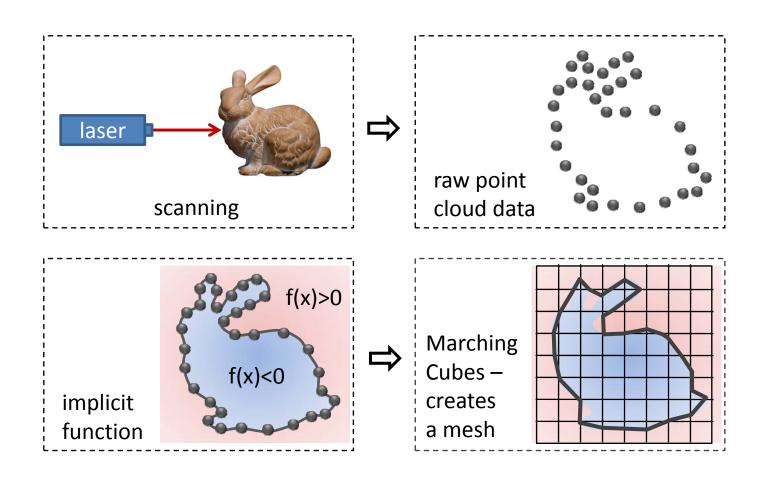
G22.3033-004, Spring 2009 Interactive Shape Modeling

Linear algebra tools for geometric modeling

Surface acquisition and reconstruction



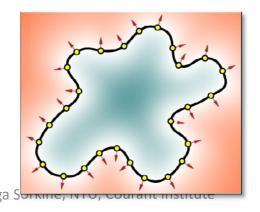
Implicit functions

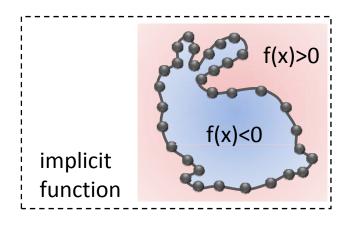
Implicit function?

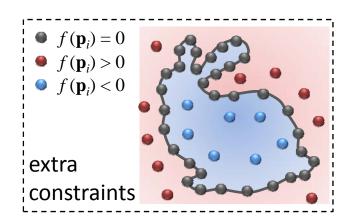
$$f(\mathbf{p}_i) = 0$$

 Need extra constraints to avoid trivial solution

$$f(\mathbf{p}_i + \varepsilon \mathbf{n}_i) = +\varepsilon$$
$$f(\mathbf{p}_i - \varepsilon \mathbf{n}_i) = -\varepsilon$$



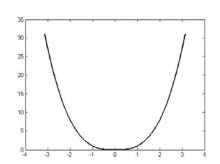




Implicit functions

Radial basis function

$$f_j = \sum_i w_i \, \mathbf{r} \Big(\Big\| \mathbf{p}_i - \mathbf{p}_j \Big\| \Big)$$

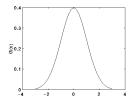


- Constraints: $f(\mathbf{p}_j) = 0$, $f(\mathbf{p}_i + \alpha \mathbf{n}_i) = \alpha$
- Need to solve for w_i

$$\begin{pmatrix} \mathbf{r}(0) & \mathbf{r}(\|\mathbf{p}_{0} - \mathbf{p}_{1}\|) & \mathbf{r}(\|\mathbf{p}_{0} - \mathbf{p}_{2}\|) & \cdots \\ \mathbf{r}(\|\mathbf{p}_{1} - \mathbf{p}_{0}\|) & \mathbf{r}(0) & \mathbf{r}(\|\mathbf{p}_{1} - \mathbf{p}_{2}\|) & w_{1} \\ \mathbf{r}(\|\mathbf{p}_{2} - \mathbf{p}_{0}\|) & \mathbf{r}(\|\mathbf{p}_{2} - \mathbf{p}_{1}\|) & \mathbf{r}(0) & \vdots \end{pmatrix} = \begin{pmatrix} f_{0} \\ w_{1} \\ w_{2} \\ \vdots \end{pmatrix}$$
 Linear problem

Implicit functions

Moving least squares



$$f(\mathbf{x}) = f_{\mathbf{x}}(\mathbf{x}); \quad f_{\mathbf{x}}(\mathbf{x}) = \underset{f_{\mathbf{x}} \in \Pi_k^d}{\arg\min} \sum_{i=0}^n \left\| f_{\mathbf{x}}(\mathbf{p}_i) - f_i \right\|^2 \theta \left(\left\| \mathbf{p}_i - \mathbf{x} \right\| \right)$$

• Need to solve locally for f_x , where f_x is a polynomial (solve for the coefficients c_k)

$$f_{\mathbf{x}}(\mathbf{x}) = c_0 + c_1 x + c_2 y + c_3 x^2 + c_4 xy + c_5 y^2 \dots$$

= $\mathbf{c}^{\mathrm{T}} \mathbf{b}(\mathbf{x})$.

$$\min_{\mathbf{c}} \sum_{i=0}^{n} \left\| \mathbf{c}^{T} \mathbf{b}(\mathbf{p}_{i}) - f_{i} \right\|^{2} w_{i}(\mathbf{x})$$
 Weighted linear least squares problem

RBF vs. MLS

$$f(\mathbf{x}) = \sum_{i=1}^{n} w_i r(||\mathbf{x} - \mathbf{p}_i||)$$

- Need to solve for the weights w_i
- Closed formulation

Requires solving a linear system of size $n \times n$ (n is the number of points!)

$$f(\mathbf{x}) = f_{\mathbf{x}}(\mathbf{x});$$

$$f_{\mathbf{x}}(\mathbf{x}) = \underset{f_{\mathbf{x}} \in \Pi_k^d}{\min} \sum_{i=1}^n ||f_{\mathbf{x}}(\mathbf{p}_i) - f_i||^2 \theta(||\mathbf{x} - \mathbf{p}_i||)$$

- Solve for the local polynomial in each x
- No global closed formula

 each point has its own
 function fit
- Requires solving a linear system of size k×k (k is the order of the polynomial) for each evaluation

Algebraic tools

Linear least squares

But first reminder: vectors/points,
inner product, projection

Points and Vectors

Basic definitions

- Points specify *location* in space (or in the plane).
- Vectors have magnitude and direction (like velocity).

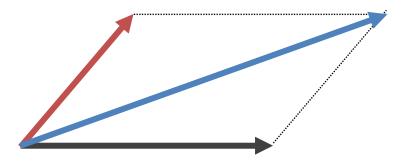
Points ≠ Vectors

Point + vector = point

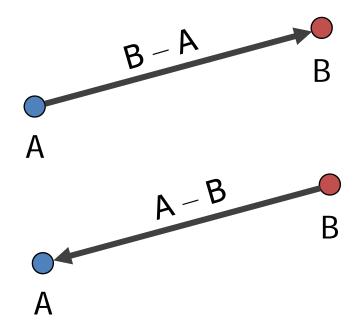


vector + vector = vector

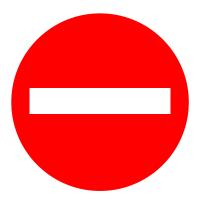
Parallelogram rule



point – point = vector

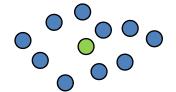


point + point: not defined!!



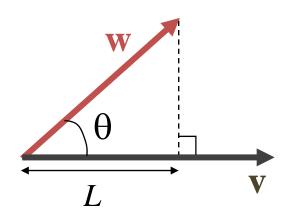
- Unless we are computing a weighted average of points (weighted centroid).
 - If the weights sum up to one, the average is meaningful.

$$\mathbf{c} = \sum_{i=1}^{n} w_i \, \mathbf{p}_i$$



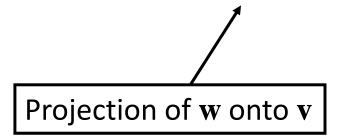
Defined for vectors:

$$\langle \mathbf{v}, \mathbf{w} \rangle = ||\mathbf{v}|| \cdot ||\mathbf{w}|| \cdot \cos \theta$$

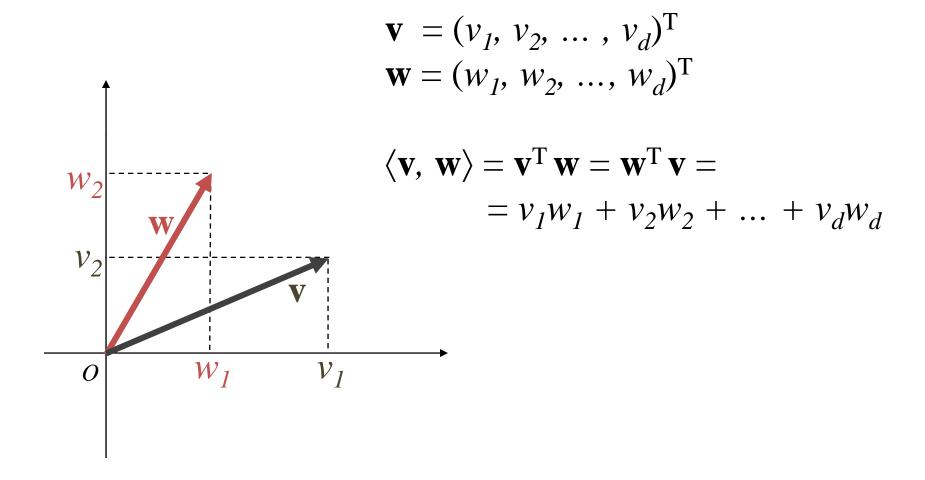


$$\cos\theta = L/\|\mathbf{w}\|$$

$$L = ||\mathbf{w}|| \cos \theta = \langle \mathbf{v}, \mathbf{w} \rangle / ||\mathbf{v}||$$



in coordinates



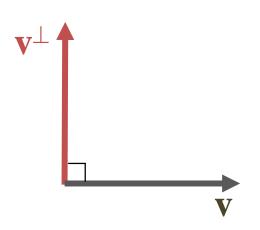
names, notations

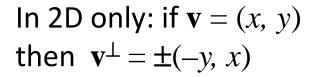
Dot product is also called inner product

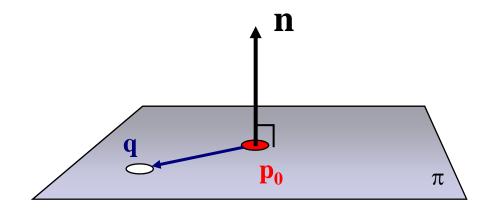
■ Notations: $\langle \mathbf{v}, \mathbf{w} \rangle$ or $\mathbf{v} \cdot \mathbf{w}$ or $\mathbf{v}^T \mathbf{w} (= \mathbf{w}^T \mathbf{v})$

Perpendicular (orthogonal) vectors

$$\langle \mathbf{v}, \ \mathbf{w} \rangle = \mathbf{v}^{\mathrm{T}} \ \mathbf{w} = 0$$







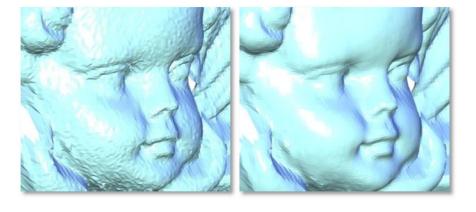
General hyper-plane: all points \mathbf{q} such that $\langle \mathbf{q} - \mathbf{p}_0, \mathbf{n} \rangle = 0$

Least squares fitting

Motivation

- Why are we going over this again?
 - Many of the shape modeling methods presented in later lectures minimize functionals of the form

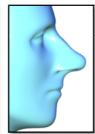
$$\mathbf{c}_{opt} = \underset{\mathbf{c}}{\operatorname{argmin}} \|\mathbf{A}\mathbf{c} - \mathbf{b}\|^2$$







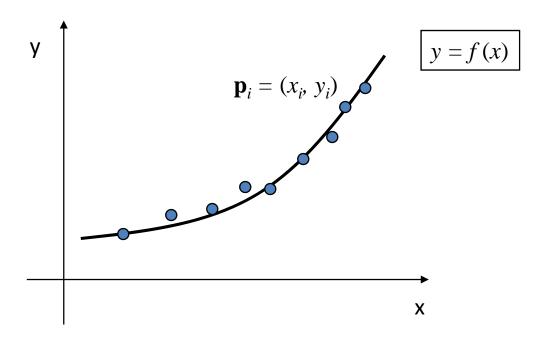




Least squares fitting

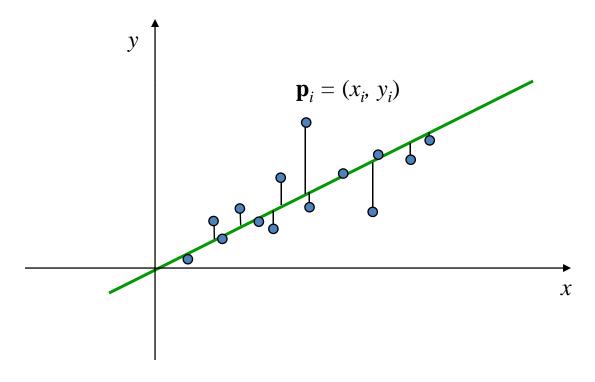
Motivation

 Given data points, fit a function that is "close" to the points



line fitting – 1st order polynomial in 2D

y-offsets minimization



line fitting – 1st order polynomial in 2D

• Find a line y = ax + b that minimizes

$$E(a,b) = \sum_{i=1}^{n} [y_i - (ax_i + b)]^2$$

- E(a,b) is quadratic in the unknown parameters a, b
- Another option would be, for example:

$$AbsErr(a,b) = \sum_{i=1}^{n} |y_i - (ax_i + b)|$$

■ But – it is not differentiable, harder to minimize...

line fitting – LS minimization

• To find optimal a, b we differentiate E(a, b):

$$E(a,b) = \sum_{i=1}^{n} [y_i - (ax_i + b)]^2$$

$$\frac{\partial}{\partial a}E(a, b) = \sum_{i=1}^{n}(-2x_i)[y_i - (ax_i + b)] = 0$$

$$\frac{\partial}{\partial b}E(a, b) = \sum_{i=1}^{n} (-2)[y_i - (ax_i + b)] = 0$$

line fitting – LS minimization

• We obtain two linear equations for a, b:

$$\sum_{i=1}^{n} (-2x_i)[y_i - (ax_i + b)] = 0$$

$$\sum_{i=1}^{n} (-2)[y_i - (ax_i + b)] = 0$$

line fitting – LS minimization

We get two linear equations for a, b:

(1)
$$\sum_{i=1}^{n} \left[x_i y_i - a x_i^2 - b x_i \right] = 0$$

(2)
$$\sum_{i=1}^{n} [y_i - ax_i - b] = 0$$

line fitting – LS minimization

We get two linear equations for a, b:

$$(\sum_{i=1}^{n} x_i^2) a + (\sum_{i=1}^{n} x_i) b = \sum_{i=1}^{n} x_i y_i$$

$$(\sum_{i=1}^{n} x_i) a + (\sum_{i=1}^{n} 1) b = \sum_{i=1}^{n} y_i$$

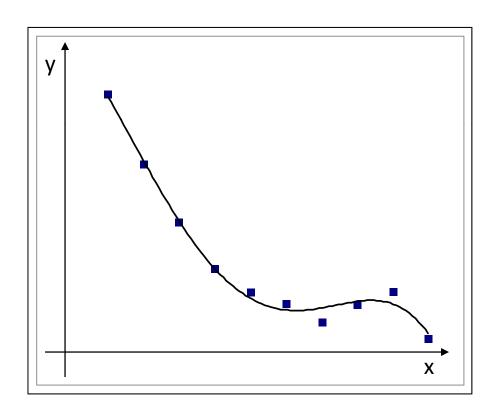
line fitting – LS minimization

Solve for a, b using e.g. Gauss elimination

• Question: why the solution is the *minimum* for the error function?

$$E(a, b) = \sum_{i=1}^{n} [y_i - (ax_i + b)]^2$$

Fitting polynomials



Fitting polynomials

- Decide on the degree of the polynomial, k
- Want to fit $f(x) = a_k x^k + a_{k-1} x^{k-1} + ... + a_1 x + a_0$
- Minimize:

$$E(a_0, a_1, ..., a_k) = \sum_{i=1}^n [y_i - (a_k x_i^k + a_{k-1} x_i^{k-1} + ... + a_1 x_i + a_0)]^2$$

$$\frac{\partial}{\partial a_m} E(a_0, ..., a_k) = \sum_{i=1}^n (-2x^m) [y_i - (a_k x_i^k + a_{k-1} x_i^{k-1} + ... + a_0)] = 0$$

Fitting polynomials

• We get a linear system of k+1 equations in k+1 variables

$$\begin{pmatrix}
\sum_{i=1}^{n} 1 & \sum_{i=1}^{n} x_{i} & \cdots & \sum_{i=1}^{n} x_{i}^{k} \\
\sum_{i=1}^{n} x_{i} & \sum_{i=1}^{n} x_{i}^{2} & \cdots & \sum_{i=1}^{n} x_{i}^{k+1} \\
\vdots & \vdots & \ddots & \vdots \\
\sum_{i=1}^{n} x_{i}^{k} & \sum_{i=1}^{n} x_{i}^{k+1} & \cdots & \sum_{i=1}^{n} x_{i}^{2k}
\end{pmatrix}
\begin{pmatrix}
a_{0} \\
a_{1} \\
\vdots \\
\vdots \\
a_{k}
\end{pmatrix}
=
\begin{pmatrix}
\sum_{i=1}^{n} 1 \cdot y_{i} \\
a_{1} \\
\vdots \\
a_{k}
\end{pmatrix}$$

General parametric fitting

- We can use this approach to fit any function $f(\mathbf{x})$
 - Specified by parameters c_1 , c_2 , c_3 , ...
 - The expression $f(\mathbf{x})$ linearly depends on the parameters.

$$f(\mathbf{x}) = c_1 f_1(\mathbf{x}) + c_2 f_2(\mathbf{x}) + \dots + c_k f_k(\mathbf{x})$$

• Minimize – find best c_1 , c_2 , c_3 ...:

$$\sum_{i=1}^{n} ||f(\mathbf{p}_i) - f_i||^2 = \sum_{i=1}^{n} ||\sum_{j=1}^{k} \mathbf{c}_j f_j(\mathbf{p}_i) - f_i||^2$$

- Let's look at the problem a little differently:
 - We have data points \mathbf{p}_i and desired function values f_i
 - We would like :

$$\forall i = 1, ..., n: f(\mathbf{p}_i) = f_i$$

- Strict interpolation is in general not possible
 - In polynomials: n+1 points define a unique interpolation polynomial of degree n.
 - So, if we have 1000 points and want a cubic polynomial, we probably won't find it...

• We have an over-determined linear system $n \times k$:

$$f(\mathbf{p}_{1}) = c_{1} f_{1}(\mathbf{p}_{1}) + c_{2} f_{2}(\mathbf{p}_{1}) + \dots + c_{k} f_{k}(\mathbf{p}_{1}) = f_{1}$$

$$f(\mathbf{p}_{2}) = c_{1} f_{1}(\mathbf{p}_{2}) + c_{2} f_{2}(\mathbf{p}_{2}) + \dots + c_{k} f_{k}(\mathbf{p}_{2}) = f_{2}$$
...
$$f(\mathbf{p}_{n}) = c_{1} f_{1}(\mathbf{p}_{n}) + c_{2} f_{2}(\mathbf{p}_{n}) + \dots + c_{k} f_{k}(\mathbf{p}_{n}) = f_{n}$$

In matrix form:

In matrix form:

$$Ac = b$$

where $A = (f_j(\mathbf{p}_i))_{i,j}$ is a rectangular $n \times k$ matrix, n > k

$$\mathbf{c} = (c_1, c_2, ..., c_k)^{\mathrm{T}}$$
 $\mathbf{b} = (f_1, f_2, ..., f_n)^{\mathrm{T}}$

$$egin{array}{c} \mathbf{c} = \mathbf{b} \end{array}$$

- More constrains than variables no exact solutions generally exist
- We want to find something that is an "approximate solution":

$$\mathbf{c}_{opt} = \underset{\mathbf{c}}{\operatorname{argmin}} \|\mathbf{A}\mathbf{c} - \mathbf{b}\|^2$$

Finding the LS solution

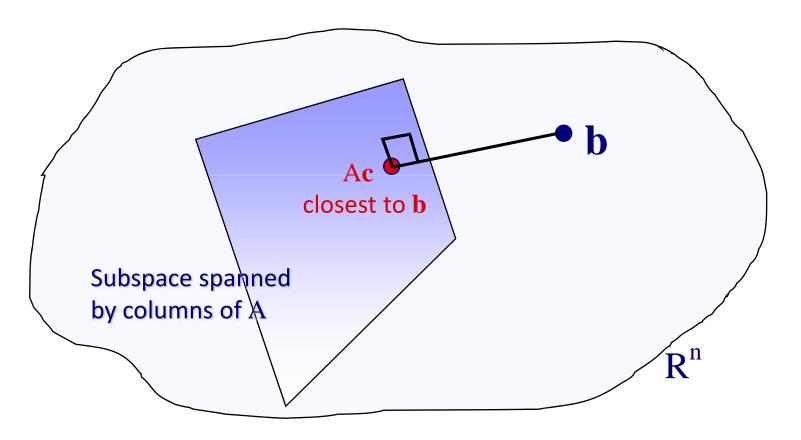
- $\mathbf{c} \in \mathbb{R}^k$
- $Ac \in R^n$
- As we vary c, Ac varies over the linear subspace of Rⁿ spanned by the columns of A:

$$\mathbf{Ac} = \left(\begin{array}{c|c} A_1 & A_2 & A_k & \hline \\ C_1 & C_2 \\ \vdots & \vdots & \vdots \\ C_k & C_k \end{array} \right) = c_1 A_1 + c_2 A_2 + \ldots + c_k A_k$$

This is also known as the column space of A

Finding the LS solution

• We want to find the closest \mathbf{Ac} to \mathbf{b} : $\min_{\mathbf{c}} ||\mathbf{Ac} - \mathbf{b}||^2$



Finding the LS solution

■ The point Ac closest to **b** satisfies:

 $(Ac - b) \perp \{subspace of A's columns\}$



$$\forall$$
 column A_i : $\langle A_i, A\mathbf{c} - \mathbf{b} \rangle = 0$

$$\forall i, A_i^{\mathrm{T}}(\mathbf{Ac} - \mathbf{b}) = 0$$

These are called the normal equations

$$\frac{\mathbf{A}^{\mathrm{T}}(\mathbf{A}\mathbf{c} - \mathbf{b}) = 0}{(\mathbf{A}^{\mathrm{T}}\mathbf{A})\mathbf{c} = \mathbf{A}^{\mathrm{T}}\mathbf{b}}$$

Finding the LS solution

• We have a square symmetric system $(A^{T}A)\mathbf{c} = A^{T}\mathbf{b}$

$$(k \times k)$$

■ If A has full rank (the columns of A are linearly independent) then (A^TA) is invertible.

$$\min_{\mathbf{c}} \|\mathbf{A}\mathbf{c} - \mathbf{b}\|^{2}$$

$$\downarrow \downarrow$$

$$\mathbf{c} = (\mathbf{A}^{T} \mathbf{A})^{-1} \mathbf{A}^{T} \mathbf{b}$$

Weighted least squares

If each constraint has a weight in the energy:

$$\min_{\mathbf{c}} \sum_{i=1}^{n} w_i \left(f_{\mathbf{c}}(\mathbf{p}_i) - f_i \right)^2$$

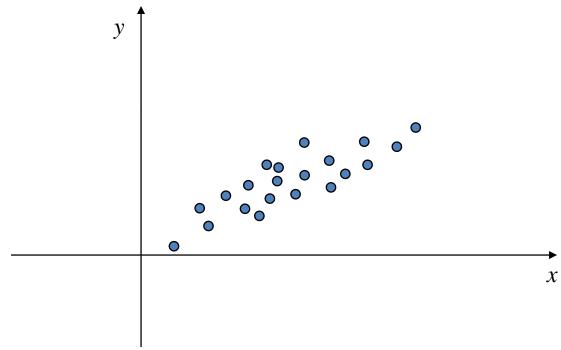
- The weights $w_i > 0$ and don't depend on \mathbf{c}
- Then:

min
$$(\mathbf{A}\mathbf{c} - \mathbf{b})^{\mathrm{T}} \mathbf{W}^{\mathrm{T}} \mathbf{W} (\mathbf{A}\mathbf{c} - \mathbf{b})$$
 where $\mathbf{W} = (w_i)_{ii}$

$$(A^{T}W^{2}A) \mathbf{c} = A^{T}W^{2} \mathbf{b}$$

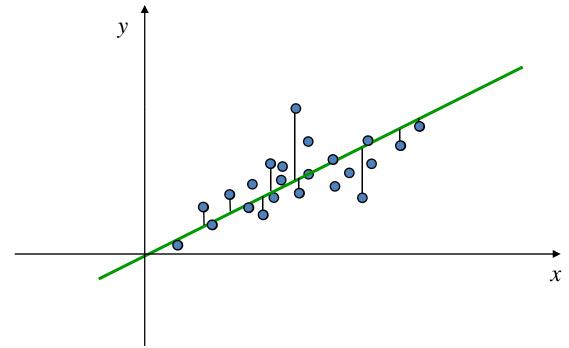
But first, reminder about eigenvectors and eigenvalues

Motivation



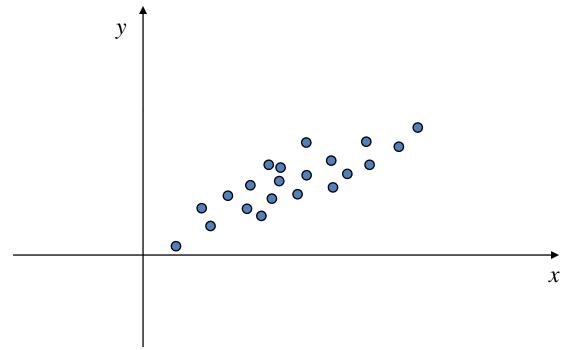
 Given a set of points, find the best line that approximates them

Motivation

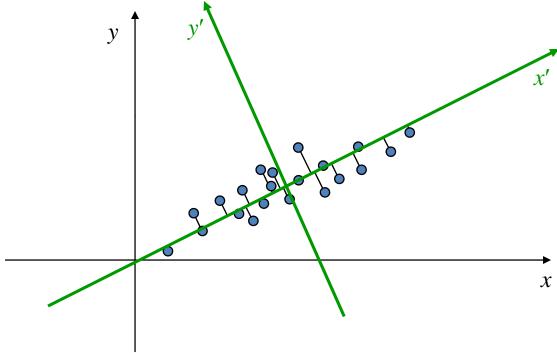


• We just saw how to fit a parametric line y = ax + b, but this does not work for vertical lines

Motivation



How to fit a line such that the true (orthogonal) distances are minimized?



PCA finds axes that minimize the sum of distances²

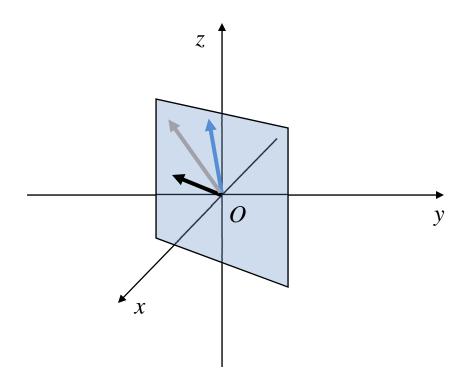
Vector space

Informal definition:

- $\blacksquare V \neq \emptyset$ (a non-empty set of vectors)
- $\mathbf{v}, \mathbf{w} \in V \implies \mathbf{v} + \mathbf{w} \in V$ (closed under addition)
- $\mathbf{v} \in V, \, \alpha \text{ is scalar } \Rightarrow \alpha \mathbf{v} \in V \text{ (closed under multiplication by scalar)}$
- Formal definition includes axioms about associativity and distributivity of the + and · operators.
- $0 \in V$ always!

Vector space – example

- Let π be a plane through the origin in 3D
- $V = \{\mathbf{p} O / \mathbf{p} \in \pi\}$ is a linear subspace of \mathbb{R}^3



Linear independence

■ The vectors $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_k\}$ are a linearly independent set if:

$$\alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \dots + \alpha_k \mathbf{v}_k = 0 \iff \alpha_i = 0 \quad \forall i$$

It means that none of the vectors can be obtained as a linear combination of the others.

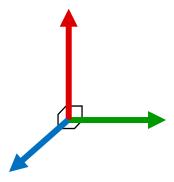
Linear independence

Parallel vectors are always dependent:



$$\mathbf{v} = 2.4 \ \mathbf{w} \implies \mathbf{v} + (-2.4)\mathbf{w} = 0$$

Orthogonal vectors are always independent.



Basis of a vector space V

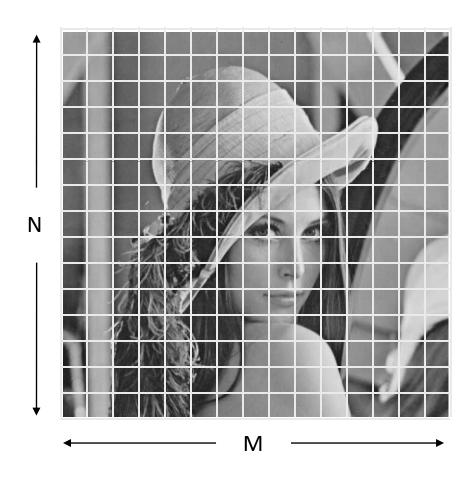
- $\{v_1, v_2, ..., v_n\}$ are linearly independent
- $\{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_n\}$ span the whole vector space V:

$$V = \{ \alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \dots + \alpha_n \mathbf{v}_n / \alpha_i \text{ is scalar} \}$$

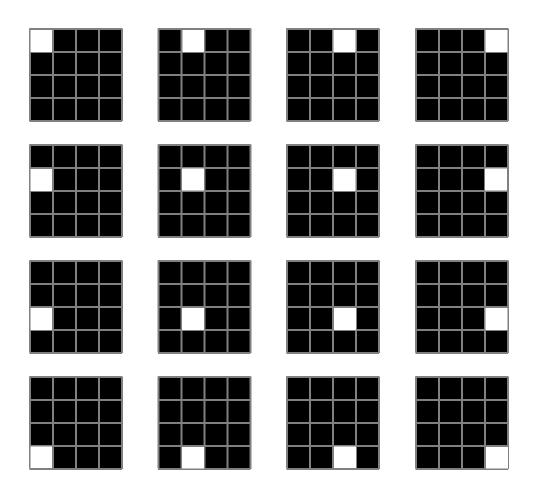
- Any vector in V is a unique linear combination of the basis.
- The number of basis vectors is called the dimension of V.

Basis example

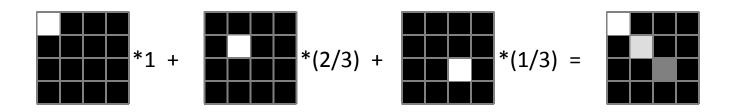
- Grayscale N×M images:
 - Each pixel has value between 0 (black) and 1 (white)
 - The image can be interpreted as a vector $\in \mathbb{R}^{N \cdot M}$



The "standard" basis (4×4)

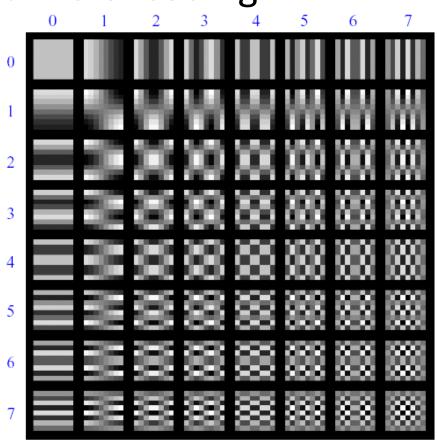


The "standard" basis (4×4) – linear combinations



Discrete cosine basis

Used for JPEG encoding



Orthogonal matrices (orthonormal basis)

- Matrix A $(n \times n)$ is orthogonal if $A^{-1} A^{T}$
- Follows: $AA^{T} = A^{T}A = I$
- The rows of A are orthonormal vectors!

$$\mathbf{I} = \mathbf{A}^{\mathrm{T}} \mathbf{A} = \begin{bmatrix} \mathbf{v}_{1} \\ \mathbf{v}_{2} \\ \mathbf{v}_{n} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{1} \\ \mathbf{v}_{2} \end{bmatrix} \begin{bmatrix} \mathbf{v}_{1} \\ \mathbf{v}_{1} \end{bmatrix} = \begin{bmatrix} \mathbf{v}_{i}^{\mathrm{T}} \mathbf{v}_{j} \\ \mathbf{v}_{i} \end{bmatrix} = \begin{bmatrix} \delta_{ij} \end{bmatrix}$$

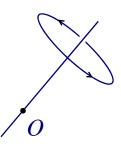
$$\Rightarrow \langle \mathbf{v}_i, \mathbf{v}_i \rangle = 1 \Rightarrow ||\mathbf{v}_i|| = 1; \langle \mathbf{v}_i, \mathbf{v}_i \rangle = 0$$

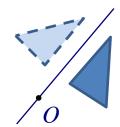
Orthogonal transformations

■ A is orthogonal matrix ⇒ A represents a linear transformation that preserves dot product (i.e., preserves lengths and angles):

$$(\mathbf{A}\mathbf{v})^{\mathrm{T}}(\mathbf{A}\mathbf{w}) = \mathbf{v}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{A}\mathbf{w} = \mathbf{v}^{\mathrm{T}}\mathbf{w}$$

■ Therefore, $||A\mathbf{v}|| = ||\mathbf{v}||$ and $\angle(A\mathbf{v},A\mathbf{w}) = \angle(\mathbf{v},\mathbf{w})$



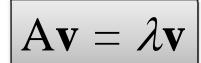


Eigenvectors and eigenvalues

- A is a square $n \times n$ matrix
- v is called eigenvector of A if:

•
$$A\mathbf{v} = \lambda \mathbf{v}$$
 (λ is a scalar)

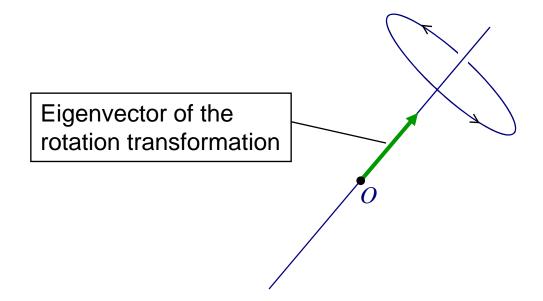
•
$$\mathbf{v} \neq 0$$



- The scalar λ is called eigenvalue
- $A\mathbf{v} = \lambda \mathbf{v} \implies A(\alpha \mathbf{v}) = \lambda(\alpha \mathbf{v}) \implies \alpha \mathbf{v}$ is also eigenvector
- $A\mathbf{v} = \lambda \mathbf{v}, A\mathbf{w} = \lambda \mathbf{w} \implies A(\mathbf{v} + \mathbf{w}) = \lambda(\mathbf{v} + \mathbf{w})$
- Therefore, eigenvectors of the same λ form a linear subspace.

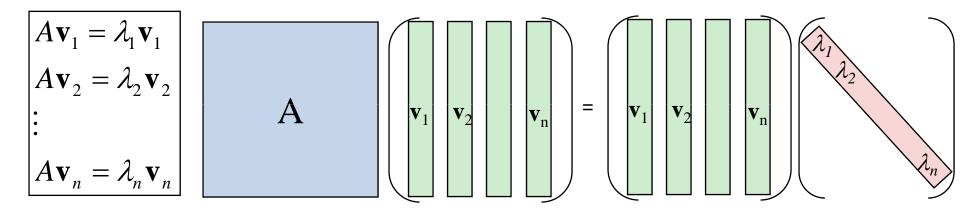
Eigenvectors and eigenvalues

- An eigenvector spans an axis (subspace of dimension 1) that remains the same under the transformation A.
- Example the axis of rotation:



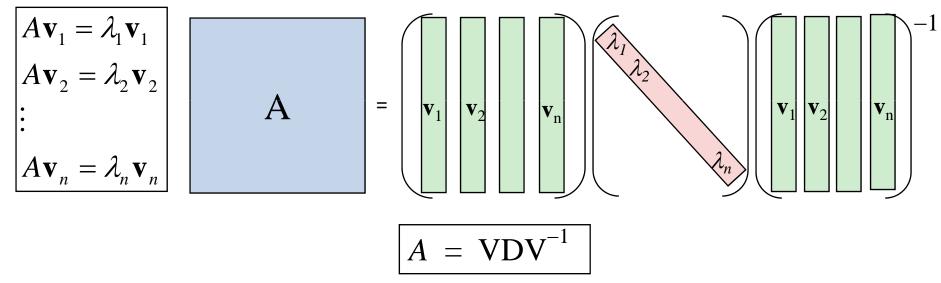
Spectrum and diagonalization

- The set of all the eigenvalues of A is called the spectrum of A.
- A is diagonalizable if A has n independent eigenvectors. Then: AV = VD



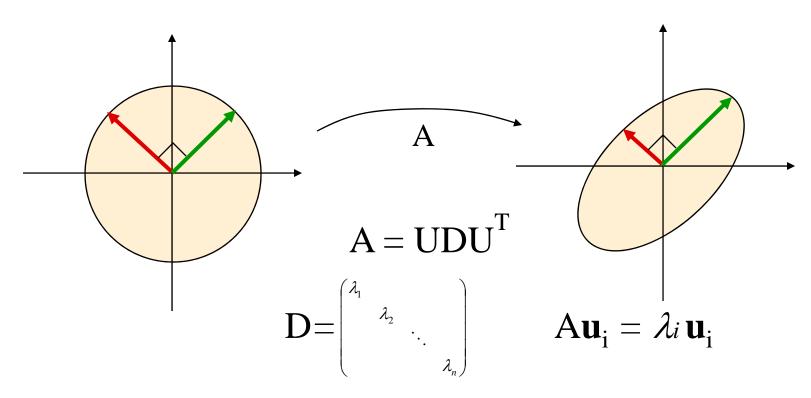
Spectrum and diagonalization

- Therefore, $A VDV^{-1}$, where D is diagonal
- A represents a scaling along the eigenvector axes!



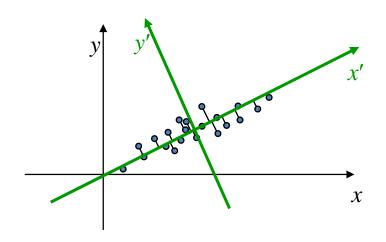
Symmetric matrices

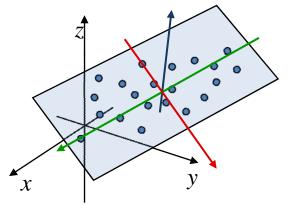
 If A is symmetric, the eigenvectors are orthogonal and there's always an eigenbasis.



Basic idea

 PCA finds an orthogonal basis that best represents given data set

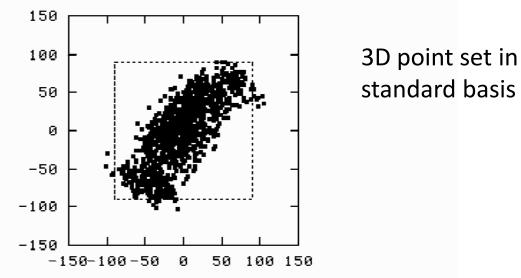




■ PCA finds a best approximating line/plane/axes... (in terms of $\Sigma_{distances}^2$)

Basic idea

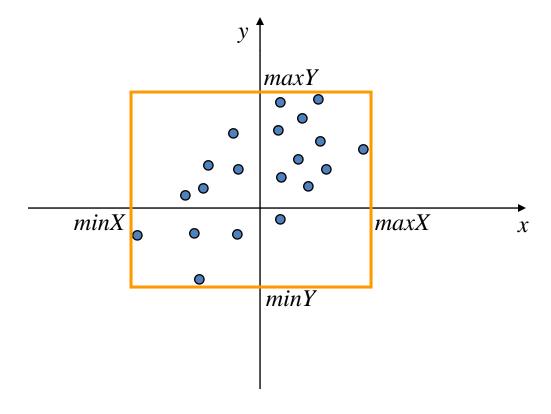
 PCA finds an orthogonal basis that best represents given data set



■ PCA finds a best approximating line/plane/axes... (in terms of $\Sigma distances^2$)

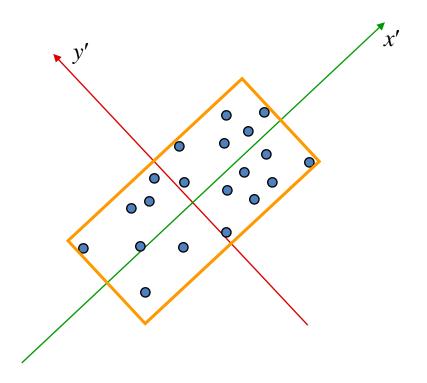
Applications

 An axis-aligned bounding box: agrees with the standard axes



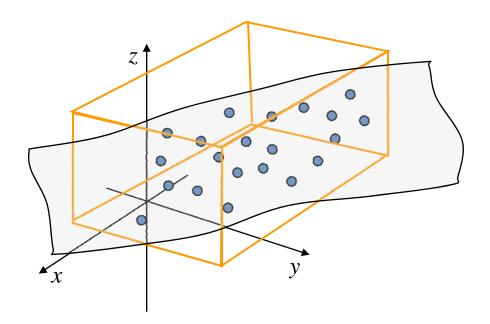
Application: oriented bounding box

Tighter fit



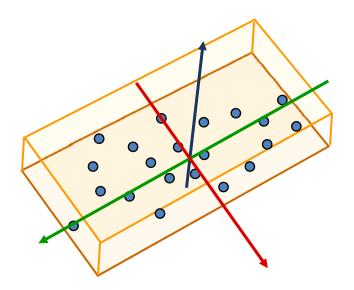
Application: oriented bounding box

Axis aligned bounding box



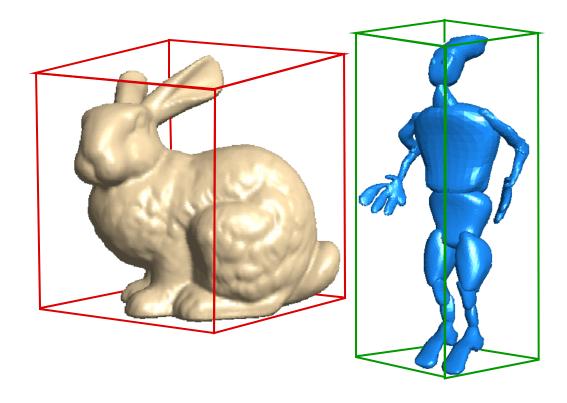
Application: oriented bounding box

Oriented bounding box by PCA

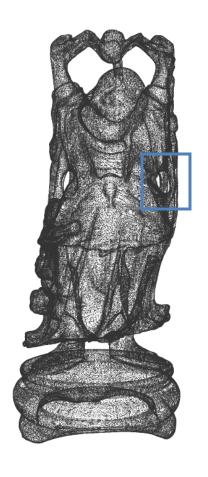


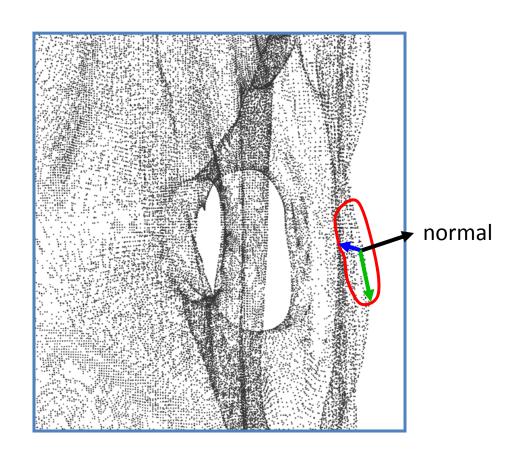
Application: oriented bounding box

- Serve as very simple "approximation" of the object
- Fast collision detection, visibility queries
- Whenever we need to know the dimensions (size) of the object
- The models consist of thousands of polygons
- To quickly test that they don't intersect, the bounding boxes are tested
- Sometimes a hierarchy of BB's is used
- The tighter the BB the less "false alarms" we have

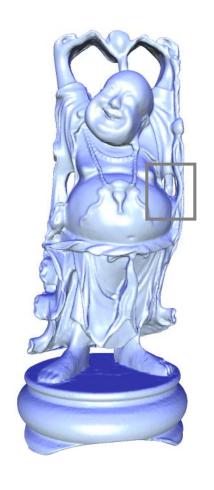


Application: local frame fitting





Application: estimate normals

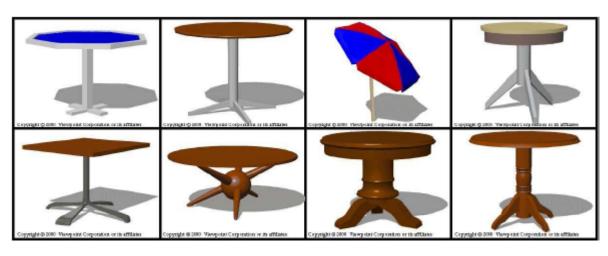




Application: shape alignment

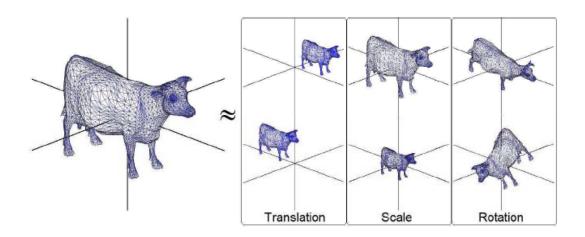
3D search engines (see http://shape.cs.princeton.edu/)





Application: shape alignment

 Can use PCA to find canonical axes and scale for shape comparison

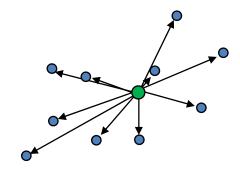


Notations

■ Denote our data points by \mathbf{x}_1 , \mathbf{x}_2 , ..., $\mathbf{x}_n \in R^d$

Center of mass:

$$\mathbf{m} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_{i}$$



Vectors from the centroid:

$$\mathbf{y}_i = \mathbf{x}_i - \mathbf{m}$$

The origin of the new axes

 The origin of the new axes will be the center of mass m

It can be shown that:

$$\mathbf{m} = \underset{\mathbf{x}}{\operatorname{argmin}} \sum_{i=1}^{n} \|\mathbf{x}_{i} - \mathbf{x}\|^{2}$$

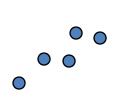
$$\mathbf{m} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{x}_{i}$$

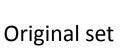
Variance of projected points

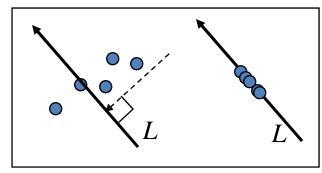
- Let us measure the variance (scatter) of our points in different directions
- Let's look at a line L through the center of mass m, and project our points x_i onto it. The variance of the projected points x'_i is:

Want to find directions of maximal/minimal variance

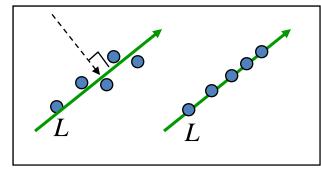
$$\operatorname{var}(L) = \frac{1}{n} \sum_{i=1}^{n} ||\mathbf{x}'_i - \mathbf{m}||^2$$







Small variance

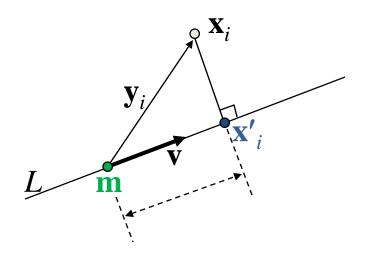


Large variance

Variance of projected points

- Given a direction \mathbf{v} , $||\mathbf{v}|| = 1$
- Line L through \mathbf{m} in the direction of \mathbf{v} is $L(t) = \mathbf{m} + \mathbf{v}t$.

$$||\mathbf{x'}_i - \mathbf{m}|| = \langle \mathbf{v}, \mathbf{x}_i - \mathbf{m} \rangle / ||\mathbf{v}|| = \langle \mathbf{v}, \mathbf{y}_i \rangle = \mathbf{v}^{\mathrm{T}} \mathbf{y}_i = \mathbf{y}_i^{\mathrm{T}} \mathbf{v}$$



Variance of projected points

So,
$$\operatorname{var}(L) = \frac{1}{n} \sum_{i=1}^{n} \|\mathbf{x}_{i}' - \mathbf{m}\|^{2} = \frac{1}{n} \sum_{i=1}^{n} (\mathbf{y}_{i}^{\mathrm{T}} \mathbf{v})^{2} = \frac{1}{n} \|\mathbf{Y}^{\mathrm{T}} \mathbf{v}\|^{2} = \frac{1}{n} (\mathbf{Y}^{\mathrm{T}} \mathbf{v})^{\mathrm{T}} (\mathbf{Y}^{\mathrm{T}} \mathbf{v}) = \frac{1}{n} \mathbf{v}^{\mathrm{T}} \mathbf{Y} \mathbf{Y}^{\mathrm{T}} \mathbf{v} = \mathbf{v}^{\mathrm{T}} S \mathbf{v}.$$

$$S = (1/n) Y Y^T$$
 Scatter matrix

where Y is a $d \times n$ matrix with $\mathbf{y}_k = \mathbf{x}_k - \mathbf{m}$ as columns.

■ The scatter matrix S measures the variance of our points

Directions of maximal variance

- So, we have: $var(L) = \mathbf{v}^T \mathbf{S} \mathbf{v}$
- Theorem:

Let
$$f: \{\mathbf{v} \in R^d \ / \ //\mathbf{v}// = 1\} \to R$$
, $f(\mathbf{v}) = \mathbf{v}^T \mathbf{S} \mathbf{v}$ (and S is a symmetric matrix).

Then, the extrema of f are attained at the eigenvectors of S.

So, eigenvectors of S are directions of maximal/minimal variance!

Directions of maximal variance

- Find extrema of $\mathbf{v}^{\mathrm{T}} \mathbf{S} \mathbf{v}$
- side condition $\mathbf{v}^{\mathrm{T}}\mathbf{v}=1$
- Lagrange Multipliers: $\nabla f + \lambda \nabla g = 0$

$$\nabla (\mathbf{v}^{\mathrm{T}} \mathbf{S} \mathbf{v}) + \lambda \nabla (\mathbf{v}^{\mathrm{T}} \mathbf{v} - 1) = 0$$

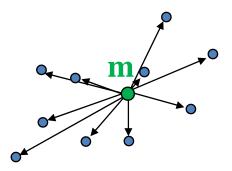
$$\mathbf{S} \mathbf{v} + \lambda \mathbf{v} = 0$$

$$\mathbf{S} \mathbf{v} = -\lambda \mathbf{v}$$

This is the definition of an eigenvector of S

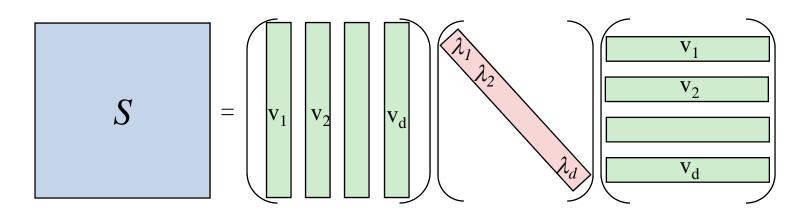
Summary so far

- We take the centered data vectors \mathbf{y}_1 , \mathbf{y}_2 , ..., $\mathbf{y}_n \in R^d$
- Construct the scatter matrix $S = Y Y^T$
- S measures the variance of the data points
- Eigenvectors of S are directions of maximal variance.



Scatter matrix eigendecomposition

- S is symmetric
- \Rightarrow S has eigendecomposition: $S = VDV^T$

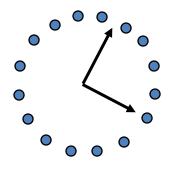


The eigenvectors form orthogonal basis

Principal components

- Eigenvectors that correspond to big eigenvalues are the directions in which the data has strong components (= large variance).
- If the eigenvalues are more or less the same there is no preferable direction.
- Note: the eigenvalues are always nonnegative. Think why...

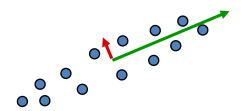
Principal components



- There's no preferable direction
- S looks like this:

$$\mathbf{V} \begin{pmatrix} \lambda & \\ & \lambda \end{pmatrix} \mathbf{V}^{\mathrm{T}}$$

Any vector is an eigenvector



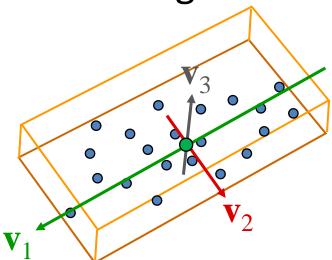
- There's a clear preferable direction
- S looks like this:

$$\mathbf{V} \begin{pmatrix} \lambda & \\ & \mu \end{pmatrix} \mathbf{V}^{\mathrm{T}}$$

 μ is close to zero, much smaller than λ

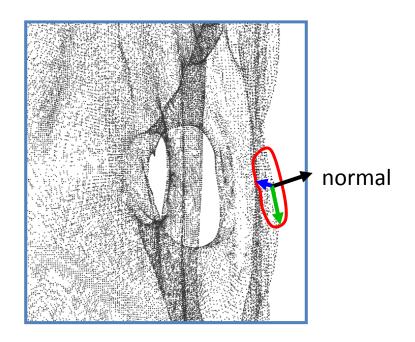
Oriented bounding box

■ For finding oriented bounding box or alignment — we simply compute the bounding box with respect to the axes defined by the eigenvectors. The origin is at the centroid **m**.

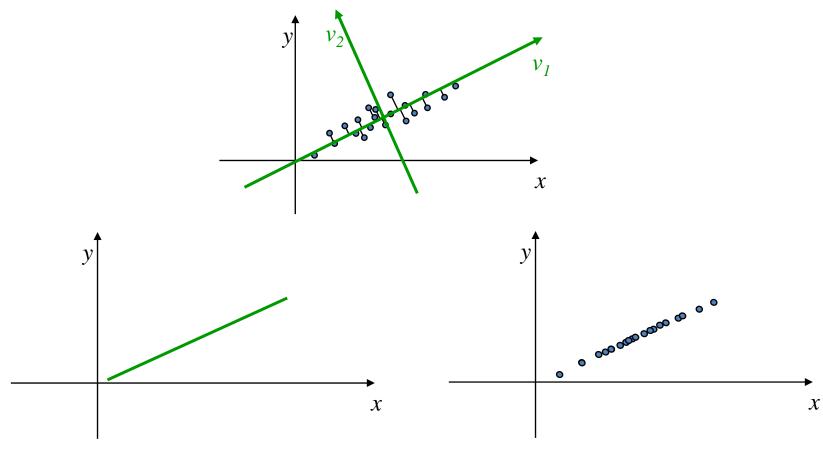


Local frame/normal estimation

- Sort the eigenvectors by ascending eigenvalues
- The eigenvector with $\lambda \approx 0$ is the normal



Dimensionality reduction / approximation

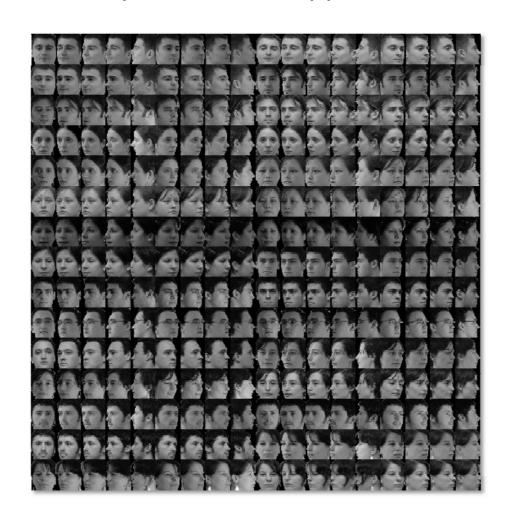


This line segment approximates the original data set

The projected data set approximates the original data set

Dimensionality reduction / approximation

- Each image is 64x64
- Vector in R^{64.64}
- But in fact all the faces live on a lowdimensional subspace
- Can find meaningful axes with PCA and other methods
 - face pose
 - expression
 - **-** ...



Dimensionality reduction / approximation

In general dimension d, the eigenvalues are sorted in descending order:

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$$

- The eigenvectors are sorted accordingly.
- To get an approximation of dimension d' < d, we take the d' first eigenvectors and look at the subspace they span (d' = 1 is a line, d' = 2 is a plane...)

Dimensionality reduction / approximation

To get an approximating set, we project the original data points onto the chosen subspace:

$$\mathbf{x}_i = \mathbf{m} + \alpha_1 \mathbf{v}_1 + \alpha_2 \mathbf{v}_2 + \dots + \alpha_{d'} \mathbf{v}_{d'} + \dots + \alpha_d \mathbf{v}_d$$

Projection:

$$\mathbf{x}_{i}' = \mathbf{m} + \alpha_{1}\mathbf{v}_{1} + \alpha_{2}\mathbf{v}_{2} + \dots + \alpha_{d'}\mathbf{v}_{d'} + \mathbf{0}\cdot\mathbf{v}_{d'+1} + \dots + \mathbf{0}\cdot\mathbf{v}_{d}$$

Technical remarks:

- $\lambda_i \ge 0$, i = 1,...,d (such matrices are called positive semi-definite). So we can indeed sort by the magnitude of λ_i
- Theorem: $\lambda_i \geq 0 \iff \langle \mathbf{S}\mathbf{v}, \mathbf{v} \rangle \geq 0 \quad \forall \mathbf{v}$ Proof: $\mathbf{S} = \mathbf{V}\mathbf{D}\mathbf{V}^T \Rightarrow \langle \mathbf{S}\mathbf{v}, \mathbf{v} \rangle = \mathbf{v}^T\mathbf{S}\mathbf{v} = \mathbf{v}^T\mathbf{V}\mathbf{D}\mathbf{V}^T\mathbf{v} = (\mathbf{V}^T\mathbf{v})^T\mathbf{D}(\mathbf{V}^T\mathbf{v}) = \mathbf{w}^T\mathbf{D}\mathbf{w} = 2 \mathbf{v}^T\mathbf{v} + 2 \mathbf{v}^T\mathbf{v$

Therefore, $\lambda_i \ge 0 \iff \langle \mathbf{S}\mathbf{v}, \mathbf{v} \rangle \ge 0 \quad \forall \mathbf{v}$