# Dimensionality Reduction: Principle Component Analysis

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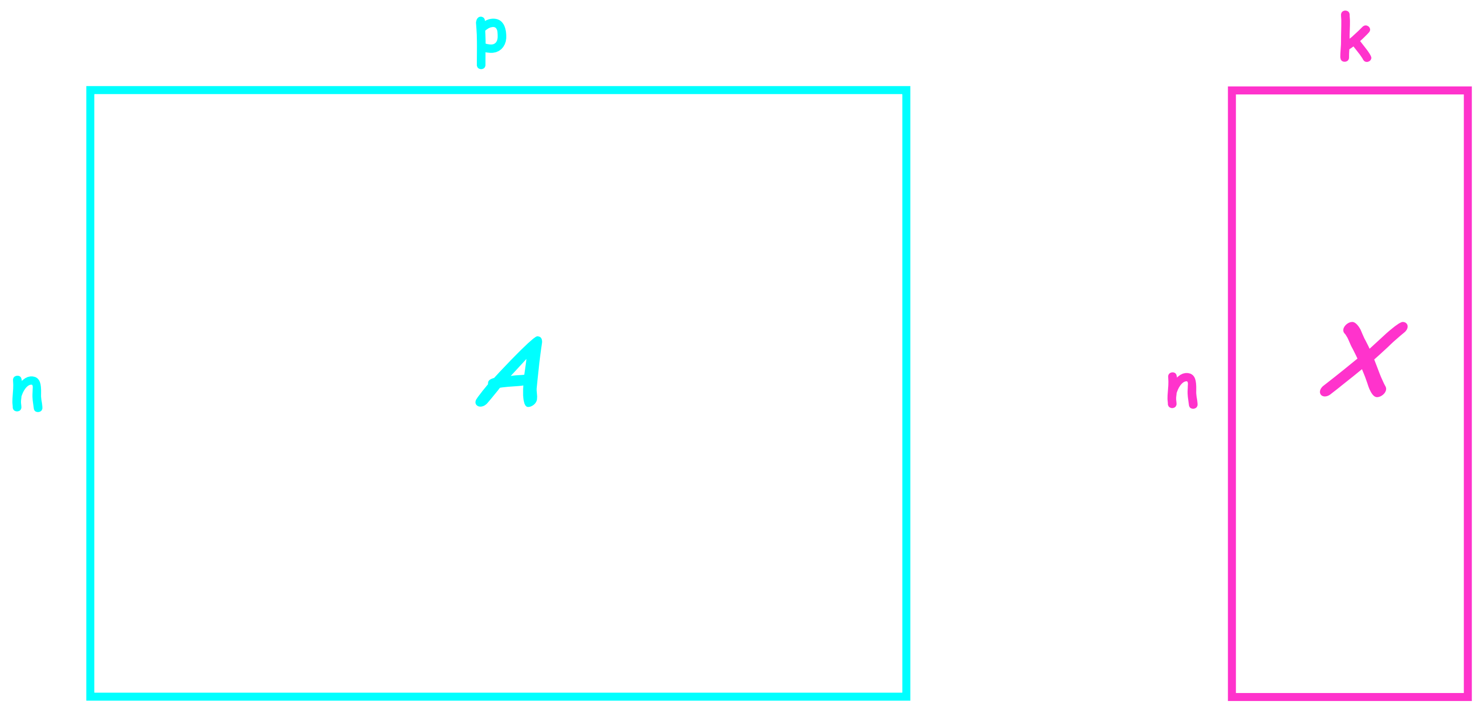
# What is dimensionality reduction?



# Dimensionality Reduction: why?

- Extract underlying factors

| | Disagree | | Neutral | | Agree |
|---|---|---|---|---|---|
| I am the life of the party. | | | | | |
| I feel little concern for others. | | | | | |
| I am always prepared. | | | | | |
| I get stressed out easily. | | | | | |
| I have a rich vocabulary. | | | | | |
| I don't talk a lot. | | | | | |
| I am interested in people. | | | | | |
| I leave my belongings around. | | | | | |
| I am relaxed most of the time. | | | | | |
| I have difficulty understanding abstract ideas. | | | | | |
| I feel comfortable around people. | | | | | |
| I insult people. | | | | | |
| I pay attention to details. | | | | | |
| I worry about things. | | | | | |
| I have a vivid imagination. | | | | | |

## The five factors [edit]

A summary of the factors of the Big Five and their co

- **Openness to experience**: (*inventive/curious* vs intellectual curiosity, creativity and a preference f preference for a variety of activities over a strict r experience.
- **Conscientiousness**: (*efficient/organized* vs. *eas* spontaneous behavior.
- **Extraversion**: (*outgoing/energetic* vs. *solitary/re* talkativeness.
- **Agreeableness**: (*friendly/compassionate* vs. *an* one's trusting and helpful nature, and whether a p
- **Neuroticism**: (*sensitive/nervous* vs. *secure/conf* degree of emotional stability and impulse control

# Dimensionality Reduction: why?

- Reduce data noise
  - Face recognition
  - Applied to image de-noising

(a) Noisy image (b) NL means (PSNR=32.90) (c) Local PCA (PSNR=33.70)

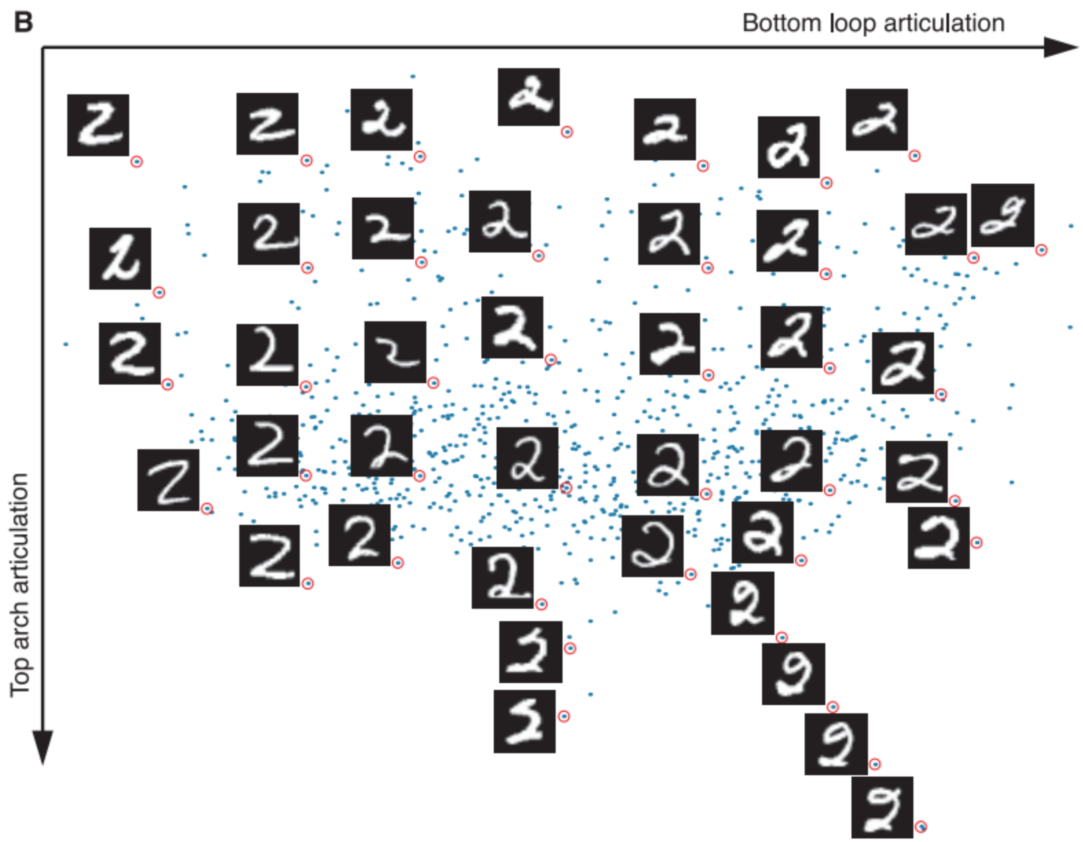
Image courtesy of Charles-Alban Deledalle, Joseph Salmon, Arnak Dalalyan; BMVC 2011
Image denoising with patch-based PCA: local versus global

# Dimensionality Reduction: why?

- Reduce the number of model parameters
  - Avoid over-fitting
  - Reduce the computational load

# Dimensionality Reduction: why?

- Visualization



# Dimensionality Reduction

- General principle:
  - Preserve "useful" information in low dimensional data
- How to define "usefulness"?
  - Many
  - An active research direction in machine learning
- Taxonomy
  - Supervised or Unsupervised
  - Linear or nonlinear
- Commonly used methods:
  - PCA, LDA (linear discriminant analysis), local linear embedding and more.

# Outline

- Theoretic Part
  - PCA explained: two perspectives
  - Mathematic basics
  - PCA objective and solution
- Application Example
  - Eigen face
  - Handle high feature dimensionality
- Extensions:
  - Kernel PCA

# PCA explained: Two perspectives

- Data correlation and information redundancy
- Signal-noise ratio maximization

# PCA explained: Data correlation and information redundancy

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I don't talk a lot.

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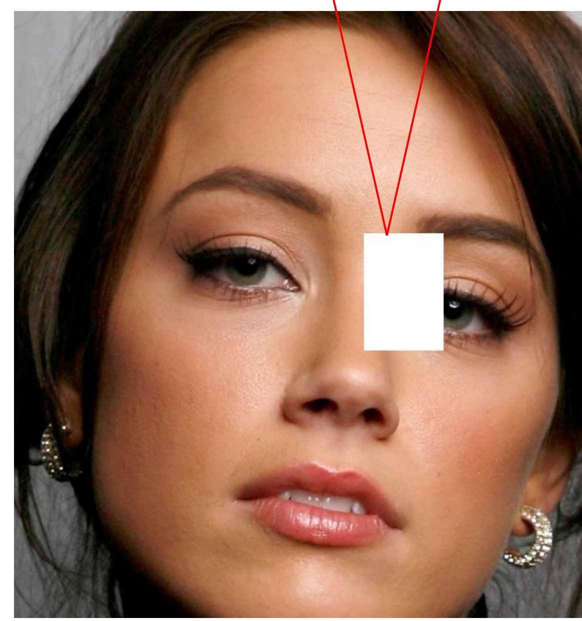
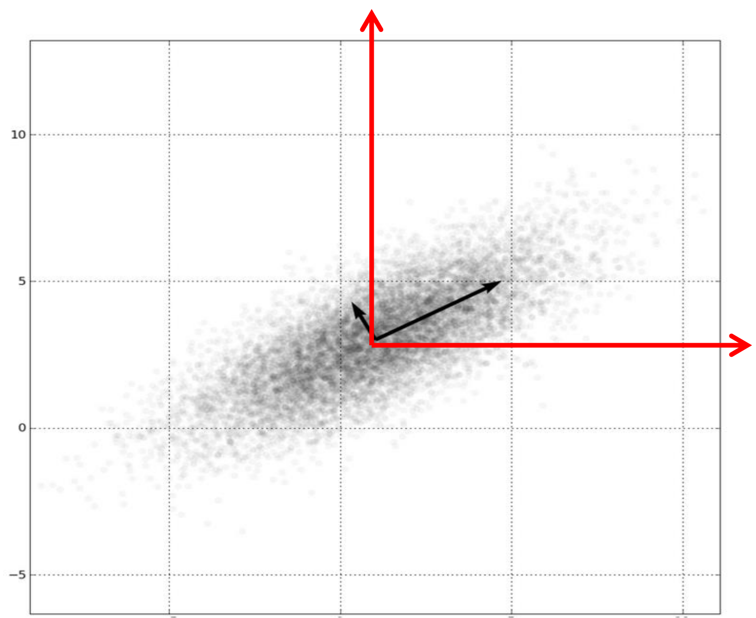


# PCA explained: Data correlation and information redundancy

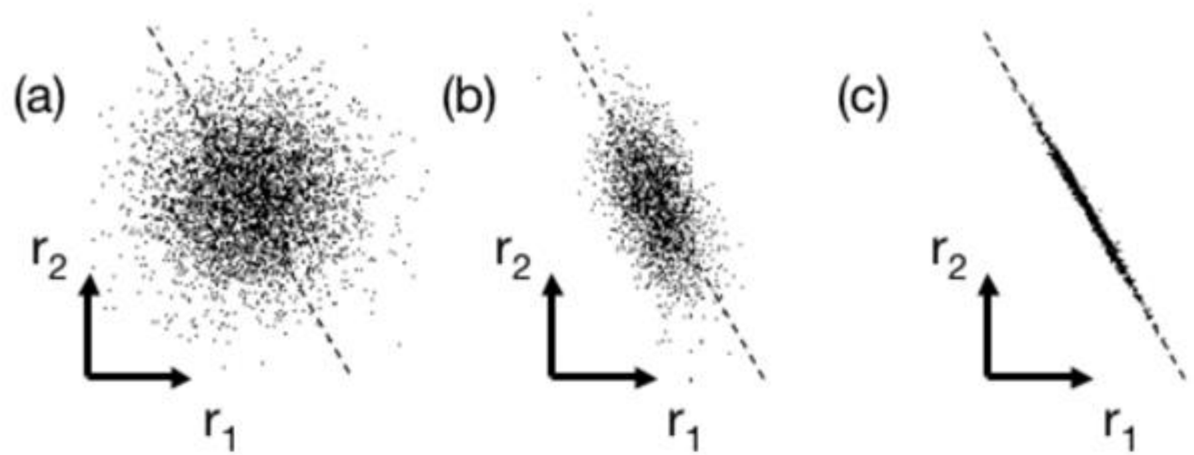
- Dependency vs. Correlation
  - Dependent is a stronger criterion
- Equivalent when data follows Gaussian distribution
- PCA only de-correlates data
  - One limitation of PCA
  - ICA, but it is more complicate

# PCA explained: Data correlation and information redundancy

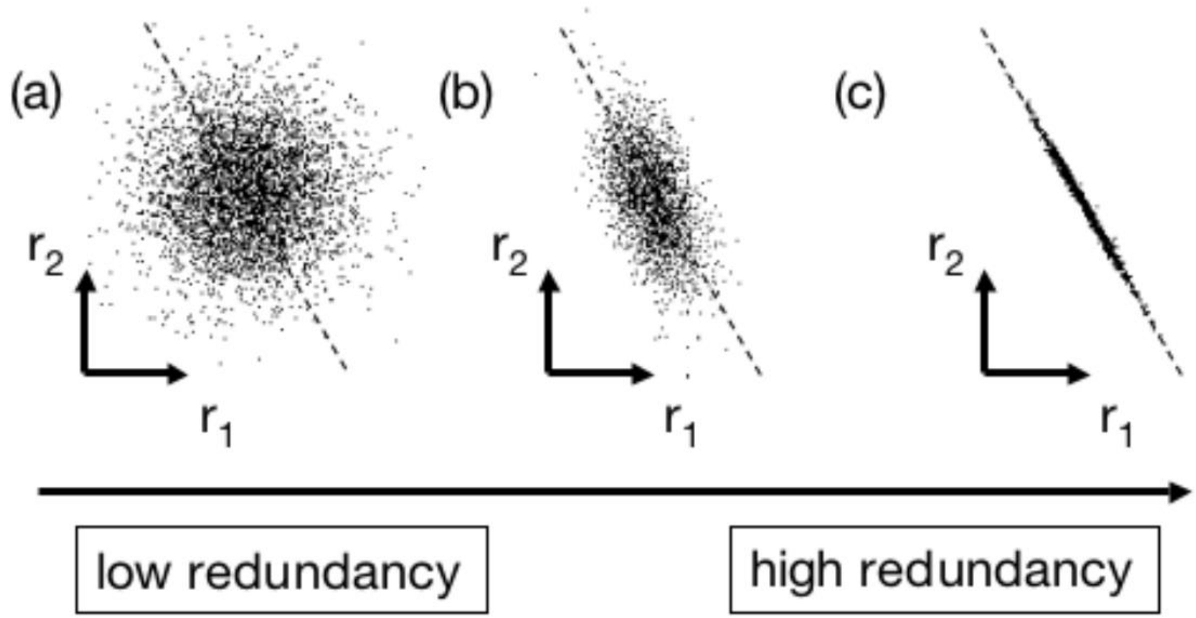
- Geometric interpretation of correlation



# PCA explained: Data correlation and information redundancy

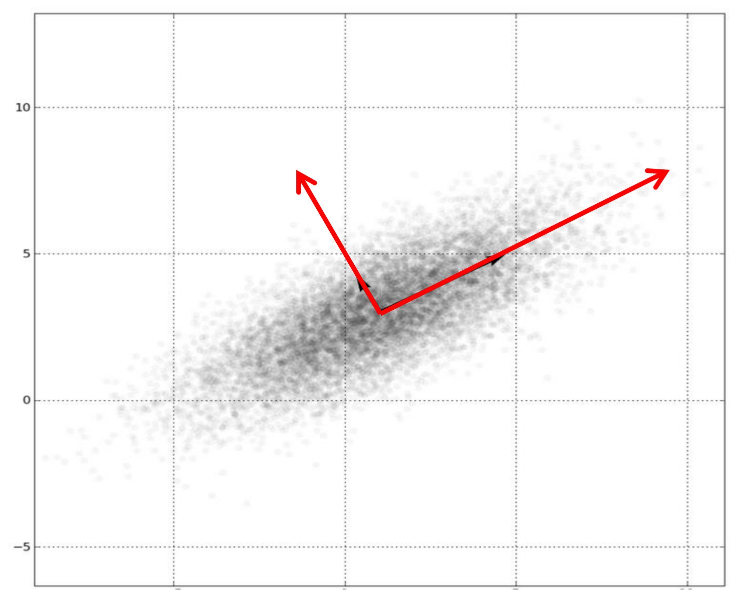


# PCA explained: Data correlation and information redundancy

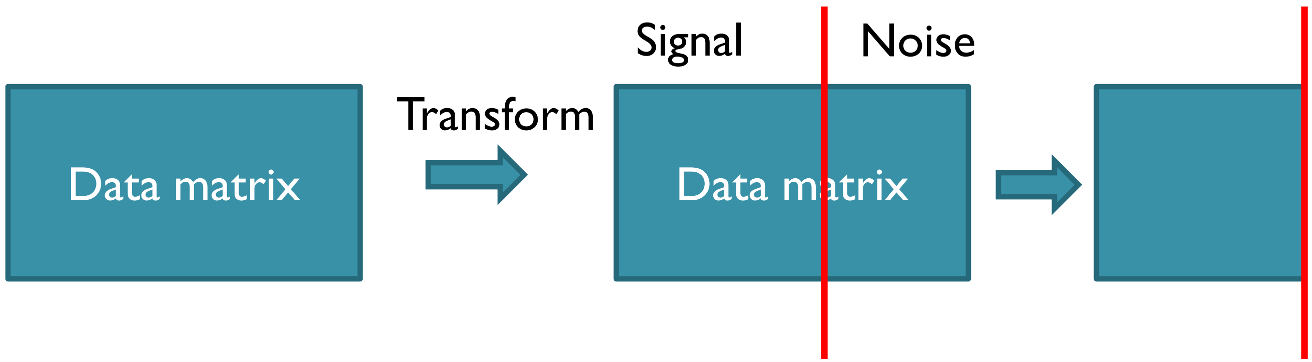


# PCA explained: Data correlation and information redundancy

- Correlation can be removed by rotating the data point or coordinate



# PCA explained: Signal-noise ratio maximization

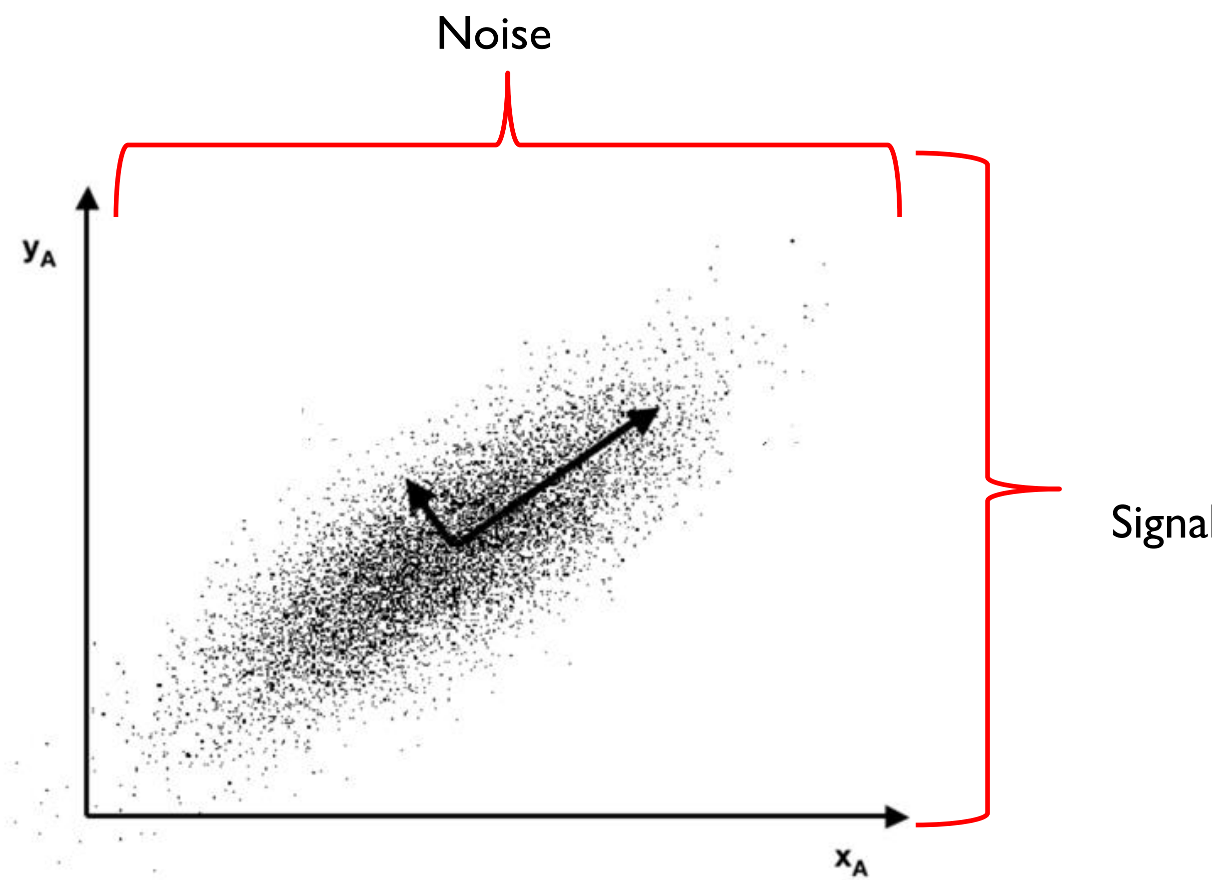



- Maximize

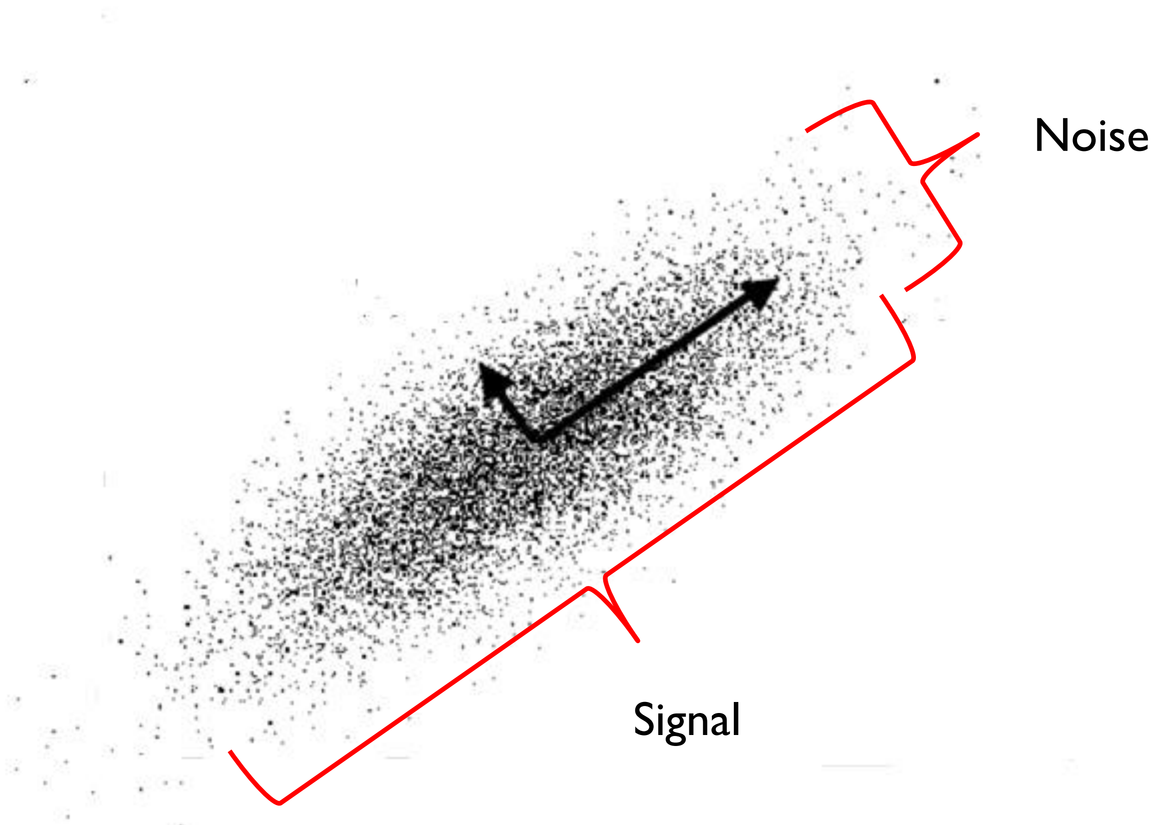
$$SNR = \frac{\sigma^2_{signal}}{\sigma^2_{noise}}.$$

# PCA explained: Signal-noise ratio maximization

- Keep one signal dimension, discard one noisy dimension



# PCA explained: Signal-noise ratio maximization



# PCA explained

- Target
  - 1: Find a new coordinate system which makes different dimensions zero correlated
  - 2: Find a new coordinate system which aligns (top-k) largest variance
- Method
  - Rotate the data point or coordinate
- Mathematically speaking…
  - How to rotate?
  - How to express our criterion

# Mathematatic Basics

- Mean, Variance, Covariance
- Matrix norm, trace,
- Orthogonal matrix, basis
- Eigen decomposition

# Mathematic Basics

- (Sample) Mean

$$\bar{X} = \frac{\sum_{i=1}^{n} X_i}{n}$$

- (Sample) Variance

$$s^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{(n-1)}$$

- (Sample) Covariance

$$cov(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{(n-1)}$$

# Mathematic Basics

- Covariance Matrix

$$C = \begin{pmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{pmatrix}$$

$$\mathbf{C} = \frac{1}{n-1}\sum_{i=1}^{n}(\mathbf{X}_i - \bar{\mathbf{X}})(\mathbf{X}_i - \bar{\mathbf{X}})^T$$

# Mathematatic Basics

- Frobenius norm

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2}$$

- Trace

$$\operatorname{tr}(A) = a_{11} + a_{22} + \cdots + a_{nn} = \sum_{i=1}^{n} a_{ii}$$

$$\operatorname{tr}(X^{\mathrm{T}}Y) = \operatorname{tr}(XY^{\mathrm{T}}) = \operatorname{tr}(Y^{\mathrm{T}}X) = \operatorname{tr}(YX^{\mathrm{T}})$$

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n}|a_{ij}|^2} = \sqrt{\operatorname{trace}(A^*A)}$$

# Mathematic Basics

- Symmetric Matrix $\mathbf{A} = \mathbf{A}^T$
- Covariance matrix is symmetric

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

$$\mathbf{C} = \mathbf{C}^T$$

# Mathematic Basics

- Orthogonal matrix

$$Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = I,$$

- Rotation effect

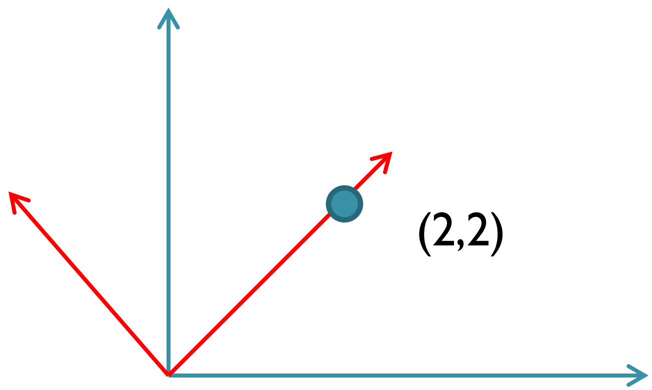
$$\|\mathbf{Qx}\|_F = \sqrt{\mathrm{trace}(\mathbf{x}^T\mathbf{Q}^T\mathbf{Qx})} = \sqrt{\mathrm{trace}(\mathbf{x}^T\mathbf{x})} = \|\mathbf{x}\|_F$$

$$\mathbf{x} = \mathbf{Q}^T\mathbf{Qx}$$

# Mathematic Basics

- Relationship to coordinate system
  - A point = linear combination of bases
  - Combination weight = coordinate
- Each row (column) of Q = basis
  - Not unique
  - Relation to coordinate rotation
- New coordinate $Qx$

# Mathematic Basics




$$\begin{pmatrix}2\\2\end{pmatrix} = 2\begin{pmatrix}1\\0\end{pmatrix} + 2\begin{pmatrix}0\\1\end{pmatrix}$$

$$\begin{pmatrix}2\\2\end{pmatrix} = 2\sqrt{2}\begin{pmatrix}\frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}}\end{pmatrix} + 0\begin{pmatrix}\frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}}\end{pmatrix}$$

New coordinate

$$\begin{pmatrix}2\sqrt{2}\\0\end{pmatrix} = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\\\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}2\\2\end{pmatrix}$$

Old coordinate

# Mathematic Basics

- Eigenvalue and Eigenvector

$$\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$$

- Properties
  - Multiple solutions
  - Scaling invariant
  - Relation to the rank of A

# Mathematatic Basics

## Eigen-decomposition

- If $\mathbf{A}$ is symmetric

$$\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T \qquad Q^{\mathrm{T}}Q = QQ^{\mathrm{T}} = I,$$

# PCA: solution

- Target 1: de-correlation

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

$$\mathbf{Y} = \mathbf{P}\mathbf{X}$$

$$\begin{aligned}\mathbf{C}_Y &= \frac{1}{n-1}\mathbf{P}\mathbf{X}(\mathbf{P}\mathbf{X})^T \\ &= \frac{1}{n-1}\mathbf{P}\mathbf{X}\mathbf{X}^T\mathbf{P}^T \\ &= \frac{1}{n-1}\mathbf{P}\mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{\mathbf{T}}\mathbf{P}^{\mathbf{T}}\end{aligned}$$

# PCA: solution

$$\mathbf{C}_Y = \frac{1}{n-1}\mathbf{PX}(\mathbf{PX})^T$$
$$= \frac{1}{n-1}\mathbf{PXX}^T\mathbf{P}^T$$
$$= \frac{1}{n-1}\mathbf{PQ\Lambda Q^T P^T}$$

$$\text{if} \quad \mathbf{P} = \mathbf{Q}^T$$

$$\mathbf{C}_Y = \frac{1}{n-1}\mathbf{\Lambda}$$

# PCA: solution

- Variance of each dimension

$$\begin{aligned}\mathrm{Var}(y_k) &= \frac{1}{n-1}\mathbf{P}_k\mathbf{X}\mathbf{X}^T\mathbf{P}_k^T \\ &= \frac{1}{n-1}\mathbf{p}_k\mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^{\mathbf{T}}\mathbf{p}_k^T \\ &= \frac{1}{n-1}\lambda_k\end{aligned}$$

- Rank dimensions according to their corresponding eigenvalues

# PCA: algorithm

- 1. Subtract mean
- 2. Calculate the covariance matrix
- 3. Calculate eigenvectors and eigenvalues of the covariance matrix
- 4. Rank eigenvectors by its corresponding eigenvalues
- 4. Obtain P with its column vectors corresponding to the top k eigenvectors

# PCA: MATLAB code

```
Mu = mean(fea);
fea = fea - repmat(Mu,[size(fea,1),1]);
Cov = fea'*fea;
[V,D] = eig(Cov);
[value,rank_idx] = sort(diag(D),'descend');
P = V(:,rank_idx(1:10));
```

# PCA: reconstruction

- Reconstruct x

$$\hat{\mathbf{x}} = \hat{\mathbf{P}}^T \hat{\mathbf{P}} \mathbf{x}$$

- Derive PCA through minimizing the reconstruction error

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

# PCA: reconstruction

- Reighley Quotient

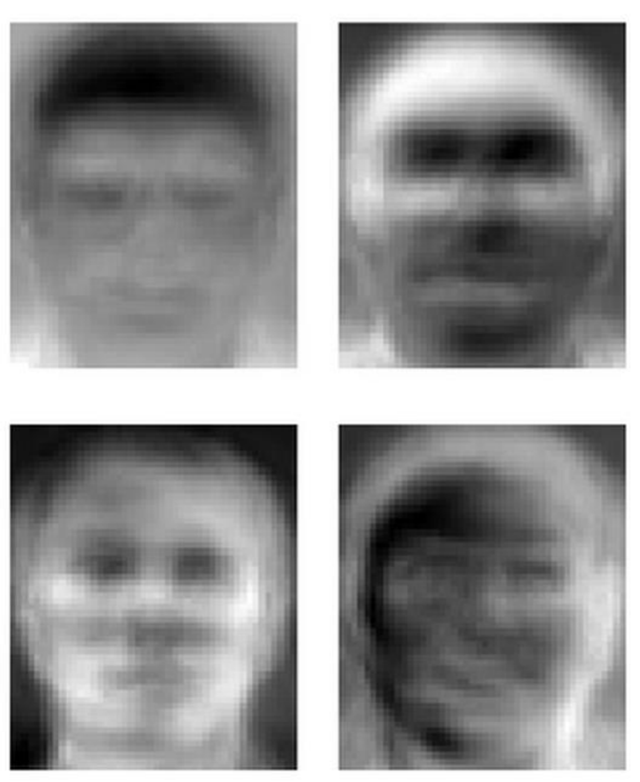
$$\max_{\mathbf{P}} \ \mathrm{trace}(\mathbf{P}\mathbf{X}\mathbf{X}^T\mathbf{P}^T)$$
$$s.t. \ \mathbf{P}\mathbf{P}^T = \mathbf{I}$$

- Solution = PCA

# Application: Eigen-face method

- Sirovich and Kirby (1987) showed that PCA could be used on a collection of face images to form a set of basis features.
- Not only limited to face recognition
- Steps
  - Image as high-dimensional feature
  - PCA

# Application: Eigen-face method



Some eigenfaces from AT&T Laboratories Cambridge

# Application: Reconstruction

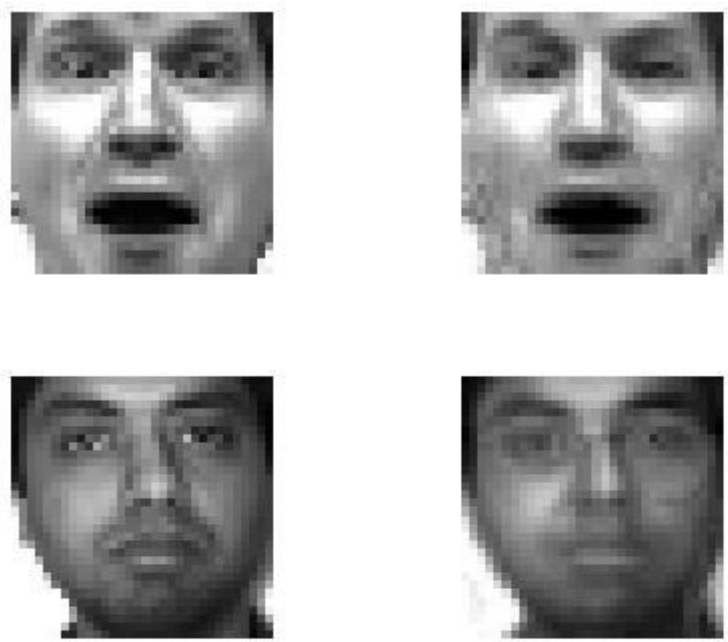
Reconstructed from top-2 eigenvectors

# Application: Reconstruction

- Reconstructed from top-15 eigenvectors

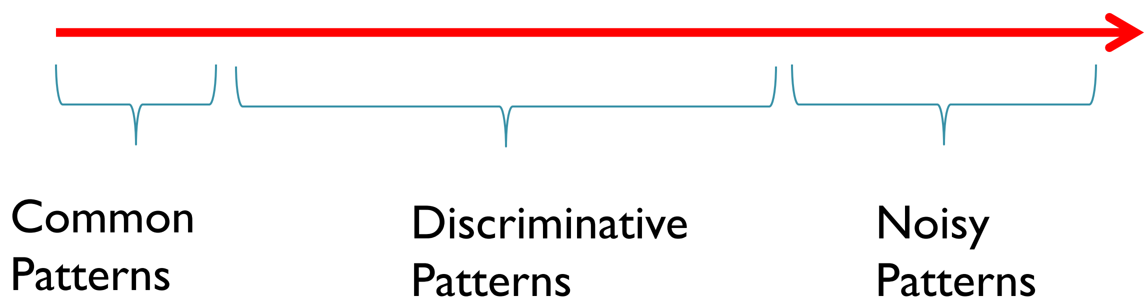
# Application: Reconstruction

- Reconstructed from top-40 eigenvectors



# Application: Eigen-face method

- From large to small eigenvalues



# Eigen-face method: How to handle high dimensionality

- For high-dimensional data $\mathbf{C}_X = \frac{1}{n-1}\mathbf{X}\mathbf{X}^T$ can be too large
- The number of samples is relatively small

$$d \gg N$$

$$\mathbf{X}^T\mathbf{X}\mathbf{v} = \lambda\mathbf{v}$$

$$\mathbf{X}\mathbf{X}^T(\mathbf{X}\mathbf{v}) = \lambda(\mathbf{X}\mathbf{v})$$

$$\text{Define} \quad \mathbf{u} = \mathbf{X}\mathbf{v}$$

$$\mathbf{X}\mathbf{X}^T\mathbf{u} = \lambda\mathbf{u}$$

# Eigen-face method: How to handle high dimensionality

- 1. Centralize data
- 2. Calculate the kernel matrix
- 3. Perform Eigen-decomposition on the kernel matrix and obtain its eigenvector $\mathbf{v}$
- 4. Obtain the Eigenvector of the covariance matrix by $\mathbf{u} = \mathbf{X}\mathbf{v}$
- Question? How many eigenvectors you can obtain in this way?

# Extension: Kernel PCA

- Kernel Method

$$\mathbf{x} \to \phi(\mathbf{x})$$

- You do not have access to $\phi(\mathbf{x})$ but you know

$$k(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle$$

# Extension: Kernel PCA

- Use the same way as how we handle high-dimensional data

$$\mathbf{u} = \phi(\mathbf{X})\mathbf{v}$$

$$\mathbf{u}^T\mathbf{x}^* = (\phi(\mathbf{X})\mathbf{v})^T\mathbf{x}_i = \sum_{j=1}^{N} v_j \langle \phi(\mathbf{x_j}), \phi(\mathbf{x}^*) \rangle = \sum_{j=1}^{N} v_j k(\mathbf{x}_j, \mathbf{x}^*)$$