Chapter 8: Unsupervised Learning: Dimensionality Reduction

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Introduction to Machine Learning

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- Difficult (if not impossible) to visualize.
- Increased number of features can dramatically increase the computational cost of ML algorithms.
- Notions of Euclidean distance and orthogonolity differ significantly in higher dimensions.

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In words this means that in high dimensions, random points drawn from the unit ball lie close to its boundary (have length near 1), and they are nearly orthogonal to each other.

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- Nonlinear methods can detects nonlinear transformations of features as well, e.g. nonlinear mappings of pictures.

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- Alternatively we can keep as many coordinates v₁, v₂,..., v_d, (with d < D) that contain most (e.g. 95%) of the variance of the data and discard the rest.
- We can think of PCA as a linear transformation $T : \mathbb{R}^D \to \mathbb{R}^D$ that sends the standard basis vectors $\{\mathbf{e}_i\}_{i=1}^D$ to $\{\mathbf{v}_i\}_{i=1}^D$.

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- If D = {x_i}ⁿ_{i=1} ⊂ ℝ^D is a dataset and F_i is the n-dimensional vector whose components are the i'th component (feature) of datapoints, then the covariance matrix of D is the matrix C such that C_{i,j} = ⟨F_i, F_j⟩/(n-1).

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- C is symmetric and therefore it is diagonalizable i.e. $C = VLV^t$ where $L = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_D)$.
- We can sort the eigenvectors so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$.

The math of PCA cont.

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• We can see that
$$C = V \frac{S^2}{n-1} V^t$$
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• Once we apply PCA and choose a number *d* < *D* of the coordinates to keep, we can map the dimensionaly reduced data

$$\bar{\mathbf{x}} = \sum_{i=1}^{d} x_i' \mathbf{v}_i \tag{3}$$

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- We can use the error $\sum_i ||\mathbf{x}_i T^{-1} \bar{\mathbf{x}}_i||^2$ to choose the value of d.
- Note: not all dimensionality reduction methods have an inverse map!

• Kernel PCA is a nonlinear dimensionality reduction method.

Image: Image:

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- Remember that in the kernel method for SVM, we had a mapping $\Phi : \mathbb{R}^d \to \mathbb{R}^D$ and a kernel function $K(\mathbf{x}, \mathbf{y})$ such that $K(\mathbf{x}, \mathbf{y}) = \langle \Phi(\mathbf{x}), \Phi(\mathbf{y}) \rangle$.

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