MATH 567: Mathematical Techniques in Data Science
Principal component analysis

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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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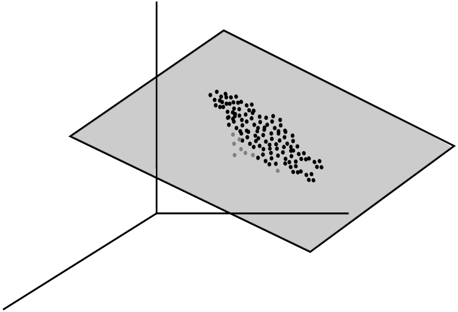

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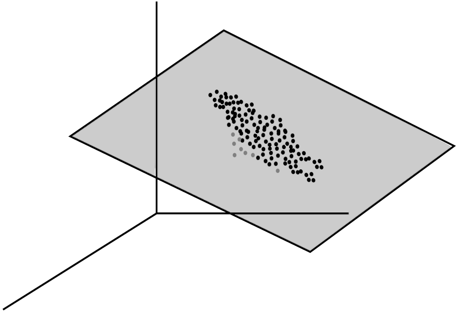

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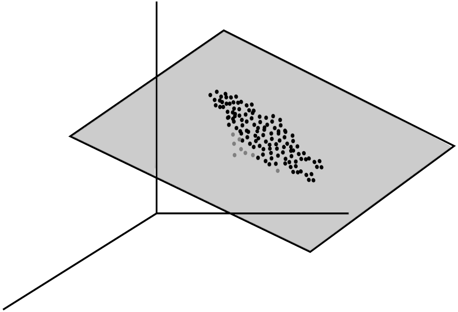

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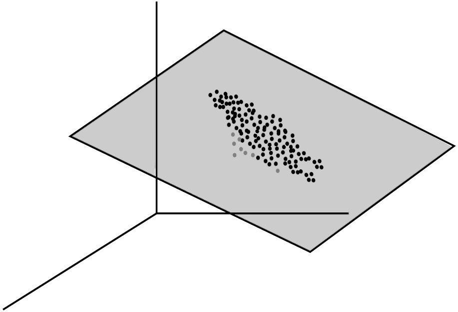

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- Principal components analysis: construct projections of the data that capture most of the *variability* in the data.
- Provides a low-rank approximation to the data.
- Can lead to a significant dimensionality reduction.

Principal component analysis (PCA)

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

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We solve:

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

(Note: $\sum_{i=1}^n (x_i^T w)^2$ is proportional to the sample variance of the data since we assume each column of X has mean 0.)

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Equivalently, we solve:

$$w = \underset{\|w\|_2=1}{\operatorname{argmax}} (Xw)^T (Xw) = \underset{\|w\|_2=1}{\operatorname{argmax}}\, w^T X^T X w$$

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

Back to PCA

Previous argument shows that

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

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- The linear combination $\sum_{i=1}^{p} w_i^{(1)} X_i$ is the *first principal component* of $(X_1, \ldots, X_p)$.
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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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- Write $U = (u_1, \ldots, u_p)$. Then the variance of the i-th principal component is

$$(Xu_i)^T (Xu_i) = u_i^T X^T X u_i = (U^T X^T X U)_{ii} = \Lambda_{ii}.$$

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

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

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^TX.)

- Recall that the columns of U are the eigenvectors of X^TX and the diagonal of Λ contains the eigenvalues of X^TX (i.e., the (square of the) singular values of X).
- Then the *principal components* of X are the columns of XU.
- Write $U = (u_1, \ldots, u_p)$. Then the variance of the i-th principal component is

$$(Xu_i)^T(Xu_i) = u_i^TX^TXu_i = (U^TX^TXU)_{ii} = \Lambda_{ii}.$$

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

- 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.

We use PCA to project the data onto a 2-dim subspace of $\mathbb{R}^{256}$.

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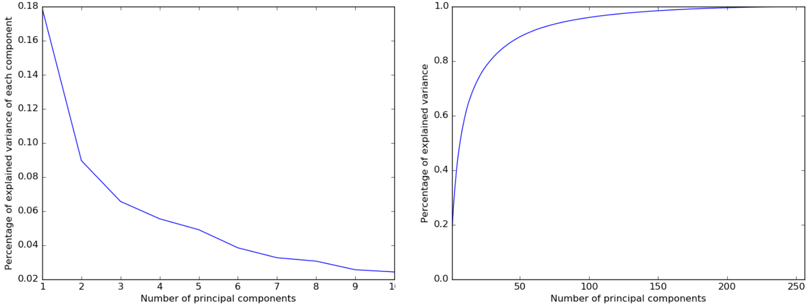

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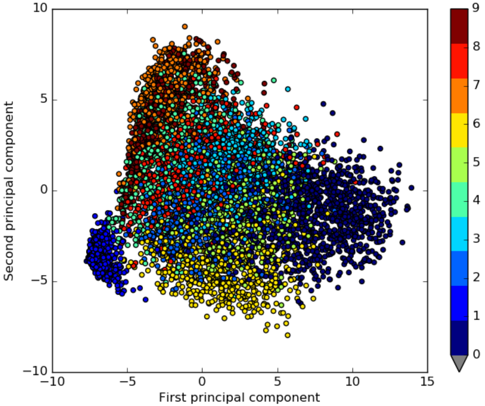

- Note: $\approx 27\%$ variance explained by the first two PCAs.
- $\approx 90\%$ variance explained by first 55 components.

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

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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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- Recall: The marginals of the multivariate Gaussian distribution are Gaussian.
- Can maximize/minimize the kurtosis to find subspaces where data looks Gaussian/non-Gaussian (e.g. to detect outliers).