Principal Component Analysis: The Algorithm & Important Properties



Objective



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Implement the PCA algorithm



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Discuss some important properties of PCA

Principal Components

We found e₁, which gives the direction of the largest variance after projection

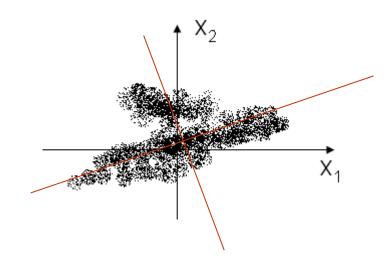
→ The first principal component.

The process can be continued in the subspace orthogonal to e_1 , and so on and so forth.

 \rightarrow Obtaining other principal components: \mathbf{e}_2 , \mathbf{e}_3 , etc., corresponding to other eigenvectors of C, ordered by the corresponding eigenvalues λ_i

Principal Components (cont'd)

The principal components are orthogonal to each other $\rightarrow \{e_i\}$ forms an orthonormal basis in the *d*-dimensional space.



The total variance is given by the sum of the variances of the projections.

$$\sigma^2 = \sum_{j=1}^d \lambda_j$$

How Many Principal Components to Keep?

To reduce dimensions, we will need to keep only $d' \ll d$ projections.

We can measure how much of the total variance a *d'*-dimensional subspace captures, by the ratio

$$\sum_{j=1}^{d'} \lambda_j / \sum_{j=1}^{d} \lambda_j$$

- Variance may be related to the "energy" of a signal: how accurately we want to represent the data.
- → The ratio can be used to guide in choosing a proper d' for desired accuracy.

The PCA Algorithm

- 1. Compute the *dxd* sample covariance matrix *C*
- 2. Find the eigenvalues and corresponding eigenvectors of *C*
- 3. Project the original data onto the space spanned by the eigenvectors
 - The projection may be done onto a d'-dimensional subspace spanned by the first d' eigenvectors (ordered by the eigenvalue in descending order)
 - d'is determined by the desired accuracy

Important Properties of PCA

- PCA represents the data in a new space, in which the components of the data is ordered by their "significance".
 - → Dimension reduction can be done by simply discarding less significant dimensions.
- Linearity assumption → extensions exist
- "Variance ≈ Importance" is meaningful only under large signal-to-noise ratio

PCA as Feature Mapping

When we use only d dimensions from PCA (with original dimension d > d), this may look like feature section.

But in general they are different approaches.

PCA

- Unsupervised (in general)
- Generates new features (linear combination of original ones)

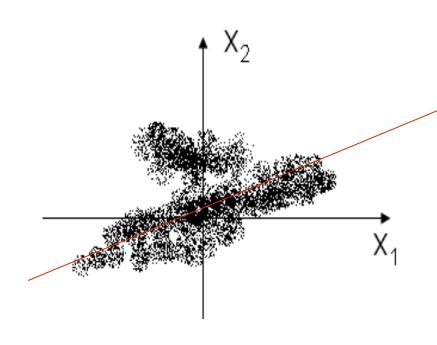
Feature Selection

- -Supervised (in general)
- Selects a few original features (e.g., for better classification)

Can PCA help classification?

Can we do better classification in a lower-dimensional space from *d'* principal components given by PCA?

→ Not necessarily.



LDA may be better posed for such a task.