MATH 829: Introduction to Data Mining and Analysis
Principal component analysis

Dominique Guillot

Departments of Mathematical Sciences
University of Delaware

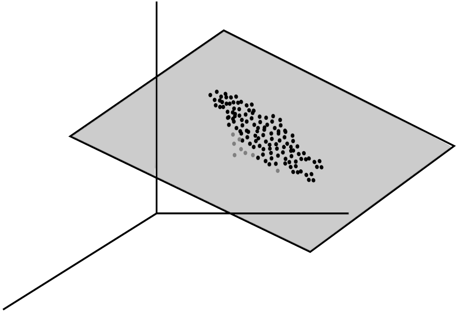
April 4, 2016

Motivation

- High-dimensional data often has a low-rank structure.
- Most of the “action” may occur in a subspace of $\mathbb{R}^p$.

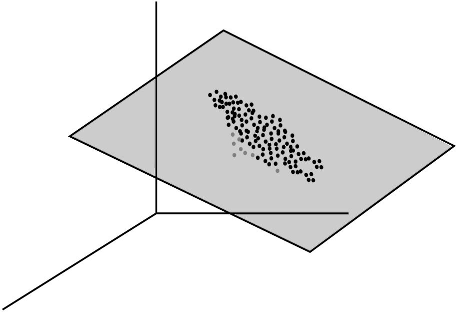
Motivation

- High-dimensional data often has a low-rank structure.
- Most of the “action” may occur in a subspace of $\mathbb{R}^p$.



Motivation

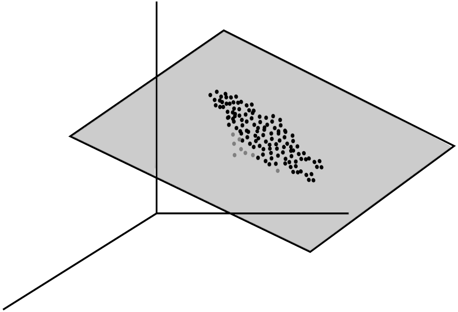
- High-dimensional data often has a low-rank structure.
- Most of the “action” may occur in a subspace of $\mathbb{R}^p$.



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

Motivation

- High-dimensional data often has a low-rank structure.
- Most of the "action" may occur in a subspace of $\mathbb{R}^p$.

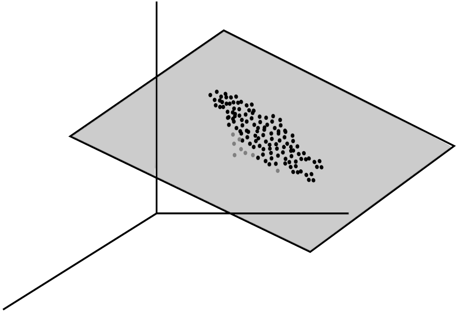


Problem: How can we discover low dimensional structures in data?

- Principal components analysis: construct projections of the data that capture most of the *variability* in the data.

Motivation

- High-dimensional data often has a low-rank structure.
- Most of the "action" may occur in a subspace of $\mathbb{R}^p$.



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 $(X_1, \ldots, X_p) \in \mathbb{R}^p$.

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 $(X_1, \dots, X_p) \in \mathbb{R}^p$.
- Suppose each column has mean 0, i.e., $\sum_{i=1}^n x_i = \mathbf{0}_{1\times p}$.

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 $(X_1, \ldots, X_p) \in \mathbb{R}^p$.
- Suppose each column has mean 0, i.e., $\sum_{i=1}^n x_i = \mathbf{0}_{1 \times p}$.
- We want to find a linear combination $w_1 X_1 + \cdots + w_p X_p$ with maximum variance. (Intuition: we look for a direction in $\mathbb{R}^p$ where the data varies the most.)

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 $(X_1, \dots, X_p) \in \mathbb{R}^p$.
- Suppose each column has mean 0, i.e., $\sum_{i=1}^n x_i = \mathbf{0}_{1 \times p}$.
- We want to find a linear combination $w_1 X_1 + \cdots + w_p X_p$ with maximum variance. (Intuition: we look for a direction in $\mathbb{R}^p$ where the data varies the most.)

We solve:

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

(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.)

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 $(X_1, \ldots, X_p) \in \mathbb{R}^p$.
- Suppose each column has mean 0, i.e., $\sum_{i=1}^n x_i = \mathbf{0}_{1\times p}$.
- We want to find a linear combination $w_1 X_1 + \cdots + w_p X_p$ with maximum variance. (Intuition: we look for a direction in $\mathbb{R}^p$ where the data varies the most.)

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.)

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

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

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

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

Observations:

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

$$\sup_{x \neq \mathbf{0}} R(A, x) \geq \lambda_{\max}(A).$$

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

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

Observations:

1. If $Ax = \lambda x$ with $\|x\|_2 = 1$, then $R(A,x) = \lambda$. Thus,
$$\sup_{x\neq \mathbf{0}} R(A,x) \geq \lambda_{\max}(A).$$

2. Let $\{\lambda_1, \dots, \lambda_p\}$ denote the eigenvalues of A, and let $\{v_1, \dots, v_p\} \subset \mathbb{R}^p$ be an orthonormal basis of eigenvectors of A. If $x = \sum_{i=1}^p \theta_i v_i$, then $R(A,x) = \frac{\sum_{i=1}^p \lambda_i \theta_i^2}{\sum_{i=1}^n \theta_i^2}$.

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

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

Observations:

1. If $Ax = \lambda x$ with $\|x\|_2 = 1$, then $R(A, x) = \lambda$. Thus,
$$\sup_{x \neq \mathbf{0}} R(A, x) \geq \lambda_{\max}(A).$$

2. Let $\{\lambda_1, \dots, \lambda_p\}$ denote the eigenvalues of A, and let $\{v_1, \dots, v_p\} \subset \mathbb{R}^p$ be an orthonormal basis of eigenvectors of A. If $x = \sum_{i=1}^p \theta_i v_i$, then $R(A, x) = \frac{\sum_{i=1}^p \lambda_i \theta_i^2}{\sum_{i=1}^n \theta_i^2}$.
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

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

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

Back to PCA

Previous argument shows that

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

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

First principal component:

- The linear combination $\sum_{i=1}^{p} w_i^{(1)} X_i$ is the *first principal component* of $(X_1, \dots, X_p)$.
- Alternatively, we say that $X w^{(1)}$ is the first (sample) principal component of X.

Back to PCA

Previous argument shows that

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

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

First principal component:

- The linear combination $\sum_{i=1}^{p} w_i^{(1)} X_i$ is the *first principal component* of $(X_1, \ldots, X_p)$.
- Alternatively, we say that $Xw^{(1)}$ is the first (sample) principal component of X.
- It is the linear combination of the columns of X having the "most variance".

Previous argument shows that

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

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

First principal component:

- The linear combination $\sum_{i=1}^p w_i^{(1)} X_i$ is the *first principal component* of $(X_1, \dots, X_p)$.
- Alternatively, we say that $X w^{(1)}$ is the first (sample) principal component of X.
- It is the linear combination of the columns of X having the "most variance".

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:

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

In other words:

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

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

Back to PCA (cont.)

In other words:

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

- 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 $w^{(1)}, \dots, w^{(k)}$, we define

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

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 $X^T X$.)

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 $X^T X$.)

- Recall that the columns of U are the eigenvectors of $X^T X$ and the diagonal of Λ contains the eigenvalues of $X^T X$ (i.e., the singular values of 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 $X^T X$.)

- Recall that the columns of U are the eigenvectors of $X^T X$ and the diagonal of Λ contains the eigenvalues of $X^T X$ (i.e., the singular values of X).
- Then the *principal components* of X are the columns of XU.

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 $X^T X$.)

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

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

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 $X^T X$.)

- Recall that the columns of U are the eigenvectors of $X^T X$ and the diagonal of Λ contains the eigenvalues of $X^T X$ (i.e., 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

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

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

- Recall that the columns of U are the eigenvectors of $X^T X$ and the diagonal of Λ contains the eigenvalues of $X^T X$ (i.e., 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

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

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.

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

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 $\mathbb{R}^{256}$.

```
from sklearn.decomposition import PCA
pc = PCA(n_components=10)
pc.fit(X_train)

print(pc.explained_variance_ratio_)
plt.plot(range(1,11), np.cumsum(pc.explained_variance_ratio_))
```

Example: zip dataset

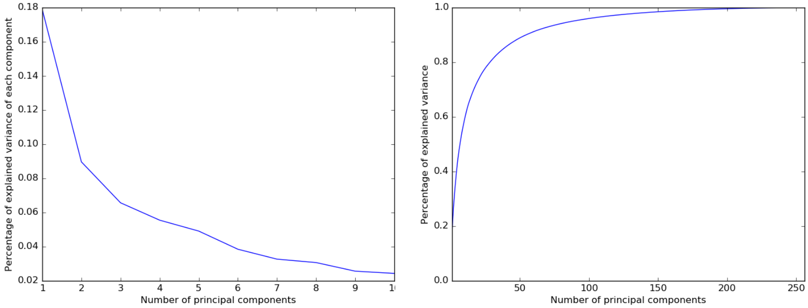
Recall the zip dataset:

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 $\mathbb{R}^{256}$.

```
from sklearn.decomposition import PCA
pc = PCA(n_components=10)
pc.fit(X_train)

print(pc.explained_variance_ratio_)
plt.plot(range(1,11), np.cumsum(pc.explained_variance_ratio_))
```



Example: zip dataset (cont.)

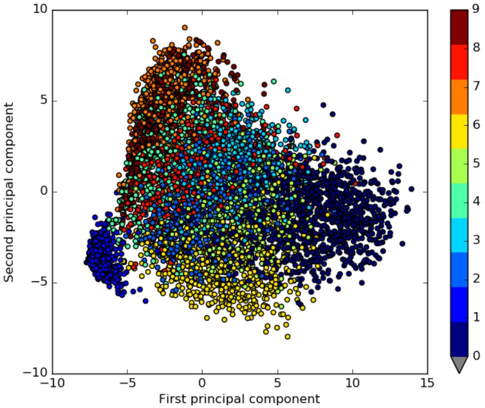
Projecting the data on the first two principal components:

```
Xt = pc.fit_transform(X_train).
```

Example: zip dataset (cont.)

Projecting the data on the first two principal components:

```
Xt = pc.fit_transform(X_train).
```



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

Principal component regression

- PCAs can be directly used in a regression context.

Principal component regression

- PCAs can be directly used in a regression context.

Principal component regression: $y \in \mathbb{R}^{n\times 1}$, $X \in \mathbb{R}^{n\times p}$.

1. Center y and each column of X (i.e., subtract mean from the columns)

Principal component regression

- PCAs can be directly used in a regression context.

Principal component regression: $y \in \mathbb{R}^{n\times 1}$, $X \in \mathbb{R}^{n\times p}$.

1. Center y and each column of X (i.e., subtract mean from the columns)
2. Compute the eigen-decomposition of $X^T X$:

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

Principal component regression

- PCAs can be directly used in a regression context.

Principal component regression: $y \in \mathbb{R}^{n\times 1}$, $X \in \mathbb{R}^{n\times p}$.

1. Center y and each column of X (i.e., subtract mean from the columns)
2. Compute the eigen-decomposition of $X^T X$:
$$X^T X = U \Lambda U^T.$$
3. Compute $k \geq 1$ principal components:
$$W_k := (Xu_1, \dots, Xu_k) = XU_k,$$
where $U = (u_1, \dots, u_p)$, and $U_k = (u_1, \dots, u_k) \in \mathbb{R}^{p\times k}$.

Principal component regression

- PCAs can be directly used in a regression context.

Principal component regression: $y \in \mathbb{R}^{n\times 1}$, $X \in \mathbb{R}^{n\times p}$.

1. Center y and each column of X (i.e., subtract mean from the columns)
2. Compute the eigen-decomposition of $X^T X$:
$$X^T X = U\Lambda U^T.$$
3. Compute $k \geq 1$ principal components:
$$W_k := (Xu_1, \ldots, Xu_k) = XU_k,$$
where $U = (u_1, \ldots, u_p)$, and $U_k = (u_1, \ldots, u_k) \in \mathbb{R}^{p\times k}$.
4. Regress y on the principal components:
$$\hat{\gamma}_k := (W_k^T W_k)^{-1} W_k^T y.$$

Principal component regression

- PCAs can be directly used in a regression context.

Principal component regression: $y \in \mathbb{R}^{n\times 1}$, $X \in \mathbb{R}^{n\times p}$.

1. Center y and each column of X (i.e., subtract mean from the columns)
2. Compute the eigen-decomposition of $X^T X$:
$$X^T X = U\Lambda U^T.$$
3. Compute $k \geq 1$ principal components:
$$W_k := (Xu_1, \dots, Xu_k) = XU_k,$$
where $U = (u_1, \dots, u_p)$, and $U_k = (u_1, \dots, u_k) \in \mathbb{R}^{p\times k}$.
4. Regress y on the principal components:
$$\hat{\gamma}_k := (W_k^T W_k)^{-1} W_k^T y.$$
5. The PCR estimator is:
$$\hat{\beta}_k := U_k \hat{\gamma}_k, \qquad \hat{y}^{(k)} := X\hat{\beta}_k = XU_k\hat{\beta}_k.$$

Principal component regression

- PCAs can be directly used in a regression context.

Principal component regression: $y \in \mathbb{R}^{n\times 1}$, $X \in \mathbb{R}^{n\times p}$.

1. Center y and each column of X (i.e., subtract mean from the columns)
2. Compute the eigen-decomposition of $X^T X$:
$$X^T X = U \Lambda U^T.$$
3. Compute $k \geq 1$ principal components:
$$W_k := (Xu_1, \ldots, Xu_k) = XU_k,$$
where $U = (u_1, \ldots, u_p)$, and $U_k = (u_1, \ldots, u_k) \in \mathbb{R}^{p\times k}$.
4. Regress y on the principal components:
$$\hat{\gamma}_k := (W_k^T W_k)^{-1} W_k^T y.$$
5. The PCR estimator is:
$$\hat{\beta}_k := U_k \hat{\gamma}_k, \qquad \hat{y}^{(k)} := X\hat{\beta}_k = XU_k\hat{\beta}_k.$$

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.

Projection pursuit

- PCA looks for subspaces with the most variance.

Projection pursuit

- PCA looks for subspaces with the most variance.
- Can also optimize other criteria.

Projection pursuit

- PCA looks for subspaces with the most variance.
- Can also optimize other criteria.

Projection pursuit (PP):

1. Set up a projection "index" to judge the merit of a particular one or two-dimensional projection of a given set of multivariate data.

Projection pursuit

- PCA looks for subspaces with the most variance.
- Can also optimize other criteria.

Projection pursuit (PP):

1. Set up a projection “index” to judge the merit of a particular one or two-dimensional projection of a given set of multivariate data.
2. Use an optimization algorithm to find the global and local extrema of that projection index over all 1/2-dimensional projections of the data.

Projection pursuit

- PCA looks for subspaces with the most variance.
- Can also optimize other criteria.

Projection pursuit (PP):

1. Set up a projection "index" to judge the merit of a particular one or two-dimensional projection of a given set of multivariate data.
2. Use an optimization algorithm to find the global and local extrema of that projection index over all 1/2-dimensional projections of the data.

Example:(Izenman, 2013) The absolute value of kurtosis, $|\kappa_4(Y)|$, of the one-dimensional projection $Y = w^T X$ has been widely used as a measure of non-Gaussianity of Y.

Projection pursuit

- PCA looks for subspaces with the most variance.
- Can also optimize other criteria.

Projection pursuit (PP):

1. Set up a projection "index" to judge the merit of a particular one or two-dimensional projection of a given set of multivariate data.
2. Use an optimization algorithm to find the global and local extrema of that projection index over all 1/2-dimensional projections of the data.

Example:(Izenman, 2013) The absolute value of kurtosis, $|\kappa_4(Y)|$, of the one-dimensional projection $Y = w^T X$ has been widely used as a measure of non-Gaussianity of Y.

- Recall: The marginals of the multivariate Gaussian distribution are Gaussian.

Projection pursuit

- PCA looks for subspaces with the most variance.
- Can also optimize other criteria.

Projection pursuit (PP):

1. Set up a projection "index" to judge the merit of a particular one or two-dimensional projection of a given set of multivariate data.
2. Use an optimization algorithm to find the global and local extrema of that projection index over all 1/2-dimensional projections of the data.

Example:(Izenman, 2013) The absolute value of kurtosis, $|\kappa_4(Y)|$, of the one-dimensional projection $Y = w^T X$ has been widely used as a measure of non-Gaussianity of Y.

- 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).