Principal Component Analysis

CSci 5525: Machine Learning

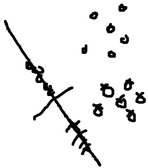
Instructor: Nicholas Johnson

November 19, 2020

Announcements

- Exam 2 posted on Monday (Nov 23) by 11:15 AM CST
  - Due Wednesday (Nov 25) at 11:15 AM CST (48 hours)
  - Covers lectures 11 (Deep Learning I) - 21 (PCA)
- No lecture next Tue (Nov 24), focus on exam 2
- No lecture/QA session/office hours next Thu (Nov 26, Thanksgiving break)
- Homework 4 posted on Dec 1 (due Dec 10)

The Main Idea

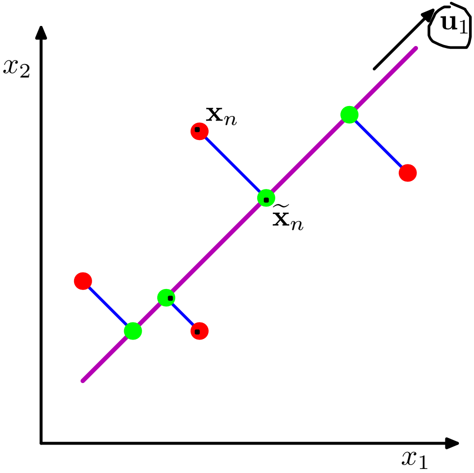


- Given a dataset $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$
- Find a low-dimensional linear projection
- Two possible formulations
  - The variance in low-d is maximized
  - The average projection objective is minimized
- Both are equivalent

Two viewpoints

$d=2$

$m=1$



$u_1^T x_n = c_n$

Maximum Variance Formulation

- Consider $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$
- With $\mathbf{x}_i \in \mathbb{R}^d$, goal is to get a projection in $\mathbb{R}^m$, $m < d$
- Consider $m = 1$, need a projection vector $\mathbf{u}_1 \in \mathbb{R}^d$
- Each datapoint $\mathbf{x}_i$ gets projected to $\mathbf{u}_1^\top \mathbf{x}_i$
- Mean of the projected data $\mathbf{u}_1^\top \bar{\mathbf{x}}$ where

$$\bar{\mathbf{x}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n$$

- Variance of the projected data

$$\frac{1}{N} \sum_{n=1}^{N} (\underbrace{\mathbf{u}_1^\top \mathbf{x}_n}_{\text{proj.}} - \underbrace{\mathbf{u}_1^\top \bar{\mathbf{x}}}_{\text{mean proj.}})^2 = \mathbf{u}_1^\top S \mathbf{u}_1$$

where

Covariance matrix →
$$S = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}_n - \bar{\mathbf{x}})(\mathbf{x}_n - \bar{\mathbf{x}})^\top$$

Maximum Variance Formulation (cont.)

- Maximize $\mathbf{u}_1^\top S \mathbf{u}_1$ w.r.t. $\mathbf{u}_1$
- Need to have a constraint to prevent $||\mathbf{u}_1|| \to \infty$
- Normalization constraint $||\mathbf{u}_1||^2 = 1$

$$u = \underset{||u_1||^2=1}{\operatorname{argmax}} \; u_1^T S u_1$$

- The Lagrangian for the problem

$$\mathbf{u}_1^\top S \mathbf{u}_1 + \lambda_1 (1 - \mathbf{u}_1^\top \mathbf{u}_1)$$

$$||u_1||^2 = u_1^T u_1 = 1$$

Lagrange multiplier

- First order necessary condition

$$u_1^T \quad u^T$$

$$S \mathbf{u}_1 = \lambda_1 \mathbf{u}_1$$

- $\mathbf{u}_1$ must be '<u>largest</u>' eigenvector of S since

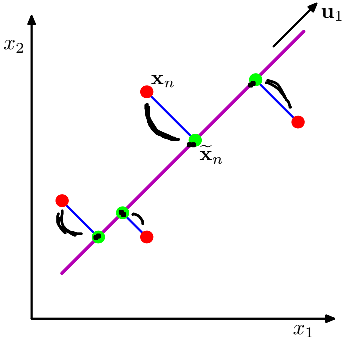
$$\mathbf{u}_1^\top S \mathbf{u}_1 = \lambda_1$$

- The eigenvector $\mathbf{u}_1$ is called a principal component

Maximum Variance Formulation (cont.)

- Subsequent principal components must be orthogonal to $\mathbf{u}_1$
- Maximize $\mathbf{u}_2^\top S\mathbf{u}_2$ s.t. $||\mathbf{u}_2||^2 = 1, \mathbf{u}_2 \perp \mathbf{u}_1$
- Turns out to be the second eigenvector, and so on
- The top-m eigenvectors give the 'best' m-dimensional projection

Minimum Error Formulation



- Idea: Pythagorean theorem
  - Maximize variance of green points
  - Minimize squared distance of blue lines
- Analysis: Next few slides

Minimum Error Formulation

- Consider a complete basis $\{\mathbf{u}_i\}$ in $\mathbb{R}^d$
- Each data point can be written as $\mathbf{x}_n = \sum_{i=1}^{d} \alpha_{ni}\mathbf{u}_i$
- Note that $\alpha_{ni} = \mathbf{x}_n^\top \mathbf{u}_i$ so that

$$\mathbf{x}_n = \sum_{i=1}^{d} (\mathbf{x}_n^\top \mathbf{u}_i)\mathbf{u}_i$$

- Our goal is to obtain a lower dimensional subspace $m < d$
- A generic representation of a low-d point

$$\text{proj. data} \longrightarrow \tilde{\mathbf{x}}_n = \underbrace{\sum_{i=1}^{m} z_{ni}\mathbf{u}_i}_{\text{low-d}} + \underbrace{\sum_{i=m+1}^{d} b_i\mathbf{u}_i}_{\text{high-d}}$$

- Coefficients z_{ni} depend on the data point $\mathbf{x}_n$
- Free to choose $z_{ni}, b_i, \mathbf{u}_i$ to get $\tilde{\mathbf{x}}_n$ close to $\mathbf{x}_n$

Minimum Error Formulation (cont.)

- The objective is to minimize

arg min J
z_{ni}, b_i, u_i

$$J = \frac{1}{N}\sum_{n=1}^{N} \|\mathbf{x}_n - \tilde{\mathbf{x}}_n\|^2$$

- Taking derivative w.r.t. z_{ni} we get $z_{ni} = \mathbf{x}_n^\top \mathbf{u}_i, i = 1, \ldots, m$
- Taking derivative w.r.t. b_i we get $b_i = \bar{\mathbf{x}}^\top \mathbf{u}_i, i = m+1, \ldots, d$
- Then we have

$$\mathbf{x}_n - \tilde{\mathbf{x}}_n = \sum_{i=m+1}^{d} \{(\mathbf{x}_n - \bar{\mathbf{x}})^\top \mathbf{u}_i\}\mathbf{u}_i$$

- Lies in the space orthogonal to the principal subspace
- The distortion measure to be minimized

covar.

$$J = \frac{1}{N}\sum_{n=1}^{N}\sum_{i=m+1}^{d} (\mathbf{x}_n^\top \mathbf{u}_i - \bar{\mathbf{x}}^\top \mathbf{u}_i)^2 = \sum_{i=m+1}^{d} \mathbf{u}_i^\top S \mathbf{u}_i$$

- Need orthonormality constraints on $\mathbf{u}_i$ to prevent $\mathbf{u}_i = 0$ solution

Minimum Error Formulation (cont.)

- Consider special case $d = 2, m = 1$
- The Lagrangian of the objective

$$L = \mathbf{u}_2^\top S \mathbf{u}_2 + \lambda_2(1 - \mathbf{u}_2^\top \mathbf{u}_2)$$

- First order condition is $S\mathbf{u}_2 = \lambda_2 \mathbf{u}_2$
- In general, the condition is $S\mathbf{u}_i = \lambda_i \mathbf{u}_i$
- Given by the eigenvectors corresponding to the smallest $(d - m)$ eigenvalues
- So the principal space $\mathbf{u}_i, i = 1, \ldots, m$ are the 'largest' eigenvectors

Kernel PCA

- In PCA, the principal components $\mathbf{u}_i$ are given by

$$S\mathbf{u}_i = \lambda_i \mathbf{u}_i$$

where

$$S = \frac{1}{N}\sum_{n=1}^{N} \mathbf{x}_n \mathbf{x}_n^\top$$

- Consider a feature mapping $\phi(\mathbf{x})$
- Want to implicitly perform PCA in the feature space
- Assume the features have zero mean $\sum_n \phi(\mathbf{x}_n) = 0$

Kernel PCA (cont.)

- The sample covariance matrix in the feature space

$$C = \frac{1}{N}\sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^\top$$

$S = \frac{1}{N}\sum_i x_i x_i^T$

- The eigenvectors are given by

$$C\mathbf{v}_i = \lambda_i \mathbf{v}_i$$

$S v_i = \lambda_i v_i$

- We want to avoid computing C explicitly
- Note that the eigenvectors satisfy

$$\frac{1}{N}\sum_{n=1}^{N} \phi(\mathbf{x}_n)\left\{\phi(\mathbf{x}_n)^\top \mathbf{v}_i\right\} = \lambda_i \mathbf{v}_i$$

c

- Since the inner product is a scaler, we have

$$\mathbf{v}_i = \sum_{n=1}^{N} a_{in}\phi(\mathbf{x}_n)$$

Kernel PCA (cont.)

- Substituting back into the eigenvalue equation

$\phi(x_l)^T$ $\phi(x_l)^T$

$$\frac{1}{N}\sum_{n=1}^{N}\phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^\top \underbrace{\sum_{m=1}^{N} a_{im}\phi(\mathbf{x}_m)}_{v_i} = \lambda_i \sum_{n=1}^{N} a_{in}\phi(\mathbf{x}_n)$$

- Multiplying both sides by $\phi(\mathbf{x}_l)^\top$ and using $K(\mathbf{x}_n,\mathbf{x}_m) = \phi(\mathbf{x}_n)^\top\phi(\mathbf{x}_m)$, we have

$k(x,x') = \phi(x)^T\phi(x')$

$$\frac{1}{N}\sum_{n=1}^{N}K(\mathbf{x}_l,\mathbf{x}_n)\sum_{m=1}^{N} a_{im}K(\mathbf{x}_n,\mathbf{x}_m) = \lambda_i \sum_{n=1}^{N} a_{in}K(\mathbf{x}_l,\mathbf{x}_n)$$

- In matrix notation, we have

$$K^2\mathbf{a}_i = \lambda_i N \cancel{K}\mathbf{a}_i$$

- Except for eigenvectors with 0 eigenvalues, we can solve

$$\longrightarrow \qquad K\mathbf{a}_i = \lambda_i N\mathbf{a}_i$$

Kernel PCA (cont.)

$\underset{\|v_i\|^2=1}{\operatorname{argmax}}\ v_i^\top S v_i$

- Since the original $\mathbf{v}_i$ are normalized, we have

$$1 = \mathbf{v}_i^\top \mathbf{v}_i = \mathbf{a}_i^\top K \mathbf{a}_i = \lambda_i N \mathbf{a}_i^\top \mathbf{a}_i$$

$\|v_i\|^2 = v_i^\top v_i = 1$

- Gives a normalization condition for $\mathbf{a}_i$
- Compute $\mathbf{a}_i$ by solving the eigenvalue decomposition

$$K\mathbf{a}_i = \lambda_i N \mathbf{a}_i$$

- The 'projection' of a point is given by

$$y_i(\mathbf{x}) = \phi(\mathbf{x})^\top \mathbf{v}_i = \sum_{n=1}^{N} a_{in}\phi(\mathbf{x})^\top \phi(\mathbf{x}_n) = \sum_{n=1}^{N} a_{in} K(\mathbf{x}, \mathbf{x}_n)$$

Illustration of Kernel PCA (Data Space)

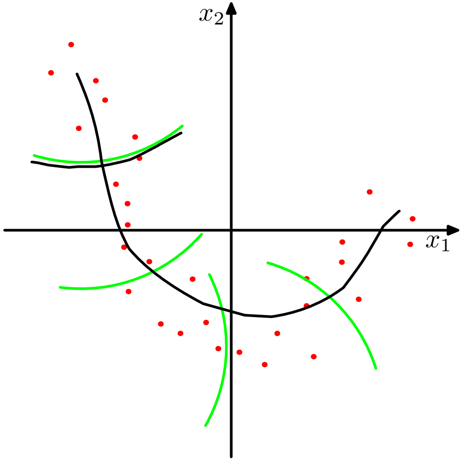
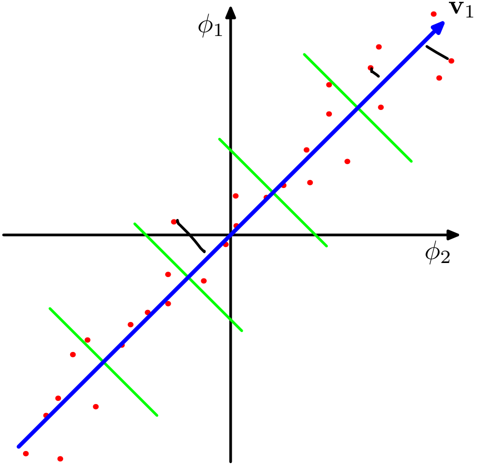


Illustration of Kernel PCA (Feature Space)



Dimensionality of Projection

- Original $\mathbf{x}_i \in \mathbb{R}^d$, feature $\phi(\mathbf{x}_i) \in \mathbb{R}^D$
- Possibly $D >> d$ so that the number of principal components can be greater than d
- However, the number of nonzero eigenvalues cannot exceed N
- The covariance matrix C has rank at most N, even if $D >> d$
- Kernel PCA involves eigenvalue decomposition of a $N \times N$ matrix

Kernel PCA: Non-zero Mean

- The features need not have zero mean
- Note that the features cannot be explicitly centered
- The centralized data would be of the form

$$\tilde{\phi}(\mathbf{x}_n) = \phi(\mathbf{x}_n) - \underbrace{\frac{1}{N}\sum_{l=1}^{N}\phi(\mathbf{x}_l)}_{\text{mean}}$$

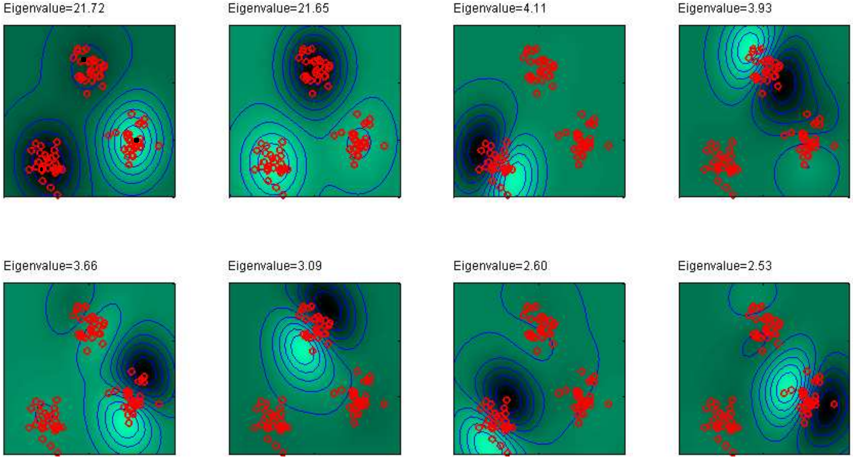
1_N = NxN matrix $\frac{1}{N}$

- The corresponding gram matrix

$$\longrightarrow \quad \tilde{K} = K - 1_N K - K 1_N + 1_N K 1_N$$

- Use $\tilde{K}$ in the basic kernel PCA formulation

Kernel PCA on Artificial Data



Kernel PCA Properties

- Computes eigenvalue decomposition of $N \times N$ matrix
  - Standard PCA computes it for $d \times d$
  - For large datasets $N >> d$, Kernel PCA is more expensive
- Standard PCA gives projection to a low dimensional principal subspace

$$\hat{\mathbf{x}}_n = \sum_{i=1}^{\ell} (\mathbf{x}_n^\top \mathbf{u}_i)\mathbf{u}_i$$

- Kernel PCA cannot do this
  - $\phi(\mathbf{x})$ forms a d-dimensional manifold in $\mathbb{R}^D$
  - PCA projection $\hat{\phi}$ of $\phi(\mathbf{x})$ need not be in the manifold
  - May not have a pre-image $\hat{\mathbf{x}}$ in the data space