Dimensionality reduction

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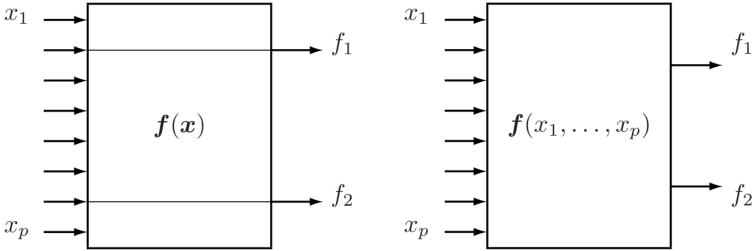
Dimensionality reduction

Feature selection / Feature extraction



(a) feature selector (b) feature extractor

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

We will consider unsupervised dimensionality reduction methods, which try to preserve geometrical properties of the data.

Applications of dimensionality reduction

Applications:

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

Categorization

Supervision in dimensionality reduction:

- supervised (such as Fisher's direction)
- unsupervied

Mapping to reduced space:

- linear
- non-linear

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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 $|\langle x, a\rangle| \,/\, \|a\|$

Useful properties

- For any matrix $X\in\mathbb{R}^{NxD}$ $X^TX\in\mathbb{R}^{DxD}$ is symmetric and positive semi-definite:
    - $\left(X^TX\right)^T=X^TX$ - symmetric matrix
    - $\forall a\in\mathbb{R}^D:\ \langle a,X^TXa\rangle=a^TX^TXa=\|Xa\|^2\geq 0$
- General properties:
    - if all eigenvalues are unique, eigenvectors are also unique (up to scalar multipliers).
    - if $A\succeq 0$ then all its eigenvalues are non-negative
- Since $X^TX\succeq 0$ it follows that all its eigenvalues are non-negative.
- We will assume that eigenvalues of X^TX are $\lambda_1\geq\lambda_2\geq ...\geq\lambda_D\geq 0$.

Useful properties

For any $x, b \in \mathbb{R}^D$ it holds that[1]:

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

For any $x \in \mathbb{R}^D$ and symmetric $B \in \mathbb{R}^{DxD}$ it holds that[2]:

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

[1] prove it
[2] prove it

Best hyperplane fit

- For point x and subspace L denote:
  - p-the projection of x on L
  - h-orthogonal complement
- $x = p + h$, $\langle p, h \rangle = 0$.

Proposition 1

For x, its projection p and orthogonal complement h

$$\|x\|^2 = \|p\|^2 + \|h\|^2 .$$

- Prove proposition 1.
- For training set $x_1, x_2, ... x_N$ and subspace L we can also find:
  - projections: $p_1, p_2, ... p_N$
  - orthogonal complements: $h_1, h_2, ... h_N$.

Best subspace fit

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 2

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.

- Prove 2 using proposition 1.

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.

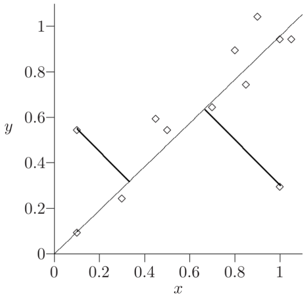
- Properties:
  - Not invariant to translation:
    - Before applying PCA, it is recommended to center objects:

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

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

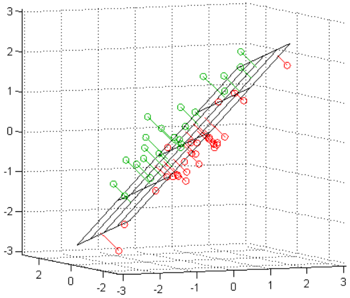
Example: line of best fit

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



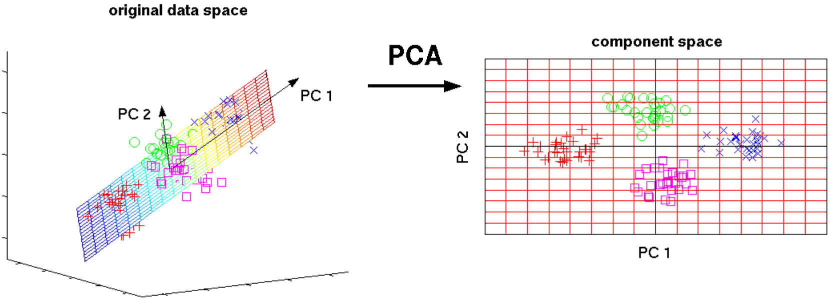
- *What is the difference with least squares minimization in regression?*

Best hyperplane fit



Subspace L_k or rank k best fits points $x_1, x_2, ...x_D$.

Visualization



Economic description of data

Faces database:

Eigenfaces

Eigenvectors are called eigenfaces. Projections on first several eigenfaces describe most of face variability.

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

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

or relative score

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

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:

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

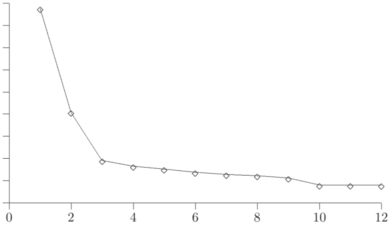
Explained variance ratio:

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

- 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 variance falls sharply down:



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

2 Principal component analysis

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

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.

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:

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

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

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

Lagrangian of optimization problem (7):

$$L(a_k, \mu) = a_k^T X^T X a_k - \mu(a_k^T a_k - 1) - \sum_{j=1}^{k-1} \alpha_j a_k^T a_j \to \text{extr}_{a_k, \mu, \alpha_1, \dots \alpha_{k-1}}$$

$$\frac{\partial L}{\partial a_k} = 2X^T X a_k - 2\mu a_k - \sum_{j=1}^{k-1} \alpha_j a_j = 0 \tag{8}$$

Derivation: k-th component

By multiplying by a_i^T for any $i = 1, 2, ...k-1$ we obtain:

$$a_i^T \frac{\partial L}{\partial a_1} = 2a_i^T X^T X a_k - 2\mu a_i^T a_k - \alpha_1 a_i^T a_1 - ... - \alpha_{k-1} a_i^T a_{k-1} = 0 \tag{9}$$

Since a_i and a_j are selected to be orthogonal for $i \neq j$, we have:

$$2\mu a_i^T a_k = 0, \quad \alpha_j a_i^T a_j = 0 \; \forall i \neq j$$

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

$$a_i^T X^T X a_2 = \left(a_i^T X^T X a_k\right)^T = a_k^T X^T X a_i = \lambda_i a_k^T a_i = 0$$

It follows that (9) simplifies to $\alpha_i a_i^T a_i = \alpha_i = 0$. Since i was selected arbitrary from $i = 1, 2, ...k-1$, $\alpha_1 = \alpha_2 = ... = \alpha_{k-1} = 0$ and (8) becomes

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

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

Derivation: k-th component

Since

$$\|Xa_k\|^2 = (Xa_k)^T Xa_k = a_k^T X^T Xa_k = \lambda a_k^T a_k = \lambda$$

a_k should be the eigenvector, corresponding to the k-th largest eigenvalue λ_k.

Comment: If many many eigenvector directions corrsponding to λ_k exist, select arbitrary eigenvector, satisfying constraints of (7).

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

$$\begin{cases} \|b_k\| = 1 \\ b_k \perp a_1, b_k \perp a_2, ... b_k \perp a_{k-1} \end{cases} \tag{10}$$

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 (10) satisfies constraints of optimization problem (7) and a_k is its optimal solution.

Conclusion

- For $x \in \mathbb{R}^D$ there exist D principal components.
- Principal component a_i is the i-th eigenvector of $X^T X$, corresponding to i-th largest eigenvalue λ_i.
- Sum of squared projections onto a_i is $\|Xa_i\|^2 = \lambda_i$.
- *Explained variance ratio* by component a_i is equal to

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