CSE176 Introduction to Machine Learning Spring semester 2023

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**Exercise 1: Euclidean distance classifier (10 points).** A Euclidean distance classifier represents each class  $k = 1, \ldots, K$  by a prototype vector  $\boldsymbol{\mu}_k \in \mathbb{R}^D$  and classifies a pattern  $\mathbf{x} \in \mathbb{R}^D$  as the class of its closest prototype:  $k^* = \arg\min_{k=1,\ldots,K} \|\mathbf{x} - \boldsymbol{\mu}_k\|$ . Prove that a Gaussian classifier with shared isotropic covariances (i.e., of the form  $\boldsymbol{\Sigma}_k = \sigma^2 \mathbf{I}$  for  $k = 1, \ldots, K$ , where  $\sigma > 0$ ) and equal class priors (i.e.,  $p(C_1) = \cdots = p(C_K) = \frac{1}{K}$ ) is equivalent to a Euclidean distance classifier. Prove the class discriminant functions  $g_1(\mathbf{x}), \ldots, g_K(\mathbf{x})$  are linear and give the expression that defines them.

Exercise 2: variation of k-means clustering (20 points). Consider the k-means error function:

$$E(\{\boldsymbol{\mu}_k\}_{k=1}^{K}, \mathbf{Z}) = \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2 \quad \text{s.t.} \quad \mathbf{Z} \in \{0, 1\}^{NK}, \ \mathbf{Z} \, \mathbf{1} = \mathbf{1}$$

over the centroids  $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K$  and cluster assignments  $\mathbf{Z}_{N \times K}$ , given training points  $\mathbf{x}_1, \ldots, \mathbf{x}_N \in \mathbb{R}^D$ .

- Variation: in k-means, the centroids can take any value in  $\mathbb{R}^D$ :  $\mu_k \in \mathbb{R}^D \ \forall k = 1, \dots, K$ . Now we want the centroids to take values from among the training points only:  $\mu_k \in \{\mathbf{x}_1, \dots, \mathbf{x}_N\} \ \forall k = 1, \dots, K$ .
  - 1. (15 points) Design a clustering algorithm that minimizes the k-means error function but respecting the above constraint. Your algorithm should converge to a local optimum of the error function. Give the steps of the algorithm explicitly.
  - 2. (5 points) Can you imagine when this algorithm would be useful, or preferable to k-means?

**Exercise 3: mixture distributions (10 points).** Let  $p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k p(\mathbf{x}|k)$  for  $\mathbf{x} \in \mathbb{R}^D$  be a mixture of K densities, where  $\pi_1, \ldots, \pi_K \in [0, 1]$  and  $\sum_{k=1}^{K} \pi_k = 1$  are the component proportions (prior probabilities) and  $p(\mathbf{x}|k)$ , for  $k = 1, \ldots, K$ , the component densities (e.g. Gaussian, but not necessarily). Let  $\boldsymbol{\mu}_k = \mathbb{E}_{p(\mathbf{x}|k)} \{\mathbf{x}\}$  and  $\boldsymbol{\Sigma}_k = \mathbb{E}_{p(\mathbf{x}|k)} \{(\mathbf{x} - \boldsymbol{\mu}_k)(\mathbf{x} - \boldsymbol{\mu}_k)^T\}$  be the mean and covariance of component density k, for  $k = 1, \ldots, K$ .

1. (5 points) Prove that the mean and covariance of the mixture are:

$$\boldsymbol{\mu} = \mathbf{E}_{p(\mathbf{x})} \left\{ \mathbf{x} \right\} = \sum_{k=1}^{K} \pi_k \boldsymbol{\mu}_k \qquad \boldsymbol{\Sigma} = \mathbf{E}_{p(\mathbf{x})} \left\{ (\mathbf{x} - \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu})^T \right\} = \sum_{k=1}^{K} \pi_k \left( \boldsymbol{\Sigma}_k + \boldsymbol{\mu}_k \boldsymbol{\mu}_k^T \right) - \boldsymbol{\mu} \boldsymbol{\mu}^T.$$

2. (5 points) Imagine the component covariances  $\Sigma_1, \ldots, \Sigma_K$  are all diagonal. Is the mixture covariance diagonal? Explain.

Exercise 4: mean-shift algorithm (10 points). Consider a Gaussian kernel density estimate

$$p(\mathbf{x}) = \sum_{n=1}^{N} p(\mathbf{x}|n) p(n) = \frac{1}{N(2\pi\sigma^2)^{D/2}} \sum_{n=1}^{N} e^{-\frac{1}{2} \left\| \frac{\mathbf{x} - \mathbf{x}_n}{\sigma} \right\|^2} \qquad \mathbf{x} \in \mathbb{R}^D.$$

Derive the mean-shift algorithm, which iterates the following expression:

$$\mathbf{x} \leftarrow \sum_{n=1}^{N} p(n|\mathbf{x})\mathbf{x}_{n} \quad \text{where} \quad p(n|\mathbf{x}) = \frac{p(\mathbf{x}|n)p(n)}{p(\mathbf{x})} = \frac{\exp\left(-\frac{1}{2}\|(\mathbf{x}-\mathbf{x}_{n})/\sigma\|^{2}\right)}{\sum_{n'=1}^{N} \exp\left(-\frac{1}{2}\|(\mathbf{x}-\mathbf{x}_{n'})/\sigma\|^{2}\right)}$$

until convergence to a maximum of p (or, in general, a stationary point of p, satisfying  $\nabla p(\mathbf{x}) = \mathbf{0}$ ). *Hint*: take the gradient of p wrt  $\mathbf{x}$ , equate it to zero and rearrange the resulting expression.

Exercise 5: nonparametric regression (20 points). Consider the Gaussian kernel smoother

$$\mathbf{g}(\mathbf{x}) = \sum_{n=1}^{N} \frac{K(\|(\mathbf{x} - \mathbf{x}_n)/h\|)}{\sum_{n'=1}^{N} K(\|(\mathbf{x} - \mathbf{x}_{n'})/h\|)} \mathbf{y}_n \quad \text{where} \quad K\left(\left\|\frac{\mathbf{x} - \mathbf{x}_n}{\sigma}\right\|\right) \propto \exp\left(-\frac{1}{2}\|(\mathbf{x} - \mathbf{x}_n)/\sigma\|^2\right)$$

estimated on a training set  $\{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N \subset \mathbb{R}^{D_x} \times \mathbb{R}^{D_y}$ .

- 1. (7 points) What is  $\mathbf{g}(\mathbf{x})$  if the training set has only one point (N=1)? Explain. Sketch the solution in 1D (i.e., when both  $\mathbf{x}_n, \mathbf{y}_n \in \mathbb{R}$ ). Compare with using a least-squares linear regression.
- 2. (13 points) Prove that, with N = 2 points, we can write  $\mathbf{g}(\mathbf{x}) = \alpha(\mathbf{x}) \mathbf{y}_1 + (1 \alpha(\mathbf{x})) \mathbf{y}_2$  where  $\alpha(\mathbf{x})$  can be written using the logistic function. Give the detailed expression for  $\alpha(\mathbf{x})$ . Sketch the solution in 1D.

Compare with using a least-squares linear regression.

Exercise 6: PCA and LDA (30 points). Consider 2D data points coming from a mixture of two Gaussians with equal proportions, different means, and equal, diagonal covariances (where  $\mu, \sigma_1, \sigma_2 > 0$ ):

$$\mathbf{x} \in \mathbb{R}^2: \ p(\mathbf{x}) = \pi_1 \ p(\mathbf{x}|1) + \pi_2 \ p(\mathbf{x}|2) \qquad p(\mathbf{x}|1) \sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1), \quad p(\mathbf{x}|2) \sim \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2),$$
$$\pi_1 = \pi_2 = \frac{1}{2}, \quad \boldsymbol{\mu}_1 = \mathbf{0}, \ \boldsymbol{\mu}_2 = \begin{pmatrix} \mu \\ 0 \end{pmatrix}, \quad \boldsymbol{\Sigma}_1 = \boldsymbol{\Sigma}_2 = \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}.$$

1. (5 points) Compute the mean  $\mu$  and covariance  $\Sigma$  of the mixture distribution  $p(\mathbf{x})$ .

*Hint*: let  $p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \, p(\mathbf{x}|k)$  for  $\mathbf{x} \in \mathbb{R}^D$  be a mixture of K densities, where  $\pi_1, \ldots, \pi_K \in [0, 1]$  and  $\sum_{k=1}^{K} \pi_k = 1$  are the component proportions (prior probabilities) and  $p(\mathbf{x}|k)$ , for  $k = 1, \ldots, K$ , the component densities (e.g. Gaussian, but not necessarily). Let  $\boldsymbol{\mu}_k = \mathbb{E}_{p(\mathbf{x}|k)} \{\mathbf{x}\}$ and  $\Sigma_k = \mathbb{E}_{p(\mathbf{x}|k)} \left\{ (\mathbf{x} - \boldsymbol{\mu}_k) (\mathbf{x} - \boldsymbol{\mu}_k)^T \right\}$  be the mean and covariance of component density k, for k = 1, ..., K. Then, the mean and covariance of the mixture are (you should be able to prove this statement):

$$\boldsymbol{\mu} = \mathbf{E}_{p(\mathbf{x})} \left\{ \mathbf{x} \right\} = \sum_{k=1}^{K} \pi_k \boldsymbol{\mu}_k \qquad \boldsymbol{\Sigma} = \mathbf{E}_{p(\mathbf{x})} \left\{ (\mathbf{x} - \boldsymbol{\mu}) (\mathbf{x} - \boldsymbol{\mu})^T \right\} = \sum_{k=1}^{K} \pi_k \left( \boldsymbol{\Sigma}_k + \boldsymbol{\mu}_k \boldsymbol{\mu}_k^T \right) - \boldsymbol{\mu} \boldsymbol{\mu}^T$$

- 2. (5 points) Compute the eigenvalues  $\lambda_1 \geq \lambda_2 \geq 0$  and corresponding eigenvectors  $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^2$  of  $\Sigma$ . Can we have  $\lambda_2 > 0?$
- 3. (2 points) Find the PCA projection to dimension 1.
- 4. (5 points) Compute the within-class and between-class scatter matrices  $\mathbf{S}_W$ ,  $\mathbf{S}_B$  of p.
- 5. (6 points) Compute the eigenvalues  $\nu_1 \geq \nu_2 \geq 0$  and corresponding eigenvectors  $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^2$  of  $\mathbf{S}_W^{-1} \mathbf{S}_B$ . Can we have  $\nu_2 > 0$ ?
- 6. (2 points) Compute the LDA projection.
- 7. (5 points) When does PCA find the same projection as LDA? Give a condition and explain it.