

Fifth practice exercises in Machine learning 1 – 2025 – Paper 1

1 Principal component analysis (October)

Suppose we have a data set $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ of D -dimensional vectors, which have a zero mean for each dimension. Assume we perform a complete eigenvalue decomposition of the empirical covariance matrix $\mathbf{S} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^T$. You are interested in only a single projection of your data such that the variance of this projection is maximized. Let \mathbf{u}_i be the direction vector of a particular projection. Assume that $\mathbf{u}_i^T \mathbf{u}_i = 1$.

- (a) What is the projection z_{ni} of a given point \mathbf{x}_n under the particular vector \mathbf{u}_i ?
- (b) What is the empirical mean of the projection z_i across all points \mathbf{x}_n ?
- (c) What is the empirical variance of the projection z_i ? Provide your answer in terms of the empirical covariance matrix \mathbf{S}
- (d) Replace \mathbf{S} with its eigenvalue decomposition and simplify the aforementioned expression. What is the variance now?

with \mathbf{e}_i to be a vector with zeros except the position with index i .

- (e) Suppose that you are interested in reducing the dimensionality from D to K , such that 99% of the variance is maintained. How can you select an appropriate K ?

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2 Introduction to backpropagation (October)

Consider a two-layer neural network, defined as follows

$$\begin{aligned}\mathbf{z}^{(1)} &= \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}, & \mathbf{a}^{(1)} &= \tanh(\mathbf{z}^{(1)}), \\ \mathbf{z}^{(2)} &= \mathbf{W}^{(2)}\mathbf{a}^{(1)} + \mathbf{b}^{(2)}, & \hat{\mathbf{y}} &= \text{softmax}(\mathbf{z}^{(2)}),\end{aligned}$$

where

- $\mathbf{x} \in \mathbb{R}^D$ is a single input example.
 - $\hat{\mathbf{y}} \in \mathbb{R}^K$ is the predicted output vector.
 - The first hidden layer (1) has H neurons.
- (a) What are the shapes of $\mathbf{W}^{(1)}$, $\mathbf{b}^{(1)}$, $\mathbf{a}^{(1)}$, $\mathbf{W}^{(2)}$, $\mathbf{b}^{(2)}$?
- (b) We feed the neural network with a sample \mathbf{x} , obtaining the prediction $\hat{\mathbf{y}}$. We assume we have the ground truth label \mathbf{y} for that sample \mathbf{x} . Write down the formula for the cross-entropy loss $L(\mathbf{y}, \hat{\mathbf{y}})$ for that sample.
- (c) Compute $\frac{\partial L}{\partial \hat{y}_i}$.
- (d) Compute $\frac{\partial L}{\partial z_i^{(2)}}$.
- (e) Compute $\frac{\partial L}{\partial W_{ij}^{(2)}}$.