Chapter 8: Unsupervised Learning: Dimensionality Reduction

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Reza Rezazadegan (Sharif University) [Introduction to Machine Learning](#page-49-0) December 14, 2022 1/9

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- **•** 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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Theorem: In d-dimensional Euclidean space, if we randomly pick n points x_1, x_2, \ldots, x_n from the unit ball $||x|| \leq 1$ then with probability $1 - \mathcal{O}(1/n)$ we have:

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Theorem: In d-dimensional Euclidean space, if we randomly pick n points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ from the unit ball $||\mathbf{x}|| \leq 1$ then with probability $1 - \mathcal{O}(1/n)$ we have:

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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[.](#page-20-0)g. nonlinear mappings of pictures. QQ Reza Rezazadegan (Sharif University) [Introduction to Machine Learning](#page-0-0) December 14, 2022 4/9

• PCA is a linear dimensionality reduction method.

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PCA is a linear dimensionality reduction method. For a dataset $\mathcal{D} \subset \mathbb{R}^D$, it finds an orthonormal basis $\mathsf{v}_1,\mathsf{v}_2,\ldots,\mathsf{v}_D$ of \mathbb{R}^D such that the variance of ${\cal D}$ along the coordinates ${\sf v}_1,\ldots,{\sf v}_i,\ldots,{\sf v}_D$ is monotonically decreasing in *i*.

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- We can think of PCA as a linear transformation $\,\mathcal{T}:\mathbb{R}^D\to\mathbb{R}^D\,$ that sends the standard basis vectors $\{{\bf e}_i\}_{i=1}^D$ to $\{{\bf v}_i\}_{i=1}^D.$

• Remember that the *covariance* of two random variables X, Y is defined as

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cov(X, Y) = E[(X - E(X))(Y - E(Y))]
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- If $\mathcal{D} = \{\mathbf{x}_i\}_{i=1}^n \subset \mathbb{R}^D$ is a dataset and \mathcal{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 $C_{i,j} = \langle \mathcal{F}_i, \mathcal{F}_j \rangle / (n-1).$

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- In other words, if X is the $n \times D$ matrix whose rows are the x_i then $C = \frac{X^t X}{n-1}$ $\frac{\lambda^{\prime} \lambda}{n-1}$.

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- C is symmetric and therefore it is diagonalizable i.e. $C = V L V^t$ where $L = diag(\lambda_1, \lambda_2, \ldots, \lambda_D).$
- We can sort the eigenvectors so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$ $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$ $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$ $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_D$ [.](#page-0-0)

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• We can see that
$$
C = V \frac{S^2}{n-1} V^t
$$
.

• Once we apply PCA and choose a number $d < D$ of the coordinates to keep, we can map the dimensionaly reduced data

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

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

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