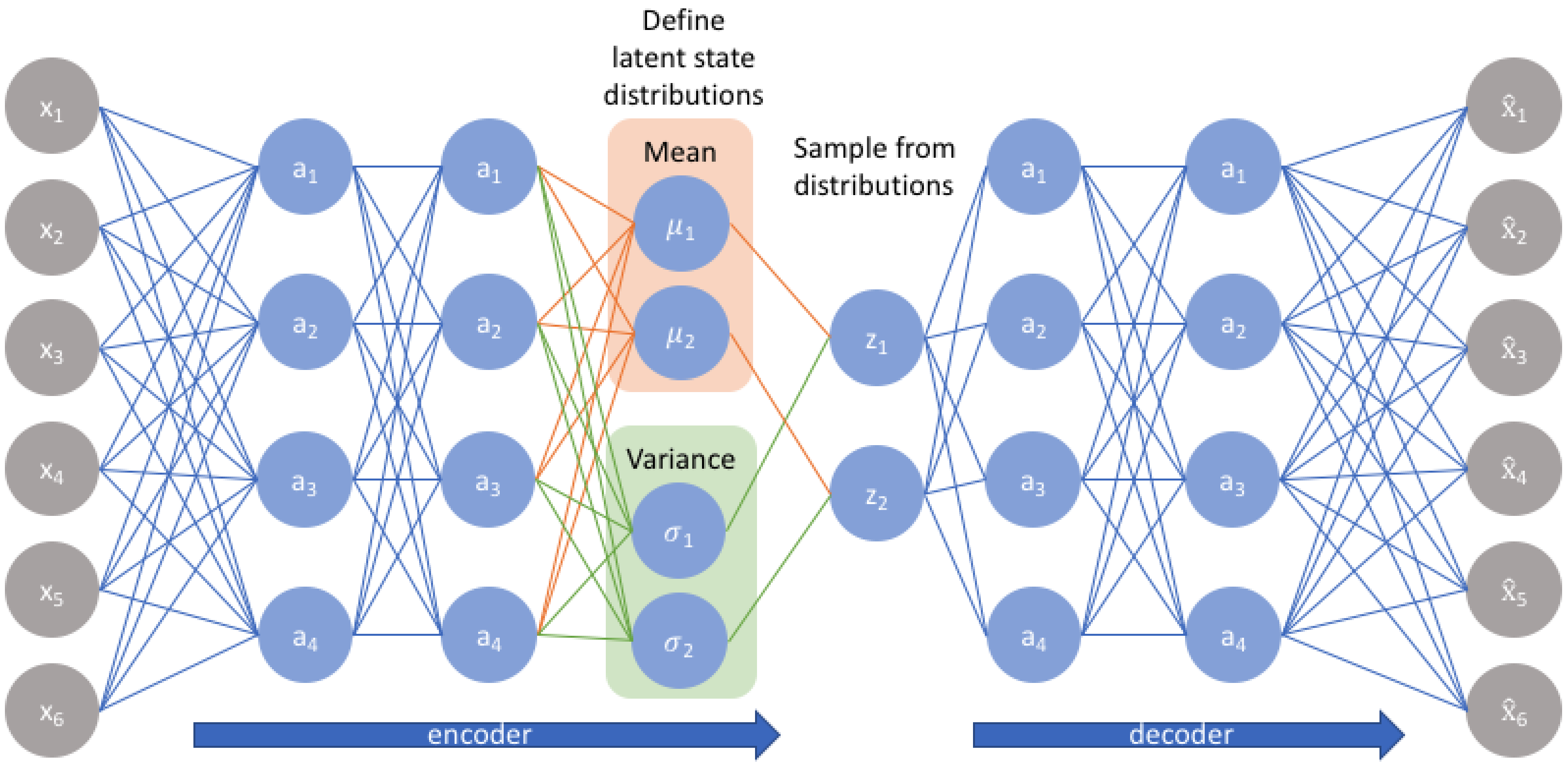
and check for convergence of either the parameters or the log likelihood. If the convergence criterion is not satisfied return to step 2.

Expectation–Maximization

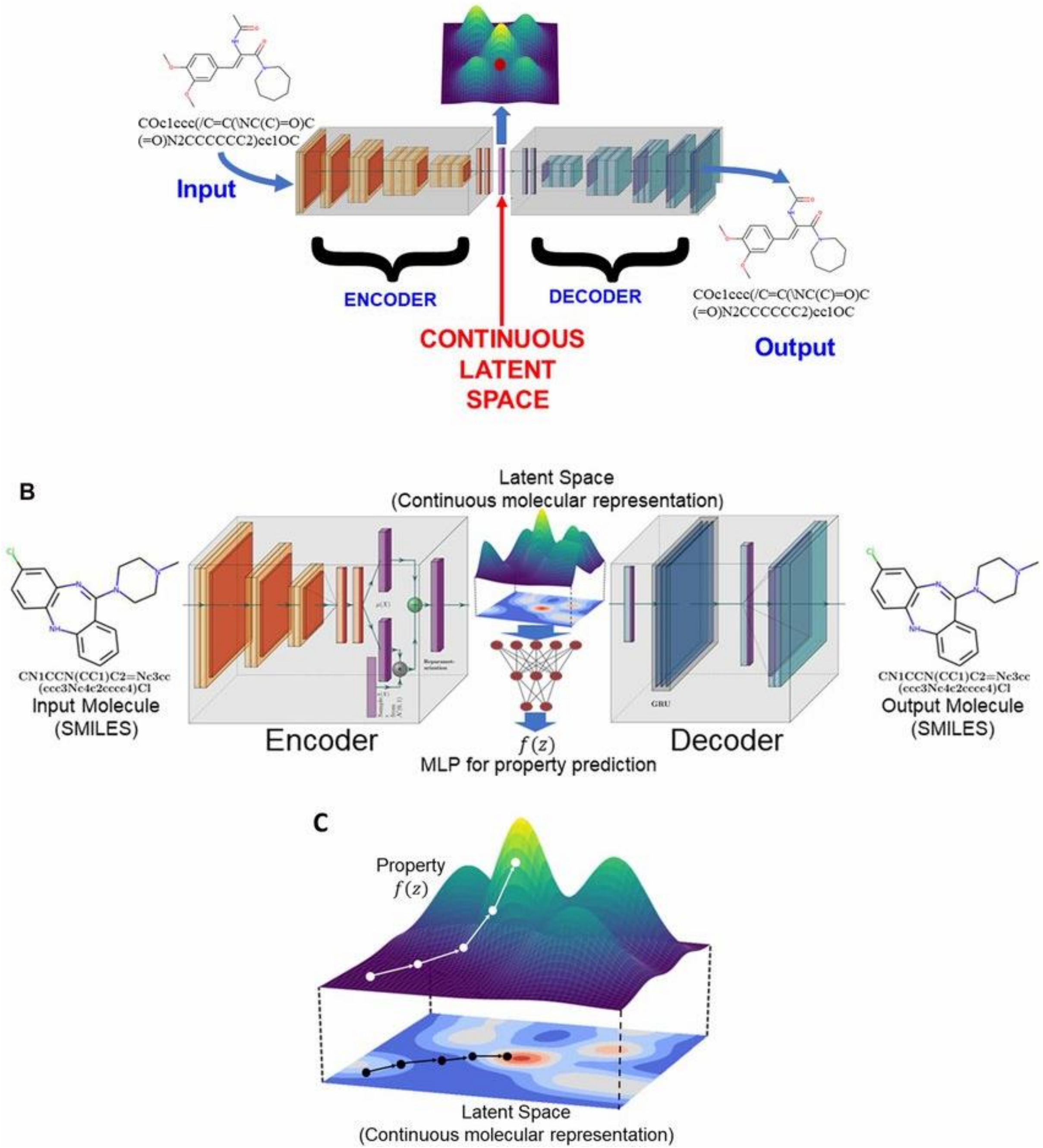


GMM

- # components?
- parameter initialization
- model evaluation
- why probabilistic models?

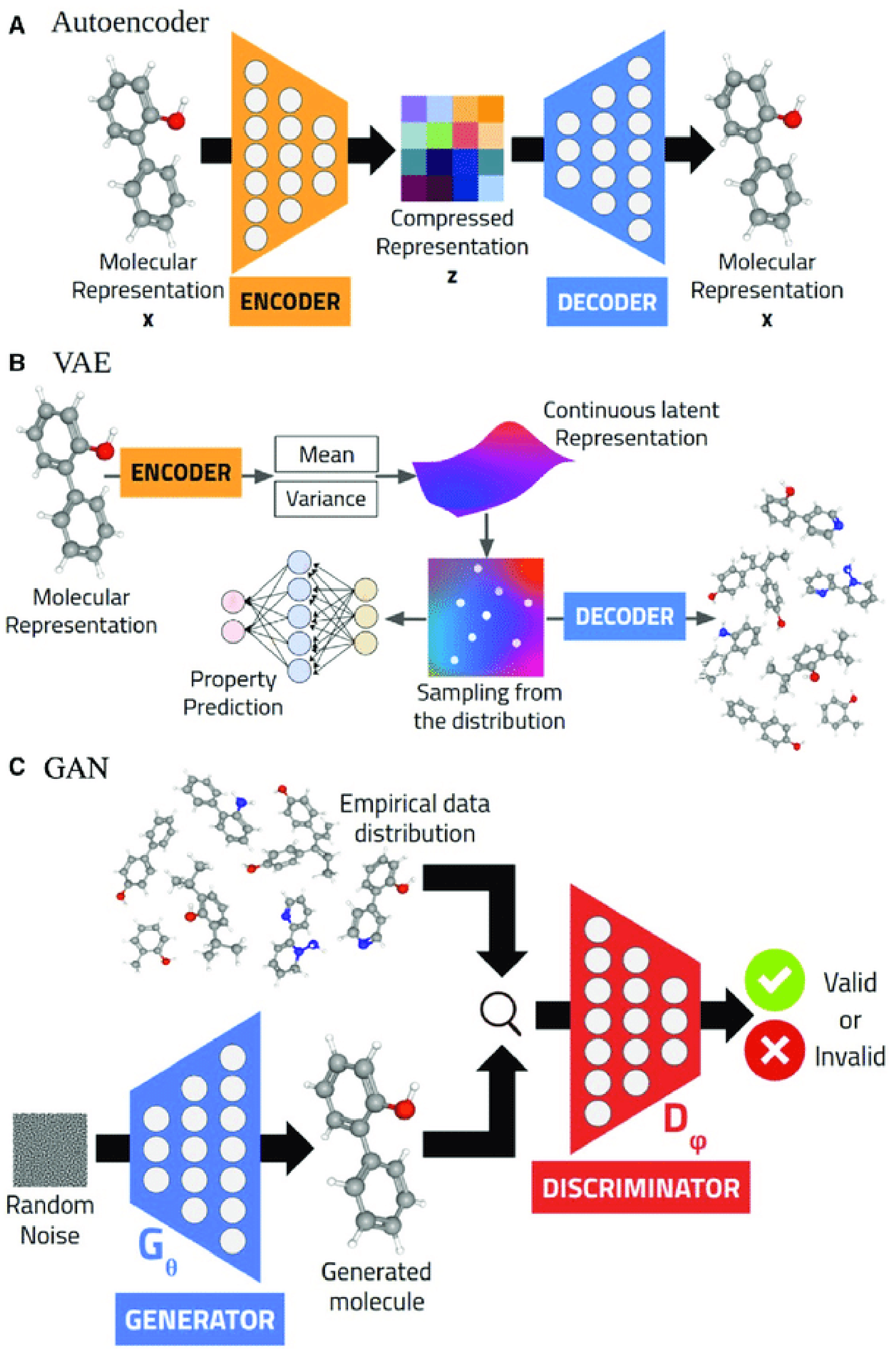


Variational autoencoder



my humble ML course

Generative networks



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