Linear Dimensionality Reduction

Practical Machine Learning (CS294-34)

September 24, 2009

Percy Liang

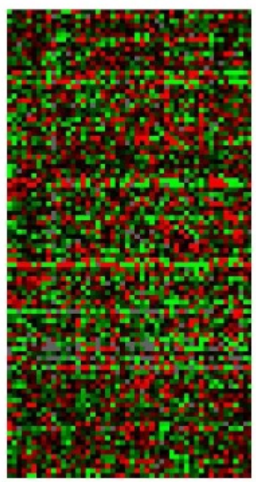
Lots of high-dimensional data...

face images

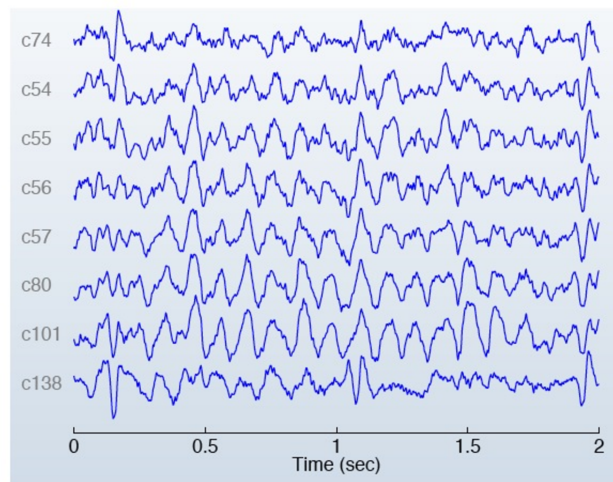
Zambian President Levy Mwanawasa has won a second term in office in an election his challenger Michael Sata accused him of rigging, official results showed on Monday.

According to media reports, a pair of hackers said on Saturday that the Firefox Web browser, commonly perceived as the safer and more customizable alternative to market leader Internet Explorer, is critically flawed. A presentation on the flaw was shown during the ToorCon hacker conference in San Diego.

documents



gene expression data



MEG readings

Motivation and context

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Dimensionality reduction in this course:

- Linear methods (this week)
- Clustering (last week)
- Feature selection (next week)
- Nonlinear methods (later)

Types of problems

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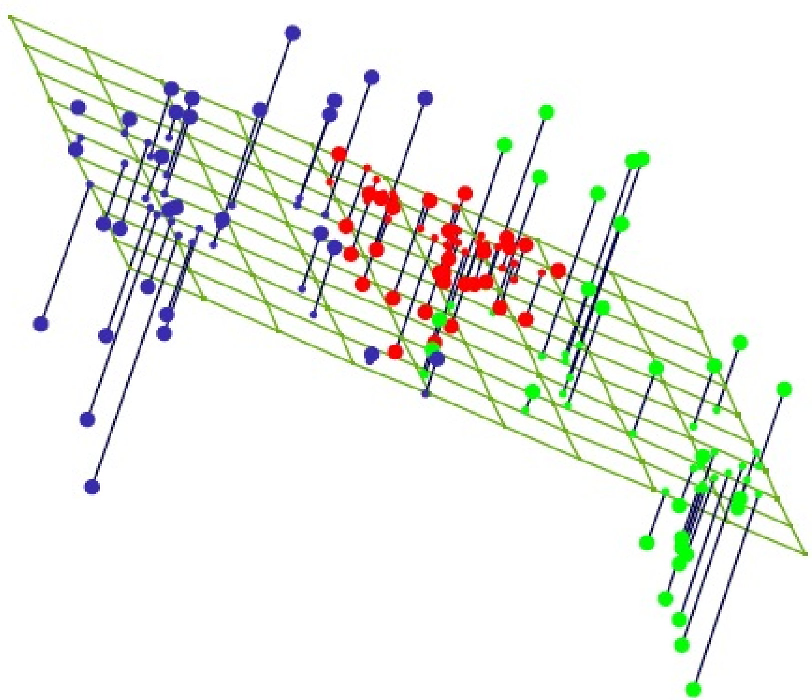

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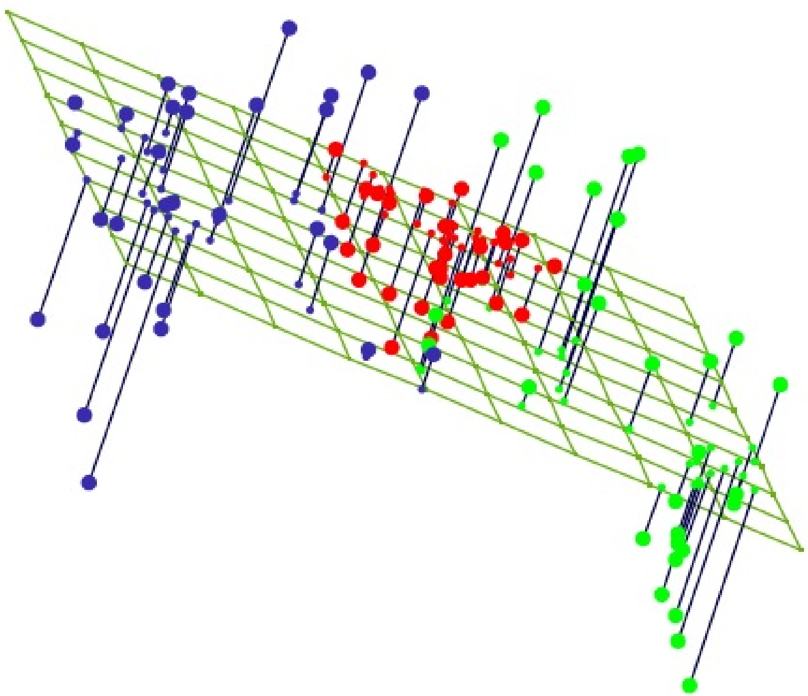

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How do we choose $\mathbf{U}$?

Outline

- Principal component analysis (PCA)
  - Basic principles
  - Case studies
  - Kernel PCA
  - Probabilistic PCA
- Canonical correlation analysis (CCA)
- Fisher discriminant analysis (FDA)
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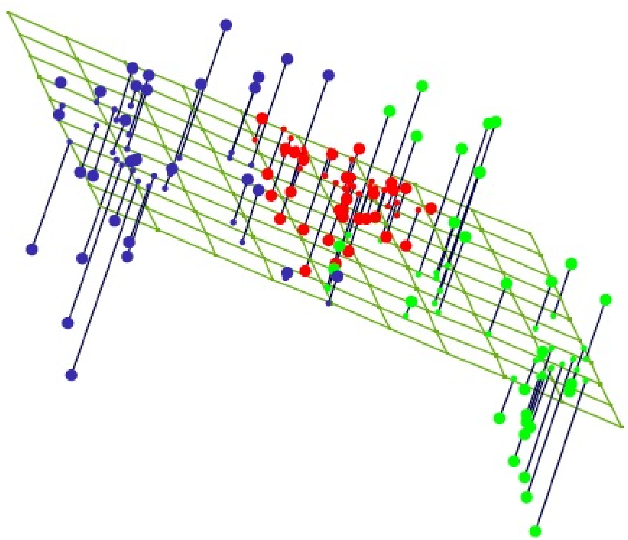
Objective: minimize total squared reconstruction error



$$\min_{\mathbf{U} \in \mathbb{R}^{d \times k}} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{U}\mathbf{U}^\top \mathbf{x}_i\|^2$$

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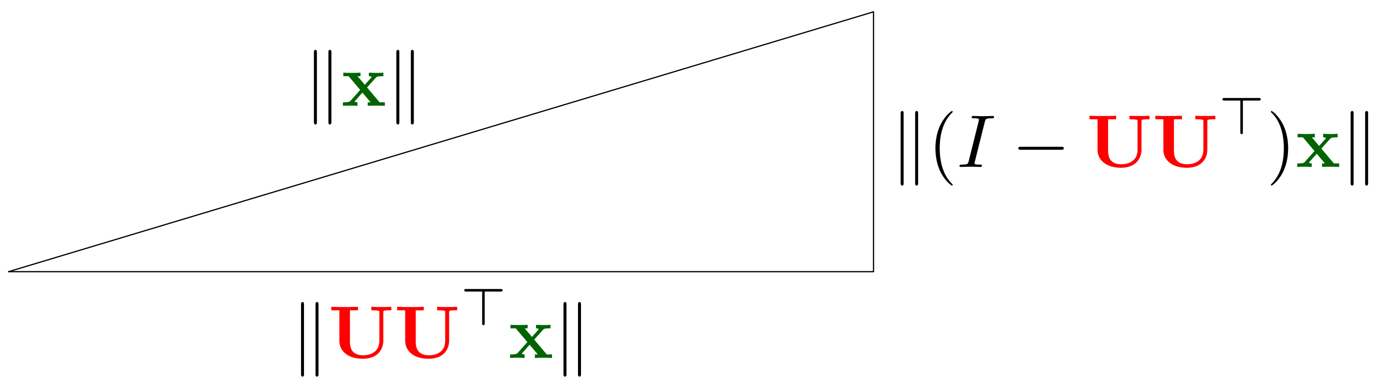

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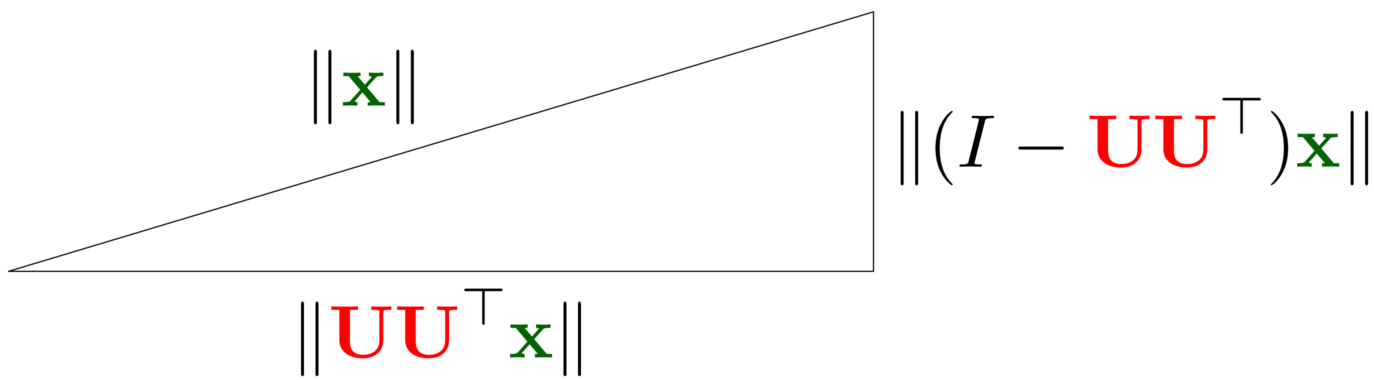

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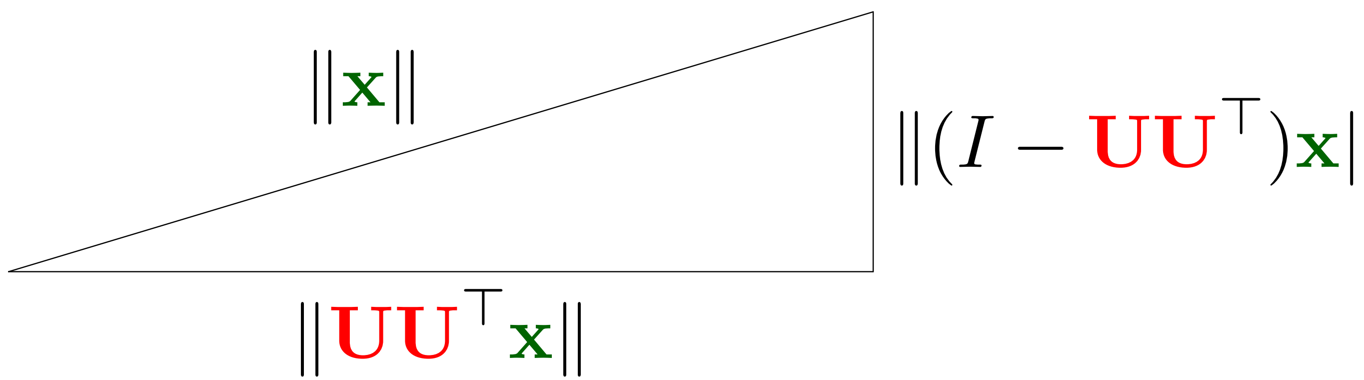

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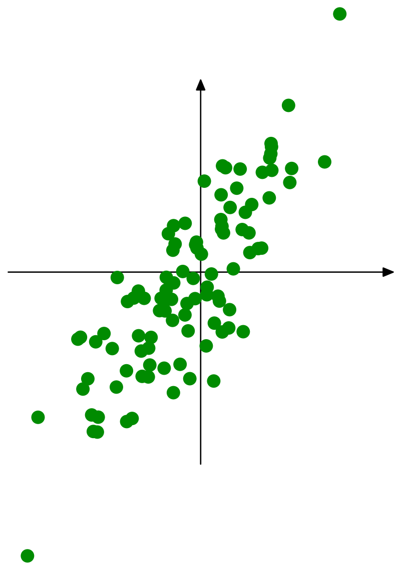
Minimize reconstruction error $\leftrightarrow$ Maximize captured variance

Finding one principal component



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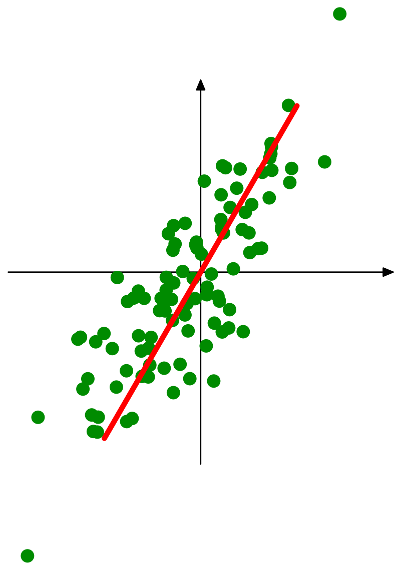

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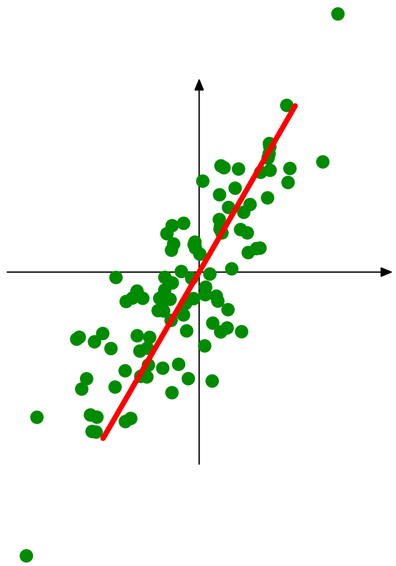

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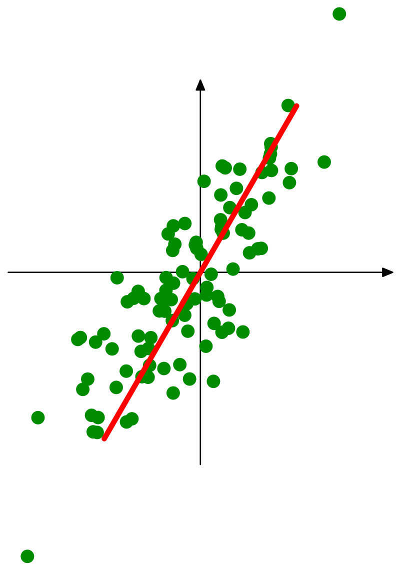

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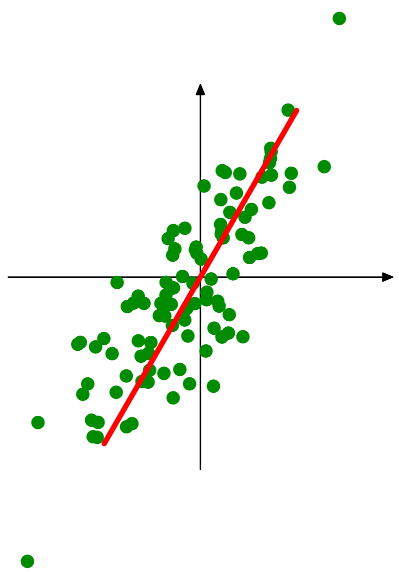

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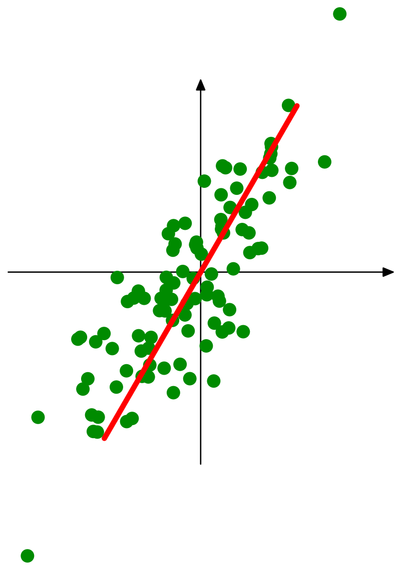

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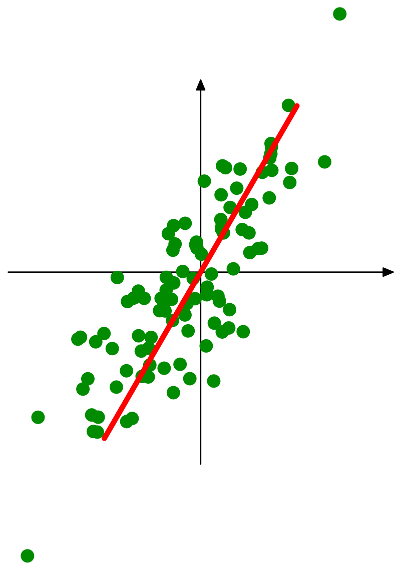

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$=$ largest eigenvalue of $C \stackrel{\text{def}}{=} \frac{1}{n}\mathbf{X}\mathbf{X}^\top$

(C is covariance matrix of data)

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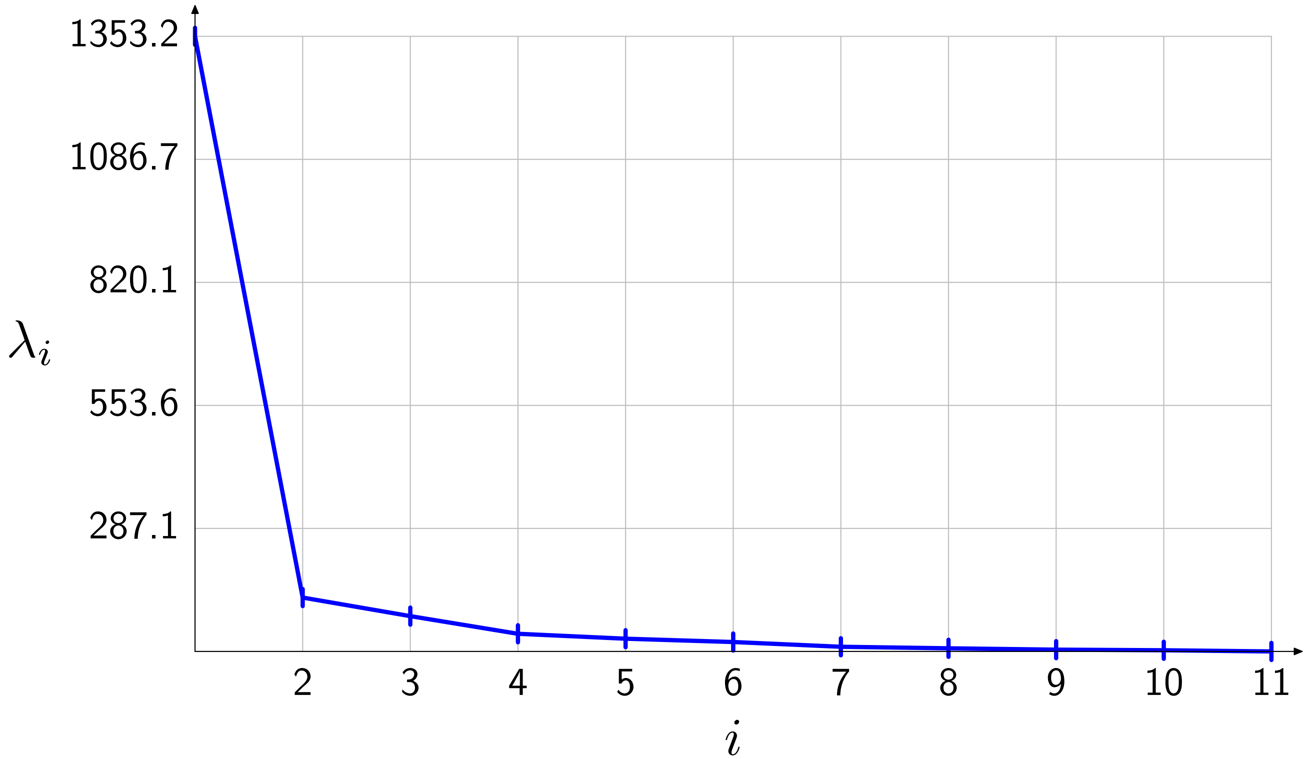

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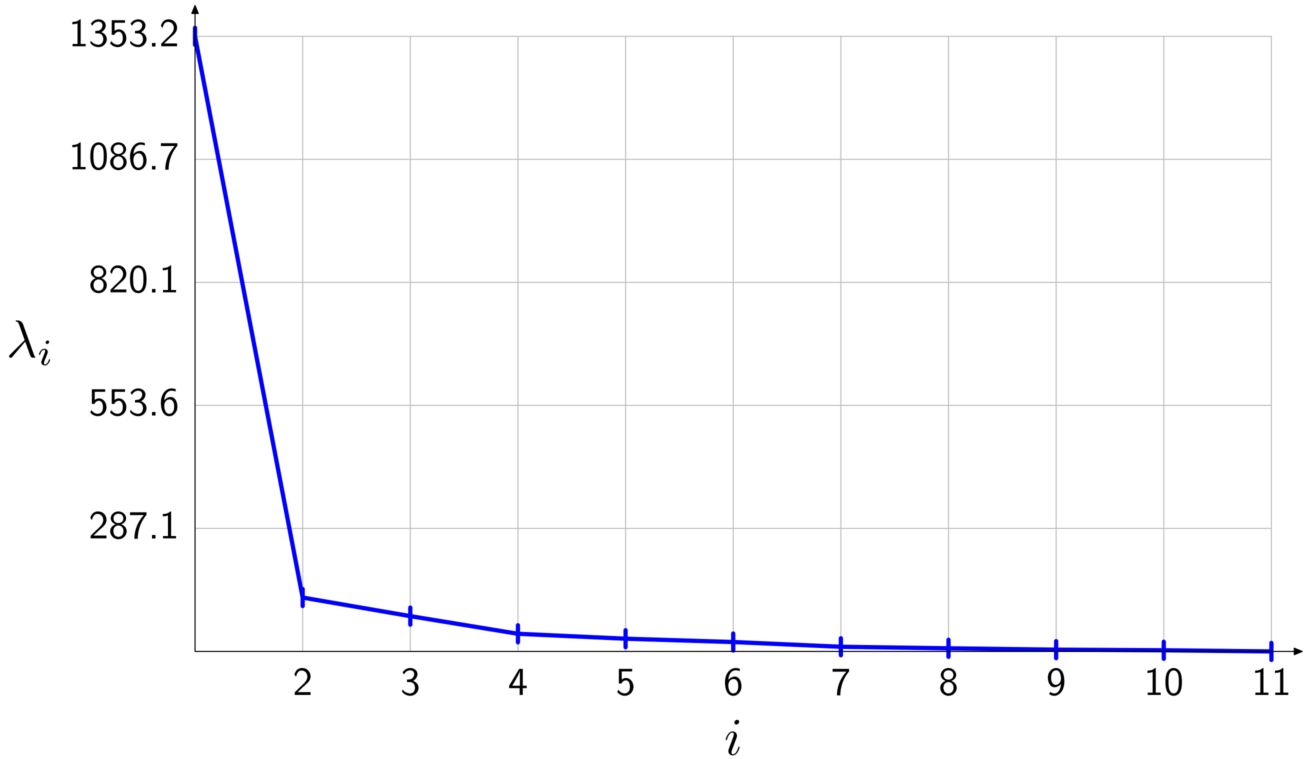

- Eigenvalues typically drop off sharply, so don't need that many.
- Of course variance isn't everything...

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Method 2: singular value decomposition (SVD)

Find $\mathbf{X} = \mathbf{U}_{d\times d}\Sigma_{d\times n}\mathbf{V}_{n\times n}^\top$

where $\mathbf{U}^\top\mathbf{U} = I_{d\times d}$, $\mathbf{V}^\top\mathbf{V} = I_{n\times n}$, Σ is diagonal

Computing top k singular vectors takes only $O(ndk)$

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Method 2: singular value decomposition (SVD)

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where $\mathbf{U}^\top\mathbf{U} = I_{d\times d}$, $\mathbf{V}^\top\mathbf{V} = I_{n\times n}$, Σ is diagonal

Computing top k singular vectors takes only $O(ndk)$

Relationship between eigendecomposition and SVD:

Left singular vectors are principal components ($C = \mathbf{U}\Sigma^2\mathbf{U}^\top$)

Roadmap

- Principal component analysis (PCA)
  - Basic principles
  - Case studies
  - Kernel PCA
  - Probabilistic PCA
- Canonical correlation analysis (CCA)
- Fisher discriminant analysis (FDA)
- Summary

Eigen-faces [Turk and Pentland, 1991]

- d = number of pixels
- Each $\mathbf{x}_i \in \mathbb{R}^d$ is a face image
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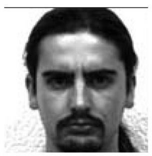
( $\cdots$ ) $\approx$ () $\begin{pmatrix} | & & | \\ \mathbf{z}_1 & \cdots & \mathbf{z}_n \\ | & & | \end{pmatrix}$

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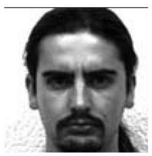
( $\cdots$ ) $\cong$ () $\begin{pmatrix} | & & | \\ \mathbf{z}_1 & \cdots & \mathbf{z}_n \\ | & & | \end{pmatrix}$

Idea: $\mathbf{z}_i$ more "meaningful" representation of i-th face than $\mathbf{x}_i$

Can use $\mathbf{z}_i$ for nearest-neighbor classification

Much faster: $O(dk + nk)$ time instead of $O(dn)$ when $n, d \gg k$

Why no time savings for linear classifier?

Latent Semantic Analysis [Deerwater, 1990]

- d = number of words in the vocabulary
- Each $\mathbf{x}_i \in \mathbb{R}^d$ is a vector of word counts
- $\mathbf{x}_{ji}$ = frequency of word j in document i

$$\mathbf{X}_{d\times n} \approxeq \mathbf{U}_{d\times k} \quad \mathbf{Z}_{k\times n}$$

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How to measure similarity between two documents?

$\mathbf{z}_1^\top \mathbf{z}_2$ is probably better than $\mathbf{x}_1^\top \mathbf{x}_2$

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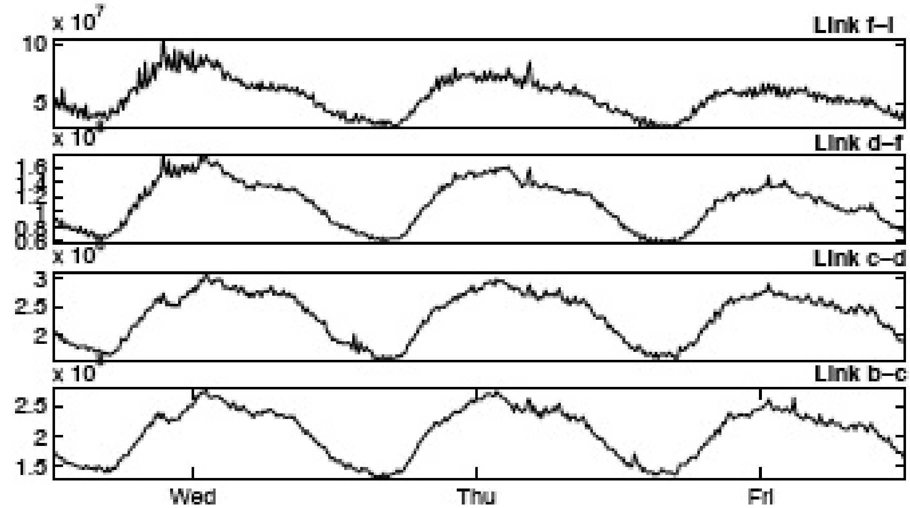
Note: no computational savings; original $\mathbf{x}$ is already sparse

Network anomaly detection [Lakhina, '05]

$\mathbf{x}_{ji}$ = amount of traffic on link j in the network during each time interval i



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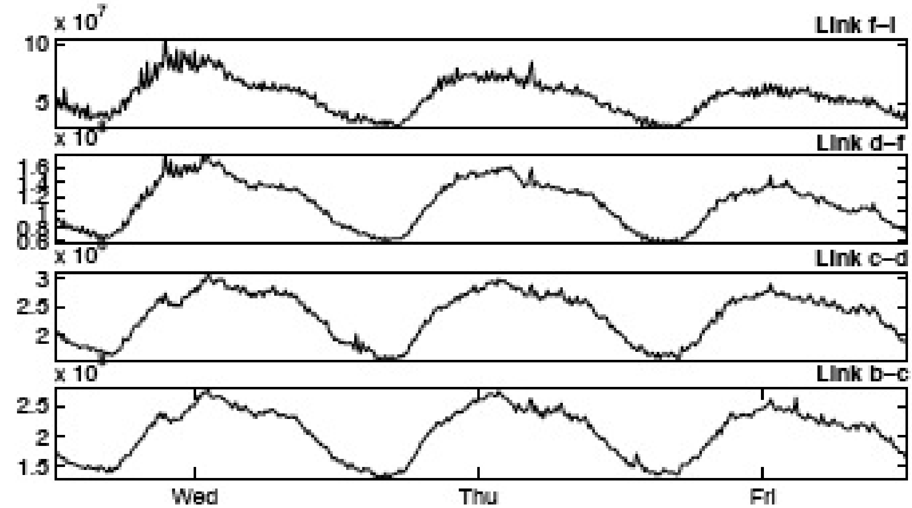

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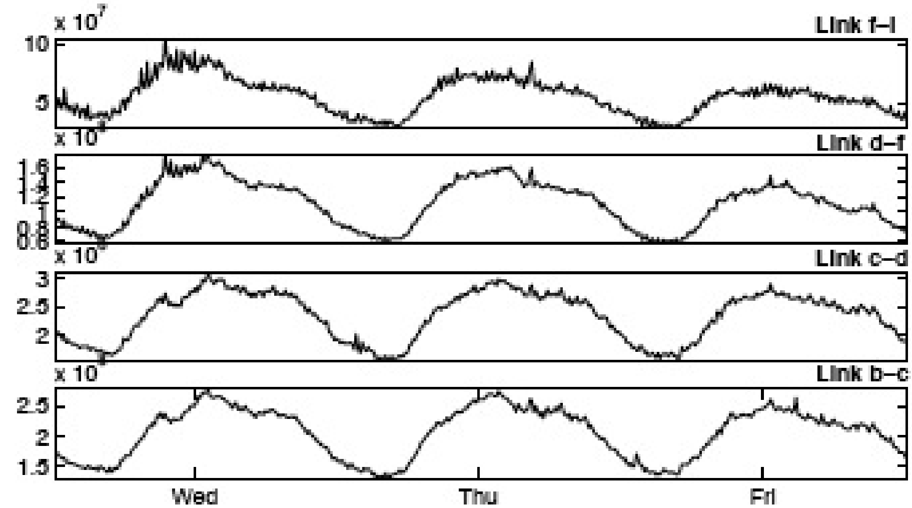

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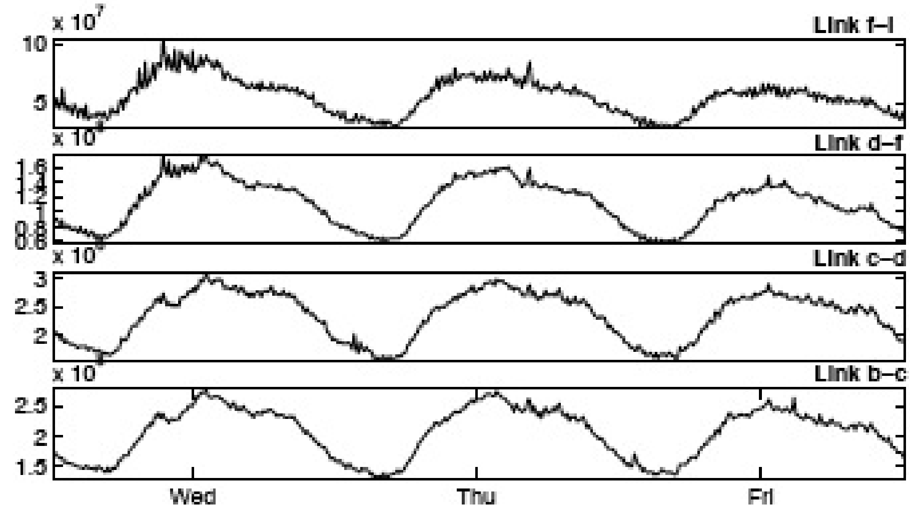

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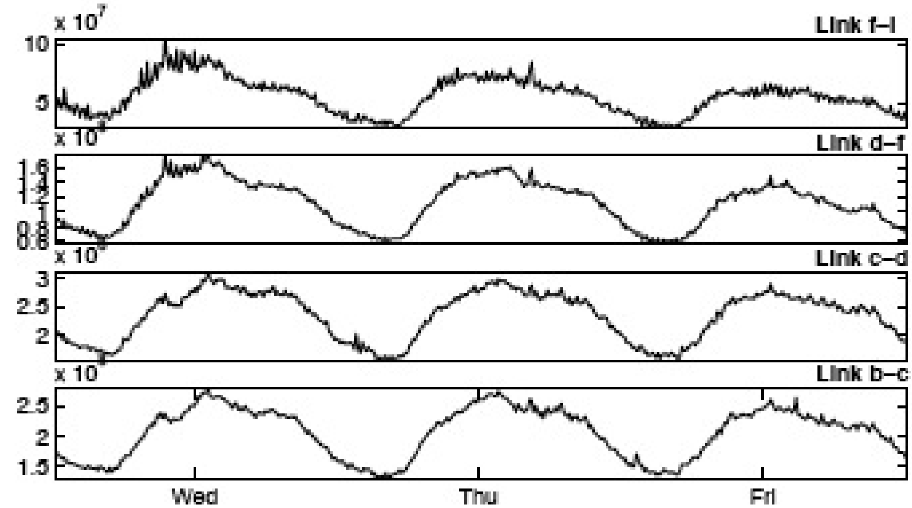

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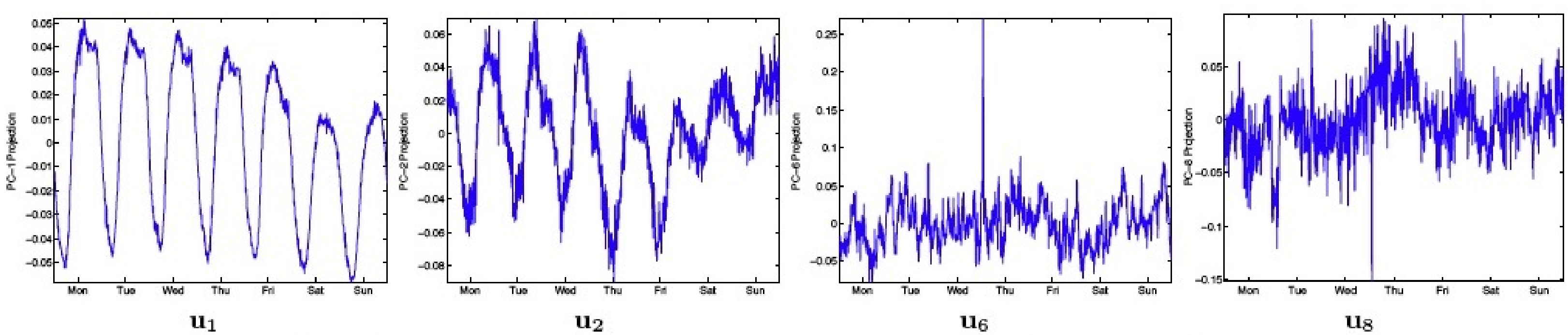

(a) Normal Behavior (b) Anomalous Behavior

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Part-of-speech (POS) tagging task:

Input:	I	like	reducing	the	dimensionality	of	data	.
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Key idea: words appearing in similar contexts
tend to have the same POS tags;
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Solution: run PCA first,
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Other step of their procedure:
Retrain classifiers, regularizing towards subspace $\mathbf{U}$

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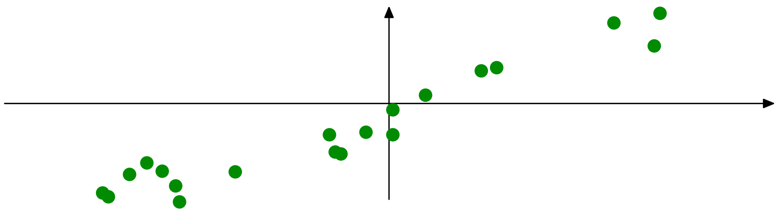

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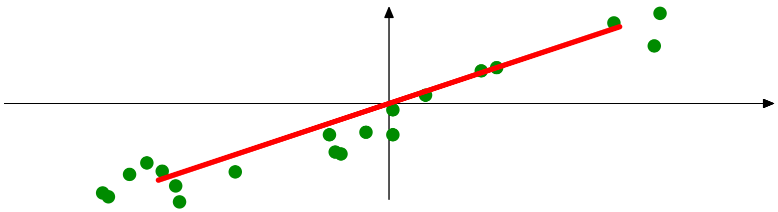

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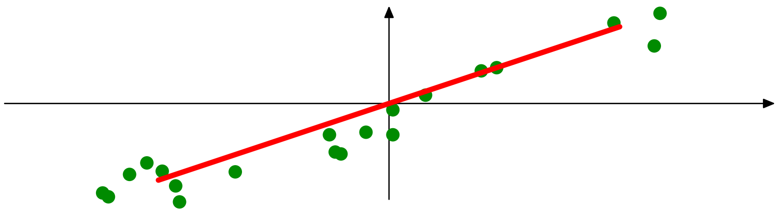

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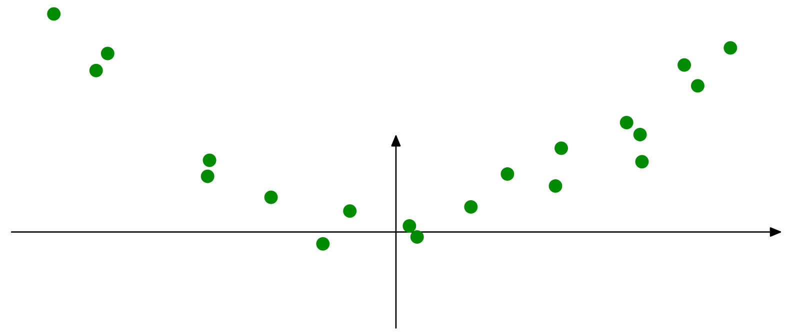

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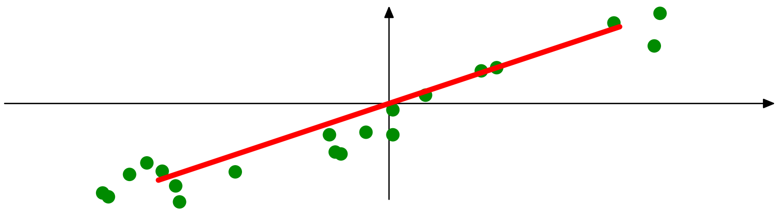

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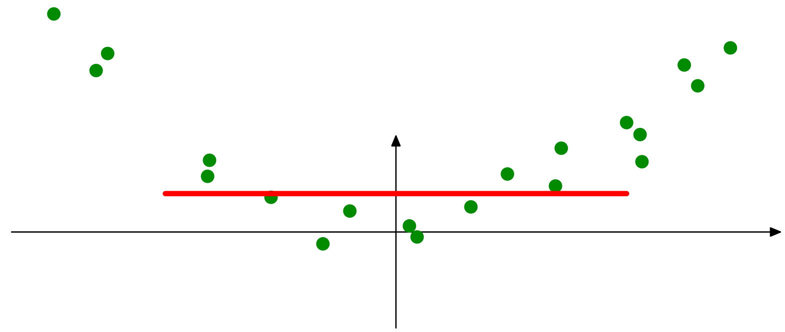

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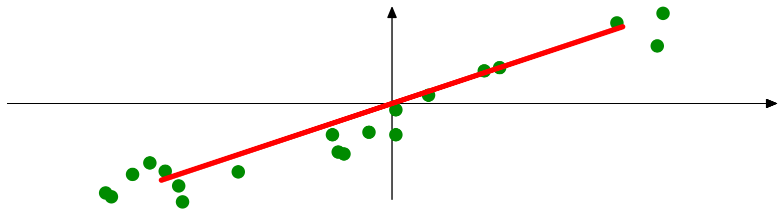

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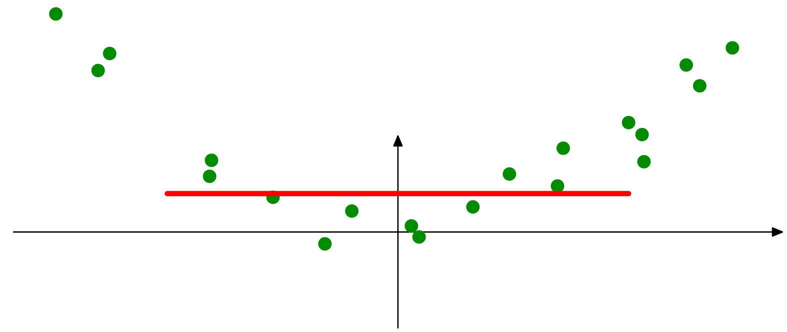

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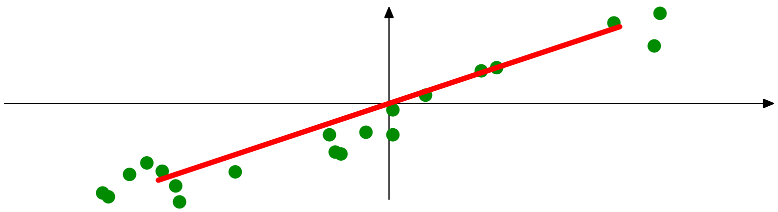

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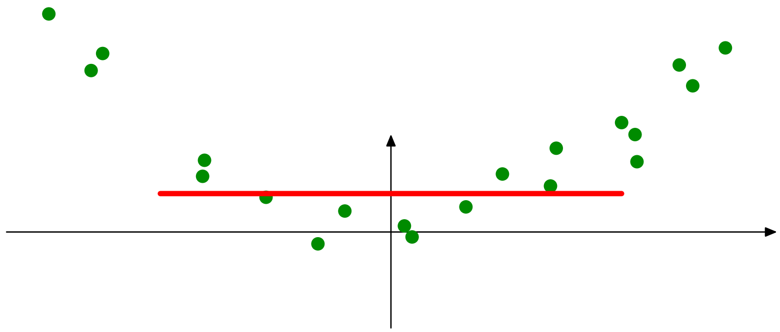

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In this example:

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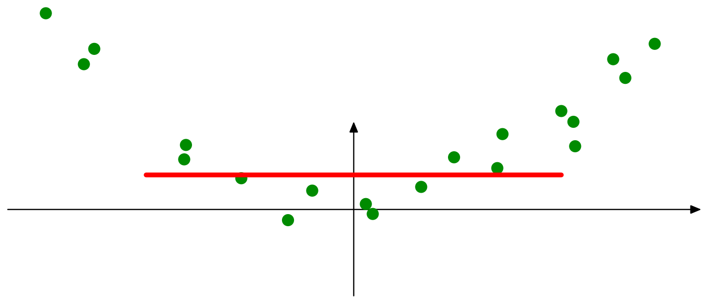
Going beyond linearity: quick solution



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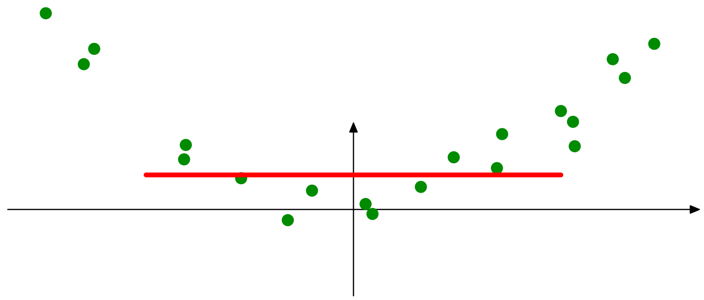

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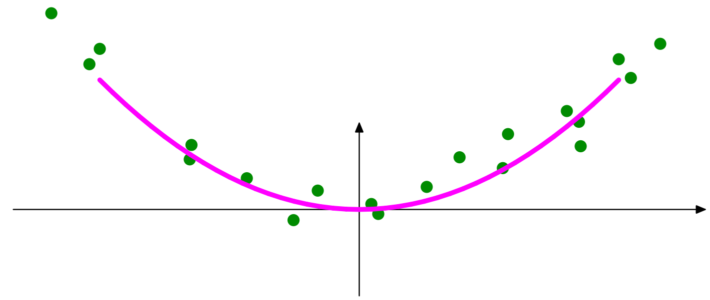

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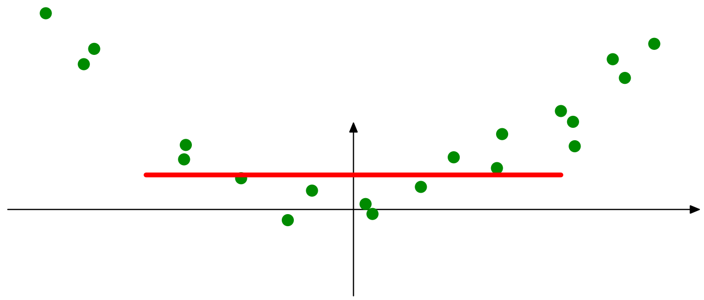

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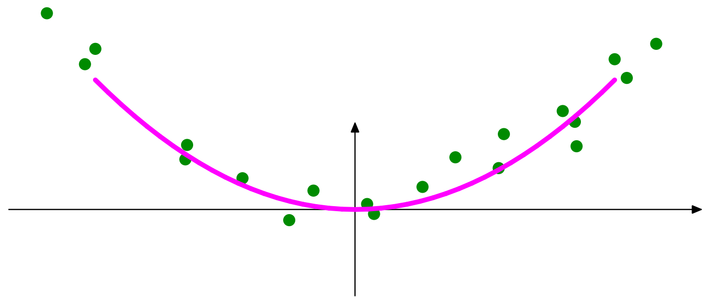

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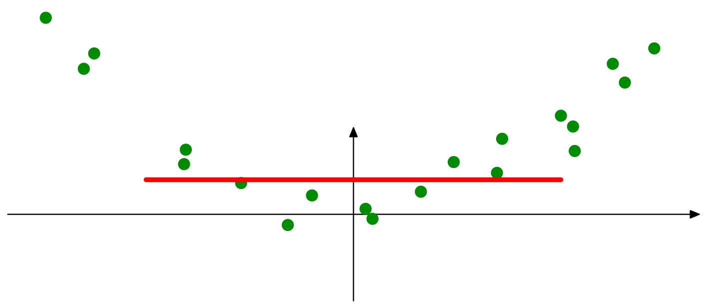

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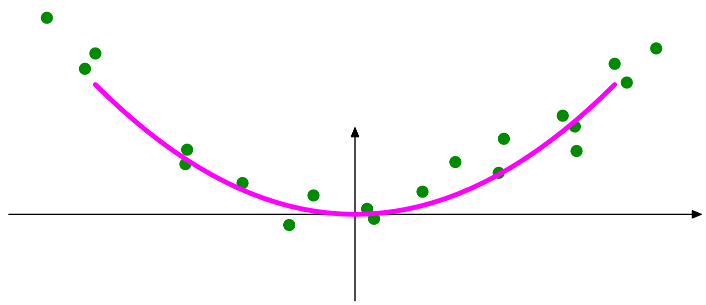

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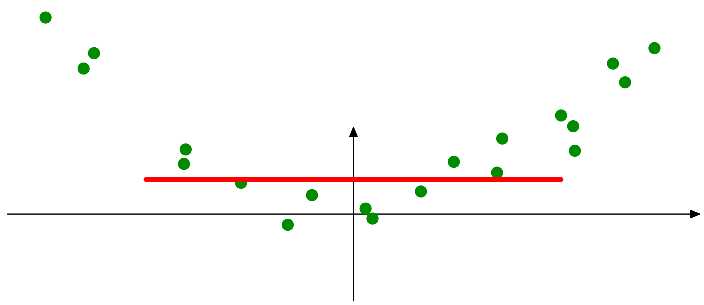

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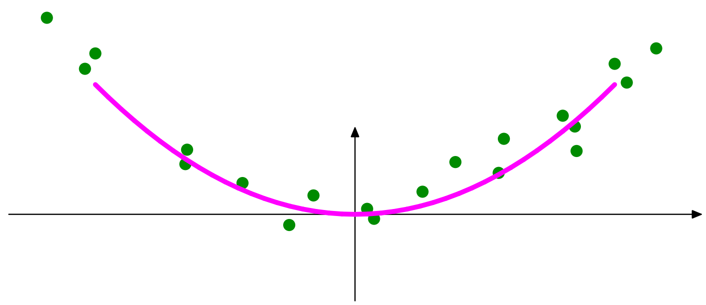

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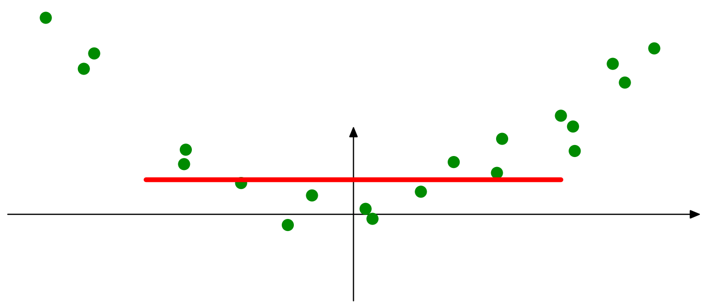

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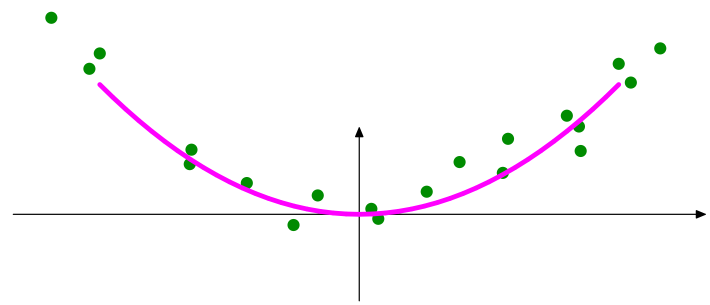

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Problems: (1) ad-hoc and tedious
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Analogy with SVMs: weight vector $\mathbf{w} = \mathbf{X}\alpha$

Towards kernels

Representer theorem:

PCA solution is linear combination of $\mathbf{x}_i$s

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Use representer theorem on PCA objective:

$$\max_{\|\mathbf{u}\|=1} \mathbf{u}^\top \mathbf{X}\mathbf{X}^\top \mathbf{u} = \max_{\boldsymbol{\alpha}^\top \mathbf{X}^\top \mathbf{X}\boldsymbol{\alpha}=1} \boldsymbol{\alpha}^\top (\mathbf{X}^\top \mathbf{X})(\mathbf{X}^\top \mathbf{X})\boldsymbol{\alpha}$$

Kernel PCA

Kernel function: $k(\mathbf{x}_1, \mathbf{x}_2)$ such that

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Mercer's theorem (using kernels is sensible)

Exists high-dimensional feature space ϕ such that

$k(\mathbf{x}_1, \mathbf{x}_2) = \phi(\mathbf{x}_1)^\top \phi(\mathbf{x}_2)$ (like quick solution earlier!)

Solving kernel PCA

Direct method:

Kernel PCA objective:

$$\max_{\boldsymbol{\alpha}^\top K \boldsymbol{\alpha} = 1} \boldsymbol{\alpha}^\top K^2 \boldsymbol{\alpha}$$

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One possibility is Cholesky decomposition $K = \mathbf{X}^\top \mathbf{X}$

Roadmap

- Principal component analysis (PCA)
  - Basic principles
  - Case studies
  - Kernel PCA
  - Probabilistic PCA

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- Fisher discriminant analysis (FDA)

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$$\min_{\mathbf{U}} f(\mathbf{X}, \mathbf{U})$$

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Example from last lecture: k-means $\Rightarrow$ GMMs

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- Extension to factor analysis: allow non-isotropic noise (replace $\sigma^2 I_{d \times d}$ with arbitrary diagonal matrix)

Probabilistic latent semantic analysis (pLSA)

Motivation: in text analysis, $\mathbf{X}$ contains word counts; PCA (LSA) is bad model as it allows negative counts; pLSA fixes this

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E-step: fix parameters, choose best topics

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More sophisticated methods: EM, Latent Dirichlet Allocation

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More sophisticated methods: EM, Latent Dirichlet Allocation

Comparison to a mixture model for clustering:
  Mixture model: assume a single topic for entire document
  pLSA: allow multiple topics per document

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Motivation for CCA [Hotelling, 1936]

Often, each data point consists of two views:

- Image retrieval: for each image, have the following:
  - $\mathbf{x}$: Pixels (or other visual features)
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Goal: reduce the dimensionality of the two views jointly

An example

Setup:

Input data: $(\mathbf{x}_1, \mathbf{y}_1), \ldots, (\mathbf{x}_n, \mathbf{y}_n)$ (matrices $\mathbf{X}$, $\mathbf{Y}$)

Goal: find pair of projections $(\mathbf{u}, \mathbf{v})$

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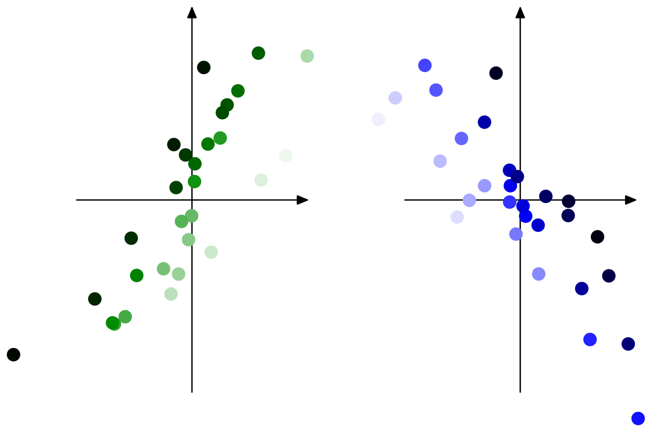
In figure, $\mathbf{x}$ and $\mathbf{y}$ are paired by brightness



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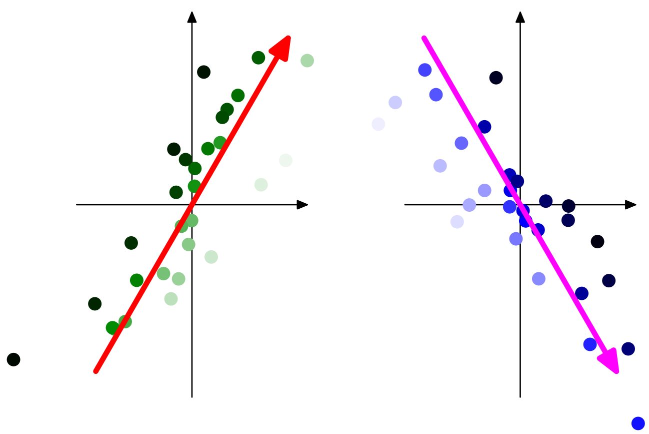

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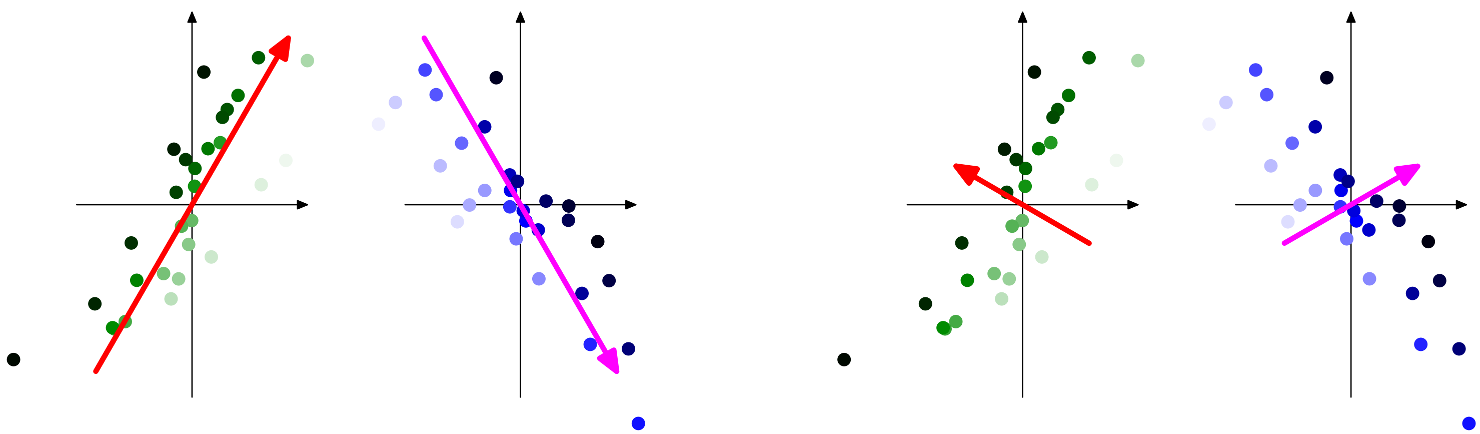

Independent　　　　Joint

From PCA to CCA

PCA on views separately: no covariance term

$$\max_{\mathbf{u},\mathbf{v}} \frac{\mathbf{u}^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}}{\mathbf{u}^\top \mathbf{u}} + \frac{\mathbf{v}^\top \mathbf{Y}\mathbf{Y}^\top \mathbf{v}}{\mathbf{v}^\top \mathbf{v}}$$

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PCA on concatenation $(\mathbf{X}^\top, \mathbf{Y}^\top)^\top$: includes covariance term

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Maximum covariance: drop variance terms

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Maximum correlation (CCA): divide out variance terms

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Variance: $\widehat{\text{var}}(\mathbf{u}^\top \mathbf{x}) = \mathbf{u}^\top \mathbf{X}\mathbf{X}^\top \mathbf{u}$

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Properties:

- Focus on how variables are related, not how much they vary

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Objective: maximize correlation between projected views

$$\max_{\mathbf{u},\mathbf{v}} \widehat{\text{corr}}(\mathbf{u}^\top \mathbf{x}, \mathbf{v}^\top \mathbf{y})$$

Properties:

- Focus on how variables are related, not how much they vary
- Invariant to any rotation and scaling of data

Canonical correlation analysis (CCA)

Definitions:

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Solved via a generalized eigenvalue problem ($A\mathbf{w} = \lambda B\mathbf{w}$)

Regularization is important

Extreme examples of degeneracy:

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Solution: regularization (interpolate between maximum covariance and maximum correlation)

$$\max_{\mathbf{u},\mathbf{v}} \frac{\mathbf{u}^\top \mathbf{X}\mathbf{Y}^\top \mathbf{v}}{\sqrt{\mathbf{u}^\top(\mathbf{X}\mathbf{X}^\top + \lambda I)\mathbf{u}}\sqrt{\mathbf{v}^\top(\mathbf{Y}\mathbf{Y}^\top + \lambda I)\mathbf{v}}}$$

Kernel CCA

Two kernels: k_x and k_y

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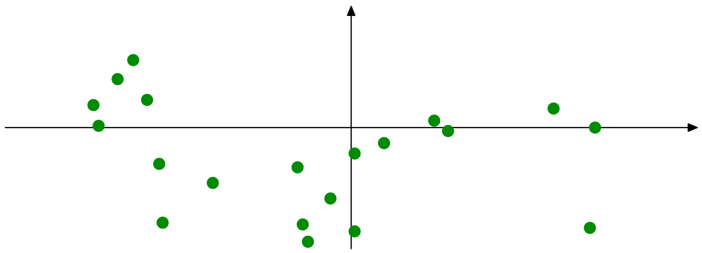
Regularization is especially important for kernel CCA!

Roadmap

- Principal component analysis (PCA)
  - Basic principles
  - Case studies
  - Kernel PCA
  - Probabilistic PCA
- Canonical correlation analysis (CCA)
- Fisher discriminant analysis (FDA)
- Summary

Motivation for FDA [Fisher, 1936]

What is the best linear projection?



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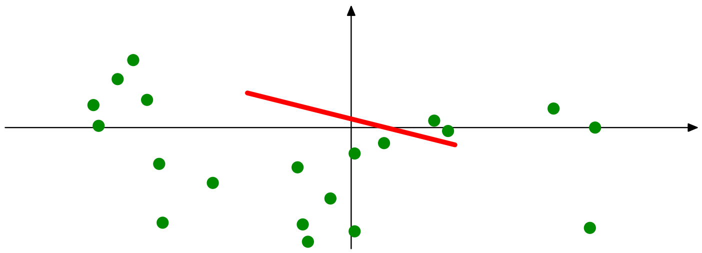

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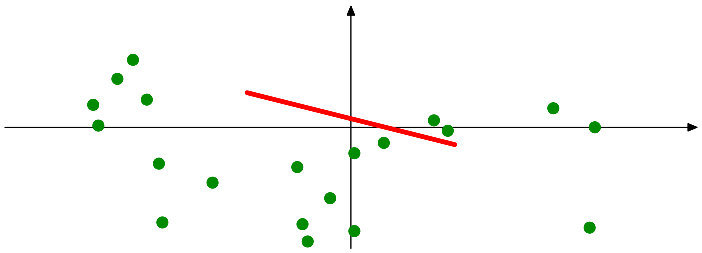

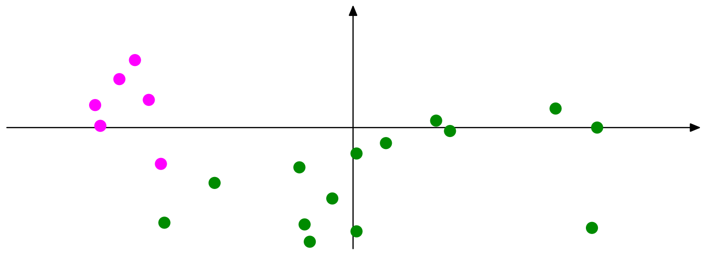

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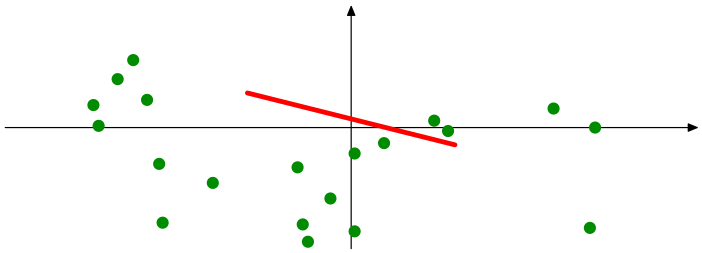

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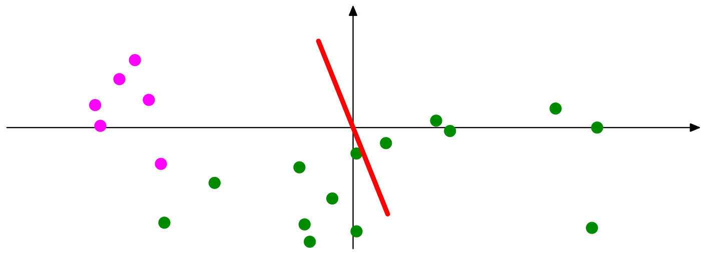

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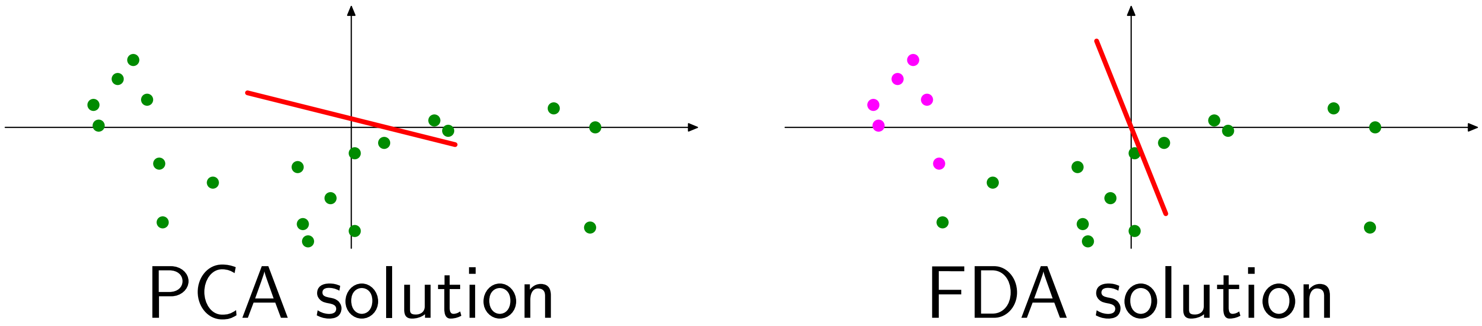

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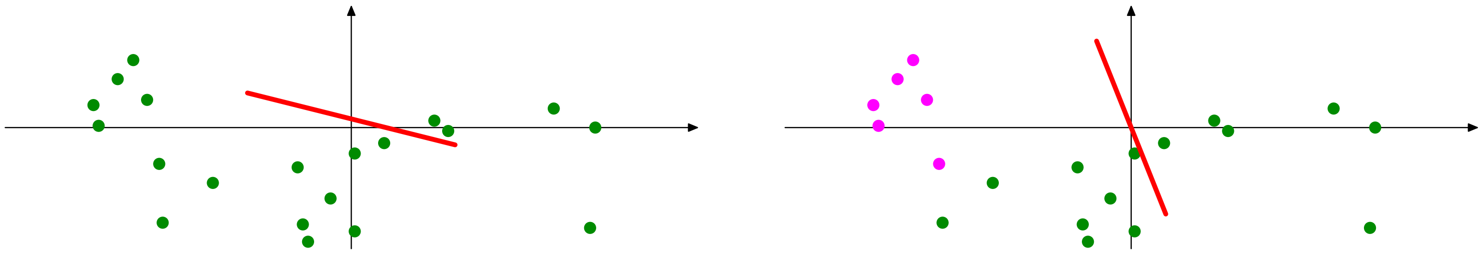

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Linear classifiers (logistic regression, SVMs) have similar feel:

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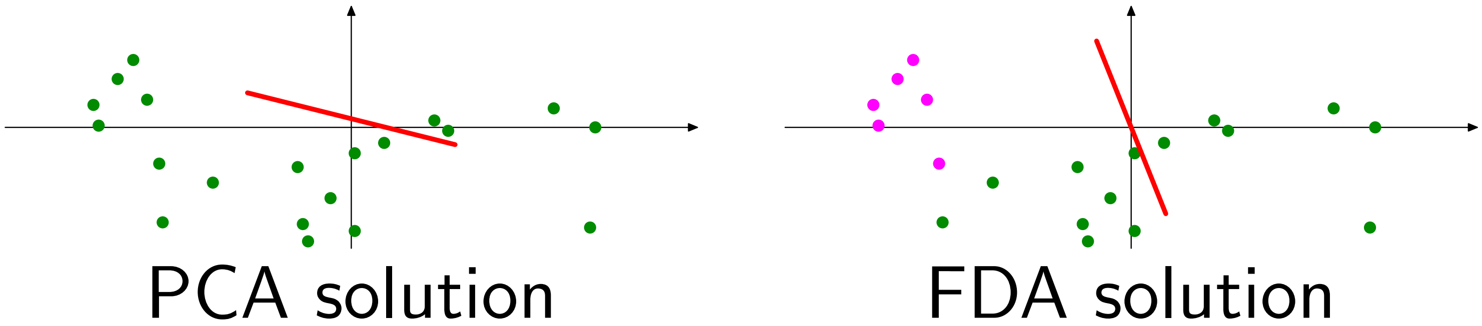

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FDA handles multiple classes, allows multiple dimensions

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Setup: $\mathbf{x}_i \in \mathbb{R}^d, y_i \in \{1, \ldots, m\}$, for $i = 1, \ldots, n$

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Extensions:

non-linear using kernels (using same linear framework)

probabilistic, sparse, robust (hard optimization)