Lecture #19: Least Squares & Gram-Schmidt Algorithm

Date: Thu. 11/29/18

Least Squares

Idea: Finding something "close" to a soln.

Question: what does "close" mean?

This is Known as a least squares problem

Recall: A system of eqns $A\vec{x}=\vec{b}$ has a soln iff $\vec{b} \in \text{Col}(A)$

What if there is no soln? In real world we may need an approx soln. even if actual soln DNE. i.e. want

$A\vec{x}$ as close as possible to $\vec{b}$.

Need a way to measure distance btwn 2 vectors: $\|\vec{u}-\vec{v}\|$

i.e. want $\|A\vec{x}-\vec{b}\|$ as small as possible

i.e. want a $\vec{u}=A\vec{x} \in \text{Col}(A)$ s.t. $\|\vec{u}-\vec{b}\|$ small as possible

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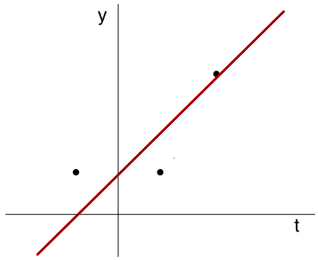
Ex. Given data

t	-1	1	2
y	1	1	3

Which we assume to be linear.
Want a line that passes thru these pts (or as close as possible to these pts)

If these pts lie on a line then $\exists$ an eqn s.t. $y = mt + c$



So we need to find m & c (given t & y)

i.e. solving system

$$1 = -m + c$$
$$1 = m + c$$
$$3 = 2m + c$$

There is not a unique soln to this system b/c there are 3 eqns & 2 unknowns

System is

$$\begin{bmatrix} -1 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 3 \end{bmatrix}$$

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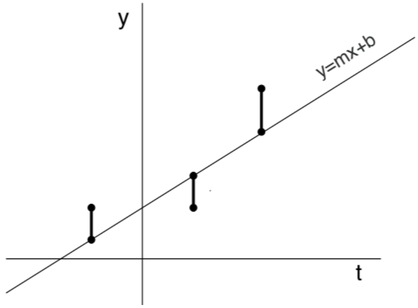
We'll use $\|A\vec{x}-\vec{b}\|^2$ rather than $\|A\vec{x}-\vec{b}\|$

Suppose that $A\vec{x} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}$

want d_1, d_2, d_3 s.t.

$$\|A\vec{x}-\vec{b}\|^2 = (d_1-1)^2 + (d_2-1)^2 + (d_3-3)^2$$

is as small as possible



The vector $\hat{x}$ for which $\|A\vec{x}-\vec{b}\|^2$ is minimized is the least squares soln. where $\vec{x} \approx \hat{x}$

(i.e. $\hat{x}$ is approx. soln to system
& $\vec{x}$ is exact soln to system)

$$A\vec{x} = \vec{b}$$

mult. by A^T on each side

$$A^TA\vec{x} = A^T\vec{b}$$

Thm. If $A \in \mathbb{R}^{m\times n}$ & $\vec{b} \in \mathbb{R}^n$, then the system

$$A^TA\vec{x} = A^T\vec{b}$$

normal eqns for $A\vec{x}=\vec{b}$

has a soln.

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<u>Thm.</u> Suppose $\vec{x} = \hat{x}$ is a soln to $A^T A\vec{x} = A^T\vec{b}$. Then $A\hat{x}$ is the vector in Col(A) that is closes to $\vec{b}$. i.e.

$$\|A\hat{x} - \vec{b}\| \leq \|\vec{w} - \vec{b}\| \quad \forall\, w \in \text{Col}(A)$$

So $\hat{x}$ is the least squares soln to $A\vec{x} = \vec{b}$

<u>Back to Ex.</u>

$$\begin{bmatrix} -1 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 3 \end{bmatrix}$$

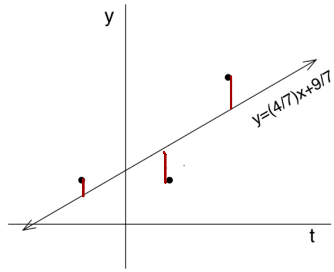
Normal Eqns are

$$\underbrace{\begin{bmatrix} -1 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}}_{A^T} \underbrace{\begin{bmatrix} -1 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} m \\ c \end{bmatrix}}_{\vec{x}} = \underbrace{\begin{bmatrix} -1 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}}_{A^T} \underbrace{\begin{bmatrix} 1 \\ 1 \\ 3 \end{bmatrix}}_{\vec{b}}$$

$$\Longrightarrow \begin{bmatrix} 6 & 2 \\ 2 & 3 \end{bmatrix} \begin{bmatrix} m \\ c \end{bmatrix} = \begin{bmatrix} 6 \\ 5 \end{bmatrix}$$

Solving this system we obtain

$m = \frac{4}{7}$, $c = \frac{9}{7}$



Gram-Schmidt Algorithm

Process to obtain an orthogonal or orthonormal basis for a space

Given $\vec{v}_1, \vec{v}_2, \vec{v}_k$ are Lin. indep. vectors in some space S.

We want vectors $\vec{q}_1, \vec{q}_2, \dots \vec{q}_k$ that

- span S (b/c $\vec{v}_i$ span S)
- are orthonormal $\Rightarrow$ lin. indep.

i.e. $\{\vec{q}_1, \vec{q}_2, \dots \vec{q}_k\}$ is an orthonormal basis for S

Steps

1) Let $\vec{q}_1 = \frac{1}{\|\vec{v}_1\|}\vec{v}_1$

2) Repeat following steps for $i = 2$ to k

i) Let $\vec{w}_i = \vec{v}_i - (\vec{q}_1 \cdot \vec{v}_i)\vec{q}_1 - (\vec{q}_2 \cdot \vec{v}_i)\vec{q}_2 - \dots - (\vec{q}_{i-1} \cdot \vec{v}_i)\vec{q}_{i-1}$

ii) Let $\vec{q}_i = \frac{1}{\|\vec{w}_i\|}\vec{w}_i$

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Ex. Given basis $\vec{v}_1 = \begin{bmatrix} 2 \\ 2 \\ 1 \\ 0 \end{bmatrix}$, $\vec{v}_2 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$ of S

Find orthonormal basis for S.

Find $\vec{q}_1$:

$$\|\vec{v}_1\| = \sqrt{\vec{v}_1 \cdot \vec{v}_1} = (2^2 + 2^2 + 1^2 + 0^2)^{1/2} = 3$$

$$\vec{q}_1 = \frac{1}{\|\vec{v}_1\|}\vec{v}_1 = \frac{1}{3}(2, 2, 1, 0)^T$$

Find $\vec{q}_2$:

Find $\vec{w}_2 = \vec{v}_2 - (\vec{q}_1 \cdot \vec{v}_2)\vec{q}_1$

$$= \underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}}_{\vec{v}_2} - \frac{1}{3}\underbrace{(2+2+1+0)}_{\vec{q}_1 \cdot \vec{v}_2}\underbrace{\begin{bmatrix} 2 \\ 2 \\ 1 \\ 0 \end{bmatrix}}_{\vec{q}_1} = \begin{bmatrix} -\frac{1}{9} \\ -\frac{1}{9} \\ \frac{4}{9} \\ 1 \end{bmatrix}$$

$$\|\vec{w}_2\| = \left[\left(-\tfrac{1}{9}\right)^2 + \left(-\tfrac{1}{9}\right)^2 + \left(\tfrac{4}{9}\right)^2 + 1\right]^{1/2} = \frac{\sqrt{11}}{3}$$

$$\Rightarrow \vec{q}_2 = \frac{1}{\|\vec{w}_2\|}\vec{w}_2 = \frac{\sqrt{11}}{3}\left(-\tfrac{1}{9}, -\tfrac{1}{9}, \tfrac{4}{9}, 1\right)^T$$

So orthonormal basis is

$$\{\vec{q}_1, \vec{q}_2\} = \left\{ \frac{1}{3}\begin{bmatrix} 2 \\ 2 \\ 1 \\ 0 \end{bmatrix}, \frac{\sqrt{11}}{3}\begin{bmatrix} -\frac{1}{9} \\ -\frac{1}{9} \\ \frac{4}{9} \\ 1 \end{bmatrix} \right\}$$