Scientific Computing: An Introductory Survey

Chapter 3 – Linear Least Squares

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Outline

Method of Least Squares

- Measurement errors are inevitable in observational and experimental sciences
- Errors can be smoothed out by averaging over many cases, i.e., taking more measurements than are strictly necessary to determine parameters of system
- Resulting system is *overdetermined*, so usually there is no exact solution
- In effect, higher dimensional data are projected into lower dimensional space to suppress irrelevant detail
- Such projection is most conveniently accomplished by method of *least squares*

Linear Least Squares

- For linear problems, we obtain *overdetermined* linear system $\boldsymbol{Ax} = \boldsymbol{b}$, with $m \times n$ matrix $\boldsymbol{A}$, $m > n$
- System is better written $\boldsymbol{Ax} \cong \boldsymbol{b}$, since equality is usually not exactly satisfiable when $m > n$
- Least squares solution $\boldsymbol{x}$ minimizes squared Euclidean norm of residual vector $\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{Ax}$,

$$\min_{\boldsymbol{x}} \|\boldsymbol{r}\|_2^2 = \min_{\boldsymbol{x}} \|\boldsymbol{b} - \boldsymbol{Ax}\|_2^2$$

Data Fitting

- Given m data points (t_i, y_i), find n-vector $\boldsymbol{x}$ of parameters that gives "best fit" to model function $f(t, \boldsymbol{x})$,

$$\min_{\boldsymbol{x}} \sum_{i=1}^{m} (y_i - f(t_i, \boldsymbol{x}))^2$$

- Problem is *linear* if function f is linear in components of $\boldsymbol{x}$,

$$f(t, \boldsymbol{x}) = x_1\phi_1(t) + x_2\phi_2(t) + \cdots + x_n\phi_n(t)$$

  where functions ϕ_j depend only on t
- Problem can be written in matrix form as $\boldsymbol{Ax} \cong \boldsymbol{b}$, with $a_{ij} = \phi_j(t_i)$ and $b_i = y_i$

Data Fitting

- Polynomial fitting

$$f(t, \boldsymbol{x}) = x_1 + x_2 t + x_3 t^2 + \cdots + x_n t^{n-1}$$

  is linear, since polynomial linear in coefficients, though nonlinear in independent variable t
- Fitting sum of exponentials

$$f(t, \boldsymbol{x}) = x_1 e^{x_2 t} + \cdots + x_{n-1} e^{x_n t}$$

  is example of nonlinear problem
- For now, we will consider only linear least squares problems

Example: Data Fitting

- Fitting quadratic polynomial to five data points gives linear least squares problem

$$\boldsymbol{Ax} = \begin{bmatrix} 1 & t_1 & t_1^2 \\ 1 & t_2 & t_2^2 \\ 1 & t_3 & t_3^2 \\ 1 & t_4 & t_4^2 \\ 1 & t_5 & t_5^2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \cong \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \boldsymbol{b}$$

- Matrix whose columns (or rows) are successive powers of independent variable is called *Vandermonde matrix*

Example, continued

- For data

t	-1.0	-0.5	0.0	0.5	1.0
y	1.0	0.5	0.0	0.5	2.0

  overdetermined 5×3 linear system is

$$\boldsymbol{Ax} = \begin{bmatrix} 1 & -1.0 & 1.0 \\ 1 & -0.5 & 0.25 \\ 1 & 0.0 & 0.0 \\ 1 & 0.5 & 0.25 \\ 1 & 1.0 & 1.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \cong \begin{bmatrix} 1.0 \\ 0.5 \\ 0.0 \\ 0.5 \\ 2.0 \end{bmatrix} = \boldsymbol{b}$$

- Solution, which we will see later how to compute, is

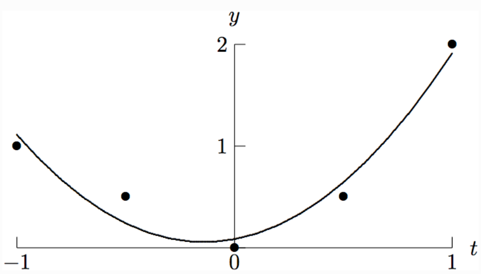
$$\boldsymbol{x} = \begin{bmatrix} 0.086 & 0.40 & 1.4 \end{bmatrix}^T$$

  so approximating polynomial is

$$p(t) = 0.086 + 0.4t + 1.4t^2$$

Example, continued

- Resulting curve and original data points are shown in graph



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Existence and Uniqueness

- Linear least squares problem $\boldsymbol{Ax} \cong \boldsymbol{b}$ *always* has solution
- Solution is *unique* if, and only if, columns of $\boldsymbol{A}$ are *linearly independent*, i.e., $\operatorname{rank}(\boldsymbol{A}) = n$, where $\boldsymbol{A}$ is $m \times n$
- If $\operatorname{rank}(\boldsymbol{A}) < n$, then $\boldsymbol{A}$ is *rank-deficient*, and solution of linear least squares problem is not unique
- For now, we assume $\boldsymbol{A}$ has full column rank n

Normal Equations

- To minimize squared Euclidean norm of residual vector

$$\begin{aligned}\|\boldsymbol{r}\|_2^2 &= \boldsymbol{r}^T\boldsymbol{r} = (\boldsymbol{b} - \boldsymbol{Ax})^T(\boldsymbol{b} - \boldsymbol{Ax}) \\ &= \boldsymbol{b}^T\boldsymbol{b} - 2\boldsymbol{x}^T\boldsymbol{A}^T\boldsymbol{b} + \boldsymbol{x}^T\boldsymbol{A}^T\boldsymbol{Ax}\end{aligned}$$

take derivative with respect to $\boldsymbol{x}$ and set it to $\boldsymbol{0}$,

$$2\boldsymbol{A}^T\boldsymbol{Ax} - 2\boldsymbol{A}^T\boldsymbol{b} = \boldsymbol{0}$$

which reduces to $n \times n$ linear system of *normal equations*

$$\boldsymbol{A}^T\boldsymbol{Ax} = \boldsymbol{A}^T\boldsymbol{b}$$

Orthogonality

- Vectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ are *orthogonal* if their inner product is zero, $\boldsymbol{v}_1^T\boldsymbol{v}_2 = 0$
- Space spanned by columns of $m \times n$ matrix $\boldsymbol{A}$, $\operatorname{span}(\boldsymbol{A}) = \{\boldsymbol{Ax} : \boldsymbol{x} \in \mathbb{R}^n\}$, is of dimension at most n
- If $m > n$, $\boldsymbol{b}$ generally does not lie in $\operatorname{span}(\boldsymbol{A})$, so there is no exact solution to $\boldsymbol{Ax} = \boldsymbol{b}$
- Vector $\boldsymbol{y} = \boldsymbol{Ax}$ in $\operatorname{span}(\boldsymbol{A})$ closest to $\boldsymbol{b}$ in 2-norm occurs when residual $\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{Ax}$ is *orthogonal* to $\operatorname{span}(\boldsymbol{A})$,

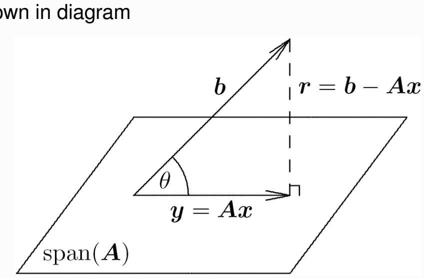
$$\boldsymbol{0} = \boldsymbol{A}^T\boldsymbol{r} = \boldsymbol{A}^T(\boldsymbol{b} - \boldsymbol{Ax})$$

again giving system of *normal equations*

$$\boldsymbol{A}^T\boldsymbol{Ax} = \boldsymbol{A}^T\boldsymbol{b}$$

Orthogonality, continued

- Geometric relationships among $\boldsymbol{b}$, $\boldsymbol{r}$, and $\operatorname{span}(\boldsymbol{A})$ are shown in diagram



Orthogonal Projectors

- Matrix $\boldsymbol{P}$ is *orthogonal projector* if it is *idempotent* ($\boldsymbol{P}^2 = \boldsymbol{P}$) and *symmetric* ($\boldsymbol{P}^T = \boldsymbol{P}$)
- Orthogonal projector onto orthogonal complement $\operatorname{span}(\boldsymbol{P})^\perp$ is given by $\boldsymbol{P}_\perp = \boldsymbol{I} - \boldsymbol{P}$
- For any vector $\boldsymbol{v}$,

$$\boldsymbol{v} = (\boldsymbol{P} + (\boldsymbol{I} - \boldsymbol{P}))\,\boldsymbol{v} = \boldsymbol{Pv} + \boldsymbol{P}_\perp\boldsymbol{v}$$

- For least squares problem $\boldsymbol{Ax} \cong \boldsymbol{b}$, if $\operatorname{rank}(\boldsymbol{A}) = n$, then

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

is orthogonal projector onto $\operatorname{span}(\boldsymbol{A})$, and

$$\boldsymbol{b} = \boldsymbol{Pb} + \boldsymbol{P}_\perp\boldsymbol{b} = \boldsymbol{Ax} + (\boldsymbol{b} - \boldsymbol{Ax}) = \boldsymbol{y} + \boldsymbol{r}$$

Pseudoinverse and Condition Number

- Nonsquare $m \times n$ matrix $\boldsymbol{A}$ has no inverse in usual sense
- If $\operatorname{rank}(\boldsymbol{A}) = n$, *pseudoinverse* is defined by

$$\boldsymbol{A}^+ = (\boldsymbol{A}^T\boldsymbol{A})^{-1}\boldsymbol{A}^T$$

and condition number by

$$\operatorname{cond}(\boldsymbol{A}) = \|\boldsymbol{A}\|_2 \cdot \|\boldsymbol{A}^+\|_2$$

- By convention, $\operatorname{cond}(\boldsymbol{A}) = \infty$ if $\operatorname{rank}(\boldsymbol{A}) < n$
- Just as condition number of square matrix measures closeness to singularity, condition number of rectangular matrix measures closeness to rank deficiency
- Least squares solution of $\boldsymbol{Ax} \cong \boldsymbol{b}$ is given by $\boldsymbol{x} = \boldsymbol{A}^+\boldsymbol{b}$

Sensitivity and Conditioning

- Sensitivity of least squares solution to $\boldsymbol{Ax} \cong \boldsymbol{b}$ depends on $\boldsymbol{b}$ as well as $\boldsymbol{A}$
- Define angle θ between $\boldsymbol{b}$ and $\boldsymbol{y} = \boldsymbol{Ax}$ by

$$\cos(\theta) = \frac{\|\boldsymbol{y}\|_2}{\|\boldsymbol{b}\|_2} = \frac{\|\boldsymbol{Ax}\|_2}{\|\boldsymbol{b}\|_2}$$

- Bound on perturbation $\Delta\boldsymbol{x}$ in solution $\boldsymbol{x}$ due to perturbation $\Delta\boldsymbol{b}$ in $\boldsymbol{b}$ is given by

$$\frac{\|\Delta\boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} \le \operatorname{cond}(\boldsymbol{A})\,\frac{1}{\cos(\theta)}\,\frac{\|\Delta\boldsymbol{b}\|_2}{\|\boldsymbol{b}\|_2}$$

Sensitivity and Conditioning, contnued

- Similarly, for perturbation $\boldsymbol{E}$ in matrix $\boldsymbol{A}$,

$$\frac{\|\Delta \boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} \lessapprox \left([\mathrm{cond}(\boldsymbol{A})]^2 \tan(\theta) + \mathrm{cond}(\boldsymbol{A})\right) \frac{\|\boldsymbol{E}\|_2}{\|\boldsymbol{A}\|_2}$$

- Condition number of least squares solution is about $\mathrm{cond}(\boldsymbol{A})$ if residual is small, but can be squared or arbitrarily worse for large residual

Normal Equations Method

- If $m \times n$ matrix $\boldsymbol{A}$ has rank n, then symmetric $n \times n$ matrix $\boldsymbol{A}^T\boldsymbol{A}$ is positive definite, so its Cholesky factorization

$$\boldsymbol{A}^T\boldsymbol{A} = \boldsymbol{L}\boldsymbol{L}^T$$

can be used to obtain solution $\boldsymbol{x}$ to system of normal equations

$$\boldsymbol{A}^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{A}^T\boldsymbol{b}$$

which has same solution as linear least squares problem $\boldsymbol{A}\boldsymbol{x} \cong \boldsymbol{b}$

- Normal equations method involves transformations

rectangular $\longrightarrow$ square $\longrightarrow$ triangular

Example: Normal Equations Method

- For polynomial data-fitting example given previously, normal equations method gives

$$\boldsymbol{A}^T\boldsymbol{A} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ -1.0 & -0.5 & 0.0 & 0.5 & 1.0 \\ 1.0 & 0.25 & 0.0 & 0.25 & 1.0 \end{bmatrix} \begin{bmatrix} 1 & -1.0 & 1.0 \\ 1 & -0.5 & 0.25 \\ 1 & 0.0 & 0.0 \\ 1 & 0.5 & 0.25 \\ 1 & 1.0 & 1.0 \end{bmatrix} = \begin{bmatrix} 5.0 & 0.0 & 2.5 \\ 0.0 & 2.5 & 0.0 \\ 2.5 & 0.0 & 2.125 \end{bmatrix},$$

$$\boldsymbol{A}^T\boldsymbol{b} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ -1.0 & -0.5 & 0.0 & 0.5 & 1.0 \\ 1.0 & 0.25 & 0.0 & 0.25 & 1.0 \end{bmatrix} \begin{bmatrix} 1.0 \\ 0.5 \\ 0.0 \\ 0.5 \\ 2.0 \end{bmatrix} = \begin{bmatrix} 4.0 \\ 1.0 \\ 3.25 \end{bmatrix}$$

Example, continued

- Cholesky factorization of symmetric positive definite matrix $\boldsymbol{A}^T\boldsymbol{A}$ gives

$$\boldsymbol{A}^T\boldsymbol{A} = \begin{bmatrix} 5.0 & 0.0 & 2.5 \\ 0.0 & 2.5 & 0.0 \\ 2.5 & 0.0 & 2.125 \end{bmatrix} = \begin{bmatrix} 2.236 & 0 & 0 \\ 0 & 1.581 & 0 \\ 1.118 & 0 & 0.935 \end{bmatrix} \begin{bmatrix} 2.236 & 0 & 1.118 \\ 0 & 1.581 & 0 \\ 0 & 0 & 0.935 \end{bmatrix} = \boldsymbol{L}\boldsymbol{L}^T$$

- Solving lower triangular system $\boldsymbol{L}\boldsymbol{z} = \boldsymbol{A}^T\boldsymbol{b}$ by forward-substitution gives $\boldsymbol{z} = \begin{bmatrix} 1.789 & 0.632 & 1.336 \end{bmatrix}^T$
- Solving upper triangular system $\boldsymbol{L}^T\boldsymbol{x} = \boldsymbol{z}$ by back-substitution gives $\boldsymbol{x} = \begin{bmatrix} 0.086 & 0.400 & 1.429 \end{bmatrix}^T$

Shortcomings of Normal Equations

- Information can be lost in forming $\boldsymbol{A}^T\boldsymbol{A}$ and $\boldsymbol{A}^T\boldsymbol{b}$
- For example, take

$$\boldsymbol{A} = \begin{bmatrix} 1 & 1 \\ \epsilon & 0 \\ 0 & \epsilon \end{bmatrix}$$

where ϵ is positive number smaller than $\sqrt{\epsilon_{\text{mach}}}$
- Then in floating-point arithmetic

$$\boldsymbol{A}^T\boldsymbol{A} = \begin{bmatrix} 1+\epsilon^2 & 1 \\ 1 & 1+\epsilon^2 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

which is singular
- Sensitivity of solution is also worsened, since

$$\mathrm{cond}(\boldsymbol{A}^T\boldsymbol{A}) = [\mathrm{cond}(\boldsymbol{A})]^2$$

Augmented System Method

- Definition of residual together with orthogonality requirement give $(m+n) \times (m+n)$ augmented system

$$\begin{bmatrix} \boldsymbol{I} & \boldsymbol{A} \\ \boldsymbol{A}^T & \boldsymbol{O} \end{bmatrix} \begin{bmatrix} \boldsymbol{r} \\ \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix}$$

- Augmented system is not positive definite, is larger than original system, and requires storing two copies of $\boldsymbol{A}$
- But it allows greater freedom in choosing pivots in computing $\boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^T$ or $\boldsymbol{L}\boldsymbol{U}$ factorization

Augmented System Method, continued

- Introducing scaling parameter α gives system

$$\begin{bmatrix} \alpha\boldsymbol{I} & \boldsymbol{A} \\ \boldsymbol{A}^T & \boldsymbol{O} \end{bmatrix} \begin{bmatrix} \boldsymbol{r}/\alpha \\ \boldsymbol{x} \end{bmatrix} = \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix}$$

which allows control over relative weights of two subsystems in choosing pivots
- Reasonable rule of thumb is to take

$$\alpha = \max_{i,j} |a_{ij}|/1000$$

- Augmented system is sometimes useful, but is far from ideal in work and storage required

Orthogonal Transformations

- We seek alternative method that avoids numerical difficulties of normal equations
- We need numerically robust transformation that produces easier problem without changing solution
- What kind of transformation leaves least squares solution unchanged?
- Square matrix $\boldsymbol{Q}$ is *orthogonal* if $\boldsymbol{Q}^T\boldsymbol{Q} = \boldsymbol{I}$
- Multiplication of vector by orthogonal matrix preserves Euclidean norm

$$\|\boldsymbol{Q}\boldsymbol{v}\|_2^2 = (\boldsymbol{Q}\boldsymbol{v})^T\boldsymbol{Q}\boldsymbol{v} = \boldsymbol{v}^T\boldsymbol{Q}^T\boldsymbol{Q}\boldsymbol{v} = \boldsymbol{v}^T\boldsymbol{v} = \|\boldsymbol{v}\|_2^2$$

- Thus, multiplying both sides of least squares problem by orthogonal matrix does not change its solution

Triangular Least Squares Problems

- As with square linear systems, suitable target in simplifying least squares problems is triangular form
- Upper triangular overdetermined ($m > n$) least squares problem has form
$$\begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix} \boldsymbol{x} \cong \begin{bmatrix} \boldsymbol{b}_1 \\ \boldsymbol{b}_2 \end{bmatrix}$$
where $\boldsymbol{R}$ is $n \times n$ upper triangular and $\boldsymbol{b}$ is partitioned similarly
- Residual is
$$\|\boldsymbol{r}\|_2^2 = \|\boldsymbol{b}_1 - \boldsymbol{R}\boldsymbol{x}\|_2^2 + \|\boldsymbol{b}_2\|_2^2$$

Triangular Least Squares Problems, continued

- We have no control over second term, $\|\boldsymbol{b}_2\|_2^2$, but first term becomes zero if $\boldsymbol{x}$ satisfies $n \times n$ triangular system
$$\boldsymbol{R}\boldsymbol{x} = \boldsymbol{b}_1$$
which can be solved by back-substitution
- Resulting $\boldsymbol{x}$ is least squares solution, and minimum sum of squares is
$$\|\boldsymbol{r}\|_2^2 = \|\boldsymbol{b}_2\|_2^2$$
- So our strategy is to transform general least squares problem to triangular form using orthogonal transformation so that least squares solution is preserved

QR Factorization

- Given $m \times n$ matrix $\boldsymbol{A}$, with $m > n$, we seek $m \times m$ orthogonal matrix $\boldsymbol{Q}$ such that
$$\boldsymbol{A} = \boldsymbol{Q} \begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix}$$
where $\boldsymbol{R}$ is $n \times n$ and upper triangular
- Linear least squares problem $\boldsymbol{A}\boldsymbol{x} \cong \boldsymbol{b}$ is then transformed into triangular least squares problem
$$\boldsymbol{Q}^T\boldsymbol{A}\boldsymbol{x} = \begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix} \boldsymbol{x} \cong \begin{bmatrix} \boldsymbol{c}_1 \\ \boldsymbol{c}_2 \end{bmatrix} = \boldsymbol{Q}^T\boldsymbol{b}$$
which has same solution, since
$$\|\boldsymbol{r}\|_2^2 = \|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}\|_2^2 = \|\boldsymbol{b} - \boldsymbol{Q}\begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix}\boldsymbol{x}\|_2^2 = \|\boldsymbol{Q}^T\boldsymbol{b} - \begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix}\boldsymbol{x}\|_2^2$$

Orthogonal Bases

- If we partition $m \times m$ orthogonal matrix $\boldsymbol{Q} = [\boldsymbol{Q}_1 \; \boldsymbol{Q}_2]$, where $\boldsymbol{Q}_1$ is $m \times n$, then
$$\boldsymbol{A} = \boldsymbol{Q}\begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix} = [\boldsymbol{Q}_1 \; \boldsymbol{Q}_2]\begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix} = \boldsymbol{Q}_1\boldsymbol{R}$$
is called *reduced* QR factorization of $\boldsymbol{A}$
- Columns of $\boldsymbol{Q}_1$ are orthonormal basis for span($\boldsymbol{A}$), and columns of $\boldsymbol{Q}_2$ are orthonormal basis for span$(\boldsymbol{A})^\perp$
- $\boldsymbol{Q}_1\boldsymbol{Q}_1^T$ is orthogonal projector onto span($\boldsymbol{A}$)
- Solution to least squares problem $\boldsymbol{A}\boldsymbol{x} \cong \boldsymbol{b}$ is given by solution to square system
$$\boldsymbol{Q}_1^T\boldsymbol{A}\boldsymbol{x} = \boldsymbol{R}\boldsymbol{x} = \boldsymbol{c}_1 = \boldsymbol{Q}_1^T\boldsymbol{b}$$

Computing QR Factorization

- To compute QR factorization of $m \times n$ matrix $\boldsymbol{A}$, with $m > n$, we annihilate subdiagonal entries of successive columns of $\boldsymbol{A}$, eventually reaching upper triangular form
- Similar to LU factorization by Gaussian elimination, but use orthogonal transformations instead of elementary elimination matrices
- Possible methods include
  - Householder transformations
  - Givens rotations
  - Gram-Schmidt orthogonalization

Householder Transformations

- *Householder transformation* has form
$$\boldsymbol{H} = \boldsymbol{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}$$
for nonzero vector $\boldsymbol{v}$
- $\boldsymbol{H}$ is orthogonal and symmetric: $\boldsymbol{H} = \boldsymbol{H}^T = \boldsymbol{H}^{-1}$
- Given vector $\boldsymbol{a}$, we want to choose $\boldsymbol{v}$ so that
$$\boldsymbol{H}\boldsymbol{a} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha\boldsymbol{e}_1$$
- Substituting into formula for $\boldsymbol{H}$, we can take
$$\boldsymbol{v} = \boldsymbol{a} - \alpha\boldsymbol{e}_1$$
and $\alpha = \pm\|\boldsymbol{a}\|_2$, with sign chosen to avoid cancellation

Example: Householder Transformation

- If $\boldsymbol{a} = \begin{bmatrix} 2 & 1 & 2 \end{bmatrix}^T$, then we take
$$\boldsymbol{v} = \boldsymbol{a} - \alpha\boldsymbol{e}_1 = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \alpha\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \begin{bmatrix} \alpha \\ 0 \\ 0 \end{bmatrix}$$
where $\alpha = \pm\|\boldsymbol{a}\|_2 = \pm 3$
- Since a_1 is positive, we choose negative sign for α to avoid cancellation, so $\boldsymbol{v} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix}$
- To confirm that transformation works,
$$\boldsymbol{H}\boldsymbol{a} = \boldsymbol{a} - 2\frac{\boldsymbol{v}^T\boldsymbol{a}}{\boldsymbol{v}^T\boldsymbol{v}}\boldsymbol{v} = \begin{bmatrix} 2 \\ 1 \\ 2 \end{bmatrix} - 2\,\frac{15}{30}\begin{bmatrix} 5 \\ 1 \\ 2 \end{bmatrix} = \begin{bmatrix} -3 \\ 0 \\ 0 \end{bmatrix}$$

< interactive example >

Householder QR Factorization

- To compute QR factorization of $\boldsymbol{A}$, use Householder transformations to annihilate subdiagonal entries of each successive column
- Each Householder transformation is applied to entire matrix, but does not affect prior columns, so zeros are preserved
- In applying Householder transformation $\boldsymbol{H}$ to arbitrary vector $\boldsymbol{u}$,
$$\boldsymbol{H}\boldsymbol{u} = \left(\boldsymbol{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}\right)\boldsymbol{u} = \boldsymbol{u} - \left(2\frac{\boldsymbol{v}^T\boldsymbol{u}}{\boldsymbol{v}^T\boldsymbol{v}}\right)\boldsymbol{v}$$
which is much cheaper than general matrix-vector multiplication and requires only vector $\boldsymbol{v}$, not full matrix $\boldsymbol{H}$

Householder QR Factorization, continued

- Process just described produces factorization

$$H_n \cdots H_1 A = \begin{bmatrix} R \\ O \end{bmatrix}$$

where R is $n \times n$ and upper triangular

- If $Q = H_1 \cdots H_n$, then $A = Q \begin{bmatrix} R \\ O \end{bmatrix}$
- To preserve solution of linear least squares problem, right-hand side b is transformed by same sequence of Householder transformations
- Then solve triangular least squares problem $\begin{bmatrix} R \\ O \end{bmatrix} x \cong Q^T b$

Householder QR Factorization, continued

- For solving linear least squares problem, product Q of Householder transformations need not be formed explicitly
- R can be stored in upper triangle of array initially containing A
- Householder vectors v can be stored in (now zero) lower triangular portion of A (almost)
- Householder transformations most easily applied in this form anyway

Example: Householder QR Factorization

- For polynomial data-fitting example given previously, with

$$A = \begin{bmatrix} 1 & -1.0 & 1.0 \\ 1 & -0.5 & 0.25 \\ 1 & 0.0 & 0.0 \\ 1 & 0.5 & 0.25 \\ 1 & 1.0 & 1.0 \end{bmatrix}, \quad b = \begin{bmatrix} 1.0 \\ 0.5 \\ 0.0 \\ 0.5 \\ 2.0 \end{bmatrix}$$

- Householder vector v_1 for annihilating subdiagonal entries of first column of A is

$$v_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} -2.236 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 3.236 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Example, continued

- Applying resulting Householder transformation H_1 yields transformed matrix and right-hand side

$$H_1 A = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & -0.191 & -0.405 \\ 0 & 0.309 & -0.655 \\ 0 & 0.809 & -0.405 \\ 0 & 1.309 & 0.345 \end{bmatrix}, \quad H_1 b = \begin{bmatrix} -1.789 \\ -0.362 \\ -0.862 \\ -0.362 \\ 1.138 \end{bmatrix}$$

- Householder vector v_2 for annihilating subdiagonal entries of second column of $H_1 A$ is

$$v_2 = \begin{bmatrix} 0 \\ -0.191 \\ 0.309 \\ 0.809 \\ 1.309 \end{bmatrix} - \begin{bmatrix} 0 \\ 1.581 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -1.772 \\ 0.309 \\ 0.809 \\ 1.309 \end{bmatrix}$$

Example, continued

- Applying resulting Householder transformation H_2 yields

$$H_2 H_1 A = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & 1.581 & 0 \\ 0 & 0 & -0.725 \\ 0 & 0 & -0.589 \\ 0 & 0 & 0.047 \end{bmatrix}, \quad H_2 H_1 b = \begin{bmatrix} -1.789 \\ 0.632 \\ -1.035 \\ -0.816 \\ 0.404 \end{bmatrix}$$

- Householder vector v_3 for annihilating subdiagonal entries of third column of $H_2 H_1 A$ is

$$v_3 = \begin{bmatrix} 0 \\ 0 \\ -0.725 \\ -0.589 \\ 0.047 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0.935 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -1.660 \\ -0.589 \\ 0.047 \end{bmatrix}$$

Example, continued

- Applying resulting Householder transformation H_3 yields

$$H_3 H_2 H_1 A = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & 1.581 & 0 \\ 0 & 0 & 0.935 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad H_3 H_2 H_1 b = \begin{bmatrix} -1.789 \\ 0.632 \\ 1.336 \\ 0.026 \\ 0.337 \end{bmatrix}$$

- Now solve upper triangular system $Rx = c_1$ by back-substitution to obtain $x = \begin{bmatrix} 0.086 & 0.400 & 1.429 \end{bmatrix}^T$

< interactive example >

Givens Rotations

- *Givens rotations* introduce zeros one at a time
- Given vector $\begin{bmatrix} a_1 & a_2 \end{bmatrix}^T$, choose scalars c and s so that

$$\boxed{\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}}$$

with $c^2 + s^2 = 1$, or equivalently, $\alpha = \sqrt{a_1^2 + a_2^2}$

- Previous equation can be rewritten

$$\begin{bmatrix} a_1 & a_2 \\ a_2 & -a_1 \end{bmatrix} \begin{bmatrix} c \\ s \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}$$

- Gaussian elimination yields triangular system

$$\begin{bmatrix} a_1 & a_2 \\ 0 & -a_1 - a_2^2/a_1 \end{bmatrix} \begin{bmatrix} c \\ s \end{bmatrix} = \begin{bmatrix} \alpha \\ -\alpha a_2/a_1 \end{bmatrix}$$

Givens Rotations, continued

- Back-substitution then gives

$$s = \frac{\alpha a_2}{a_1^2 + a_2^2} \quad \text{and} \quad c = \frac{\alpha a_1}{a_1^2 + a_2^2}$$

- Finally, $c^2 + s^2 = 1$, or $\alpha = \sqrt{a_1^2 + a_2^2}$, implies

$$\boxed{c = \frac{a_1}{\sqrt{a_1^2 + a_2^2}}} \quad \text{and} \quad \boxed{s = \frac{a_2}{\sqrt{a_1^2 + a_2^2}}}$$

Example: Givens Rotation

- Let $\boldsymbol{a} = \begin{bmatrix} 4 & 3 \end{bmatrix}^T$
- To annihilate second entry we compute cosine and sine

$$c = \frac{a_1}{\sqrt{a_1^2 + a_2^2}} = \frac{4}{5} = 0.8 \quad \text{and} \quad s = \frac{a_2}{\sqrt{a_1^2 + a_2^2}} = \frac{3}{5} = 0.6$$

- Rotation is then given by

$$\boldsymbol{G} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} = \begin{bmatrix} 0.8 & 0.6 \\ -0.6 & 0.8 \end{bmatrix}$$

- To confirm that rotation works,

$$\boldsymbol{G}\boldsymbol{a} = \begin{bmatrix} 0.8 & 0.6 \\ -0.6 & 0.8 \end{bmatrix} \begin{bmatrix} 4 \\ 3 \end{bmatrix} = \begin{bmatrix} 5 \\ 0 \end{bmatrix}$$

Givens QR Factorization

- More generally, to annihilate selected component of vector in n dimensions, rotate target component with another component

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & c & 0 & s & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -s & 0 & c & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} = \begin{bmatrix} a_1 \\ \alpha \\ a_3 \\ 0 \\ a_5 \end{bmatrix}$$

- By systematically annihilating successive entries, we can reduce matrix to upper triangular form using sequence of Givens rotations
- Each rotation is orthogonal, so their product is orthogonal, producing QR factorization

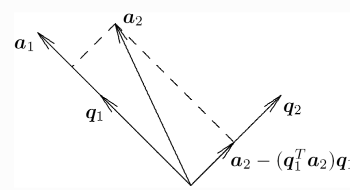
Givens QR Factorization

- Straightforward implementation of Givens method requires about 50% more work than Householder method, and also requires more storage, since each rotation requires two numbers, c and s, to define it
- These disadvantages can be overcome, but requires more complicated implementation
- Givens can be advantageous for computing QR factorization when many entries of matrix are already zero, since those annihilations can then be skipped

< interactive example >

Gram-Schmidt Orthogonalization

- Given vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$, we seek orthonormal vectors $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ having same span
- This can be accomplished by subtracting from second vector its projection onto first vector and normalizing both resulting vectors, as shown in diagram



< interactive example >

Gram-Schmidt Orthogonalization

- Process can be extended to any number of vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_k$, orthogonalizing each successive vector against all preceding ones, giving *classical Gram-Schmidt* procedure

for $k = 1$ **to** n
  $\boldsymbol{q}_k = \boldsymbol{a}_k$
  for $j = 1$ **to** $k - 1$
    $r_{jk} = \boldsymbol{q}_j^T \boldsymbol{a}_k$
    $\boldsymbol{q}_k = \boldsymbol{q}_k - r_{jk}\boldsymbol{q}_j$
  end
  $r_{kk} = \|\boldsymbol{q}_k\|_2$
  $\boldsymbol{q}_k = \boldsymbol{q}_k / r_{kk}$
end

- Resulting $\boldsymbol{q}_k$ and r_{jk} form reduced QR factorization of $\boldsymbol{A}$

Modified Gram-Schmidt

- Classical Gram-Schmidt procedure often suffers loss of orthogonality in finite-precision
- Also, separate storage is required for $\boldsymbol{A}$, $\boldsymbol{Q}$, and $\boldsymbol{R}$, since original $\boldsymbol{a}_k$ are needed in inner loop, so $\boldsymbol{q}_k$ cannot overwrite columns of $\boldsymbol{A}$
- Both deficiencies are improved by *modified Gram-Schmidt* procedure, with each vector orthogonalized in turn against all *subsequent* vectors, so $\boldsymbol{q}_k$ can overwrite $\boldsymbol{a}_k$

Modified Gram-Schmidt QR Factorization

- Modified Gram-Schmidt algorithm

for $k = 1$ **to** n
  $r_{kk} = \|\boldsymbol{a}_k\|_2$
  $\boldsymbol{q}_k = \boldsymbol{a}_k / r_{kk}$
  for $j = k + 1$ **to** n
    $r_{kj} = \boldsymbol{q}_k^T \boldsymbol{a}_j$
    $\boldsymbol{a}_j = \boldsymbol{a}_j - r_{kj}\boldsymbol{q}_k$
  end
end

< interactive example >

Rank Deficiency

- If $\operatorname{rank}(\boldsymbol{A}) < n$, then QR factorization still exists, but yields singular upper triangular factor $\boldsymbol{R}$, and multiple vectors $\boldsymbol{x}$ give minimum residual norm
- Common practice selects minimum residual solution $\boldsymbol{x}$ having smallest norm
- Can be computed by QR factorization with column pivoting or by singular value decomposition (SVD)
- Rank of matrix is often not clear cut in practice, so relative tolerance is used to determine rank

Example: Near Rank Deficiency

- Consider 3×2 matrix

$$A = \begin{bmatrix} 0.641 & 0.242 \\ 0.321 & 0.121 \\ 0.962 & 0.363 \end{bmatrix}$$

- Computing QR factorization,

$$R = \begin{bmatrix} 1.1997 & 0.4527 \\ 0 & 0.0002 \end{bmatrix}$$

- R is extremely close to singular (exactly singular to 3-digit accuracy of problem statement)
- If R is used to solve linear least squares problem, result is highly sensitive to perturbations in right-hand side
- For practical purposes, $\text{rank}(A) = 1$ rather than 2, because columns are nearly linearly dependent

QR with Column Pivoting

- Instead of processing columns in natural order, select for reduction at each stage column of remaining unreduced submatrix having maximum Euclidean norm
- If $\text{rank}(A) = k < n$, then after k steps, norms of remaining unreduced columns will be zero (or "negligible" in finite-precision arithmetic) below row k
- Yields orthogonal factorization of form

$$Q^T A P = \begin{bmatrix} R & S \\ O & O \end{bmatrix}$$

where R is $k \times k$, upper triangular, and nonsingular, and permutation matrix P performs column interchanges

QR with Column Pivoting, continued

- *Basic solution* to least squares problem $Ax \cong b$ can now be computed by solving triangular system $Rz = c_1$, where c_1 contains first k components of $Q^T b$, and then taking

$$x = P \begin{bmatrix} z \\ 0 \end{bmatrix}$$

- *Minimum-norm solution* can be computed, if desired, at expense of additional processing to annihilate S
- $\text{rank}(A)$ is usually unknown, so rank is determined by monitoring norms of remaining unreduced columns and terminating factorization when maximum value falls below chosen tolerance

< interactive example >

Singular Value Decomposition

- Singular value decomposition (SVD) of $m \times n$ matrix A has form

$$A = U \Sigma V^T$$

where U is $m \times m$ orthogonal matrix, V is $n \times n$ orthogonal matrix, and Σ is $m \times n$ diagonal matrix, with

$$\sigma_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ \sigma_i \geq 0 & \text{for } i = j \end{cases}$$

- Diagonal entries σ_i, called *singular values* of A, are usually ordered so that $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$
- Columns u_i of U and v_i of V are called left and right *singular vectors*

Example: SVD

- SVD of $A = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{bmatrix}$ is given by $U\Sigma V^T =$

$$\begin{bmatrix} .141 & .825 & -.420 & -.351 \\ .344 & .426 & .298 & .782 \\ .547 & .0278 & .664 & -.509 \\ .750 & -.371 & -.542 & .0790 \end{bmatrix} \begin{bmatrix} 25.5 & 0 & 0 \\ 0 & 1.29 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} .504 & .574 & .644 \\ -.761 & -.057 & .646 \\ .408 & -.816 & .408 \end{bmatrix}$$

< interactive example >

Applications of SVD

- *Minimum norm solution* to $Ax \cong b$ is given by

$$x = \sum_{\sigma_i \neq 0} \frac{u_i^T b}{\sigma_i} v_i$$

For ill-conditioned or rank deficient problems, "small" singular values can be omitted from summation to stabilize solution

- *Euclidean matrix norm*: $\|A\|_2 = \sigma_{\max}$
- *Euclidean condition number of matrix*: $\text{cond}(A) = \dfrac{\sigma_{\max}}{\sigma_{\min}}$
- *Rank of matrix*: number of nonzero singular values

Pseudoinverse

- Define pseudoinverse of scalar σ to be $1/\sigma$ if $\sigma \neq 0$, zero otherwise
- Define pseudoinverse of (possibly rectangular) diagonal matrix by transposing and taking scalar pseudoinverse of each entry
- Then *pseudoinverse* of general real $m \times n$ matrix A is given by

$$A^+ = V \Sigma^+ U^T$$

- Pseudoinverse always exists whether or not matrix is square or has full rank
- If A is square and nonsingular, then $A^+ = A^{-1}$
- In all cases, minimum-norm solution to $Ax \cong b$ is given by $x = A^+ b$

Orthogonal Bases

- SVD of matrix, $A = U\Sigma V^T$, provides orthogonal bases for subspaces relevant to A
- Columns of U corresponding to nonzero singular values form orthonormal basis for span(A)
- Remaining columns of U form orthonormal basis for orthogonal complement span$(A)^\perp$
- Columns of V corresponding to zero singular values form orthonormal basis for null space of A
- Remaining columns of V form orthonormal basis for orthogonal complement of null space of A

Lower-Rank Matrix Approximation

- Another way to write SVD is
$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T = \sigma_1 \boldsymbol{E}_1 + \sigma_2 \boldsymbol{E}_2 + \cdots + \sigma_n \boldsymbol{E}_n$$
with $\boldsymbol{E}_i = \boldsymbol{u}_i \boldsymbol{v}_i^T$
- $\boldsymbol{E}_i$ has rank 1 and can be stored using only $m+n$ storage locations
- Product $\boldsymbol{E}_i \boldsymbol{x}$ can be computed using only $m+n$ multiplications
- Condensed approximation to $\boldsymbol{A}$ is obtained by omitting from summation terms corresponding to small singular values
- Approximation using k largest singular values is closest matrix of rank k to $\boldsymbol{A}$
- Approximation is useful in image processing, data compression, information retrieval, cryptography, etc.

< interactive example >

Total Least Squares

- Ordinary least squares is applicable when right-hand side $\boldsymbol{b}$ is subject to random error but matrix $\boldsymbol{A}$ is known accurately
- When all data, including $\boldsymbol{A}$, are subject to error, then total least squares is more appropriate
- Total least squares minimizes orthogonal distances, rather than vertical distances, between model and data
- Total least squares solution can be computed from SVD of $[\boldsymbol{A}, \boldsymbol{b}]$

Comparison of Methods

- Forming normal equations matrix $\boldsymbol{A}^T\boldsymbol{A}$ requires about $n^2m/2$ multiplications, and solving resulting symmetric linear system requires about $n^3/6$ multiplications
- Solving least squares problem using Householder QR factorization requires about $mn^2 - n^3/3$ multiplications
- If $m \approx n$, both methods require about same amount of work
- If $m \gg n$, Householder QR requires about twice as much work as normal equations
- Cost of SVD is proportional to $mn^2 + n^3$, with proportionality constant ranging from 4 to 10, depending on algorithm used

Comparison of Methods, continued

- Normal equations method produces solution whose relative error is proportional to $[\mathrm{cond}(\boldsymbol{A})]^2$
- Required Cholesky factorization can be expected to break down if $\mathrm{cond}(\boldsymbol{A}) \approx 1/\sqrt{\epsilon_{\text{mach}}}$ or worse
- Householder method produces solution whose relative error is proportional to
$$\mathrm{cond}(\boldsymbol{A}) + \|\boldsymbol{r}\|_2 \, [\mathrm{cond}(\boldsymbol{A})]^2$$
which is best possible, since this is inherent sensitivity of solution to least squares problem
- Householder method can be expected to break down (in back-substitution phase) only if $\mathrm{cond}(\boldsymbol{A}) \approx 1/\epsilon_{\text{mach}}$ or worse

Comparison of Methods, continued

- Householder is more accurate and more broadly applicable than normal equations
- These advantages may not be worth additional cost, however, when problem is sufficiently well conditioned that normal equations provide sufficient accuracy
- For rank-deficient or nearly rank-deficient problems, Householder with column pivoting can produce useful solution when normal equations method fails outright
- SVD is even more robust and reliable than Householder, but substantially more expensive