Linear Least Squares

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Orthogonal and Hermitian Matrix

A square matrix Q is *orthogonal* iff $Q^{-1}=Q^{T}$

$\Rightarrow Q^{T}Q = QQ^{T} = I$

$\Rightarrow$ its rows are orthonormal

$\Rightarrow$ its columns are orthonormal

note: orthogonal matrices are often named Q

generalization: a matrix is *Hermitian* iff $Q^{-1}=Q^{H}$ where superscript ^{H} denotes complex conjugate transpose

Householder Transformations

The *Householder transformation* determined by vector *v* is:

$$H = I - 2\frac{vv^T}{v^T v}$$

outer product, n×n matrix

inner product, scalar

To apply it to a vector *x*, compute:

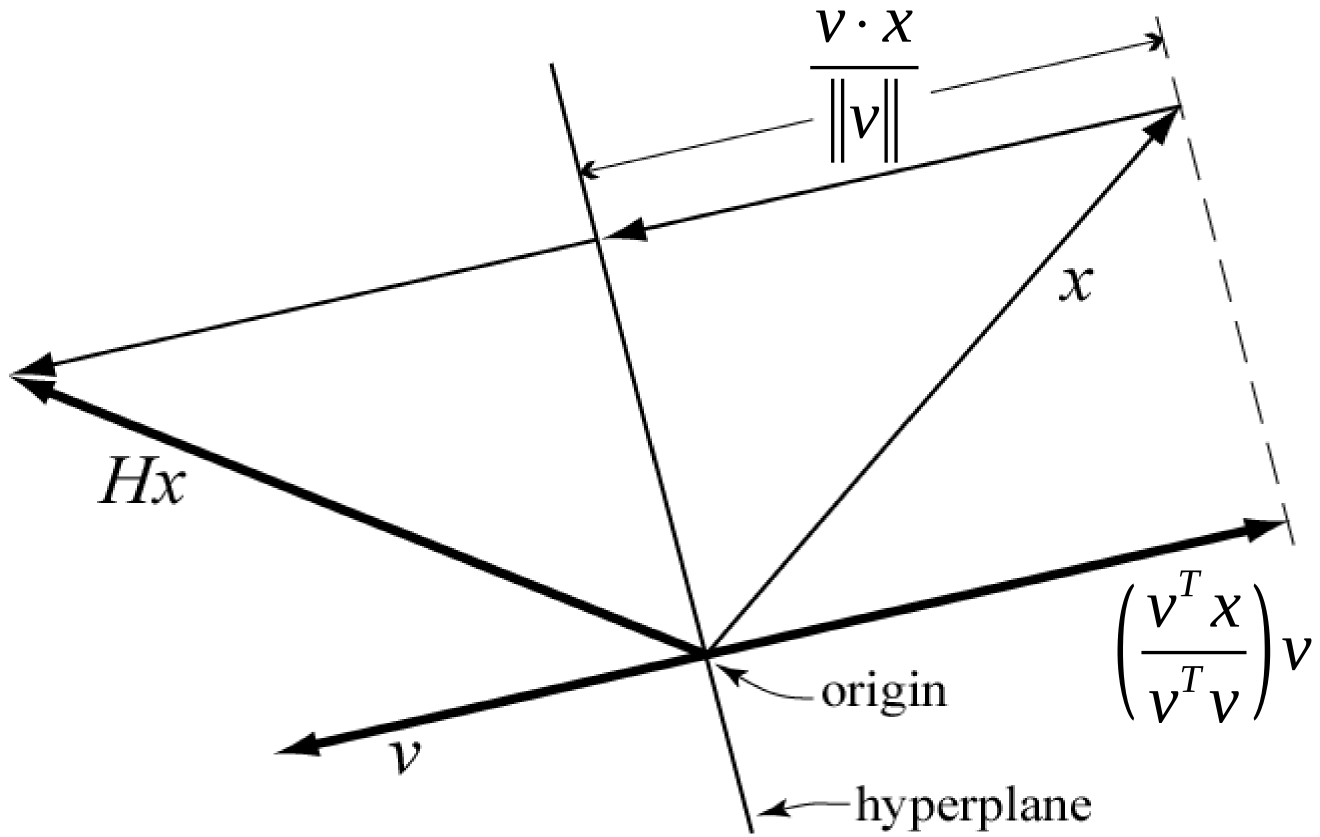
$$Hx = \left(I - 2\frac{vv^T}{v^T v} \right) x = x - 2\frac{v(v^T x)}{v^T v}$$

$$\boxed{Hx = x - \left(2\frac{v^T x}{v^T v} \right) v}$$

scalar

Householder Geometry

- ***Hx* is *x* reflected through the hyperplane perpendicular to *v*** ($p : p^{\mathrm{T}}v=0$)



Householder Properties

- H is symmetric, since

$$H^T = \left(I - 2\frac{vv^T}{v^T v} \right)^T = I^T - 2\frac{(vv^T)^T}{v^T v} = I - 2\frac{v^{T^T} v^T}{v^T v} = H$$

- H is orthogonal, since

$$H^T H = HH = \left(I - 2\frac{vv^T}{v^T v} \right)\left(I - 2\frac{vv^T}{v^T v} \right)$$

$$= I - 4\frac{vv^T}{v^T v} + 4\frac{v(v^T v)v^T}{(v^T v)^2} = I - 4\frac{vv^T}{v^T v} + 4\frac{vv^T}{v^T v} = I$$

and $H^T H = I$ implies $H^T = H^{-1}$

Householder to Zero Matrix Elements

We'll use Householder transformations to zero subdiagonal elements of a matrix.

Given any vector *a*, find the *v* that determines an *H* such that,

$$Ha = \alpha e_1 = \alpha[1, 0, 0, ..., 0]^T$$

Now solve for *v*:

$$Ha = a - \left(2\frac{v^T a}{v^T v}\right)v = a - \mu v = \alpha e_1$$

where μ is parenthesized scalar, related to length of v

$$\Rightarrow \; v = (a - \alpha e_1) / \mu$$

We're free to choose $\mu = 1$, since $\|v\|$ does not affect H

Choosing the Vector v

So $v = a - \alpha e_1$ for some scalar α.

But $\|Ha\|_2 = \|a\|_2$

(prove this by expanding $\|Ha\|_2^2 = (Ha)^T Ha$)

and $\|Ha\|_2 = |\alpha|$ by design, so $\alpha = \pm\|a\|_2$

(either sign will work).

To avoid $v \approx 0$ we choose $\alpha = -\text{sign}(a_1)\|a\|_2$,

so $v = a + \text{sign}(a_1)\|a\|_2 e_1$ is our answer.

Applying Householder Transforms

- Don’t compute Hx explicitly, that costs $3n^2$ flops.
- Instead use the formula given previously,

$$Hx = x - \left(2 \frac{v^T x}{v^T v} \right) v$$

which costs $4n$ flops (if you pre-compute $v^T v$ or pre-normalize $v^T v=2$).

- Typically, when using Householder transformations, you never compute the matrix H; it’s only used in derivation and analysis.

QR Decomposition

- Householder transformations are a good way to zero out subdiagonal elements of a matrix.
- A is decomposed:

$$Q^T A = \begin{bmatrix} R \\ 0 \end{bmatrix} \quad \text{or} \quad QQ^T A = A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$$

- where $Q^{\mathrm{T}} = H_n \ldots H_2 H_1$ is the orthogonal (prove!) product of Householders and R is upper triangular.
- Overdetermined system $Ax=b$ is transformed into the easy-to-solve

$$\begin{bmatrix} R \\ 0 \end{bmatrix} x = Q^T b$$