Dimensionality Reduction
PCA

Aarti Singh

Machine Learning 10-315
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Slides Courtesy: Tom Mitchell, Eric Xing, Lawrence Saul

High-Dimensional data

- High-Dimensions = Lot of Features

Document classification

Features per document =

thousands of words/unigrams

millions of bigrams, contextual information

Surveys - Netflix

480189 users x 17770 movies

	movie 1	movie 2	movie 3	movie 4	movie 5	movie 6
Tom	5	?	?	1	3	?
George	?	?	3	1	2	5
Susan	4	3	1	?	5	1
Beth	4	3	?	2	4	2

High-Dimensional data

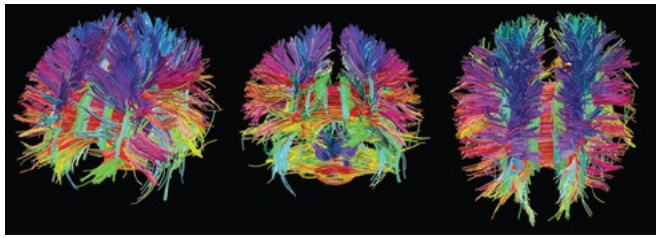
- High-Dimensions = Lot of Features

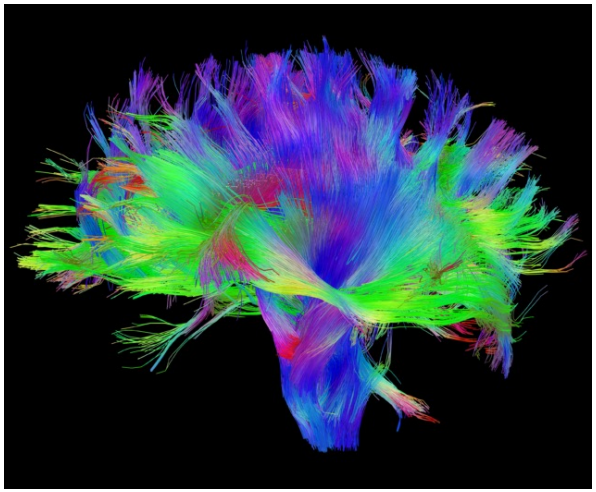
High resolution images

millions of pixels

Diffusion scans of Brain

300,000 brain fibers



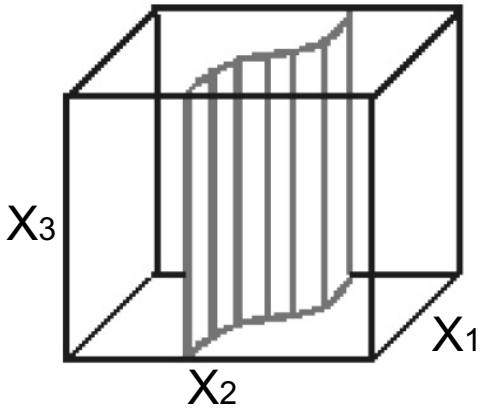


Curse of Dimensionality

- Why are more features bad?
  - Redundant features (not all words are useful to classify a document) more noise added than signal
  - Hard to interpret and visualize
  - Hard to store and process data (computationally challenging)
  - Complexity of decision rule tends to grow with # features. Hard to learn complex rules as it needs more data (statistically challenging)

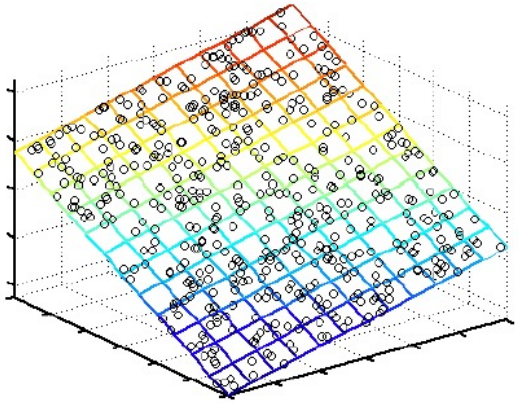
Dimensionality Reduction

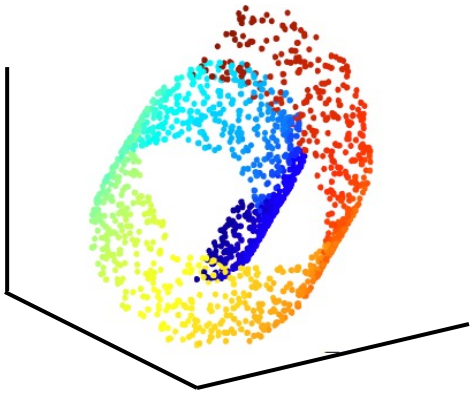
- Feature Selection – Only a few features are relevant to the learning task



X_3 - Irrelevant

- Latent features – Some linear/nonlinear combination of features provides a more efficient representation than observed features





Feature Selection

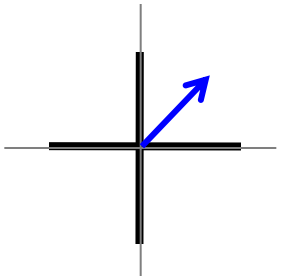
- One Approach: **Regularization (MAP)**

  Integrate feature selection into learning objective by penalizing number of features with non-zero weights

$$\widehat{W} = \arg\min_{W} \sum_{i=1}^{n} -\log P(Y_i|X_i; W) + \lambda\|W\|$$

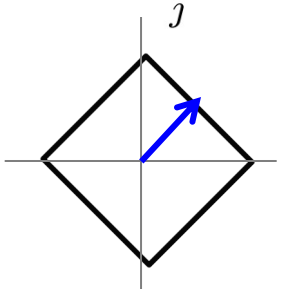
-ve log likelihood — penalty

$\|W\|_0 = \#\{W_j > 0\}$



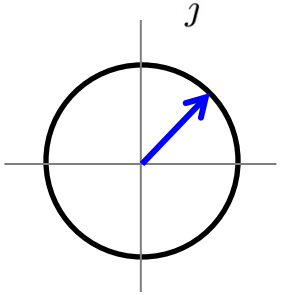
Minimizes # features chosen

$\|W\|_1 = \sum_j |W_j|$



Convex compromise

$\|W\|_2 = \sum_j W_j^2$



Small weights of features chosen

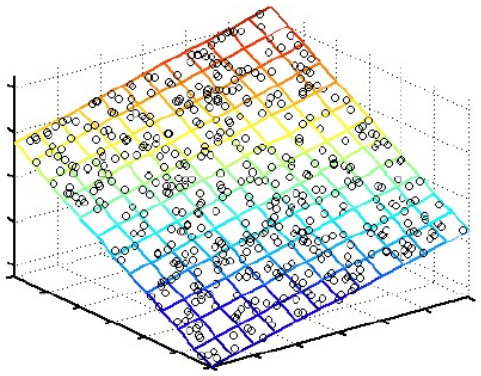
Latent Features

Combinations of observed features provide more efficient representation, and capture underlying relations that govern the data

E.g. Ego, personality and intelligence are hidden attributes that characterize human behavior instead of survey questions

Topics (sports, science, news, etc.) instead of documents

Often may not have physical meaning

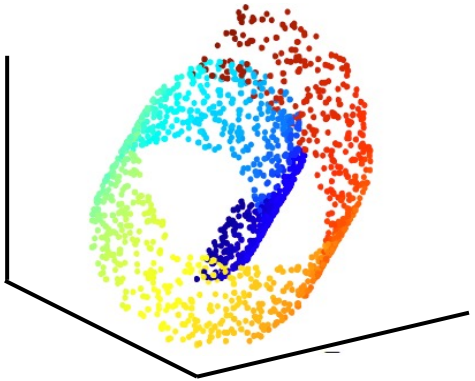


- Linear

  Principal Component Analysis (PCA)

  Factor Analysis

  Independent Component Analysis (ICA)



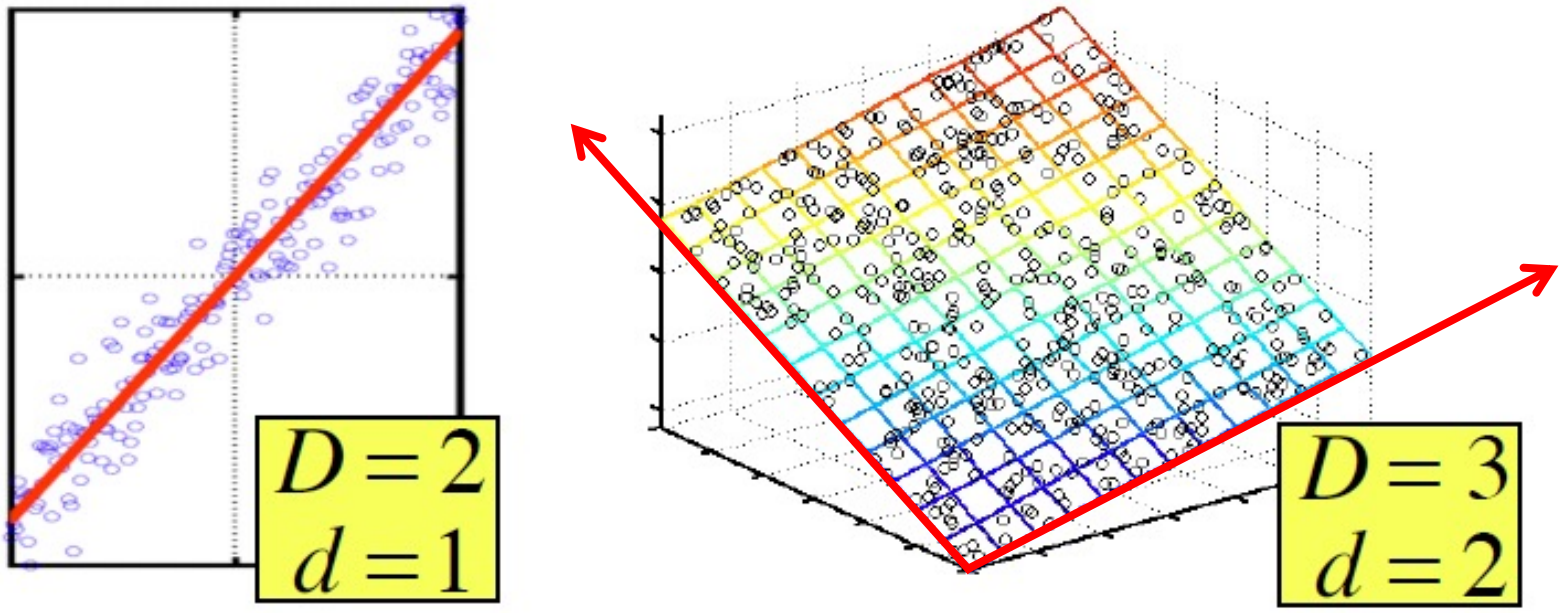
- Nonlinear

  Kernel PCA

  Laplacian Eigenmaps, ISOMAP, LLE

  Autoencoders

Principal Component Analysis (PCA)



When data lies on or near a low d-dimensional linear subspace, axes of this subspace are an effective representation of the data

Identifying the axes is known as Principal Components Analysis, and can be obtained by Eigen or Singular value decomposition

Data for PCA

Data X = $[x_1, x_2, \ldots, x_n]$ where each data point x_i is D-dimensional vector

X is D x n matrix

Assume data are centered i.e. sample mean $\frac{1}{n}\sum_{i=1}^{n} x_i = 0$

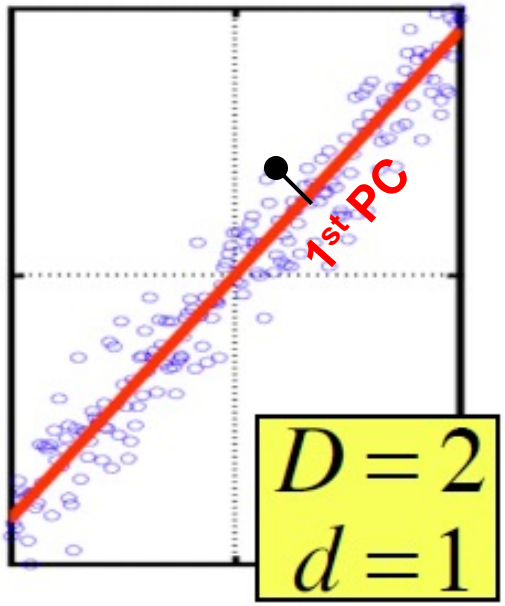
What if data is not centered?

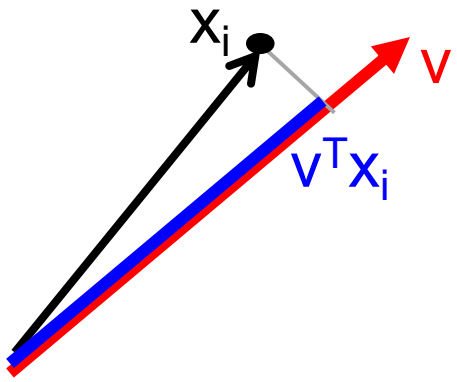
Subtract off sample mean from each data point

Since data matrix is centered, sample covariance matrix can be written as

$$S = \frac{1}{n} X X^\top$$

Principal Component Analysis (PCA)





Principal Components (PC) are orthogonal directions that capture most of the variance in the data

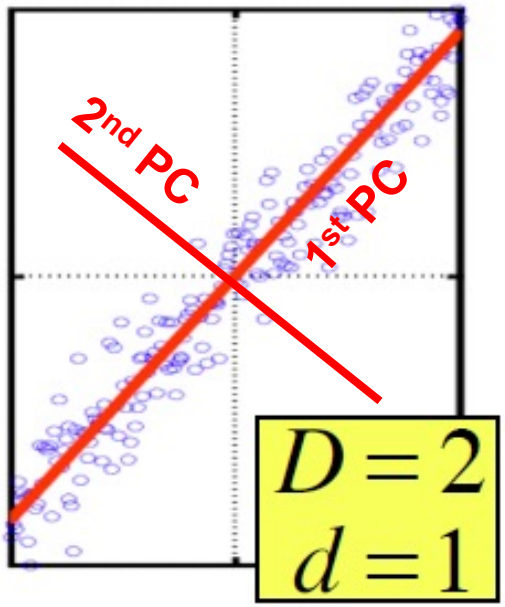
1st PC – direction of greatest variability in data

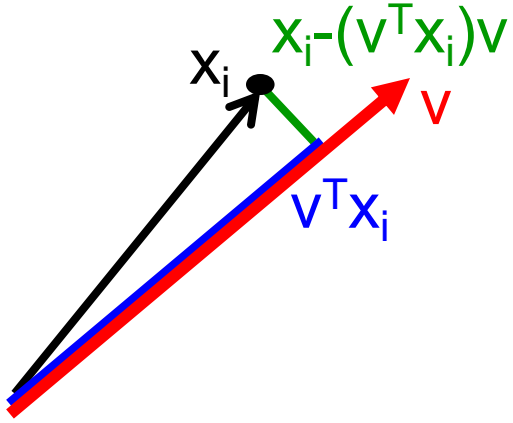
Projection of data points along 1st PC discriminate the data most along any one direction

Take a data point x_i (D-dimensional vector)

Projection of x_i onto the 1st PC v is $v^T x_i$

Principal Component Analysis (PCA)





Principal Components (PC) are orthogonal unit norm directions that capture most of the variance in the data

1st PC – direction of greatest variability in data

2nd PC – Next orthogonal (uncorrelated) direction of greatest variability

(remove all variability in first direction, then find next direction of greatest variability)

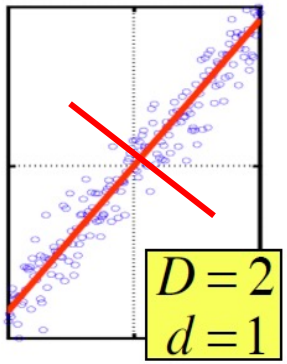
And so on …

Principal Component Analysis (PCA)

Let $v_1, v_2, \ldots, v_d$ denote the principal components

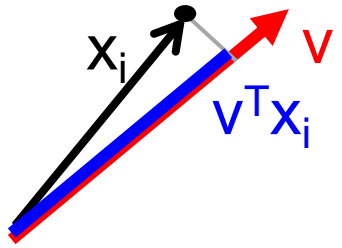
Orthogonal and unit norm $v_i^T v_j = 0 \quad i \neq j$

$v_i^T v_i = 1$



Find vector that maximizes sample variance of projection

$$\frac{1}{n}\sum_{i=1}^{n}(\mathbf{v}^T\mathbf{x}_i)^2 = \frac{\mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v}}{n}$$



$$\max_{\mathbf{v}} \ \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} \quad \text{s.t.} \quad \mathbf{v}^T\mathbf{v} = 1$$

Poll:

- Is this a convex optimization problem?

Principal Component Analysis (PCA)

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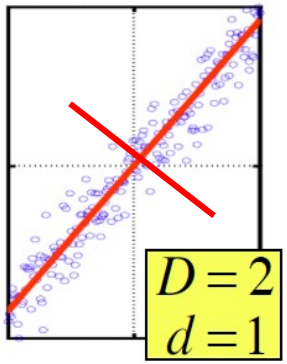

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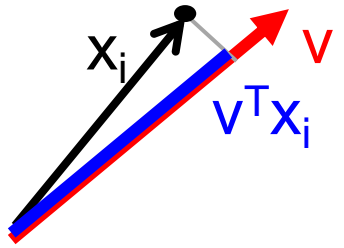


$$\max_{\mathbf{v}} \ \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} \quad \text{s.t.} \quad \mathbf{v}^T\mathbf{v} = 1$$

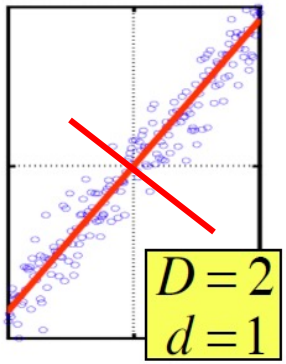
Lagrangian: $\max_{\mathbf{v}} \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} - \lambda\mathbf{v}^T\mathbf{v}$

Wrap constraints into the objective function

$$\partial/\partial\mathbf{v} = 0 \qquad (\mathbf{X}\mathbf{X}^T - \lambda\mathbf{I})\mathbf{v} = 0 \qquad \Rightarrow \boxed{(\mathbf{X}\mathbf{X}^T)\mathbf{v} = \lambda\mathbf{v}}$$

Principal Component Analysis (PCA)

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



Therefore, v is the eigenvector of sample covariance matrix XX^T

Sample variance of projection = $\mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v} = \lambda\mathbf{v}^T\mathbf{v} = \lambda$

Thus, the eigenvalue λ denotes the amount of variability captured along that dimension (aka amount of energy along that dimension).

Eigenvalues $\lambda_1 > \lambda_2 > \lambda_3 > \ldots$

The 1st Principal component v_1 is the eigenvector of the sample covariance matrix XX^T associated with the largest eigenvalue λ_1

The 2nd Principal component v_2 is the eigenvector of the sample covariance matrix XX^T associated with the second largest eigenvalue λ_2

And so on …

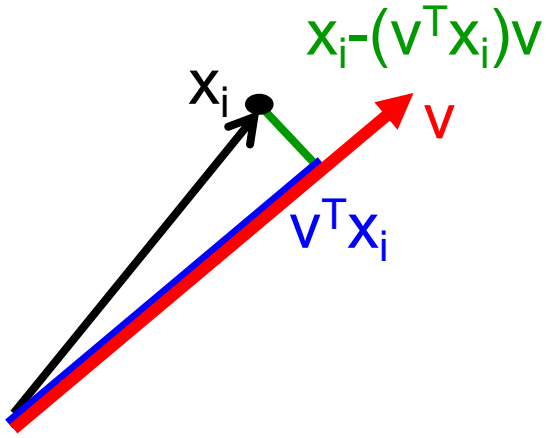
Another interpretation

Maximum Variance Subspace: PCA finds vectors v such that projections on to the vectors capture maximum variance in the data

$$\frac{1}{n}\sum_{i=1}^{n}(\mathbf{v}^T\mathbf{x}_i)^2 = \mathbf{v}^T\mathbf{X}\mathbf{X}^T\mathbf{v}$$

Minimum Reconstruction Error: PCA finds vectors v such that projection on to the vectors yields minimum MSE reconstruction

$$\frac{1}{n}\sum_{i=1}^{n}\|\mathbf{x}_i - (\mathbf{v}^T\mathbf{x}_i)\mathbf{v}\|^2$$



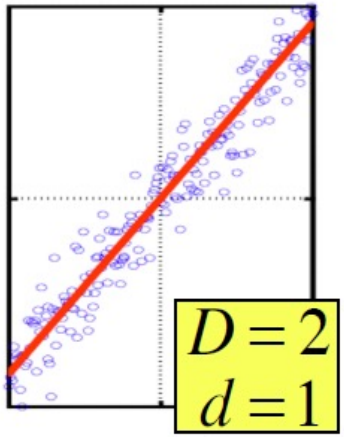
$$\frac{1}{n}\sum_{i=1}^{n} \|\mathbf{x}_i - (\mathbf{v}^T\mathbf{x}_i)\mathbf{v}\|^2$$

Dimensionality Reduction using PCA

The eigenvalue λ denotes the amount of variability captured along that dimension.

Zero eigenvalues indicate no variability along those directions => data lies exactly on a linear subspace

Only keep data projections onto principal components with non-zero eigenvalues, say $v_1, \ldots, v_d$ where d = rank (XX^T)



Original Representation

data point

$x_i = [x_i^1, x_i^2, \ldots. x_i^D]^T$

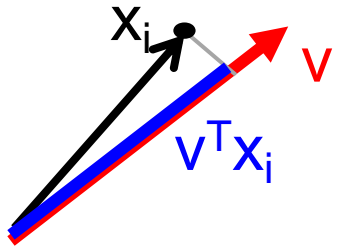
(D-dimensional vector)

Transformed representation

projections

$[v_1^T x_i, v_2^T x_i, \ldots v_d^T x_i]$

(d-dimensional vector)

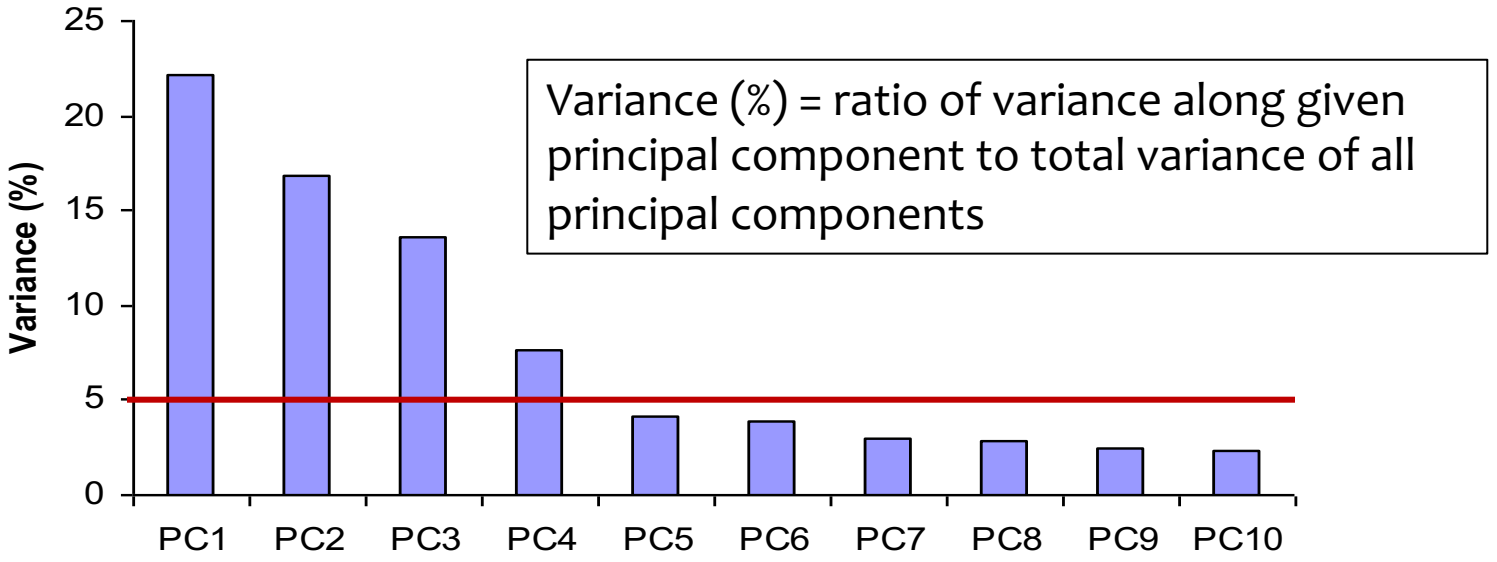


Dimensionality Reduction using PCA

In high-dimensional problem, data usually lies near a linear subspace, as noise introduces small variability

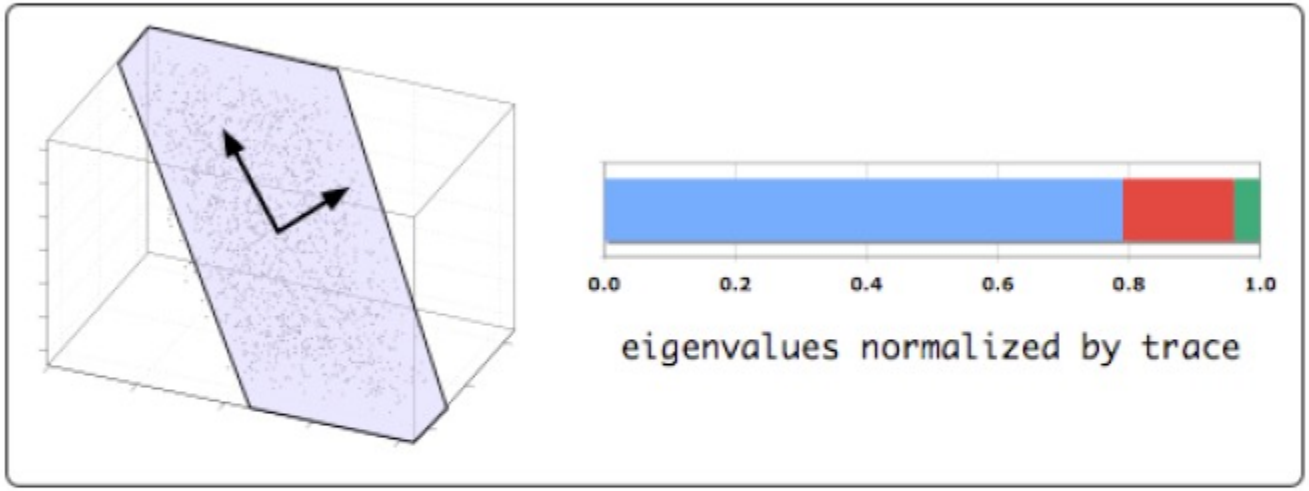
Only keep data projections onto principal components with **large** eigenvalues

Can *ignore* the components of lesser significance.



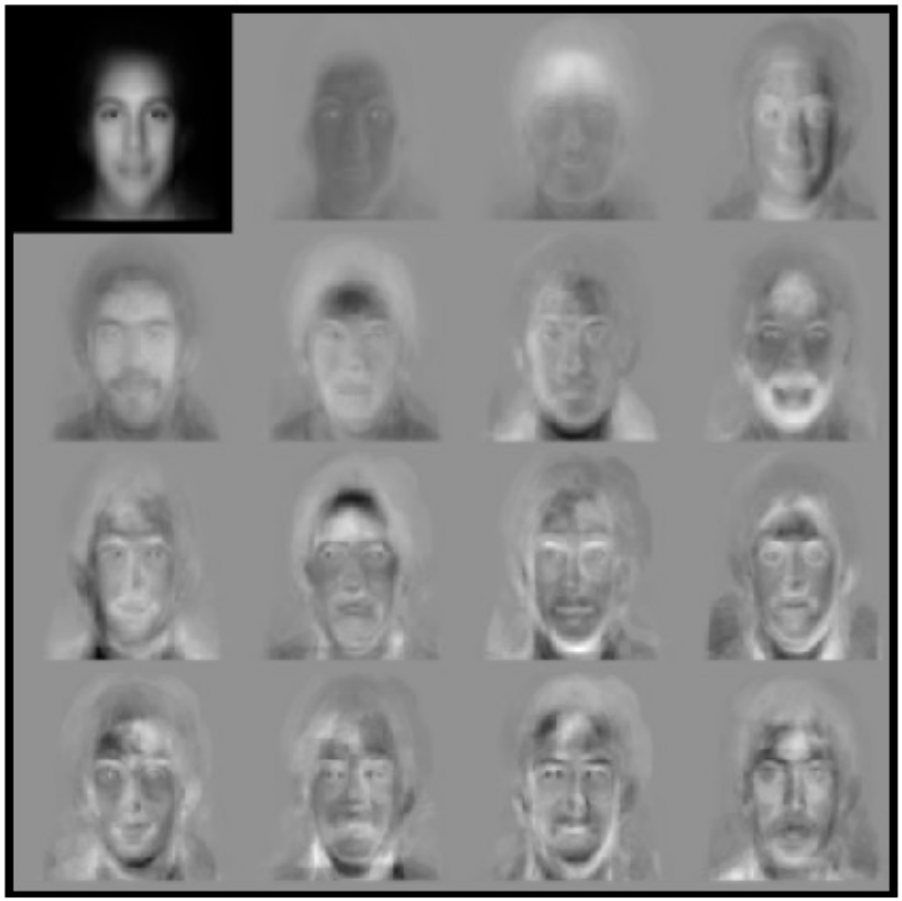
You might lose some information, but if the eigenvalues are small, you don't lose much

Example of PCA



Eigenvectors and eigenvalues of covariance matrix for $n=1600$ inputs in $d=3$ dimensions.

Example: faces



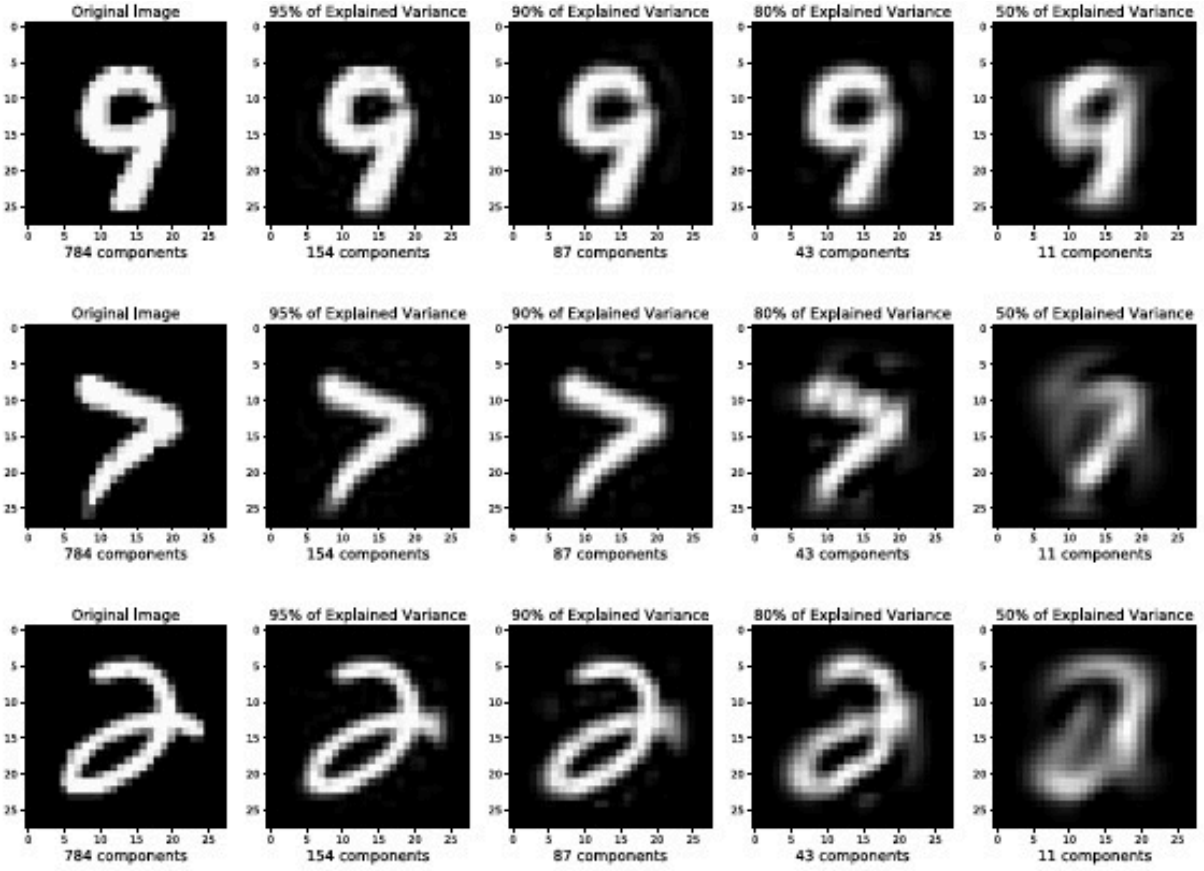
Eigenfaces from 7562 images:

top left image is linear combination of rest.

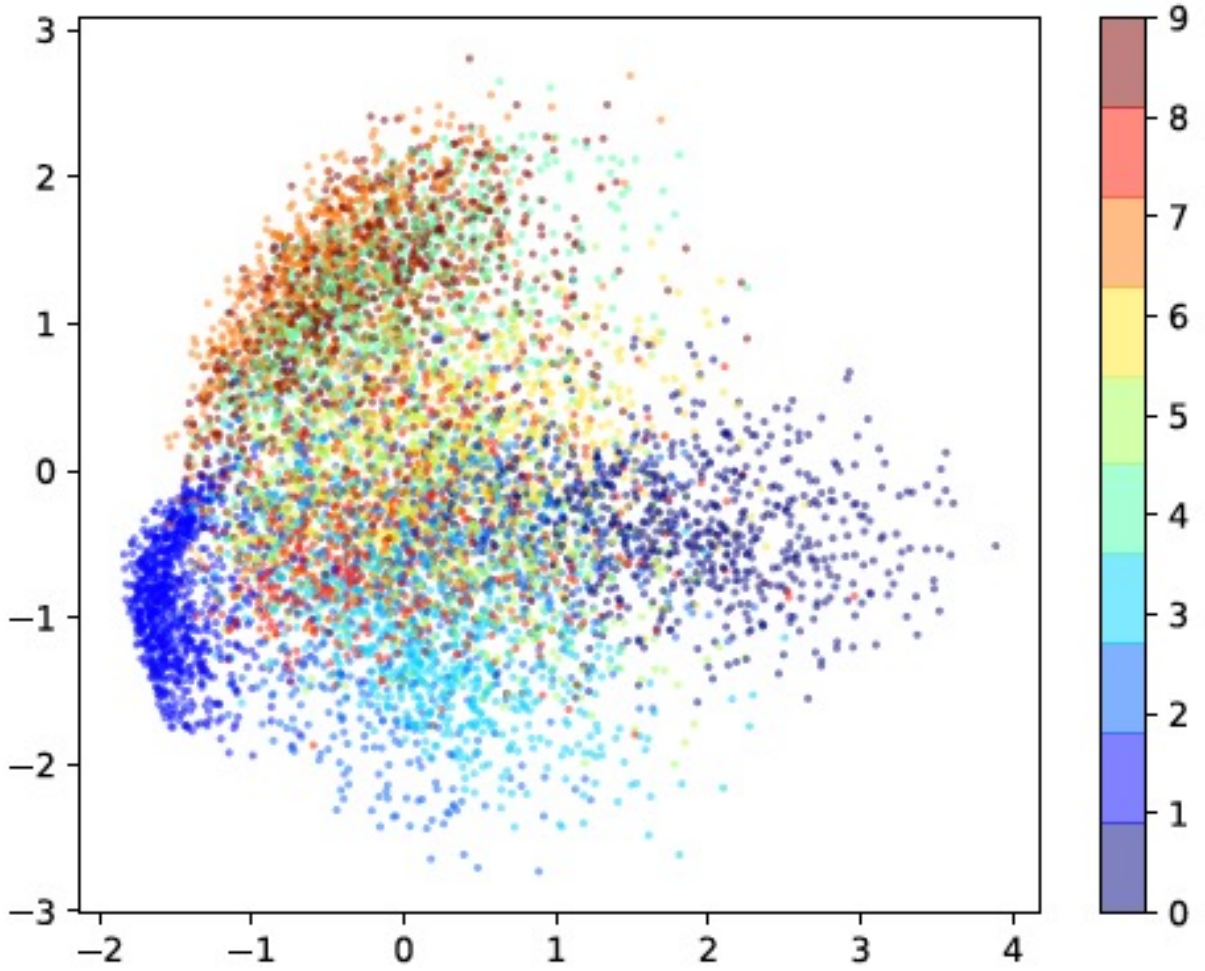
Sirovich & Kirby (1987)
Turk & Pentland (1991)

Example: MNIST digits

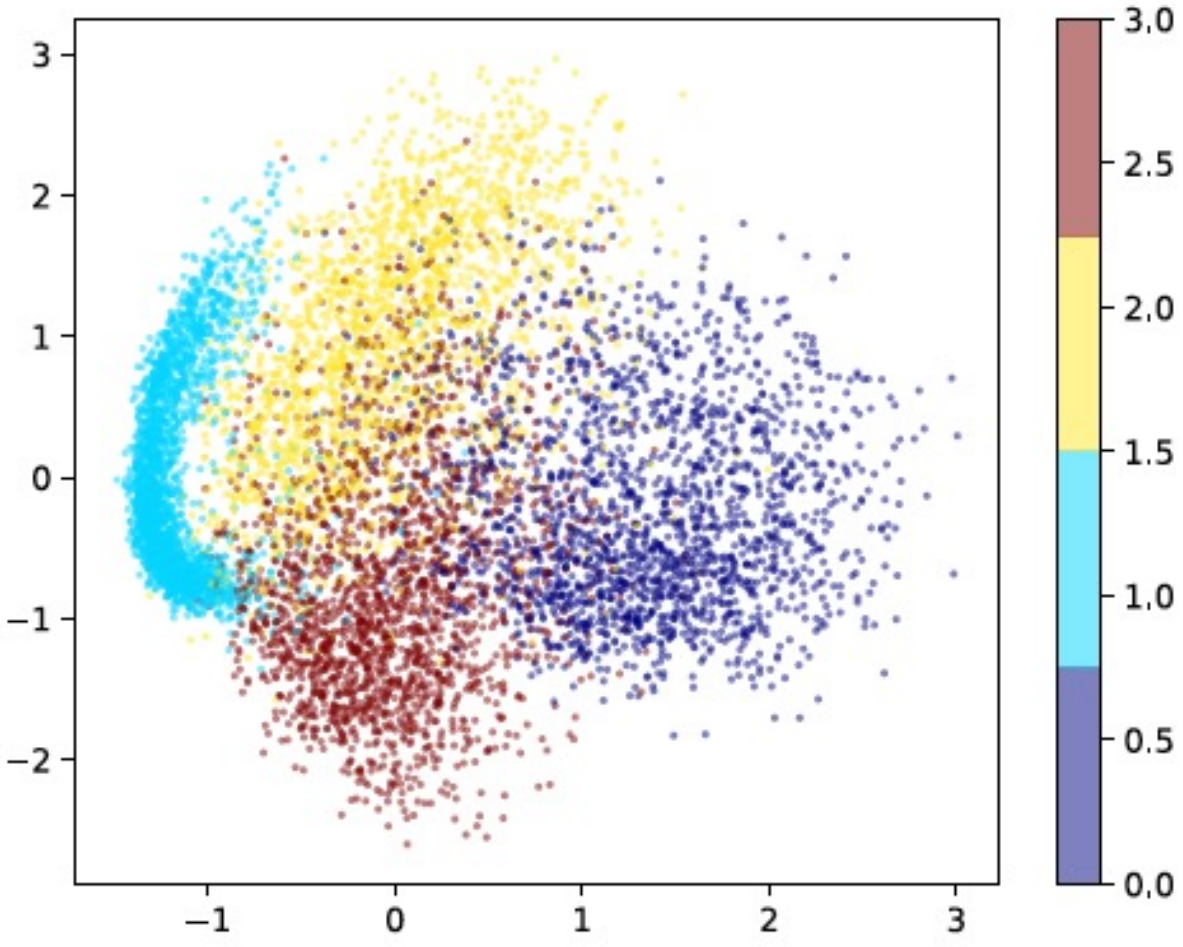
- 28x28 images = 784 PCA vectors
- Project to K dimensional space and then project back up



Projecting MNIST digits

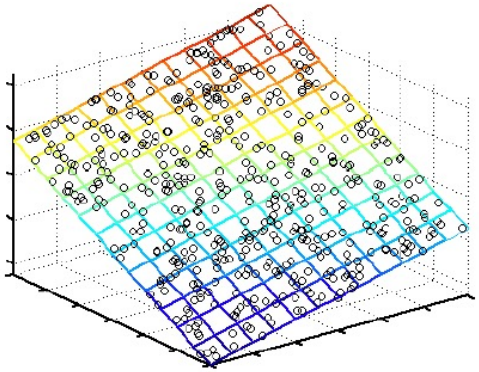


Projecting MNIST digits

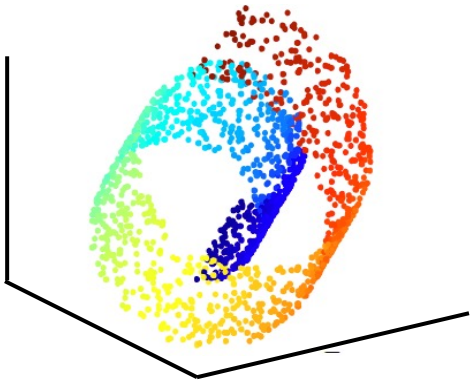


Unsupervised Dimensionality Reduction

- Linear
  - **Principal Component Analysis (PCA)**
  - Factor Analysis
  - Independent Component Analysis (ICA)



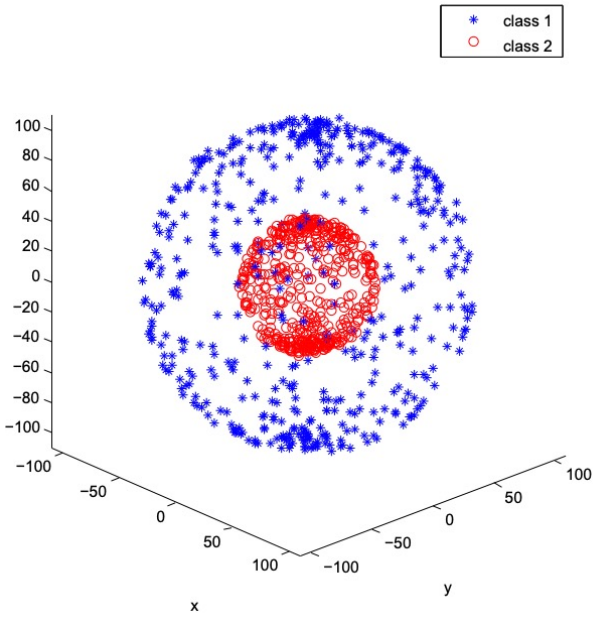
- Nonlinear
  - **Kernel PCA**
  - Laplacian Eigenmaps, ISOMAP, LLE
  - Autoencoders



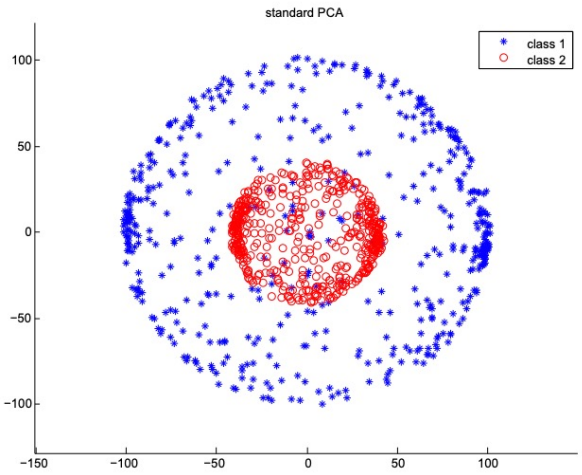
Kernel PCA

HW4!

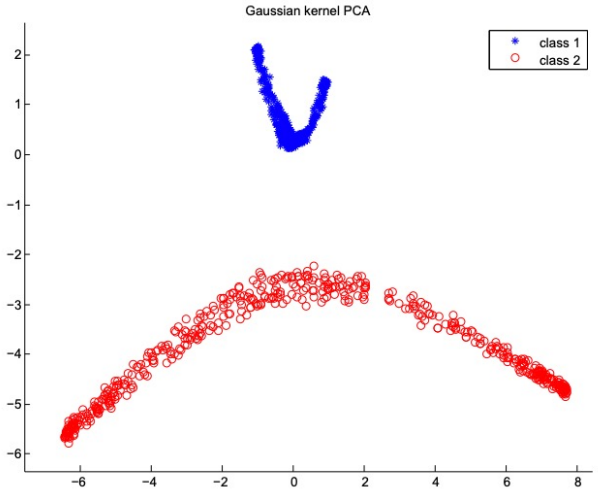
Latent features: linear in $\phi(x)$ where $\phi(x).\ \phi(x') = K(x,x')$ that capture maximum variance or minimum reconstruction error



Original data points



PCA



Kernel PCA
Gaussian/RBF kernel

Src: ArXiv 1207.3538

Kernel PCA

HW4!

Latent features: linear in $\phi(x)$ where $\phi(x).\ \phi(x') = K(x,x')$ that capture maximum variance or minimum reconstruction error

PCA:

Top d eigenvectors (each D dimensional) of sample covariance XX^T

Low d-dimensional embedding of a point: $[v_1^T x_i,\ v_2^T x_i,\ \ldots\ v_d^T x_i]$

Kernel PCA:

Top d eigenvectors (each n dimensional) of kernel matrix K(X,X)

Low d-dimensional embedding of a point: $[v_1(i),\ v_2(i),\ \ldots,\ v_d(i)]$

Eigenvectors are not PCs but projections of data points

PCA Summary

- PCA finds latent features linear in original features x that capture
  - Maximum variance amongst all linear features
  - Minimum reconstruction error when recovering points from PC projections

- Non-convex problem with simple solution:

  PCs = eigenvectors of sample covariance matrix

  Lower ($d < D$) dimensional embedding of data point = projection of data point onto d PCs

- Kernel PCA: latent features linear in $\phi(x)$ where $\phi(x).\ \phi(x') = K(x,x')$ that capture maximum variance or minimum reconstruction error
  - Directly get projections of data points