Dimensionality Reduction

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Learning Objectives

- Explain and Apply Principal Component Analysis (PCA)
- Explain Multidimensional Scaling (MDS)
- Apply Intel® Extension for Scikit-learn* to leverage underlying compute capabilities of hardware
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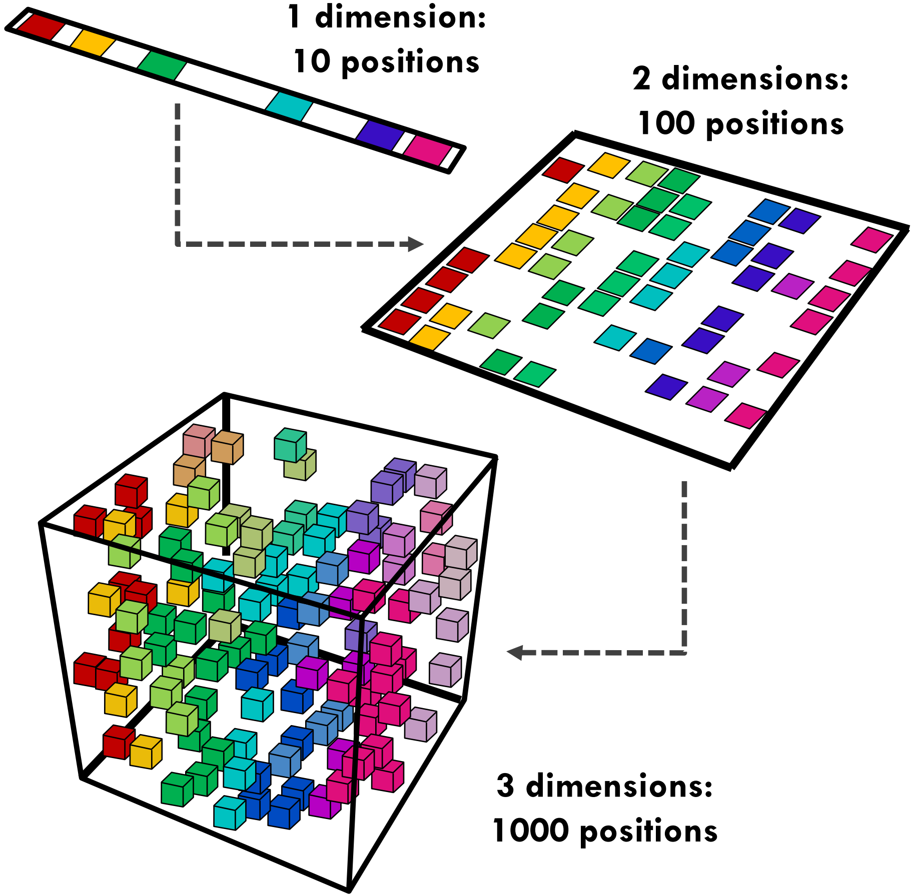
Curse of Dimensionality

- Theoretically, increasing features should improve performance



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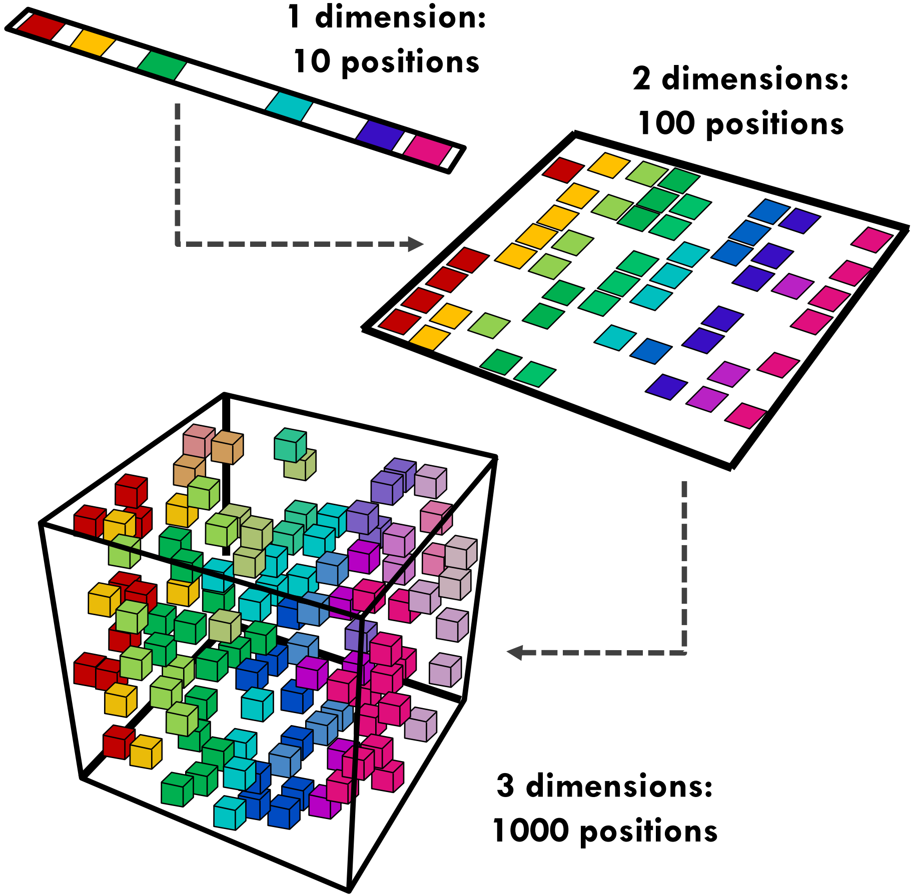
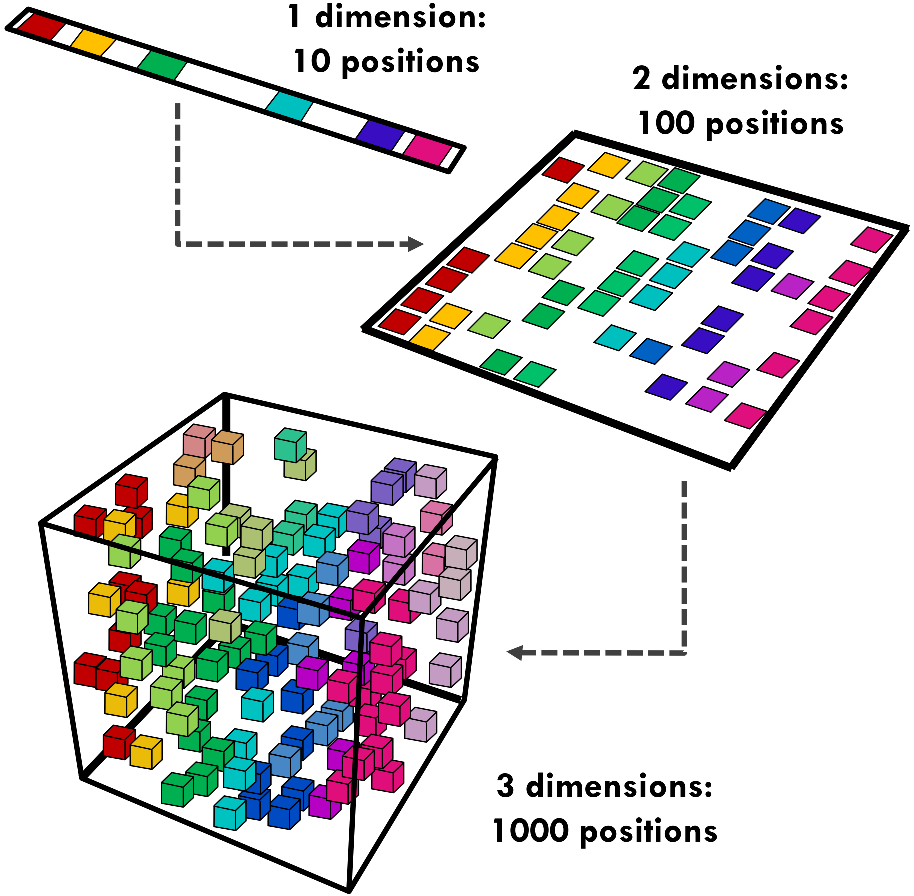


Curse of Dimensionality

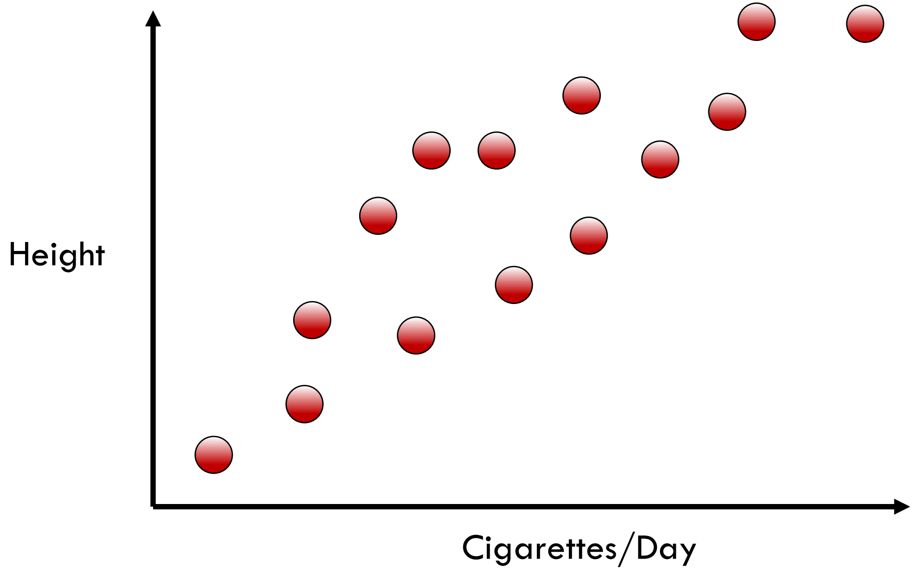
- Theoretically, increasing features should improve performance
- In practice, too many features leads to worse performance
- Number of training examples required increases exponentially with dimensionality



Solution: Dimensionality Reduction

- Data can be represented by fewer dimensions (features)

- Reduce dimensionality by



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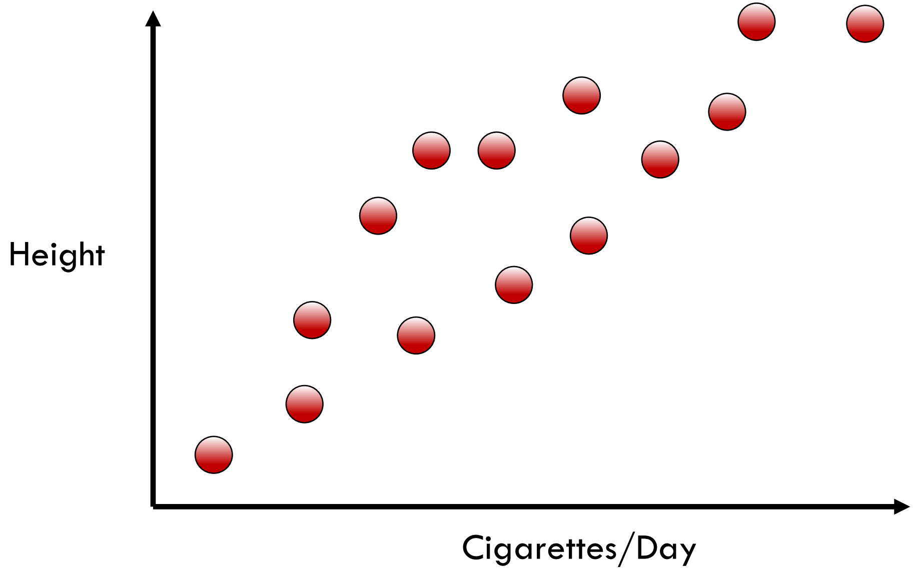
- Data can be represented by fewer dimensions (features)
- Reduce dimensionality by selecting subset (feature elimination)
- Combine with linear and non-



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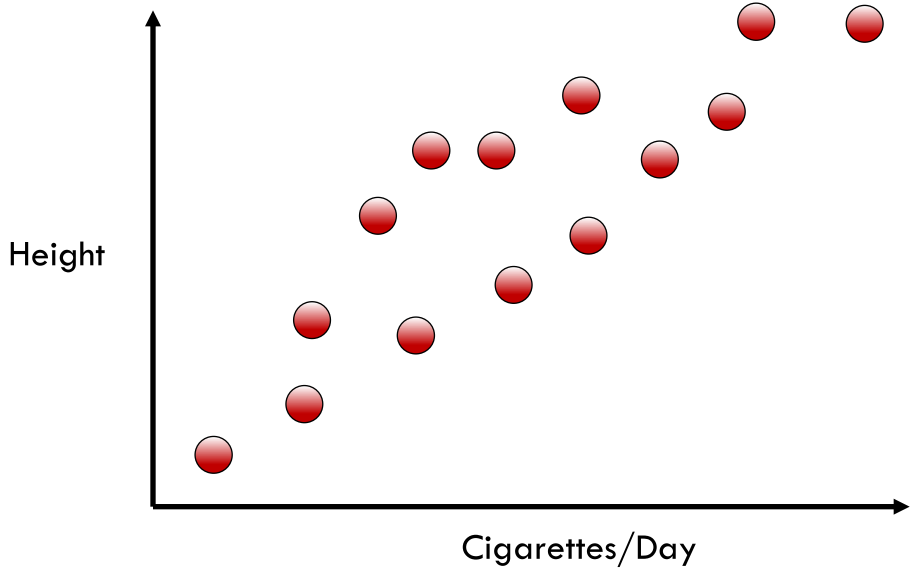
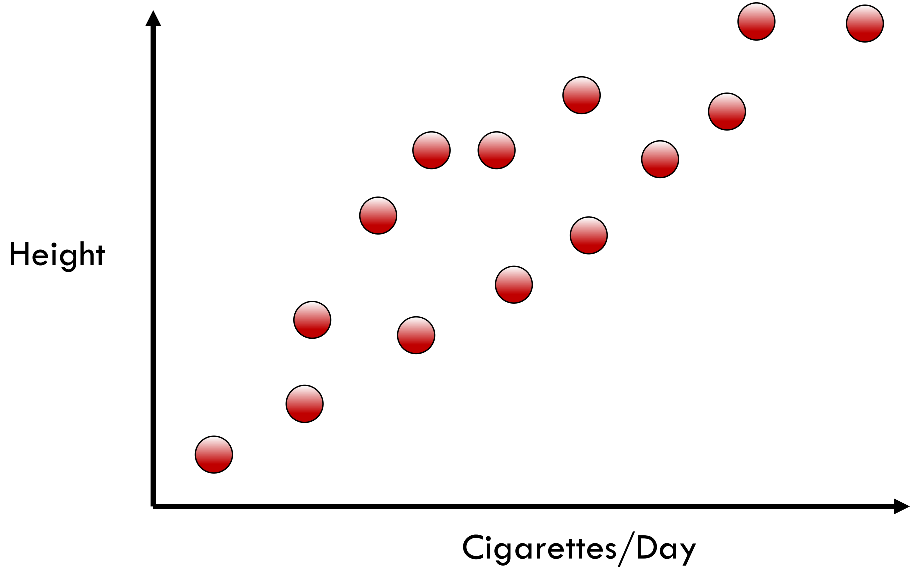


Solution: Dimensionality Reduction

- Two features: height and cigarettes per day

- Both features increase together (correlated)

- Can we reduce number of features to one?



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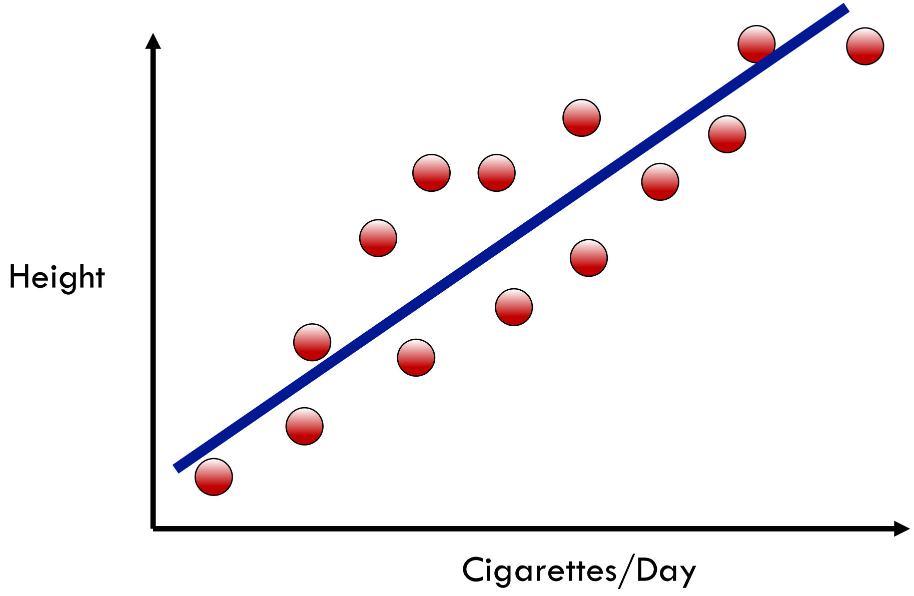

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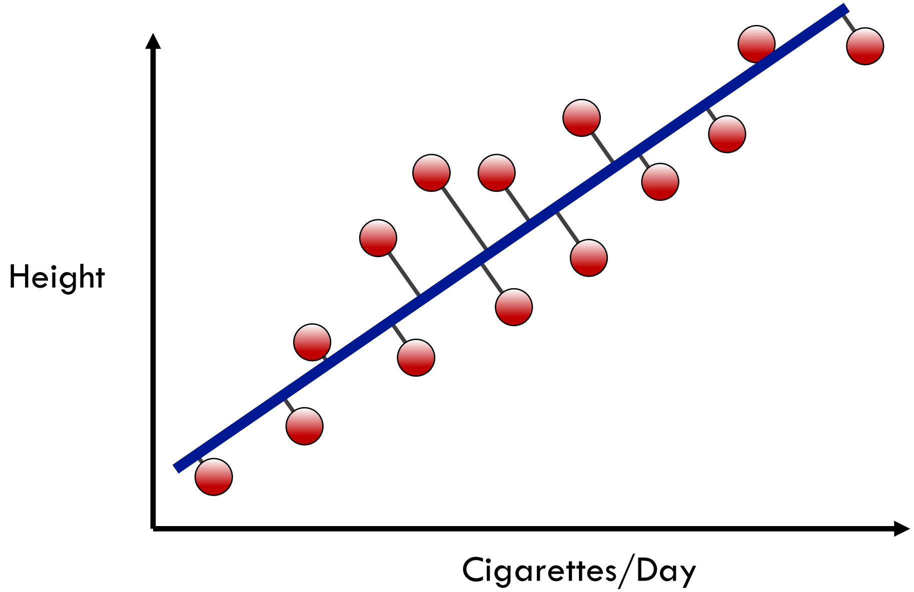

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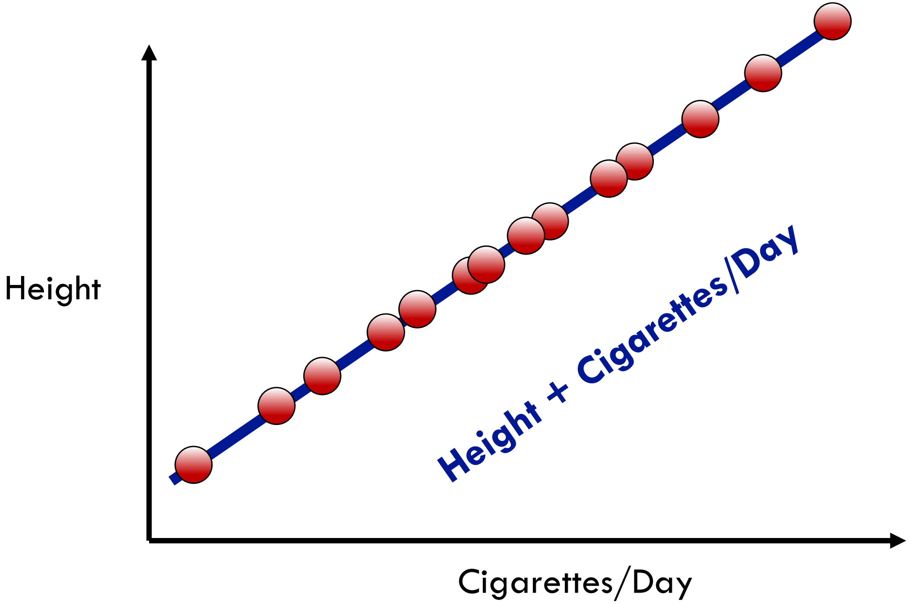
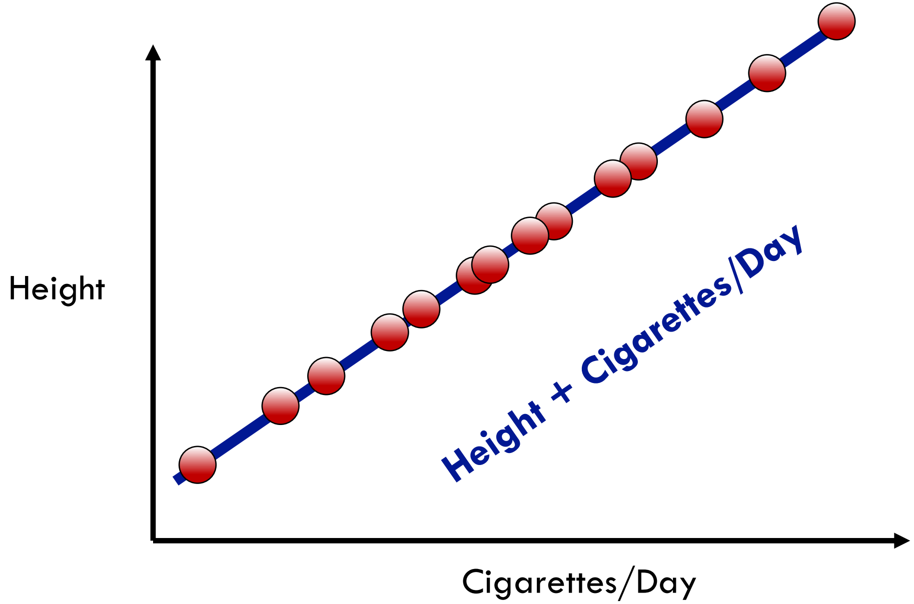


Solution: Dimensionality Reduction

- Create single feature that is combination of height and cigarettes
- This is Principal Component Analysis (PCA)



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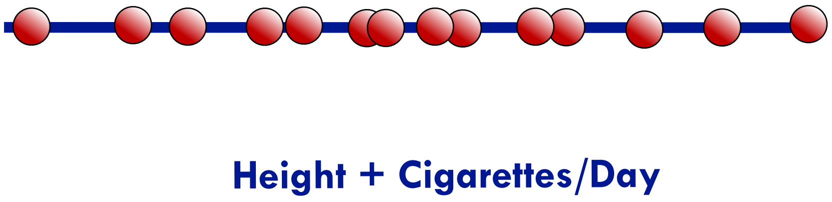


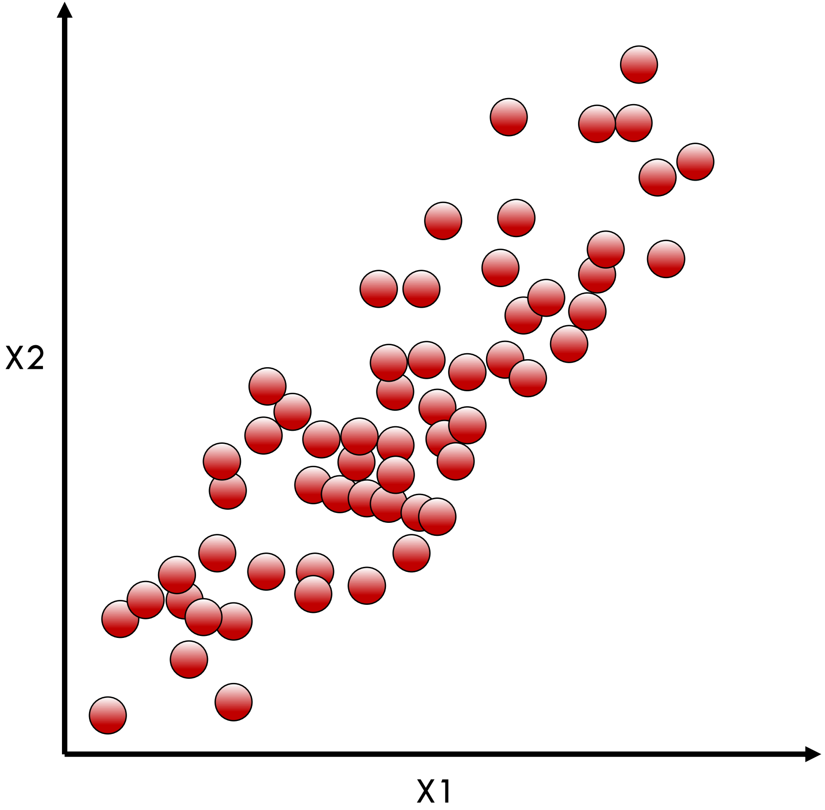
Dimensionality Reduction

Given an N-dimensional data set (x), find a $N \times K$ matrix (U):

$$y = U^T x, \text{ where } y \text{ has } K \text{ dimensions and } K < N$$

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix} \xrightarrow{U^T} y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_k \end{bmatrix} (K < N)$$

Principal Component Analysis (PCA)



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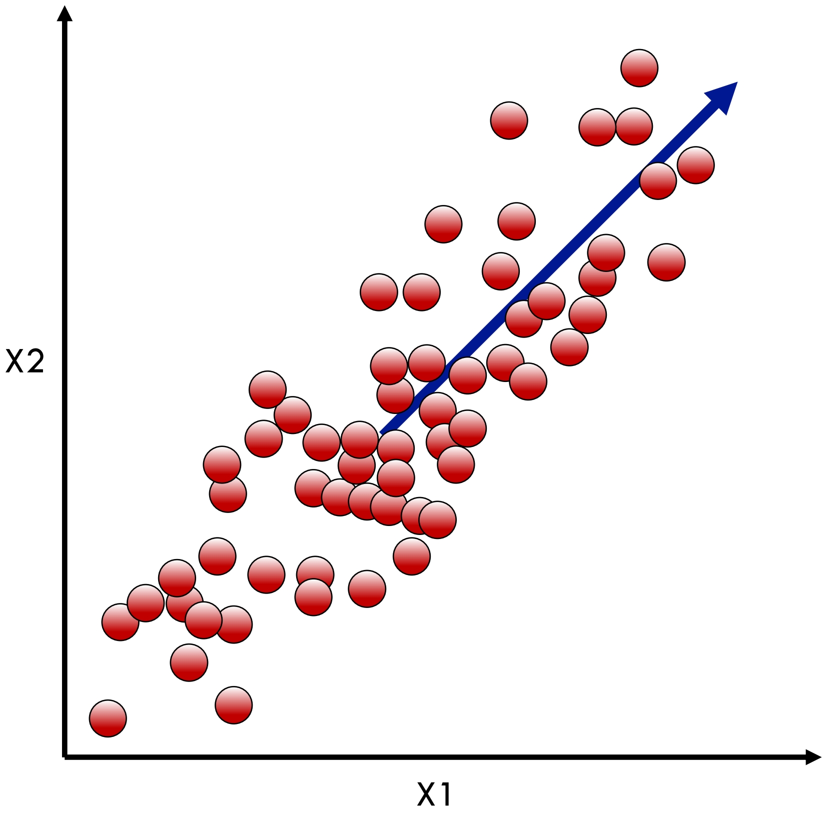

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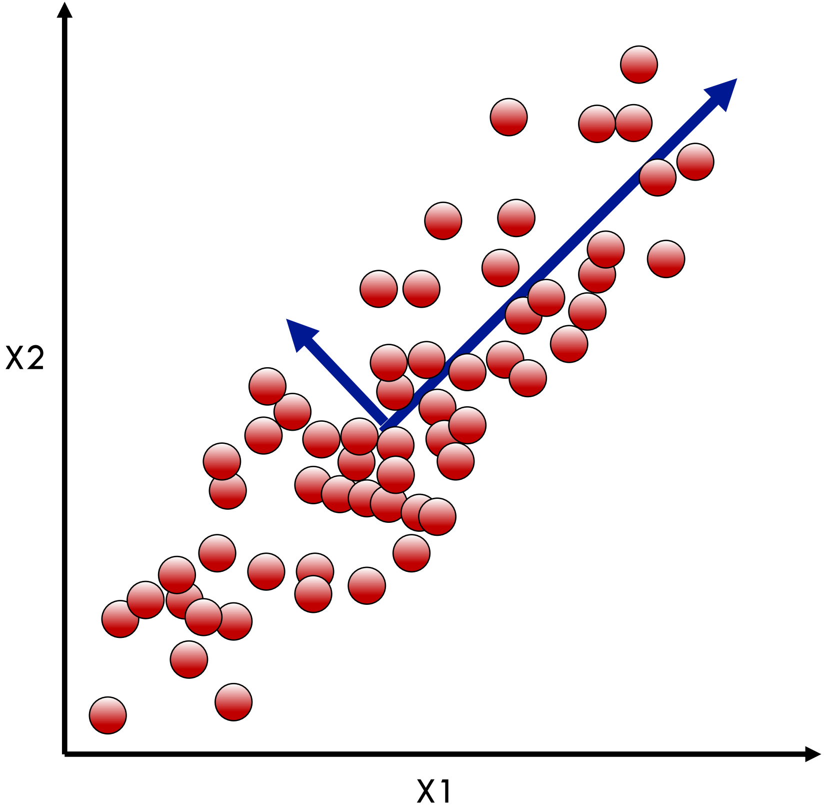

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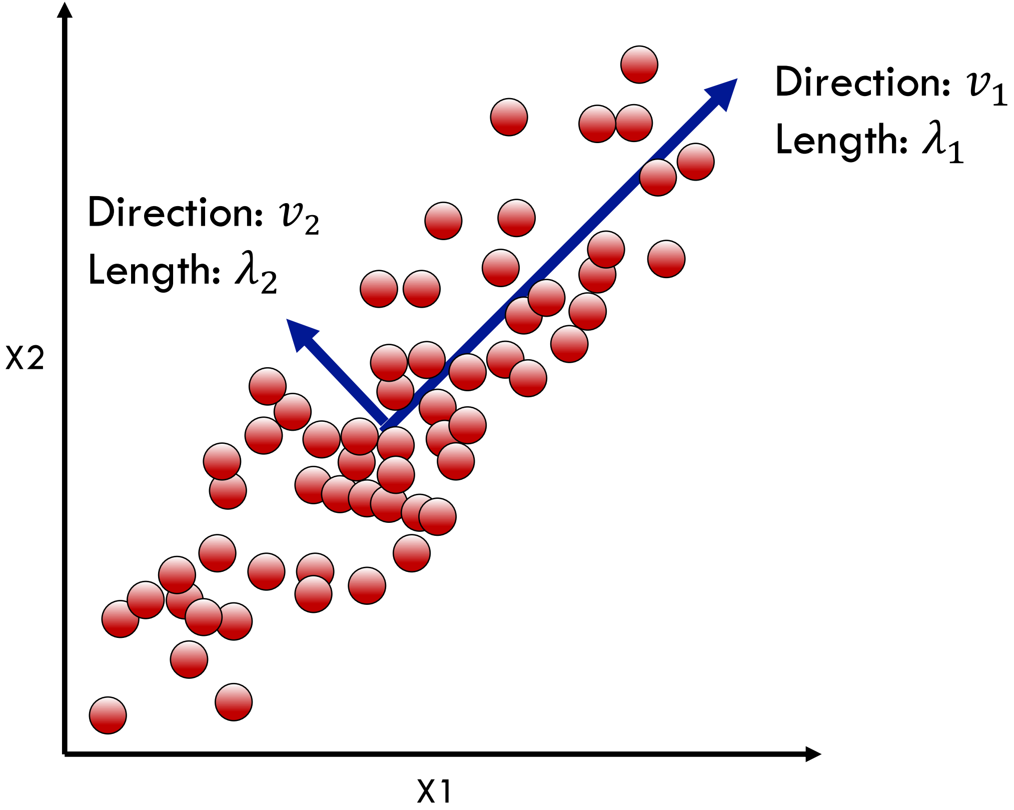


Single Value Decomposition (SVD)

- SVD is a matrix factorization method normally used for PCA
- Does not require a square data set
- SVD is used by Scikit-learn for PCA

$$\begin{bmatrix} \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \end{bmatrix} = \begin{bmatrix} \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \end{bmatrix} \begin{bmatrix} \star & 0 & 0 \\ 0 & \star & 0 \\ 0 & 0 & \star \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \end{bmatrix}$$

$$A_{m\times n} \qquad U_{m\times m} \qquad S_{m\times n} \qquad V^T_{n\times n}$$

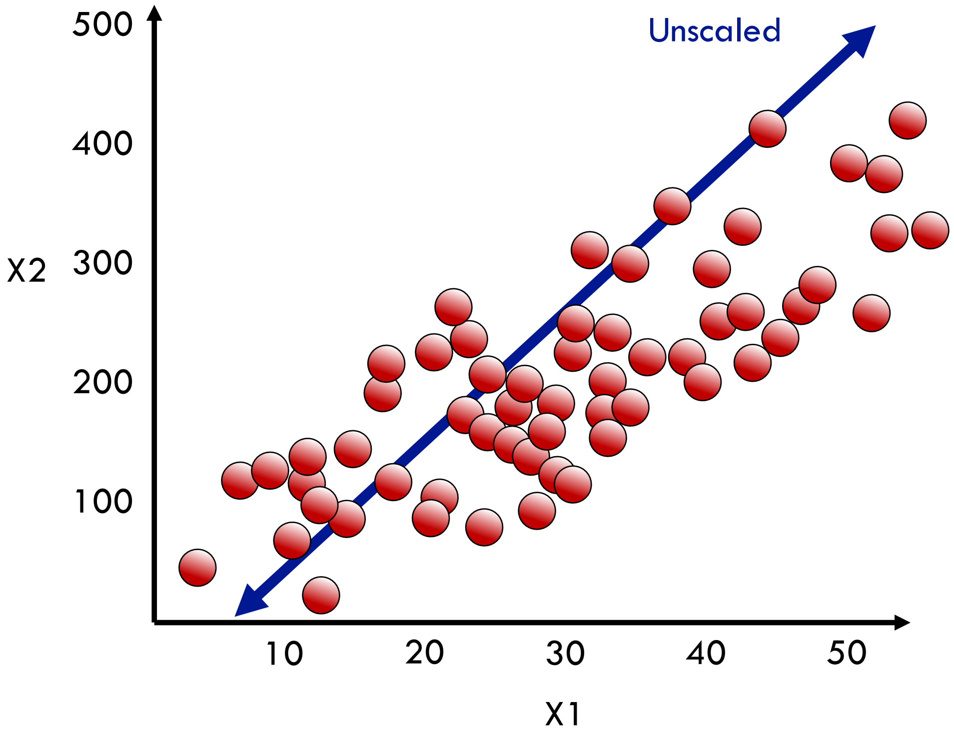
Truncated Single Value Decomposition

- How can SVD be used for dimensionality reduction?
- Principal components are calculated from US
- "Truncated SVD" used for dimensionality reduction ($n \rightarrow k$)

$$\underset{A_{m\times n}}{\begin{bmatrix} \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \end{bmatrix}} \approx \underset{U_{m\times k}}{\begin{bmatrix} \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \\ \star & \star & \star & \star & \star \end{bmatrix}} \underset{S_{k\times k}}{\begin{bmatrix} \mathbf{9} & 0 & 0 \\ 0 & \mathbf{7} & 0 \\ 0 & 0 & \mathbf{1} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}} \underset{V^T_{k\times n}}{\begin{bmatrix} \star & \star & \star \\ \star & \star & \star \\ \star & \star & \star \end{bmatrix}}$$

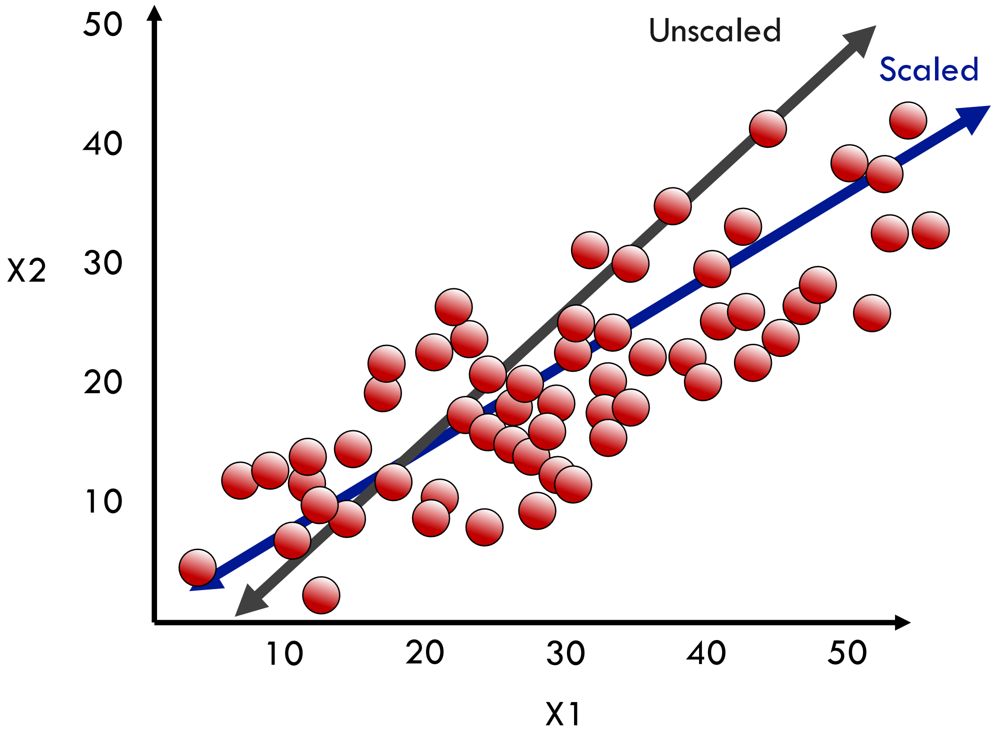
Importance of Feature Scaling

- PCA and SVD seek to find the vectors that capture the most variance
- Variance is sensitive to axis scale



Importance of Feature Scaling

- PCA and SVD seek to find the vectors that capture the most variance
- Variance is sensitive to axis scale
- Must scale data!



PCA: The Syntax

Import the class containing the dimensionality reduction method

```
from sklearn.decomposition import PCA
```

To use the Intel® Extension for Scikit-learn* variant of this algorithm:

- **Install Intel® oneAPI AI Analytics Toolkit (AI Kit)**
- **Add the following two lines of code after the above code:**

```
import patch_sklearn
patch_sklearn()
```

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final number of dimensions

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whiten = scale and center data

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Fit the instance on the data and then transform the data

```
X_trans = PCAinst.fit_transform(X_train)
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Does not work with sparse matrices

Truncated SVD: The Syntax

Import the class containing the dimensionality reduction method

```
from sklearn.decomposition import TruncatedSVD
```

Create an instance of the class

```
SVD = TruncatedSVD(n_components=3)
```

Fit the instance on the data and then transform the data

```
X_trans = SVD.fit_transform(X_sparse)
```

Works with sparse matrices—used with text data for Latent Semantic Analysis (LSA)

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does not center data

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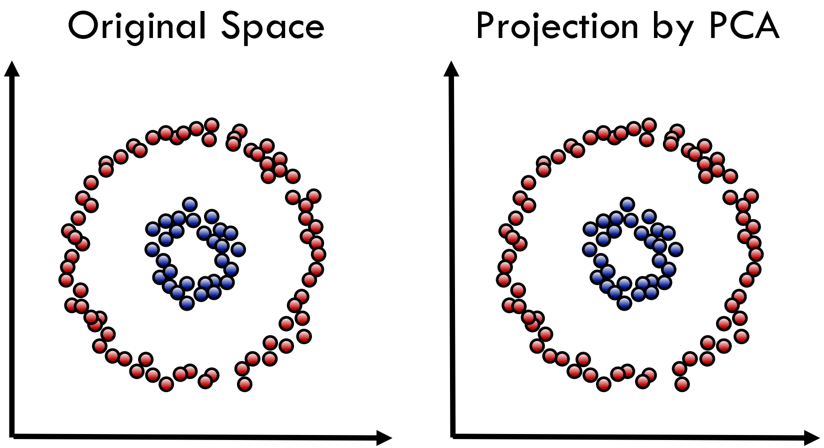
Moving Beyond Linearity

- Transformations calculated with PCA/SVD are linear
- Data can have non-linear features
- This can cause dimensionality



Moving Beyond Linearity

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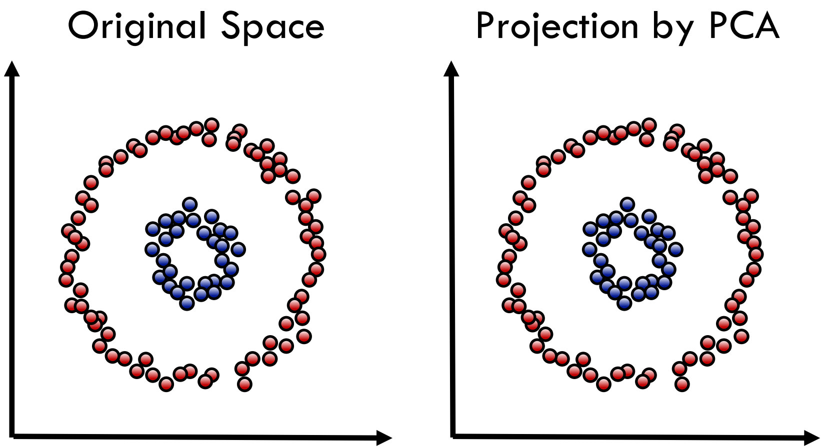

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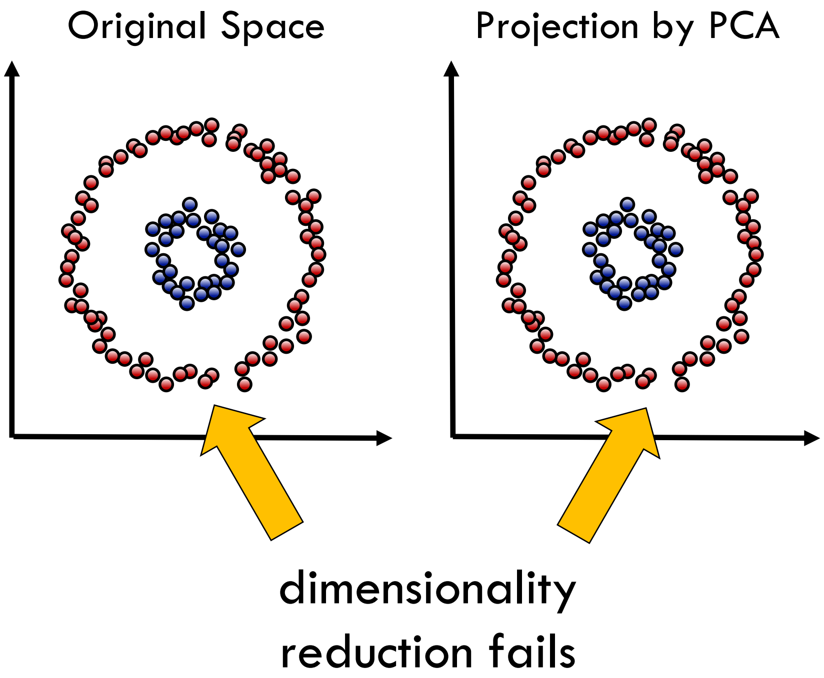
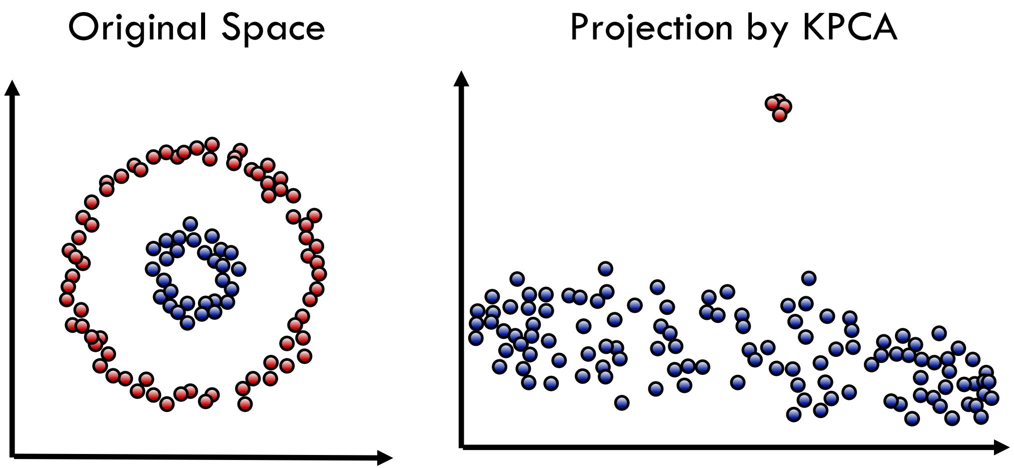


Kernel PCA

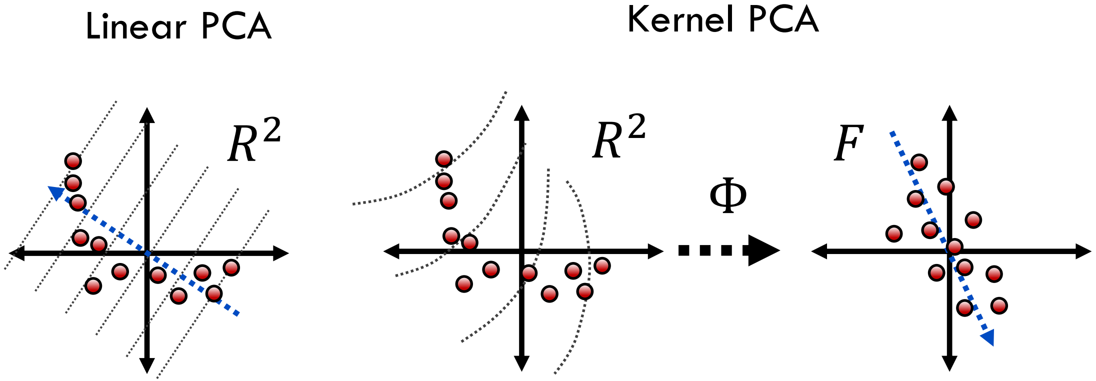
- **Solution:** kernels can be used to perform non-linear PCA



Kernel PCA

- **Solution:** kernels can be used to perform non-linear PCA

- Like the kernel trick introduced for SVMs



Kernel PCA: The Syntax

Import the class containing the dimensionality reduction method

```
from sklearn.decomposition import KernelPCA
```

Create an instance of the class

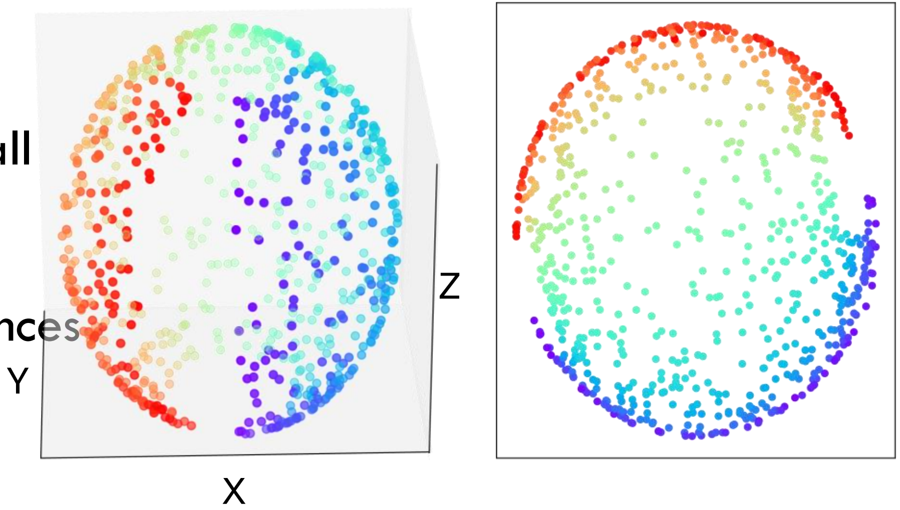
```
kPCA = KernelPCA(n_components=3, kernel='rbf', gamma=1.0)
```

Fit the instance on the data and then transform the data

```
X_trans = kPCA.fit_transform(X_train)
```

Multi-Dimensional Scaling (MDS)

- Non-linear transformation
- Doesn't focus on maintaining overall variance
- Instead, maintains geometric distances between points



MDS: The Syntax

Import the class containing the dimensionality reduction method

```
from sklearn.manifold import MDS
```

Create an instance of the class

```
mdsMod = MDS(n_components=2)
```

Fit the instance on the data and then transform the data

```
X_trans = mdsMod.fit_transform(X_sparse)
```

Many other manifold dimensionality methods exist: Isomap, TSNE.

Uses of Dimensionality Reduction

- Frequently used for high dimensionality data
- Natural language processing (NLP)—many word combinations
- Image-based data sets—pixels are features

Image Source: https://commons.wikimedia.org/wiki/File:Monarch_In_May.jpg

Uses of Dimensionality Reduction

- Divide image into 12 x 12 pixel sections

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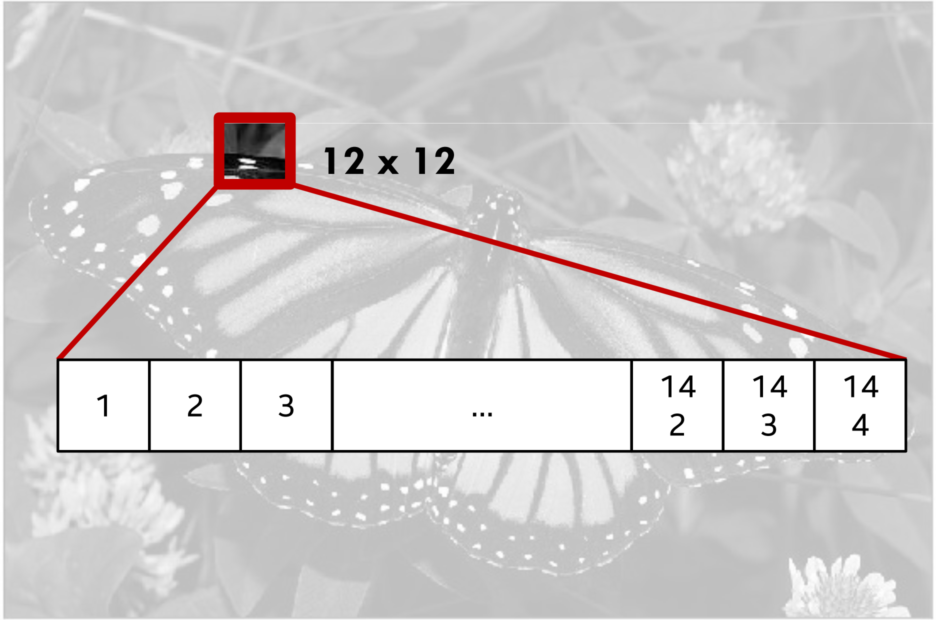
- Divide image into 12 x 12 pixel sections
- Flatten section to create row of data with 144 features



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Uses of Dimensionality Reduction

- Divide image into 12 x 12 pixel sections
- Flatten section to create row of data with 144 features
- Perform PCA on all data points

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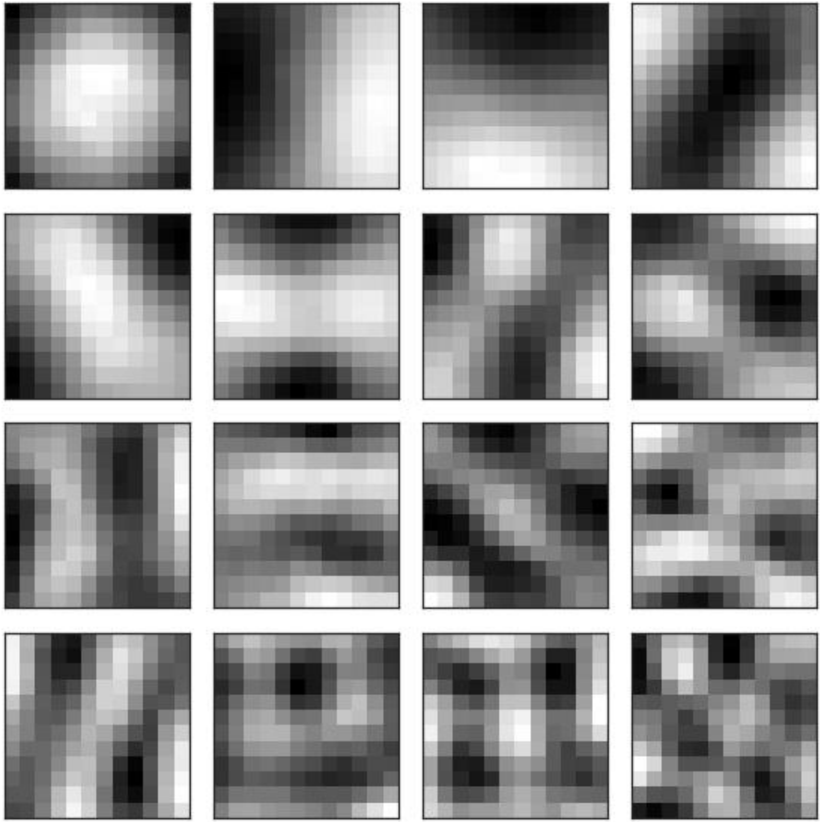
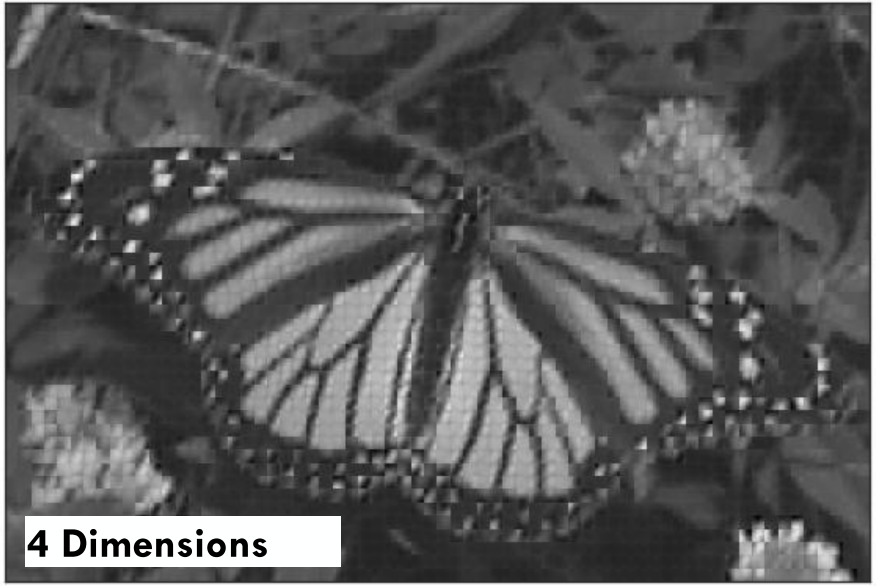
PCA Compression: 144 → 60 Dimensions

PCA Compression: 144 → 16 Dimensions

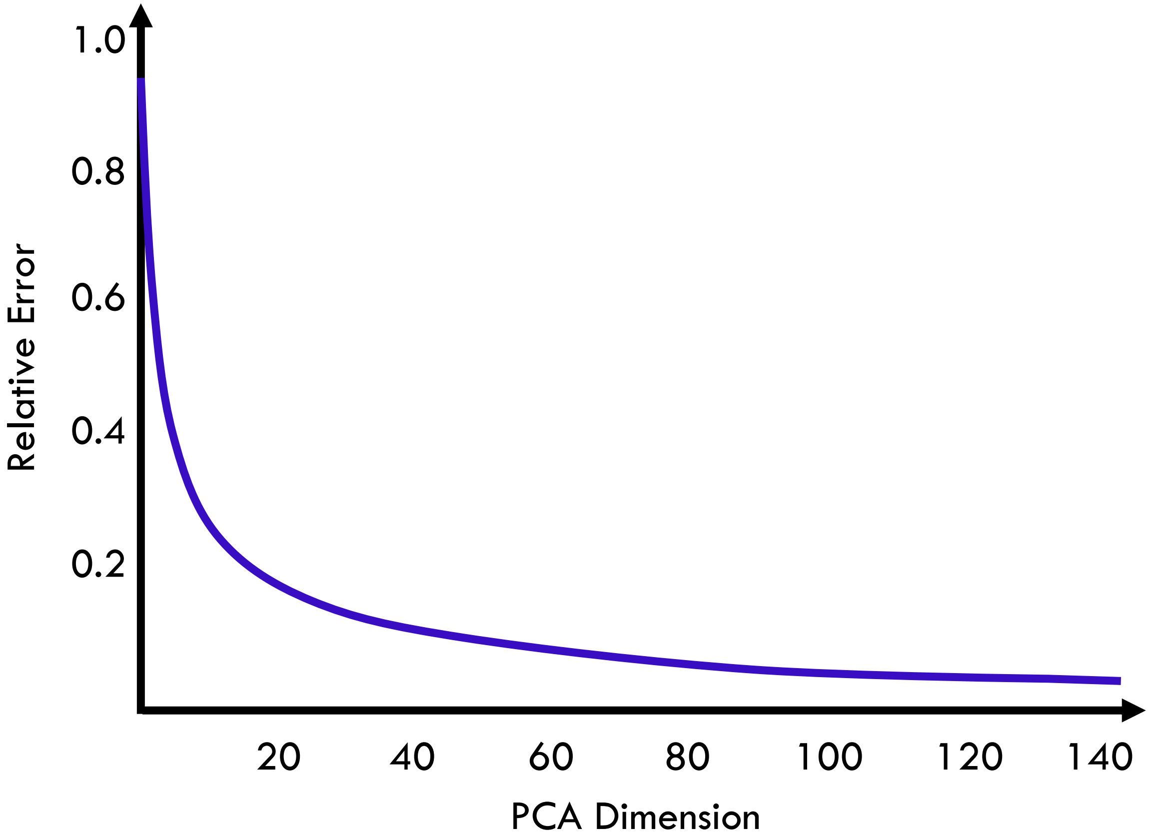
Sixteen Most Important Eigenvectors



PCA Compression: 144 → 4 Dimensions



L2 Error and PCA Dimension



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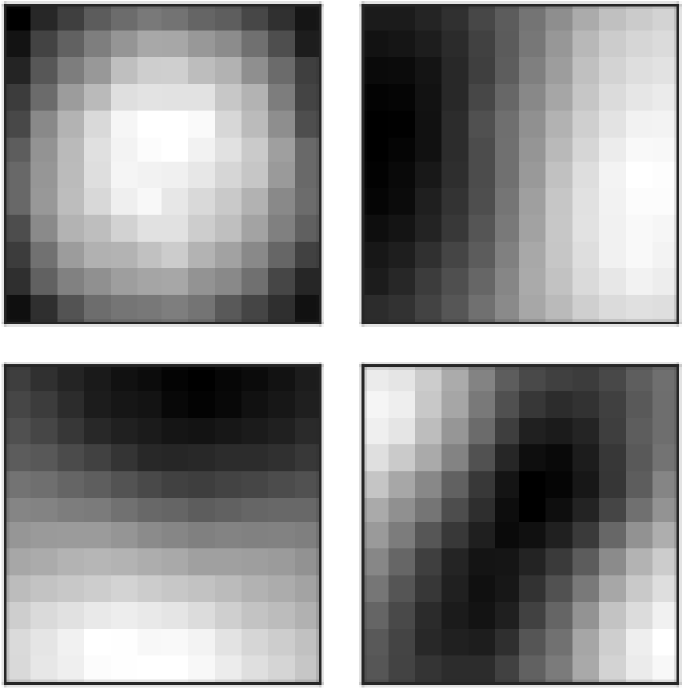

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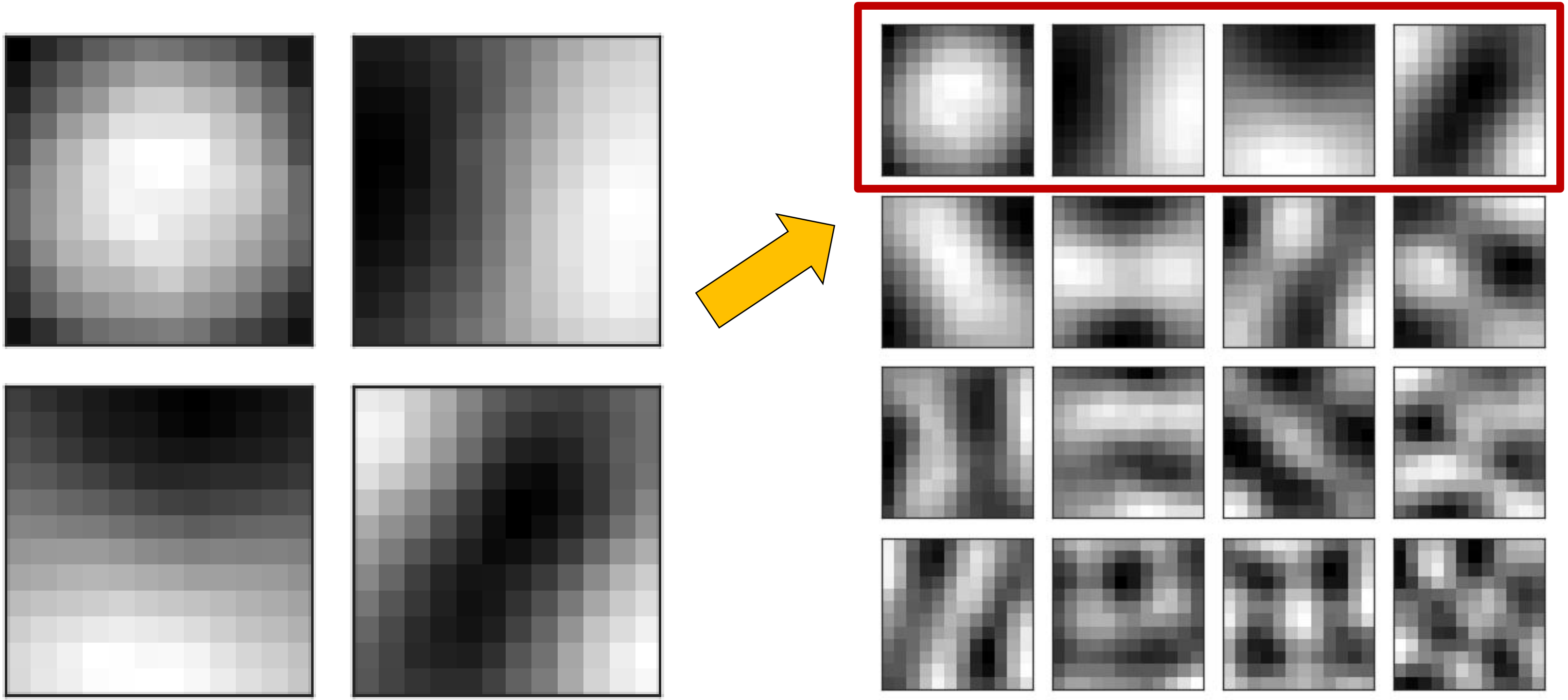
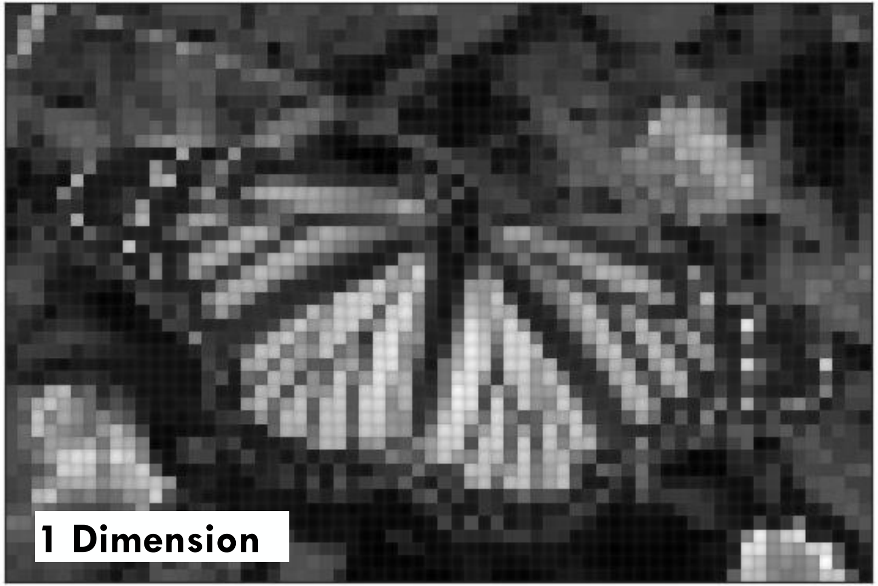


PCA Compression: 144 → 1 Dimension



Software