Exercise 1: Maximum Likelihood vs. Bayes

An unfair coin is tossed seven times and the event (head or tail) is recorded at each iteration. The observed sequence of events is

$$\mathcal{D} = (x_1, x_2, \dots, x_7) = (\text{head}, \text{head}, \text{tail}, \text{tail}, \text{head}, \text{head}, \text{head}).$$

We assume that all tosses $x_1, x_2, \dots$ have been generated independently following the Bernoulli probability distribution

$$P(x \mid \theta) = \begin{cases} \theta & \text{if} \quad x = \text{head} \\ 1-\theta & \text{if} \quad x = \text{tail}, \end{cases}$$

where $\theta \in [0,1]$ is an unknown parameter.

(a) *State* the likelihood function $P(\mathcal{D}|\theta)$, that depends on the parameter θ.

$$P(D|\theta) = \prod_{i=1}^{7} p(x_i|\theta) = \theta^5 \cdot (1-\theta)^2$$

(b) *Compute* the maximum likelihood solution $\hat{\theta}$, and *evaluate* for this parameter the probability that the next two tosses are "head", that is, evaluate

$$P(x_8 = \text{head}\,,\ x_9 = \text{head} \mid \hat{\theta}).$$

$$P(D|\theta) = \theta^5(1-\theta)^2$$

$$\log P(D|\theta) = 5 \cdot \log\theta + 2 \cdot \log(1-\theta) \qquad \text{concave}$$

$$\frac{\partial}{\partial\theta}\log P(D|\theta) = \frac{5}{\theta} - \frac{2}{1-\theta} \overset{!}{=} 0 \Rightarrow \hat{\theta} = \frac{5}{7}$$

$$P(h,h|\hat{\theta}) = \hat{\theta}\cdot\hat{\theta} = \frac{25}{49}$$

(c) We now adopt a Bayesian view on this problem, where we assume a prior distribution for the parameter θ defined as:

$$p(\theta) = \begin{cases} 1 & \text{if} \quad 0 \le \theta \le 1 \\ 0 & \text{else.} \end{cases}$$

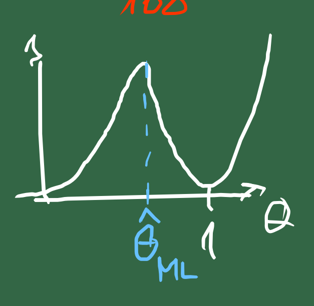
Compute the posterior distribution $p(\theta|\mathcal{D})$, and *evaluate* the probability that the next two tosses are head, that is,

$$\int P(x_8 = \text{head}\,,\ x_9 = \text{head} \mid \theta)\, p(\theta|\mathcal{D})\, d\theta.$$

$$p(\theta|D) = \frac{p(D|\theta)\,p(\theta)}{\int_0^1 p(D|\theta)\,p(\theta)\,d\theta} = \frac{\theta^5(1-\theta)^2}{\int_0^1 \theta^5(1-\theta)^2\,d\theta} \qquad (0 \le \theta \le 1)$$

$$\int_0^1 \theta^5(1-\theta)^2\,d\theta = \frac{1}{168}$$

$$= 168 \cdot \theta^5(1-\theta)^2$$



$$\int_0^1 P(h,h|\theta)\,p(\theta|D)\,d\theta$$

$$= \int_0^1 \theta^2 \cdot 168 \cdot \theta^5(1-\theta)^2\,d\theta$$

$$= \frac{7}{15}$$

$$\int_0^1 \theta^5 - 2\theta^6 + \theta^7\,d\theta = \left[\frac{\theta^6}{6} - 2\cdot\frac{\theta^7}{7} + \frac{\theta^8}{8}\right]_0^1$$

$$= \frac{1}{6} - \frac{2}{7} + \frac{1}{8} = \frac{56}{336} - \frac{96}{336} + \frac{42}{336} = \frac{2}{336} = \frac{1}{168}$$

Exercise 2: Principal Component Analysis

We consider an unsupervised dataset $\boldsymbol{x}_1, \dots, \boldsymbol{x}_N \in \mathbb{R}^d$, where $\bar{\boldsymbol{x}} = \frac{1}{N}\sum_{k=1}^N \boldsymbol{x}_k$ is the empirical mean. The principal component analysis problem consists of finding the vector $\boldsymbol{e} \in \mathbb{R}^d$ of norm 1 such that the data projected in this space has maximum variance, i.e. is a solution of the optimization problem

$$\max_{\boldsymbol{e}\in\mathbb{R}^d} \frac{1}{N}\sum_{k=1}^{N} (\boldsymbol{e}^\top \boldsymbol{x}_k - m)^2 \qquad \text{subject to} \quad \|\boldsymbol{e}\|^2 = 1$$

where $m = \frac{1}{N}\sum_{k=1}^N \boldsymbol{e}^\top \boldsymbol{x}_k$ is the mean of the projected data.

(a) *Show* that the problem can be rewritten as the quadratic program

$$\max_{\boldsymbol{e}\in\mathbb{R}^d} \boldsymbol{e}^\top C \boldsymbol{e} \qquad \text{subject to} \quad \|\boldsymbol{e}\|^2 = 1$$

where $C = \frac{1}{N}\sum_{k=1}^N (\boldsymbol{x}_k - \bar{\boldsymbol{x}}) \cdot (\boldsymbol{x}_k - \bar{\boldsymbol{x}})^\top$ is the empirical covariance matrix.

$$\frac{1}{N}\sum_k \Big[e^\top x_k - \underbrace{\frac{1}{N}\sum_{k'} e^\top x_{k'}}_{e^\top \bar{x}}\Big]^2 = \frac{1}{N}\sum_k e^\top x_k x_k^\top e - 2e^\top x_k \bar{x}^\top e + e^\top \bar{x}\bar{x}^\top e$$

$$= \frac{1}{N}\sum_k e^\top (x_k x_k^\top - 2x_k\bar{x}^\top + \bar{x}\bar{x}^\top) e$$

$$= e^\top \Big(\frac{1}{N}\sum_k (x_k - \bar{x})(x_k - \bar{x})^\top\Big) e$$

$$= e^\top C e$$

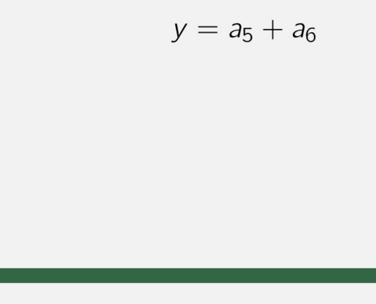
(b) *Show* using the method of Lagrange multipliers that the solution of the optimization problem above is an eigenvector of the matrix C.

$$\mathcal{L}(e,\lambda) = e^\top C e - \lambda(\|e\|^2 - 1)$$

$$\frac{\partial \mathcal{L}}{\partial e} = 2Ce - 2\lambda e \overset{!}{=} 0 \iff Ce = \lambda e$$

(c) *Show* that, among all possible eigenvectors of C, the solution of the optimization problem above is the one with highest associated eigenvalue.

$$e^\top C e = e^\top (\lambda e) = \lambda \cdot \|e\|^2 = \lambda$$



Exercise 3: Neural Networks

We consider a neural network that takes two inputs x_1 and x_2 and produces an output y based on the following set of computations:

$$z_3 = x_1 \cdot w_{13} + x_2 \cdot w_{23} \qquad z_5 = a_3 \cdot w_{35} + a_4 \cdot w_{45} \qquad y = a_5 + a_6$$
$$a_3 = \tanh(z_3) \qquad a_5 = \tanh(z_5)$$
$$z_4 = x_1 \cdot w_{14} + x_2 \cdot w_{24} \qquad z_6 = a_3 \cdot w_{36} + a_4 \cdot w_{46}$$
$$a_4 = \tanh(z_4) \qquad a_6 = \tanh(z_6)$$

(a) *Draw* the neural network graph associated to this set of computations.

(b) *Write* the set of backward computations that leads to the evaluation of the partial derivative $\partial y / \partial w_{13}$. Your answer should avoid redundant computations. Hint: $\tanh'(t) = 1 - (\tanh(t))^2$.

$$\delta_j = \frac{\partial y}{\partial z_j}$$

$$\delta_6 = 1 - a_6^2$$

$$\delta_5 = 1 - a_5^2$$

$$\delta_3 = (\delta_5 \cdot w_{35} + \delta_6 \cdot w_{36}) \cdot (1 - a_3^2)$$

$$\frac{\partial y}{\partial w_{13}} = x_1 \cdot \delta_3$$

Regarding **Slater's condition**, since the constraints are linear and the two hyperplanes typically do not coincide, there exists a **strictly feasible point** satisfying $w_1^\top x > 1, w_2^\top x < -1$. Thus, Slater's condition holds, ensuring **strong duality**, and we can solve the problem using **Lagrangian duality**.

then Strong duality hold

Slater: linear seperability of two hyperplanes

Exercise 4: Support Vector Machines

The primal program for the linear hard margin SVM is

$$\min_{\boldsymbol{w},\theta} \|\boldsymbol{w}\|^2 \qquad \text{subject to} \quad y_i(\boldsymbol{w}^\top \boldsymbol{x}_i + \theta) \ge 1, \quad \text{for } 1 \le i \le N,$$

where $\|.\|$ denotes the Euclidean norm, and the minimization is performed in $\boldsymbol{w} \in \mathbb{R}^d, \theta \in \mathbb{R}$, while the data $\boldsymbol{x}_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$ are regarded as fixed constants.

(a) *State* the Lagrangian ~~dual~~ of the constrained optimization problem above and determine when the Slater's conditions for strong duality are satisfied.

$$\mathcal{L}(w,\theta,\vec{\alpha}) = \frac{1}{2}\|w\|^2 - \sum_i \alpha_i \left[y_i(w^\top x_i + \theta) - 1\right]$$

$$\max_{\alpha} \min_{w,\theta} \mathcal{L}(w,\theta,\alpha) \quad \text{s.t.} \quad \forall_i \ \alpha_i \ge 0$$

Slater: linear separability of the two classes

(b) *Show* that the Lagrange dual takes the form of a quadratic optimization problem w.r.t. the dual variables $\alpha_1, \dots, \alpha_N$.

$$\frac{\partial \mathcal{L}}{\partial w} = w - \sum_i \alpha_i y_i x_i \overset{!}{=} 0 \Rightarrow w = \sum_i \alpha_i y_i x_i$$

$$\frac{\partial \mathcal{L}}{\partial \theta} = -\sum_i \alpha_i y_i \overset{!}{=} 0 \Rightarrow \sum_i \alpha_i y_i = 0$$

$$\mathcal{L}(\vec{\alpha}) = -\frac{1}{2}\sum_i\sum_j \alpha_i\alpha_j y_i y_j x_i^\top x_j + \sum_i \alpha_i$$

$$\max_{\alpha} -\frac{1}{2}\sum_i\sum_j \alpha_i\alpha_j y_i y_j x_i^\top x_j + \sum_i \alpha_i$$

$$\text{s.t.} \quad \forall_i \ \alpha_i \ge 0$$

$$\sum_i \alpha_i y_i = 0$$

The **dual formulation** is preferred when the number of constraints is much smaller than the number of primal variables (i.e., when d is large). This is because solving the dual problem involves optimizing over a lower-dimensional space, making it computationally more efficient. However, if d is small or the number of constraints is large, solving the **primal problem** directly may be more straightforward.

当约束的数量远小于原始变量的数量时（即 whenis large），则首选对偶公式。这是因为解决对偶问题涉及在较低维空间上进行优化，从而提高计算效率。但是，如果很小或者 constraints 的数量很多，直接解决 theprimal problem 可能更直接。

Exercise 5: Kernels

A kernel function $k\colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ generalizes the linear scalar product between two vectors. The kernel must satisfy positive semi-definiteness, that is, for any sequence of data points $\boldsymbol{x}_1, \dots, \boldsymbol{x}_n \in \mathbb{R}^d$ and coefficients $c_1, \dots, c_n \in \mathbb{R}$ the following inequality should hold:

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_i\, c_j\, k(\boldsymbol{x}_i, \boldsymbol{x}_j) \ge 0 \qquad K_{ij} = k(x_i, x_j)$$

$$c^\top K c \ge 0$$

We consider the kernel function $k(\boldsymbol{x}, \boldsymbol{x}') = \langle \boldsymbol{x}, \boldsymbol{x}' \rangle^2$.

(a) *Show* that this kernel is positive semi-definite.

$$\sum_i\sum_j c_i c_j \Big(\sum_d x_{id} \cdot x_{jd}\Big)^2$$

$$= \sum_i\sum_j c_i c_j \Big(\sum_k x_{ik} x_{jk}\Big)\Big(\sum_\ell x_{i\ell} x_{j\ell}\Big)$$

$$= \sum_i\sum_j c_i c_j \sum_k\sum_\ell x_{ik} x_{jk} x_{i\ell} x_{j\ell}$$

$$= \sum_k\sum_\ell\sum_i\sum_j c_i x_{ik} x_{i\ell} \cdot c_j x_{jk} x_{j\ell}$$

$$= \sum_k\sum_\ell \Big(\sum_i c_i x_{ik} x_{i\ell}\Big)^2 \ge 0$$