Tutorial 12: Nonlinear Dimensionality Reduction

Kernel PCA, distance embeddings, and local reconstruction

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Task 1: Kernel PCA

Consider three scalar training observations

$$x_1 = -1, \qquad x_2 = 0, \qquad x_3 = 1,$$

with kernel $k(x, z) = (1 + xz)^2$. Define the Gram matrix by $K_{ij} = k(x_i, x_j)$ and its centered form by

$$\boldsymbol{K}_c = \boldsymbol{H}\boldsymbol{K}\boldsymbol{H}, \qquad \boldsymbol{H} = \boldsymbol{I} - \tfrac{1}{3}\mathbf{1}\mathbf{1}^{\mathsf{T}}.$$

(a) Compute the 3×3 Gram matrix $\boldsymbol{K}$.

(b) Compute $\boldsymbol{K}_c$ and verify that its rows sum to zero.

(c) Verify that $\boldsymbol{u} = (-1, 0, 1)^{\mathsf{T}}/\sqrt{2}$ is an eigenvector of $\boldsymbol{K}_c$. Find its eigenvalue κ and the three training scores $\boldsymbol{z} = \sqrt{\kappa}\,\boldsymbol{u}$.

(d) For a new input $x_* = 1/2$, compute its centered kernel vector $\boldsymbol{k}_{*,c}$ using training means and its score $z_* = (\boldsymbol{u}/\sqrt{\kappa})^{\mathsf{T}}\boldsymbol{k}_{*,c}$.

Task 2: MDS and ISOMAP

Three observations have the squared-distance matrix

$$\boldsymbol{\Delta} = \begin{bmatrix} 0 & 4 & 16 \\ 4 & 0 & 4 \\ 16 & 4 & 0 \end{bmatrix}.$$

Classical MDS uses $\boldsymbol{B} = -\frac{1}{2}\boldsymbol{H}\boldsymbol{\Delta}\boldsymbol{H}$, with $\boldsymbol{H} = \boldsymbol{I} - \mathbf{1}\mathbf{1}^{\mathsf{T}}/3$.

(a) Compute the centered Gram matrix $\boldsymbol{B}$.

(b) Find its largest eigenvalue and a corresponding unit eigenvector. Obtain one-dimensional coordinates and verify the distance between points 1 and 3.

Separately, an undirected graph has edges $AB = 2$, $BC = 3$, $CD = 2$, $AC = 4$, and $BD = 4$, with no other edges.

(c) Find shortest-path distances $d_G(A, C)$ and $d_G(A, D)$. Give the shortest routes.

(d) An incorrect edge $AD = 1$ is added. Recompute $d_G(A, C)$ and $d_G(A, D)$, and state how this shortcut affects ISOMAP.

Task 3: Local reconstruction

A target point and its three neighbors are

$$\boldsymbol{p} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}, \quad \boldsymbol{a} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 4 \\ 0 \end{bmatrix}, \quad \boldsymbol{c} = \begin{bmatrix} 0 \\ 3 \end{bmatrix}.$$

Use weights satisfying $\boldsymbol{p} = w_A\boldsymbol{a} + w_B\boldsymbol{b} + w_C\boldsymbol{c}$ and $w_A + w_B + w_C = 1$.

(a) Find the three reconstruction weights w_A, w_B, w_C.

(b) Shift all four points by $\boldsymbol{t} = (2, -1)^\mathsf{T}$. Verify that the *same* weights reconstruct the shifted target.

(c) Suppose the neighbors have one-dimensional coordinates $(z_A, z_B, z_C) = (-2, 2, 1)$. If the target coordinate is $z_p = 0$, find its squared reconstruction error and the value of z_p that makes this error zero.

(d) For a different target $\boldsymbol{q} = (5, 1)^\mathsf{T}$, find the three weights using the same neighbors. Explain the sign of any negative weight.

Tutorial 12 complete

Questions and discussion