IAML: Dimensionality Reduction

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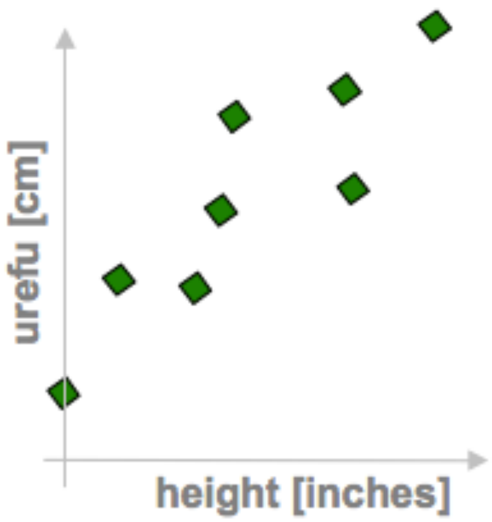
Semester 1

Overview

- Curse of dimensionality
- Different ways to reduce dimensionality
- Principal Components Analysis (PCA)
- Example: Eigen Faces
- PCA for classification
- Witten & Frank section 7.3
  - only the PCA section required

True vs. observed dimensionality

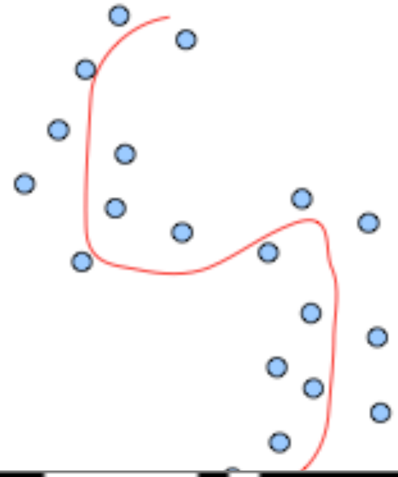
- Get a population, predict some property
  - instances represented as {urefu, height} pairs
  - what is the dimensionality of this data?



- Data points over time from different geographic areas over time:
  - X_1: # of skidding accidents
  - X_2: # of burst water pipes
  - X_3: snow-plow expenditures
  - X_4: # of school closures
  - X_5: # patients with heat stroke

Temperature?

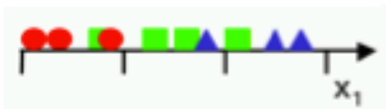
Curse of dimensionality

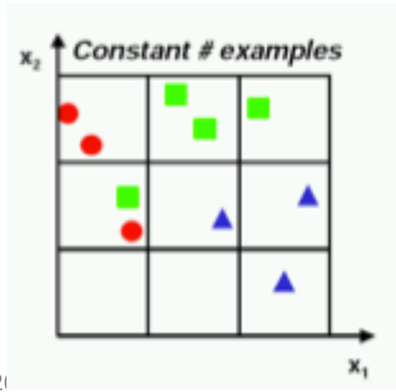


- Datasets typically high dimensional
  - vision: 10^4 pixels, text: 10^6 words
    - the way we observe / record them
  - true dimensionality often much lower
    - a manifold (sheet) in a high-d space
- Example: handwritten digits
  - 20 x 20 bitmap: $\{0,1\}^{400}$ possible events
    - will never see most of these events
    - actual digits: tiny fraction of events
  - true dimensionality:
    - possible variations of the pen-stroke

Curse of dimensionality (2)

- Machine learning methods are statistical by nature
  - count observations in various regions of some space
  - use counts to construct the predictor f(x)
  - e.g. decision trees: p_+/p_- in {o=rain,w=strong,T>28°}
  - text: #documents in {“hp” and “3d” and not “$” and …)
- As dimensionality grows: fewer observations per region
  - 1d: 3 regions, 2d: 3^2 regions, 1000d – hopeless
  - statistics need repetition
    - flip a coin once → head
    - P(head) = 100%?





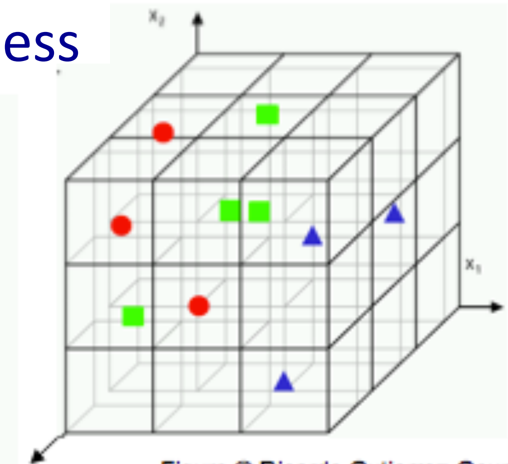
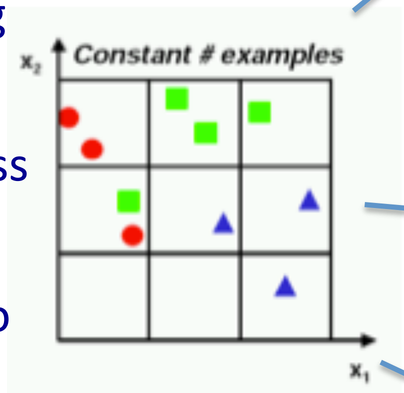
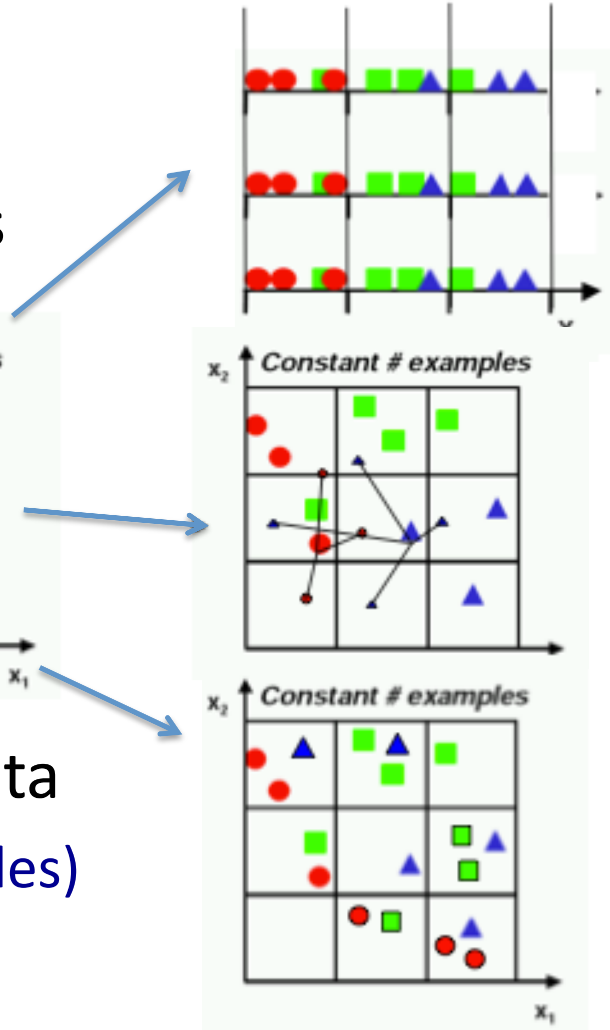


Figure © Ricardo Gutierrez-Osuna

Dealing with high dimensionality

- Use domain knowledge
  - feature engineering: SIFT, MFCC
- Make assumption about dimensions
  - independence: count along each dimension separately
  - smoothness: propagate class counts to neighboring regions
  - symmetry: e.g. invariance to order of dimensions: $x_1 \Leftrightarrow x_2$
- Reduce the dimensionality of the data
  - create a new set of dimensions (variables)

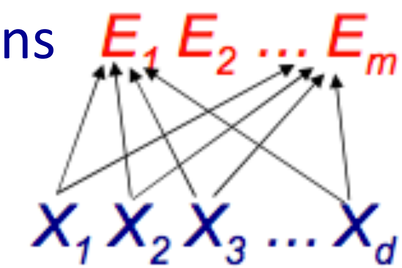




Dimensionality reduction

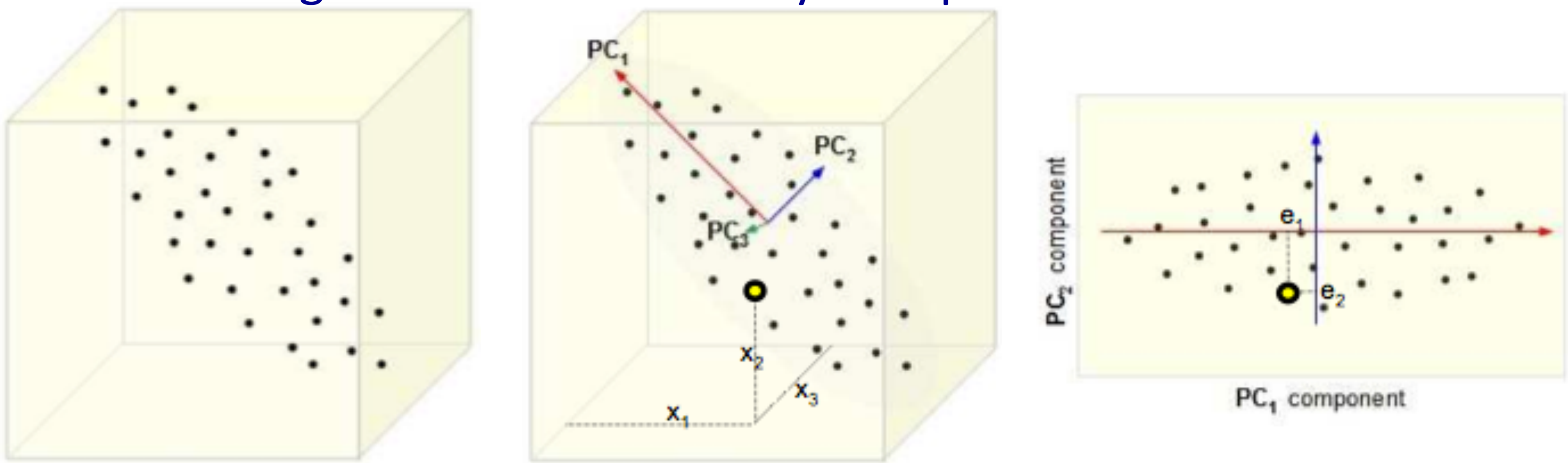
- Goal: represent instances with fewer variables
  - try to preserve as much structure in the data as possible
  - discriminative: only structure that affects class separability
- Feature selection
  - pick a subset of the original dimensions $X_1\ X_2\ X_3 \ldots X_{d-1}\ X_d$
  - discriminative: pick good class "predictors" (e.g. gain)
- Feature extraction
  - construct a new set of dimensions

    $E_i = f(X_1 \ldots X_d)$
  - (linear) combinations of original



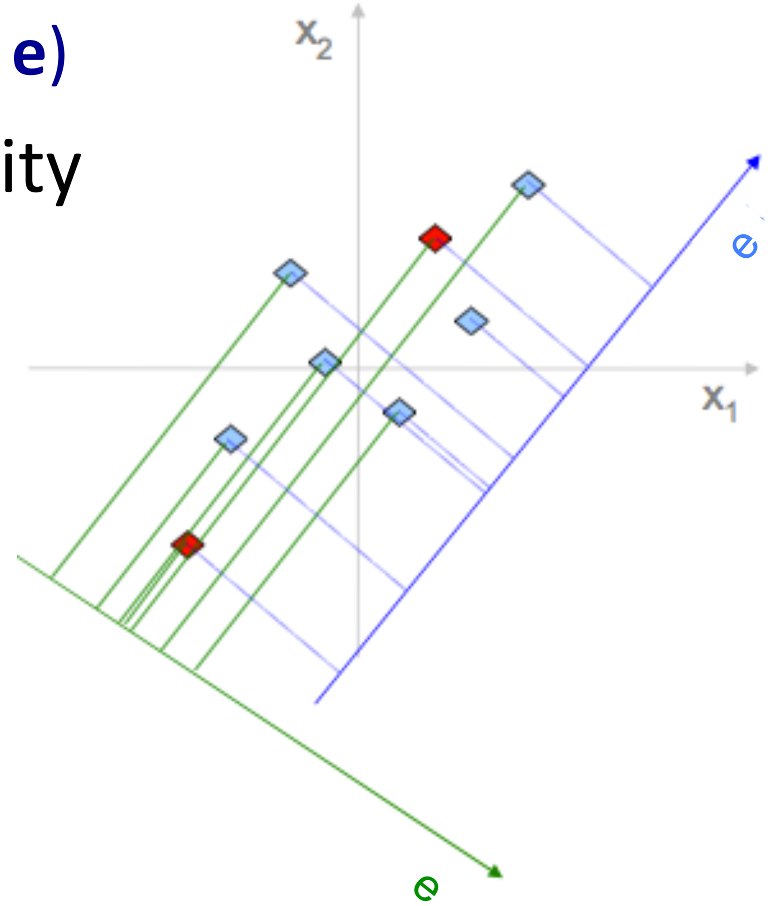
Principal Components Analysis

- Defines a set of principal components
  - 1st: direction of the greatest variability in the data
  - 2nd: perpendicular to 1st, greatest variability of what's left
  - ... and so on until d (original dimensionality)
- First *m<<d* components become *m* new dimensions
  - change coordinates of every data point to these dimensions

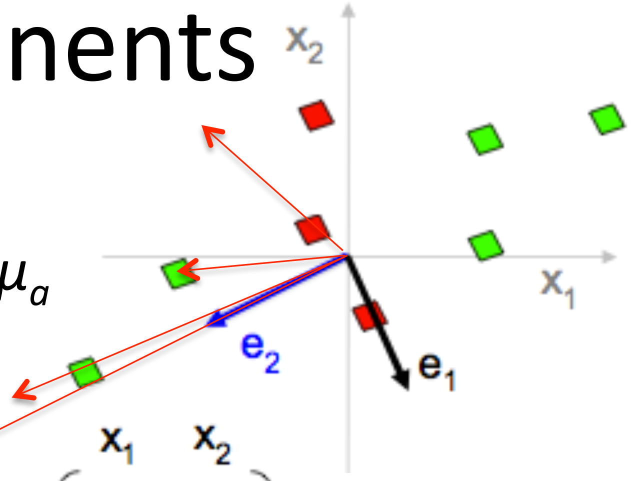


Why greatest variability?

- Example: reduce 2-dimensional data to 1-d
  - $\{x_1,x_2\} \rightarrow e'$ (along new axis **e**)
- Pick *e* to maximize variability
- Reduces cases when two points are close in **e**-space but very far in (x,y)-space
- Minimizes distances between original points and their projections



Principal components



- "Center" the data at zero: $x_{i,a} = x_{i,a} - \mu_a$
  - subtract mean from each attribute
- Compute covariance matrix Σ
  - covariance of dimensions x_1 and x_2:
    - do x_1 and x_2 tend to increase together?
    - or does x_2 decrease as x_1 increases?

$$\begin{array}{c|cc} & x_1 & x_2 \\ \hline x & 2.0 & 0.8 \\ x_2^1 & 0.8 & 0.6 \end{array}$$

$$\mathrm{var}(a) = \frac{1}{n}\sum_{i=1}^{n} x_{ia}^2$$

$$\mathrm{cov}(b,a) = \frac{1}{n}\sum_{i=1}^{n} x_{ib}x_{ia}$$

- Multiply a vector by Σ: $\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} -1 \\ +1 \end{pmatrix} \rightarrow \begin{pmatrix} -1.2 \\ -0.2 \end{pmatrix}$ again $\rightarrow \begin{pmatrix} -2.5 \\ -1.0 \end{pmatrix} \rightarrow \begin{pmatrix} -6.0 \\ -2.7 \end{pmatrix} \rightarrow \begin{pmatrix} -14.1 \\ -6.4 \end{pmatrix} \rightarrow \begin{pmatrix} -33.3 \\ -15.1 \end{pmatrix}$
  - turns towards direction of variance

slope: 0.400 0.450 0.454 0.454

- Want vectors **e** which aren't turned: Σ **e** = λ **e**
  - e … eigenvectors of Σ, λ … corresponding eigenvalues
  - principal components = eigenvectors w. largest eigenvalues

Finding Principal Components

1. find eigenvalues by solving: det(Σ – λI) = 0

$$\det\begin{pmatrix} 2.0-\lambda & 0.8 \\ 0.8 & 0.6-\lambda \end{pmatrix} = (2-\lambda)(0.6-\lambda)-(0.8)(0.8) \;= \lambda^2 - 2.6\lambda + 0.56 = 0$$

$$\{\lambda_1, \lambda_2\} = \tfrac{1}{2}\left(2.6 \pm \sqrt{2.6^2 - 4 * 0.56}\right) = \{2.36, 0.23\}$$

2. find i^{th} eigenvector by solving: $\Sigma\, \mathbf{e}_i = \lambda_i\, \mathbf{e}_i$

$$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} e_{1,1} \\ e_{1,2} \end{pmatrix} = 2.36\begin{pmatrix} e_{1,1} \\ e_{1,2} \end{pmatrix} \Rightarrow \begin{matrix} 2.0e_{1,1} + 0.8e_{1,2} = 2.36e_{1,1} \\ 0.8e_{1,1} + 0.6e_{1,2} = 2.36e_{1,2} \end{matrix} \Rightarrow e_{1,1} = 2.2e_{1,2}$$

$$\Downarrow$$

$$e_1 \sim \begin{bmatrix} 2.2 \\ 1 \end{bmatrix}$$

$$\Downarrow$$ want: $\|e_1\| = 1$

$$e_1 = \begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix}$$

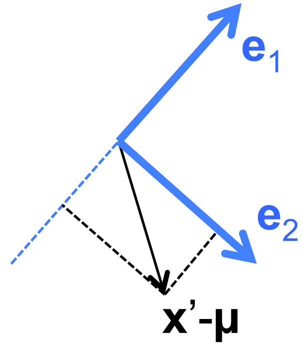
slope: 0.454

$$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix}\begin{pmatrix} e_{2,1} \\ e_{2,2} \end{pmatrix} = 0.23\begin{pmatrix} e_{2,1} \\ e_{2,2} \end{pmatrix} \Rightarrow e_2 = \begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$$

3. 1^{st} PC: $\begin{bmatrix} 0.91 \\ 0.41 \end{bmatrix}$, 2^{nd} PC: $\begin{bmatrix} -0.41 \\ 0.91 \end{bmatrix}$

Projecting to new dimensions

- $\mathbf{e}_1 \ldots \mathbf{e}_m$ are new dimension vectors
- Have instance $\mathbf{x} = \{x_1 \ldots x_d\}$ (original coordinates)
- Want new coordinates $\mathbf{x}' = \{x'_1 \ldots x'_m\}$:
  1. "center" the instance (subtract the mean): $\mathbf{x}'-\boldsymbol{\mu}$
  2. "project" to each dimension: $(\mathbf{x}'-\boldsymbol{\mu})^T\mathbf{e}_j$ for j=1…m

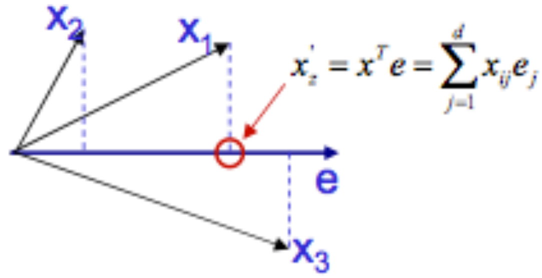


$$(\vec{x}-\vec{\mu}) = \begin{bmatrix}(x_1-\mu_1) & (x_2-\mu_2) & \cdots & (x_d-\mu_d)\end{bmatrix}$$

$$\begin{bmatrix} x_1' \\ x_2' \\ \vdots \\ x_m' \end{bmatrix} = \begin{bmatrix} (\vec{x}-\vec{\mu})^T\vec{e}_1 \\ (\vec{x}-\vec{\mu})^T\vec{e}_2 \\ \vdots \\ (\vec{x}-\vec{\mu})^T\vec{e}_m \end{bmatrix} = \begin{bmatrix} (x_1-\mu_1)e_{1,1} + (x_2-\mu_2)e_{1,2} + \cdots + (x_d-\mu_d)e_{1,d} \\ (x_1-\mu_1)e_{2,1} + (x_2-\mu_2)e_{2,2} + \cdots + (x_d-\mu_d)e_{2,d} \\ \vdots \\ (x_1-\mu_1)e_{m,1} + (x_2-\mu_2)e_{m,2} + \cdots + (x_d-\mu_d)e_{m,d} \end{bmatrix}$$

Direction of greatest variability

- Select dimension **e** which maximizes the variance
- Points $\boldsymbol{x}_i$ "projected" onto vector **e**:



- Variance of projections: $\frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j - \mu\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j\right)^2$
- Maximize variance
  - want unit length: ||**e**||=1
  - add Lagrange multiplier

$$V = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j\right)^2 - \lambda\left(\left(\sum_{k=1}^{d} e_j^2\right) - 1\right)$$

$$\frac{\partial V}{\partial e_a} = \frac{2}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j\right)x_{ia} - 2\lambda e_a = 0$$

$$2\sum_{j=1}^{d} e_j \underbrace{\left(\frac{1}{n}\sum_{i=1}^{n} x_{ia}x_{ij}\right)}_{\text{covariance of a,j}} = 2\lambda e_a$$

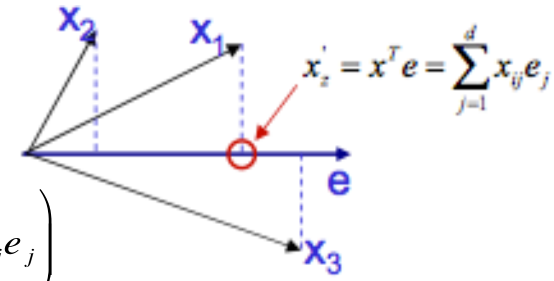
hold for *a=1..d*

$$\left\{\begin{array}{c} \sum_{j=1}^{d} \mathrm{cov}(1,j)e_j = \lambda e_1 \\ \vdots \\ \sum_{j=1}^{d} \mathrm{cov}(d,j)e_j = \lambda e_d \end{array}\right\}$$

$$\Sigma e = \lambda e$$

e must be an eigenvector

Variance along eigenvector



Variance of projected points ($\mathbf{x}^T\mathbf{e}$):

$$\frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j - \mu\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j\right)^2$$

$$\mu = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j\right) = \sum_{j=1}^{d}\left(\frac{1}{n}\sum_{i=1}^{n} x_{ij}\right)e_j$$

$$= \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{d} x_{ij}e_j\right)\left(\sum_{a=1}^{d} x_{ia}e_a\right)$$

$$= \sum_{a=1}^{d}\sum_{j=1}^{d}\left(\frac{1}{n}\sum_{i=1}^{n} x_{ia}x_{ij}\right)e_j e_a$$

$$= \sum_{a=1}^{d}\left(\sum_{j=1}^{d} \mathrm{cov}(a,j)e_j\right)e_a$$

$$\mathrm{cov}(a,j) = \frac{1}{n}\sum_{i=1}^{n} x_{ia}x_{ij}$$

$$= \sum_{a=1}^{d}(\lambda e_a)e_a$$

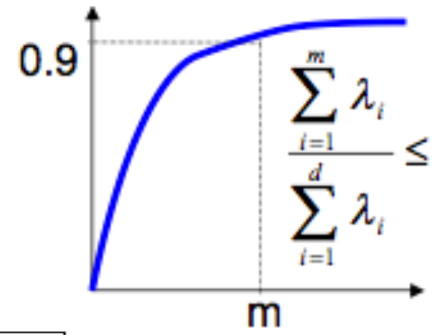
$$\sum_{j=1}^{d} \mathrm{cov}(a,j)e_j = \lambda e_a$$

e is an eigenvector of the covariance matrix

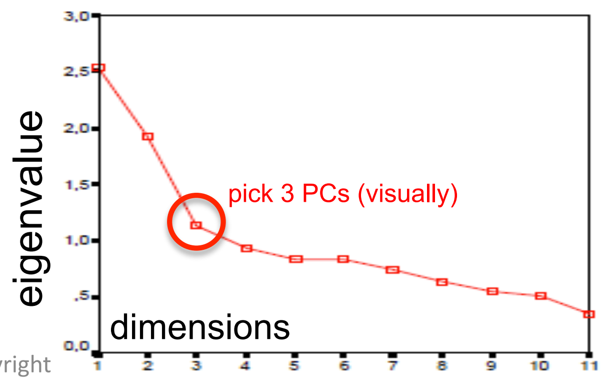
$$= \lambda\|e\|^2 = \lambda$$

How many dimensions?

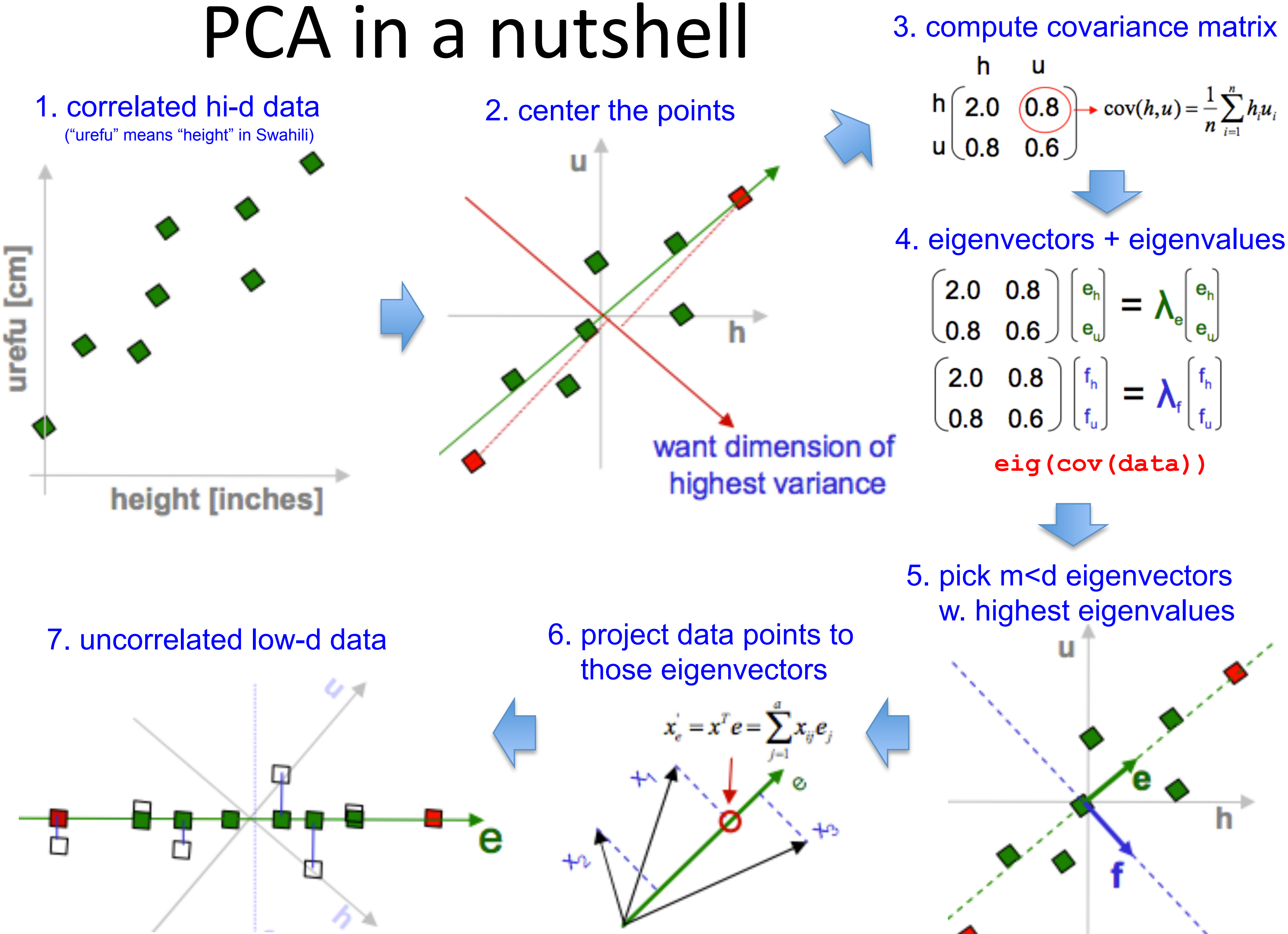
- Have: eigenvectors $\mathbf{e}_1 \ldots \mathbf{e}_d$ want: $m << d$
- Proved: eigenvalue λ_i = variance along $\mathbf{e}_i$
- Pick $\mathbf{e}_i$ that “explain” the most variance
  - sort eigenvectors s.t. $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$
  - pick first m eigenvectors which explain 90% or the total variance
    - typical threshold values: 0.9 or 0.95



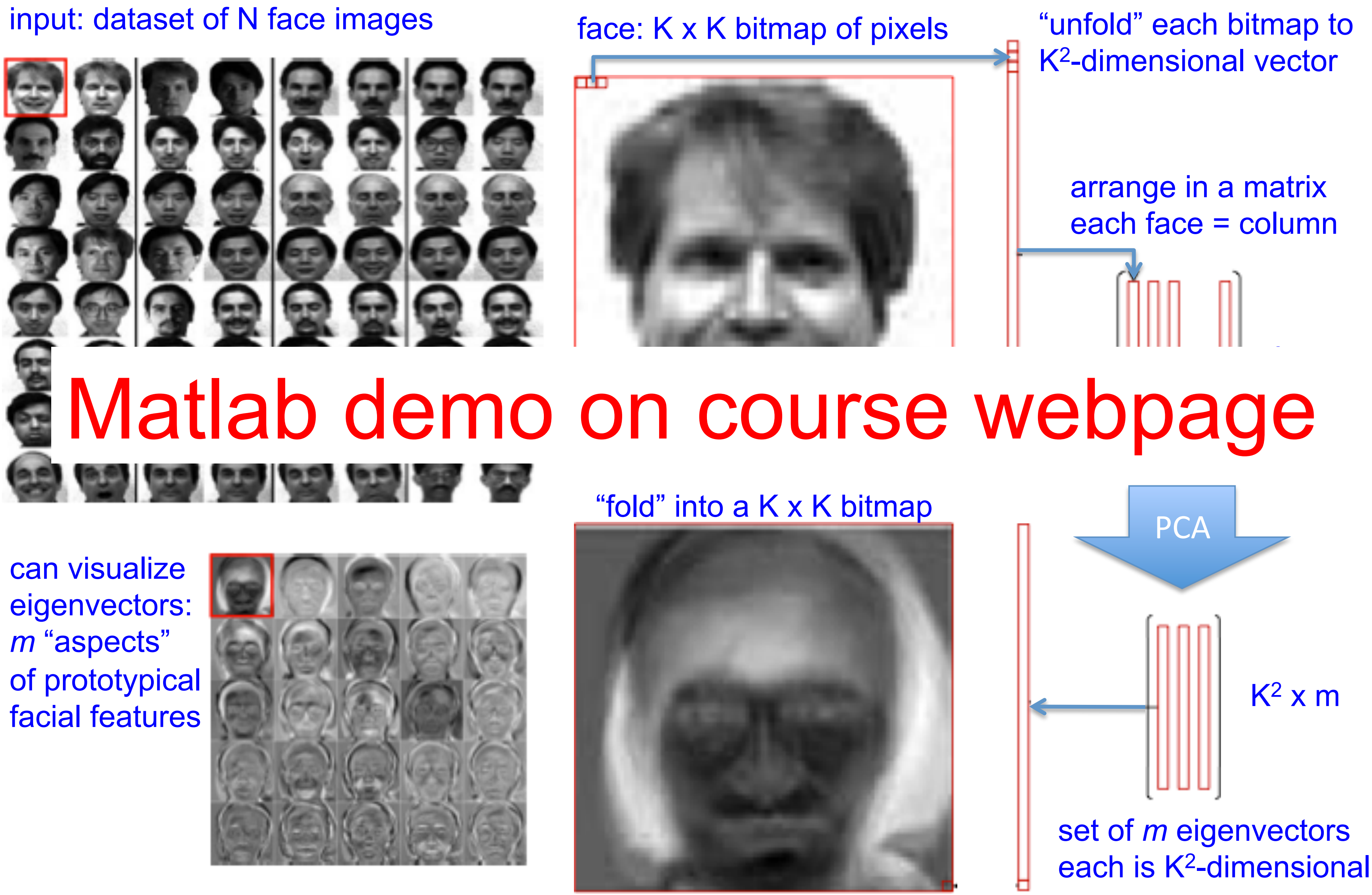
- Or use a scree plot:
  - like K-means



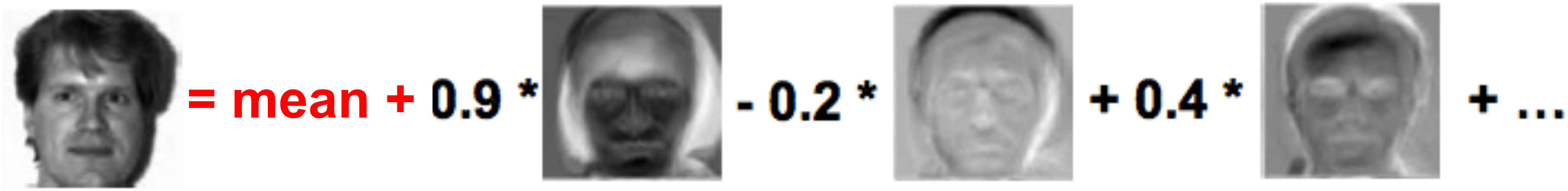
PCA in a nutshell

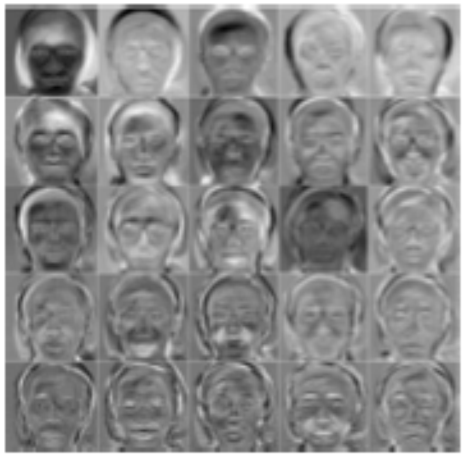


PCA example: Eigen Faces

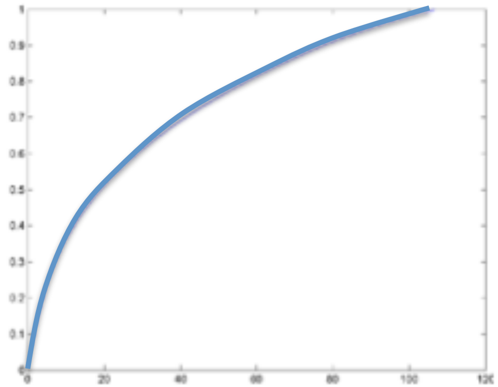


Eigen Faces: Projection





- Project new face to space of eigen-faces
- Represent vector as a linear combination of principal components
- How many do we need?



(Eigen) Face Recognition

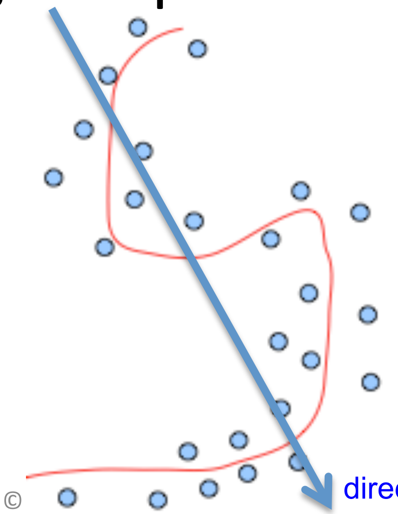
- Face similarity
  - in the reduced space
  - insensitive to lighting expression, orientation
- Projecting new "faces"
  - everything is a face

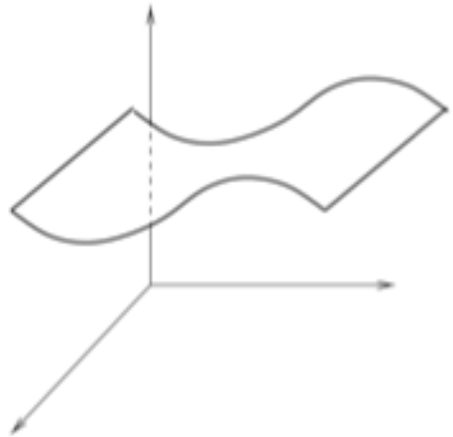
new face

projected to eigenfaces

PCA: practical issues

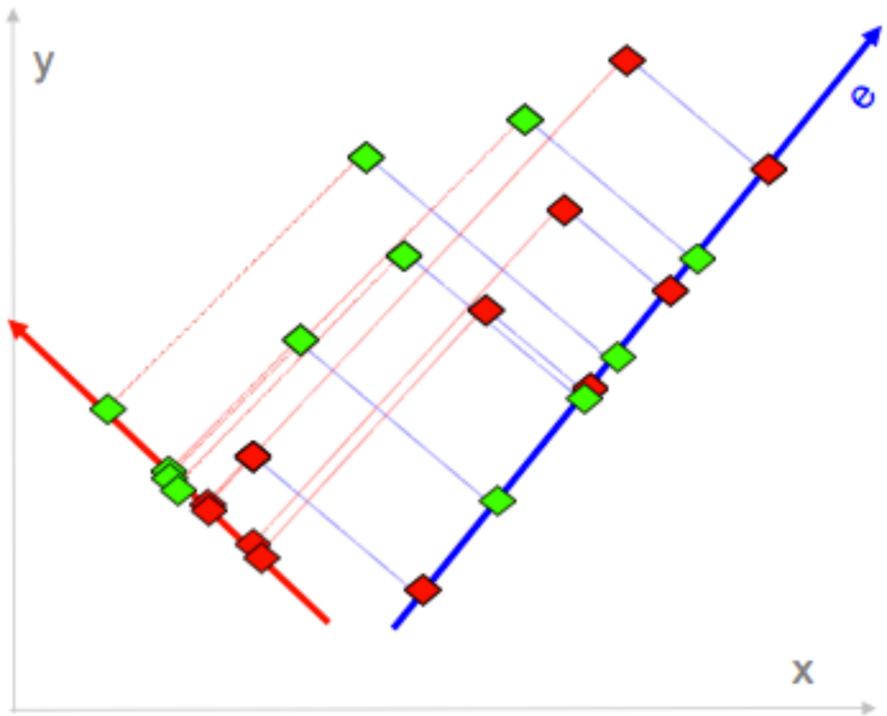
- Covariance extremely sensitive to large values
  - multiply some dimension by 1000
    - dominates covariance
    - becomes a principal component
  - normalize each dimension to zero mean and unit variance:
    $\boldsymbol{x}' = (\boldsymbol{x} - \text{mean}) / \text{st.dev}$
- PCA assumes underlying subspace is linear
  - 1d: straight line
    2d: flat sheet
  - transform to handle
    non-linear spaces
    (manifolds)





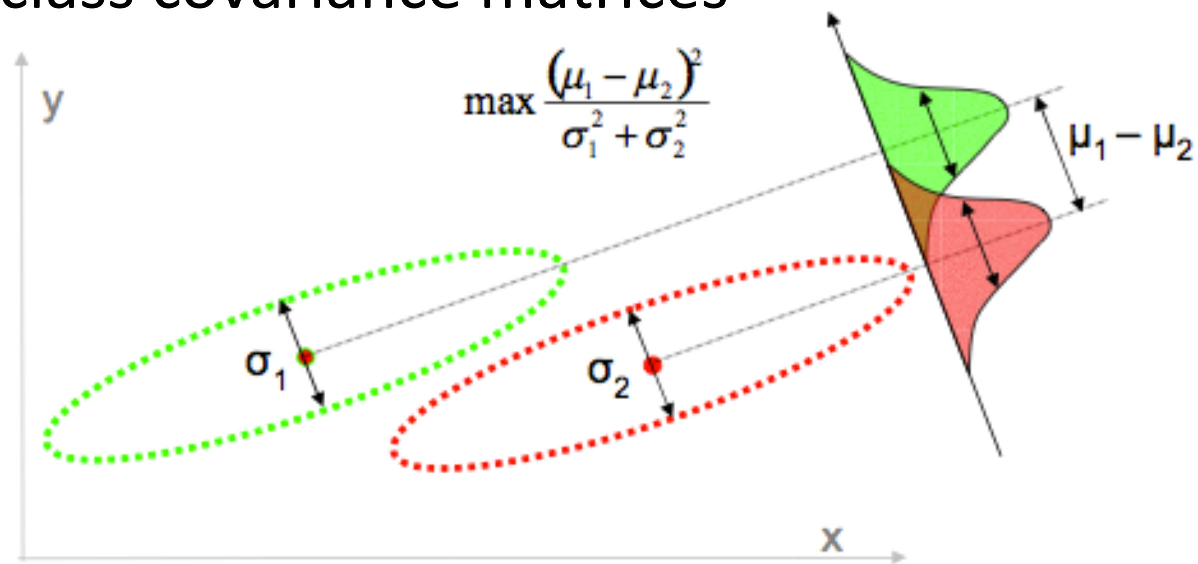
PCA and classification

- PCA is unsupervised
  - maximizes overall variance of the data along a small set of directions
  - does not know anything about class labels
  - can pick direction that makes it hard to separate classes
- Discriminative approach
  - look for a dimension that makes it easy to separate classes



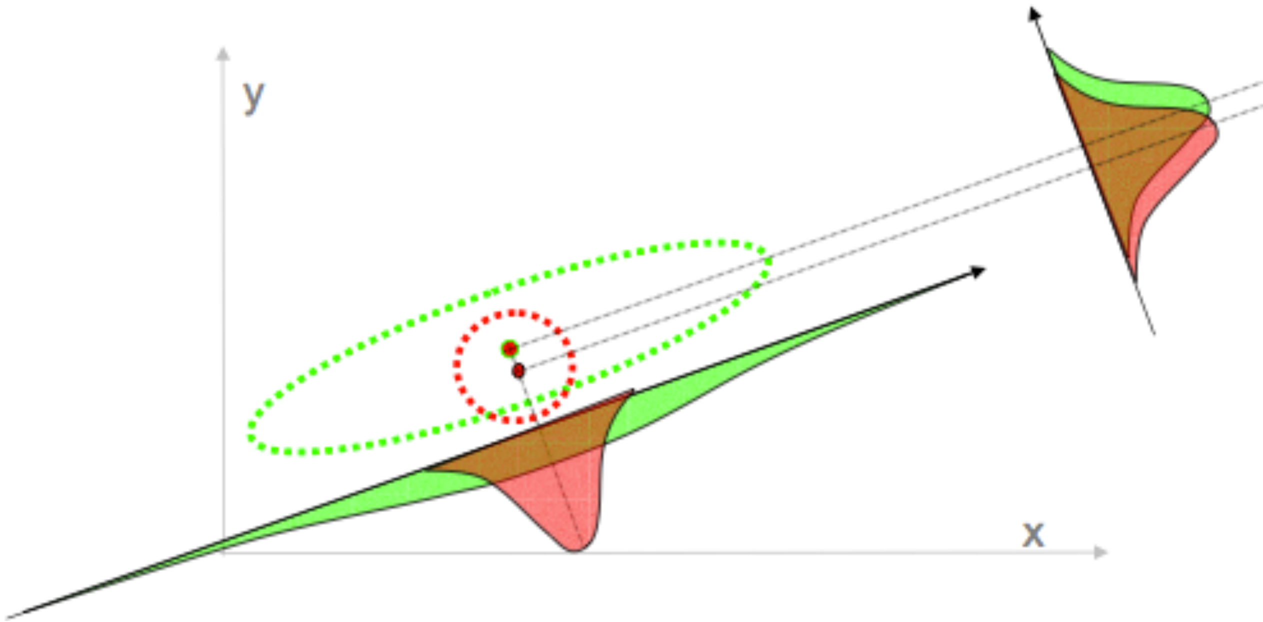
Linear Discriminant Analysis

- LDA: pick a new dimension that gives:
  - maximum separation between means of projected classes
  - minimum variance within each projected class
- Solution: eigenvectors based on between-class and within-class covariance matrices



PCA vs. LDA

- LDA not guaranteed to be better for classification
  - assumes classes are unimodal Gaussians
  - fails when discriminatory information is not in the mean, but in the variance of the data
- Example where PCA gives a better projection:



Dimensionality reduction

- Pros
  - reflects our intuitions about the data
  - allows estimating probabilities in high-dimensional data
    - no need to assume independence etc.
  - dramatic reduction in size of data
    - faster processing (as long as reduction is fast), smaller storage
- Cons
  - too expensive for many applications (Twitter, web)
  - disastrous for tasks with fine-grained classes
  - understand assumptions behind the methods (linearity etc.)
    - there may be better ways to deal with sparseness

Summary

- True dimensionality << observed dimensionality
- High dimensionality ➔ sparse, unstable estimates
- Dealing with high dimensionality:
  - use domain knowledge
  - make an assumption: independence / smoothness / symmetry
  - dimensionality reduction: feature selection / feature extraction
- Principal Components Analysis (PCA)
  - picks dimensions that maximize variability
    - eigenvectors of the covariance matrix
  - examples: Eigen Faces
  - variant for classification: Linear Discriminant Analysis