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.

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

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:

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

Covariances:

Definition 1.3 — Variance is defined as

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

Covariance (random variables) is defined as

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

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

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

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:

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

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: $p(w|\alpha) = N(w|0, \alpha^{-1})$

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

   Then, we can estimate

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

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

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

§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,

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

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)

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

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

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

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

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

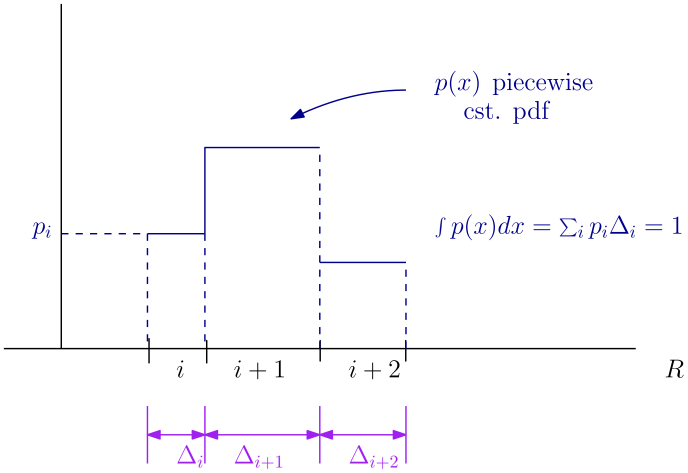
$$\implies \mu_{\text{MAP}} = \left(N\Sigma^{-1} + \Sigma_0^{-1}\right)^{-1} \left(N\Sigma^{-1}\overline{x} + \Sigma_0^{-1}\mu_0\right)$$

§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,

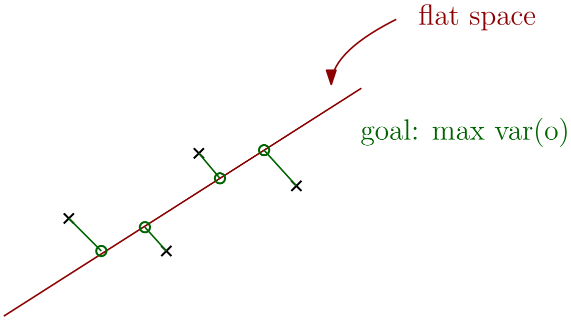
$$\begin{cases} k(u) \geq 0 \\ \int k(u)\, du = 1 \end{cases}$$

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

$$\begin{aligned} \frac{\partial L}{\partial u_1} : \; & 2Su_1 - 2\lambda_1 u_1 = 0 \\ & Su_1 = \lambda_1 u_1 \end{aligned}$$

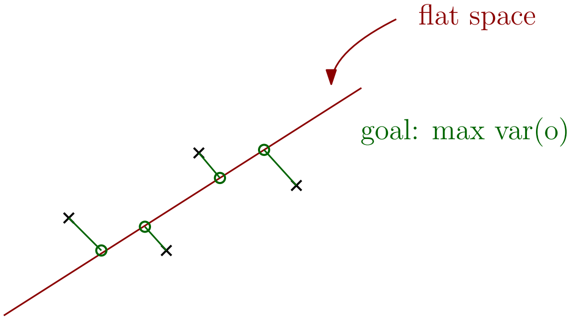
So, the eigen-problem: (λ_1, u_1) is eigenpair of S.

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

$\implies$ 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

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

Minimum Error Formulation:



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

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

Then each data point x_n has unique expansion in that basis

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

where

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

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, $S = \frac{1}{N} x^\top x$

$$X = \begin{bmatrix} \rule{1.5cm}{0.4pt} \\ \rule{1.5cm}{0.4pt} \\ \rule{1.5cm}{0.4pt} \\ \\ \end{bmatrix}$$

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

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

$\Longrightarrow$ 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,

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

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

□

Note: 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.