COMPSCI 589
Lecture 19: Principal Components Analysis

Benjamin M. Marlin

College of Information and Computer Sciences
University of Massachusetts Amherst

Slides by Benjamin M. Marlin (marlin@cs.umass.edu).
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Outline

The Dimensionality Reduction Task

Definition: The Dimensionality Reduction Task

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

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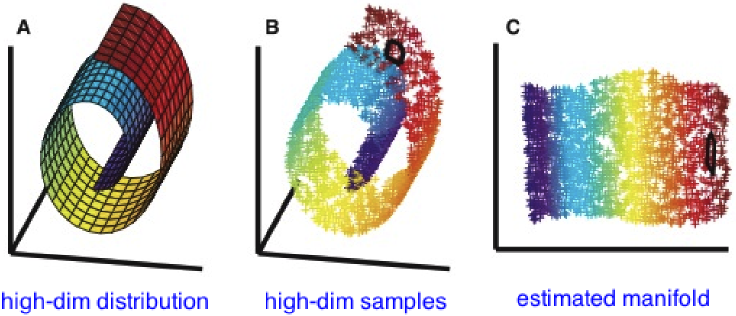
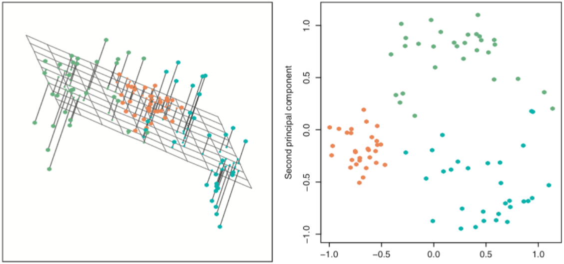


Linear Dimensionality Reduction

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



Learning

- The learning problem for linear dimensionality reduction is to estimate values for both $\mathbf{Z}$ and $\mathbf{B}$ given only the noisy observations $\mathbf{X}$.
- One possible learning criteria is to minimize the sum of squared errors when reconstructing $\mathbf{X}$ from $\mathbf{Z}$ and $\mathbf{B}$. This leads to:

$$\arg\min_{\mathbf{Z},\mathbf{B}} ||\mathbf{X} - \mathbf{ZB}||_F$$

where $||\mathbf{A}||_F$ is the Frobenius norm of matrix $\mathbf{A}$ (the sum of the squares of all matrix entries).

Singular Value Decomposition

- We can pick a unique representation for the subspace by specifying additional criteria. Classical Rank-K Singular Value Decomposition (K-SVD) corresponds to the following restriction:

$$\arg\min_{\mathbf{U},\mathbf{S},\mathbf{V}} ||\mathbf{X} - \mathbf{U}\mathbf{S}\mathbf{V}^T||_F$$

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

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- The matrix product $\mathbf{Z} = \mathbf{U}\mathbf{S}$ gives the optimal rank-K representation of $\mathbf{X}$ with respect to Frobenius norm minimization, with $\mathbf{V}^T$ acting as the basis for the space.

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Eigenvectors

- Let $\mathbf{A} \in \mathbb{R}^{DxD}$ be a matrix, $\mathbf{v} \in \mathbb{R}^{D}$ be a vector, and λ be scalar.

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

Eigendecomposition

- Let $\mathbf{V} \in \mathbb{R}^{DxD}$ be a matrix whose columns $\mathbf{v}_d$ are D 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 $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_D$.

Eigendecomposition of a Symmetric Matrix

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

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

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Representation of a Vector in the Eigen Basis

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

$$\mathbf{a} = \sum_{d=1}^{D} \alpha_d \mathbf{v}_d \quad (1)$$

$$\alpha_d = \mathbf{a}^T \mathbf{v}_d \quad (2)$$

Geometry

- If $\mathbf{A}$ is a real symmetric matrix with positive eigenvalues, then the quadratic equation $\mathbf{x}^T\mathbf{A}\mathbf{x} = 0$ defines an ellipsoid in a D-dimensional space, which provides a different way of thinking about these operations:

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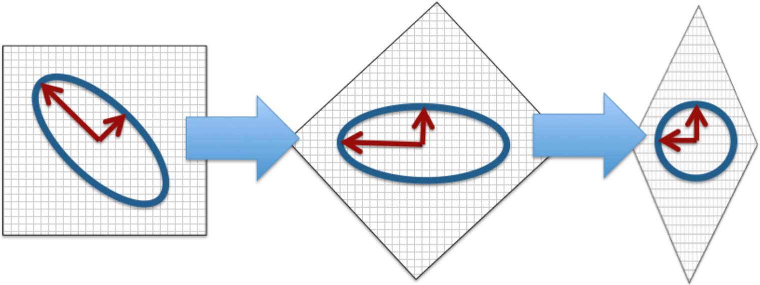

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Principal Component Analysis

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

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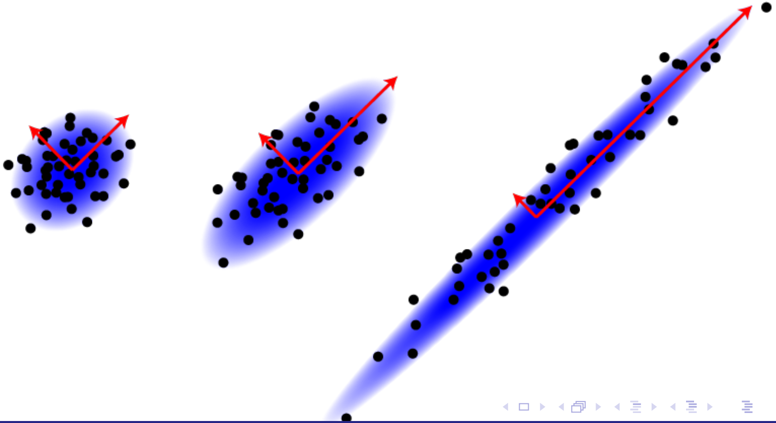

Sample Variance in a Given Direction

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- Let $\mathbf{w} \in \mathbb{R}^D$ 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:

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

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

The Direction of Maximum Variance

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

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- The constraint that $||\mathbf{w}||_2 = 1$ becomes $\sqrt{\sum_{d=1}^{D} \omega_d^2} = 1$.
- This means $\sum_{d=1}^{D} \omega_d^2 = 1$ 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 $\mathbf{w} = \sum_{d=1}^{D} \omega_d \mathbf{V}_d = \mathbf{V}_1$.
- **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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- Suppose instead of just the direction of maximum variance, we want the K largest directions of variance that are all mutually orthogonal.
- Finding the second-largest direction of variance corresponds to solving the problem:

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- It's easy to see that this is going to be the eigenvector corresponding to the second largest eigenvalue.
- **In general, the top K directions of variance $\mathbf{w}_1, \ldots, \mathbf{w}_K$ are given by the K eigenvectors corresponding to the K largest eigenvalues of $\mathbf{X}^T\mathbf{X}$.**

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3. Stack the eigenvectors together into a $D \times K$ matrix $\mathbf{W}$ where each column k of $\mathbf{W}$ corresponds to $\mathbf{w}_k$.
4. Project the matrix $\mathbf{X}$ into the rank-K 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 the rank-K SVD of **X**:

$$\arg\min_{\mathbf{U},\mathbf{S},\mathbf{V}} ||\mathbf{X} - \mathbf{U}\mathbf{S}\mathbf{V}^T||_F$$

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

Connection to SVD

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

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- According to PCA, the projection operation is $\mathbf{Z} = \mathbf{XW}$.
- Using $\mathbf{X} = \mathbf{USV}^T$ and $\mathbf{V} = \mathbf{W}$ we have:

$$\mathbf{Z} = \mathbf{XW} = (\mathbf{USV}^T)(\mathbf{V}) = \mathbf{US}$$

- Finally, note that if the decompositions are based only on the K leading basis vectors, which are identical under both PCA and SVD, the projections $\mathbf{Z} = \mathbf{XW}$ and $\mathbf{Z} = \mathbf{US}$ 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.

Issues

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- If $K << D$, then PCA can also be computed iteratively, as can SVD.
- The basic SVD and PCA algorithms are not suitable for large-scale data. Instead, randomized algorithms are often used.
- The value of K can sometimes be chosen based on looking for eigenvalue gaps in the eigenspectrum of the covariance matrix. Otherwise, a supervised end/side-task is needed or a criteria like AIC/BIC must be applied.