Machine Learning (CE 40717)

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2. Principal Component Analysis (PCA)
3. Choose PCs
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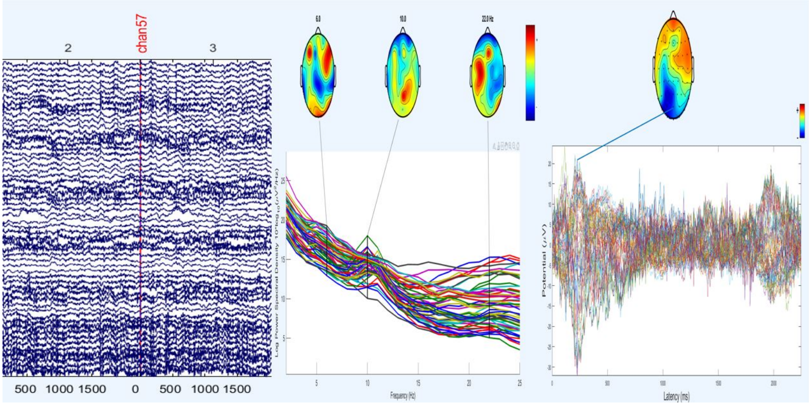
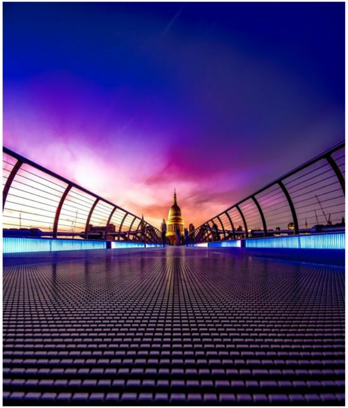
High Dimensional Data

- High-Dimensions = Lots of Features
- EEG Signals of Brain 64 Channels $*$ 3000 Time Points For Each Trial



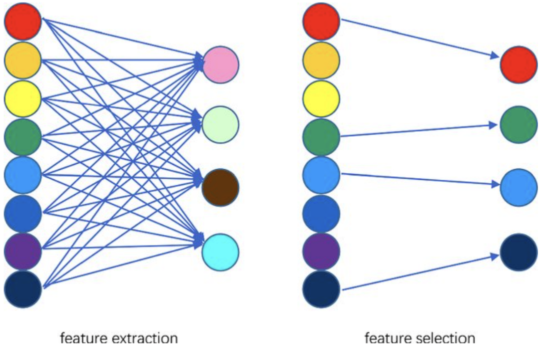
High Dimensional Data

- High-Dimensions = Lots of Features
- High Resolution Images (Millions of Pixels)



Dimensionality Reduction

- **Feature Selection**
  - Select a subset of a given feature set
- **Feature Extraction**
  - A linear or non-linear transform on the original feature space



Dimensionality Reduction Benefits

- **Visualization**
  - Project high dimensional data into 2D or 3D
- **More efficient use of resources**
  - Time, Memory, CPU
- **Statistical**
  - Fewer dimensions leads to better generalization
- **Removing Noise**
- **Pre-Process**
  - Improve accuracy by reducing features
  - As a Preprocessing step to reduce dimensions for supervised learning tasks
  - Helps avoiding overfitting

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  - Sample Covariance Matrix Algorithm

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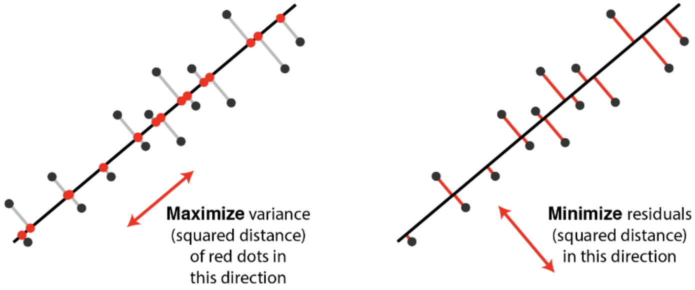
Definition

- **Goal** is reducing the dimensionality of the data while preserving important aspects of the data
- **Principal Components (PCs)** are orthogonal vectors that are ordered by the fraction of the total information (variation) in the corresponding directions
  - Find the directions at which data approximately lie

Definition

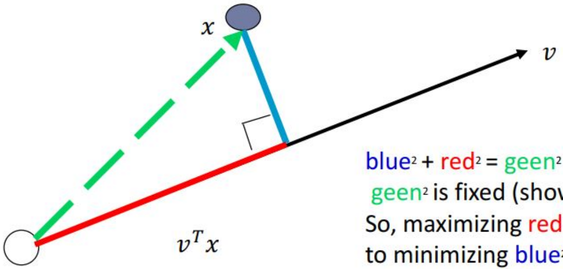
Orthogonal projection of the data onto a **lower-dimensional** linear space that:

- Maximizes variance of projected data
- Minimizes sum of squared distances to the line



Definition

- Minimizing sum of square distances to the line is **equivalent** to maximizing the sum of squares of the projections on that line.



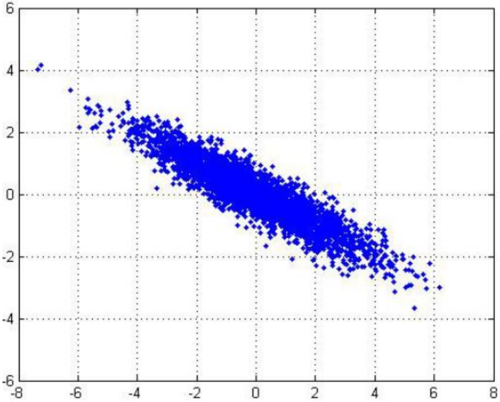
blue² + red² = geen²
geen² is fixed (shows data)
So, maximizing red² is equivalent to minimizing blue²

Idea

- Given data points in a d-dimensional space, project them into a lower dimensional space while preserving as much information as possible,
  - Find best planar approximation of 3D data
  - Find best 12-D approximation of 104-D data
- In particular, choose projection that minimizes squared error in reconstructing the original data

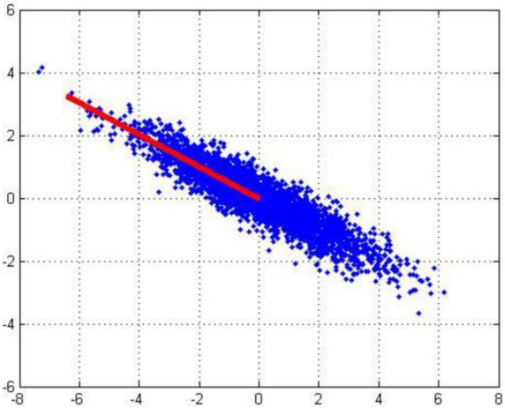
Idea

- 2D Gaussian dataset



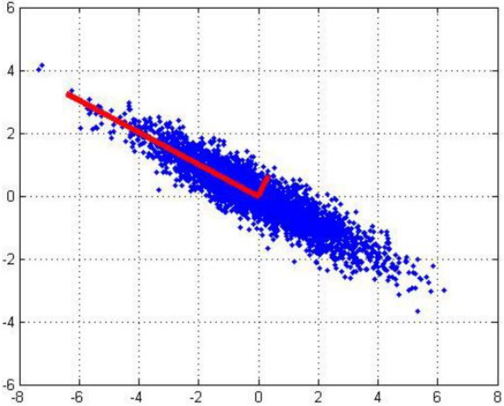
Idea

- 2D Gaussian dataset
- First PCA axis



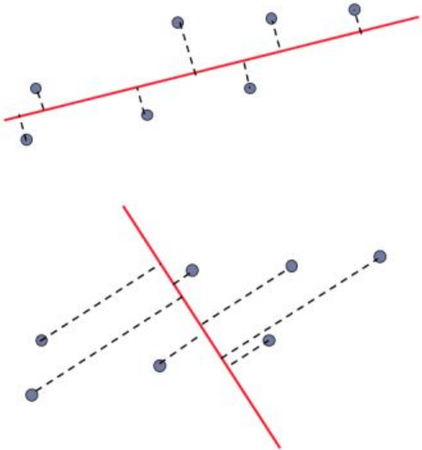
Idea

- 2D Gaussian dataset
- First and second PCA axes



Random vs Principal Projection

- Random direction vs. principal component

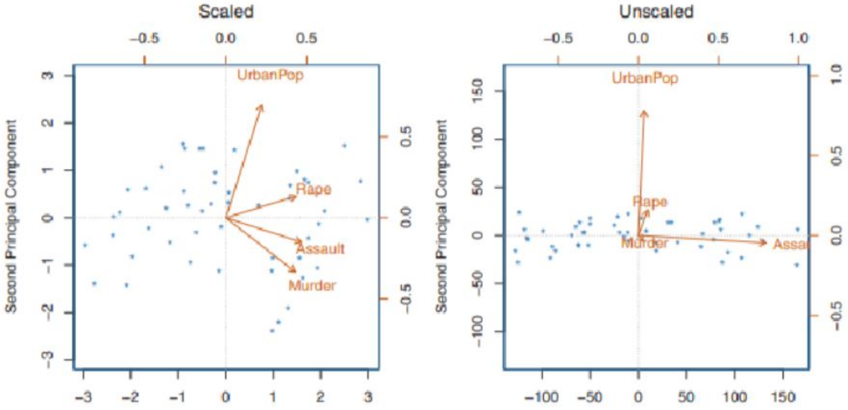


Pre-processing

- **Center the data**
  - **Zero**ing out the **mean** of each feature
- **Scaling to normalize each feature to have variance 1**
  - An arbitrary step (May affect the final result!)
  - It helps when unit of measurements of features are different and some features may be ignored without normalization

Pre-processing

- Scaling to normalize each feature may affect the final result!!



Algorithms

- Algorithm 1: sequential
- Algorithm 2: sample covariance matrix

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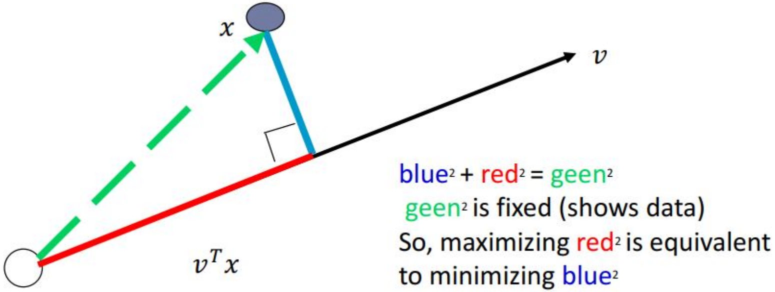
Sequential Algorithm

- First view
  - Find directions with the maximum variations

$$\max_{v_1} \frac{1}{N}\sum_{n=1}^{N}(v_1^T x_n)^2 = \frac{1}{N}\sum_{n=1}^{N} v_1^T (x_n x_n^T) v_1 = v_1^T \left(\frac{1}{N}\sum_{n=1}^{N}(x_n x_n^T)\right) v_1 = v_1^T S v_1$$

$$\text{s.t. } v_1^T v_1 = 1$$



Sequential Algorithm

- First view
- why $v_1^T v_1 = 1$?
- Eigenvector with maximum eigenvalue maximizes the objective
  - Using Lagrangian multiplier technique

$$L(v_1, \lambda) = v_1^T S v_1 + \lambda(1 - v_1^T v_1)$$

$$\frac{\partial L}{\partial v_1} = 0 \Rightarrow 2Sv_1 - 2\lambda v_1 = 0$$

$$\Rightarrow Sv_1 = \lambda v_1$$

Sequential Algorithm

- First view
- To find v_2, we maximize the variance of the projection in the residual subspace

$$v_2 = max_{v_2}\left(\frac{1}{N}\sum_{i=1}^{N}(x_i - v_1^T x_i)^2\right)$$

$$\text{s.t. } v_2^T v_2 = 1$$

- To find v_k, we maximize the variance of the projection in the residual subspace

$$v_k = max_{v_k}\left(\frac{1}{N}\sum_{i=1}^{N}\left(x_i - \sum_{j=1}^{k-1} W_j^T x_i\right)^2\right)$$

$$\text{s.t. } v_k^T v_k = 1$$

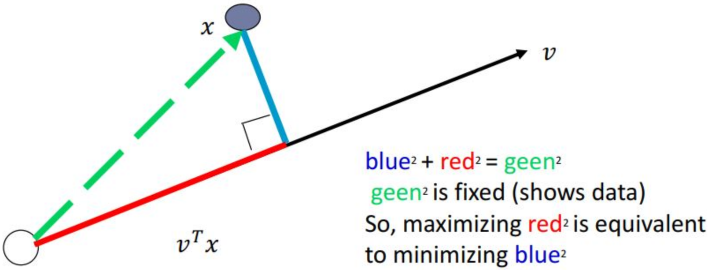
Sequential Algorithm

- Second view
  - Find directions with the minimum reconstruction error

$$\min_{v1} \sum_{n=1}^{N} \|x_n - (v_1^T x_n) v_1\|_2^2$$

$$\text{s.t. } v_1^T v_1 = 1$$

- Show this has an equal solution with the first view



Sequential Algorithm

- As we have $Sv_j = \lambda_j v_j$,

$$\Rightarrow \mathrm{var}(v_j^T x) = v_j^T x x^T v_j = v_j^T S v_j = \lambda_j v_j^T v_j = \lambda_j$$

.

- The variance along an eigenvector v_j equals the eigenvalue λ_j.

Sequential Algorithm

- Eigenvalues: $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots$
  - The first PC v_1 is the the eigenvector of the sample covariance matrix S associated with the largest eigenvalue
  - The 2nd PC v_2 is the the eigenvector of the sample covariance matrix S associated with the second largest eigenvalue
  - And so on ...
- To reduce the dimension of the data to k, we select eigenvectors with the top k eigenvalues

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   - **Sample Covariance Matrix Algorithm**
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Sample Covariance Matrix

- Given data $x_1, \ldots, x_n$, compute covariance matrix Σ

$$\Sigma = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T \text{ where } \bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

- PCA basis vectors = the eigenvectors of Σ
- Larger eigenvalue → more important eigenvectors

Sample Covariance Matrix

Algorithm 1 Sample Covariance Matrix

1: **Input:** $X \in \mathbb{R}^{N \times d}$ (data matrix with N data points and d dimensions)
2: Compute the mean of each feature: $\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$
3: Subtract the mean from each data point (center the data): $\tilde{X} \leftarrow X - 1_N \bar{x}^T$
4: Compute the covariance matrix: $S = \frac{1}{N} \tilde{X}^T \tilde{X}$
5: Compute the eigenvalues and eigenvectors of S: $[\lambda_1, \lambda_2, \ldots, \lambda_d], [v_1, v_2, \ldots, v_d] = \text{eig}(S)$
6: Select the top K eigenvectors corresponding to the largest eigenvalues: $A \leftarrow [v_1, v_2, \ldots, v_K]$
7: Transform the data into the new subspace: $X' \leftarrow X \cdot A$
8: **Output:** $X' \in \mathbb{R}^{N \times K}$ (transformed data with reduced dimensions)

Sample Covariance Matrix

- Eigen-vectors of symmetric matrices are orthogonal
- Covariance matrix is symmetric
  - Principal component are orthonormal
- We have

$$v_i^T v_j = 0, \quad \forall i \neq j$$

$$v_i^T v_i = 1, \quad \forall i$$

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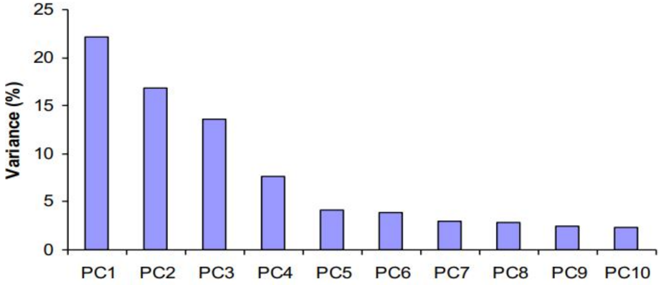
How many PCs?

- For n original dimensions, sample covariance matrix is $n * n$, and has up to n eigenvectors. So n PCs
- Can ignore the components of lesser significance



- You do lose some information, but if the eigenvalues are small, you don't lose much

How many PCs?

$$\frac{\sum_{i=d-k+1}^{d} \lambda_i}{\sum_{i=1}^{d} \lambda_i}$$

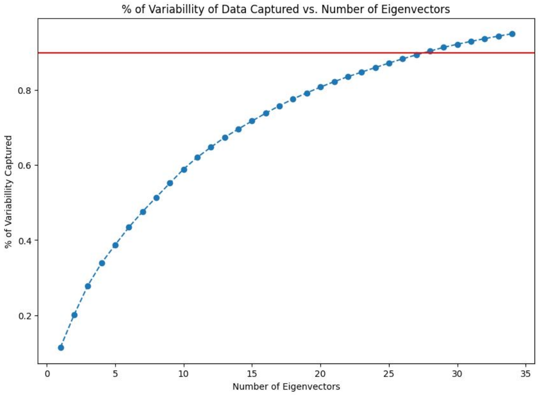


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Image Compression

- Divide the original 372x492 image into patches
  - Each patch is an instance that contains 12x12 pixels on a grid
- Consider each as a 144-D vector

Image Compression

- 144D ⇒ 60D

Image Compression

- 144D ⇒ 16D

Image Compression

- 16 most important eigenvectors

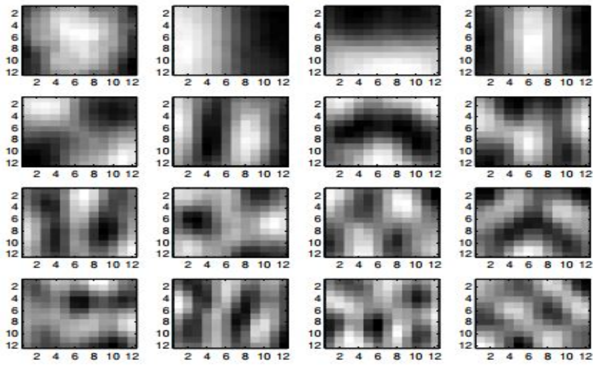


Image Compression

- 144D ⇒ 3D

Image Compression

- 3 most important eigenvectors

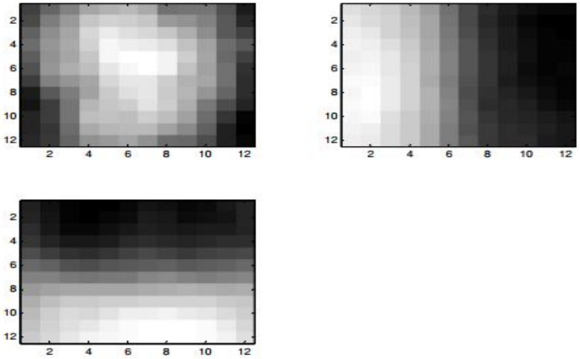
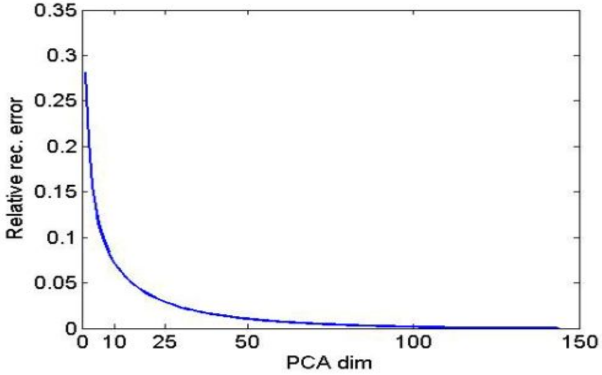


Image Compression

- L2 error and PCA dim



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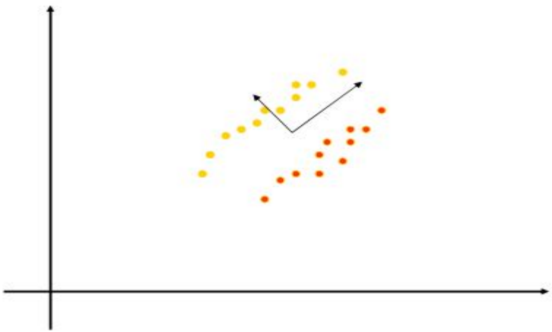
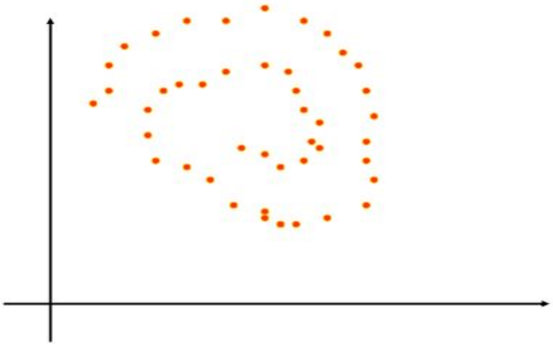
Class Labels

- PCA doesn't know about class labels!



Non-Linear

- PCA cannot capture Non-Linear structure!



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Conclusion

- PCA
  - finds orthonormal basis for data
  - Sorts dimensions in order of “importance”
  - Discard low significance dimensions
- Applications
  - Get compact description
  - Remove noise
  - Improve classification (hopefully)
  - More efficient use of resources
  - Statistical
- Not magic
  - Doesn’t know class labels
  - Can only capture linear variations
- One of many tricks to reduce dimensionality!

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References

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