Numerical Linear Algebra
Chap. 2: Least Squares Problems

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Projection onto a line

Problem: Given a point $b \in \mathbb{R}^m$ and a line through the origin in the direction of $a \in \mathbb{R}^m$

Find the point p on the line closest to the point b

Observations:

- p has a representattion αa for some $\alpha \in \mathbb{R}$
- The line connecting b to p is perpendicular to the vector a

Hence

$$0 = a^T(b - p) = a^T(b - \alpha a) = a^T b - \alpha a^T a \quad \Rightarrow \quad \alpha = \frac{a^T b}{a^T a}.$$

Projection matrix

$$p = \alpha a = a\alpha = a\frac{a^T b}{a^T a} = \frac{aa^T}{a^T a} b =: Pb$$

The projection of some b onto the direction of some a is obtained by multiplying the vector b by the rank-one matrix

$$P = \frac{aa^T}{a^T a}$$

Projection onto a subspace

Problem: Given a point $b \in \mathbb{R}^m$ and n linearly independent vectors $a^1, \dots, a^n \in \mathbb{R}^m$

Find the linear combination $p = \sum_{j=1}^n x_j a^j \in \text{span}\{a^1, \dots, a^n\}$ which is closest to the point b

p is called projection of b onto $\text{span}\{a^1, \dots, a^n\}$.

p is characterized by the condition that the error $b - p$ is perpendicular to the subspace, and this is equivalent to: $b - p$ is perpendicular to $a^1, \dots, a^n$.

Projection onto a subspace ct.

$b - p = b - Ax$ is perpendicular to $a^1, \dots, a^n$ if and only if

$$\begin{aligned} (a^1)^T(b - Ax) &= 0 \\ (a^2)^T(b - Ax) &= 0 \\ &\vdots \\ (a^n)^T(b - Ax) &= 0 \end{aligned}$$

$$\iff A^T(b - Ax) = 0 \quad \iff \quad A^TAx = A^Tb.$$

Theorem

$A^T A$ is nonsingular if and only if the columns of A are linearly independent

Let x be in the nullspace of A. Then it holds

$$Ax = 0 \quad \Rightarrow \quad A^T Ax = 0.$$

Hence, x is in the nullspace of $A^T A$.

If x is in the nullspace of $A^T A$, then it holds

$$A^T Ax = 0 \quad \Rightarrow 0 = x^T A^T Ax = (Ax)^T (Ax) = \|Ax\|^2 \quad \Rightarrow Ax = 0.$$

If the columns of A are linearly independent, then it follows $x = 0$.

Projection onto a subspace

If $a^1, \dots, a^n$ are linearly independent, then the projection p of some vector b onto $\text{span}\{a1, \dots, a^n\}$ is given by $p = Ax$ where x is the unique solution of

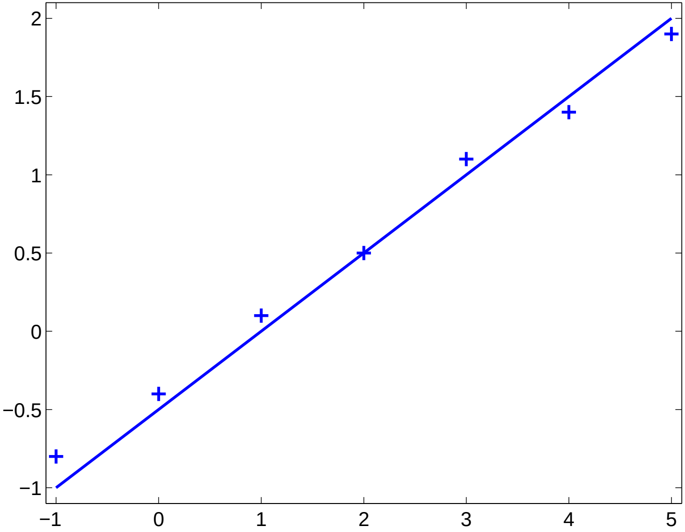
$$A^T Ax = A^T b \quad \Longleftrightarrow \quad x = (A^T A)^{-1} A^T b$$

The projector is given by $P = A(A^T A)^{-1} A^T$

P is symmetric, and it holds $P^2 = P$

The distance from b to the subspace is $\|b - Pb\|$

Least squares problem



Least squares problem ct.

Given are measurements (t_j, b_j), $j = 1, \dots, m$.
Find straight line $f(t) = x_1 + x_2 t$ which matches the measurements best

Try to solve the linear system

$$x_1 + x_2 t_j = b_j, \quad j = 1, \dots, m$$

as good as possible.

Solve the linear system

$$\begin{pmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \\ 1 & t_m \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}$$

as good as possible.

Least squares problem ct.

Replace problem $Ax = b$ by: Find x such that the error $\|Ax - b\|$ is as small as possible. The (unique) solution is called least squares solution.

Solution: The nearest point in the space $\{Ax : x \in \mathbb{R}^n\}$ to the point b is the projection of b onto this space.

Hence the solution of the least squares problem is

$$\bar{x} = (A^T A)^{-1} Ab.$$

Fitting a straight line

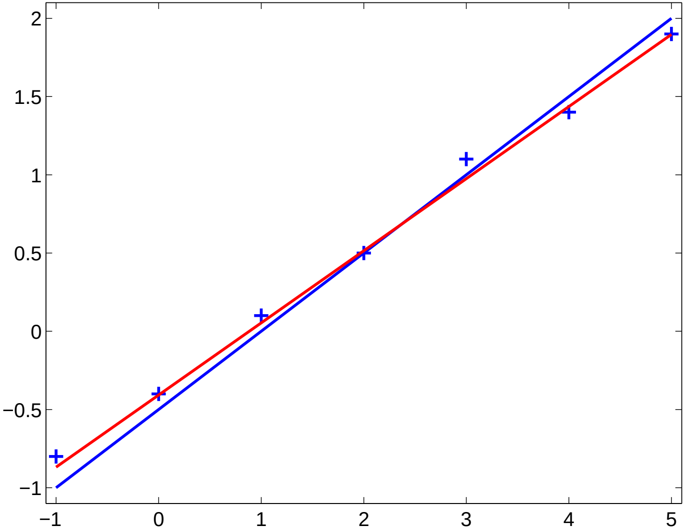
Measurements

t_j	-1	0	1	2	3	4	5
b_j	-0.8	-0.4	0.1	0.5	1.1	1.4	1.9

$$A = \begin{pmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \\ 1 & 5 \end{pmatrix}, \quad b = \begin{pmatrix} -0.8 \\ -0.4 \\ 0.1 \\ 0.5 \\ 1.1 \\ 1.4 \\ 1.9 \end{pmatrix}$$

$$A^T A x = \begin{pmatrix} 7 & 14 \\ 14 & 56 \end{pmatrix} x = A^T b = \begin{pmatrix} 3.8 \\ 20.3 \end{pmatrix} \quad \Rightarrow \quad x = \begin{pmatrix} -0.3643 \\ 0.4536 \end{pmatrix}$$

Least squares problem



Fitting a straight line

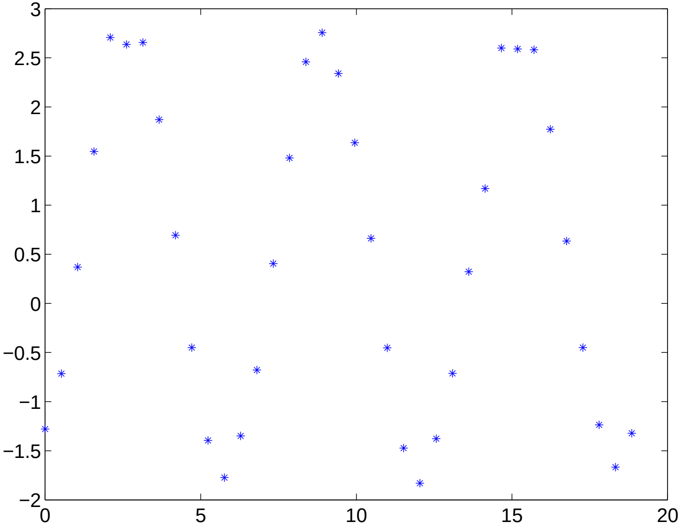
Given m points (t_j, b_j), $j = 1, dots, m$ in the plane. Find a straight line $x_1 + x_2 t$, $t \in \mathbb{R}$ fitting the data in the least squares sense.

$$A = \begin{pmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \\ 1 & t_m \end{pmatrix}, \quad \Rightarrow \quad A^T b = \begin{pmatrix} 1 & 1 & \dots & 1 \\ t_1 & t_2 & \dots & t_m \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = \begin{pmatrix} \sum_{j=1}^m b_j \\ \sum_{j=1}^m t_j b_j \end{pmatrix}$$

$$A^T A = \begin{pmatrix} 1 & 1 & \dots & 1 \\ t_1 & t_2 & \dots & t_m \end{pmatrix} \begin{pmatrix} 1 & t_1 \\ 1 & t_2 \\ \vdots & \\ 1 & t_m \end{pmatrix} = \begin{pmatrix} m & \sum_{j=1}^m t_j \\ \sum_{j=1}^m t_j & \sum_{j=1}^m t_j^2 \end{pmatrix}$$

$$\Rightarrow \quad A^T A x = \begin{pmatrix} m & \sum_{j=1}^m t_j \\ \sum_{j=1}^m t_j & \sum_{j=1}^m t_j^2 \end{pmatrix} x = \begin{pmatrix} \sum_{j=1}^m b_j \\ \sum_{j=1}^m t_j b_j \end{pmatrix} = A^T b$$

Trigonometric polynomial



Trigonometric polynomial ct.

Given measurements (t_j, b_j), $j = 1, \dots, n$. Find trigonometric polynomial

$$f(t) = x_1 + x_2 \sin(t) + x_3 \cos(t)$$

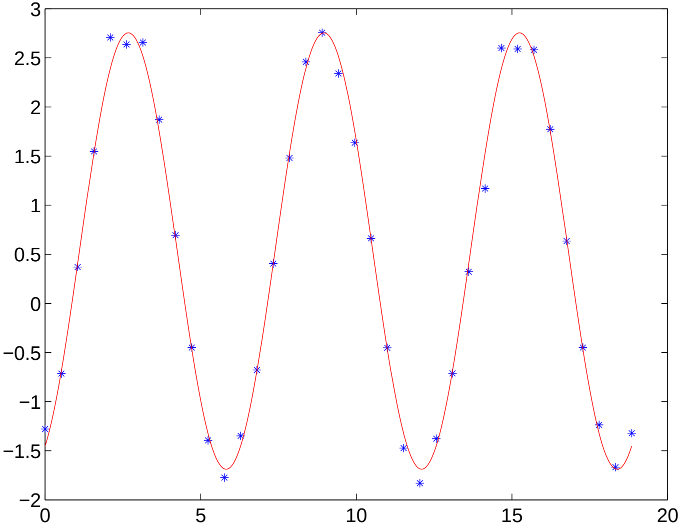
such that the measurements are closest to the graph of f

$$A = \begin{pmatrix} 1 & \sin(t_1) & \cos(t_1) \\ 1 & \sin(t_2) & \cos(t_2) \\ & \vdots & \\ 1 & \sin(t_n) & \cos(t_n) \end{pmatrix}$$

Solve

$$\|Ax - b\| = \min! \quad \iff \quad A^T Ax = A^T b$$

Trigonometric polynomial ct.



Orthonormal vectors

$q^1, q^2, \dots, q^n \in \mathbb{R}^m$ are orthonormal if

$$(q^j)^T q^k = \begin{cases} 0 & \text{when} \quad j \neq k \\ 1 & \text{when} \quad j = k \end{cases}$$

Orthonormal vectors are linearly independent:

$$\sum_{j=1}^{n} \alpha_j q^j = 0 \quad \Rightarrow \quad 0 = (q^k)^T \sum_{j=1}^{n} \alpha_j q^j = \sum_{j=1}^{n} \alpha_j (q^k)^T q^j = \alpha_k, \; k = 1, \dots, n$$

If $n = m$ then $q^1, \dots, q^n$ is an orthonormal basis.

If $q^1, \dots, q^n$ is an orthonormal basis of $\mathbb{R}^n$, then $x \in \mathbb{R}^n$ has the representation

$$x = \sum_{j=1}^{n} \alpha_j q^j \quad \Rightarrow \quad (q^k)^T x = \sum_{j=1}^{n} \alpha_j (q^k)^T q^j = \alpha_k \quad \Rightarrow \quad x = \sum_{j=1}^{n} x^T q^j \cdot q^j.$$

Example

$$q^1 = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \; q^2 = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}, \; x = \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix}$$

$$\begin{aligned} x &= x^T q^1 \cdot q^1 + x^T q^2 \cdot q^2 \\ &= ((\cos\alpha\cos\theta + \sin\alpha\sin\theta) q^1 + (-\cos\alpha\sin\theta + \sin\alpha\cos\theta) q^2 \\ &= \cos(\alpha - \theta) \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} + \sin(\alpha - \theta) \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}. \end{aligned}$$

Orthogonal matrix

An $n \times n$ matrix with orthonormal columns is called orthogonal matrix. It is usually denoted by Q.

Every orthogonal matrix Q is nonsingular.

$$Q^T Q = I \quad \Rightarrow \quad Q^{-1} = Q^T.$$

If Q is orthogonal then Q^T is orthogonal:

$$(Q^T)^T Q^T = QQ^T = QQ^{-1} = I$$

Rotation

$$Q = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

rotates every vector in the plane through the angle θ

$$Q^T = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} \cos(-\theta) & -\sin(-\theta) \\ \sin(-\theta) & \cos(-\theta) \end{pmatrix} = Q^{-1}$$

rotates every vector in the plane through the angle $-\theta$

Permutation

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

obviously is an orthogonal matrix.

$$Px = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} x_2 \\ x_4 \\ x_1 \\ x_3 \end{pmatrix}$$

$$P^T = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} = P^{-1} \Rightarrow \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_2 \\ x_4 \\ x_1 \\ x_3 \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}$$

puts the components back into their original order

Reflection

If u is any unit vector, then $Q = I - 2uu^T$ is orthogonal:

$$\begin{aligned} Q^T &= I - 2(uu^T)^T = I - 2(u^T)^T u^T = I - 2uu^T = Q, \\ Q^T Q &= (I - 2uu^T)(I - 2uu^T) = I - 4uu^T + 4uu^T uu^T = I \end{aligned}$$

since $u^T u = 1$.

Q defines a refection at the hyperplane $u^\perp$: Let $x = u^T x \cdot u + v$, $u^T v = 0$. Then it follows

$$\begin{aligned} Qx &= (u^T x)(I - 2uu^T)u + (I - 2uu^T)v \\ &= (u^T x)(u - 2uu^T u) + (v - 2uu^T v) = -(u^T x)u + v \end{aligned}$$

Now it is obvious, that $Q^2 = Q$: reflecting twice through a mirror brings back the original.

Orthogonal matrices

If Q is orthogonal, then it leaves lengths unchanged:

$$\|Qx\|^2 = (Qx)^T(Qx) = x^T Q^T Qx = x^T x = \|x\|^2.$$

It also leaves angles unchanged

$$\cos(x, y) = \frac{x^T y}{\|x\| \cdot \|y\|} = \frac{x^T Q^T Qy}{\|Qx\| \cdot \|Qy\|} = \frac{(Qx)^T (Qy)}{\|Qx\| \cdot \|Qy\|}.$$

Orthogonal matrices are excellent for computations: numbers never grow too large when lengths are fixed.

Projection

Let $q^1, \dots, q^n \in \mathbb{R}^m$ orthonormal vectors (how do we know that $m \geq n$?)

Then with $Q := [q^1, \dots, q^n] \in \mathbb{R}^{m \times n}$ the projector onto $V := \text{span}\{q^1, \dots, q^n\}$ is

$$P = Q(Q^T Q)^{-1} Q^T = QQ^T$$

and the projection of $x \in \mathbb{R}^m$ onto V is

$$Px = QQ^T x = \sum_{j=1}^{n} (x^T q^j) q^j,$$

the truncation of the Fourier development with respect to an orthonormal basis containing $q^1, \dots, q^n$.

Least squares problem

Consider the least squares problem $\|Qx - b\| = \min!$, where the system matrix has orthonormal columns:

Solution: $\bar{x} = Q^T b$

Example

$$Q = \frac{1}{13}\begin{pmatrix} 3 & -12 & 4 \\ 4 & -3 & -12 \\ 12 & 4 & 3 \end{pmatrix}$$

is an orthogonal matrix

Represent the vector $x = (1, 1, 1)^T$ as a linear combination of the columns q^j of Q.

$$x^T q^1 = \frac{19}{13},\ x^T q^2 = \frac{-11}{13},\ x^T q^3 = \frac{-5}{13}$$

$$\Rightarrow x = \frac{19}{169}\begin{pmatrix} 3 \\ 4 \\ 12 \end{pmatrix} - \frac{11}{169}\begin{pmatrix} -12 \\ -3 \\ 4 \end{pmatrix} - \frac{5}{13}\begin{pmatrix} 4 \\ -12 \\ 3 \end{pmatrix}$$

Fitting a straight line

Given measurements (t_j, b_j), $j = 1, \dots, m$. Assume that the measurement times t_j add to zero.

Since the scalar product of $(t_j)_{j=1,\dots,m}$ and $(1, 1, \dots, 1)^T$ is zero the normal equations

$$A^T A x = \begin{pmatrix} m & \sum_{j=1}^m t_j \\ \sum_{j=1}^m t_j & \sum_{j=1}^m t_j^2 \end{pmatrix} x = \begin{pmatrix} \sum_{j=1}^m b_j \\ \sum_{j=1}^m t_j b_j \end{pmatrix} = A^T b$$

obtain the form

$$\begin{pmatrix} m & 0 \\ 0 & \sum_{j=1}^m t_j^2 \end{pmatrix} x = \begin{pmatrix} \sum_{j=1}^m b_j \\ \sum_{j=1}^m t_j b_j \end{pmatrix}$$

and the solution is

$$\bar{x} = \begin{pmatrix} \sum_{j=1}^m b_j / m \\ \sum_{j=1}^m t_j b_j / \sum_{j=1}^m t_j^2 \end{pmatrix}$$

Fitting a straight line

Orthogonal columns are so helpful that it is worth moving the time origing to produce them.

To this end subtract the average time $\bar{t} = \frac{1}{m}\sum_{j=1}^{m} t_j$. Then the shifted measurement times $\tilde{t}_j := t_j - \bar{t}$ add to zero.

The solution of the least squares problem is

$$\tilde{x}_1 + \tilde{x}_2\tilde{t} = \tilde{x}_1 + \tilde{x}_2(t - \bar{t}) = (\tilde{x}_1 - \tilde{x}_2\bar{t}) + \tilde{x}_2 t$$

where

$$\tilde{x}_1 = \frac{1}{m}\sum_{j=1}^{m} b_j \quad \text{and} \quad \tilde{x}_2 = \frac{\sum_{j=1} b_j\tilde{t}_j}{\sum_{j=1}^{m} \tilde{t}_j^2}.$$

Example ct.

Measurements

t_j	-1	0	1	2	3	4	5
b_j	-0.8	-0.4	0.1	0.5	1.1	1.4	1.9

The average time is $\bar{t} = 2$, and $\tilde{t} = (-3, -2, -1, 0, 1, 2, 3)^T$, and

$$\tilde{x}_1 = \frac{1}{7}\sum_{j=1}^{7} b_j = \frac{3.8}{7}, \quad \tilde{x}_2 = \frac{\sum_{j=1} b_j \tilde{t}_j}{\sum_{j=1}^{m} \tilde{t}_j^2} = \frac{12.9}{28}$$

Therefore, the solution of the least equares problem is

$$(\tilde{x}_1 - \tilde{x}_2 \bar{t}) + \tilde{x}_2 t = -\frac{5.9}{14} + \frac{12.9}{28} t = -0.3643 + 0.4536t.$$

Gram Schmidt process

Assume that $a^1, \dots, a^n \in \mathbb{R}^m$ are given linearly independent vectors.
Problem: Determine an orthogonal basis $q^1, \dots, q^n$ of $V := \text{span}\{a^1, \dots, a^n\}$

Advantage
For $Q := [q^1, \dots, q^n]$ it holds that $Q^T Q = \text{diag}\{\|q^1\|^2, \dots, \|q^n\|^2\}$ is a diagonal matrix. Hence the orthogonal projection onto V decouples:

$$\begin{aligned} Px &:= Q(Q^T Q)^{-1} Q^T x = Q\text{diag}\{\|q^1\|^2, \dots, \|q^n\|^2\}^{-1} \left(x^T q^1, \dots, x^T q^n\right)^T \\ &= Q\left(\frac{x^T q^1}{\|q^1\|^2}, \dots, \frac{x^T q^n}{\|q^n\|^2}\right)^T = \sum_{j=1}^n \frac{x^T q^j}{\|q^j\|^2} q^j. \end{aligned}$$

Example

Project $x = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}$ to the subspace spanned by $q^1 = \begin{pmatrix} 1 \\ 2 \\ 3 \\ -1 \end{pmatrix}$ and $q^2 = \begin{pmatrix} -1 \\ 1 \\ 0 \\ 1 \end{pmatrix}$.

Since q^1 and q^2 are orthogonal, the projection is

$$p = \frac{x^T q^1}{\|q^1\|^2} q^1 + \frac{x^T q^2}{\|q^2\|^2} q^2 = \frac{10}{15} \begin{pmatrix} 1 \\ 2 \\ 3 \\ -1 \end{pmatrix} + \frac{5}{3} \begin{pmatrix} -1 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 \\ 3 \\ 2 \\ 1 \end{pmatrix}$$

Indeed, $p - x = \begin{pmatrix} -2 \\ 1 \\ -1 \\ -3 \end{pmatrix}$ is orthogonal to q^1 and q^2.

Gram–Schmidt process

Assume that $a^1, \dots, a^n \in \mathbb{R}^m$ are given linearly independent vectors.
Problem: Determine an orthogonal basis $q^1, \dots, q^n$ of $V := \mathrm{span}\{a^1, \dots, a^n\}$

Idea: Set $q^1 = a^1$, and for $j = 2, 3, \dots, n$ subtract the projection of a^j to the subspace $\mathrm{span}\{a^1, \dots, a^{j-1}\}$ from a^j. Then this difference q^j is orthogonal to $\mathrm{span}\{a^1, \dots, a^{j-1}\}$, and therefore to the previously determined vectors q^i.

Since $q^1, \dots, q^{j-1}$ is an orthogonal basis of $\mathrm{span}\{a^1, \dots, a^{j-1}\}$, the projections are decoupled. Hence,

$$q^j = a^j - \sum_{k=1}^{j-1} \frac{(a^j)^T q^k}{\|q^k\|^2} q^k, \; j = 2, \dots, n.$$

Example

Apply the Gram–Schmidt process to $a^1 = \begin{pmatrix} -3 \\ 4 \\ 0 \end{pmatrix}$, $a^2 = \begin{pmatrix} -2 \\ 11 \\ 1 \end{pmatrix}$, $a^3 = \begin{pmatrix} 5 \\ 10 \\ -24 \end{pmatrix}$

$$q^1 = a^1, \quad q^2 = a^2 - \frac{(a^2)^T(q^1)}{\|q^1\|^2} q^1 = \begin{pmatrix} -2 \\ 11 \\ 1 \end{pmatrix} - \frac{50}{25} \begin{pmatrix} -3 \\ 4 \\ 0 \end{pmatrix} = \begin{pmatrix} 4 \\ 3 \\ 1 \end{pmatrix}$$

$$q^3 = a^3 - \frac{(a^3)^T(q^1)}{\|q^1\|^2} q^1 - \frac{(a^3)^T(q^2)}{\|q^2\|^2} q^2 = \begin{pmatrix} 5 \\ 10 \\ -24 \end{pmatrix} - \frac{25}{25} \begin{pmatrix} -3 \\ 4 \\ 0 \end{pmatrix} - \frac{26}{26} \begin{pmatrix} 4 \\ 3 \\ 1 \end{pmatrix} = \begin{pmatrix} 4 \\ 3 \\ -25 \end{pmatrix}$$

Factorization

Remember

$$q^j = a^j - \sum_{k=1}^{j-1} \frac{(a^j)^T q^k}{\|q^k\|^2} q^k,\ j = 2, \dots, n.$$

It is more convenient to normalize the q–vectors in the course of the algorithm and to get rid of the denominators.

The Gram–Schmidt algorithm then reads

$$\begin{aligned} q^1 &= \frac{1}{\|a^1\|} a^1 \\ q^j &= \left(a^j - \sum_{k=1}^{j-1} (a^j)^T q^k q^k \right) \Big/ \left\| a^j - \sum_{k=1}^{j-1} (a^j)^T q^k q^k \right\|,\ j = 2, \dots, n. \end{aligned}$$

QR Factorization

The following form is more convenient:

$$\begin{aligned} a^1 &= \|a^1\| q^1 \\ a^j &= \sum_{k=1}^{j-1} (a^j)^T q^k q^k + \left\| a^j - \sum_{k=1}^{j-1} (a^j)^T q^k q^k \right\| q^j, \; j = 2, \dots, n. \end{aligned}$$

Since at every step a^j is a linear combination of $q^1, \dots, q^j$, and later q^i:s are not involved:

$$A = (a^1, \dots, a^n) = (q^1, \dots, q^n) \begin{pmatrix} r_{11} & r_{12} & r_{13} & \dots & r_{1n} \\ & r_{22} & r_{23} & \dots & r_{2n} \\ & & \ddots & & \\ & & & \ddots & \\ & & & & r_{nn} \end{pmatrix} = QR$$

where $r_{ij} = (a^j)^T q^i$, $i = 1, \dots, j-1$ and $r_{jj} = \|a^j - \sum_{k=1}^{j-1} (a^j)^T q^k q^k\|$.

Example

Determine the *QR*-factorization of

$$A = [a^1, a^2, a^3] = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 2 & -1 \\ 0 & 2 & 1 \\ 3 & 3 & 4 \end{pmatrix}$$

$$q^1 = \frac{1}{\|a^1\|} a^1 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\|q^2\| q^2 = a^2 - (a^2)^T q^1 q^1 = \begin{pmatrix} 1 \\ 2 \\ 2 \\ 3 \end{pmatrix} - 3 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 2 \\ 0 \end{pmatrix} \Rightarrow \frac{1}{3} \begin{pmatrix} 1 \\ 2 \\ 2 \\ 0 \end{pmatrix}$$

Example ct.

$$
\begin{aligned}
\|q^3\| q^3 &= a^3 - (a^3)^T q^1 q^1 - (a^3)^T q^2 q^2 \\
&= \begin{pmatrix} 0 \\ -1 \\ 1 \\ 4 \end{pmatrix} - 4 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} - 0 \begin{pmatrix} 1 \\ 2 \\ 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix} \Rightarrow q^3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}
\end{aligned}
$$

Hence the QR–factorization of A is

$$
\begin{pmatrix} 0 & 1 & 0 \\ 0 & 2 & -1 \\ 0 & 2 & 1 \\ 3 & 3 & 4 \end{pmatrix} = \begin{pmatrix} 0 & 1/3 & 0 \\ 0 & 2/3 & -1/\sqrt{2} \\ 0 & 2/3 & 1/\sqrt{2} \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 3 & 3 & 4 \\ 0 & 3 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}
$$

Least squares problems

Any matrix $A \in \mathbb{R}^{m\times n}$ with linearly independent columns can be factored into QR.
$Q \in \mathbb{R}^{m\times n}$ has orthonormal columns, and $R \in \mathbb{R}^{n\times n}$ is upper triangular with positive diagonal.

Given the QR–factorization of A a least squares problem with system matrix A can be solved easily:

$$\begin{aligned} A^TAx = A^Tb \quad &\iff \quad (QR)^T(QR)x = (QR)^Tb \\ &\iff \quad R^TQ^TQRx = R^TQ^Tb \\ &\iff \quad R^TRx = R^TQ^Tb \\ &\iff \quad Rx = Q^Tb. \end{aligned}$$

Instead of solving the normal equations $A^TAx = A^Tb$ by Gaussian elimination one just solves $Rx = Q^Tb$ by back substitution.

Example

Solve the least squares problem $Ax \approx b$ where

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 2 & -1 \\ 0 & 2 & 1 \\ 3 & 3 & 4 \end{pmatrix} \quad \text{and} \quad b = \begin{pmatrix} 4 \\ 3 \\ 2 \\ 1 \end{pmatrix}.$$

Normal equations:

$$A^T A x = \begin{pmatrix} 9 & 9 & 12 \\ 9 & 18 & 12 \\ 12 & 12 & 18 \end{pmatrix} x = A^T b = \begin{pmatrix} 3 \\ 17 \\ 3 \end{pmatrix} \Rightarrow x = \frac{1}{18} \begin{pmatrix} -10 \\ 28 \\ -9 \end{pmatrix}$$

Example ct.

Taking advantage of the known QR–factorization

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 2 & -1 \\ 0 & 2 & 1 \\ 3 & 3 & 4 \end{pmatrix} = \begin{pmatrix} 0 & 1/3 & 0 \\ 0 & 2/3 & -1/\sqrt{2} \\ 0 & 2/3 & 1/\sqrt{2} \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 3 & 3 & 4 \\ 0 & 3 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}$$

we have to solve

$$Rx = \begin{pmatrix} 3 & 3 & 4 \\ 0 & 3 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} x = Q^T b = \begin{pmatrix} 1 \\ 14/3 \\ -1/\sqrt{2} \end{pmatrix} \Rightarrow x = \frac{1}{18} \begin{pmatrix} -10 \\ 28 \\ -9 \end{pmatrix}$$

Gram–Schmidt algorithm

1: $q^1 = a^1 / \|a^1\|$
2: **for** j=2,...,n **do**
3: $\quad q^j = a^j$
4: $\quad$ **for** k=1,...,j-1 **do**
5: $\qquad r_{kj} = (a^j)^T q^k;$
6: $\qquad q^j = q^j - r_{kj} q^k;$
7: $\quad$ **end for**
8: $\quad q^j = q^j / \|q^j\|$
9: **end for**

In steps 5 and 6 the projection of a^j onto spanq^k is subtracted from q^j for $k = 1, \dots, j-1$. At that time

$$q^j = a^j - \sum_{\ell=1}^{k-1} (a^j)^T q^\ell q^\ell$$

and from $(q^\ell)^T q^k = 0$ for $\ell = 1, \dots, k-1$ it follows that we can replace step 5 by $r_{kj} = (q^j)^T q^k$.

This version is called modified Gram–Schmidt method. It is numerically more stable than the original Gram–Schmidt factorization.

Householder transformation

Although the modified Gram–Schmidt method is knwon to be more stable than the original Gram–Schmidt method, there is a better way to solve least square problems by Householder transformation.

Problem: Given a vector $a \in \mathbb{R}^m$; find a refection $H = I - 2uu^T$, $\|u\| = 1$ such that Ha is a multiple of the first unit vector $e := (1, 0, \ldots, 0)^T$.

From the orthogonality of H it follows that $\|Ha\| = \|a\|$. Hence, $Ha = a - 2u^T a \cdot u = \pm\|a\|e$, and therefore u and $a \pm \|a\|e$ are parallel.

If a is not a multiple of e then there are two solutions of our problem:

$$u = \frac{a + \|a\|e}{\|a + \|a\|e\|} \quad \text{and} \quad u = \frac{a - \|a\|e}{\|a - \|a\|e\|},$$

for $a = \|a\|e$ the first solution is defined, for $a = -\|a\|e$ only the second one.

Householder transformation ct.

In any case the Householder transformation

$$H = I - 2\frac{ww^T}{w^T w} \quad \text{with} \quad w = a + \text{sign}(a_1)\|a\|e$$

exists. For stability reasons (cancellation!) we always choose this one.

Let $a = (2, 2, 1)^T$. Then $\|a\| = 3$, and $w = (5, 2, 1)^T$, and

$$H = I - \frac{1}{\|w\|^2} ww^T = I - \frac{1}{15}\begin{pmatrix}5\\2\\1\end{pmatrix}\begin{pmatrix}5 & 2 & 1\end{pmatrix} \Rightarrow Ha = -3\begin{pmatrix}1\\0\\0\end{pmatrix}$$

A second solution is defined by $w_- = (-1, 2, 1)^T$:

$$H = I - \frac{1}{\|w_-\|^2} w_- w_-^T = I - \frac{1}{3}\begin{pmatrix}-1\\2\\1\end{pmatrix}\begin{pmatrix}-1 & 2 & 1\end{pmatrix} \Rightarrow Ha = 3\begin{pmatrix}1\\0\\0\end{pmatrix}$$

Least equares problem

Consider the least square problem

$$\|Ax - b\| = \min! \quad \text{where } A \in \mathbb{R}^{m\times n},\ b \in \mathbb{R}^n.$$

Since orthogonal matrices do not change the length of a vector, it follows

$$\|Ax - b\| = \|Q(Ax - b)\| \quad \text{for every orthogonal matrix } Q \in \mathbb{R}^{m\times m}.$$

Assume that $QA = \begin{pmatrix} R \\ O \end{pmatrix}$ where $Q^TQ = I$, $R \in \mathbb{R}^{n\times n}$ is upper triangular and $O \in \mathbb{R}^{m-n,n}$ denotes the nullmatrix. Then we obtain

$$\|Ax - b\|^2 = \|QAx - Qb\|^2 = \left\| \begin{pmatrix} R \\ O \end{pmatrix} x - Qb \right\|^2 = \|Rx - \tilde{b}^1\|^2 + \|\tilde{b}^2\|^2$$

where $\tilde{b}^1 \in \mathbb{R}^n$ contains the leading n components of Qb, and $\tilde{b}^2$ the remaining ones.

Least equares problem ct.

From

$$\|Ax - b\|^2 = \|Rx - \tilde{b}^1\|^2 + \|\tilde{b}^2\|^2$$

it is obvious that $x = R^{-1}\tilde{b}^1$ is the solution of the least squares problem, and that $\|\tilde{b}^2\|$ is the residuum.

Q is constructed step by step using Householder transformations.

Let H_1 be a Householder transformation such that $Ha^1 = \pm\|a^1\|e$, where a^1 denotes the first column of A. Then

$$A_1 := H_1 A = \begin{pmatrix} r_{11} & r_{12} \dots r_{1n} \\ 0 & \\ \vdots & \tilde{A}_1 \\ 0 & \end{pmatrix}$$

Least equares problem ct.

Next we annihilate the subdiagonal elements of the second column.

Let $\tilde{H}_2$ be the Householder matrix wich maps the first column of $\tilde{A}_1$ to a multiple of the first unit vector (in $\mathbb{R}^{m-1}$), and let

$$H_2 = \begin{pmatrix} 1 & 0 \dots 0 \\ 0 & \\ \vdots & \tilde{H}_2 \\ 0 & \end{pmatrix}$$

Then we obtain

$$H_2 H_1 A = H_2 A_1 =: A_2 = \begin{pmatrix} r_{11} & r_{12} & r_{13} \dots r_{1n} \\ 0 & r_{22} & r_{23} \dots r_{2n} \\ 0 & 0 & \\ \vdots & \vdots & \tilde{A}_2 \\ 0 & 0 & \end{pmatrix}$$

Least equares problem ct.

Continuing that way we finally arrive at

$$H_n H_{n-1} \cdots H_1 A =: A_n = \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ 0 & r_{22} & \dots & r_{2n} \\ 0 & 0 & \ddots & \\ 0 & 0 & \dots & r_{nn} \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix} =: \begin{pmatrix} R \\ O \end{pmatrix}$$

With $\tilde{b} := H_n H_{n-1} \cdots H_1 b := \begin{pmatrix} \tilde{b}^1 \\ \tilde{b}^n \end{pmatrix}$, $\tilde{b}^1 \in \mathbb{R}^n$ the least squares problem obtains the form

$$\|Ax - b\| = \|A_n x - \tilde{b}\|$$

with the unique solution

$$x = R^{-1}\tilde{b}^1.$$

Example

$$A = [a^1, a^2] = \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 2 \\ 1 & 5 \end{pmatrix}, \quad b = \begin{pmatrix} 2.9 \\ 5.1 \\ 5.2 \\ 11.9 \end{pmatrix}$$

From $\|a^1\| = 2$ it follows that the Householder method mapping the first column a^1 of A to a multiple of the first unit vector is

$$H_1 = I - 2\frac{ww^T}{w^T w} \quad \text{where } w = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} + 2 \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

$$A_1 = H_1 A = \begin{pmatrix} -3 & -5 \\ 0 & 0 \\ 0 & 0 \\ 0 & 3 \end{pmatrix}, \quad H_1 b = \begin{pmatrix} -12.55 \\ -0.05 \\ 0.05 \\ 6.75 \end{pmatrix}$$

Example ct.

Obviously, this problem is equivalent to

$$\left\| \begin{pmatrix} -2 & -5 \\ 0 & 3 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} x - \begin{pmatrix} -12.55 \\ 6.75 \\ -0.05 \\ 0.05 \end{pmatrix} \right\| = \text{min!}$$

which is solved by

$$\begin{pmatrix} -2 & -5 \\ 0 & 3 \end{pmatrix} x = \begin{pmatrix} -12.55 \\ 6.75 \end{pmatrix} \quad \Rightarrow \quad x = \begin{pmatrix} 0.65 \\ 2.25 \end{pmatrix}$$

For didactic reasons we solve the transformed problem

$$\|A_1 x - H_1 b\| = \left\| \begin{pmatrix} -3 & -5 \\ 0 & 0 \\ 0 & 0 \\ 0 & 3 \end{pmatrix} x - \begin{pmatrix} -12.55 \\ -0.05 \\ 0.05 \\ 6.75 \end{pmatrix} \right\| = \text{min!}$$

using a Householder transformation.

$$\tilde{H}_2 = I - 2\frac{vv^T}{v^T v}, \quad v = \begin{pmatrix} 0 \\ 0 \\ 3 \end{pmatrix} + 3 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 3 \\ 0 \\ 3 \end{pmatrix}$$

maps the first column of $\tilde{A}_2$ to a multiple of the first unit vector in $\mathbb{R}^3$

Hence

$$\tilde{H}_2 \begin{pmatrix} 0 \\ 0 \\ 3 \end{pmatrix} = \begin{pmatrix} -3 \\ 0 \\ 0 \end{pmatrix}, \; H_2 A_1 = \begin{pmatrix} 1 & 0 \\ 0 & \tilde{H}_2 \end{pmatrix} A_1 = \begin{pmatrix} -2 & -5 \\ 0 & -3 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$H_2 \begin{pmatrix} -0.05 \\ 0.05 \\ 6.75 \end{pmatrix} = \begin{pmatrix} -0.05 \\ 0.05 \\ 6.75 \end{pmatrix} - \frac{2}{9} \begin{pmatrix} 3 \\ 0 \\ 3 \end{pmatrix} \begin{pmatrix} 3 & 0 & 3 \end{pmatrix} \begin{pmatrix} -0.05 \\ 0.05 \\ 6.75 \end{pmatrix} = \begin{pmatrix} -6.75 \\ 0.05 \\ 0.05 \end{pmatrix}$$

and we obtain the equivalent problem

$$\left\| \begin{pmatrix} -2 & -5 \\ 0 & -3 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} x - \begin{pmatrix} -6.75 \\ 0.05 \\ 0.05 \end{pmatrix} \right\| = \min!$$

which is solved by

$$\begin{pmatrix} -2 & -5 \\ 0 & -3 \end{pmatrix} x = \begin{pmatrix} -6.75 \end{pmatrix} \quad \Rightarrow \quad x = \begin{pmatrix} 0.65 \\ 2.25 \end{pmatrix}$$