Curse of Dimensionality, Dimensionality Reduction with PCA

Curse of Dimensionality: Overfitting

- If the number of features ***d*** is large, the number of samples ***n***, may be too small for accurate parameter estimation.

- For example, covariance matrix has ***d*²** parameters:

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \cdots & \sigma_{1d} \\ \vdots & \ddots & \vdots \\ \sigma_{d1} & \cdots & \sigma_d^2 \end{bmatrix}$$

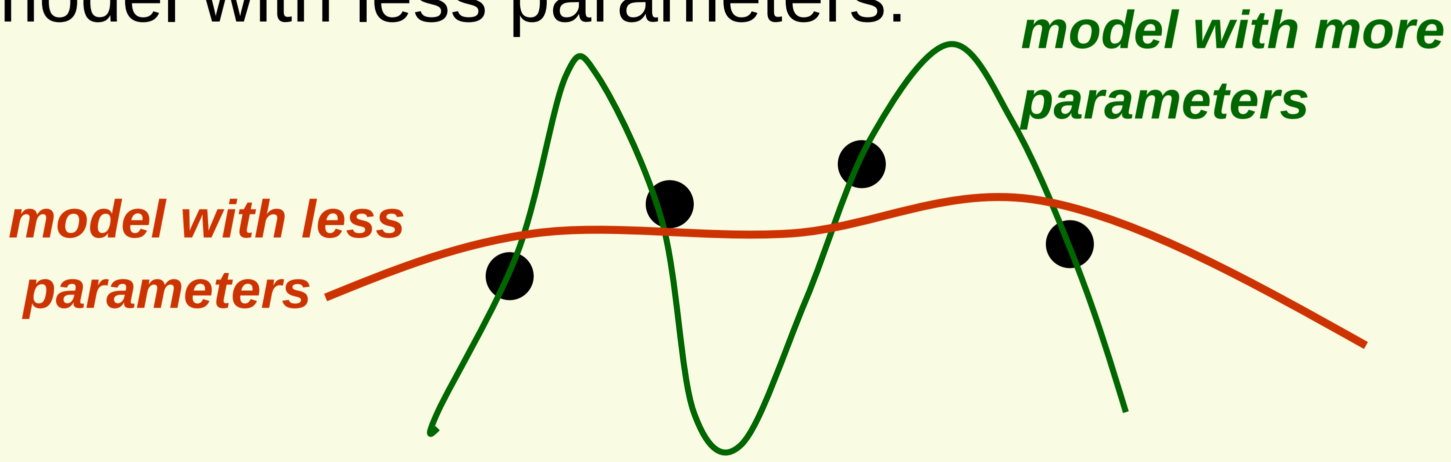
- For accurate estimation, ***n*** should be much bigger than ***d*²**, otherwise model is too complicated for the data, ***overfitting***:

Curse of Dimensionality: Overfitting

- Paradox: If $\boldsymbol{n} < \boldsymbol{d}^2$ we are better off assuming that features are uncorrelated, even if we know this assumption is wrong
- In this case, the covariance matrix has only $\boldsymbol{d}$ parameters:

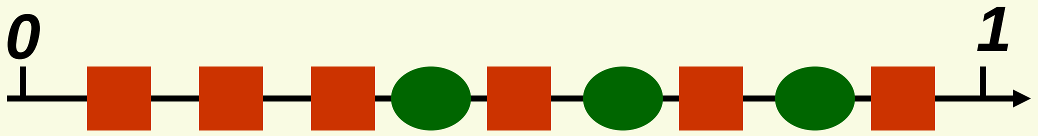
$$\Sigma = \begin{bmatrix} \sigma_1^2 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_d^2 \end{bmatrix}$$

- We are likely to avoid overfitting because we fit a model with less parameters:



Curse of Dimensionality: Number of Samples

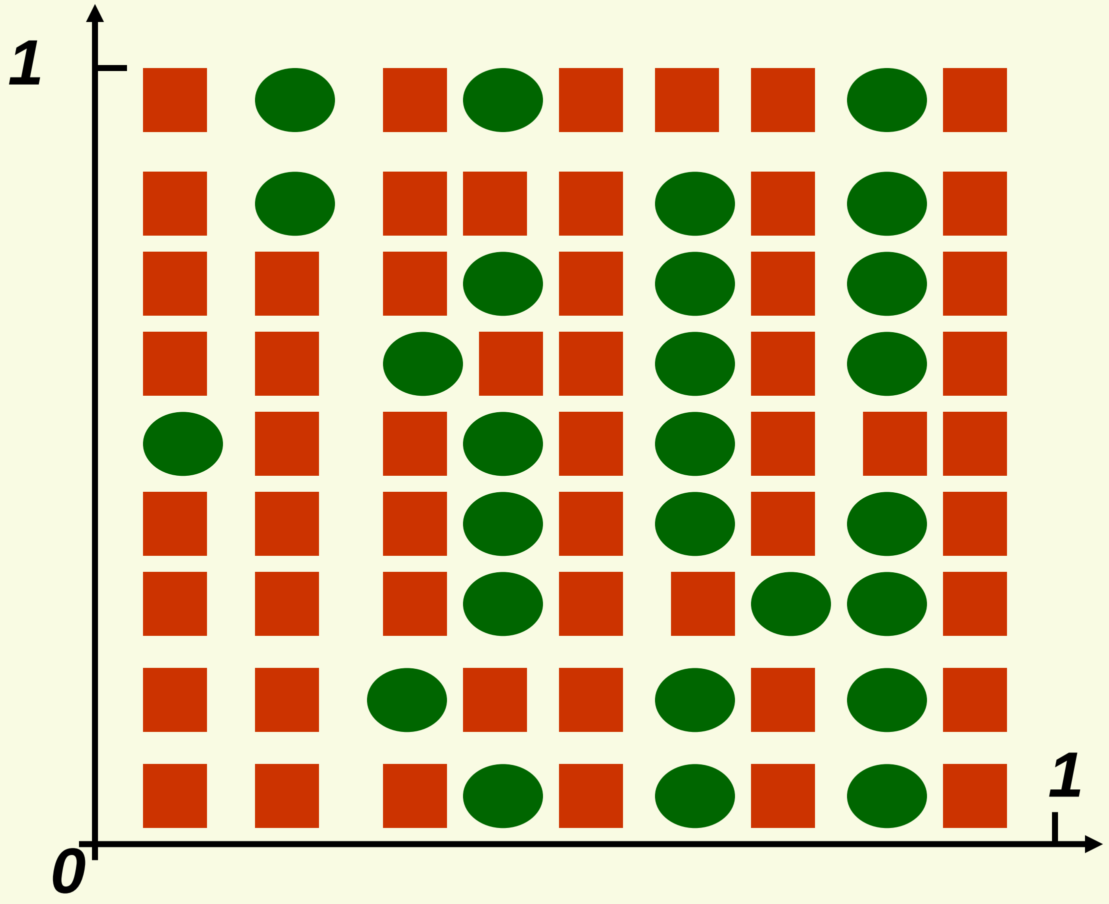
- Suppose we want to use the nearest neighbor approach with ***k*** = 1 (***1NN***)
- Suppose we start with only one feature



- This feature is not discriminative, i.e. it does not separate the classes well
- We decide to use 2 features. For the 1NN method to work well, need a lot of samples, i.e. samples have to be dense
- To maintain the same density as in 1D (9 samples per unit length), how many samples do we need?

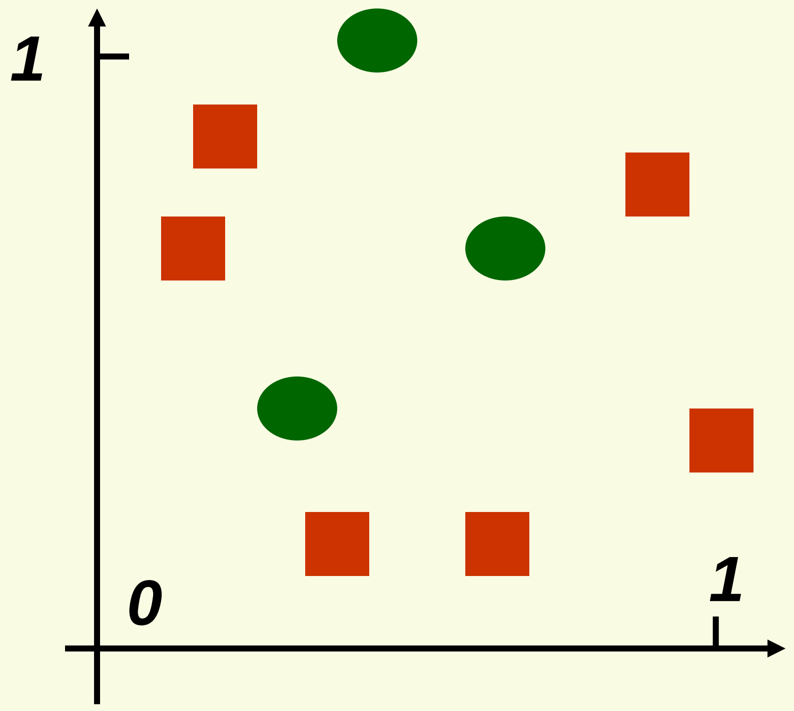
Curse of Dimensionality: Number of Samples

- We need $\boldsymbol{9^2}$ samples to maintain the same density as in ***1D***



Curse of Dimensionality: Number of Samples

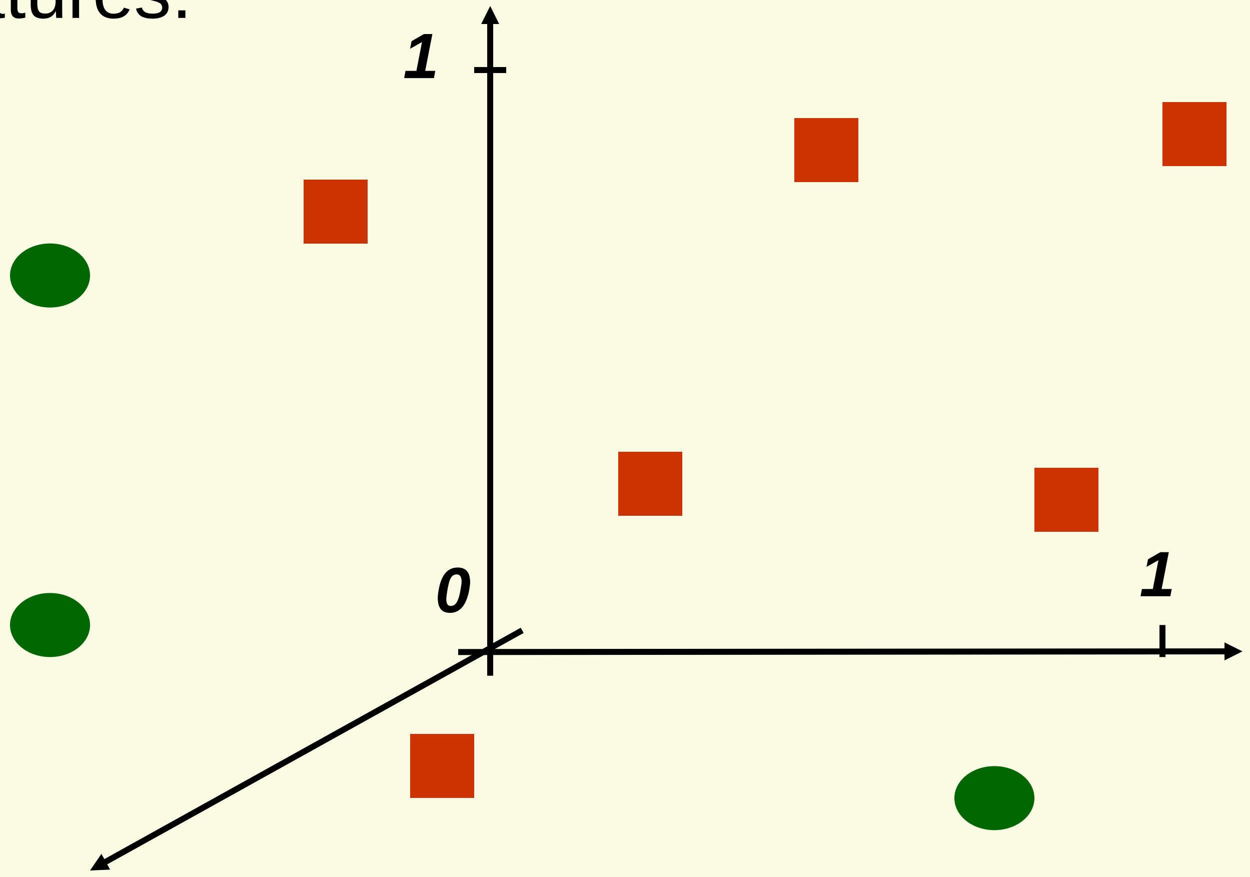
- Of course, when we go from 1 feature to 2, no one gives us more samples, we still have 9



- This is way too sparse for ***1NN*** to work well

Curse of Dimensionality: Number of Samples

- Things go from bad to worse if we decide to use 3 features:



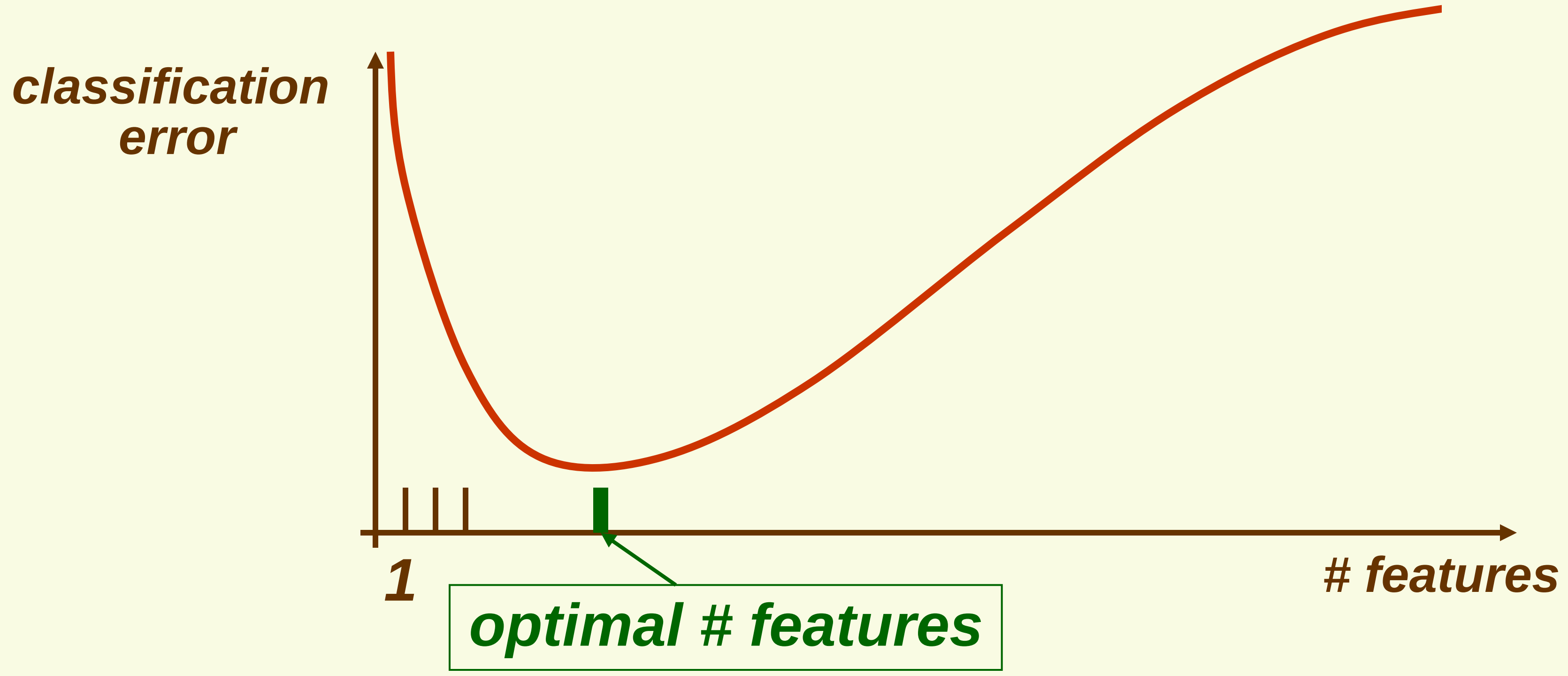
- If ***9*** was dense enough in 1D, in 3D we need ***9^3=729*** samples!

Curse of Dimensionality: Number of Samples

- In general, if ***n*** samples is dense enough in ***1D***
- Then in ***d*** dimensions we need $\boldsymbol{n^d}$ samples!
- And $\boldsymbol{n^d}$ grows really really fast as a function of ***d***
- Common pitfall:
  - If we can’t solve a problem with a few features, adding more features seems like a good idea
  - However the number of samples usually stays the same
  - The method with more features is likely to perform worse instead of expected better

Curse of Dimensionality: Number of Samples

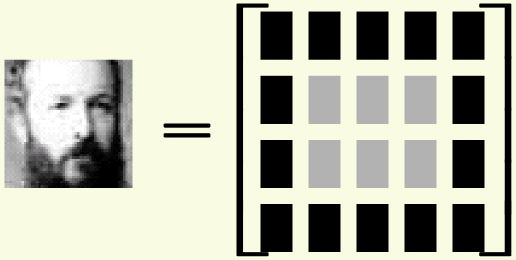
- For a fixed number of samples, as we add features, the graph of classification error:



- Thus for each fixed sample size ***n***, there is the optimal number of features to use

The Curse of Dimensionality

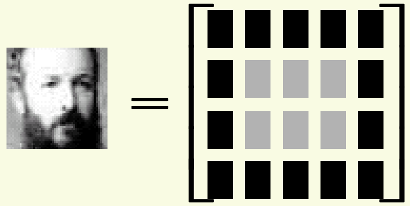
- We should try to avoid creating lot of features
- Often no choice, problem starts with many features
- Example: Face Detection
    - One sample point is ***k*** by ***m*** array of pixels



    - Feature extraction is not trivial, usually every pixel is taken as a feature
    - Typical dimension is 20 by 20 = 400
    - Suppose ***10*** samples are dense enough for 1 dimension. Need only $\boldsymbol{10^{400}}$ samples

The Curse of Dimensionality

- Face Detection, dimension of one sample point is ***km***



- The fact that we set up the problem with ***km*** dimensions (features) does not mean it is really a ***km***-dimensional problem
- Space of all ***k*** by ***m*** images has ***km*** dimensions
- Space of all ***k*** by ***m*** faces must be much smaller, since faces form a tiny fraction of all possible images
- Most likely we are not setting the problem up with the right features
- If we used better features, we are likely need much less than ***km***-dimensions

Dimensionality Reduction

- High dimensionality is challenging and redundant
- It is natural to try to reduce dimensionality
- Reduce dimensionality by feature combination: combine old features ***x*** to create new features ***y***

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} \rightarrow f\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix}\right) = \begin{bmatrix} y_1 \\ \vdots \\ y_k \end{bmatrix} = \mathbf{y} \quad \text{with } k < d$$

- For example,

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \rightarrow \begin{bmatrix} x_1 + x_2 \\ x_3 + x_4 \end{bmatrix} = \mathbf{y}$$

- Ideally, the new vector ***y*** should retain from ***x*** all information important for classification

Dimensionality Reduction

- The best ***f***(***x***) is most likely a non-linear function
- Linear functions are easier to find though
- For now, assume that ***f***(***x***) is a linear mapping
- Thus it can be represented by a matrix ***W***:

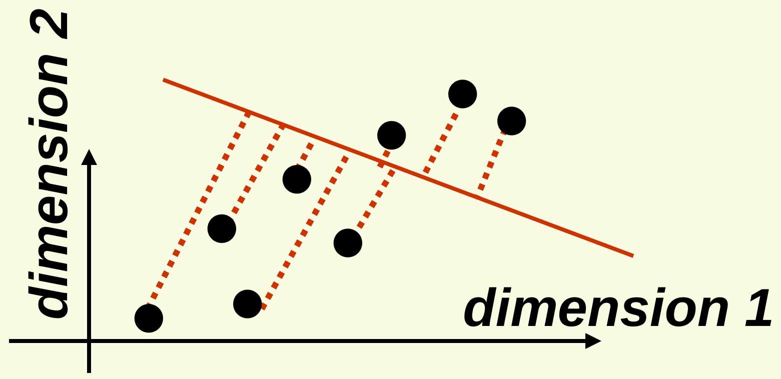
$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} \Rightarrow W \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} = \begin{bmatrix} w_{11} & \cdots & w_{1d} \\ \vdots & & \vdots \\ w_{k1} & \cdots & w_{kd} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_k \end{bmatrix} \quad \textbf{\textit{with } } k < d$$

Feature Combination

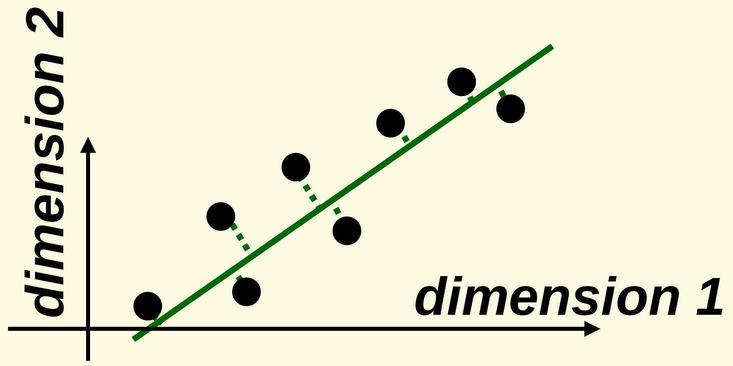
- We will look at 2 methods for feature combination
  - Principle Component Analysis (PCA)
  - Fischer Linear Discriminant (next lecture)

Principle Component Analysis (PCA)

- Main idea: seek most accurate data representation in a lower dimensional space
- Example in 2-D
  - Project data to 1-D subspace (a line) which minimize the projection error



large projection errors, bad line to project to

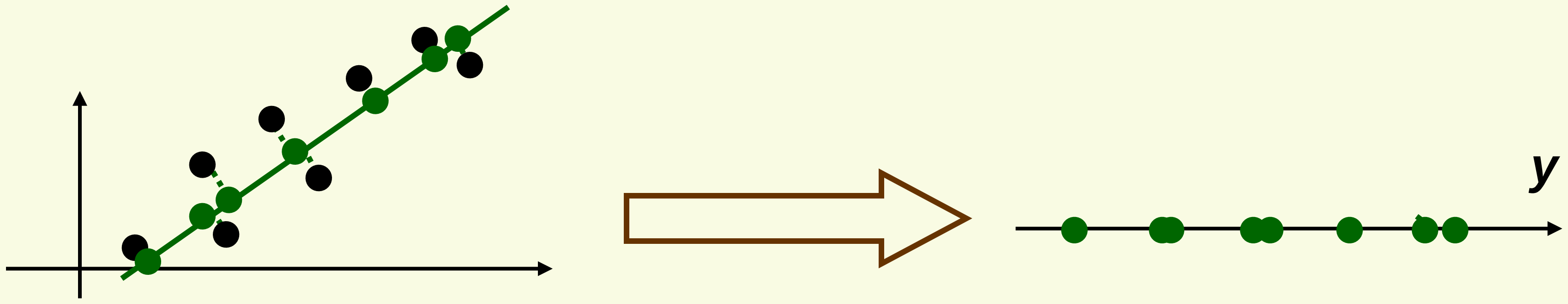


small projection errors, good line to project to

- Notice that the good line to use for projection lies in the direction of largest variance

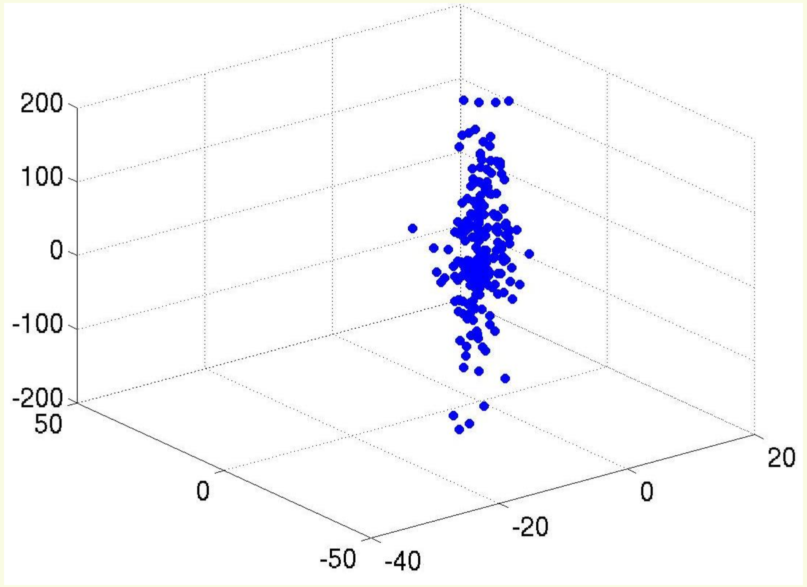
PCA

- After the data is projected on the best line, need to transform the coordinate system to get 1D representation for vector ***y***

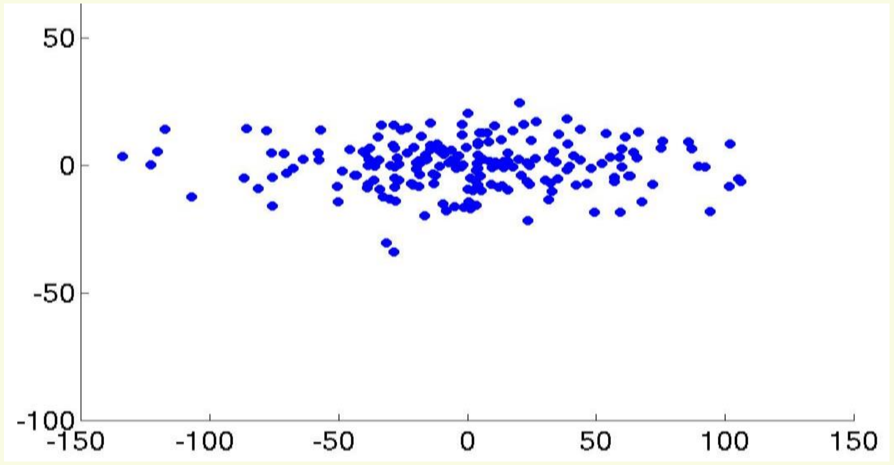


- Note that new data ***y*** has the same variance as old data ***x*** in the direction of the green line
- PCA preserves largest variances in the data. We will prove this statement, for now it is just an intuition of what PCA will do

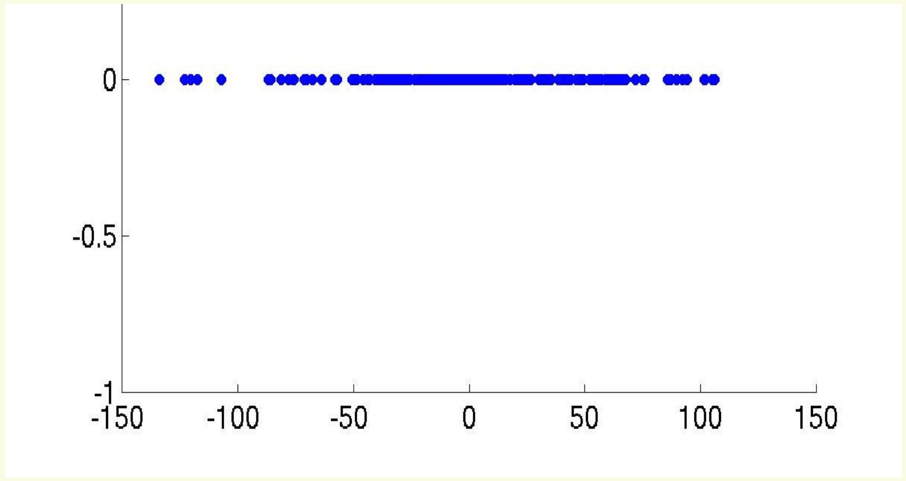
PCA: Approximation of Elliptical Cloud in 3D



best 2D approximation



best 1D approximation



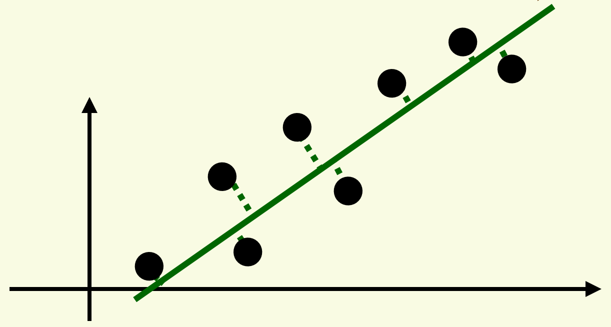
PCA: Linear Algebra for Derivation

- Let ***V*** be a ***d*** dimensional linear space, and ***W*** be a ***k*** dimensional linear subspace of ***V***
- We can always find a set of ***d*** dimensional vectors $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_k\}$ which forms an orthonormal basis for ***W***
  - $\langle \mathbf{e}_i, \mathbf{e}_j \rangle = 0$ if ***i*** is not equal to ***j*** and $\langle \mathbf{e}_i, \mathbf{e}_i \rangle = 1$
- Thus any vector in ***W*** can be written as

$$\alpha_1 \mathbf{e}_1 + \alpha_2 \mathbf{e}_2 + \ldots + \alpha_k \mathbf{e}_k = \sum_{i=1}^{k} \alpha_i \mathbf{e}_i \quad \textit{for scalars } \alpha_1, \ldots, \alpha_k$$

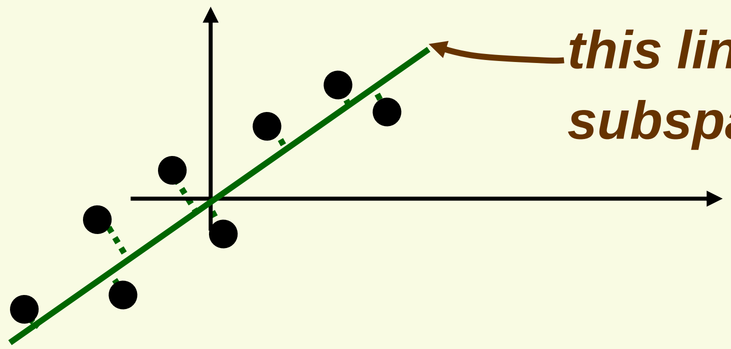
PCA: Linear Algebra for Derivation

- Recall that subspace ***W*** contains the zero vector, i.e. it goes through the origin



this line is not a subspace of R^2

- For derivation, it will be convenient to project to subspace ***W***: thus we need to shift everything



this line is a subspace of R^2

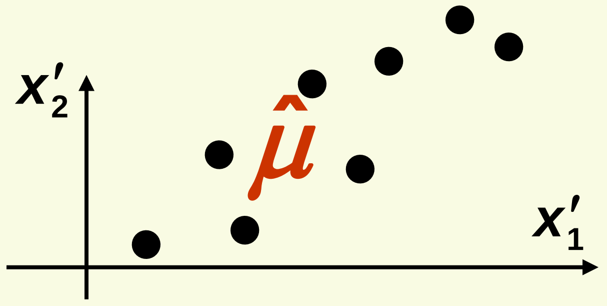
PCA Derivation: Shift by the Mean Vector

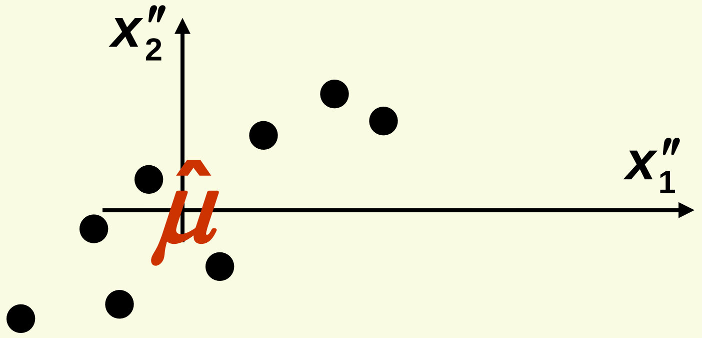
- Before PCA, subtract sample mean from the data

$$x - \frac{1}{n}\sum_{i=1}^{n} x_i = x - \hat{\mu}$$

- The new data has zero mean.

- All we did is change the coordinate system





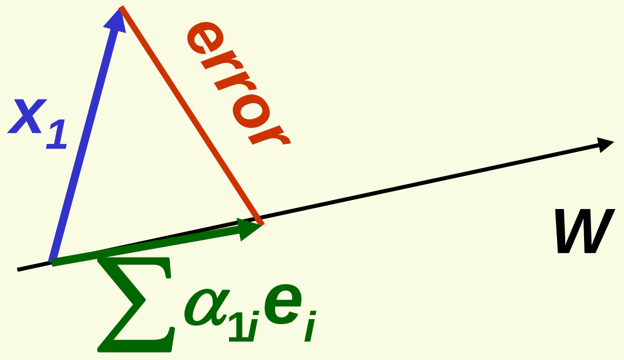
PCA: Derivation

- We want to find the most accurate representation of data $\boldsymbol{D}=\{\boldsymbol{x_1},\boldsymbol{x_2},\ldots,\boldsymbol{x_n}\}$ in some subspace $\boldsymbol{W}$ which has dimension $\boldsymbol{k} < \boldsymbol{d}$
- Let $\{\boldsymbol{e_1},\boldsymbol{e_2},\ldots,\boldsymbol{e_k}\}$ be the orthonormal basis for $\boldsymbol{W}$. Any vector in $\boldsymbol{W}$ can be written as $\sum_{i=1}^{k} \alpha_i \boldsymbol{e}_i$
- Thus $\boldsymbol{x_1}$ will be represented by some vector in $\boldsymbol{W}$

$$\sum_{i=1}^{k} \alpha_{1i} \boldsymbol{e}_i$$

- Error of this representation:

$$\boldsymbol{error} = \left\| \boldsymbol{x}_1 - \sum_{i=1}^{k} \alpha_{1i} \boldsymbol{e}_i \right\|^2$$



PCA: Derivation

- To find the total error, we need to sum over all $\boldsymbol{x}_j$'s
- Any $\boldsymbol{x}_j$ can be written as $\sum_{i=1}^{k} \alpha_{ji} \mathbf{e}_i$
- Thus the total error for representation of all data ***D*** is:

$$\underbrace{J(\mathbf{e}_1,\ldots,\mathbf{e}_k,\alpha_{11},\ldots\alpha_{nk})}_{\text{unknowns}} = \overset{\text{sum over all data points}}{\downarrow}\sum_{j=1}^{n} \underbrace{\boxed{\left\| \mathbf{x}_j - \sum_{i=1}^{k} \alpha_{ji}\mathbf{e}_i \right\|}^2}_{\text{error at one point}}$$

PCA: Derivation

- To minimize ***J***, need to take partial derivatives and also enforce constraint that $\{\mathbf{e}_1,\mathbf{e}_2,\ldots,\mathbf{e}_k\}$ are orthogonal

$$J(\mathbf{e}_1,\ldots,\mathbf{e}_k,\alpha_{11},\ldots\alpha_{nk}) = \sum_{j=1}^{n}\left\|\mathbf{x}_j - \sum_{i=1}^{k}\alpha_{ji}\mathbf{e}_i\right\|^2$$

- Let us simplify ***J*** first:

$$J(\mathbf{e}_1,\ldots,\mathbf{e}_k,\alpha_{11},\ldots\alpha_{nk}) = \sum_{j=1}^{n}\left\|\mathbf{x}_j\right\|^2 - 2\sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}\mathbf{x}_j^t\mathbf{e}_i + \sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}^2$$

PCA: Derivation

$$J(\mathbf{e}_1,\dots,\mathbf{e}_k,\alpha_{11},\dots\alpha_{nk}) = \sum_{j=1}^{n}\|\mathbf{x}_j\|^2 - 2\sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}\mathbf{x}_j^t\mathbf{e}_i + \sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}^2$$

- First take partial derivatives with respect to α_{ml}

$$\frac{\partial}{\partial\alpha_{ml}} J(\mathbf{e}_1,\dots,\mathbf{e}_k,\alpha_{11},\dots\alpha_{nk}) = -2\mathbf{x}_m^t\mathbf{e}_l + 2\alpha_{ml}$$

- Thus the optimal value for α_{ml} is

$$-2\mathbf{x}_m^t\mathbf{e}_l + 2\alpha_{ml} = 0 \;\Rightarrow\; \alpha_{ml} = \mathbf{x}_m^t\mathbf{e}_l$$

PCA: Derivation

$$J(e_1,\dots,e_k,\alpha_{11},\dots\alpha_{nk}) = \sum_{j=1}^{n}\|x_j\|^2 - 2\sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}x_j^t e_i + \sum_{j=1}^{n}\sum_{i=1}^{k}\alpha_{ji}^2$$

- Plug the optimal value for $\alpha_{ml} = x^t{}_m e_l$ back into J

$$J(e_1,\dots,e_k) = \sum_{j=1}^{n}\|x_j\|^2 - 2\sum_{j=1}^{n}\sum_{i=1}^{k}(x_j^t e_i)x_j^t e_i + \sum_{j=1}^{n}\sum_{i=1}^{k}(x_j^t e_i)^2$$

- Can simplify J

$$J(e_1,\dots,e_k) = \sum_{j=1}^{n}\|x_j\|^2 - \sum_{j=1}^{n}\sum_{i=1}^{k}(x_j^t e_i)^2$$

PCA: Derivation

$$J(e_1,\dots,e_k)=\sum_{j=1}^{n}\|x_j\|^2-\sum_{j=1}^{n}\sum_{i=1}^{k}\left(x_j^t e_i\right)^2$$

- Rewrite ***J*** using $(a^t b)^2 = (a^t b)(a^t b) = (b^t a)(a^t b) = b^t(aa^t)b$

$$J(e_1,\dots,e_k)=\sum_{j=1}^{n}\|x_j\|^2-\sum_{i=1}^{k}e_i^t\left(\sum_{j=1}^{n}\left(x_j x_j^t\right)\right)e_i$$

$$=\sum_{j=1}^{n}\|x_j\|^2-\sum_{i=1}^{k}e_i^t S e_i$$

- Where $S=\sum_{j=1}^{n}x_j x_j^t$
- ***S*** is called the scatter matrix, it is just n-1 times the sample covariance matrix we have seen before

$$\hat{\Sigma}=\frac{1}{n-1}\sum_{j=1}^{n}\left(x_j-\hat{\mu}\right)\left(x_j-\hat{\mu}\right)^t$$

PCA: Derivation

$$J(\mathbf{e}_1,\ldots,\mathbf{e}_k) = \underbrace{\sum_{j=1}^{n}\left\|\mathbf{x}_j\right\|^2}_{\text{constant}} - \sum_{i=1}^{k}\mathbf{e}_i^t S\,\mathbf{e}_i$$

- Minimizing J is equivalent to maximizing $\sum_{i=1}^{k}\mathbf{e}_i^t S\,\mathbf{e}_i$
- We should also enforce constraints $\mathbf{e}_i^t\mathbf{e}_i = 1$ for all i
- Use the method of Lagrange multipliers, incorporate the constraints with undetermined $\lambda_1, \ldots, \lambda_k$
- Need to maximize new function u

$$u(\mathbf{e}_1,\ldots,\mathbf{e}_k) = \sum_{i=1}^{k}\mathbf{e}_i^t S\,\mathbf{e}_i - \sum_{j=1}^{k}\lambda_j\left(\mathbf{e}_j^t\mathbf{e}_j - 1\right)$$

PCA: Derivation

$$u(\mathbf{e}_1,\ldots,\mathbf{e}_k) = \sum_{i=1}^{k} \mathbf{e}_i^t S\,\mathbf{e}_i - \sum_{j=1}^{k} \lambda_j \left(\mathbf{e}_j^t \mathbf{e}_j - 1\right)$$

- Compute the partial derivatives with respect to $\mathbf{e}_m$

$$\frac{\partial}{\partial \mathbf{e}_m} u(\mathbf{e}_1,\ldots,\mathbf{e}_k) = 2S\mathbf{e}_m - 2\lambda_m \mathbf{e}_m = 0$$

Note: *$\mathbf{e}_m$ is a vector, what we are really doing here is taking partial derivatives with respect to each element of $\mathbf{e}_m$ and then arranging them up in a linear equation*

- Thus λ_m and $\mathbf{e}_m$ are eigenvalues and eigenvectors of scatter matrix S

$$S\mathbf{e}_m = \lambda_m \mathbf{e}_m$$

PCA: Derivation

$$J(\mathbf{e}_1,\dots,\mathbf{e}_k) = \sum_{j=1}^{n} \|\mathbf{x}_j\|^2 - \sum_{i=1}^{k} \mathbf{e}_i^t \mathbf{S}\, \mathbf{e}_i$$

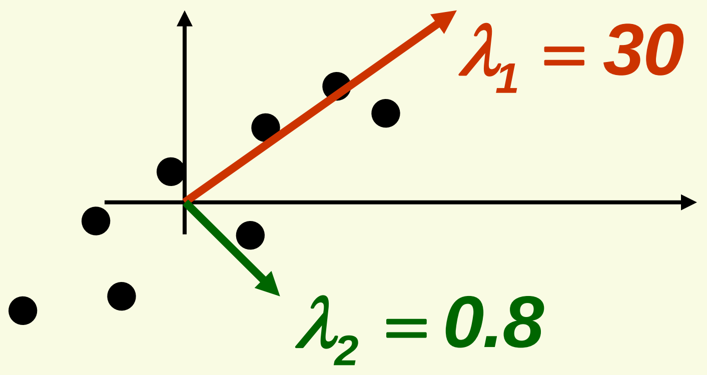
- Let's plug $\mathbf{e}_m$ back into ***J*** and use $\mathbf{S}\mathbf{e}_m = \lambda_m \mathbf{e}_m$

$$J(\mathbf{e}_1,\dots,\mathbf{e}_k) = \sum_{j=1}^{n} \|\mathbf{x}_j\|^2 - \sum_{i=1}^{k} \lambda_i \|\mathbf{e}_i\|^2 = \underbrace{\sum_{j=1}^{n} \|\mathbf{x}_j\|^2}_{\text{constant}} - \sum_{i=1}^{k} \lambda_i$$

- Thus to minimize ***J*** take for the basis of ***W*** the ***k*** eigenvectors of ***S*** corresponding to the ***k*** largest eigenvalues

PCA

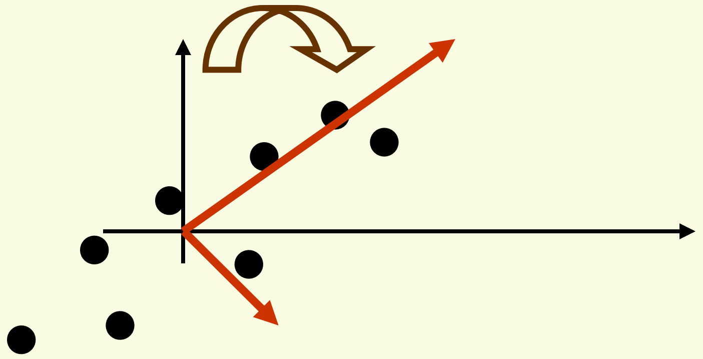
- The larger the eigenvalue of ***S***, the larger is the variance in the direction of corresponding eigenvector



- This result is exactly what we expected: project ***x*** into subspace of dimension ***k*** which has the largest variance
- This is very intuitive: restrict attention to directions where the scatter is the greatest

PCA

- Thus PCA can be thought of as finding new orthogonal basis by rotating the old axis until the directions of maximum variance are found



PCA as Data Approximation

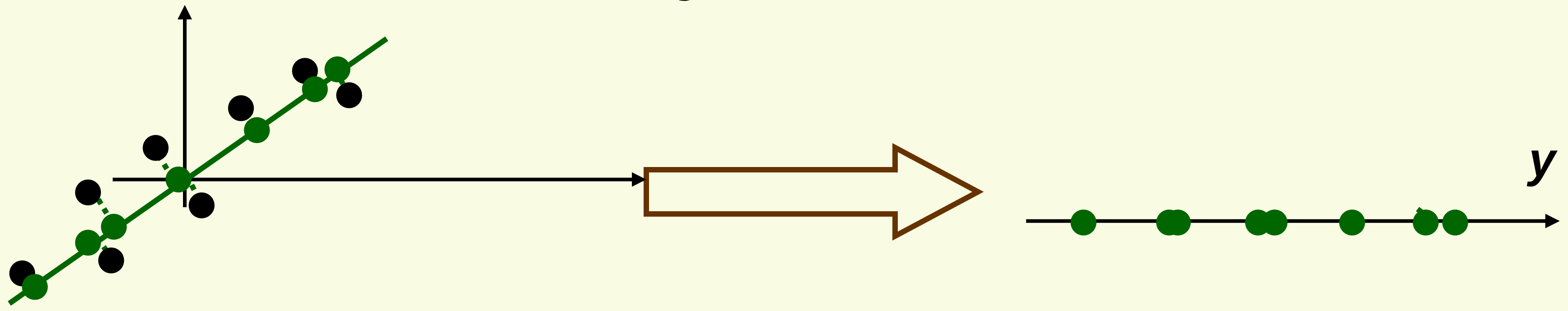
- Let $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_d\}$ be all ***d*** eigenvectors of the scatter matrix ***S***, sorted in order of decreasing corresponding eigenvalue
- Without any approximation, for any sample $\boldsymbol{x}_i$:

$$\boldsymbol{x}_i = \sum_{j=1}^{d} \alpha_j \boldsymbol{e}_j = \underbrace{\alpha_1 \boldsymbol{e}_1 + \ldots + \alpha_k \boldsymbol{e}_k}_{\text{approximation of } x_i} + \overbrace{\alpha_{k+1} \boldsymbol{e}_{k+1} \ldots + \alpha_d \boldsymbol{e}_d}^{\text{error of approximation}}$$

- coefficients $\alpha_m = \boldsymbol{x}^t_i \boldsymbol{e}_m$ are called *principle components*
  - The larger ***k***, the better is the approximation
  - Components are arranged in order of importance, more important components come first
- Thus PCA takes the first ***k*** most important components of $\boldsymbol{x}_i$ as an approximation to $\boldsymbol{x}_i$

PCA: Last Step

- Now we know how to project the data
- Last step is to change the coordinates to get final ***k***-dimensional vector ***y***



- Let matrix $\boldsymbol{E} = [\boldsymbol{e}_1 \cdots \boldsymbol{e}_k]$
- Then the coordinate transformation is $\boldsymbol{y} = \boldsymbol{E}^t \boldsymbol{x}$
- Under $\boldsymbol{E}^t$, the eigenvectors become the standard basis:

$$\boldsymbol{E}^t \boldsymbol{e}_i = \begin{bmatrix} \boldsymbol{e}_1 \\ \vdots \\ \boldsymbol{e}_i \\ \vdots \\ \boldsymbol{e}_k \end{bmatrix} \boldsymbol{e}_i = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

Recipe for Dimension Reduction with PCA

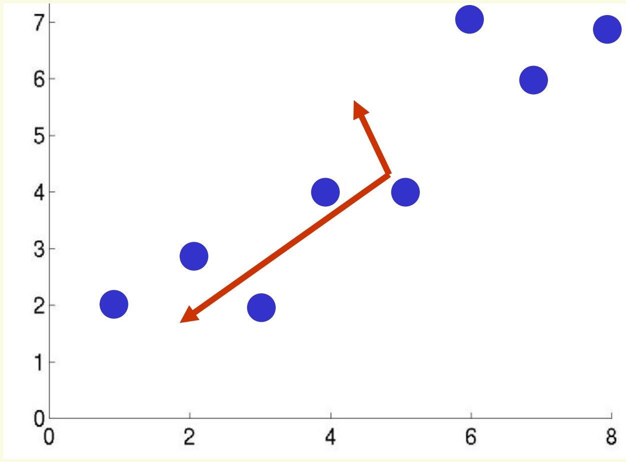
Data $\boldsymbol{D}=\{\boldsymbol{x_1},\boldsymbol{x_2},\ldots,\boldsymbol{x_n}\}$. Each $\boldsymbol{x_i}$ is a $\boldsymbol{d}$-dimensional vector. Wish to use PCA to reduce dimension to $\boldsymbol{k}$

1. Find the sample mean $\hat{\mu}=\frac{1}{n}\sum_{i=1}^{n}x_i$
2. Subtract sample mean from the data $z_i = x_i - \hat{\mu}$
3. Compute the scatter matrix $S=\sum_{i=1}^{n} z_i z_i^t$
4. Compute eigenvectors $\boldsymbol{e_1},\boldsymbol{e_2},\ldots,\boldsymbol{e_k}$ corresponding to the $\boldsymbol{k}$ largest eigenvalues of $\boldsymbol{S}$
5. Let $\boldsymbol{e_1},\boldsymbol{e_2},\ldots,\boldsymbol{e_k}$ be the columns of matrix $E=\left[e_1 \cdots e_k\right]$
6. The desired $\boldsymbol{y}$ which is the closest approximation to $\boldsymbol{x}$ is $y = E^t z$

PCA Example Using Matlab

- Let $\boldsymbol{D} = \{(1,2),(2,3),(3,2),(4,4),(5,4),(6,7),(7,6),(9,7)\}$
- Convenient to arrange data in array

$$X = \begin{bmatrix} 1 & 2 \\ \vdots & \vdots \\ 9 & 7 \end{bmatrix} = \begin{bmatrix} x_1 \\ \vdots \\ x_8 \end{bmatrix}$$



- Mean $\mu = mean(X) = [4.6 \ \ 4.4]$
- Subtract mean from data to get new data array Z

$$Z = X - \begin{bmatrix} \mu \\ \vdots \\ \mu \end{bmatrix} = X - repmat(\mu,8,1) = \begin{bmatrix} -3.6 & -4.4 \\ \vdots & \vdots \\ 4.4 & 2.6 \end{bmatrix}$$

- Compute the scatter matrix ***S***

$$S = 7 * cov(Z) = [-3.6 \ \ -4.4]\begin{bmatrix} -3.6 \\ -4.4 \end{bmatrix} + \ldots + [4.4 \ \ 2.6]\begin{bmatrix} 4.4 \\ 2.6 \end{bmatrix} = \begin{bmatrix} 57 & 40 \\ 40 & 34 \end{bmatrix}$$

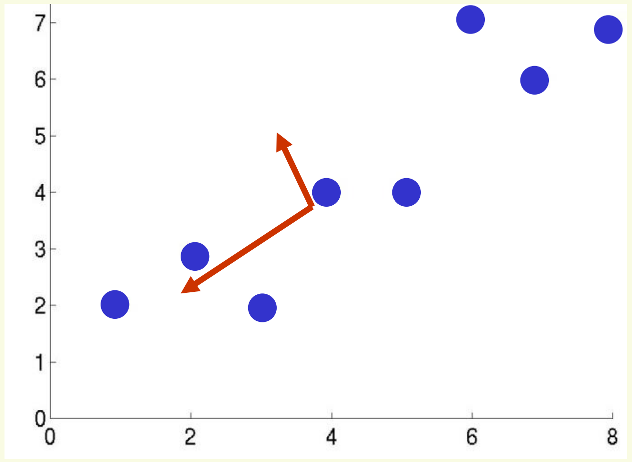
*matlab uses unbiased estimate for covariance, so S=(n-1)*cov(Z)*

PCA Example Using Matlab

- Use [V,D] =eig(***S***) to get eigenvalues and eigenvectors of ***S***

$$\lambda_1 = 87 \text{ and } e_1 = \begin{bmatrix} -0.8 \\ -0.6 \end{bmatrix}$$

$$\lambda_2 = 3.8 \text{ and } e_2 = \begin{bmatrix} 0.6 \\ -0.8 \end{bmatrix}$$



- Projection to 1D space in the direction of $\boldsymbol{e_1}$

$$Y = e_1^t Z^t = \left(\begin{bmatrix} -0.8 & -0.6 \end{bmatrix} \begin{bmatrix} -3.6 & \cdots & 4.4 \\ -4.4 & \cdots & 2.6 \end{bmatrix} \right) = \begin{bmatrix} 4.3 & \cdots & -5.1 \end{bmatrix}$$
$$= \begin{bmatrix} y_1 & \cdots & y_8 \end{bmatrix}$$