MATH 637: Mathematical Techniques in Data Science
Principal component analysis

Dominique Guillot

Departments of Mathematical Sciences
University of Delaware

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Motivation

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- Most of the "action" may occur in a subspace of $\mathbb{R}^p$.

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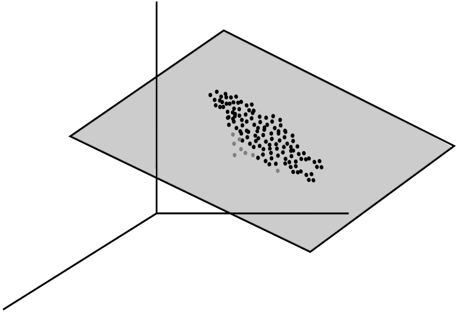

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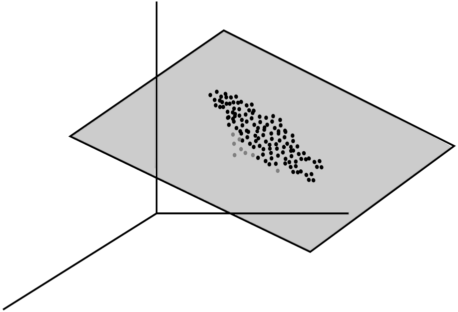

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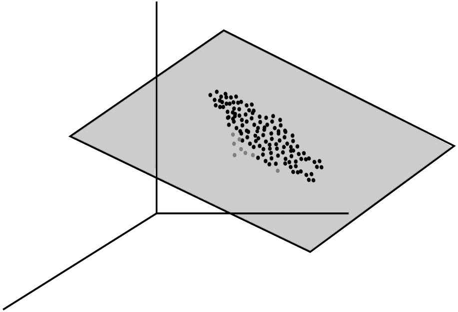

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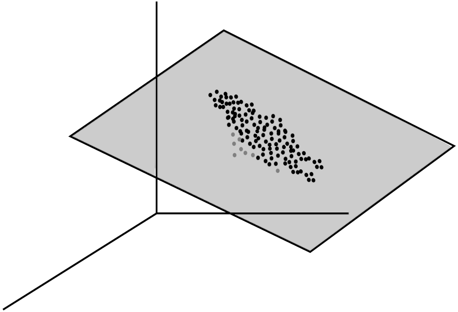

Problem: How can we discover low dimensional structures in data?

- Principal components analysis: construct projections of the data that capture most of the *variability* in the data.
- Provides a low-rank approximation to the data.
- Can lead to a significant dimensionality reduction.

Principal component analysis (PCA)

- Let $X \in \mathbb{R}^{n \times p}$ with rows $x_1, \ldots, x_n \in \mathbb{R}^p$. We think of X as n observations of a random vector $(X_1, \ldots, X_p) \in \mathbb{R}^p$.

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We solve:

$$w^* = \underset{\|w\|_2 = 1}{\operatorname{argmax}} \sum_{i=1}^n (x_i^T w)^2.$$

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Claim: w is an eigenvector associated to the largest eigenvalue of $X^T X$.

Proof of claim: Rayleigh quotients

Let $A \in \mathbb{R}^{p\times p}$ be a symmetric (or Hermitian) matrix. The *Rayleigh quotient* is defined by

$$R(A, x) = \frac{x^T A x}{x^T x} = \frac{\langle Ax, x\rangle}{\langle x, x\rangle}, \qquad (x \in \mathbb{R}^p, x \neq \mathbf{0}_{p\times 1}).$$

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Observations:

1. If $Ax = \lambda x$ with $\|x\|_2 = 1$, then $R(A,x) = \lambda$. Thus,

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It follows that
$$\sup_{x\neq \mathbf{0}} R(A,x) \leq \lambda_{\max}(A).$$

Thus, $\sup_{x\neq \mathbf{0}} R(A,x) = \sup_{\|x\|_2=1} x^T Ax = \lambda_{\max}(A)$.

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Previous argument shows that

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Second principal component: We look for a new linear combination of the X_i's that

1. Is orthogonal to the first principal component, and
2. Maximizes the variance.

Back to PCA (cont.)

In other words:

$$w^{(2)} := \underset{\substack{\|w\|_2=1 \\ w \perp w^{(1)}}}{\operatorname{argmax}} \sum_{i=1}^{n} (x_i^T w)^2 = \underset{\substack{\|w\|_2=1 \\ w \perp w^{(1)}}}{\operatorname{argmax}} w^T X^T X w.$$

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- Using a similar argument as before with Rayleigh quotients, we conclude that $w^{(2)}$ is an eigenvector associated to the second largest eigenvalue of $X^T X$.
- Similarly, given $w^{(1)}, \ldots, w^{(k)}$, we define

$$w^{(k+1)} := \underset{\substack{\|w\|_2=1 \\ w\perp w^{(1)},w^{(2)},\ldots,w^{(k)}}}{\operatorname{argmax}} \sum_{i=1}^{n} (x_i^T w)^2 = \underset{\substack{\|w\|_2=1 \\ w\perp w^{(1)},w^{(2)},\ldots,w^{(k)}}}{\operatorname{argmax}} w^T X^T X w.$$

As before, the vector $w^{(k+1)}$ is an eigenvector associated to the $(k+1)$-th largest eigenvalue of $X^T X$.

PCA: summary

In summary, suppose

$$X^T X = U \Lambda U^T$$

where $U \in \mathbb{R}^{p \times p}$ is an orthogonal matrix and $\Lambda \in \mathbb{R}^{p \times p}$ is diagonal. (Eigendecomposition of $X^T X$.)

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Conclusion: The variance of the i-th principal component is the i-th eigenvalue of $X^T X$.

- We say that the first k PCs *explain* $(\sum_{i=1}^k \Lambda_{ii}) / (\sum_{i=1}^p \Lambda_{ii}) \times 100$ percent of the variance.

Example: zip dataset

Recall the `zip` dataset:

1. 9298 images of digits $0 - 9$.
2. Each image is in black/white with $16 \times 16 = 256$ pixels.

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pc = PCA(n_components=10)
pc.fit(X_train)

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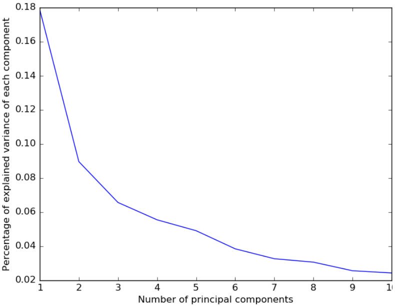

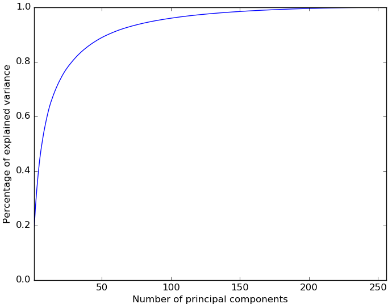

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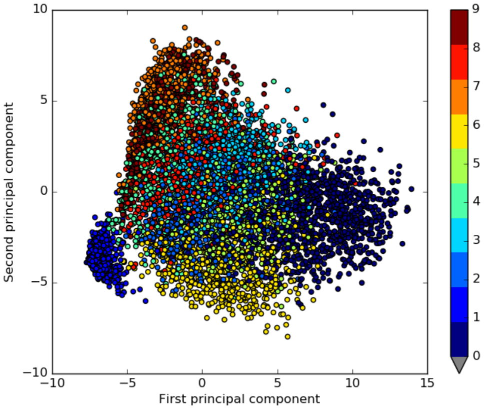

- Note: $\approx 27\%$ variance explained by the first two PCAs.
- $\approx 90\%$ variance explained by first 55 components.

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3. Compute $k \geq 1$ principal components:
$$W_k := (Xu_1, \dots, Xu_k) = XU_k,$$
where $U = (u_1, \dots, u_p)$, and $U_k = (u_1, \dots, u_k) \in \mathbb{R}^{p \times k}$.

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Note: k is a parameter that needs to be chosen (using CV or another method). Typically, one picks k to be significantly smaller than p.

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- Can maximize/minimize the kurtosis to find subspaces where data looks Gaussian/non-Gaussian (e.g. to detect outliers).