Overdetermined Systems

measurements of unknown function $y(t)$

$y(t_1) = y_1$

$y(t_m) = y_m$

approximate $y(t)$ by linear combination of basis functions:

$$y(t) \simeq \sum_{i=1}^{n} \varphi_i(t)\, x_i$$

$$\varphi_1(t_1)x_1 + \varphi_2(t_1)x_2 + \varphi_3(t_1)x_3 + \cdots + \varphi_n(t_1)x_n = y_1$$

$$\varphi_1(t_2)x_1 + \varphi_2(t_2)x_2 + \varphi_3(t_2)x_3 + \cdots + \varphi_n(t_2)x_n = y_2$$

$$\vdots$$

$$\varphi_1(t_m)x_1 + \varphi_2(t_m)x_2 + \varphi_3(t_m)x_3 + \cdots + \varphi_n(t_m)x_n = y_m$$

Best choice for coefficients $x_1, x_2, \cdots, x_n$?

Notation $Ax \simeq y \rightarrow$

$$x = \arg\min_{\tilde{x} \in \mathbb{R}^n} \| y - A\tilde{x} \|$$

(in some norm)

$$A = \begin{pmatrix} \varphi_1(t_1) & \cdots & \varphi_n(t_1) \\ \vdots & & \vdots \\ \varphi_1(t_m) & \cdots & \varphi_n(t_m) \end{pmatrix}$$

We can choose norm based on application, purpose, etc. Not all norms are equally nice (in making problem easy to solve).

1

2-norm : $\min \|y - Ax\|_2 \Longleftrightarrow \min \|y - Ax\|_2^2$

$\min (y - Ax)^T (y - Ax) \rightarrow$

$\min\ y^T y - 2y^T A x + x^T A^T A x$

poss. $\frac{\partial}{\partial x_i} \left(y^T y - 2y^T A x + x^T A^T A x \right) = 0$

for $i = 1..n$

$\rightarrow$ n equations in n unknowns.

Alternative : $R(x) \equiv \|y - Ax\|_2^2$

If minimum obtained for $\hat{x}$, then $R(x)$ must increase in any arbitrary direction from $\hat{x}$.

So, directional derivative for any vector p at $\hat{x}$ must vanish. (quadratic problem)

$$\lim_{\alpha \to 0} \frac{1}{\alpha} \left(R(\hat{x} + \alpha p) - R(\hat{x}) \right) = 0$$

$$\frac{1}{\alpha} \left(R(\hat{x} + \alpha p) - R(\hat{x}) \right) =$$

$$\frac{1}{\alpha} \left(y^T y - 2(\hat{x} + \alpha p)^T A^T y + (\hat{x} + \alpha p)^T A^T A (\hat{x} + \alpha p) - y^T y + 2\hat{x}^T A^T y - \hat{x}^T A^T A \hat{x} \right) =$$

$$\frac{1}{\alpha} \left(-2\alpha p^T A^T y + 2\alpha p^T A^T A \hat{x} + \alpha^2 p^T A^T A p \right) =$$

$$-2p^T A^T y + 2p^T A^T A x + \alpha p^T A^T A p$$

$$\lim_{\alpha \to 0} \frac{1}{\alpha} \left(R(\hat{x} + \alpha p) - R(\hat{x}) \right) = 0 \Longleftrightarrow$$

$$2p^T A^T (y - A\hat{x}) = 0$$

Same equation can be derived by taking arbitrary $p \neq 0$ and setting

$$\tilde{R}(\alpha) \equiv R(\hat{x} + \alpha p)$$

If $\min R(x)$ is obtained at $\hat{x}$, then $\frac{d}{d\alpha}\tilde{R}(\alpha) = 0$ for $\alpha = 0$ (only).

We can simplify the condition on $\hat{x}$ above to:

$$p^T A^T (y - A\hat{x}) = 0 \quad \text{(for any } p \neq 0\text{)}$$

This defines solution in 2 different ways.

1) $p^T (A^T y - A^T A \hat{x}) = 0$ for any $p \neq 0$

~~[illegible] for~~

This indicates $A^T y - A^T A \hat{x} = 0$.
If not, take $p = A^T y - A^T A \hat{x} \Rightarrow$

$$p^T p = \sum p_i^2 = 0 \Rightarrow p = 0 \quad \text{(contradiction)} \; *$$

$\hat{x}$ determined by normal equations:

$$A^T A \hat{x} = A^T y$$

(if columns of A independent, well-defined)

* Put another way, the only vector orthogonal to all other (nonzero) vectors is the zero vector itself.

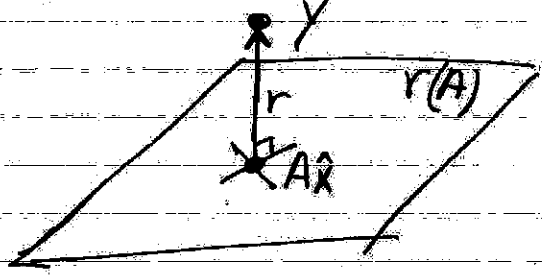
2) $p^T A^T (y - A\hat{x}) = 0 \iff$

$$(Ap)^T (y - A\hat{x}) = 0 \quad \text{for any } p$$

That means $y - A\hat{x} \perp$ range(A)

(range$(A) \equiv \{z : z = Ap$ for some $p\}$)

Note that $(Ap)^T(y - A\hat{x})$ is the Euclidean inner product of Ap and $y - A\hat{x}$.



$r = y - A\hat{x}$

So, $\hat{x}$ is defined by orthogonality property.

We say $x \perp y$ (in Euclidean inner prod) if $y^T x = 0$.

The orthogonality property of $\hat{x}$ leads to better solution methods than solving the normal equations.

An inner product of $x, y \in \mathbb{R}^n$, $\langle x, y \rangle$, has the following properties:

1) $\langle x, y \rangle = \langle y, x \rangle$

2) $\langle \alpha_1 x_1 + \alpha_2 x_2, y \rangle = \alpha_1 \langle x_1, y \rangle + \alpha_2 \langle x_2, y \rangle$

3) $\langle x, \alpha_1 y_1 + \alpha_2 y_2 \rangle = \alpha_1 \langle x, y_1 \rangle + \alpha_2 \langle x, y_2 \rangle$

4) $\langle x, x \rangle \geq 0$ and $\langle x, x \rangle = 0$ iff $x = 0$

for all $x, x_1, x_2, y, y_1, y_2 \in \mathbb{R}^n$, $\alpha_1, \alpha_2 \in \mathbb{R}$

Note (3) can be derived from (1) and (2).

A function $f : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ that satisfies (2) and (3) is called a bilinear form.

An inner product induces a norm:

$$\|x\|_\alpha = \langle x, x \rangle_\alpha^{1/2}$$

Example:

Euclidean inner product: $\langle x, y \rangle = y^T x$

Euclidean norm $\|x\|_2 = (x^T x)^{1/2}$

Not all norms have an associated inner product (are induced by an inner product).

In many ways those norms that can be defined in terms of an inner product are nicer.

A norm has an associated inner product if it satisfies the parallelogram equality:

$$\|x+y\|^2 + \|x-y\|^2 = 2(\|x\|^2 + \|y\|^2)$$

In that case we can find the associated inner product from the norm.

$$\langle x,y \rangle = \frac{1}{4}(\|x+y\|^2 - \|x-y\|^2) \quad \text{(real inner product space)}$$

For complex inner product space we have:

$$\mathrm{Re}\,\langle x,y \rangle = \frac{1}{4}(\|x+y\|^2 - \|x-y\|^2)$$

$$\mathrm{Im}\,\langle x,y \rangle = \frac{1}{4}(\|x+iy\|^2 - \|x-iy\|^2)$$

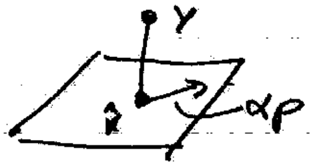
(polarization identity)

An important property of norms induced by an inner product is that the best approximation in such a norm is characterized by an equivalent orthogonality property.

The orthogonality property can typically be used to define set of simple, linear equations. It is generally much easier to solve these equations than minimize the corresponding directly.

Ex. let $y \in \mathbb{R}^n$ and $y \notin S$.

Find $x \in S$ such that $\|y-x\|$ minimal.



Let $\hat{x} \in S$ be the point in S closest to y.

Then for any $p \neq 0 \in S$ we must have

$$\frac{d}{d\alpha} \|y - (\hat{x} + \alpha p)\|^2 = 0 \text{ at } \alpha = 0 \quad (\to \text{at } \hat{x})$$

$$\Rightarrow \frac{d}{d\alpha}\left(\langle y,y\rangle - 2\langle y, \hat{x}+\alpha p\rangle + \langle \hat{x}+\alpha p, \hat{x}+\alpha p\rangle\right) = 0$$

at $\alpha = 0$

$$\Rightarrow -2\langle y,p\rangle + 2\langle \hat{x},p\rangle + 2\alpha\langle p,p\rangle\Big|_{\alpha=0} = 0$$

$$\Rightarrow \langle y-\hat{x}, p\rangle = 0 \text{ for any } p \neq 0 \in S$$

So, $\hat{x}$ is the point in S such that

$$y - \hat{x} \perp S$$

The reverse is easy to show as well (Pythagoras). Hence, the orthogonality property and the minimum norm property are equivalent.

Now, let $s_1 \cdots s_m$ form a basis for S.

$$\min_{x = \underbrace{[s_1 \cdots s_m]}_{S_m}\xi} \|y - x\| \Longleftrightarrow \min_{\xi \in \mathbb{R}^m} \|y - S_m\xi\| \Longleftrightarrow$$

$$y - S_m\xi \perp s_i \quad \text{for } i = 1..m$$

$$\to \langle y - \sum_{i=1}^{m} s_i\xi_i, s_j\rangle = 0 \quad \text{for } j = 1..m$$

System of m equations in m unknowns.

7

We can use the inner product to define angles between vectors more generally:

$$\cos\vartheta(x,y) = \frac{\langle x,y\rangle}{\|x\|\cdot\|y\|}$$

$$\vartheta(x,y) = \arccos\frac{\langle x,y\rangle}{\|x\|\cdot\|y\|}$$

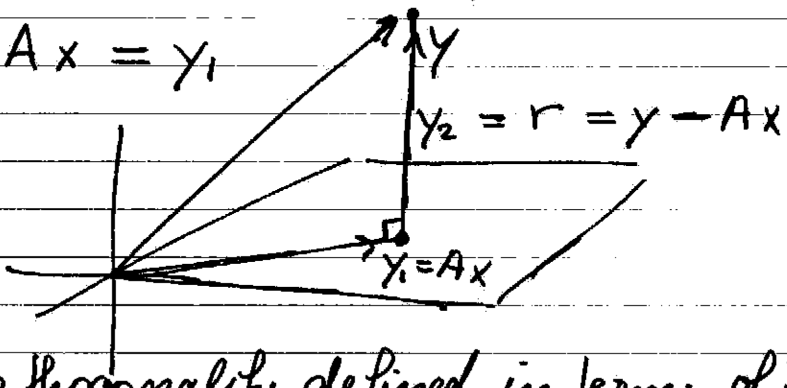
Note, factors $\|x\|^{-1}$, $\|y\|^{-1}$ simply <u>normalize</u> vectors (make unit vectors)

$$\cos\vartheta(x,y) = \left\langle \frac{x}{\|x\|}, \frac{y}{\|y\|} \right\rangle$$

So, in solution $Ax \simeq y$ $\rightarrow$

$$y = y_1 + y_2 \quad \begin{cases} y_1 \in \text{range}(A) \\ y_2 \perp A \end{cases}$$

$Ax = y_1$



orthogonality defined in terms of inner product associated with norm we want to minimize.

We will use orthogonality relations to derive solution algorithm.

y_1 is the orthogonal projection of y onto range(A)

y_2 is orthog. projection of y onto range$(A)^\perp$

For a space S,

$$S^\perp = \{z : \langle z, s\rangle = 0 \text{ forall } s \in S\}$$

working/solving using 2-norm:

$$Ax \simeq y \rightarrow A^T(y - Ax) = 0$$

$$A^TAx = A^Ty \quad (A \text{ independent columns})$$

$$x = (A^TA)^{-1}A^Ty$$

$$\rightarrow y_1 = Ax = A(A^TA)^{-1}A^Ty$$

$$y_2 = y - y_1 = (I - A(A^TA)^{-1}A^T)y$$

$A(A^TA)^{-1}A^T$ orthog. projector onto range(A)

$I - A(A^TA)^{-1}A^T$ orthog. projector onto range$(A)^\perp$

$$P = A(A^TA)^{-1}A^T$$

for any y: $A^T(y - Py) = A^Ty - A^Ty = 0$

and $\underbrace{Py}_{y_1} + \underbrace{(I-P)y}_{y_2} = y$

$P^2 = P$ (defining property of projector)

$P = P^T$ (symmetry)

A symmetric projector is orthogonal projector:

$$y - Py \perp \text{range}(P)$$

Matrix $Q \in \mathbb{R}^{n \times n}$ orthogonal if $Q^T Q = Q Q^T = I$

$\rightarrow Q^{-1} = Q^T$

If Q orthogonal then for Euclidean inner product $\langle x, y \rangle = y^T x$ we get

a) $\langle Qx, Qy \rangle = y^T Q^T Q x = y^T x = \langle x, y \rangle$

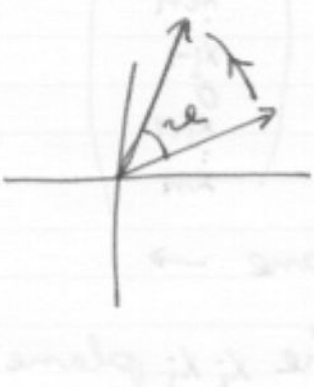
b) $\|Qx\|_2 = (x^T Q^T Q x)^{1/2} = \|x\|_2$

$\rightarrow$ Orthogonal transformations preserve lengths and angles (inner product)

$$\cos \vartheta(x,y) = \frac{\langle x, y \rangle}{\|x\| \, \|y\|} = \frac{\langle Qx, Qy \rangle}{\|Qx\| \cdot \|Qy\|}$$

Cauchy-Schwartz

$$|\langle x, y \rangle| \leq \|x\|_2 \cdot \|y\|_2$$



Consider vectors in $\mathbb{R}^2$

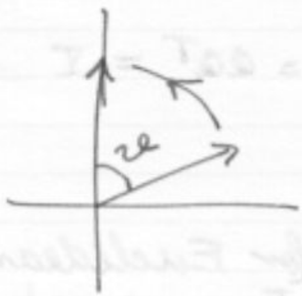
We call the matrix $Q = \begin{pmatrix} \cos\vartheta & -\sin\vartheta \\ \sin\vartheta & \cos\vartheta \end{pmatrix}$

a rotation or rotator as it rotates each vector in $\mathbb{R}^2$ throug angle ϑ around origin. $Q\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos\vartheta \\ \sin\vartheta \end{pmatrix}$ $Q\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\sin\vartheta \\ \cos\vartheta \end{pmatrix}$

We can use (plane) rotations to selectively create zeros in a vector or matrix without changing length of vector (~~[illegible]~~ or 2-norm of matrix.

Verify $QQ^T = Q^T Q = I$

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \rightarrow Q^T x = \begin{pmatrix} y \\ 0 \end{pmatrix} \quad \text{(some } y\text{)}$$



$$\begin{pmatrix} \cos\vartheta & \sin\vartheta \\ -\sin\vartheta & \cos\vartheta \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} y \\ 0 \end{pmatrix}$$

$$-\sin\vartheta\, x_1 + \cos\vartheta\, x_2 = 0 \quad \Rightarrow$$

i) $x_1 \sin\vartheta = x_2 \cos\vartheta$

ii) $(\sin\vartheta)^2 + (\cos\vartheta)^2 = 1$

$$\rightarrow \cos\vartheta = \frac{x_1}{\sqrt{x_1^2 + x_2^2}}, \quad \sin\vartheta = \frac{x_2}{\sqrt{x_1^2 + x_2^2}}$$

$$\rightarrow y = \cos\vartheta\, x_1 + \sin\vartheta\, x_2 = \sqrt{x_1^2 + x_2^2}$$

$$= \|x\|_2$$

$$\rightarrow \|y\|_2 = \|Q^T x\|_2 = \|x\|_2$$

More generally

$$\begin{array}{c c} & \begin{array}{ccccccc} & & i & & j & & \end{array} \\ \begin{array}{c} \\ \\ i \\ \\ j \\ \\ \end{array} & \begin{pmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & c & & +s & & \\ & & & 1 & & & \\ & & & & \ddots & & \\ & & & & & 1 & \\ & & -s & & c & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \end{pmatrix} \end{array} \begin{pmatrix} x_1 \\ \vdots \\ x_i \\ \vdots \\ x_j \\ \vdots \end{pmatrix} = \begin{pmatrix} x_1 \\ \vdots \\ x_{i-1} \\ y \\ x_{i+1} \\ \vdots \\ x_{j-1} \\ 0 \\ x_{j+1} \\ \vdots \\ x_m \end{pmatrix}$$

Plane rotation in $x_i x_j$ plane $\rightarrow$

rotates component of x in the $x_i x_j$ plane just as rotation in $\mathbb{R}^2$

We can use plane rotations to selectively create zeros in matrix A $\quad (Ax \simeq b)$

Solution algorithm for least squares problem.

Let Q^T be product of rotations such that $Q^T A$ upper triangular (easy to solve)

Note that product of orthogonal matrices is orthogonal:

$$Q_1^T Q_1 = I, \quad Q_2^T Q_2 = I$$

$$(Q_1 Q_2)^T (Q_1 Q_2) = Q_2^T Q_1^T Q_1 Q_2 = Q_2^T Q_2 = I$$

$$\underset{m\times m}{Q^T}\ \underset{m\times n}{A} = \underset{m\times n}{R} = \begin{pmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \\ & O & \end{pmatrix}$$

and so $A = QR$

$Ax \simeq b \rightarrow$ find x s.t. $\|b - Ax\|_2$ minimal

This gives $\|b - QRx\|_2$ minimal $\Leftrightarrow$

$\|QQ^T b - QRx\|_2 = \|Q(Q^T b - Rx)\|_2 \Leftrightarrow$

$\|Q^T b - Rx\|_2$ minimal $\quad (\|Qz\|_2 = \|z\|_2)$

$$\begin{pmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \\ & O & \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} \tilde{b}_1 \\ \vdots \\ \tilde{b}_n \\ \tilde{b}_{n+1} \\ \vdots \\ \tilde{b}_m \end{pmatrix} \qquad (\tilde{b} = Q^T b)$$

Best we can do is solve for top n coefficients of $\tilde{b} = Q^T b$. Not possible to approximate "remaining" vector as corresponding coefficients of R are zero.

Alternative view:

$$A^{m\times n} = Q^{m\times m} R^{m\times n}$$

$$Q = [q_1\, q_2 \cdots q_m] \longrightarrow$$

$QR = [q_1\, q_2 \cdots q_m]\, R^{m\times n}$ since all coeff.s of R below row n are zero.

$$\text{let} \begin{cases} Q_n = [q_1 \cdots q_n] \rightarrow A = QR = Q_n R_n \\ R_n = \begin{pmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ & & r_{nn} \end{pmatrix} \end{cases}$$

$A = Q_n R_n \longrightarrow$ <u>reduced</u> <u>QR</u> <u>decomposition</u>

$A = QR \longrightarrow$ <u>QR decomposition</u>

$Ay = Q_n(R_n y)$ and R_n invertible if columns A independent (assumed)

$\text{Range}(A) = \text{Range}(Q_n) \longrightarrow$

Q_n provides orthogonal basis for Range(A)

$$\min_x \|b - Ax\|_2 \Longleftrightarrow \cancel{x \text{ s.t. } b - Ax \perp}$$

x such that $b - Ax \perp \text{Range}(A)$

$\Longleftrightarrow$ x s.t. $b - Ax \perp Q_n$ $(\text{Range}(Q_n))$

$\Longleftrightarrow$ $Q_n^T(b - Ax) = 0$

$\Longleftrightarrow$ $Q_n^T b - R_n x = 0$

Solve $n\times n$ upper triangular system

Computing Q from A can be done in many ways (see book pp. 193-194)

$$\begin{pmatrix} x & x \\ x & x \\ x & x \\ x & x \end{pmatrix} \to \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & c_1 & s_1 \\ & & -s_1 & c_1 \end{pmatrix} \begin{pmatrix} x & x \\ x & x \\ x & x \\ x & x \end{pmatrix} = \begin{pmatrix} x & * \\ x & * \\ * & * \\ 0 & * \end{pmatrix}$$

$$\begin{pmatrix} 1 & & & \\ & c_2 & s_2 & \\ & -s_2 & c_2 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} x & x \\ x & x \\ x & x \\ 0 & x \end{pmatrix} = \begin{pmatrix} x & x \\ * & * \\ 0 & * \\ 0 & x \end{pmatrix}$$

$$\begin{pmatrix} c_3 & s_3 & & \\ -s_3 & c_3 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} x & x \\ x & x \\ 0 & x \\ 0 & x \end{pmatrix} = \begin{pmatrix} * & * \\ 0 & * \\ 0 & x \\ 0 & x \end{pmatrix}$$

$$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & c_4 & s_4 \\ & & -s_4 & c_4 \end{pmatrix} \begin{pmatrix} x & x \\ 0 & x \\ 0 & x \\ 0 & x \end{pmatrix} = \begin{pmatrix} x & x \\ 0 & x \\ 0 & * \\ 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & & & \\ & c_5 & s_5 & \\ & -s_5 & c_5 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} x & x \\ 0 & x \\ 0 & x \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} x & x \\ 0 & * \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{(done)}$$

Also possible

$$\begin{pmatrix} c_1 & s_1 & & \\ -s_1 & c_1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} x & x \\ x & x \\ x & x \\ x & x \end{pmatrix} = \begin{pmatrix} * & * \\ 0 & * \\ x & x \\ x & x \end{pmatrix}$$

$$\begin{pmatrix} c_2 & 0 & s_2 & \\ 0 & 1 & 0 & \\ -s_2 & 0 & c_2 & \\ & & & 1 \end{pmatrix} \begin{pmatrix} x & x \\ 0 & x \\ x & x \\ x & x \end{pmatrix} = \begin{pmatrix} * & * \\ 0 & x \\ 0 & * \\ x & x \end{pmatrix} \quad \text{etc}$$

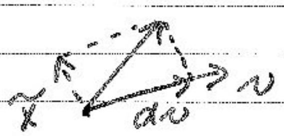
$$\to Q_5^T Q_4^T Q_3^T Q_2^T Q_1^T A = R \to Q = Q_1 Q_2 \cdots Q_5$$

(Q not assembled in practice)

(14)

Given a vector $v \neq 0$ we can always decompose x into $x = \alpha v + \tilde{x}$ such that

$$\tilde{x} \perp v$$



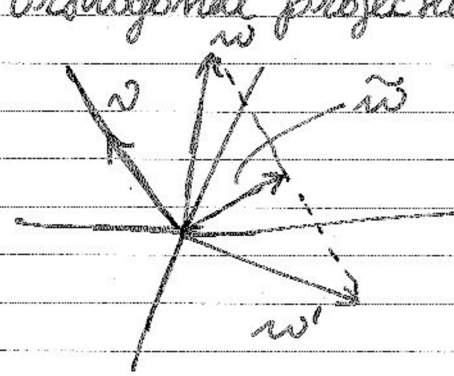
α ?

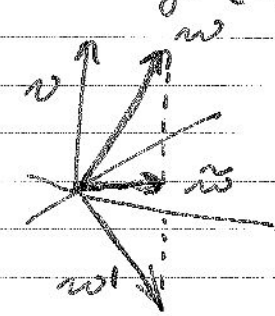
$$\tilde{x} = x - \alpha v \perp v \iff v^T x - \alpha v^T v = 0$$

$$\Rightarrow \alpha = \frac{v^T x}{v^T v} \quad \left(\text{more general } \alpha = \frac{\langle x, v \rangle}{\langle v, v \rangle}\right)$$

Just simple form of $A(A^T A)^{-1} A^T \rightarrow$

orthogonal projection onto Range (A)





Reflection of vector w in plane

orthogonal to v (unit vector $\rightarrow v^T v = 1$)

$$w = \alpha v + \tilde{w} \longrightarrow w' = -\alpha v + \tilde{w}$$

where $\alpha = v^T w$ $\left(\frac{v^T w}{v^T v} \text{ where } v^T v = 1\right)$

$$w' = w - 2\alpha v = w - 2 v v^T w$$

$$= (I - 2 v v^T) w$$

Matrix $I - 2vv^T$ is called reflection or reflector.

$(v^T v = 1) \quad Q = I - 2vv^T$
$\qquad\qquad\qquad Q^T = I - 2vv^T$

$$QQ^T = (I - 2vv^T)(I - 2vv^T)$$

$$= I - 2vv^T - 2vv^T + 4v\overset{1}{\cancel{v^T v}}v^T = I$$

Q orthogonal.

For $v^T v \neq 1$ (not 0) $\quad Q = \left(I - 2\dfrac{vv^T}{v^T v}\right)$

For $v^T v = 1 \rightarrow P = vv^T$ orthogonal proj.

$P(\alpha v) = \alpha v$
$Pu = 0$ if $u \perp v \quad \langle v, u \rangle = 0$
$P^2 = P \rightarrow$ projection
$P = P^T \rightarrow$ symmetric projection is orthogonal projection

$Q = I - 2vv^T$

$Qv = -v$
$Qu = u \quad u \perp v$

$Q = Q^T$
$Q^T = Q^{-1}$
$Q = Q^{-1}$

We can also use reflections to transform A into upper triangular form.

$Q_1^T A = A^{(1)} \qquad Q_1 = (I - 2v_1 v_1^T)$

$$Q_1^T \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & & \vdots \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix} = \left(\begin{array}{c|ccc} \alpha_1 & a_{12}^{(1)} & \cdots & a_{1n}^{(1)} \\ \hline 0 & a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\ \vdots & \vdots & & \\ 0 & a_{m2}^{(1)} & \cdots & a_{mn}^{(1)} \end{array}\right)$$

Next. $Q_2^T A^{(1)} = A^{(2)}$ where Q_2^T acts only on part $\begin{pmatrix} a_{22}^{(1)} & \cdots & a_{2n}^{(1)} \\ \vdots & & \vdots \\ a_{m2}^{(1)} & \cdots & a_{mn}^{(1)} \end{pmatrix} \equiv \tilde{A}_1^{(1)}$

$$Q_2^T A^{(1)} = \left(\begin{array}{c|c} 1 & 0 \cdots 0 \\ \hline 0 & \\ \vdots & \tilde{Q}_2^T \\ 0 & \end{array}\right) \left(\begin{array}{c|c} \alpha_1 & a_{12}^{(1)} \cdots a_{1n}^{(1)} \\ \hline 0 & \\ \vdots & \tilde{A}^{(1)} \\ 0 & \end{array}\right)$$

$$= \left(\begin{array}{c|c} \alpha_1 \cancel{e_1} & a_{12}^{(1)} \cdots a_{1n}^{(1)} \\ \hline & \alpha_2 \tilde{e}_1 \; a_{23}^{(2)} \cdots a_{2n}^{(2)} \\ & 0 \quad \vdots \\ & \vdots \quad \vdots \\ & 0 \quad a_{m3}^{(2)} \cdots a_{mn}^{(3)} \end{array}\right)$$

$$A^{(2)} = \left(\begin{array}{cc|c} \alpha_1 & a_{12}^{(1)} & \cdots \quad a_{1n}^{(1)} \\ 0 & \alpha_2 & a_{23}^{(2)} \cdots a_{2n}^{(2)} \\ \hline 0 & 0 & \\ \vdots & \vdots & \tilde{A}^{(2)} \\ \vdots & \vdots & \end{array}\right)$$

Next reflection acts only on $\tilde{A}^{(2)}$, and so on.

$$Q_n^T Q_{n-1}^T \cdots Q_1^T A = R^{m \times n} \longrightarrow A = QR$$

where $Q^{m \times m} = Q_1 Q_2 \cdots Q_n$

Again we can consider the reduced QR decomposition

$$A = [q_1 \cdots q_n] \begin{pmatrix} r_{11} & \cdots & r_{1n} \\ & \ddots & \vdots \\ 0 & & r_{nn} \end{pmatrix} = Q_n^{m \times n} R_n^{n \times n}$$

This QR decomposition can be used in same fashion to solve least squares problem.

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Again, in general, Q not stored explicitly (just v_i)

Computation of Q_i :

need v such that $(I - 2vv^T)x = \alpha e_1$

$\longrightarrow x - 2vv^Tx = \alpha e_1 \Longleftrightarrow$

$$v(2v^Tx) = x - \alpha e_1 = \begin{pmatrix} x_1 - \alpha_1 \\ x_2 \\ \vdots \end{pmatrix}$$

where $|\alpha| = \|x\|_2$ (Q_i orthogonal)

$\longrightarrow \alpha = \pm \|x\|_2$

For accuracy we give α opposite sign of x_1 so that no cancellation occurs in $x_1 - \alpha$

Set $\tilde{v} = x - \alpha e_1$ and $v = \frac{\tilde{v}}{\|\tilde{v}\|_2}$

See book pp. 201 - 204 for QR decomposition using reflectors

(Naming:
reflectors $\rightarrow$ Householder reflections/transformations

rotators $\rightarrow$ Givens rotations)

~~Alternative~~
<u>Theorem:</u>

Let $A \in \mathbb{R}^{m \times n}$ be nonsingular. There exist unique $Q, R \in \mathbb{R}^{n \times n}$ such that $Q^TQ = I$, R upper triangular with positive real diagonal entries, and $A = QR$

$\rightarrow$ uniqueness of QR decomposition for $A \in \mathbb{R}^{m \times n}$

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Complex case

Inner product $\langle \cdot, \cdot \rangle : \mathbb{C}^n \times \mathbb{C}^n \to \mathbb{C}^n$

$$\langle x, y \rangle = \overline{\langle y, x \rangle}$$

$$\langle \alpha x_1 + \beta x_2, y \rangle = \alpha \langle x_1, y \rangle + \beta \langle x_2, y \rangle$$

$\langle x, x \rangle \in \mathbb{R} \geq 0$ and

$$\langle x, x \rangle = 0 \iff x = 0$$

Euclidean inner product:

$$\langle x, y \rangle = y^H x = \sum_i x_i \overline{y_i}$$

($\overline{\alpha}$ complex conjugate of α)

$\|x\|_2 = \langle x, x \rangle^{1/2}$ (still holds)

$A \in \mathbb{C}^{m \times n}$, $b \in \mathbb{C}^{m}$

$Ax \simeq b \longrightarrow \|b - Ax\|$ minimum

in some norm. Typically (if no other statement) 2-norm

With respect to complex inner product all earlier theory still holds.

$\|b - Ax\|_2$ min iff $b - Ax \perp \text{Range}(A)$

$\rightarrow (Ap)^H (b - Ax) = 0$ for all p

$\langle b - Ax, Ap \rangle = 0$ all p

The complex equivalent of an orthogonal matrix is a unitary matrix :

$$A A^H = A^H A = I$$

If U is unitary, we have

$\langle Ux, Uy \rangle = \langle x, y \rangle$ (Euclidean inn.pr.)

$\|Ux\|_2 = \|x\|_2$

$\|U\|_2 = \|U^{-1}\|_2 = \kappa_2(U) = 1$

Unitary matrices preserve the Euclidean inner product, and hence the 2-norm. So, complex least-squares problems can be solved same way as real least-squares problems (based on complex inner product and unitary matrices)

Theorem

Let $A \in \mathbb{C}^{m \times m}$ be nonsingular. There exist unique $Q, R \in \mathbb{C}^{m \times m}$ such that Q is unitary, R is uppertriangular with real positive diagonal entries, and $A = QR$.

Existence and uniqueness of solution of least squares problem.

Since Range (A) is a (complex) subspace of $\mathbb{R}^m$ or $\mathbb{C}^m$ the orthogonal projection of a given right hand side onto Range (A) always exist (even for singular A). ~~For~~ Furthermore, by definition for every point/vector y_1 in Range (A) there exists an $x \in \mathbb{R}^n$ such that $Ax = y_1$. Hence, solution always exists.

If the columns of A are independent the solution is unique since the columns of A form a basis for the Range (A).
(and orthogonal projection is unique)

If the columns of A are dependent, the solution is not unique since there is a vector $z \in \mathbb{R}^n$ ($\mathbb{C}^n$) such that $Az = 0$. Given a solution $\hat{x} \in \mathbb{R}^n$ ($\mathbb{C}^n$) all vectors $\hat{x} + \alpha z$ are also solutions.

We say a matrix $A \in \mathbb{R}^{m \times n}$ $(m \geq n)$ is singular if its columns are dependent, nonsingular if its columns are independent.

Clearly, there is no inverse of A (for the nonsingular case) in the sense of the inverse in the $n \times n$ case. However, one can think of $R_n^{-1} Q_n^T$ as an inverse in the sense of giving the solution.

Here $\overset{m\times n}{Q_n} \overset{n\times n}{R_n}$ is the reduced QR decomposition of A. (condensed QR decomp. in the book)

book pp. 216ff.

<u>The singular / rank-deficient case</u>

Two main ~~ways~~ ways of handling the rank-deficient (or near rank-def.) case.

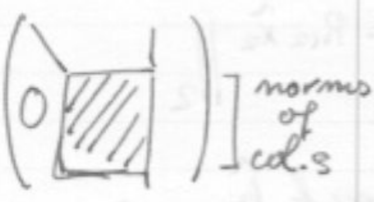
- Column pivoting

- Singular value decomposition (SVD)
  ↳ discussed later in detail

The idea of column pivoting is quite simple.

Before we start working on the "next" column (setting coefficients below diagonal to zero), we select the remaining column with largest norm *1 and exchange columns.

*1 norm taken only over lower right block of matrix on which we work



Effect is that of making all column exchanges first and then carrying out the QR-decomposition without column pivoting:

$$AP = QR$$

where P is a permutation matrix defining the column exchanges.

Procedure guarantees that diagonal coefficients of R, in absolute sense, decrease monotonically.

If A singular, at some step, all remaining columns below current diagonal coefficient will be zero.

$$Q_r^T Q_{r-1}^T \cdots Q_1^T A = \begin{pmatrix} \underset{r\times r}{R_{11}} & R_{12} \\ 0 & 0 \end{pmatrix} = R$$

where R_{11} is upper triangular and nonsingular.

$$\mathrm{Rank}(R) = \mathrm{Rank}(A) = r$$

$$A = \overset{m\times m}{Q} \; \overset{m\times n}{R} \qquad \text{QR-decomp.}$$

$$A = \cancel{Q_r R_r} \; \overset{m\times r}{Q_r} \; \overset{r\times n}{R_n} \qquad \text{reduced QR-decomp.}$$

See theorem 3.3.11 (book)

Solution of rank-deficient least-squares problem.

$$A x \simeq b$$

$$A P P^T x = b \iff Q R \hat{x} = b$$

$$\begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{x}_1 \\ \hat{x}_2 \end{pmatrix} \simeq Q^T b = \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \end{pmatrix}$$

a) minimise $\left\| \begin{matrix} \hat{b}_1 - R_{11} \hat{x}_1 - R_{12} \hat{x}_2 \\ \hat{b}_2 \end{matrix} \right\|_2$

nothing to be done about $\hat{b}_2 \longrightarrow$

minimise $\| \hat{b}_1 - R_{11} \hat{x}_1 - R_{12} \hat{x}_2 \|_2$

infinite possibilities; R_{11} nonsingular:

For any $\hat{x}_2$: Solve $R_{11} \hat{x}_1 = \hat{b}_1 - R_{12} \hat{x}_2$

Obvious choice $\hat{x}_2 = 0$

b) $b - A x \perp$ Range (A)

$AP = Q_r R_n \rightarrow Q_r^T (b - AP\hat{x}) = 0$

$Q_r^T b - R_n \hat{x} = 0 \iff \hat{b}_1 - R_{11} \hat{x}_1 - R_{12} \hat{x}_2 = 0$

(same as above)

At end, we set $x = P \hat{x}$

In practice we will not get $R_{22} = 0$ exactly. (rounding errors)

We have to decide on "effective" rank of A, in other words when R_{22} is numerically zero.

In general, if largest column in R_2 has norm below $\varepsilon \|A\|$ we stop

ε depends on machine precision and accuracy of the data.

Cost of QR-decomposition using Householder reflections.

We'll ignore the cost of constructing the reflector and count only the cost of multiplying the reflector times the (sub) matrix

1) $(I - 2q_1 q_1^T) A^{m \times n}$ where q_1 m-vector

$\rightarrow$ $4mn$ floating point operations

2) $(I - 2q_2 q_2^T) \hat{A}_2^{(m-1)\times(n-1)}$ and q_2 $(m-1)$ vector

$\rightarrow 4(m-1)(n-1)$

etc. taking n steps $\rightarrow$

$$4mn + 4(m-1)(n-1) + 4(m-2)(n-2) + \cdots + 4(m-n+1)\cdot 1$$

$$= 4\left[mn + m(n-1) + \cdots + m - 1\cdot(n-1) - 2(n-2) - 3(n-3) - 4(n-4) - \cdots - (n-1)\cdot 1\right]$$

$$f_n = 1\cdot(n-1) + 2(n-2) + 3(n-3) + \cdots + (n-1)\cdot 1$$

$$f_{n-1} = 1\cdot(n-2) + 2(n-3) + \cdots + (n-2)\cdot 1$$

$$f_n - f_{n-1} = (n-1) + (n-2) + (n-3) + \cdots + 1 + n - 1$$

$f_n - f_{n-1} = \frac{1}{2}n(n+1) - 1 = \frac{1}{2}n^2 + \frac{1}{2}n - 1$

$f_n = an^3 + bn^2 + cn + d \rightarrow \frac{1}{6}n^3 + \cdots$

Total cost:

$4 \cdot m \cdot \frac{1}{2}n(n+1) - \frac{4}{6}n^3 \cdots$

$\simeq 2mn^2 - \frac{2}{3}n^3$

If $m \gg n \rightarrow 2mn^2$

$m = n \rightarrow \frac{4}{3}n^3$ (twice as expensive as LU)

Gram-Schmidt process

We say a set of vectors $q_1, q_2, \ldots, q_k \in \mathbb{R}^k$ are orthonormal if they are unit vectors and pairwise orthogonal:

$$\langle q_i, q_j \rangle = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

theorem 3.4.2

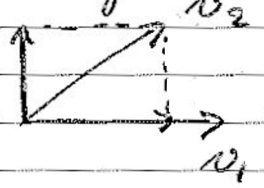
An orthogonal matrix has orthonormal columns (as follows from $Q^T Q = I$)

$Q^{m\times n}$ is isometric (or isometry) if columns are orthonormal

theorem 3.4.8

Let $A \in \mathbb{R}^{m\times n}$ with $\operatorname{rank}(A) = n$. There exists unique $\hat{Q}^{m\times n}$ and $\hat{R}^{n\times n}$, such that $\hat{Q}$ is isometric, $\hat{R}$ is upper triangular with positive entries on main diagonal and $A = \hat{Q}\hat{R}$.

Orthogonalise vector v_2 wrt v_1



$v_2 - \alpha v_1 \perp v_1 \rightarrow v_1^T v_2 - \alpha v_1^T v_1 = 0$

$$\Rightarrow \alpha = \frac{v_1^T v_2}{v_1^T v_1}$$

So orthonormalise columns of A:

1) $q_1 = a_1$; $r_{11} = \|q_1\|$; $q_1 = q_1 / r_{11}$

2) $q_2 = a_2$; $r_{12} = q_1^T q_2$; $q_2 = q_2 - q_1 r_{12}$

$r_{22} = \|q_2\|$; $q_2 = q_2 / r_{22}$

k) $q_k = a_k$; $r_{ik} = q_i^T q_k$ for $i = 1 .. k-1$

$q_k = q_k - \sum_{i=1}^{k-1} q_i r_{ik}$

$r_{kk} = \|q_k\|$; $q_k = q_k / r_{kk}$

Easy to verify that $A = QR$ ($Q^{m \times n}$, $R^{n \times n}$)

Unfortunately, this algorithm is unstable. $\rightarrow$ Better Modified Gram-Schmidt

<u>MGS</u>

k: $q_k = a_k$;
for $i = 1 .. k-1$
$r_{ik} = q_i^T q_k$; $q_k = q_k - q_i r_{ik}$
end
$r_{kk} = \|q_k\|$; $q_k = q_k / r_{kk}$

The crucial difference between (classical) Gram-Schmidt and modified Gram-Schmidt is that in the latter the inner products are taken with the updated vector rather than the initial vector.

We can measure the orthogonality of the computed columns of $\hat{Q}_n$ by computing

$$\| I_n - \hat{Q}_n^T \hat{Q}_n \|_2$$

For Householder reflectors we find

$$\| I_n - \hat{Q}_n^T \hat{Q}_n \|_2 \approx c u$$

(a modest multiple of unit round-off)

For MGS we find

$$\| I_n - \hat{Q}_n^T \hat{Q}_n \|_2 \simeq u \kappa_2(A)$$

where
$$\kappa(A) = \frac{\max_{x \neq 0} \|Ax\| / \|x\|}{\min_{y \neq 0} \|Ay\| / \|y\|}$$

So, MGS may not produce (near) orthogonal vectors if the columns of A are nearly dependent.

So, if orthogonality is really important (for solving least squares problems it is not), we may want to improve orthogonality.

A simple approach is to orthogonalize each vector twice against all previous vectors.

This is, of course, expensive. A better approach is to reorthogonalise a vector only when necessary. ~~If a vector is nearly~~

The key idea is that MGS produces a poorly orthogonalized vector only when the original vector was nearly dependent with the previous vectors. We can monitor this by comparing the original length of the vector (before any orthogonalization) with the final length. If this ratio is too large, we reorthogonalize the vector.
(see, for example, G.W. Stewart, Matrix Algorithms, vol 1, SIAM)

In computational work, solving the LS problem by MGS, is more expensive than solving it by Householder reflections.
On the other hand, if we assemble the Q matrix from Householder reflections, the algorithm becomes more expensive than MGS.

Note that in general for solving the LS problem we do not need Q explicitly.