Feature Learning

Finding the diamonds in the rough

High Dimensionality

Higher Dimensionality

More Data

Feature 1	Feature 2	Feature 3	Feature 4
Value 1, 1	Value 1, 2	Value 1, 3	Value 1, 4
Value 2, 1	Value 2, 2	Value 2, 3	Value 2, 4
Value 3, 1	Value 3, 2	Value 3, 3	Value 3, 4
Value 4, 1	Value 4, 2	Value 4, 3	Value 4, 4
Value 5, 1	Value 5, 2	Value 5, 3	Value 5, 4
Value 6, 1	Value 6, 2	Value 6, 3	Value 6, 4

Feature Extraction

$$\min_{\mathbf{U},\mathbf{V}} ||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2,$$
$$s.t.\ \mathbf{U}^T\mathbf{U} = \mathbf{I}.$$

where **X** is our $d \times n$ data matrix, **U** is a $d \times r$ matrix of the principal components, and **V** is an $n \times r$ matrix of the data in the new principal components' space.

PCA's Goals

- Minimize reconstruction error
- Maximize variance along each principal component

PCA Goal

$$\min_{\mathbf{U},\mathbf{V}} ||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2,$$
$$s.t.\ \mathbf{U}^T\mathbf{U} = \mathbf{I}.$$

$$\mathbf{U}\mathbf{V}^T \approx \mathbf{X}.$$

PCA Goal

$$\begin{aligned} \mathbf{U}\mathbf{V}^T &= \mathbf{X}, \\ \mathbf{U}^T\mathbf{U}\mathbf{V}^T &= \mathbf{U}^T\mathbf{X}, \\ \mathbf{V}^T &= \mathbf{U}^T\mathbf{X}. \end{aligned}$$

PCA Alternative Definition

$$\min_{\mathbf{W}} ||\mathbf{X} - \mathbf{W}\mathbf{W}^T\mathbf{X}||_F^2,$$
$$s.t.\ \mathbf{W}^T\mathbf{W} = \mathbf{I}.$$

Covariance

$$\mathbf{C} = \frac{\mathbf{X}^T\mathbf{X}}{n-1}.$$

Covariance Relationship to Frobenius

$$\mathbf{C} = \frac{\mathbf{X}^T\mathbf{X}}{n-1}.$$

$$||\mathbf{X}||_F^2 = \mathbf{tr}(\mathbf{X}^T\mathbf{X}).$$

$$\mathbf{C} \propto ||\mathbf{X}||_F^2.$$

PCA Objective Reformulation (1)

$$||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 = \mathbf{tr}((\mathbf{X} - \mathbf{U}\mathbf{V}^T)(\mathbf{X} - \mathbf{U}\mathbf{V}^T)^T),$$

Using $||\mathbf{A}||_F^2 = \mathbf{tr}(\mathbf{A}^T\mathbf{A})$.

PCA Objective Reformulation (2)

$$\begin{aligned}||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}((\mathbf{X} - \mathbf{U}\mathbf{V}^T)(\mathbf{X} - \mathbf{U}\mathbf{V}^T)^T), \\ &= \mathbf{tr}((\mathbf{X} - \mathbf{U}\mathbf{V}^T)(\mathbf{X}^T - (\mathbf{U}\mathbf{V}^T)^T))\end{aligned}$$

Using $(\mathbf{A} + \mathbf{B})^T = \mathbf{A}^T + \mathbf{B}^T$.

PCA Objective Reformulation (3)

$$\begin{aligned} ||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}((\mathbf{X} - \mathbf{U}\mathbf{V}^T)(\mathbf{X}^T - (\mathbf{U}\mathbf{V}^T)^T)) \\ &= \mathbf{tr}((\mathbf{X} - \mathbf{U}\mathbf{V}^T)(\mathbf{X}^T - \mathbf{V}\mathbf{U}^T)) \end{aligned}$$

Using $(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$.

PCA Objective Reformulation (4)

$$\begin{aligned}||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}((\mathbf{X} - \mathbf{U}\mathbf{V}^T)(\mathbf{X}^T - \mathbf{V}\mathbf{U}^T)) \\ &= \mathbf{tr}(\mathbf{X}\mathbf{X}^T - \mathbf{X}\mathbf{V}\mathbf{U}^T - \mathbf{U}\mathbf{V}^T\mathbf{X}^T + \mathbf{U}\mathbf{V}^T\mathbf{V}\mathbf{U}^T)\end{aligned}$$

Using $(a - b)(c - d) = ac - ad - bc + bd$.

PCA Objective Reformulation (5)

$$
\begin{aligned}
||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}(\mathbf{X}\mathbf{X}^T - \mathbf{X}\mathbf{V}\mathbf{U}^T - \mathbf{U}\mathbf{V}^T\mathbf{X}^T + \mathbf{U}\mathbf{V}^T\mathbf{V}\mathbf{U}^T) \\
&= \mathbf{tr}(-\mathbf{X}\mathbf{V}\mathbf{U}^T - \mathbf{U}\mathbf{V}^T\mathbf{X}^T + \mathbf{U}\mathbf{V}^T\mathbf{V}\mathbf{U}^T)
\end{aligned}
$$

Ignoring constants in objective function.

PCA Objective Reformulation (6)

$$
\begin{aligned}
||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}(-\mathbf{X}\mathbf{V}\mathbf{U}^T - \mathbf{U}\mathbf{V}^T\mathbf{X}^T + \mathbf{U}\mathbf{V}^T\mathbf{V}\mathbf{U}^T) \\
&= \mathbf{tr}(-\mathbf{X}\mathbf{X}^T\mathbf{U}\mathbf{U}^T - \mathbf{U}\mathbf{U}^T\mathbf{X}\mathbf{X}^T + \mathbf{U}\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}\mathbf{U}^T)
\end{aligned}
$$

Using $\mathbf{V}^T = \mathbf{U}^T\mathbf{X}, \mathbf{V} = \mathbf{X}^T\mathbf{U}$.

PCA Objective Reformulation (7)

$$
\begin{aligned}
||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}(-\mathbf{X}\mathbf{X}^T\mathbf{U}\mathbf{U}^T - \mathbf{U}\mathbf{U}^T\mathbf{X}\mathbf{X}^T + \mathbf{U}\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}\mathbf{U}^T) \\
&= \mathbf{tr}(-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U} - \mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U} + \mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}\mathbf{U}^T\mathbf{U})
\end{aligned}
$$

Using $\mathbf{tr}(\mathbf{AB}) = \mathbf{tr}(\mathbf{BA})$.

PCA Objective Reformulation (8)

$$\begin{aligned}||\mathbf{X}-\mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}(-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}+\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}\mathbf{U}^T\mathbf{U})\\ &= \mathbf{tr}(-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}+\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U})\end{aligned}$$

Using $\mathbf{U}^T\mathbf{U}=\mathbf{I}$.

PCA Objective Reformulation (9)

$$
\begin{aligned}
||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}(-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U} - \mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U} + \mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}) \\
&= \mathbf{tr}(-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U})
\end{aligned}
$$

Using summation.

PCA Objective Reformulation (10)

$$\begin{aligned} ||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= \mathbf{tr}(-\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}) \\ &= -\mathbf{tr}(\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}) \end{aligned}$$

Using $\mathbf{tr}(-\mathbf{A}) = -\mathbf{tr}(\mathbf{A})$.

PCA Objective Reformulation (11)

$$\begin{aligned} \|\mathbf{X} - \mathbf{U}\mathbf{V}^T\|_F^2 &= -\mathbf{tr}(\mathbf{U}^T\mathbf{X}\mathbf{X}^T\mathbf{U}) \\ &= -\mathbf{tr}(\mathbf{U}^T\mathbf{X}(\mathbf{U}^T\mathbf{X})^T) \end{aligned}$$

Using $(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$.

PCA Objective Reformulation (12)

$$
\begin{aligned}
||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2 &= -\mathbf{tr}(\mathbf{U}^T\mathbf{X}(\mathbf{U}^T\mathbf{X})^T) \\
&= -||\mathbf{U}^T\mathbf{X}||_F^2
\end{aligned}
$$

Using $||\mathbf{A}||_F^2 = \mathbf{tr}(\mathbf{A}^T\mathbf{A})$.

PCA Objective

$$
\begin{aligned}
&\min_{\mathbf{U},\mathbf{V}} \; ||\mathbf{X} - \mathbf{U}\mathbf{V}^T||_F^2, && s.t.\ \mathbf{U}^T\mathbf{U} = \mathbf{I}. \\
=&\min_{\mathbf{U}} \; -||\mathbf{U}^T\mathbf{X}||_F^2, && s.t.\ \mathbf{U}^T\mathbf{U} = \mathbf{I}. \\
=&\max_{\mathbf{U}} \; ||\mathbf{U}^T\mathbf{X}||_F^2, && s.t.\ \mathbf{U}^T\mathbf{U} = \mathbf{I}. \\
\approx&\max_{\mathbf{U}} \; cov(\mathbf{U}^T\mathbf{X}), && s.t.\ \mathbf{U}^T\mathbf{U} = \mathbf{I}.
\end{aligned}
$$

Singular Value Decomposition

$$\mathbf{X} = \mathbf{USV}^T,$$

where $\mathbf{X}$ is a $d \times n$ matrix, $\mathbf{U}$ is a unitary $d \times d$ matrix, $\mathbf{S}$ is a diagonal matrix of singular values, which are the square root of the respective eigenvalues, and $\mathbf{V}$ is a unitary $n \times n$ matrix.

Covariance Matrix SVD Representation

$$\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^T.$$

$$\begin{aligned}
\mathbf{C} &= \frac{\mathbf{X}^T\mathbf{X}}{n-1}, \\
&= \frac{\mathbf{V}\mathbf{S}\mathbf{U}^T\mathbf{U}\mathbf{S}\mathbf{V}^T}{n-1}, \\
&= \mathbf{V}\frac{\mathbf{S}^2}{n-1}\mathbf{V}^T.
\end{aligned}$$

Eigenvalue Decomposition

$$\mathbf{A} = \mathbf{Q}\Lambda\mathbf{Q}^T,$$

where $\mathbf{Q}$ is a matrix of eigenvector columns and Λ is a diagonal of the eigenvalues of $\mathbf{A}$.

Covariance Eigenvalue Decomposition

$$\mathbf{C} = \mathbf{V}\Lambda\mathbf{V}^T,$$

where $\mathbf{V}$ contains the eigenvector columns and Λ is the diagonal of eigenvalues of $\mathbf{C}$.

Singular Value, Eigenvalue Relationship

$$\frac{\mathbf{S}^2}{n-1} = \Lambda.$$

Solving PCA

We can calculate the principal components of a matrix by calculating the eigenvectors of its covariance matrix with the largest r eigenvalues,

$$\mathbf{U} = eig(\mathbf{C}, r). \tag{1}$$

Demo

Kernel PCA

Allows for non-linear transformations using the kernel trick.

$$\mathbf{C} = \phi(\mathbf{X})^T \phi(\mathbf{X}).$$

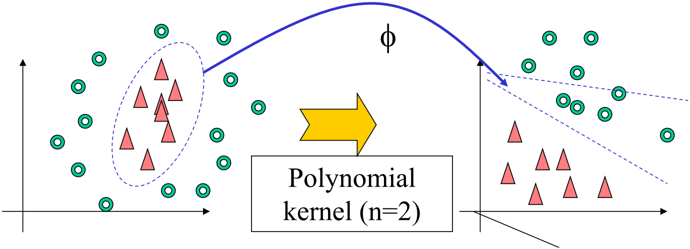
C is an $m \times m$ matrix.

Polynomial Kernel

$$\underbrace{K(\mathbf{x}_i, \mathbf{x_j})}_{\textit{Polynomial}} = (\mathbf{x}_i^T \mathbf{x}_j + 1)^d,$$

with degree d.

Polynomial Kernel

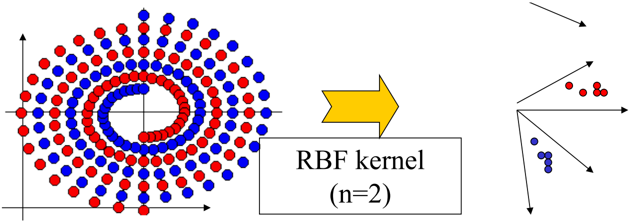


Radial Basis Function Kernel

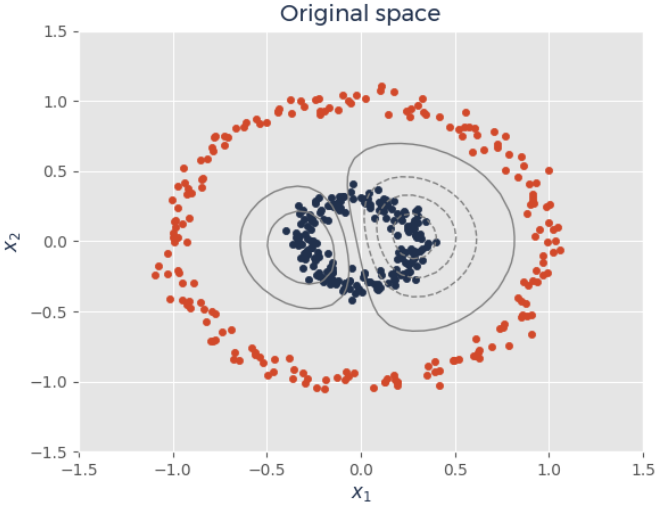
$$\underset{RBF}{K}(\mathbf{x}_i, \mathbf{x_j}) = \exp(\frac{-||\mathbf{x}_i - \mathbf{x}_j||^2}{2\sigma^2}),$$

with width σ.

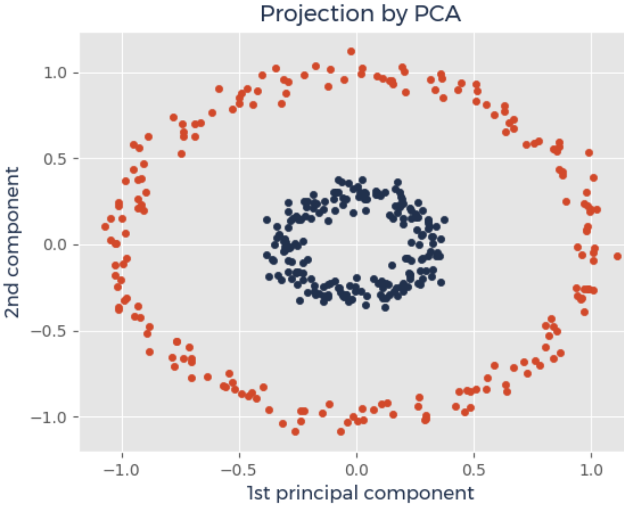
Radial Basis Function Kernel



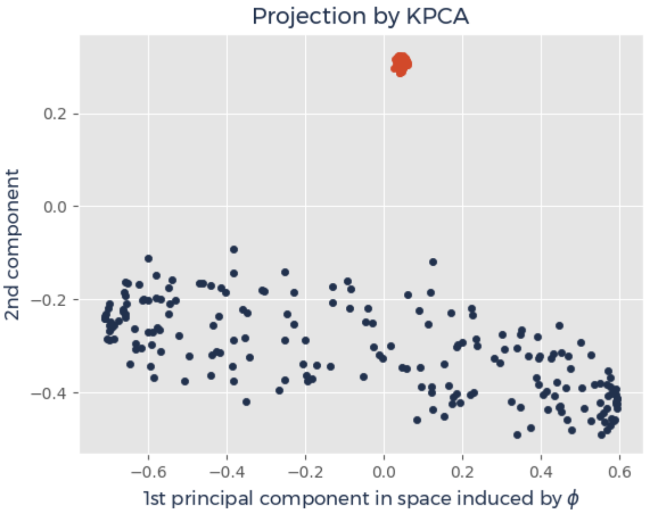
Kernel PCA Example



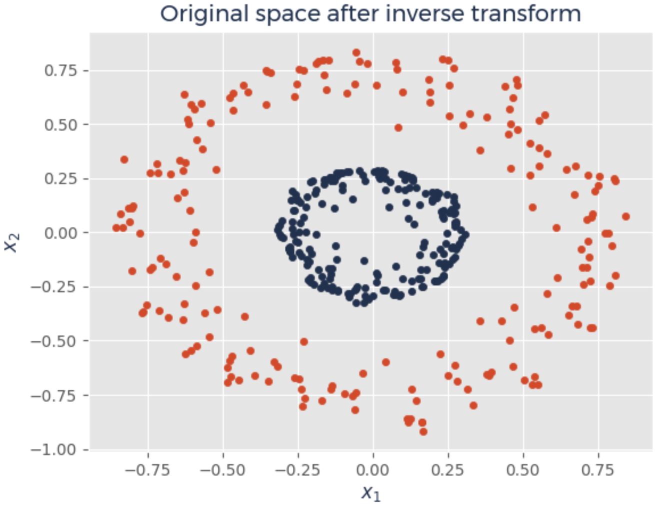
Kernel PCA Example



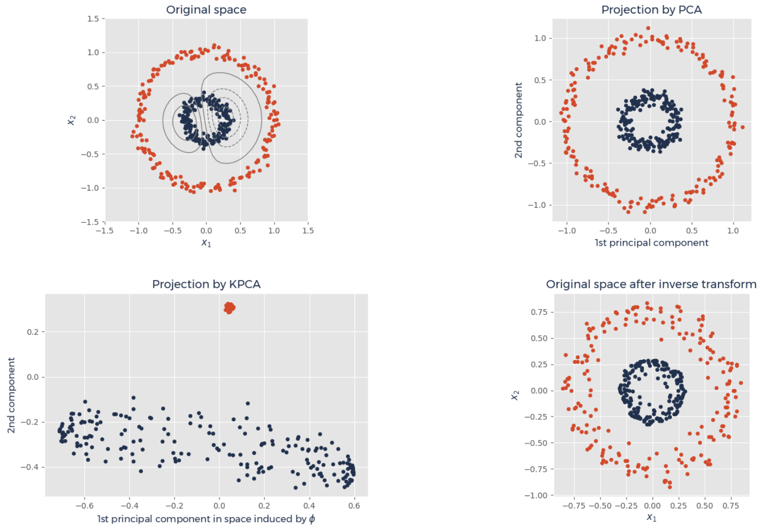
Kernel PCA Example



Kernel PCA Example



Kernel PCA Example



Questions

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