COMPSCI 589
Lecture 24: Principal Components Analysis

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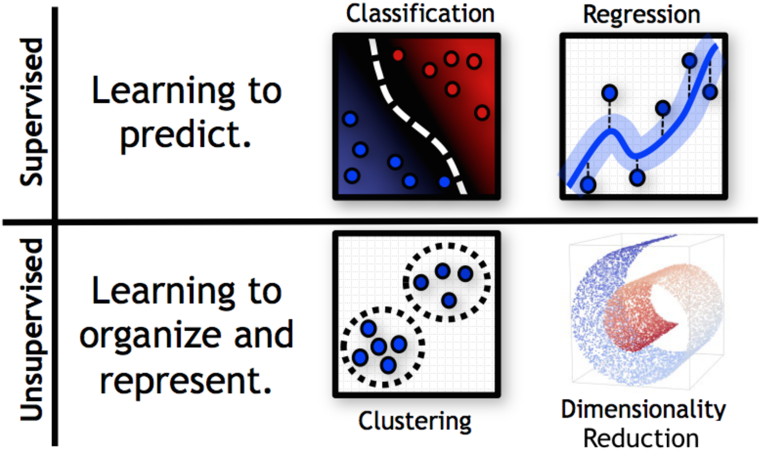
Outline

Machine Learning Tasks



The Dimensionality Reduction Task

Definition: The Dimensionality Reduction Task

Given a collection of feature vectors $\mathbf{x}_i \in \mathbb{R}^p$, map the feature vectors into a lower dimensional space $\mathbf{z}_i \in \mathbb{R}^q$ where $q < p$ while preserving certain properties of the data.

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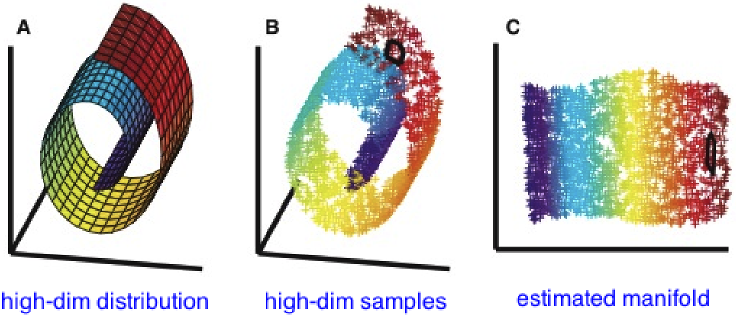
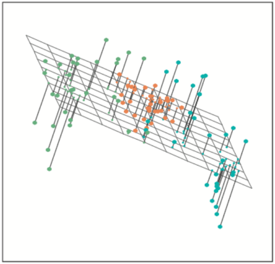
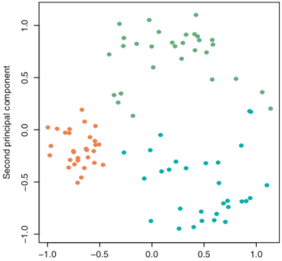


Linear Dimensionality Reduction

- The simplest dimensionality reduction methods assume that the observed high dimensional data vectors $\mathbf{x}_i \in \mathbb{R}^p$ lie on a q-dimensional linear manifold within $\mathbb{R}^p$.
- Mathematically, the linear sub-space assumption can be written as $\mathbf{X} = \mathbf{Z} \times \mathbf{B}$





Learning

- Minimize reconstruction error as

$$\min \|\mathbf{X} - \tilde{\mathbf{X}}\|_F^2$$

- Using encoder ($t(\mathbf{X})$) and decoder (S):

$$\min \sum_{i=1}^{N} \|X_i - S(t(X_i))\|_F^2$$

- Best encoder for fixed decoder $S(\lambda) = \mu + V_q\lambda$ is $\lambda = V_q^T(X - \mu)$
- Updated reconstruction error:

$$\min_{V_q} \sum_{i=1}^{N} \|X_i - V_q V_q^T(X_i)\|_F^2$$

Singular Value Decomposition

- SVD representation of

$$\mathbf{X} = UDV^T$$

where D is a $p \times p$ diagonal matrix with positive elements, $\mathbf{U}$ is an $N \times p$ matrix such that $\mathbf{U}^T\mathbf{U} = I$, and V is a $p \times p$ matrix such that $\mathbf{V}^T\mathbf{V} = I$.

- PCA using SVD

$$\|\mathbf{X} - UD_q^T V_q^T\|_F^2$$

where $q < p$

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- A full-rank (invertible) matrix $\mathbf{A} \in \mathbb{R}^{p \times p}$ will have p linearly independent eigenvectors.

Eigendecomposition

- Let $\mathbf{V} \in \mathbb{R}^{p \times p}$ be a matrix whose columns $\mathbf{v}_d$ are p linearly independent eigenvectors of $\mathbf{A}$ with Λ the corresponding diagonal matrix of eigenvalues such that $\Lambda_{dd} = \lambda_d$.Then:

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- Without loss of generality, we can assume that $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_p$.

Eigendecomposition of a Symmetric Matrix

- If $\mathbf{A}$ is symmetric, we can choose p orthonormal eigenvectors so that $||\mathbf{v}_d||_2 = 1$, $\mathbf{v}_d^T\mathbf{v}_{d'} = 0$ and p real eigenvalues $\lambda_d \in \mathbb{R}$. This representation of $\mathbf{A}$ is unique. As a result, we have:

$$\mathbf{A} = \mathbf{V}\Lambda\mathbf{V}^T = \sum_{d=1}^{p} \lambda_d \mathbf{v}_d \mathbf{v}_d^T$$

Representation of a Vector in the Eigen Basis

- Similarly, if **a** is an arbitrary vector, then we can also represent **a** using the basis provided by the eigevectors **V** of a real symmetric matrix **A**. We obtain:

$$\mathbf{a} = \sum_{d=1}^{p} \alpha_d \mathbf{v}_d \tag{1}$$

$$\alpha_d = \mathbf{a}^T \mathbf{v}_d \tag{2}$$

Outline

Principal Component Analysis

- Given a data matrix $\mathbf{X} \in \mathbb{R}^{N \times p}$, the goal of Principal Component Analysis (PCA) is to identify the directions of maximum variance contained in the data.

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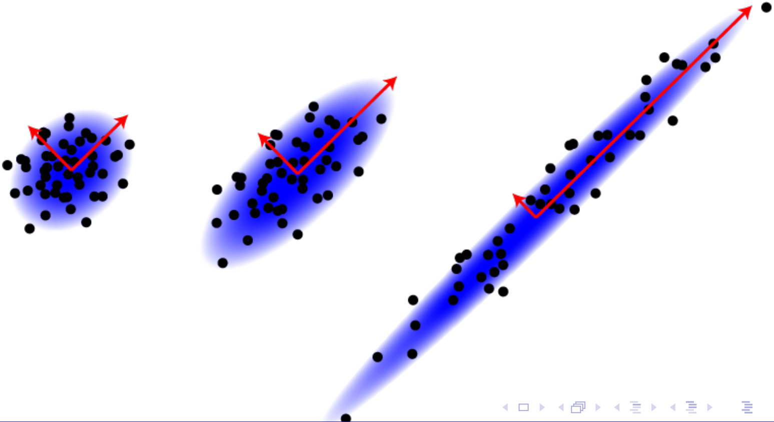

Sample Variance in a Given Direction

- Let $\mathbf{w} \in \mathbb{R}^p$ such that $||\mathbf{w}||_2 = \sqrt{\mathbf{w}^T\mathbf{w}} = 1$.

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- Let $\mathbf{w} \in \mathbb{R}^p$ such that $||\mathbf{w}||_2 = \sqrt{\mathbf{w}^T\mathbf{w}} = 1$.
- The sample estimate of the variance in the direction $\mathbf{w}$ given the data set $\mathbf{X}$ is given by the expression:

$$\frac{1}{N}\sum_{i=1}^{N}(\mathbf{X}_i\mathbf{w} - \mu)^2 \quad \text{where} \quad \mu = \frac{1}{N}\sum_{i=1}^{N}\mathbf{X}_i\mathbf{w}$$

Pre-Centering

- Under the assumption that the data are pre-centered so that $\frac{1}{N}\sum_{i=1}^{N}\mathbf{X}_i = 0$, this expression simplifies to:

$$\frac{1}{N}\sum_{i=1}^{N}(\mathbf{X}_i\mathbf{w})^2 = (\mathbf{X}\mathbf{w})^T(\mathbf{X}\mathbf{w}) = \mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w}$$

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- How can we solve this problem?

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- $\mathbf{V}_d \in \mathbb{R}^D$ are the eigenvectors of Σ. They satisfy:

$$||\mathbf{V}_d||_2 = \sqrt{\mathbf{V}_d^T \mathbf{V}_d} = 1 \text{ ... for all } d$$

$$\mathbf{V}_d^T \mathbf{V}_{d'} = 0 \text{ ... for all } d \neq d'$$

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- Using this result, we can write the optimization problem as:

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- This means $\sum_{d=1}^{p} \omega_d^2 = 1$ and $\omega_d^2 > 0$, so the ω_d^2 values act like a discrete probability distribution.

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- Plugging this back into the objective function, we have:

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- Working our way back to $\mathbf{w}_1$, we put all our weight on the maximum eigenvalue, so $\mathbf{w} = \sum_{d=1}^{p} \omega_d \mathbf{V}_d = \mathbf{V}_1$.
- **This shows that the maximum variance direction given a data matrix X is the eigenvector of $\mathbf{X}^T\mathbf{X}$ with the largest eigenvalue.**

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- Finding the second-largest direction of variance corresponds to solving the problem:

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- **In general, the top q directions of variance $\mathbf{w}_1, ..., \mathbf{w}_q$ are given by the q eigenvectors corresponding to the q largest eigenvalues of $\mathbf{X}^T\mathbf{X}$.**

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4. Project the matrix $\mathbf{X}$ into the rank-q sub-space of maximum variance by computing the matrix product $\mathbf{Z} = \mathbf{XW}$.
5. To reconstruct $\mathbf{X}$ given $\mathbf{Z}$ and $\mathbf{W}$, we use $\hat{\mathbf{X}} = \mathbf{ZW}^T$.

Outline

Connection to SVD

- Last class we saw that the minimum Frobenius norm linear dimensionality reduction problem could be solved using the rank-q SVD of $\mathbf{X}$:

$$\|\mathbf{X} - \mathbf{U}\mathbf{D_q}\mathbf{V_q}^T\|_F^2$$

where the matrix product $\mathbf{Z} = \mathbf{U}\mathbf{D_q}$ gives the optimal rank-q representation of $\mathbf{X}$ with respect to Frobenius norm minimization.

Connection to SVD

- If we let $q = p$ then $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ and $\mathbf{X}^T\mathbf{X} = \mathbf{V}\mathbf{D}\mathbf{U}^T\mathbf{U}\mathbf{D}\mathbf{V}^T$.

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- Due to orthogonality of U this gives: $\mathbf{X}^T\mathbf{X} = \mathbf{VD}^2\mathbf{V}^T$.
- This means that the right singular vectors of $\mathbf{X}$ are exactly the eigenvectors of $\mathbf{X}^T\mathbf{X}$, so SVD's $\mathbf{V}$ and PCA's $\mathbf{W}$ are identical (assuming $\mathbf{X}$ is centered).

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- If we let $q = p$ then $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ and $\mathbf{X}^T\mathbf{X} = \mathbf{V}\mathbf{D}\mathbf{U}^T\mathbf{U}\mathbf{D}\mathbf{V}^T$.
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- This means that the right singular vectors of $\mathbf{X}$ are exactly the eigenvectors of $\mathbf{X}^T\mathbf{X}$, so SVD's $\mathbf{V}$ and PCA's $\mathbf{W}$ are identical (assuming $\mathbf{X}$ is centered).
- We can also see that the eigenvalues of $\mathbf{X}^T\mathbf{X}$ are the squares of the diagonal elements of $\mathbf{D}$.

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- Finally, note that if the decompositions are based only on the q leading basis vectors, which are identical under both PCA and SVD, the projections $\mathbf{Z} = \mathbf{X}\mathbf{W}$ and $\mathbf{Z} = \mathbf{U}\mathbf{D}$ will still be identical.

Connection to SVD

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- As a result, generic linear dimensionality reduction simultaneously minimizes the Frobenius norm of the reconstruction error of $\mathbf{X}$ and maximizes the retained variance in the learned sub-space.
- Both SVD and PCA provide the same refinement of generic linear dimensionality reduction: an orthogonal basis for exactly the same optimal linear subspace.

Demo

- Demo