156 – Machine Learning

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This is math 156 – Machine Learning, an introductory course on mathematical models for pattern recognition and machine learning. It's instructed by Professor Zosso, and we meet weekly on MWTh from 9:00 am to 10:50 am. The textbook used for the class is *Pattern Recognition and Machine Learning* by *Bishop*. You can find the other course notes through my blog site. Any error appeared in this note is my responsibility and please email me if you happen to notice it.

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§1 Lec 1: Jun 21, 2021

§1.1 Introduction & Probability Review

According to Wikipedia, **Machine Learning** is a scientific discipline that deals with the construction and study of algorithms that can learn from data.

$$\text{Input(data)} \rightarrow \boxed{\text{Model}} \rightarrow \text{Output(Predictions/Decisions)}$$

From §1.2 of the book, let's review a bit on probability.

- Discrete random variable X, value $\{x_i\}$

$$\text{prob}(X = x_i) = p(x_i) = \frac{n_i}{N}$$

  and

$$\sum_i \text{prob}(X = x_i) = \sum_i p(x_i)$$

  For multiple random variables, $X, Y \in \{x_i\} \times \{y_i\}$

  1. $\text{prob}(X = x_i, Y = y_i) = \frac{n_{ij}}{N} = p(x_i, y_i)$ – joint probability
  2. $\text{prob}(X = x_i) = \sum_j \text{prob}(X = x_i, Y = y_j)$ – marginal probability
  3. $\text{prob}(X = x_i | Y = y_j) =$ conditional

$$\underbrace{p\left(x_i | y_j\right)}_{\text{conditional}} \cdot \underbrace{p(y_j)}_{\text{marginal}} = \underbrace{p(x_i, y_j)}_{\text{joint}}$$

  $\implies$ product rule

  Bayes' Rule:

$$p(y|x) = \frac{p(x|y) \cdot p(y)}{p(x)}$$

- Continuous random variable $X \in \mathbb{R}$

$$\text{prob}(X = x_i) = 0 \text{ in general}$$

  So we consider probability densities instead where

$$p(x) \geq 0$$

  s.t. $p(x)$ can be greater than 1. In addition,

$$\int_{-\infty}^{\infty} p(x) = 1$$

  Within a neighborhood $a \leq b$, we have

$$\text{prob}(a \leq x \leq b) = \int_a^b p(x)\, dx$$

  Sum rule:

$$\int \underbrace{p(x, y)}_{\text{joint pdf}}\, dy = \underbrace{p(x)}_{\text{marginal pdf}}$$

  Product rule:

$$p(x, y) = p(y|x)p(x) = p(x|y)p(y)$$

  Bayes' Rule:

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

Expectations & Covariances

Expectations:

Definition 1.1 — Expectation is defined as

$$\begin{aligned}\mathbb{E}[f] &:= \sum_i p(x_i) f(x_i) \\ \text{or} &:= \int_{\mathbb{R}} p(x) f(x)\, dx\end{aligned}$$

"Average value of a function $f : \mathbb{R} \to \mathbb{R}$ under a probability distribution $p(x)$"

In practice, we need to estimate p from data.

$$\text{Sampling Approximation: } \mathbb{E}[f] \approx \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

Definition 1.2 — Marginal expectation is defined as

$$\mathbb{E}_x[f](y) := \sum_x p(x) f(x, y)$$

Conditional expectation:

$$\mathbb{E}_x\left[f|y\right] := \sum_x p(x|y) f(x)$$

Covariances:

Definition 1.3 — Variance is defined as

$$\begin{aligned}\operatorname{var}[f] &:= \mathbb{E}\left[\left(f(x) - \mathbb{E}[f]\right)^2\right] \\ &= \mathbb{E}[f^2] - \mathbb{E}[f]^2\end{aligned}$$

Covariance (random variables) is defined as

$$\begin{aligned}\operatorname{cov}[x, y] &:= \mathbb{E}\left[\left(x - \mathbb{E}[x]\right)\left(y - \mathbb{E}[y]\right)\right] \\ &= \mathbb{E}[xy] - \mathbb{E}[x]\mathbb{E}[y]\end{aligned}$$

For vectors $\vec{x}, \vec{y} \in \mathbb{R}^D$, the covariance matrix is

$$\mathbb{E}\left[\left(\vec{x} - \mathbb{E}[\vec{x}]\right)\left(\vec{y} - \mathbb{E}[\vec{y}]\right)^\top\right]$$

Question 1.1. How does this fit in within the context of machine learning?

In machine learning, there are usually two approaches to find the "optimal prediction"

- Frequentist approach: maximize likelihood

$$\max_w p(D|w)$$

- Bayesian approach: maximize posterior

$$\text{posterior through Bayes': } p(w|D) = \frac{p(D|w) \cdot p(w)}{p(D)}$$

  s.t.

$$\max_w p(w|D) \sim p(D|w) \cdot p(w)$$

  where D represents data, and w is parameters.

Gaussian noise model:

$$p(t_n|x_n, w, \beta) = N\left(t_n|y(x_n, w), \frac{1}{\beta}\right)$$

Given training data $\{(x,t)\}$, we can determine optimal parameters w, β by

1. Frequentist: maximize likelihood

$$p(t|x, w, \beta) \overset{\text{i.i.d}}{=} \prod_{n=1}^{N} N\left(t_n|y(x_n|w), \beta^{-1}\right)$$

2. include a prior: $p(w|\alpha) = N(w|0, \alpha^{-1})$

$$\implies \text{posterior: } p(w|x, t, \alpha, \beta) \propto p(t|x, w, \beta)\, p(w|\alpha)$$

   Then, we can estimate

$$\min_w \left\{ \frac{\beta}{2} \sum_{n=1}^{N} (y(x_n, w) - t_n)^2 + \frac{\alpha}{2} w^\top w \right\}$$

3. Fully Bayesian: not just point estimates $\implies$ predictive distribution

$$p(t_i|x_i, x, t) = \int \underbrace{p(t_i|x_i, w)}_{\text{model}} \underbrace{p(w|x, t)}_{\text{posterior}} dw$$

§1.2 Gaussian Distribution

Definition 1.4 (Gaussian Distribution) — The 1-D Gaussian distribution is defined as

$$N\left(x|\mu, \sigma^2\right) := \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

where μ is the mean and σ^2 is the variance.
For D-dimensional,

$$N(\vec{x}|\vec{\mu}, \Sigma) := \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(x-\mu)^\top \sigma^{-1}(x-\mu)}$$

where Σ is the covariance matrix and $|\Sigma|$ is the determinant of Σ.

Consider $x \in \mathbb{R}^D$, $x \sim N$. Assume

$$x = \begin{bmatrix} x_a \\ x_b \end{bmatrix}$$

where x_a is unknown and x_b is given component.

$$x \sim N\left(\begin{bmatrix} \mu_a \\ \mu_b \end{bmatrix}, \Sigma = \begin{bmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{bmatrix}\right)$$

Note that

$$\Sigma = \Sigma^\top$$

Also, we define the precision matrix Λ as

$$\begin{aligned}\Lambda &\coloneqq \Sigma^{-1} \\ &= \begin{bmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{bmatrix}\end{aligned}$$

Unfortunately, $\Lambda_{aa} \neq \Sigma_{aa}^{-1}$ and similar result applies for b.

Question 1.2. What can we say about $p(x_a|x_b)$?

Use product rule:

$$p\left(x_a|x_b\right) \cdot p(x_b) = p(x_a, x_b)$$

where $p(x_b)$ is a constant w.r.t. x_a

$$\implies p(x_a|x_b) \propto p(x_a, x_b)$$

Let's look at quadratic form in exponential only.

$$\begin{aligned}-\frac{1}{2}(x-\mu)^\top \Sigma^{-1}(x-\mu) = -\frac{1}{2}(x_a-\mu_a)^\top \Lambda_{aa}(x_a-\mu_a) - \frac{1}{2}(x_a-\mu_a)^\top \Lambda_{ab}(x_b-\mu_b) \\ -\frac{1}{2}(x_b-\mu_b)^\top \Lambda_{ba}(x_a-\mu_a) - \frac{1}{2}(x_b-\mu_b)^\top \Lambda_{bb}(x_b-\mu_b)\end{aligned}$$

Also,

$$\text{other side } = -\frac{1}{2}x_a^\top \Sigma_{a|b}^{-1} x_a + x_a^\top \Sigma_{a|b}^{-1}\mu_{a|b} + \text{const}$$

- Quadratic terms need to match

$$\begin{aligned}-\frac{1}{2}x_a^\top \Sigma_{a|b}^{-1} x_a &= -\frac{1}{2}x_a^\top \Lambda_{aa} x_a \\ \implies \Sigma_{a|b}^{-1} &= \Lambda_{aa}\end{aligned}$$

- Linear terms in x_a

$$\begin{aligned}x_a^\top \Sigma_{a|b}^{-1}\mu_{a|b} &= x_a^\top \Lambda_{aa}\mu_{a|b} \\ \Lambda_{aa}\mu_{a|b} &= \Lambda_{aa}\mu_a - \Lambda_{ab}(x_b-\mu_b) \\ \implies \mu_{a|b} &= \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(x_b-\mu_b)\end{aligned}$$

Note that

$$\begin{aligned}\Lambda_{aa} &= \left(\Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}\right)^{-1} \\ \Lambda_{ab} &= -\Lambda_{aa}\Sigma_{ab}\Sigma_{bb}^{-1}\end{aligned}$$

Thus,

$$\begin{cases} \mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b-\mu_b) \\ \Sigma_{a|b} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} \end{cases}$$

§2 Lec 2: Jun 23, 2021

§2.1 Gaussian Distribution (Cont'd)

Let's start with a set of observations:

$$X = \{\vec{x}_1, \dots, \vec{x}_N\} \quad N \text{ data points where each } \vec{x}_n \in \mathbb{R}^D$$

and each $\vec{x}_n \sim N(\mu, \Sigma)$. As usual, there are two approach to this.

- Maximum likelihood: given the data, what μ, Σ are most probable/likely?

$$\max_{\mu,\Sigma} p\left(X|\mu,\Sigma\right)$$

Model assumption: $\vec{x}_n$ are i.i.d (independently, identically distributed). From i.i.d, we have

$$\begin{aligned} p\left(X|\mu,\Sigma\right) &= \prod_{n=1}^{N} p\left(\vec{x}_n|\mu,\Sigma\right) \\ &= \prod_{n=1}^{N} N\left(\vec{x}_n|\mu,\Sigma\right) \end{aligned}$$

This is tricky to do, so let's minimize the negative log likelihood

$$\begin{aligned} \min_{\mu,\Sigma} - \ln p\left(X|\mu,\Sigma\right) &= -\ln \prod_{n=1}^{N} \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(x_n-\mu)^\top \Sigma^{-1}(x_n-\mu)} \\ &= \cancel{-N \ln \frac{1}{(2\pi)^{\frac{D}{2}}}} - N \ln \frac{1}{|\Sigma|^{\frac{1}{2}}} + \frac{1}{2}\sum_{n=1}^{N}(x_n-\mu)^\top \Sigma^{-1}(x_n-\mu) \\ &= \frac{N}{2} \ln |\Sigma| + \frac{1}{2}\sum_{n=1}^{N}(x_n-\mu)^\top \Sigma^{-1}(x_n-\mu) + C \end{aligned}$$

As the domain is unbounded (unconstrained optimization problem) and objective function is convex, so to find optimal μ, we set $\frac{d}{d\mu} = 0$. Then

$$\begin{aligned} \frac{1}{2}\sum_{n=1}^{N} \Sigma^{-1}(x_n-\mu) &= 0 \\ \sum_{n=1}^{N} \Sigma^{-1} x_n &= N\Sigma^{-1}\mu \\ \implies \mu &= \frac{1}{N}\sum_{n=1}^{N} x_n \end{aligned}$$

- Maximum a posteriori (MAP)

$$\max_{\mu} p\left(\mu,\Sigma|X\right) \overset{\text{Bayes'}}{\Longrightarrow} \max_{\mu} p\left(X|\mu,\Sigma\right) \cdot p\left(\mu\right)$$

e.g., $p(\mu|\mu_0, \Sigma_0) = N(\mu|\mu_0, \Sigma_0)$. We have

$$-\ln p(X|\mu, \Sigma) \cdot p(\mu|\mu_0, \Sigma_0)$$

$$\min_{\mu} \frac{1}{2} \sum_{n=1}^{N} (x_n - \mu)^\top \Sigma^{-1} (x_n - \mu) + \frac{1}{2} (\mu - \mu_0)^\top \Sigma_0^{-1} (\mu - \mu_0)$$

$$\frac{d}{d\mu} = 0: \sum_{n=1}^{N} \Sigma^{-1} (x_n - \mu) + \Sigma_0^{-1} (\mu - \mu_0) = 0$$

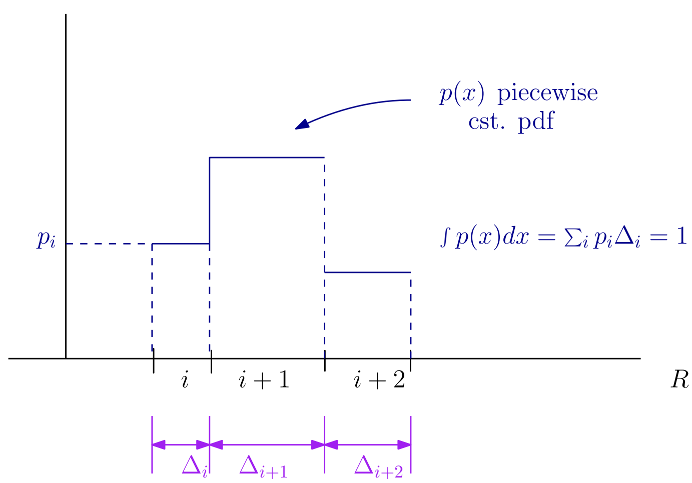
$$\implies \mu_{\mathrm{MAP}} = \left(N\Sigma^{-1} + \Sigma_0^{-1}\right)^{-1} \left(N\Sigma^{-1}\overline{x} + \Sigma_0^{-1}\mu_0\right)$$

§2.2 Non-parametric Probability Density Function (Estimation)

Let's consider the following

- Histograms
- partition domain of x into distinct bins of width $\triangle_i$
- count number of observations n_i of x falling into bin i
- divide by $N, \triangle_i$ to get a pdf.

$$p_i = \frac{n_i}{N\Delta_i} \text{ is density over bin } i$$



We often partition the domain uniformly, i.e., $\Delta_i = \Delta$

refer to fig 2.24 in textbook for other cases

Consider a region $R \subseteq \mathbb{R}^D$. The probability of a randomly chosen point will fall into R (according to pdf of $p(x)$ is

$$p = \int_R p(x)\, dx$$

Collect N samples; a fraction K of which will fall into R. So $K \sim \text{Binomial}(N, p)$

$$\mathbb{E}\left[\frac{K}{N}\right] = p$$

$$\text{var}\left[\frac{K}{N}\right] = \frac{p(1-p)}{N}$$

$$\text{var}\left[\frac{K}{N}\right] \xrightarrow[N\to\infty]{} 0$$

For large N, $\frac{K}{N} \approx P \implies K \approx N \cdot P$. Also, we want R big so that there are plenty of points in there. On the other hand, we want R small s.t. $p(x) \sim$ constant over R where $p = p(x)V$ in which V is the volume of R. Thus,

$$p(x) = \frac{K}{NV}$$

For histogram: we fix V and measure $\frac{K}{N}$. For the kernel, it's essentially the same but bin locations are not predefined.

Kernel Approach: If we want to know $p(x)$ at arbitrary x, we put a bin of predefined size around x then count $\frac{K}{N}$ for that bin.

Pick a smooth kernel, e.g., the Gaussian

$$p_h(x) \coloneqq \frac{1}{N} \sum_{n=1}^{N} \frac{1}{(2\pi h^2)^{\frac{D}{2}}} e^{-\frac{\|x-x_n\|_2^2}{2h^2}}$$

where h is standard deviation of Gaussian. Recall from 131BH that this is a convolution.

$$(f * g)(x) \coloneqq \int f(y)g(x-y)\, dy$$

So $k * \sum \delta(-x_n)$. More general,

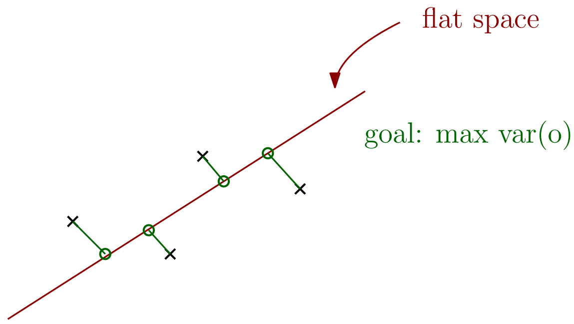
$$\begin{cases} k(u) \geq 0 \\ \int k(u)\, du = 1 \end{cases}$$

is sufficient criteria to be a kernel for kernel density estimation (KDE).

§3 Lec 3: Jun 24, 2021

§3.1 Principal Component Analysis

Maximum Variance Formulation: consider $\{x_n\}$, $n = 1, \ldots, N$, $x_n \in \mathbb{R}^D$. The goal is to project x onto a flat space with dimension $M \ll D$ while maximizing the variance of the projected data.



Let's start with $M = 1$ (a line) defined by a single vector $\vec{u} \in \mathbb{R}^D$ with unit norm, i.e.,

$$u_1^\top u_1 = \langle u_1, u_1 \rangle = \|u_1\|_2^2 = 1$$

Define: $\overline{x} = \frac{1}{N} \sum_{n=1}^N x_n$. Note that the variance before projection is

$$\text{var} = \frac{1}{N} \sum_{n=1}^N (x_n - \overline{x})^2$$

and after projection is

$$\text{var} = \frac{1}{N} \sum_{n=1}^N \left(u_1^\top x_n - u_1^\top \overline{x}\right)^2 = u_1^\top S u_1$$

with

$$\begin{aligned} S &= \frac{1}{N} \sum_{n=1}^N (x_n - \overline{x})(x_n - \overline{x})^\top \\ &= \text{cov}(x) \end{aligned}$$

Our optimization goal is

$$\max_{u_1} u_1^\top S u_1 \quad \text{s.t.} \quad u_1^\top u_1 = 1$$

This is a constrained optimization problem – let's introduce Lagrange multipliers for constraint:

$$\max_{u_1, \lambda_1} \left\{ \underbrace{u_1^\top S u_1 + \lambda_1 (1 - u_1^\top u_1)}_{=: L[u_1, \lambda_1]} \right\}$$

We have

$$\begin{aligned} \frac{\partial L}{\partial u_1} &: \ 2 S u_1 - 2\lambda_1 u_1 = 0 \\ & S u_1 = \lambda_1 u_1 \end{aligned}$$

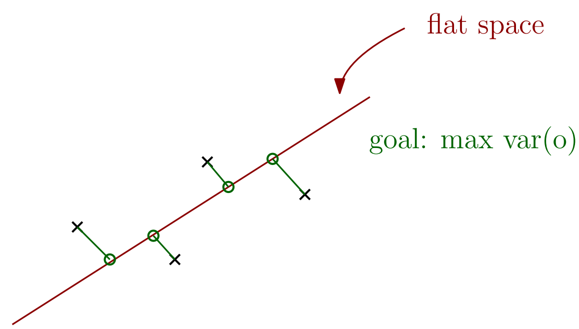
So, the eigen-problem: (λ_1, u_1) is eigenpair of S.

$$\text{var} = u_1^\top S u_1 = u_1^\top (\lambda_1 u_1) = \lambda_1 u_1^\top u_1 = \lambda_1$$

$\Longrightarrow$ we need to pick the dominant eigenpair of S. So if we want to project onto a flat with $M > 1$, we can simply pick $u_1, \ldots, u_n$ as the M leading eigenvectors of S where all u_i are orthogonal and

$$\text{var} = \sum_{i=1}^{N} \lambda_i$$

<u>**Minimum Error Formulation**</u>:



Goal: introduce as little distortion as possible.
Consider: $\{u_i\}, i = 1, \ldots, D$ orthonormal basis of $\mathbb{R}^D$

$$\Longrightarrow u_i^\top u_j = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & \text{otherwise} \end{cases}$$

Then each data point x_n has unique expansion in that basis

$$x_n = \sum_{i=1}^{D} \alpha_{ni} u_i \qquad\qquad \alpha_{ni} \in \mathbb{R}$$

where

$$\begin{aligned} x_n^\top u_j = u_j^\top x_n &= u_j^\top \sum_{i=1}^{D} \alpha_{ni} u_i \\ &= \sum_{i=1}^{D} \alpha_{ni} u_j^\top u_i = \alpha_{nj} \\ \Longrightarrow x_n &= \sum_{i=1}^{D} \left(x_n^\top u_i\right) u_i \end{aligned}$$

As we project to a flat, we need only the first M terms

$$\tilde{x}_n = \sum_{i=1}^{M} z_{ni} u_i + \sum_{i=M+1}^{D} b_i u_i$$

Now, we choose z_{ni}, u_i, b_i so as to minimize the distortion.

$$J = \frac{1}{N} \sum_{n=1}^{N} \|x_n - \tilde{x}_n\|_2^2$$

The results we should've obtained are

1. $z_{ni} = x_n^\top u_i$, $i = 1, \ldots, M$
2. $b_i = \overline{x}^\top u_i$, $i = M+1, \ldots, D$

We can substitute these into the expression of $\tilde{x}_n$ as follow

$$\tilde{x}_n = \sum_{i=1}^{M} \left(x_n^\top u_i\right) u_i + \sum_{i=M+1}^{D} \left(\overline{x}^\top u_i\right) u_i$$

$$x_n - \tilde{x}_n = \sum_{i=M+1}^{D} \left(x_n^\top u_i - \overline{x}^\top u_i\right) u_i$$

In addition, the error term can be written as

$$J = \frac{1}{N} \sum_{n=1}^{N} \sum_{i=M+1}^{D} \left(x_n^\top u_i - \overline{x}^\top u_i\right)^2 = \sum_{i=M+1}^{D} u_i^\top S u_i$$

So the problem now becomes

$$\min_{u_i, i=M+1,\ldots,D} \sum_{i=M+1}^{D} u_i^\top S u_i \quad \text{s.t.} \quad u_i^\top u_i = 1$$

Analogous to the case of maximum variance, we "throw away" the weakest eigenpairs of S.

§3.2 High-Dimensional PCA

Assume we have N data points with D dimensions and $\overline{x} = 0$. Then, $S = \frac{1}{N} x^\top x$

$$X = \begin{bmatrix} \text{———} \\ \text{———} \\ \text{———} \\ \\ \end{bmatrix}$$

where each x_n is a row of X. As $\overline{x} = 0$, rows sum up to 0.
Let's examine the eigenvalues of $x^\top x$ v.s. eigenvalues of $xx^\top$.

$$\frac{1}{N} x^\top x u_i = \lambda_i u_i$$

$$\frac{1}{N} x x^\top (x u_i) = \lambda_i (\underbrace{x u_i}_{v_i})$$

$$\frac{1}{N} x x^\top v_i = \lambda_i v_i$$

§3.3 Probabilistic PCA

Consider $x_n \in \mathbb{R}^D$ where

$$x_n = Wz + \mu + \varepsilon$$

where $z \in \mathbb{R}^M$ is latent variable and μ is mean and ε is noise & $\varepsilon \sim N(0, \sigma^2 I)$; z is the coordinates within the lower-dim flat, and W is the basis of the flat. The probabilistic formulation is

$$p(z) = N\left(z | 0, I\right)$$

$\implies$ latent variable $\sim$ zero-mean, unit variance Gaussian. The conditional distribution $x|z$ is again Gaussian

$$p(x|z) = N\left(x| \underbrace{Wz + \mu}_{\text{nozzle location}}, \underbrace{\sigma^2 I}_{\text{spray size}}\right)$$

Resulting point cloud is governed by predictive density $p(x)$.

$$p(x) = \int \underbrace{p(x|z) \cdot p(z)}_{p(x,z)} \, dz$$

Claim 3.1. $p(x)$ is Gaussian, too.

$$\begin{aligned} p(x) &= N\left(x|\mu, C\right) \\ C &= WW^\top + \sigma^2 I \in \mathbb{R}^{D\times D} \end{aligned}$$

Proof. Sufficient statistics

$$\begin{aligned} \mathbb{E} &= \mathbb{E}\left[Wz + \mu + \varepsilon\right] \\ &= \mathbb{E}[Wz] + \mu + \mathbb{E}[\varepsilon] \\ &= W\mathbb{E}[z] + \mu = \mu \end{aligned}$$

For the covariance,

$$\begin{aligned} \operatorname{cov}[x] &= \mathbb{E}\left[(x-\mu)(x-\mu)^\top\right] \\ &= \mathbb{E}\left[(Wz + \mu + \varepsilon - \mu)\left(Wz + \mu + \varepsilon - \mu\right)^\top\right] \\ &= \mathbb{E}\left[(Wz + \varepsilon)(Wz+\varepsilon)^\top\right] \\ &= \mathbb{E}\left[\left(Wz(Wz)^\top\right) + Wz\varepsilon^\top + \varepsilon(Wz)^\top + \varepsilon\varepsilon^\top\right] \\ &= \mathbb{E}\left[Wzz^\top W^\top\right] + \mathbb{E}\left[Wz\varepsilon^\top\right] + \mathbb{E}\left[\varepsilon z^\top W^\top\right] + \mathbb{E}\left[\varepsilon\varepsilon^\top\right] \\ &= W\mathbb{E}\left[zz^\top\right]W^\top + \cancel{W\mathbb{E}\left[z\varepsilon^\top\right]} + \cancel{\mathbb{E}\left[\varepsilon z^\top\right]W^\top} + \mathbb{E}\left[\varepsilon\varepsilon^\top\right] \\ &= WW^\top + \sigma^2 I \end{aligned}$$

> **Remark 3.1.** $\mathbb{E}\left[z\varepsilon^\top\right] = 0 = \mathbb{E}\left[\varepsilon z^\top\right]$ because z is independent from ε.

□

<u>*Note*</u>: Redundancy w.r.t. rotations in latent space (lack of uniqueness). Let $\tilde{W} = WQ$ where Q is orthonormal.

$$\begin{aligned} C &= \tilde{W}\tilde{W}^\top + \sigma^2 I \\ &= W\underbrace{QQ^\top}_{I}W^\top + \sigma^2 I \\ &= WW^\top + \sigma^2 I \end{aligned}$$

To evaluate $p(x) = N\left(x|\mu, C\right)$. We need C^{-1}.

$$C^{-1} = \sigma^{-2}I - \sigma^2 WM^{-1}W^\top$$

for $M = W^\top W + \sigma^2 I \in \mathbb{R}^{M\times M}$.

§3.4 Maximum Likelihood PCA

We need to learn W, μ, σ^2 from given data. By i.i.d,

$$\begin{aligned} p\left(X|W,\mu,\sigma^2\right) &= \prod_{n=1}^{N} p\left(x_n|W,\mu,\sigma^2\right) \\ \implies \ln p\left(X|W,\mu,\sigma^2\right) &= \sum_{n=1}^{N} \ln N\left(x_n|\mu, WW^\top+\sigma^2 I\right) \\ &= -\frac{ND}{2}\ln(2\pi) - \frac{N}{2}\ln|C| - \frac{1}{2}\sum_{n=1}^{N}(x_n-\mu)^\top C^{-1}(x_n-\mu) \end{aligned}$$

where $C = WW^\top + \sigma^2 I$; $\frac{d}{d\mu} = 0 \to \mu = \overline{x}$.
W, σ^2 are more tricky but again

refer to Bishop's paper

$$W = \begin{bmatrix} u_1 & \dots & u_n \end{bmatrix}$$

where u_i are leading eigenvectors of S.

§4 Lec 4: Jun 30, 2021

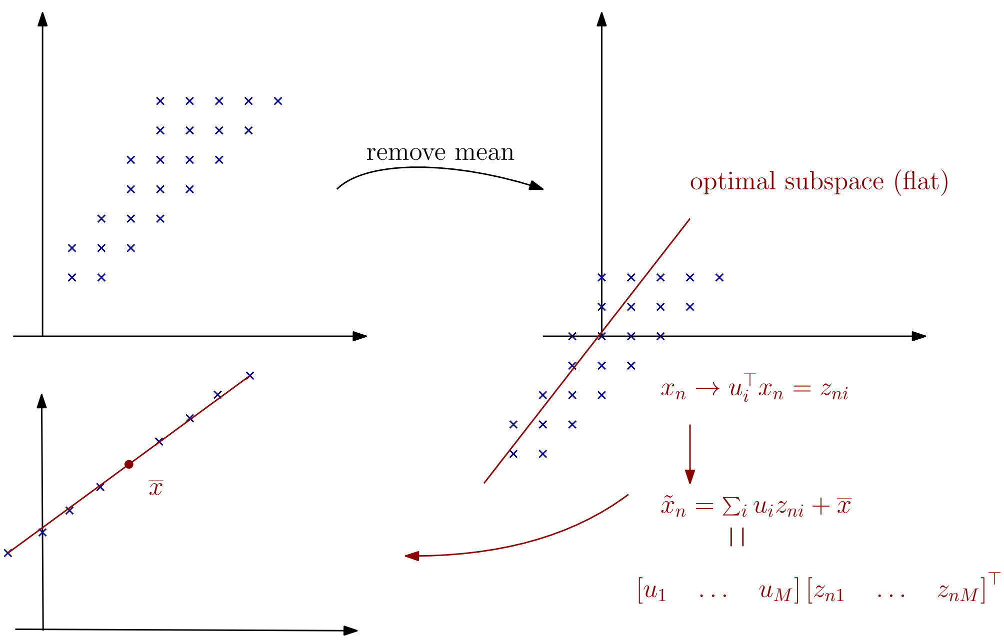
§4.1 Kernel PCA

Recap: Consider standard PCA – $\{x_n\}_{n=1}^N$ where each $x_n \in \mathbb{R}^D$. Assume w.l.o.g, $\sum \overline{x}_n = 0$, then

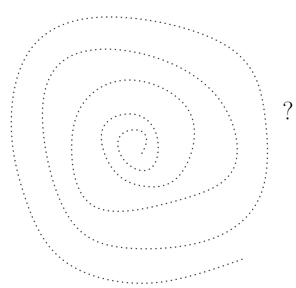
$$S = \frac{1}{N}\sum_{n=1}^{N} x_n x_n^\top$$

$\implies$ Principal components are found as leading eigenvectors of S.

$$Su_i = \lambda_i u_i \qquad \text{where oftentimes} \qquad u_i^\top u_i = 1$$



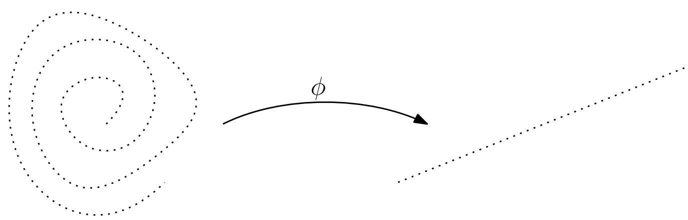
Question 4.1. What happens if we have non-flat data?



One way we can introduce non-linearity:

$$\{x_n\} \to \{\phi(x_n)\}$$

where $\phi : \mathbb{R}^D \to \mathbb{R}^E$ (E is possibly much bigger than D)



Let's assume $\{\phi(x_n)\}$ has 0 mean. Then, we can perform PCA on that data set.

$$C = \frac{1}{N}\sum_{n=1}^{N}\phi(x_n)\phi(x_n)^\top$$

is the relevant covariance matrix. We then need eigenpairs $Cv_i = \lambda_i v_i$, $i = 1, \ldots, M$. In fact,

$$k(x_n, x_m) \coloneqq \phi(x_n)^\top\phi(x_m)$$

where k is the kernel – it would be interesting if we can compute k easily even for large/infinite dimensional ϕ. more in later lecture!

$$\frac{1}{N}\sum\phi(x_n)\phi(x_n)^\top = \lambda_i v_i$$

For $\lambda_i > 0$, v_i (RHS) is a linear combination of $\phi(x_n)$. So

$$v_i = \sum_{n=1}^{N} a_{in}\phi(x_n)$$

and we don't know a yet. Let's substitute this into the eigen-equation:

$$\frac{1}{N}\sum_{n=1}^{N}\phi(x_n)\phi(x_n)^\top\sum_{m=1}^{N}a_{im}\phi(x_m) = \lambda_i\sum_{n=1}^{N}a_{in}\phi(x_n)$$

Multiply both sides with $\phi(x_l)^\top$, we have

$$\frac{1}{N}\sum_{n=1}^{N}\phi(x_l)^\top\phi(x_n)\sum_{m=1}^{N}a_{im}\phi(x_n)^\top\phi(x_m) = \lambda_i\sum_{n=1}^{N}a_{in}\phi(x_l)^\top\phi(x_n)$$

Now, we can replace all $\phi^\top\phi$ by the appropriate kernel k:

$$\frac{1}{N}\sum_{n=1}^{N}k(x_l, x_n)\sum_{m=1}^{N}a_{im}k(x_n, x_m) = \lambda_i\sum_{n=1}^{N}a_{in}k(x_l, x_n)$$

Notice that a_{in}, λ_i are the unknowns. In matrix notation,

$$K^2 a_i = \lambda_i N K a_i \implies K a_i = (\lambda_i N)\, a_i$$

where

$$\begin{cases} K_{m,n} = k(x_m, x_n) \\ a_i = \begin{bmatrix} a_{i1} \\ \vdots \\ a_{iN}\end{bmatrix} \in \mathbb{R}^N \end{cases}$$

So we just need to look for eigenpairs of K, i.e., instead of eigenpairs of $C(\mathbb{R}^{E\times E})$, we now look for eigenpairs of K $(\mathbb{R}^{N\times N})$. But we don't actually need v_i (we will project onto principal components, so all we do is compute inner products with v_i)

z – "Score" = coordinates within manifold

$$\begin{aligned} z(x) = \phi(x)^\top v_i &= \sum_{n=1}^{N} a_{in}\phi(x)^\top \phi(x_n) \\ &= \sum_{n=1}^{N} a_{in} k(x, x_n) \end{aligned}$$

<u>**Summary of Kernel PCA (kPCA)**</u>:

- Start with $\phi : \mathbb{R}^D \to \mathbb{R}^E$
- Build kernel $k(x, y) \coloneqq \phi(x)^\top \phi(y)$
- Build kernel matrix: $K_{\text{min}} \coloneqq k(x_m, x_n) \in \mathbb{R}^{N\times N}$
- Eigenpairs $(\lambda_i N, a_i)$ of $Ka_i = \lambda_i N a_i$
- For new data point x, $z_i(x) = \sum_{n=1}^{N} a_{in} k(x, x_n)$

Example 4.1

A kernel that we usually see:

$$k(x, y) = e^{-\frac{\|x-y\|^2}{\sigma^2}}$$

§4.2 Linear Basis Function Models

<u>Goal</u>: Predict the value of one or more continuous (real value) target variables t given the D-dimensional input vector x.

Example 4.2

We have

- $x \mapsto t$ is linear, $x \in \mathbb{R}^D$
- $t = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_D x_D$
- $t = w_0 + w_1\phi_1(x) + w_2\phi_2(x) + \ldots$ where $\phi(x)$ could be some <u>non-linear basis</u> function (polys, exponentials,...). The important part here is the linearity w.r.t. parameters.

Linear regression:

$$y(x, w) = w_0 + w_1 x_1 + \ldots + w_D x_D$$

where $x \in \mathbb{R}^D$ is data, and w is parameters. Extend to non-linear functions of input

$$y(x, w) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(x)$$

where

$$\begin{cases} \phi_j(x) = \text{basis function} \\ M = \text{degree of freedom} \\ w_0 = \text{offset/bias} \end{cases}$$

For convenience, we often denote

$$\phi_0(x) \coloneqq 1$$

Then

$$y(x,w) = w^\top \phi$$

where

$$\phi = \begin{bmatrix} \phi_0(x) = 1 \\ \phi_1(x) \\ \vdots \\ \phi_{n-1}(x) \end{bmatrix}, \qquad w = \begin{bmatrix} w_0 \\ \vdots \\ w_{n-1} \end{bmatrix}$$

in which $\phi, w \in \mathbb{R}^n$

Example 4.3

Consider:

- $\phi_j = x^j$
- $\phi_j = e^{-\frac{\|x-\mu_j\|^2}{2\sigma^2}}$ – Gaussian.

Question 4.2. How do we find the optimal weights, train/fit the model given the data point?

Approach 1 – Maximum Likelihood/Least Squares

Assumption: Want to find w that make the observed data most likely.

$$\text{Model}: \quad t = y(x,w) + \varepsilon$$

where $\varepsilon \sim N(0,\sigma^2)$ – Gaussian noise. Note that the book uses $\frac{1}{\beta} = \sigma^2$, $\sigma^2 =$ variance, and $\beta =$ precision.

$$p\left(t|x,w,\sigma^2\right) \coloneqq N\left(t|y(x,w),\sigma^2\right)$$

in which x : location, w : parameter, and σ^2 : noise. Next, let's look at the conditional mean

$$\begin{aligned} \mathbb{E}\left[t|x\right] &= \int tp(t|x)\,dt \\ &= y(x,w) \end{aligned}$$

We have training data $X = \{x_1 \quad \dots \quad x_N\}$ with associated target values $t = \{t_1 \quad \dots \quad t_N\}$. Observed samples are i.i.d.

$$p\left(\vec{t}|X,w,\sigma^2\right) = \prod_{n=1}^{N} N\left(t_n|y(x,w),\sigma^2\right)$$

The usual approach:

$$\begin{aligned} \ln\left(\vec{t}|X,w,\sigma^2\right) &= \sum_{n=1}^{N} \ln N\left(t_n|w^\top\phi(x_n),\sigma^2\right) \\ &= -\frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi) - \frac{1}{2\sigma^2}\sum_{n=1}^{N}\left(t_n - w^\top\phi(x_n)\right)^2 \end{aligned}$$

Thus,

$$-\ln p \cong \frac{1}{2}\sum_{n=1}^{N}\left(t_n - w^\top\phi(x_n)\right)^2 = \text{sum of squared errors}$$

i.e., maximum likelihood is equivalent to minimum squared error.

To minimize error: $\frac{d}{dw} \overset{\text{set}}{=} 0$

$$\frac{d}{dw} - \ln p\left(\vec{t}|X, w, \sigma^2\right) = \frac{1}{\sigma^2}\sum_{n=1}^{N}\left(t_n - w^\top \phi(x_n)\right)\phi(x_n)^\top$$

As LHS = 0, we have

$$\sum_{n=1}^{N} t_n \phi(x_n)^\top = w^\top \sum_{n=1}^{N}\phi(x_n)\phi(x_n)^\top$$

Let's define

$$\Phi := \begin{bmatrix} \phi_0(x_1) & \dots & \phi_{n-1}(x_1) \\ \vdots & & \vdots \\ \phi_0(x_N) & \dots & \phi_{n-1}(x_N) \end{bmatrix} \text{ – design matrix}$$

So the solution is

$$w_{ML} = \underbrace{(\Phi^\top\Phi)^{-1}\Phi^\top}_{\text{Moore Penrose pseudo inverse}} \quad \vec{t}$$

From the pseudo-inverse idea, recall that for $A\vec{x} = \vec{b}$ where $\vec{b} \notin \text{range}(A)$, we have

$$\begin{aligned} \min \frac{1}{2}\|A\vec{x} - \vec{b}\|^2 \quad &\text{(least squares problem)} \\ \implies \vec{x} = (A^\top A)^{-1}A^\top \vec{b} \end{aligned}$$

Question 4.3. What is the MLE for σ^2?

Same approach as above but we take the derivative with repspect to σ^2 and set that equal to 0.

$$\sigma^2 = \frac{1}{N}\sum_{n=1}^{N}\left(\underbrace{t_n - w_{ML}^\top\phi(x_n)}_{\text{residual(error)}}\right)^2$$

Remark 4.4. In the context of "big data" – N, D big (or M: # of basis functions big), Φ is not going to fit into memory and/or difficult to handle or data visible in portions (streaming). So we need sequential learning in which we use "gradual updates" to estimates of w_{ML}

$$\begin{aligned} w^0 &= \text{initial guess} \\ w^{n+1} &= \underbrace{w^n - \eta\frac{d}{dw}E}_{\text{gradient descent}} \end{aligned} \tag{*}$$

where E is the loss function evaluated for current batch of data points and η is the stepsize. We hope that (*) converge to optimal parameters. In details,

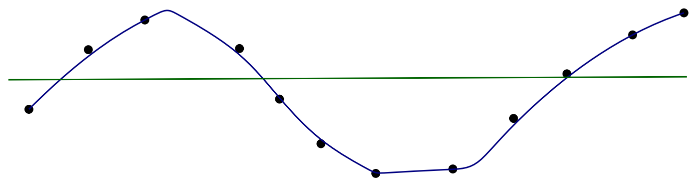
$$w^{n+1} = w^n - \eta\left(t_n - w^{nT}\phi(x_n)\right)\phi(x_n)^\top$$

One of the crucial step here is to choose the step-size carefully.

§5 Lec 5: Jul 1, 2021

§5.1 Overfitting

Consider:



Through a first glance, it might be intuitive to assume that the data is generated from the blue curve ... However, it's not that clear, and the data may actually stem from the green line. In fact, it's very difficult to tell as the data itself does not communicate well with us here (noise level?). This phenomenon, in one direction, is called overfitting.
Assume that $\{x\}$ was generated from the blue curve, and we try to fit/learn the green line instead; this is the definition of overfitting. In essence, we try to explain some of the "wiggle" (variance) we see in the data by a more complicated/unnecessary model – a very dangerous process. Overfit is a consequence of too powerful models (often too many options to learn from).
Thus, to avoid overfitting, we use 3 data sets:

1. training data set $\{x_n\}$ & $\{t_n\}$
2. validation: $\{x_n\}$ & $\{t_n\}$ (10-20 % of data not used for training)
   $\rightarrow$ run "trained" model and see how well it performs.
3. "real data": $\{x_n\} \rightarrow \{t_n\}$ inferred using trained model.

Overall, our ultimate goal is to test the model's ability to "generalize" or perform on new/unseen data.

refer to overfitting for more details on the topic

§5.2 Regularized Least Squares

Goal: we want to control overfitting – include a regularization term in addition to the data term.
Connection to linear algebra:

$$\begin{cases} A\vec{x} = \vec{b} \text{ does not have a solution} \\ A \text{ ill-conditioned (no solution, not unique solution, sensitive to } \triangle\vec{b}) \\ \implies \text{Tikhonov – regularization :} \\ \quad \min \frac{1}{2}\|A\vec{x} - \vec{b}\|_2^2 + \| \underbrace{\Gamma\vec{x}}_{\text{regularizer}} \|_2^2 \end{cases}$$

Data-term for linear regression

$$E_0(w) = \frac{1}{2}\sum_{n=1}^{N}\left(t_n - w^\top\phi(x_n)\right)^2$$

Simple regularizer: quadratic penalty on w

$$E_w(w) = \frac{1}{2}w^\top w = \frac{1}{2}\|w\|^2$$

then

$$\min_w E_0(w) + \lambda E_w(w) = \frac{1}{2}\sum_{n=1}^{N}\left(t_n - w^\top\phi(x_n)\right)^2 + \frac{\lambda}{2}w^\top w$$

Now, we can set $\frac{d}{dw} = 0$,

$$w = \left(\lambda I + \Phi^\top \Phi\right)^{-1} \Phi^\top \vec{t}$$

This shrinks the component of w towards 0 if compared to

$$w_{ML} = \left(\Phi^\top \Phi\right)^{-1} \Phi^\top \vec{t}$$

More generally (more modern),

$$E_w(w) \coloneqq \frac{1}{2} \sum_{j=1}^{M} |w_j|^q$$

- $q = 1 \to$ "LASSO" which has tendency to promote sparsity (some coeffs of w will be exactly 0)

refer to wiki for more details

- $q = 2 \to$ same as above.

To summarize, to address the problem of overfitting, we have the following ways

- Model complexity: keep model simple (restricted set of basis functions)
- Regularization: encourage simple coefficients by adding penalty to complex choices.

§5.3 Bayesian Linear Regression

Let's start by introducing a prior distribution on w (for now we consider noise $\sigma^2 = \frac{1}{\text{position}}$ known). Recall from the last lecture,

- $p(t|x_n, w, \sigma^2)$ is Gaussian, i.e., $= N\left(t_n | w^\top \phi(x_n), \sigma^2\right)$
- conjugate prior: $p(w) = N\left(w|m_0, S_0\right)$ is Gaussian too.

The posterior will also be Gaussian.

$$p\left(w|\vec{t}, x, \sigma^2\right) = N\left(w|m_N, S_N\right)$$

which is in basically through Bayes' rule

$$p\left(w|\text{data}\right) = \frac{p\left(\text{data}|w\right) p(w)}{p(\text{data})}$$

From exercise 3.7 in the book,

$$m_N = S_N \left(S_0^{-1} m_0 + \frac{1}{\sigma^2} \Phi^\top \vec{t}\right)$$

and

$$S_N^{-1} = S_0^{-1} + \frac{1}{\sigma^2} \Phi^\top \Phi \quad \text{(precision)}$$

So

$$\boxed{\text{posterior precision} = \text{prior precision} + \text{data precision}}$$

> **Remark 5.1.** If $S_0^{-1} = 0(\implies S_0 = \frac{1}{\alpha} I, \alpha \to 0)$ non-informative prior
>
> $$S_N^{-1} = \frac{1}{\sigma^2} \Phi^\top \Phi \to m_N = \sigma^2 \left(\Phi^\top \Phi\right)^{-1} \frac{1}{\sigma^2} \Phi^\top \vec{t} = \left(\Phi^\top \Phi\right) \Phi^\top \vec{t}$$

Notice that

$$\underset{w}{\operatorname{argmax}}\, p\left(w|\vec{t}, X, \sigma^2\right) = \underset{w}{\operatorname{argmax}}\, N\left(w|m_N, S_N\right)$$

Gaussian: $\operatorname{argmax}_w n\left(w|m_N, S_N\right) = m_N$

$$w_{\text{MAP}} = m_N = S_N\left(S_0^{-1}m_0 + \frac{1}{\sigma^2}\Phi^\top\vec{t}\right)$$

The second special case: $N \to 0$

$$m_N \to m_0 \qquad \text{(prior becomes dominant)}$$

Choose a special prior: $m_0 = 0; S_0 = \frac{1}{\alpha}I$ (zero mean, isotropic Gaussian prior).

$$\implies \begin{cases} m_N = \frac{1}{\sigma^2}S_N\Phi^\top\vec{t} \\ S_N^{-1} = \alpha I + \frac{1}{\sigma^2}\Phi^\top\Phi \end{cases}$$

Now, we can take $-\log$ of posterior

$$-\ln p\left(w|\vec{t}, X, \sigma^2\right) = \underbrace{\frac{1}{2\sigma^2}\sum_{n=1}^{N}\left(t_n - w^\top\phi(x_n)\right)^2 + \frac{\alpha}{2}w^\top w}_{=E_0(w)+E_w(w)} + \text{constant}(w)$$

Predictive Distribution

w is/are not actually the object of interest. Rather, we want to predict t for new x. For a new query location x and new target variable t,

$$p\left(t|x, \vec{t}, X, \alpha, \sigma^2\right) = \int p\left(t|x, w, \sigma^2\right)\cdot p\left(w|\vec{t}, X, \alpha, \sigma^2\right)\, dw$$

then

$$\int N\left(t|w^\top\phi(x), \sigma^2\right)N\left(w|m_N, S_N\right)\, dw = N * N$$

and the convolution of two Gaussians is Gaussian. So we only need to find the right parameters

$$p\left(t|x, \vec{t}, X, \alpha, \sigma^2\right) = N\left(t|m_N^\top\phi(x), \sigma_N^2(x)\right)$$

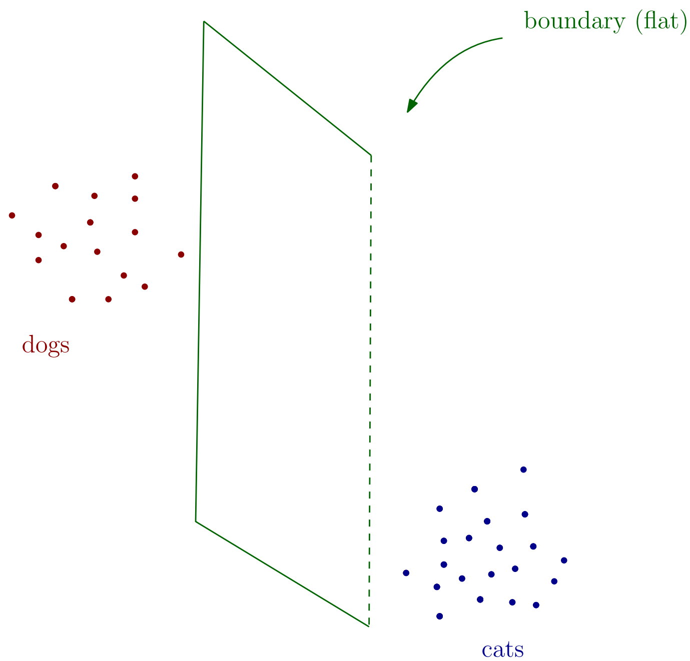
where $\sigma_N^2(x) = \sigma^2 + \phi(x)^\top S_N\phi(x)$ in which the first term is general noise, and second term is uncertainty on w due to proximity/distance of training data.

§6 Lec 6: Jul 7, 2021

§6.1 Linear Models for Classification

Goal: $\mathbb{R}^D \ni x \mapsto C_k$ one of k discrete classes $k = 1 \dots k$. Note that classes are disjoint, i.e., x belongs to exactly 1 class. Thus, classification is equivalent to partitioning of $\mathbb{R}^D$ (decision regions separated by decision boundaries/surfaces).

$$\text{linear model} \iff \text{decision surfaces are } D-1 \text{ dimensional hyperplanes}$$



Representation:

$$\begin{cases} t \in \{0;1\}, & k=2 \\ \text{or } \{-1;+1\}, & \text{“binary”} \\ t \in \{1,\dots,k\}, & k \geq 2 - \text{not use in practice} \\ t \in \{0,1\}^k;\ |t| = 1, & \text{1 in k coding (vector)} \end{cases}$$

There are 3 approaches to classification problems

1. discriminant function: $x \mapsto C_k$
2. probability based
   a) discriminative: $p(C_k|x)$
   b) generative model: $p(C_k) \cdot p(x|C_k)$

   Let's dive right into the first approach.

General form of linear model:

$$y(x) = f\left(w^\top x + w_0\right)$$

where f is an activation function.

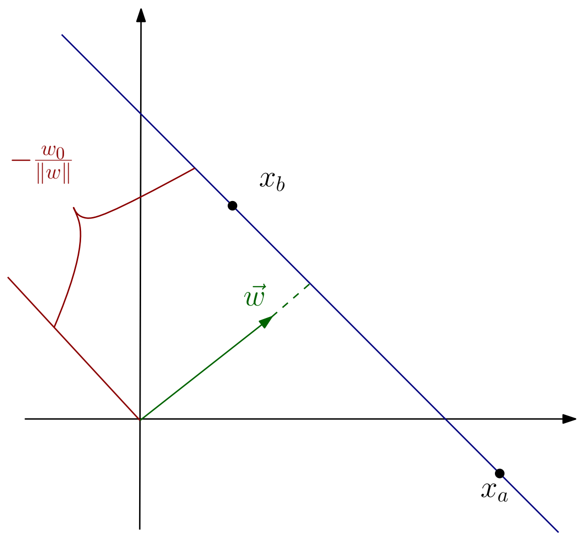
same notation later on for deep learning

Decision surface: $y(x) =$ constant which means

$$w^\top x + w_0 = \text{constant}$$

Take $k = 2$, $f :=$ sign, i.e., $y(x) \in \{-1; +1\}$.

Claim 6.1. Let x_a, x_b on decision boundary (which means $w^\top x_a + w_0 = 0$, etc). Then $w \perp x_a - x_b$.



Proof. WTS: $w^\top(x_a - x_b) = 0$.

$$\begin{aligned} w^\top(x_a - x_b) &= w^\top x_a - w^\top x_b + w_0 - w_0 \\ &= \left(w^\top x_a + w_0\right) - \left(w^\top x_b + w_0\right) \\ &= 0 - 0 = 0 \end{aligned}$$

□

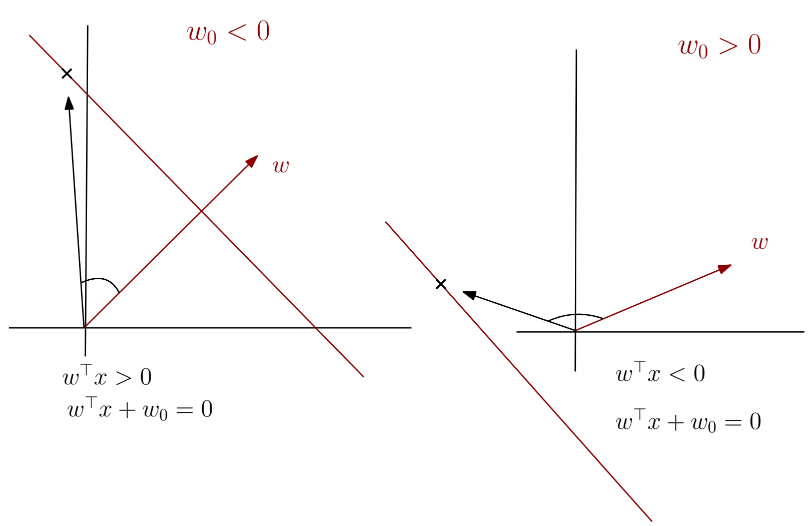
So w is orthogonal to $x_a - x_b$.

Claim 6.2. Signed distance between the origin and decision surface is $\frac{-w_0}{\|w\|}$.

Proof. As x is on decision surface, we have $w^\top x = -w_0$. Signed distance between origin and decision surface

$$\frac{w^\top}{\|w\|}x = -\frac{w_0}{\|w\|}$$

□



Claim 6.3. Signed distance between x and decision surface is $\frac{w^\top x + w_0}{\|w\|}$.

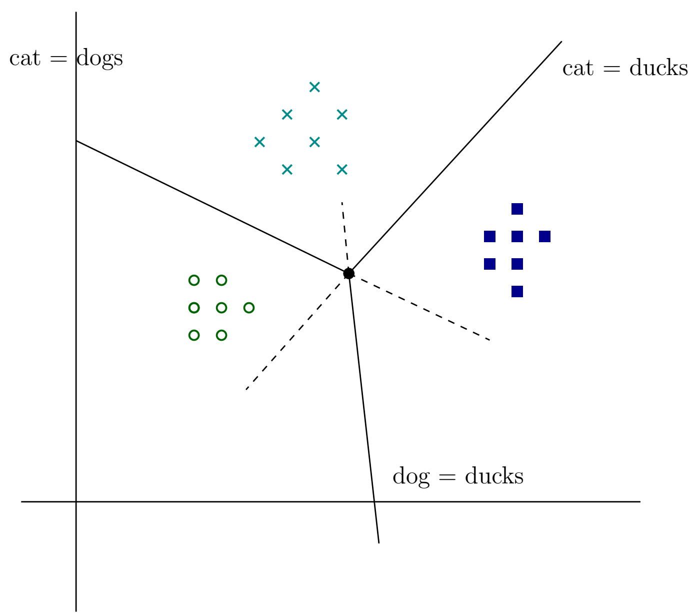
Proof. We have

$$\begin{aligned} x &= x_p + r\frac{w}{\|w\|} \\ w^\top x &= w^\top x_p + r\frac{w^\top w}{\|w\|} \\ w^\top x + w_0 &= (w^\top x_p + w_0) + r\frac{w^\top w}{\|w\|} \\ w^\top x + w_0 &= r\|w\| \\ r &= \frac{w^\top x + w_0}{\|w\|} \end{aligned}$$

□

That's all the geometry we need. Next, let's take a quick look at multiclass extension. Define $y_k(x) = w_k^\top x + w_{k0}$ for each class. Then assign class by winner takes all. For a new x: $y_1(x), y_2(x), \ldots, y_k(x)$ then say x class j if $y_i \geq y_k(x)\ \forall k$.
Decision boundary: ($b|w$ class k & j)

$$\begin{gathered} w_k^\top x + w_{k_0} = w_j^\top x + w_{j_0} \\ \underbrace{(w_k - w_j)^\top}_{\text{orth}} x + \underbrace{(w_{k_0} + w_{j_0})}_{\text{bias}} = 0 \\ \implies \text{decision surfaces} = D - 1 \text{ dimensional hyperplanes} \end{gathered}$$



Claim 6.4. Decision regions are always convex.

Proof. Let $x_a, x_b \in$ class k. Convexity means that for any $\lambda \in (0, 1]$

$$\lambda x_a + (1 - \lambda)x_b \in \text{class } k$$

We then have

$$\forall j \neq k: \; w_k^\top x_a + w_{k_0} > w_j^\top x_a + w_{j_0}$$
$$w_k^\top x_b + w_{k_0} > w_j^\top x_b + w_{j_0}$$

Consider: $x = \lambda x_a + (1-\lambda) x_b$

$$\begin{aligned} w_k^\top x + w_{k_0} &= w_k^\top (\lambda x_a + (1-\lambda)x_b) + w_{k_0} \\ &= \lambda \left(w_k^\top x_a + w_{k_0} \right) + (1-\lambda) \left(w_k^\top x_b + w_{k_0} \right) \\ w_j^\top x + w_{j_0} &= \ldots = \lambda \left(w_j^\top x_a + w_{j_0} \right) + (1-\lambda) \left(w_j^\top x_b + w_{j_0} \right) \end{aligned}$$

$\implies$ x is also in class k. □

Probabilistic Generative Models

Goal: get linear models as a result of probabilistic modeling.
Generative model:

1. class conditional probabilities: $p(x|C_k)$
2. class priors: $p(C_k)$

We want to use Bayes' to compute the estimate $p(C_k|x)$. We will consider the two-class case only.

$$p(C_1|x) = \frac{p(x|C_1) \cdot p(C_1)}{p(x|C_1)p(C_1) + p(x|C_2)p(C_2)}$$

Let's define

$$a := \ln \frac{p(x|C_1)p(C_1)}{p(x|C_2)p(C_2)}$$

Then,

$$p(C_1|x) = \frac{1}{1+e^{-a}} =: \sigma(a)$$

which we call sigmoid(a). Notice that the logistic sigmoid $\sigma : \mathbb{R} \to [0,1]$

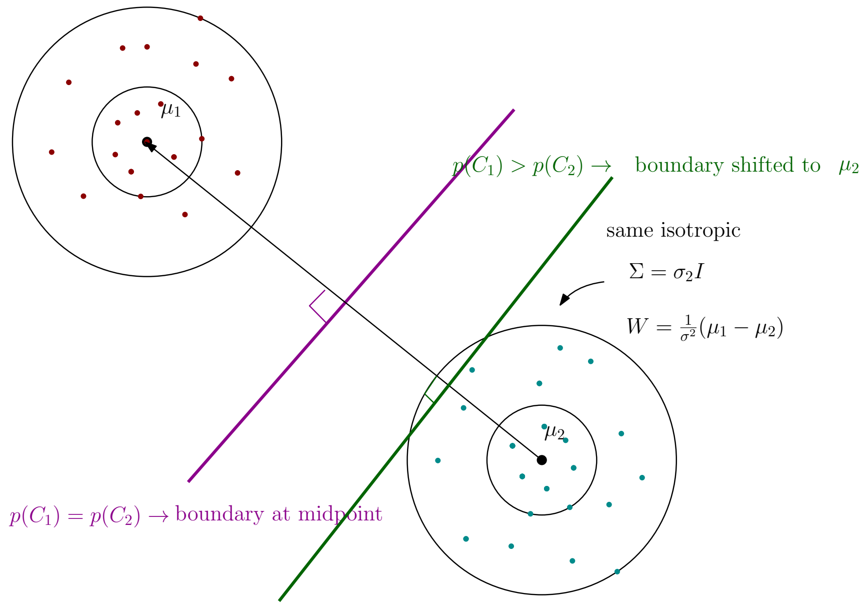
- symmetry: $\sigma(-a) = 1 - \sigma(a)$
- inverse: $a = \ln \left(\frac{\sigma}{1-\sigma} \right)$ – logit function

We now define class-conditional probability (Gaussian). Then

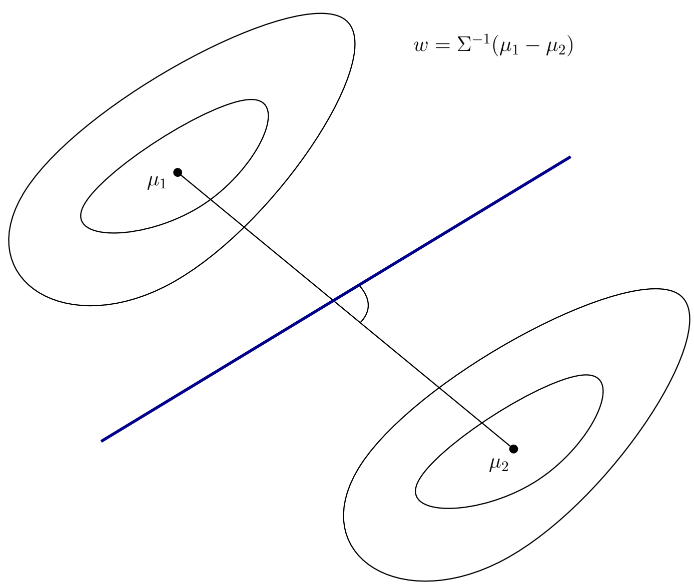
$$p(x|C_k) = \frac{1}{(2\pi)^{\frac{D}{2}}} \frac{1}{|\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k}$$

where we assume class-specific μ_k; common Σ. So

$$p(C_1|x) = \sigma(w^\top x + w_0), \quad \begin{cases} w = \Sigma^{-1}(\mu_1 - \mu_2) \\ w_0 = -\frac{1}{2}\mu_1^\top \Sigma^{-1}\mu_1 + \frac{1}{2}\mu_2^\top \Sigma^{-1}\mu_2 + \ln \frac{p(C_1)}{p(C_2)} \end{cases}$$



For a more general Σ (not necessarily isotropic)



We will use MLE to learn $\Sigma, p(C_1)/p(C_2)$, and μ_1, μ_2

$$\text{Data:} \quad X = \begin{bmatrix} x_1 & \dots & x_N \end{bmatrix}$$

$$\vec{t} = \begin{bmatrix} t_1 \\ \vdots \\ t_N \end{bmatrix}; \quad t_n \in \{0, 1\}$$

$$p(C_1) = \underbrace{\pi}_{\neq 3.14\ldots}, \quad p(C_2) = 1 - \pi$$

For $x_n \in C_1 : t_n = 1$, and

$$p(x_n, C_1) = p(C_1) p(x_n | C_1) = \pi N \left(x_n | \mu_1, \Sigma\right)$$

Similarly, for $x_n \in C_2 : t_n = 0$, and

$$p(x_n, C_2) = p(C_2)p(x_n|C_2) = (1-\pi)N(x_n|\mu_2, \Sigma)$$

Because the data is assume i.i.d:

$$p\left(\vec{t}, x|\pi, \mu_1, \mu_2, \Sigma\right) = \prod_{n=1}^{N} \left[\pi \underbrace{N\left(x_n|\mu_1, \Sigma\right)}_{N_1}\right]^{t_n} \left[(1-\pi) \underbrace{N\left(x_n|\mu_2, \Sigma\right)}_{N_2}\right]^{1-t_n}$$

As usual, we want to maximize the log-likelihood.

$$\ln p\left(\vec{t}, x|\pi, \mu_1, \mu_2, \Sigma\right) = \sum_{n=1}^{N} t_n \left[\ln \pi + \ln N_1\right] + (1-t_n)\left[\ln(1-\pi) + \ln N_2\right]$$

and set the derivatives of each term to zero.

- π

  $$\sum_{n=1}^{N} t_n \ln \pi + (1-t_n)\ln(1-\pi)$$

  Set $\frac{d}{d\pi} = 0$, then

  $$\pi = \frac{1}{N}\sum_{n=1}^{N} t_n = \frac{\text{\# of data pts in class 1}}{N}$$

- μ_k, let's consider $k = 1$, i.e., μ_1

  $$\sum_{n=1}^{N} t_n \left(-\frac{1}{2}(x_n - \mu_1)^\top \Sigma^{-1}(x_N - \mu_1)\right)$$

  Set $\frac{d}{du_1} = 0$ as before and we get

  $$\mu_1 = \frac{1}{\#1}\sum_{n=1}^{N} t_n x_n$$

  Similarly,

  $$\mu_2 = \frac{1}{\#2}\sum_{n=1}^{N}(1-t_n)x_n$$

Probabilistic Discriminative Models

Probabilities are good, but we have to deal with too many parameters, e.g., $\pi, \mu_1, \mu_2, \Sigma$. Knowing that the shared covariance matrix Σ leads to linear models we can try to learn $p(C_k|x)$ directly.

$$p(C_k|x) = \sigma\left(w_k^\top x + w_{k_0}\right) \impliedby \text{logistic regression}$$

§7 Lec 7: Jul 12, 2021

§7.1 Ensemble Methods

The basic idea of ensemble method is "pool" (average) predictions stemming from a *diverse* set of models (regression/classification). This is another way to address the issue of overfitting, in which we hope that multiple models will

1. overfit differently
2. capture the structure coherently

When trained on different parts of the data, noise realizations will hopefully cancel out (in statistical sense) in aggregation because they are statistically independent. Meanwhile, the structural components will be reinforced. There are two crucial steps to this problem.

1. **Bootstrapping**

   Given a data set D of size N (N data points in the set). We can generate M new training sets D_m each of size N' by sampling from D uniformly and with replacement.

   > **Remark 7.1.** If $N' = N$, then each D_m contains $\left(1 - \frac{1}{e}\right) \approx 63\%$ of unique elements of D and the rest is duplicates.

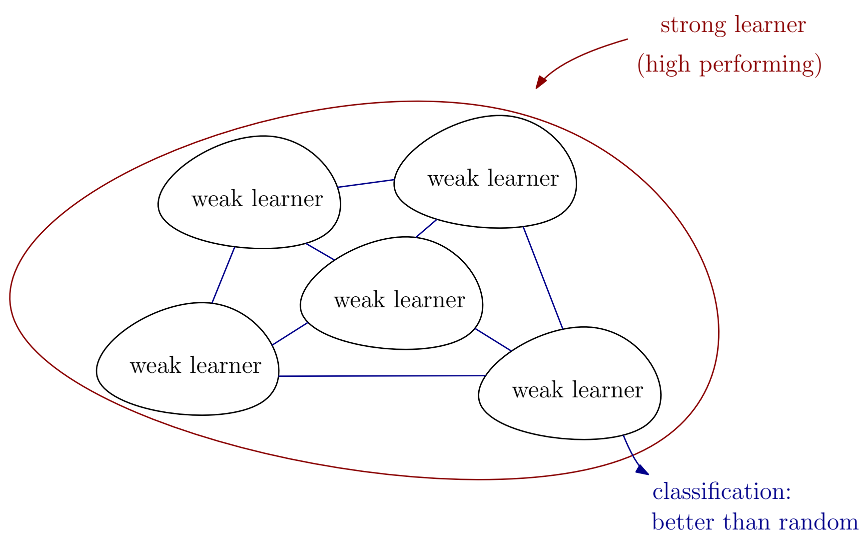
   By using the M "new" training data sets D_m, we train M models.

2. **Aggregation**

   $\rightarrow$ combine output of M models by

   - averaging (regression)
   - majority vote (classification)

This process is also known as "bagging" (bootstrap aggregating). Notice that the M models are all equally dumb as they don't learn from each other's mistakes.



<u>**Adaptive Boosting**</u> (AdaBoost for classification)
Fundamentally, we still have M weak learners (slightly better than random), and we train them in sequence where training focuses on data points that were previously misclassified. In this case, the output is weighted average; this provably results in strong learners.

Algorithm:
Input:

- location: $x_1, \ldots, x_N \in \mathbb{R}^D$
- binary targets: $t_1, \ldots, t_N \in \{-1; +1\}$

A family of weak learners: $y_w(x)$ where w is parameters (discrete/continuous) and

$$y_w(x) \in \{-1; +1\}$$

For example, $y_w(x) = \operatorname{sign}(w^\top x + w_0)$.
Initial weights:

$$w_n^{(1)} = \frac{1}{N}$$

which is not a parameter, but it's weight attached to each data point. So they all have same weight initially and add up to one. For $m = 1, \ldots, M$,

- train/select classifier $y_w^m(x)$ – minimizing:

$$J_m := \sum_{n=1}^{N} w_n^{(m)} \underbrace{\mathbf{1}\left(y_w^m(x_n) \neq t_n\right)}_{\text{error indicator}}$$

  where $w_n^{(m)}$ is the current weight of x_n, $y_w^m(x_n)$ is the current prediction for x_n, and t_n is the label. Also, when the arguments inside $\mathbf{1}$ are equal, the term becomes zero, or one otherwise.

- estimate learner performance:

$$\varepsilon_m := \frac{\sum_{n=1}^N w_n^{(m)} \mathbf{1}\left(y_w^m(x_n) \neq t_n\right)}{\sum_{n=1}^N w_n^{(m)}}$$

- weight learner:

$$\alpha_m := \ln \frac{1 - \varepsilon_m}{\varepsilon_m}$$

- update the data weighting:

$$w_n^{(m+1)} = w_n^{(m)} e^{\alpha_m \mathbf{1}(y_w^m(x_n) \neq t_n)}$$

- prediction:

$$y_m(x) = \operatorname{sign}\left(\sum_{m=1}^{M} \alpha_m y_w^m(x)\right)$$

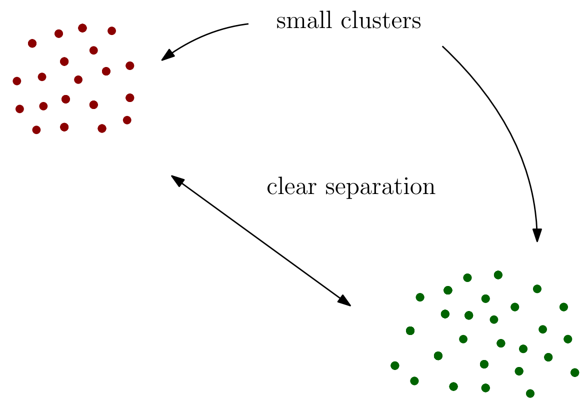
Notice that

- the perfect learner has $\varepsilon_m = 0 \implies \alpha_m \to \infty$
- the perfect liar has $\varepsilon_m = 1 \implies \alpha_m \to -\infty$
- the random learner has $\varepsilon_m = \frac{1}{2} \implies \alpha_m = 0$
- $\varepsilon_m > \frac{1}{2} \implies \alpha_m < 0$

§7.2 K-Means Clustering

Clustering is basically classification without training labels. It's the partitioning of data points into "meaningful" groups from "scratch" (no training data).
Goal: Given data $\{x_n\}_{n=1}^N$, $x_n \in \mathbb{R}^D$ group samples into K clusters s.t.

- within a cluster: distances are small
- between clusters: distances are big



The trick here is to introduce $\mu_k \in \mathbb{R}^D$, $k = 1, \ldots, K$ to represent the cluster centers. Cluster membership: $r_{nk} \in \{0, 1\}$

$$r_{nk} = 1 \text{ if } x_n \text{ belongs to class } k \text{ (1-in-k coding)}$$
$$r_{nk} = 0 \text{ otherwise}$$

We can now introduce the objective function as follow

$$\min_{r_{nk}, \mu_k} J := \frac{1}{2} \sum_{n=1}^N \sum_{k=1}^K r_{nk} \|x_n - \mu_k\|_2^2$$

Our goal here is to minimize J to make sure that each x_n is close to its assigned μ_k.
Algorithm to approximate the min:

NP-hard problem

1. Initialize with a random μ_k
2. Given μ_k, assign each x_n to closest μ_k

$$r_{nk} = \begin{cases} 1, & k = \text{argmin } \|x_n - \mu_j\|^2 \\ 0, & \text{otherwise} \end{cases}$$

3. Given r_{nk}, update the cluster centers

$$\mu_k = \frac{\sum_n r_{nk} x_n}{\sum_n r_{nk}}$$

Repeat this process until no further class reassignments happen. It can be shown that this converges but not necessarily to the global optimum, and it might be trapped in a local min.

§8 Lec 8: Jul 14, 2021

§8.1 Mixture of Gaussians

Let's first introduce a latent variable:

$$z \in \{0,1\}^k, \qquad \left(\sum_k z_k = 1\right) \text{ – 1-in-k code}$$

This latent variable describes the "inner" state of a data point (or of an observed x). We can now talk about the joint distribution. Let x be an observed data point and z be its associated latent variable.

$$p(x,z) = \underbrace{p(x|z)}_{\text{Gaussian}} \cdot p(z)$$

- Denote $p(z_k = 1) = \pi_k$, $\sum_{k=1}^{k} \pi_k = 1$, $\pi_k \in [0,1]$

$$\implies p(z) = \prod_{k=1}^{K} \pi_k^{z_k} \quad \text{– A compact notation}$$

- Class-conditional is Gaussian:

$$p(x|z_k = 1) := N\left(x|\mu_k, \Sigma_k\right)$$

  Using the same trick as above, we have

$$p(x|z) = \prod_{k=1}^{K} N\left(x|\mu_k, \Sigma_k\right)^{z_k}$$

  and the marginal is

$$\begin{aligned} p(x) &= \sum_z p(x,z) = \sum_z p(x|z)p(z) \\ &= \sum_{k=1}^{K} N\left(x|\mu_k, \Sigma_k\right)\pi_k \end{aligned}$$

From Bayes, we can find the likelihood of latent variable as follows

$$\begin{aligned} \gamma(z_n) = p(z_k = 1|x) &\frac{p(x|z_k=1)p(z_k=1)}{\underbrace{\sum_{j=1}^{k} p\left(x|z_j = 1\right) p(z_j = 1)}_{p(x)}} \\ &= \frac{\pi_k N\left(x|\mu_k, \Sigma_k\right)}{\sum_j \pi_j N\left(x|\mu_j, \Sigma_j\right)} \end{aligned}$$

Question 8.1. So how do we learn π_k, μ_k, Σ_k?

→ Maximum Likelihood Estimation (MLE). Given a point cloud $X = \{x_1, \ldots, x_N\}$, $x_n \in \mathbb{R}^D$. As the joint are i.i.d., we have

$$\begin{aligned} p(X) &= \prod_{n=1}^{N} p(x_n) \\ &= \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k N\left(x_n|\mu_k, \Sigma_k\right) \end{aligned}$$

Note: When we take the natural logarithm, we obtain

$$\ln p(X) = \sum_{n=1}^{N} \ln \sum_{k=1}^{K} \pi_k N\left(x_n | \mu_k, \Sigma_k\right)$$

Observe that setting taking the derivative and set it equal to 0 (the usual approach) fails here as the problem becomes difficult and "labor-intensive", i.e.,

$$0 = \sum_{n=1}^{N} \frac{\pi_k N\left(x_n|\mu_k, \Sigma_k\right)}{\sum_j \pi_j N\left(x_n|\mu_j, \Sigma_j\right)} \Sigma_k^{-1}(x_n - \mu_k)$$

But recall from earlier when we define $\gamma(z)$,

$$0 = \sum_{n=1}^{N} \gamma(z_{nk}) \Sigma_k^{-1}(x_n - \mu_k)$$

Keeping $\gamma(z_{nk})$ fixed, we can solve for μ_k.

$$\mu_k = \sum_{n=1}^{N} \gamma(z_{nk}) x_n / \underbrace{\sum_{n=1}^{N} \gamma(z_{nk})}_{=N_k}$$

– weighted average of data points. Also,

$$\Sigma_k = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk})(x_n - \mu_k)(x_n - \mu_k)^\top$$

Now, consider π_k s.t. $\sum \pi_k = 1$. Since this is a constraint optimization problem, we include Lagrange multiplier for this constraint in the optimization.

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

1. **Maximization Step**: Given $\gamma(z_{nk})$. We need to update
   - μ_k
   - Σ_k
   - π_k

   using MLE
2. **Expectation Step**: Given μ_k, Σ_k, π_k. We will update
   - $\gamma(z_{nk}) = p\left(z_k = 1|x_n\right) = \frac{\pi_k N(x_n|\mu_k,\Sigma_k)}{\sum_j \pi_j N(x_n|\mu_j,\Sigma_j)}$

This is an example of Expectation-Maximization Algorithm on a Gaussian mixture model.

§8.2 General Expectation-Maximization Algorithm

First, we have

$$\begin{cases} \text{observed variables } X \\ \text{latent variables } z \\ \text{parameters } \theta \end{cases}, \text{ the joint: } p\left(X, z|\theta\right)$$

Goal: maximize $p(X|\theta)$ w.r.t θ. Let's get to the steps to solve this.

1. Initialize θ^{old} (estimate)
2. E-step: evaluate $p(z|X, \theta^{\text{old}})$
3. M-step: $\theta^{\text{new}} = \text{argmax}_\theta\, Q\left(\theta|\theta^{\text{old}}\right)$ where
$$Q\left(\theta|\theta^{\text{old}}\right) := \sum_z p\left(z|X, \theta^{\text{old}}\right) \ln p\left(X, z|\theta\right)$$
4. $\theta^{\text{old}} \leftarrow \theta^{\text{new}}$ repeat if necessary.

Now, we're ready to delve into the derivation of the EM-algorithm. Let's start with the log-likelihood function.
$$L(\theta) := \ln p(X|\theta)$$
E-M is iterative: given θ^{old}, we want to find θ^{new} s.t. $L(\theta^{\text{new}}) > L(\theta^{\text{old}})$ which we can obtain by
$$\max_{\theta^{\text{new}}} L\left(\theta^{\text{new}}\right) - L\left(\theta^{\text{old}}\right) = \ln p\left(X|\theta^{\text{new}}\right) - \ln p\left(X|\theta^{\text{old}}\right)$$
The trick here is to include the latent variable z.
$$\begin{aligned}
p(X|\theta) &= \sum_z p(X, z|\theta) \\
&= \sum_z p\left(X|z, \theta\right) \cdot p(z|\theta) \\
L(\theta^{\text{new}}) - L(\theta^{\text{old}}) &= \ln \sum_z p\left(X|z, \theta^{\text{new}}\right) p\left(z|\theta^{\text{new}}\right) - \ln p\left(X|\theta^{\text{old}}\right) \\
&= \ln \sum_z p\left(z|X, \theta^{\text{old}}\right) \frac{p\left(X|z, \theta^{\text{new}}\right) p\left(z|\theta^{\text{new}}\right)}{p\left(z|X, \theta^{\text{old}}\right)} - \ln p\left(X|\theta^{\text{old}}\right)
\end{aligned}$$
Using Jensen's inequality, which is
$$\ln \sum \lambda_i x_i \geq \sum \lambda_i \ln x_i$$
provided that $\lambda_i \geq 0$ and $\sum \lambda_i = 0$.
$$\begin{aligned}
L(\theta^{\text{new}}) - L(\theta^{\text{old}}) &\geq \sum_z p\left(z|X, \theta^{\text{old}}\right) \left[\ln \frac{p\left(X|z, \theta^{\text{new}}\right) p\left(z|\theta^{\text{new}}\right)}{p\left(z|X, \theta^{\text{old}}\right)} - \ln p\left(X|\theta^{\text{old}}\right)\right] \\
&= \sum_z p\left(z|X, \theta^{\text{old}}\right) \ln \frac{p\left(X|z, \theta^{\text{new}}\right) p\left(z|\theta^{\text{new}}\right)}{p\left(z|X, \theta^{\text{old}}\right) p\left(X|\theta^{\text{old}}\right)} =: \Delta\left(\theta^{\text{new}}|\theta^{\text{old}}\right)
\end{aligned}$$
Thus,
$$\begin{aligned}
L(\theta^{\text{new}}) - L(\theta^{\text{old}}) &\geq \Delta\left(\theta^{\text{new}}|\theta^{\text{old}}\right) \\
L(\theta^{\text{new}}) &\geq \underbrace{L(\theta^{\text{old}}) + \Delta\left(\theta^{\text{new}}|\theta^{\text{old}}\right)}_{=:l\left(\theta^{\text{new}}|\theta^{\text{old}}\right)}
\end{aligned}$$
$L\left(\theta^{\text{new}}\right)$ is bounded below by $l\left(\theta^{\text{new}}|\theta^{\text{old}}\right)$. The best guess to update θ is
$$\theta^{\text{new}} = \operatorname*{argmax}_\theta l\left(\theta|\theta^{\text{old}}\right) = \operatorname*{argmax}_\theta \left\{L(\theta^{\text{old}}) + \sum_z p\left(z|X, \theta^{\text{old}}\right) \ln \frac{p\left(X|z, \theta\right) p(z|\theta)}{p\left(z|X, \theta^{\text{old}}\right) p\left(X|\theta^{\text{old}}\right)}\right\}$$
which is equivalent to
$$\operatorname*{argmax}_\theta \sum_z p\left(z|X, \theta^{\text{old}}\right) \ln p\left(X|z, \theta\right) p(z|\theta)$$

or

$$\underbrace{\underset{\theta}{\operatorname{argmax}}}_{\text{M-step}} \underbrace{\sum_z p\left(z|X,\theta^{\text{old}}\right) \ln p\left(X,z|\theta\right)}_{=:Q\left(\theta|\theta^{\text{old}}\right)}$$

Convergence:

$$\left.\begin{array}{l} \theta^{\text{new}} \text{ maximizes } \Delta\left(\theta|\theta^{\text{old}}\right) \\ \Delta\left(\theta^{\text{old}}|\theta^{\text{old}}\right) = 0 \end{array}\right\} \implies \Delta\left(\theta^{\text{new}}|\theta^{\text{old}}\right) \geq 0$$

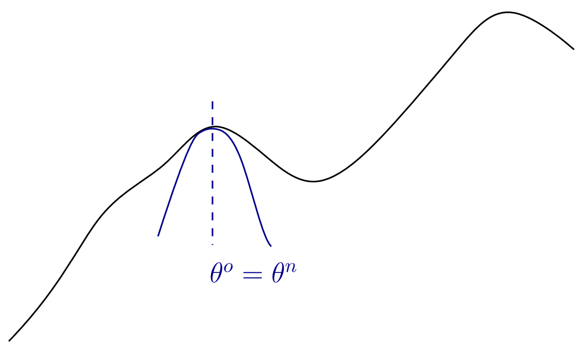
As a result,

$$L\left(\theta^{\text{new}}\right) \geq L\left(\theta^{\text{old}}\right) + \Delta\left(\theta^{\text{new}}|\theta^{\text{old}}\right)$$

Thus,

$$L\left(\theta^{\text{new}}\right) \geq L\left(\theta^{\text{old}}\right) \qquad \text{(non-decreasing)}$$

When θ reaches a fixed point on $l\left(\theta|\theta^{\text{old}}\right)$, we can only conclude that $\nabla L\left(\theta^{\text{old}}\right) = 0$ (not necessarily reach global max, could be a local max or even just a local min or saddle point).



§9 Lec 9: Jul 15, 2021

§9.1 Kernel Methods – Linear Regression

Idea: Apply a linear machine learning model onto data after non-linear preprocessing thereof.

$$x_n \overset{\phi}{\mapsto} \phi(x_n) \qquad \mathbb{R}^D \to \mathbb{R}^E$$

We want to avoid isolated $\phi(x_n)$, but we want to have $\phi(x_n)^\top \phi(x_m)$ instead. We define the kernel function as follows

$$\phi(x_n)^\top \phi(x_m) \equiv k(x_n, x_m) \qquad \text{(kernel trick)}$$

Recall: regularized least squares loss function

$$J(w) \coloneqq \frac{1}{2} \sum_{n=1}^{N} \left(w^\top \phi(x_n) - t_n\right)^2 + \frac{\lambda}{2} w^\top w$$

As this is a non-constraint optimization problem, optimality requires:

$$\Delta_w J = \sum_{n=1}^{N} \left(w^\top \phi(x_n) - t_n\right) \phi(x_n) \lambda w \overset{\text{set}}{=} 0$$

Rearrange this a bit and we obtain

$$w = -\frac{1}{\lambda} \sum_{n=1}^{N} \left(w^\top \phi(x_n) - t_n\right) \phi(x_n)$$

Notice that w is a linear combination of the non-linear transform data $\phi(x_n)$.

$$w = \sum_{n=1}^{N} a_n \phi(x_n) = \Phi^\top a$$

in which the design matrix Φ is defined as

$$\Phi = \begin{bmatrix} \phi_1(x_1) & \dots & \phi_E(x_1) \\ \vdots & & \vdots \\ \phi_1(x_N) & \dots & \phi_E(x_N) \end{bmatrix}$$

Also,

$$a_n \coloneqq -\frac{1}{\lambda} \left(w^\top \phi(x_n) - t_n\right)$$

Substitute $w = \Phi^\top a$ into $J(w)$,

$$J(a) \coloneqq \frac{1}{2} \sum_{n=1}^{N} \left(a^\top \Phi \phi(x_n) - t_n\right)^2 + \frac{\lambda}{2} a^\top \Phi \Phi^\top a$$

which is equivalent to

$$J(a) = \frac{1}{2} a^\top \Phi \Phi^\top \Phi \Phi^\top a - a^\top \Phi \Phi^\top t + \frac{1}{2} t^\top t + \frac{\lambda}{2} a^\top \Phi \Phi^\top a$$

We introduce $K \coloneqq \Phi\Phi^\top$ = Gram matrix, $N \times N$ and symmetric.

$$K_{mn} = \phi(x_m)^\top \phi(x_n) = K(x_m, x_n) \qquad (K \succeq 0)$$

So, the loss (in terms of weights a) becomes

$$J(a) = \frac{1}{2}a^\top KKa - a^\top Kt + \frac{1}{2}t^\top t + \frac{\lambda}{2}a^\top Ka$$

The optimality requires

$$\begin{gathered}\nabla_a J = KKa - Kt + \lambda ka \stackrel{\text{set}}{=} 0 \\ K^{-1}KKa - K^{-1}Kt + \lambda K^{-1}Ka = 0 \quad (\text{as } K \succ 0) \\ Ka - t + \lambda a = 0 \\ (K + \lambda I)\, a = t \\ a = (K + \lambda I)^{-1}\, t\end{gathered}$$

If $E \to \infty$ then w has ∞-dim as well. We are not actually interested in w but in using w to make predictions for new data points $\tilde{x}$ and

$$\tilde{t} = w^\top \phi(\tilde{x}) = \phi(\tilde{x})^\top w = \underbrace{\phi(\tilde{x})^\top \Phi^\top}_{\vec{K}^\top} a = K^\top (K + \lambda I)^{-1}\, t$$

where K is the kernel with $\tilde{x}$ and each sample, $K_n = K(\tilde{x}, x_n)$.
The main difference between traditional linear regression and kernel-based linear regression:

- Traditional: use training data to learn optimal parameters (then discard data)
- Kernel (no parameters): the data are in charge which needs to say in memory as we need to evaluate $K(\tilde{x}, x_n)$.

§9.2 Kernel Construction

In principle:

$$k(x, y) = \phi(x)^\top \phi(y)$$

In practice, we want to skip the ϕ-part. It's "easy" if we find a ϕ that results in k, then we have confirmation that k is indeed a kernel.

Example 9.1

$k(x, y) := \left(x^\top y\right)^2$, $x, y \in \mathbb{R}^2$

$$\begin{aligned} k(x, y) &= (x_1 y_1 + x_2 y_2)^2 = x_1^2 y_1^2 + 2x_1 y_1 x_2 y_2 + x_2^2 y_2^2 \\ &= \begin{bmatrix} x_1^2 \\ \sqrt{2} x_1 x_2 \\ x_2^2 \end{bmatrix}^\top \begin{bmatrix} y_1^2 \\ \sqrt{2} y_1 y_2 \\ y_2^2 \end{bmatrix} = \phi(x)^\top \phi(y) \end{aligned}$$

with

$$\phi(z) := \begin{bmatrix} z_1^2 \\ \sqrt{2} z_1 z_2 \\ z_2^2 \end{bmatrix}$$

Necessary and sufficient condition for $k(x, y)$ to be a kernel function: If for any $\{x_n\}$, $n = 1 \dots N$, the Gram matrix K, $(K_{mn} = K(x_m, x_n))$, is positive semidefinite. Then $k(x, y)$ s a valid kernel (however, this is not a very practical rule).
From page 296 of the textbook, given k_1, k_2 valid kernels, then the following new kernels will also be valid (kernel lego)

- $ck_1(x, y)$, $c > 0$

- $f(x)k_1(x,y)f(y)$ for any f
- $q\left(k_1(x,y)\right)$, q is a polynomial with non-negative coefficients
- $e^{k_1(x,y)}$
- $k_1(x,y) + k_2(x,y)$
- $k_1(x,y) \cdot k_2(x,y)$
- $k_1(\phi(x), \phi(y))$, $\phi : \mathbb{R}^D \to \mathbb{R}^M$
- $x^\top A y$, A is symmetric positive semidefinite.

§9.3 Gaussian Processes – Linear Regression

Linear regression: linear combination of M fixed basis functions

$$y(x) = y = w^\top \phi(x), \qquad \phi \in \mathbb{R}^M$$

We will add a prior distribution on w

$$p(w) = N\left(w \middle| 0, \frac{1}{\alpha} I\right)$$

For any given value w, $y(x)$ is a particular function. So the pdf over w defines a pdf over function $y(x)$. In practice, we evaluate $y(x)$ not on the entire $\mathbb{R}^D$ but only at discrete locations (e.g. $x_1, \ldots, x_N, \tilde{x}$).
We're interested in the joint distribution $y(x_1), \ldots, y(x_N)$. We write

$$\vec{y} : \; y_n \coloneqq y(x_n)$$

where $\vec{y} \in \mathbb{R}^N$.

$$\implies \vec{y} = \Phi w \qquad (\Phi_{nk} = \phi_k(x_n))$$

Question 9.1. What does the joint distribution of $\vec{y}$ look like?

It turns out $\vec{y}$ is multiple linear combination of Gaussian random variables $w = \begin{bmatrix} w_0 \\ \vdots \\ w_{m-1} \end{bmatrix}$ which is Gaussian itself. To find the parameters, we compute sufficient statistics.

- $\mathbb{E}[y] = \mathbb{E}\left[\Phi w\right] = \Phi \mathbb{E}[w] = 0$
- $\operatorname{cov}[\vec{y}] = \mathbb{E}\left[\left(\vec{y} - \mathbb{E}[\vec{y}]\right)\left(\vec{y} - \mathbb{E}[\vec{y}]\right)^\top\right] = \mathbb{E}\left[\vec{y}\vec{y}^\top\right]$

$$\begin{aligned} \mathbb{E}\left[\Phi w w^\top \Phi^\top\right] &= \Phi \mathbb{E}\left[w w^\top\right] \Phi^\top \\ &= \Phi \operatorname{cov}[w] \Phi^\top = \frac{1}{\alpha} \Phi \Phi^\top = k \end{aligned}$$

So, the kernel is

$$k_{mn} = \frac{1}{\alpha} \phi(x_m)^\top \phi(x_n) = k(x_m, x_n)$$

Overall, what just happens is

$$
\begin{gathered}
w \sim N\left(0, \frac{1}{\alpha} I\right) \\
\downarrow \\
y(x) = w^\top \phi(x) \\
\downarrow \\
\vec{y} = \begin{bmatrix} y(x_1) \\ \vdots \\ y(x_N) \end{bmatrix} \\
\downarrow \\
\vec{y} \sim N(0, k)
\end{gathered}
$$

Definition 9.2 (Gaussian Process) — Gaussian process is a pdf over function $y(x)$ s.t. the values evaluated at arbitrary $x_1, \ldots, x_N$ jointly have a Gaussian distribution.

Fundamental Property:

$$\mathbb{E}\left[y(x_n) y(x_m)\right] = k(x_n, x_m)$$

Now, let's get to the Gaussian processes for regression.

$$\text{Model}: \quad t_n = y_n + \varepsilon_n$$

where ε_n is the white noise and $\varepsilon_n \sim N\left(0, \sigma^2 (= \frac{1}{\beta})\right)$

$$\implies p\left(t_n | y_n, \sigma^2\right) = N\left(t_n | y_n, \sigma^2\right)$$

Then, we have

$$
\begin{aligned}
p\left(\vec{t} | \vec{y}\right) &= \prod_{n=1}^{N} p\left(t_n | y_n\right) \\
&= N\left(\vec{t} | \vec{y}, \sigma^2 I\right)
\end{aligned}
$$

From the definition of Gaussian process, we know

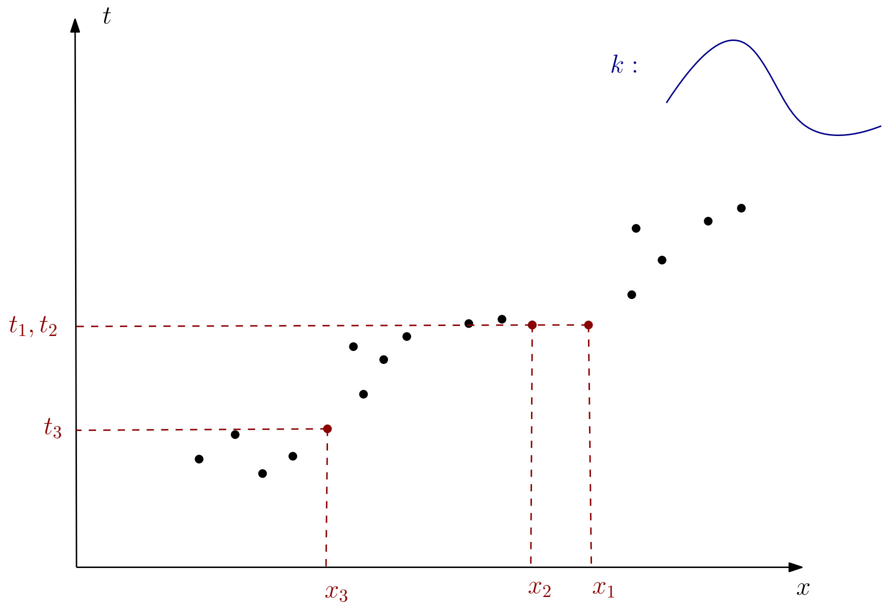
$$p(\vec{y}) = N\left(\vec{y} | 0, K\right)$$

From page 93 of the textbook, we can find the predictive distribution

$$p(\vec{t}) = \int p\left(\vec{t} | \vec{y}\right) P(\vec{y}) \, d\vec{y} = N\left(\vec{t} | 0, K + \sigma^2 I\right)$$

We can evaluate the likelihood of a given data set as follows

1. $x_n \sim x_m$, i.e., $k(x_n, x_m)$ is large $\implies t_n \sim t_m$ or "penalty" (unlikely)
2. $x_n \not\sim x_m$, i.e., $k(x_n, x_m)$ is small $\implies t_n \perp t_m$ (independent)



$k(x_1, x_2)$ is relatively large: $\exp(-\|x_1 - x_2\|^2)$

$\rightarrow$ strong correlation between t_1 & t_2 (need to be similar)

What's even more interesting is we can use this to make predictions, $p\left(\tilde{t}|\vec{t}\right)$ at $\tilde{x}$?

$$\vec{t}_{N+1} = \begin{bmatrix} t_1 \\ \vdots \\ t_N \\ \tilde{t} \end{bmatrix}, \quad \vec{y}_{N+1} = \begin{bmatrix} y(x_1) \\ \vdots \\ y(x_N) \\ y(\tilde{x}) \end{bmatrix}$$

Then,

$$p\left(\vec{t}_{N+1}\right) = N\left(\vec{t}_{N+1}|0, C_{N+1}\right)$$
$$C_{N+1} = k_{n+1} + \sigma^2 I = \begin{bmatrix} C & k \\ k^\top & c \end{bmatrix}$$

where $k_n = k\left(\tilde{x}, x_n\right)$ and $c = k\left(\tilde{x}, \tilde{x}\right) + \sigma^2$. Then, we can use page 87 to get the marginal partition as follows

$$p\left(\tilde{t}|\vec{t}\right) = N\left(\tilde{t}|m\left(\tilde{x}\right), \sigma^2(\tilde{x})\right)$$
$$m(\tilde{x}) = k^\top C^{-1}\vec{t} = k^\top \left(k + \sigma^2 I\right)^{-1}\vec{t}$$
$$\sigma^2(\tilde{x}) = c - k^\top C^{-1}k$$

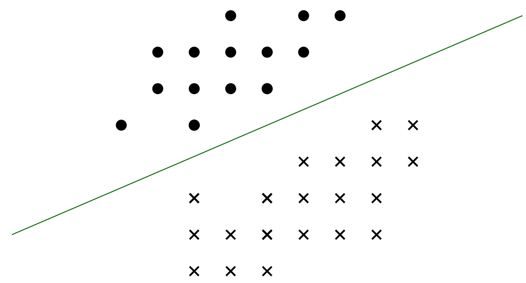
§10 Lec 10: Jul 19, 2021

§10.1 Sparse Kernel Machines – SVM for Classification

First, let's consider the following model

$$y(x) = w^\top \phi(x) + b$$

Training data (assume linear separability):



$$X = \{x_1, \ldots, x_N\}, \quad x_n \in \mathbb{R}^D$$

$$\tilde{t} = \begin{bmatrix} t_1 \\ \vdots \\ t_N \end{bmatrix}, \quad t_n \in \{-1; +1\}$$

New data is classified according to the sign of y. If data are linearly separable, there are usually more than one (w, b) that do the job. Among these choices, we want to find the one with the best generalization (doing the best job on new data).

Definition 10.1 (Margin) — Margin is the smallest distance between the decision boundary and any of the training data points.

<u>Idea</u>: Among all the decision boundary we could find, we want to find the one that has the largest margin (large margin = least generalization error). Recall that the signed distance of x from decision boundary ($y(x) = 0$) is $\frac{y(x)}{\|w\|}$. We want to have large distances with correct sign.

$$\begin{cases} t_n y(x_n) > 0 & \text{(correct sign)} \\ \max \frac{|y(x_n)|}{\|w\|} \end{cases}$$

So combining these together, we obtain the signed distance

$$\frac{t_n y(x_n)}{\|w\|} = \frac{t_n \left(w^\top \phi(x_n) + b\right)}{\|w\|}$$

Now, the margin is the least of these signed distances

$$\text{margin} := \min_n \frac{t_n \left(w^\top \phi(x_n) + b\right)}{\|w\|}$$

Also, we know that misclassified samples will have negative signed distance. On the other hand, the maximum classifier problem becomes

$$\max_{w,b} \left\{ \frac{1}{\|w\|} \min_n t_n \left(w^\top \phi(x_n) + b\right) \right\}$$

$(k \cdot w, k \cdot b)$ where $k > 0$ all describe the same decision boundary. Thus, in all cases we can rescale the problem to

$$\left[\min_n t_n \left(w^\top \phi(x_n) + b\right)\right] = 1$$

We can rephrase the interior problem into a constraint

$$\forall n : \quad t_n \left(w^\top \phi(x_n) + b\right) \geq 1$$

For support vectors (data points = 1), the constraint is active. For all other data points, the constraint is inactive. Max margin classifier becomes

$$\max_{w,b} \left\{ \frac{1}{\|w\|} \right\} \quad \text{s.t.} \quad t_n \left(w^\top \phi(x_n) + b\right) \geq 1 \ \forall n$$

Equivalently,

$$\min_{w,b} \frac{1}{2}\|w\|^2 \quad \text{s.t.} \quad t_n \left(w^\top \phi(x_n) + b\right) \geq 1 \ \forall n$$

$\implies$ quadratic program.
To solve the optimization problem, let's introduce KKT-multipliers to address the constraints

$$L(w, b, a) = \frac{1}{2}\|w\|^2 - \sum_{n=1}^{N} a_n \left(t_n \left(w^\top \phi(x_n) + b\right) - 1\right)$$

Then, we check KKT-conditions for optimality.

$$\begin{cases} \nabla_w L \overset{\text{set}}{=} 0 \implies w = \sum a_n t_n \phi(x_n) \\ \frac{dL}{db} \overset{\text{set}}{=} 0 \implies \sum_{n=1}^{N} a_n t_n = 0 \end{cases}$$

Next, we construct the dual

$$\tilde{L}(a) \coloneqq \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m k(x_n, x_m) \quad \text{s.t.} \quad \begin{cases} a_n \geq 0 \\ \sum_{n=1}^{N} a_n t_n = 0 \end{cases}$$

So the dual problem is

$$\max \tilde{L}(a) \quad \text{s.t.} \quad \begin{cases} a_n \geq 0 \\ \sum_{n=1}^{N} a_n t_n = 0 \end{cases}$$

Let' say we have a new data point: $y(x) = \sum_{n=1}^{N} a_n t_n k(x, x_n) + b(*)$. From one of the KKT conditions (complementarity), we have

$$\forall n : \quad a_n \left(t_n \left(w^\top \phi(x_n) + b\right) - 1\right) = 0$$

So either we have an inactive data point, i.e.

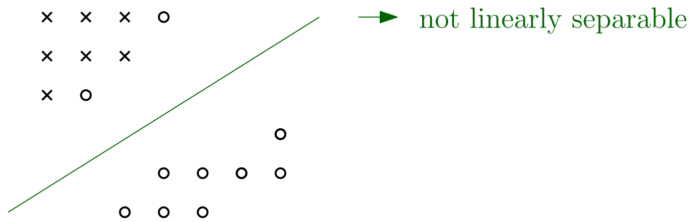
$$a_n = 0, \qquad t_n \left(w^\top \phi(x_n) + b\right) > 1$$

or an active data point (support vectors)

$$a_n > 0, \qquad t_n \left(w^\top \phi(x_n) + b\right) = 1$$

From $(*)$, we can deduce that only the support vectors need to be considered when making predictions – thus sparsity.

Let's now consider the non-linear separable case.



Specifically, no (w, b) is going to give perfect classification of training data (but it is still nearly separable).
Trick: Introduce slack variable. For each data point x_n, we now have

$$\begin{cases} \xi_n \geq 0 \\ \xi_n = 0 \text{ if } x_n \text{ is on margin or correct outside the margin} \\ \xi_n = |t_n - y(x_n)|\,, \text{ otherwise} \end{cases}$$

In essence, ξ_n captures how much we violate the constraint $t_n \left(w^\top \phi(x_n) + b\right) \geq 1$.

Fact 10.1.
- $\xi_n = 1$ if x_n on decision boundary.
- $\xi_n > 1$ if x_n is misclassified.

Question 10.1. How do we incorporate the slack variables into the problem?

We will add slack to constraints (permissible) and add slack to objective (penalty). So the soft-margin classifier problem now looks like

$$\min_{w,b,\xi_n} \gamma \sum_{n=1}^{N} \xi_n + \frac{1}{2}\|w\|^2 \quad \text{s.t.} \quad \forall n: \; t_n \left(w^\top \phi(x_n) + b\right) \geq 1 - \xi_n$$

Optimization Review: KKT-conditions for inequality constrained optimization

$$\min_{x \in \mathbb{R}^D} f(x) \quad \text{s.t.} \quad \begin{cases} g_i(x) \leq 0 \\ h_j(x) = 0 \end{cases}$$

Then, we write down the Lagrange

$$L(x, \mu_i, \lambda_i) \coloneqq f(x) + \sum_i \mu_i g_i(x) + \sum_j \lambda_j h_j(x)$$

The saddle point $(x^\star, \mu_i^\star, \lambda_j^\star)$ w.r.t. $L \left(\min_x, \max_{\mu_i,\lambda_j}\right)$ solves original problem. In addition, the saddle point must satisfy

1. Constrained stationary: $\nabla f(x) + \sum_i \mu_i \nabla g_i(x) + \sum_j \lambda_j \nabla h_j(x) = 0$
2. Primal feasibility: $g_i(x^\star) \leq 0$ and $h_j(x^\star) = 0$
3. Dual feasibility: $\mu_i \geq 0$ (only for inequality case)
4. Complementary slackness: $\mu_i^\star g_i(x^\star) = 0$

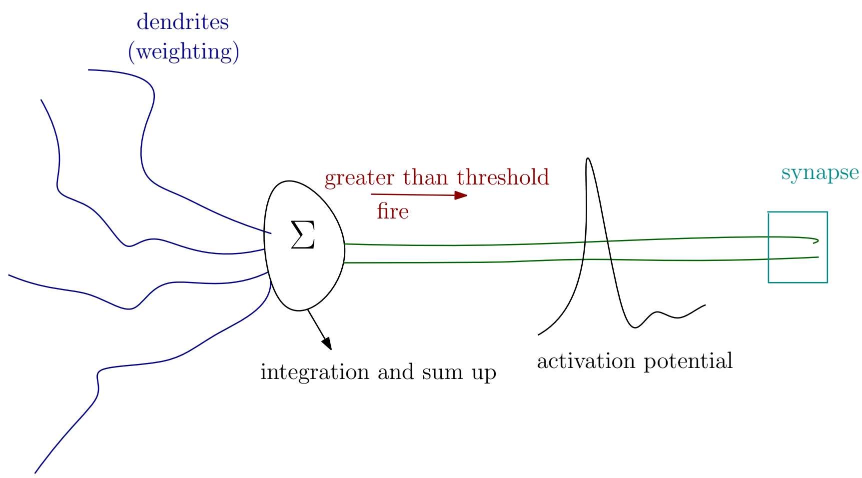
§11 Lec 11: Jul 21, 2021

§11.1 The Perceptron Algorithm

Idea: We have 2-class model which makes decision using ϕ (including bias term, $\phi_0 = 1$)

$$y(x) = f\left(w^\top \phi(x)\right)$$

where f = sign function.
We want to make connection to biology – neuron.



For an arbitrary x_n, we want

$$f\left(w^\top \phi(x_n)\right) = \begin{cases} +1 \text{ if } x_n \text{ is member of class 1} \\ -1 \text{ if } x_n \text{ is member of class -1} \end{cases}$$

which means

$$w^\top \phi(x_n) \cdot t_n > 0$$

Perceptron criterion: focus on misclassified data x_n only. More specifically,

- associate zero error with a correctly classified x_n
- associate $-w^\top \phi(x_n) \cdot t_n$ as error of misclassified patterns (error > 0)

Thus, a weakly wrong prediction is less bad than a strongly wrong prediction.

$$E_p(w) := -\sum_{n \in M} w^\top \phi(x_n) t_n$$

where M = set of misclassified data points given w and $E_p(w)$ is a function of parameters w given a fixed training set. Notice that

1. the contribution of error by x_n is 0 in regions of w where x_n is correctly classified.
2. the contribution of error is a linear function of w where x_n is misclassified.

$\implies$ the error function $E_p(w)$ is piecewise linear and continuous (no jump discontinuity, etc). Thus, gradient methods can be used for optimization almost everywhere. Instead of gradient descent, we will perform stochastic gradient descent, i.e., at each step t, we will estimate ∇E using a subset of data points only. Here, for the extreme case (with only 1 data point),

$$w^{t+1} = w^t - \eta\left(-\phi(x_n) t_n\right)$$

where η is the step size/learning rate.

Remark 11.1. 1. at each update step, pick x_n

- if x_n is correctly classified, then we move on.
- otherwise, update w.

2. pick $\eta = 1$ without loss of generality
3. the set M will change (at each step) as w is updated.

Note that perceptron algorithm may not reduce the error at each step.

There is a perceptron convergence theorem that states

Theorem 11.2

If the data are linearly separable to begin with (a solution with no misclassification error exists) then the algorithm will find it within finite numbers of update steps.

Remark 11.3. Solution may not be unique, i.e., there's no guarantee that we find a good boundary in terms of margin, for example. So which solution we find depends on

1. initial w°
2. sequence of x_n presented to the algorithm

If no solution exists (data is not linearly separable), the algorithm keeps going indefinitely.

§11.2 Neural Networks

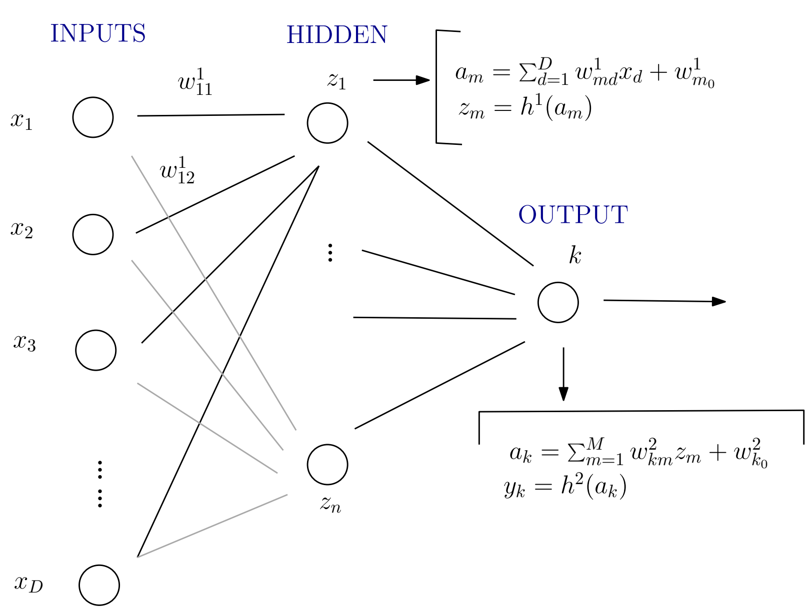
Idea: We use a fixed number of model components and/or adaptive basis functions.

1. put "a bunch" of perceptrons in parallel, train them and their aggregation simultaneously.

$$\begin{cases} \text{each individual weak learners: } y_i(x) = f\left(w^\top \phi(x) + b\right) \\ \text{aggregation: } z(x) = f\left(w^\top y + b\right) \end{cases}$$

2. make ϕ adaptive themselves; then learn $\{\phi_j\}$ along with $\{w_j\}$ s.t. $w^\top \phi(x)$ performs well. We also need to parametrize ϕ_j

$$\phi_j(x) = f\left(w^\top x + b\right)$$



We can refer to the neural networks above as

- single hidden layer
- double layers (weights)
- 3 total layers

Combining by substituting the expression from the hidden layer into the output and we obtain

$$y_k(x,w) = h^2\left(\sum_{m=1}^{M} w_{km}^2 h^1\left(\sum_{d=1}^{D} w_{md}^1 + w_{m_0}^1\right) + w_{k_0}^2\right)$$

Clearly, $y_k(x,w)$ is a non-linear function of $x \in \mathbb{R}^D$ parametrized by all the weights w and hyperparameters (number of nodes and choice of h^1, h^2).
Once the model is trained, we have forward propagation (left-to-right). More complicated architectures are possible with more layers, etc. The important thing to keep in mind is h^1 must be non-linear; otherwise, the network collapses into a single perceptron.

Question 11.1. How do we train the multilayer perceptrons model?

Given a classification/regression, the output which includes bias in the nodes x_0 is

$$y_k(x,w) = h^2\left(\sum_{m=0}^{M} w_{km}^2 h^1\left(\sum_{d=0}^{D} w_{md}^1 x_d\right)\right)$$

Consider the energy/error function

$$E(w) = \frac{1}{2}\sum_{n=1}^{N}\left\{y(x_n,w) - t_n\right\}^2$$

We can optimize E by solving $\nabla_w E = 0$, but it's unfortunately too hard to solve directly. Instead, we use gradient descent method: $\frac{dw}{dt} = -\nabla_w E$. Explicitly, we have

$$w^{t+1} = w^t - \eta \nabla_w E(w^\top)$$

We estimate $\nabla_w E$ based off just a few data points, at a time.

Question 11.2. Why stochastic gradient descent works?

1. Far from the solution, all samples/data point will want the same change.
2. Close to optimal w, ∇E will be relatively flat.
3. Data set is redundant (even smaller fractions of the data set should capture the essence).

Refer to the book for more details about backpropagation.

§12 Lec 12: Jul 22, 2021

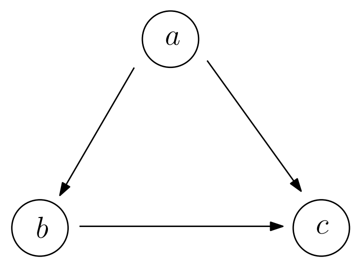
§12.1 Graphical Models

Doodle rules:

- nodes = random variables
- links/edges = probabilistic relationship

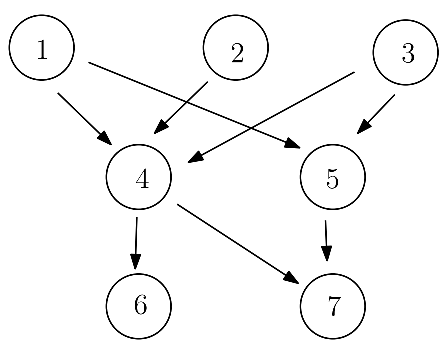
Assume a, b, c are random variables and the joint is

$$p(a,b,c) = p(c|a,b) \cdot p(a,b) = p(c|a,b) \cdot p(b|a) \cdot p(a)$$



However, an actual model might not be fully connected.

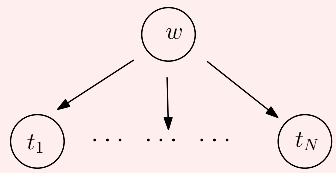
$$p(x_1,\ldots,x_7) = p(x_7|x_4,x_5)\,p(x_6|x_4)\,p(x_5|x_1,x_3)\,p(x_4|x_1,x_2,x_3)\,p(x_3)\,p(x_2)\,p(x_1)$$



Example 12.1 (Linear Regression)

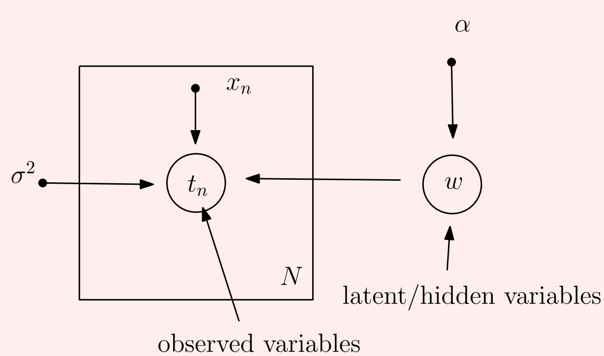
$x_n \to t_n$ with parameters w

$$p(\vec{t}, w) = p(w) \cdot \prod_{n=1}^{N} p(t_n | w)$$

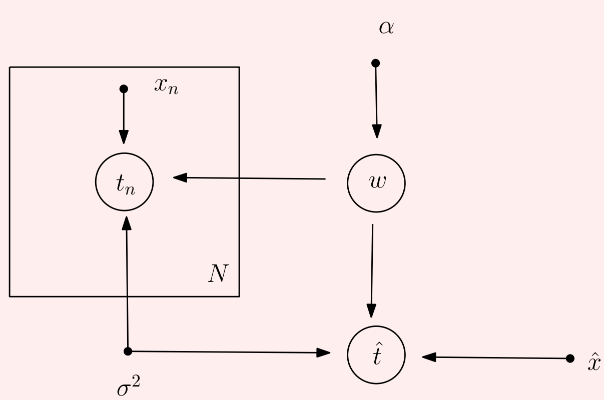


With variance and noise,

$$p(\vec{t}, w) = p(w|\alpha) \cdot \prod_{n=1}^{N} p(t_n | x_n, w, \sigma^2)$$



<u>Prediction</u>:



The joint is

$$p(\hat{t}, \vec{t}, w | \hat{x}, \vec{x}, \alpha, \sigma^2) = p(w|\alpha) \prod_{n=1}^{N} p(t_n | x_n, w, \sigma^2) \cdot p(\hat{t} | \hat{x}, w, \sigma^2)$$

Marginal:

$$p(\hat{t} | \hat{x}, \vec{x}, \vec{t}, \alpha, \sigma^2) \propto \int p(\hat{t}, \vec{t}, w | \hat{x}, \vec{x}, \alpha, \sigma^2)\, dw$$

Example 12.2 (Sampling)

Graphical models can also be used to visualize sampling: draw samples of the joint distribution by sequentially sampling from the conditional distributions (starting from the parent node).

§12.2 Markov Random Fields

Definition 12.3 (Conditional Independence) — Random variables a and b are called conditionally independent given c iff

$$p(a|b,c) = p(a|c)$$

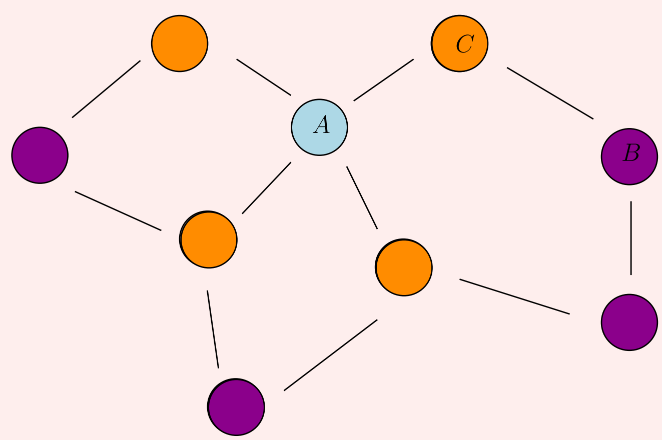
or equivalently

$$p(a,b|c) = p(a|c) \cdot p(b|c)$$

Definition 12.4 (Conditional Independence – Extended) — For graphical model with three sets of nodes A, B and C, we say A and B are conditionally independent given C iff for all paths connecting A and B we have to visit C; equivalently, if we remove C, then A is disconnected from B.

Example 12.5

Markov blanket:



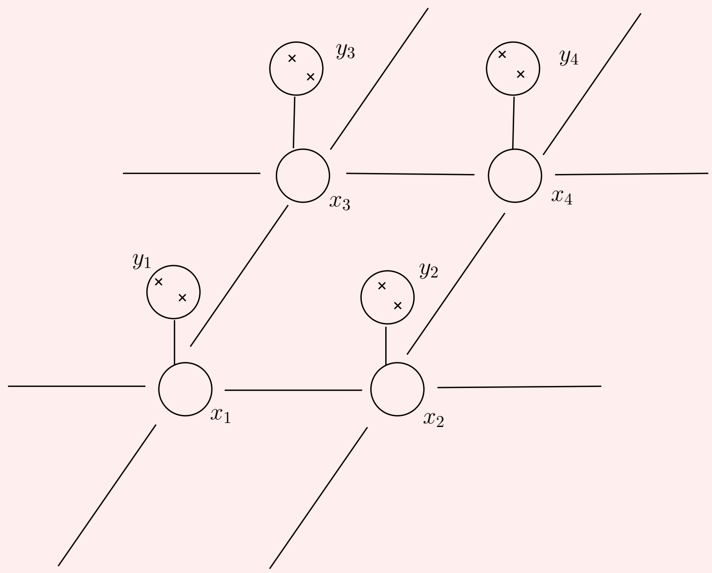
We can observe that A and B are conditionally independent given C.

Example 12.6 (Dirty Pictures)

Besag 1986: Statistical analysis of dirty pictures

- Observed: binary images $y_i \in \{-1, +1\}$
- underlying/latent/hidden image: $x_i \in \{-1, +1\}$

What happened is y_i is obtained from x_i by randomly flipping some of the pixels



1. strong correlation between x_i and y_i
2. strong correlation between neighboring x_i, x_j

For two random variables not connected by an edge or x_i, x_j are not neighbors,

$$p(x_i, x_j | x_{k \neq i,j}) = p(x_i | x_{k \neq i,j}) p(x_j | x_{k \neq i,j})$$

The factorization of the joint distribution must not contain x_i, x_j in the same factor.

Definition 12.7 (Clique) — A clique is a subset of nodes of the graph, s.t. there exists a link between each pair of nodes.

Remark 12.8.

1. - nodes = random variables
   - link = dependence between random variables
2. cliques = fully connected subgraphs

Definition 12.9 (Maximal Clique) — A clique is maximal iff it's not possible to add further nodes while still being a clique.

Then, observe that factors of the joint distribution are functions of the variables in the maximal cliques. Let C denote the set of maximal cliques, and x_c for $c \in C$ is the variables in that clique.

Then

$$p(x) = \frac{1}{z} \prod_{c \in C} \psi_c(x_c)$$

where ψ_c is a potential function (positive) and $z = \sum_x \prod_{c \in C} \psi_c(x_c)$ is a normalization constant. Factorization and conditional independence are connected through the Hammersley – Clifford theorem. Because $\psi_c > 0$, it can be expressed as

$$\psi_c(x_c) = \exp\{-E(x_c)\}$$

- $E(x_c)$ is an energy function
- the exponential representation is called Boltzmann distribution.

$$\text{joint prob} = \frac{1}{z} \prod_c \psi_c(x_c)$$

which is also the total energy $\sum_c E(x_c)$. However, ψ_c is not the probability density itself.

Example 12.10

From the Besag's example above, we have two types of maximal cliques

- $x_i \sim y_i$
- $x_i \sim x_j$

We define the clique energy as follows

- $-\eta x_i y_i$
- $-\beta x_i x_j$

which would be small when pixels values match.
Total energy:

$$E(x, y) = -\beta \sum_{(i,j) \in E} x_i x_j - \eta \sum_i x_i y_i$$

and

$$p(x, y) = \frac{1}{z} e^{-E(x,y)} = \frac{1}{z} \prod_c \psi_c(x_c)$$

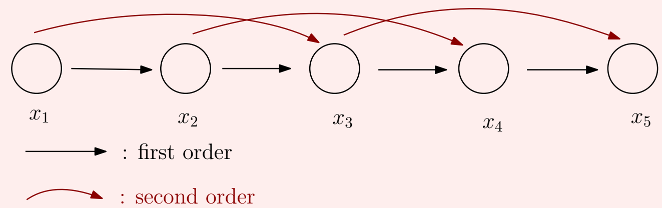
Now, given y find x s.t. $E(x, y)$ is minimal – very hard to solve. So we want to solve this optimization problem using "coordinate descent", i.e., iterative conditional models.

§13 Lec 13: Jul 26, 2021

§13.1 Hidden Markov Models/Chains

Example 13.1

Rainfall/pollen data per day



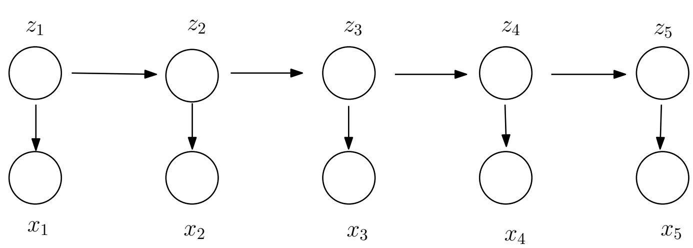
Since the data is not i.i.d., the joint looks more complicated

$$p(x_1, \ldots, x_N) = p(x_1) \prod_{n=2}^{N} p(x_n|x_{n-1})$$

Stationarity(homogeneous Markov chain): $p(x_n|x_{n-1})$ is independent of n. For 2^{nd} order model, we have

$$p(x_1)p(x_2|x_1) \prod_{n=3}^{N} p(x_n|x_{n-1}, x_{n-2})$$

Powerful idea: Markov assumption on hidden/latent data ("state variable")



1^{st} order Markov: z_{n+1} and z_{n-1} are conditionally independent given z_n.
HMM are an extension of mixture models: z_n describes which mixture component is responsible for x_n.

- x_n : $p(x_n|z_n)$
- z_n : is strutted in time: $p(z_n|z_{n-1})$

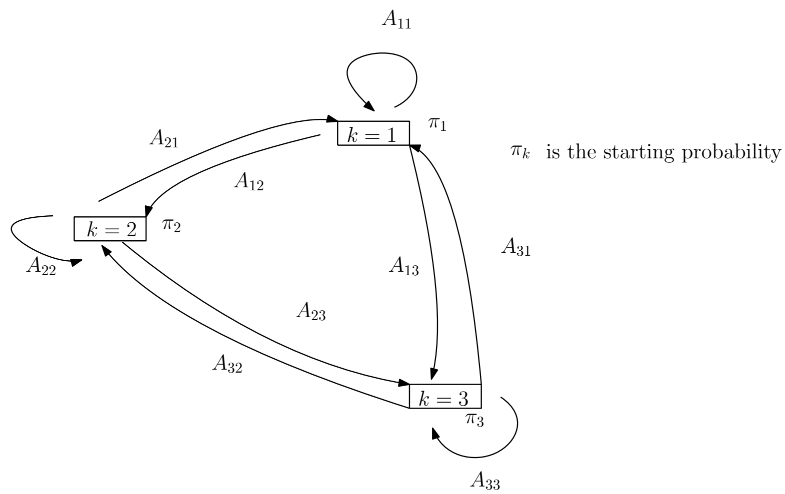
Since states z_n are discrete,

$$p(z_n = k|z_{n-1} = j) = A_{jk} =: \text{transition matrix}$$

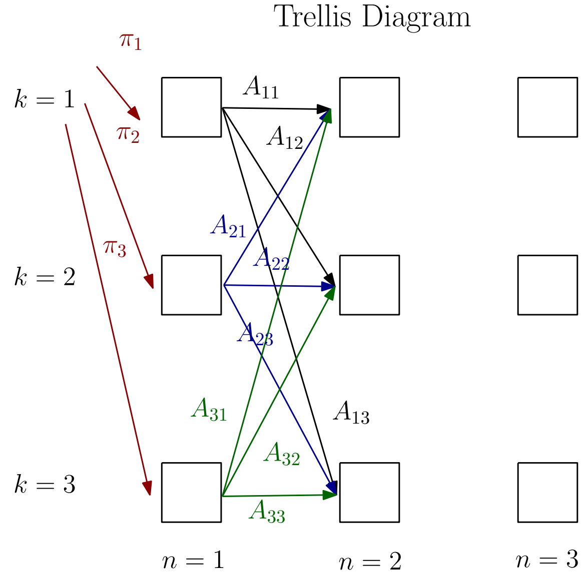
where $\sum_k A_{jk} = 1$. The initial node distribution is

$$p(z_1)?$$
$$p(z_1 = k) = \pi_k \qquad (\sum_k \pi_k = 1)$$

State Diagram



Trellis Diagram



Now, the second ingredient is emission probabilities which corresponds to class conditional densities

$$p(x_n|z_n) = p(x_n|z_n, \phi)$$

for some parameters ϕ, e.g., $\phi = \{\mu_1, \Sigma_1, \mu_2, \Sigma_2, \ldots\}$

$$p(x_n|z_n = k, \phi) = p(x_n|\phi_k)$$

So, the joint is

$$p(X, Z|\theta) = p(z_1|\pi) \prod_{n=2}^{N} p(z_n|z_{n-1}) \prod_{n=1}^{N} p(x_n|z_{n_1}\phi)$$

where $\theta = (A, \pi, \phi)$.

Question 13.1. How do we learn $\theta = \{A, \pi, \phi\}$ from a sequence of $x_1, \ldots, x_N$?

$\implies$ Maximum likelihood!

$$\max p(X|\theta) = \sum_z p(X, Z|\theta)$$

in which we sum over all the possible paths through state/trellis diagram.
Since summing over all the possible paths is a very labor-intensive task, we "need" to use E-M algorithm.

$$Q(\theta^{\text{new}}, \theta^{\text{old}}) = \sum_z p(Z|X, \theta^{\text{old}}) \ln p(X, Z|\theta^{\text{new}})$$

Notation: $\gamma(z_n)_k = p(z_n = k|X, \theta^{\text{old}})$

$$\xi \to \xi(z_{n-1}, z_n)_{jk} = p\left(z_{n-1} = j, z_n = k|X, \theta^{\text{old}}\right)$$

Thus,

$$Q(\theta^{\text{new}}, \theta^{\text{old}}) = \sum_{k=1}^K \gamma(z_1)_k \ln \pi_k + \sum_{n=2}^N \sum_{j=1}^K \sum_{k=1}^K \xi(z_{n-1}, z_n)_{jk} \ln A_{jk} + \sum_{n=1}^N \sum_{k=1}^K \gamma(z_n)_k \ln p(x_n|\phi_k)$$

- E-step: compute $\gamma(z_n)_k$ and $\xi(z_{n-1}, z_n)_{jk}$ with an efficient algorithm (Baum-Welch)
- M-step: update π, A, ϕ

$$\pi_k = \frac{\gamma(z_1)_k}{\sum_{j=1}^K \gamma(z_1)_j}; \qquad A_{jk} = \frac{\sum_{n=2}^N \xi(z_{n-1}, z_n)_{jk}}{\sum_{l=1}^K \sum_{n=2}^N \xi(z_{n-1}, z_n)_{jl}}$$

For ϕ update, it's the same as for GMM.

In order to compute γ, ξ, let's dive into the Baum-Welch algorithm. First, let's take a look at the conditional independence properties.

$$p(X|z_n) = p(x_1, \ldots, x_n|z_n)\; p(x_{n+1}, \ldots, x_N|z_n) \tag{1}$$
$$p(x_1, \ldots, x_{n-1}|x_n, z_n) = p(x_1, \ldots, x_{n-1}|z_n) \tag{2}$$
$$p(x_1, \ldots, x_{n-1}|z_{n-1}, z_n) = p(x_1, \ldots, x_{n-1}|z_{n-1}) \tag{3}$$
$$p(x_{n+1}, \ldots, x_N|z_n, z_{n+1}) = p(x_{n+1}, \ldots, x_N|z_{n+1}) \tag{4}$$
$$p(x_{n+2}, \ldots, x_N|z_{n+1}, x_{n+1}) = p(x_{n+2}, \ldots, x_N|z_{n+1}) \tag{5}$$
$$p(X|z_{n-1}, z_n) = p(x_1, \ldots, x_{n-1}|z_{n-1})\, p(x_n|z_n)\, p(x_{n+1}, \ldots, x_N|z_n) \tag{6}$$
$$p(x_{N+1}|X, z_{N+1}) = p(x_{N+1}|z_{N+1}) \tag{7}$$
$$p(z_{N+1}|z_N, X) = p(z_{N+1}|z_N) \tag{8}$$

We begin with $\gamma(z_n)_k$. By Bayes' Rules,

$$\begin{aligned}
\gamma(z_n)_k &= p(z_n = k|X) \\
&= \frac{p(X|z_n = k)\, p(z_n = k)}{p(X)} \\
&\overset{(1)}{=} \frac{p(x_1, \ldots, x_n|z_n)\, p(x_{n+1}, \ldots, x_N|z_n)\, p(z_n = k)}{p(X)} \\
&= \frac{\overbrace{p(x_1, \ldots, x_N, z_n = k)}^{\alpha(z_n)_k}\, \overbrace{p(x_{n+1}, \ldots, x_N|z_n = k)}^{\beta(z_n)_k}}{p(X)} \\
&= \frac{\alpha(z_n)_k \beta(z_n)_k}{p(X)}
\end{aligned}$$

with $\alpha(z_n)_k = p(x_1, \ldots, x_n, z_n = k)$ and $\beta(z_n)_k = p(x_{n+1}, \ldots, x_N|z_n = k)$. At this point, we want to find recursion rules for α, β.

1.

$$\begin{aligned}
\alpha(z_n)_k &= p(x_1, \dots, x_n, z_n = k) \\
&\overset{\prod}{=} p(x_1, \dots, x_n | z_n = k)\, p(z_n = k) \\
&\overset{(2)}{=} p(x_n | z_n = k)\, p(x_1, \dots, x_{n-1} | z_n = k)\, p(z_n = k) \\
&\overset{\prod}{=} p(x_n | z_n = k)\, p(x_1, \dots, x_{n-1}, z_n = k) \\
&\overset{\Sigma}{=} p(x_n | z_n = k) \sum_j p(x_1, \dots, x_{n-1}, z_{n-1} = j, z_n = k) \\
&\overset{3,\prod}{=} p(x_n | z_n = k) \sum_j p(x_1, \dots, x_{n-1} | z_{n-1} = j)\, p(z_{n-1} = j)\, p(z_n = k | z_{n-1} = j) \\
&\overset{\prod}{=} p(x_n | z_n = k) \sum_j \underbrace{p(x_1, \dots, x_{n-1}, z_{n-1} = j)}_{\alpha(z_{n-1})_j}\, p(z_n = k | z_{n-1} = j) \\
&= p(x_n | \phi_k) \sum_j \alpha(z_{n-1})_j A_{jk}
\end{aligned}$$

Recursion starts for $n = 1$:

$$\begin{aligned}
\alpha(z_1)_k = p(x_1, z_1 = k) &= p(x_1 | z_1 = k) \cdot p(z_1 = k) \\
&= p(x_1 | \phi_k) \pi_k
\end{aligned}$$

We proceed with left-to-right sweep, and it's pretty easy to compute the data. Let's now tackle the other half of the problem, β.

2.

$$\begin{aligned}
\beta(z_n)_k &= p(x_{n+1}, \dots, x_N | z_n = k) \\
&\overset{\Sigma}{=} \sum_j p(x_{n+1}, \dots, x_N, z_{n+1} = j | z_n = k) \\
&\overset{\prod}{=} \sum_j p(x_{n+1}, \dots, x_N | z_{n+1} = j, z_n = k)\, p(z_{n+1} = j | z_n = k) \\
&\overset{(4)}{=} \sum_j p(x_{n+1}, \dots, x_N | z_{n+1} = j)\, p(z_{n+1} = j | z_n = k) \\
&\overset{(5)}{=} \sum_j p(x_{n+2}, \dots, x_N | z_{n+1} = j)\, p(x_{n+1} | z_{n+1} = j)\, p(z_{n+1} = j | z_n = k) \\
&= \sum_j \beta(z_{n+1})_j p(x_{n+1} | \phi_j) A_{jk}
\end{aligned}$$

Recursion needs to start at $n = N$ for $\beta(z_N)_k$.

$$\begin{aligned}
\gamma(z_N)_k &= \frac{\alpha(z_N)_k \beta(z_N)_k}{p(X)} \\
p(z_N = k | X) &= \frac{p(X, z_N = k) \beta(z_N)_k}{p(X)} \\
\implies \beta(z_N)_k &= 1
\end{aligned}$$

We proceed right-to-left (backward) sweep to compute all β.

3. Also,

$$
\begin{aligned}
\xi(z_{n-1}, z_n)_{jk} &= p(z_{n-1} = j, z_n = k | X) \\
\text{(Bayes')} \quad &= \frac{p(X | z_{n-1} = j, z_n = k)\, p(z_{n-1} = j, z_n = k)}{p(X)} \\
&\overset{(6)}{=} p(x_1, \ldots, x_{n-1} | z_{n-1} = j)\, p(x_n | z_n = k)\, p(x_{n+1}, \ldots, x_N | z_n = k) \\
&\quad p(z_n = k | z_{n-1} = j)\, p(z_{n-1} = j) \cdot \frac{1}{p(X)} \\
&= \frac{\alpha(z_{n-1})_j\, \beta(z_n)_k\, p(x_n | \phi_k)\, A_{jk}}{p(X)}
\end{aligned}
$$

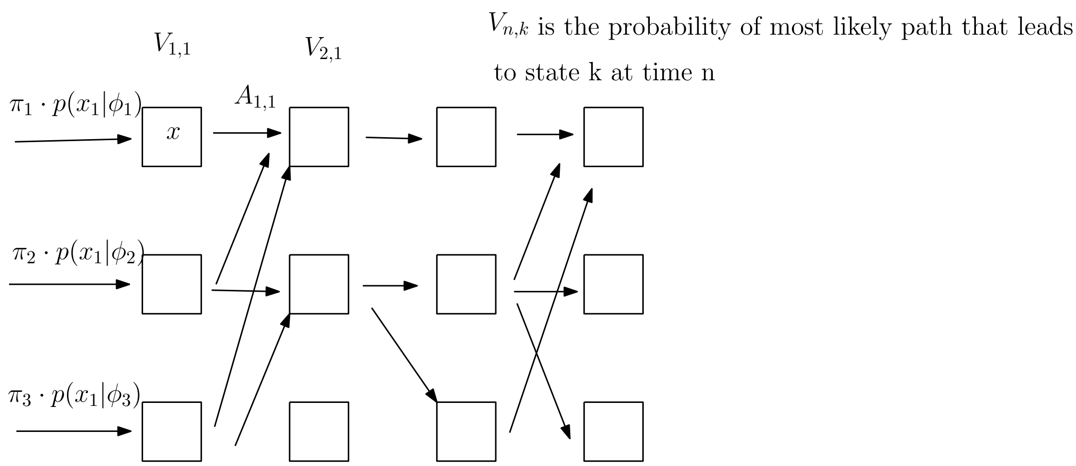
§14 Lec 14: Jul 28, 2021

§14.1 Viterbi's Algorithm

Given a fully trained model: π_k, A_{jk}, ϕ_k, and we have a new sequence of observations $x_1, \ldots, x_N$.

Question 14.1. What is the most likely sequence $z_1, \ldots, z_N$ that produces these observations? (Decoding)

The key idea is to avoid computing $p(X, Z|\pi, A, \phi)$ for all possible paths. Instead, we want to use dynamic programming-based "Viterbi" algorithm. We want to incrementally (left-to-right) compute the probability and sequence of the most likely path.



$$V_{n,k} = \max_j(v_{n-1,j} \cdot A_{jk}) \cdot p(x_n|\phi_k)$$

At the end of the sequence, we can trace back the path with the highest likelihood to obtain the most likely state.