Principal components analysis

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Scalar product reminer

- Here we will assume $\langle a, b \rangle = a^T b$
- $\|a\| = \sqrt{\langle a, a \rangle}$
- Signed projection of x on a is equal to $\langle x, a \rangle / \|a\|$
- Unsigned projection (length) of x onto a is equal to $|\langle x, a \rangle| / \|a\|$

Eigenvectors, eigenvalues

- If for some $A \in \mathbb{R}^{DxD}$ there exist scalar λ and D-dimensional vector v such that $Av = \lambda v$ then
  - v is called eigenvector of A
  - λ is called eigenvalue of A, corresponding to eigenvector v.
- $\exists v \neq 0 : \; Av = \lambda v \Leftrightarrow (A - \lambda I)\, v = 0 \Leftrightarrow det(A - \lambda I) = 0$. So all eigenvalues satisfy $det(A - \lambda I) = 0$ which
  - is a polynomial equation of order D
  - so has D solutions[1] (accounting for their multiplicity, possibly complex)

[1] According to Fundamental theorem of algebra.

Symmetric matrices

- Matrix $A \in \mathbb{R}^{DxD}$ is called *symmetric* if $A^T = A$.
- Properties:
  - All eigenvalues of symmetric matrix are real.
  - Eigenvectors, corresponding to different eigenvalues of symmetric matrix B are orthogonal to each other.
  - If $\tilde{\lambda}$ is a repeated root of $\det(A - \lambda I) = 0$ for some symmetric $A \in \mathbb{R}^{DxD}$ with multiplicity m then there exist m orthonormal eigenvectors of A, corresponding to $\tilde{\lambda}$.
  - For any symmetric matrix $A \in \mathbb{R}^{DxD}$ there exists orthonormal basis of eigenvectors of this matrix.

Vector derivatives

- Suppose $x = [x^1, ...x^D]$ and $f(x) = f(x^1, ...x^D)$. Vector derivative

$$\frac{\partial f(x)}{\partial x} := \begin{pmatrix} \frac{\partial f(x)}{\partial x^1} \\ \frac{\partial f(x)}{\partial x^2} \\ \cdots \\ \frac{\partial f(x)}{\partial x^D} \end{pmatrix}$$

- For any $x, b \in \mathbb{R}^D$ it holds that[2]:

$$\frac{\partial [b^T x]}{\partial x} = b$$

- For any $x \in \mathbb{R}^D$ and symmetric $B \in \mathbb{R}^{DxD}$ it holds that[3]:

$$\frac{\partial [x^T B x]}{\partial x} = 2Bx$$

[2] Prove it.

[3] Prove it. How will the formula change for non-symmetric B?

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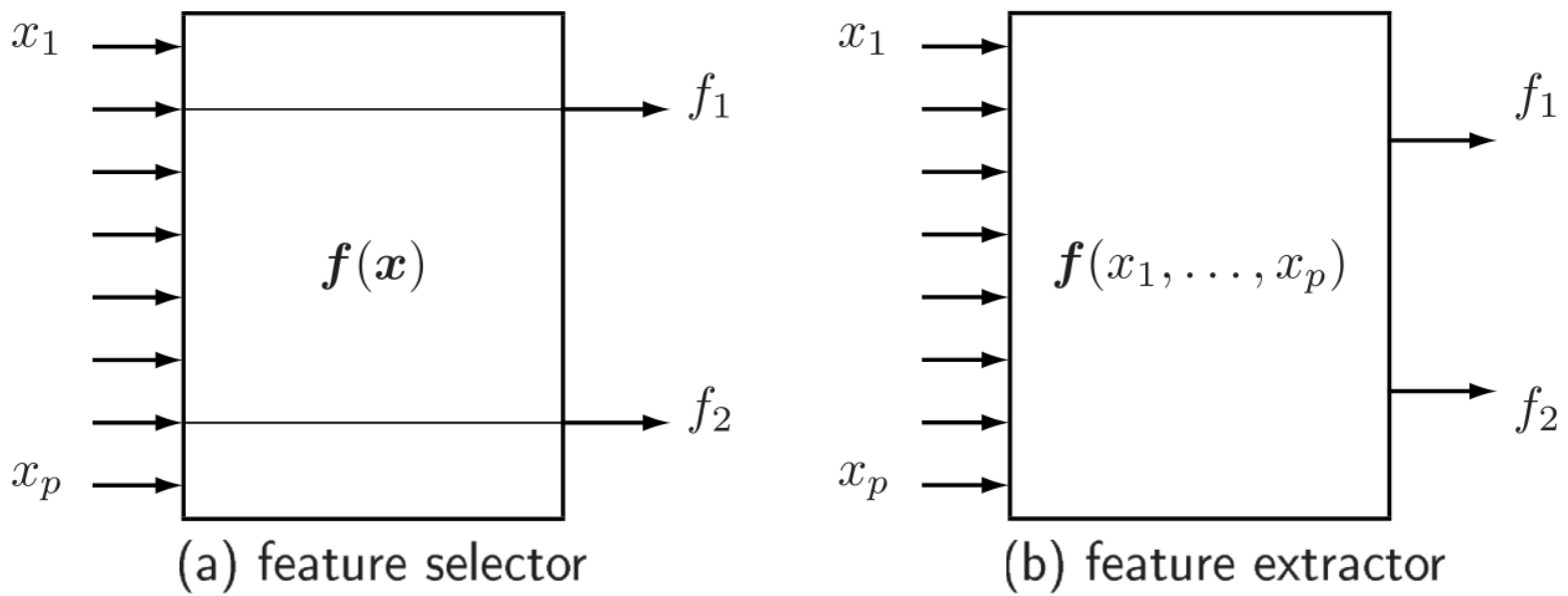
Dimensionality reduction

Feature selection / Feature extraction



Feature extraction: find transformation of original data which extracts most relevant information for machine learning task.

Applications of dimensionality reduction

Applications:

- visualization in 2D or 3D
- reduce operational costs on data storage, transfer and processing
  - memory
  - disk
  - CPU usage
- remove multi-collinearity to improve performance of some machine-learning models

Categorization of dimensionality reduction methods

Supervision:

- supervised
- unsupervied

Mapping to reduced space:

- linear
- non-linear

Principal components analysis - linear unsupervised method of dimensionality reduction.

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Projections, orthogonal complements

- For point x and subspace L denote:
  - p: the projection of x on L
  - h: orthogonal complement
  - $x = p + h$, $\langle p, h \rangle = 0$.
- For training set $x_1, x_2, ...x_N$ and subspace L find:
  - projections: $p_1, p_2, ...p_N$
  - orthogonal complements: $h_1, h_2, ...h_N$.

Best subspace fit[4]

Definition 1

Best-fit k-dimensional subspace for a set of points $x_1, x_2, ...x_N$ is a subspace, spanned by k vectors $v_1, v_2, ...v_k$, solving

$$\sum_{n=1}^{N} \|h_n\|^2 \to \min_{v_1, v_2, ...v_k}$$

Proposition 1

Vectors $v_1, v_2, ...v_k$, solving

$$\sum_{n=1}^{N} \|p_n\|^2 \to \max_{v_1, v_2, ...v_k}$$

also define best-fit k-dimensional subspace.

[4] Prove 1 using that $\|x\|^2 = \|p\|^2 + \|h\|^2$ for $x = p + h$ and $\langle p, h \rangle = 0$.

Definition of PCA

Definition 2

Principal components $a_1, a_2, ...a_k$ are vectors, forming orthonormal basis in the k-dimensional subspace of best fit.

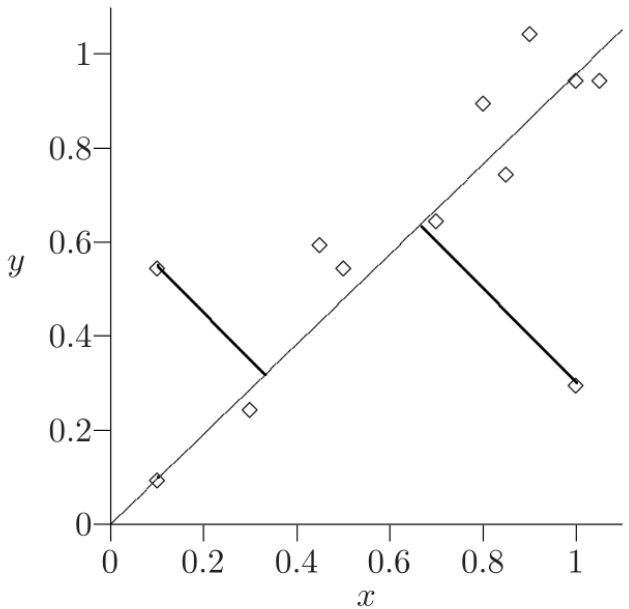
- Properties:
  - Not invariant to translation:
    - center data before PCA:

$$x \leftarrow x - \mu \text{ where } \mu = \frac{1}{N}\sum_{n=1}^{N} x_n$$

  - Not invariant to scaling:
    - scale features to have unit variance before PCA

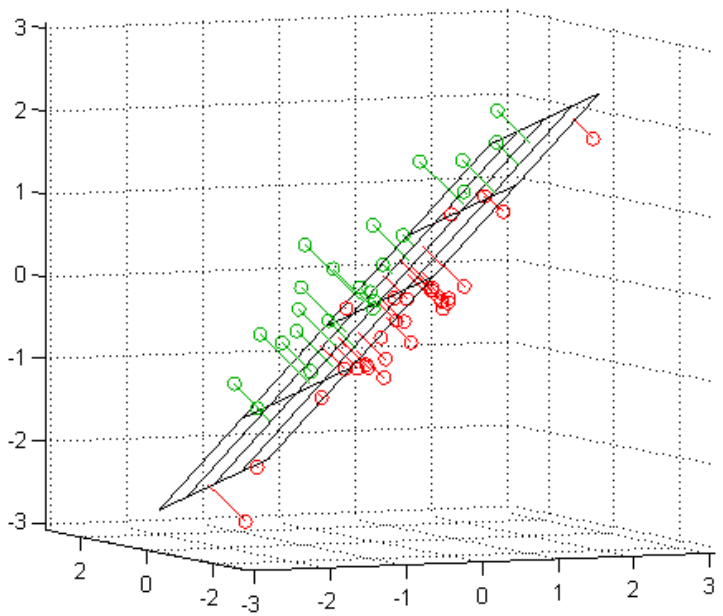
Example: line of best fit

- In PCA the sum of squared perpendicular distances to line is minimized:



- *What is the difference with least squares minimization in regression?*

Example: plane of best fit



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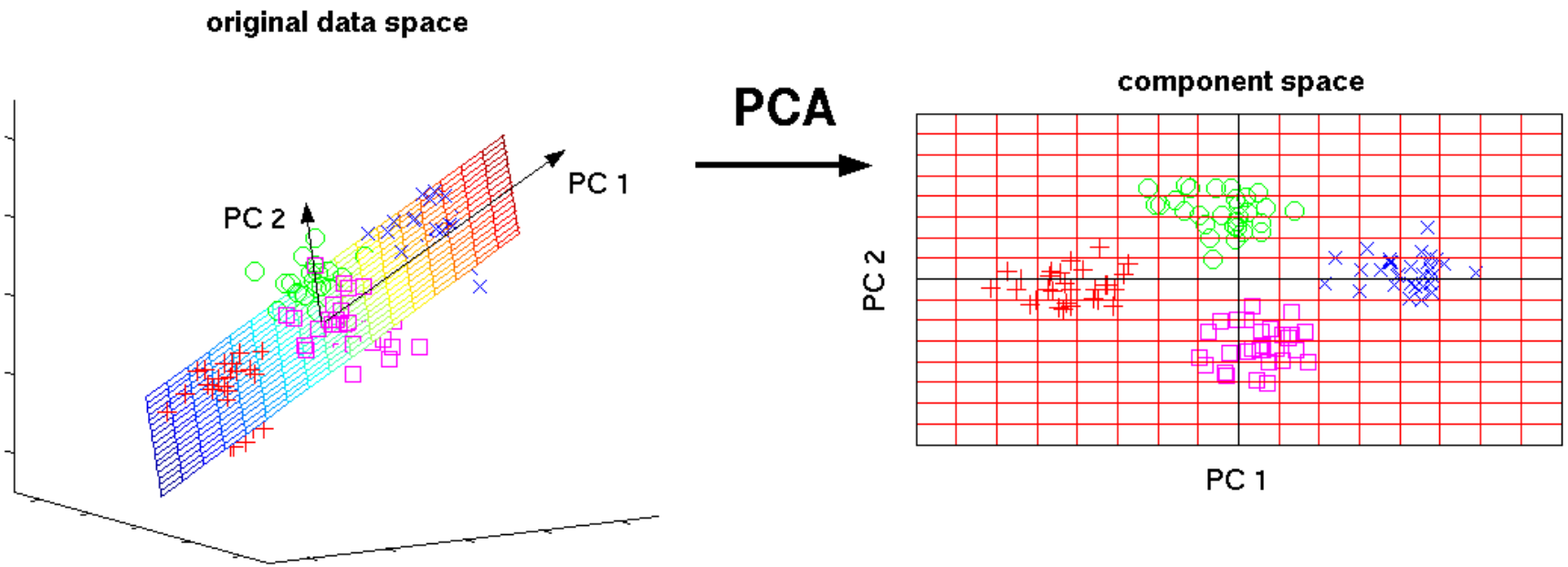
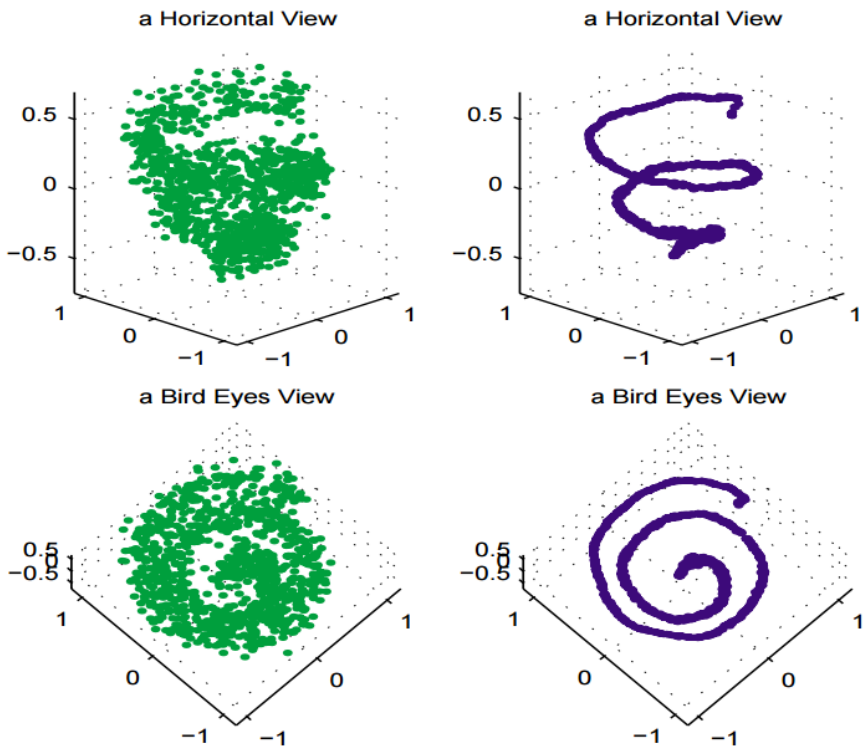
Visualization



Data filtering

Remove noise to get a cleaner picture of data distribution:



X. Huo and Jihong Chen (2002). Local linear projection (LLP). First IEEE Workshop on Genomic Signal Processing and Statistics (GENSIPS), Raleigh, NC, October. http://www.gensips.gatech.edu/proceedings/.

Economic description of data

Faces database:

Eigenvectors (called eigenfaces)

Projections on first several eigenvectors describe most of face variability.

Text analysis

- Objects=text files
- Binary, TF, TF-IDF representations have huge D.
  - math operations with X - inefficient
    - ML methods work longer
- Sparsity induces complications with query matching
  - consider query "automobile"
  - simple cosine-metric matching won't match documents with "car","bus",etc.

Latent semantic analysis (LSA)

Latent semantic analysis (LSA)

Get economical document representations with coordinates of most important PCA components found without centering.

Comments:

- usually 200-300 components are sufficient.
- Do *not* center X before computing PCA
  - otherwise will lose sparsity of X
  - $\mu \approx 0$ anyway, because most features are 0.
- Techically done with truncated SVD of X.

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Quality of approximation

Consider vector x. Since all D principal components form a full othonormal basis, x can be written as

$$x = \langle x, a_1 \rangle a_1 + \langle x, a_2 \rangle a_2 + ... + \langle x, a_D \rangle a_D$$

Let p^K be the projection of x onto subspace spanned by first K principal components:

$$p^K = \langle x, a_1 \rangle a_1 + \langle x, a_2 \rangle a_2 + ... + \langle x, a_K \rangle a_K$$

Error of this approximation is

$$h^K = x - p^K = \langle x, a_{K+1} \rangle a_{K+1} + ... + \langle x, a_D \rangle a_D$$

Quality of approximation

Using that $a_1, ...a_D$ is an orthonormal set of vectors, we get

$$\|x\|^2 = \langle x, x\rangle = \langle x, a_1\rangle^2 + ... + \langle x, a_D\rangle^2$$
$$\left\|p^K\right\|^2 = \langle p^K, p^K\rangle = \langle x, a_1\rangle^2 + ... + \langle x, a_K\rangle^2$$
$$\left\|h^K\right\|^2 = \langle h^K, h^K\rangle = \langle x, a_{K+1}\rangle^2 + ... + \langle x, a_D\rangle^2$$

We can measure how well first K components describe our dataset $x_1, x_2, ...x_N$ using relative loss

$$L(K) = \frac{\sum_{n=1}^N \left\|h_n^K\right\|^2}{\sum_{n=1}^N \|x_n\|^2} \tag{1}$$

or relative score

$$S(K) = \frac{\sum_{n=1}^N \left\|p_n^K\right\|^2}{\sum_{n=1}^N \|x_n\|^2} \tag{2}$$

Evidently $L(K) + S(K) = 1$.

Contribution of individual component

Contribution of a_k for explaining x is $\langle x, a_k \rangle^2$.
Contribution of a_k for explaining $x_1, x_2, ...x_N$ is:

$$\sum_{n=1}^{N} \langle x_n, a_k \rangle^2$$

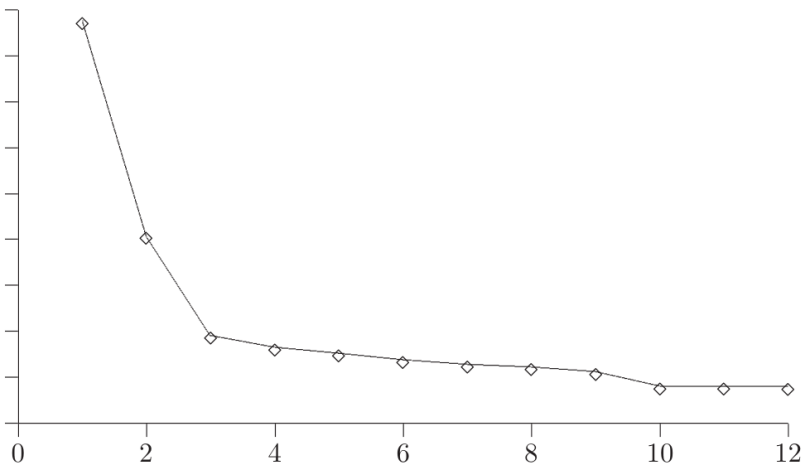
Explained variance ratio:

$$E(a_k) = \frac{\sum_{n=1}^{N} \langle x_n, a_k \rangle^2}{\sum_{d=1}^{D} \sum_{n=1}^{N} \langle x_n, a_d \rangle^2} = \frac{\sum_{n=1}^{N} \langle x_n, a_k \rangle^2}{\sum_{n=1}^{N} \|x_n\|^2}$$

- Explained variance ratio measures relative contribution of component a_k to explaining our dataset $x_1, ...x_N$.
- Note that $\sum_{k=1}^{K} E(a_k) = S(K)$.

How many principal components to select?

- Data visualization: 2 or 3 components.
- Take most significant components until their explained variance ratio falls sharply down:



- Or take minimum K such that $L(K) \leq t$ or $S(K) \geq 1 - t$, where typically $t = 0.95$.

PCA solution

- Center $x_1, ...x_N$ to have zero mean.
- Scale $x_1, ...x_N$ to have equal variance.
- Form $X = [x_1^T; ...x_N^T]^T \in \mathbb{R}^{NxD}$
- Estimate sample covariance matrix of x: $\widehat{\Sigma} = \frac{1}{N} X^T X$
- Find eigenvalues $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_D \geq 0$ and corresponding eignevectors $a_1, a_2, ...a_D$.
- $a_1, a_2, ...a_k$ are first k principal components, $k = 1, 2, ...D$.
- Sum of squared projections onto a_i is $\|Xa_i\|^2 = \lambda_i$.
- *Explained variance ratio* by component a_i is equal to

$$\frac{\lambda_i}{\sum_{d=1}^{D} \lambda_d}$$

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Constructive definition of PCA

- Principal components $a_1, a_2, ...a_D \in \mathbb{R}^D$ are found such that $\langle a_i, a_j \rangle = \begin{cases} 1, & i = j \\ 0 & i \neq j \end{cases}$
- Xa_i is a vector of projections of all objects onto the i-th principal component.
- For any object x its projections onto principal components are equal to:

$$p = A^T x = [\langle a_1, x \rangle, ...\langle a_D, x \rangle]^T$$

where $A = [a_1; a_2; ...a_D] \in \mathbb{R}^{D \times D}$.

Constructive definition of PCA

1. a_1 is selected to maximize $\|Xa_1\|$ subject to $\langle a_1, a_1 \rangle = 1$
2. a_2 is selected to maximize $\|Xa_2\|$ subject to $\langle a_2, a_2 \rangle = 1$, $\langle a_2, a_1 \rangle = 0$
3. a_3 is selected to maximize $\|Xa_3\|$ subject to $\langle a_3, a_3 \rangle = 1$, $\langle a_3, a_1 \rangle = \langle a_3, a_2 \rangle = 0$

   etc.

- It turns out that:
  - $a_1, ...a_k$ form k-dimensional subspace of best fit.
  - $a_1, a_2, ...$ are first, second,... eigenvectors of $X^T X$ (ordered by decreasing eigenvalue).

Derivation: 1st component

$$\begin{cases} \|Xa_1\|^2 \to \max_{a_k} \\ \|a_1\| = 1 \end{cases} \tag{3}$$

Lagrangian of optimization problem (3):

$$L(a_1, \mu) = a_1^T X^T X a_1 - \mu(a_1^T a_1 - 1) \to \text{extr}_{a_1, \mu}$$

$$\frac{\partial L}{\partial a_1} = 2X^T X a_1 - 2\mu a_1 = 0$$

so a_1 is selected from a set of eigenvectors of $X^T X$.

Derivation: 1st component

Since

$$\|Xa_1\|^2 = (Xa_1)^T Xa_1 = a_1^T X^T Xa_1 = \lambda a_1^T a_1 = \lambda$$

a_1 should be the eigenvector, corresponding to the largest eigenvalue λ_1.

Comment: If many many eigenvector directions corrsponding to λ_1 exist, select arbitrary eigenvector, satisfying constraint of (3).

Derivation: 2nd component

$$\begin{cases} \|Xa_2\|^2 \to \max_{a_2} \\ \|a_2\| = 1 \\ a_2^T a_1 = 0 \end{cases} \tag{4}$$

Lagrangian of optimization problem (4):

$$L(a_2, \mu) = a_2^T X^T X a_2 - \mu(a_2^T a_2 - 1) - \alpha a_1^T a_2 \to \text{extr}_{a_2,\mu,\alpha}$$

$$\frac{\partial L}{\partial a_2} = 2X^T X a_2 - 2\mu a_2 - \alpha a_1 = 0 \tag{5}$$

Derivation: 2nd component

By multiplying by a_1^T we obtain:

$$a_1^T \frac{\partial L}{\partial a_1} = 2a_1^T X^T X a_2 - 2\mu a_1^T a_2 - \alpha a_1^T a_1 = 0 \qquad (6)$$

Since a_2 is selected to be orthogonal to a_1:

$$2\mu a_1^T a_2 = 0$$

Since $a_1^T X^T X a_2$ is scalar and a_1 is eigenvector of $X^T X$:

$$a_1^T X^T X a_2 = \left(a_1^T X^T X a_2\right)^T = a_2^T X^T X a_1 = \lambda_1 a_2^T a_1 = 0$$

It follows that (6) simplifies to $\alpha a_1^T a_1 = \alpha = 0$ and (5) becomes

$$X^T X a_2 - \mu a_2 = 0$$

So a_2 is selected from a set of eigenvectors of $X^T X$.

Derivation: 2nd component

Since

$$\|Xa_2\|^2 = (Xa_2)^T Xa_2 = a_2^T X^T Xa_2 = \lambda a_2^T a_2 = \lambda$$

a_2 should be the eigenvector, corresponding to second largest eigenvalue λ_2.

Comment: If many many eigenvector directions corrsponding to λ_2 exist, select arbitrary eigenvector, satisfying constraints of (4).

Derivation: k-th component

$$\begin{cases} \|Xa_k\|^2 \to \max_{a_k} \\ \|a_k\| = 1 \\ a_k^T a_1 = ... = a_k^T a_{k-1} = 0 \end{cases} \tag{7}$$

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Componentwise optimization leads to best fit subspace

Theorem 1

Let L_k be the subspace spanned by $a_1, a_2, ...a_k$. Then for each k L_k is the best-fit k-dimensional subspace for X.

Proof: use induction. For $k = 1$ the statement is true by definition since projection maximization is equivalent to distance minimization.
Suppose theorem holds for $k-1$. Let L_k be the plane of best-fit of dimension with $\dim L = k$. We can always choose an orthonormal basis of L_k $b_1, b_2, ...b_k$ so that

$$\begin{cases} \|b_k\| = 1 \\ b_k \perp a_1, b_k \perp a_2, ...b_k \perp a_{k-1} \end{cases} \tag{8}$$

by setting b_k perpendicular to projections of $a_1, a_2, ...a_{k-1}$ on L_k.

Componentwise optimization leads to best fit subspace

Consider the sum of squared projections:

$$\|Xb_1\|^2 + \|Xb_2\|^2 + ... + \|Xb_{k-1}\|^2 + \|Xb_k\|^2$$

By induction proposition $L[a_1, a_2, ...a_{k-1}]$ is space of best fit of rank $k-1$ and $L[b_1, ...b_{k-1}]$ is some space of same rank, so sum of squared projections on it is smaller:

$$\|Xb_1\|^2+\|Xb_2\|^2+...+\|Xb_{k-1}\|^2 \leq \|Xa_1\|^2+\|Xa_2\|^2+...+\|Xa_{k-1}\|^2$$

and

$$\|Xb_k\|^2 \leq \|Xa_k\|^2$$

since b_k by (8) satisfies constraints of optimization problem (7) and a_k is its optimal solution.

Summary

- Every symmetric matrix A can be decomposed into rotation, scaling and backward rotation:

$$A = P\Lambda P^T$$

- Sample covariance matrix $\frac{1}{N}X^TX$ is symmetric and $\succcurlyeq 0$.
  - so it has non-negative eigenvalues $\lambda_1 \geq ... \geq \lambda_D \geq 0$ with corresponding eigenvectors $a_1, ...a_D$.
  - spread of distribution is characterized by eigenvalues.

Summary

- Dimensionality reduction - common preprocessing step for efficiency and numerical stability.
- Subspace of best fit of rank k for training set $x_1, ...x_N$ is k-dimensional subspace $\mathcal{L}(b_1, ...b_k)$, minimizing:

$$\|h_1\|^2 + ... + \|h_N\|^2 \to \min_{b_1,...b_k}$$

- Solution vectors are called top k principal components.
- Principal component analysis - expression of x in terms of first k principal components.
- It is unsupervised linear dimensionality reduction.
- Solution: principal components $a_1, ...a_k$ are top k eigenvectors of X^TX.