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

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

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 $\boldsymbol{A}\boldsymbol{x} \cong \boldsymbol{b}$, 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

$$\begin{array}{c|ccccc} t & -1.0 & -0.5 & 0.0 & 0.5 & 1.0 \\ y & 1.0 & 0.5 & 0.0 & 0.5 & 2.0 \end{array}$$

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

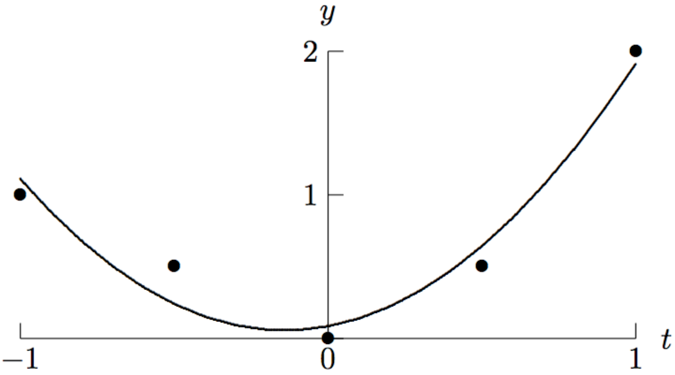
$$\boldsymbol{x} = \begin{bmatrix} 0.086 & 0.40 & 1.4 \end{bmatrix}^T$$

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., $\mathrm{rank}(\boldsymbol{A}) = n$, where $\boldsymbol{A}$ is $m \times n$
- If $\mathrm{rank}(\boldsymbol{A}) < n$, 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

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

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

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

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

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

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 $\boldsymbol{A}$, $\text{span}(\boldsymbol{A}) = \{\boldsymbol{A}\boldsymbol{x} : \boldsymbol{x} \in \mathbb{R}^n\}$, is of dimension at most n
- If $m > n$, $\boldsymbol{b}$ generally does not lie in $\text{span}(\boldsymbol{A})$, so there is no exact solution to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$
- Vector $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ in $\text{span}(\boldsymbol{A})$ closest to $\boldsymbol{b}$ in 2-norm occurs when residual $\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}$ is *orthogonal* to $\text{span}(\boldsymbol{A})$,

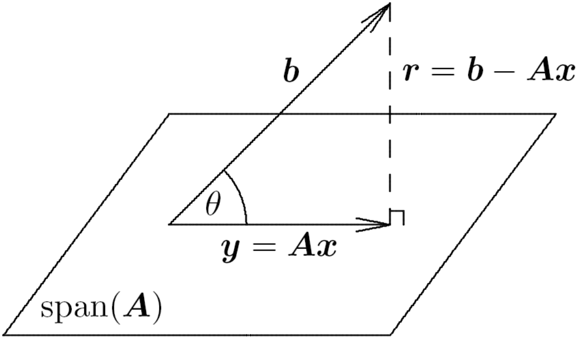
$$\boldsymbol{0} = \boldsymbol{A}^T \boldsymbol{r} = \boldsymbol{A}^T (\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x})$$

again giving system of *normal equations*

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

Orthogonality, continued

- Geometric relationships among $\boldsymbol{b}$, $\boldsymbol{r}$, and $\mathrm{span}(\boldsymbol{A})$ 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 span$(\boldsymbol{P})^\perp$ is given by $\boldsymbol{P}_\perp = \boldsymbol{I} - \boldsymbol{P}$
- For any vector $\boldsymbol{v}$,

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

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

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

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

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

Pseudoinverse and Condition Number

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

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

  and condition number by

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

- By convention, $\mathrm{cond}(\boldsymbol{A}) = \infty$ if $\mathrm{rank}(\boldsymbol{A}) < n$
- 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 $\boldsymbol{A}\boldsymbol{x} \cong \boldsymbol{b}$ 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

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

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

$$\text{rectangular} \quad \longrightarrow \quad \text{square} \quad \longrightarrow \quad \text{triangular}$$

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

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

- 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

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

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 $\boldsymbol{LDL}^T$ or $\boldsymbol{LU}$ 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 $\text{span}(\boldsymbol{A})$, and columns of $\boldsymbol{Q}_2$ are orthonormal basis for $\text{span}(\boldsymbol{A})^{\perp}$
- $\boldsymbol{Q}_1 \boldsymbol{Q}_1^T$ is orthogonal projector onto $\text{span}(\boldsymbol{A})$
- 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

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

  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

$$\boxed{\boldsymbol{v} = \boldsymbol{a} - \alpha \boldsymbol{e}_1}$$

  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

$$\boldsymbol{H}_n \cdots \boldsymbol{H}_1 \boldsymbol{A} = \begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix}$$

  where $\boldsymbol{R}$ is $n \times n$ and upper triangular

- If $\boldsymbol{Q} = \boldsymbol{H}_1 \cdots \boldsymbol{H}_n$, then $\boldsymbol{A} = \boldsymbol{Q} \begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix}$

- To preserve solution of linear least squares problem, right-hand side $\boldsymbol{b}$ is transformed by same sequence of Householder transformations

- Then solve triangular least squares problem $\begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix} \boldsymbol{x} \cong \boldsymbol{Q}^T \boldsymbol{b}$

Householder QR Factorization, continued

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

Example: Householder QR Factorization

- For polynomial data-fitting example given previously, with

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

- Householder vector $\boldsymbol{v}_1$ for annihilating subdiagonal entries of first column of $\boldsymbol{A}$ is

$$\boldsymbol{v}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} - \begin{bmatrix} -2.236 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 3.236 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

Example, continued

- Applying resulting Householder transformation $\boldsymbol{H}_1$ yields transformed matrix and right-hand side

$$\boldsymbol{H}_1\boldsymbol{A} = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & -0.191 & -0.405 \\ 0 & 0.309 & -0.655 \\ 0 & 0.809 & -0.405 \\ 0 & 1.309 & 0.345 \end{bmatrix}, \quad \boldsymbol{H}_1\boldsymbol{b} = \begin{bmatrix} -1.789 \\ -0.362 \\ -0.862 \\ -0.362 \\ 1.138 \end{bmatrix}$$

- Householder vector $\boldsymbol{v}_2$ for annihilating subdiagonal entries of second column of $\boldsymbol{H}_1\boldsymbol{A}$ is

$$\boldsymbol{v}_2 = \begin{bmatrix} 0 \\ -0.191 \\ 0.309 \\ 0.809 \\ 1.309 \end{bmatrix} - \begin{bmatrix} 0 \\ 1.581 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ -1.772 \\ 0.309 \\ 0.809 \\ 1.309 \end{bmatrix}$$

Example, continued

- Applying resulting Householder transformation $\boldsymbol{H}_2$ yields

$$\boldsymbol{H}_2\boldsymbol{H}_1\boldsymbol{A} = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & 1.581 & 0 \\ 0 & 0 & -0.725 \\ 0 & 0 & -0.589 \\ 0 & 0 & 0.047 \end{bmatrix}, \quad \boldsymbol{H}_2\boldsymbol{H}_1\boldsymbol{b} = \begin{bmatrix} -1.789 \\ 0.632 \\ -1.035 \\ -0.816 \\ 0.404 \end{bmatrix}$$

- Householder vector $\boldsymbol{v}_3$ for annihilating subdiagonal entries of third column of $\boldsymbol{H}_2\boldsymbol{H}_1\boldsymbol{A}$ is

$$\boldsymbol{v}_3 = \begin{bmatrix} 0 \\ 0 \\ -0.725 \\ -0.589 \\ 0.047 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ 0.935 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -1.660 \\ -0.589 \\ 0.047 \end{bmatrix}$$

Example, continued

- Applying resulting Householder transformation $\boldsymbol{H}_3$ yields

$$\boldsymbol{H}_3\boldsymbol{H}_2\boldsymbol{H}_1\boldsymbol{A} = \begin{bmatrix} -2.236 & 0 & -1.118 \\ 0 & 1.581 & 0 \\ 0 & 0 & 0.935 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \boldsymbol{H}_3\boldsymbol{H}_2\boldsymbol{H}_1\boldsymbol{b} = \begin{bmatrix} -1.789 \\ 0.632 \\ 1.336 \\ 0.026 \\ 0.337 \end{bmatrix}$$

- Now solve upper triangular system $\boldsymbol{R}\boldsymbol{x} = \boldsymbol{c}_1$ by back-substitution to obtain $\boldsymbol{x} = \begin{bmatrix} 0.086 & 0.400 & 1.429 \end{bmatrix}^T$

< 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

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

  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

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

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

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

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

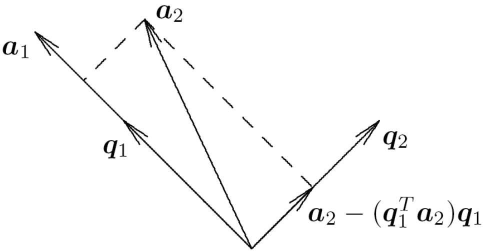
Givens QR Factorization

- 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
  $\quad \boldsymbol{q}_k = \boldsymbol{a}_k$
  $\quad$**for** $j = 1$ **to** $k - 1$
  $\quad\quad r_{jk} = \boldsymbol{q}_j^T \boldsymbol{a}_k$
  $\quad\quad \boldsymbol{q}_k = \boldsymbol{q}_k - r_{jk}\boldsymbol{q}_j$
  $\quad$**end**
  $\quad r_{kk} = \|\boldsymbol{q}_k\|_2$
  $\quad \boldsymbol{q}_k = \boldsymbol{q}_k / r_{kk}$
  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 $\mathrm{rank}(\boldsymbol{A}) < n$, 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,

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

- $\boldsymbol{R}$ is extremely close to singular (exactly singular to 3-digit accuracy of problem statement)
- If $\boldsymbol{R}$ is used to solve linear least squares problem, result is highly sensitive to perturbations in right-hand side
- For practical purposes, $\mathrm{rank}(\boldsymbol{A}) = 1$ 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 $\mathrm{rank}(\boldsymbol{A}) = k < n$, 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

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

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

QR with Column Pivoting, continued

- *Basic solution* to least squares problem $\boldsymbol{Ax} \cong \boldsymbol{b}$ can now be computed by solving triangular system $\boldsymbol{Rz} = \boldsymbol{c}_1$, where $\boldsymbol{c}_1$ contains first k components of $\boldsymbol{Q}^T\boldsymbol{b}$, and then taking

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

- *Minimum-norm solution* can be computed, if desired, at expense of additional processing to annihilate $\boldsymbol{S}$
- $\mathrm{rank}(\boldsymbol{A})$ 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 $\boldsymbol{A}$ has form

$$\boxed{\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^T}$$

where $\boldsymbol{U}$ is $m \times m$ orthogonal matrix, $\boldsymbol{V}$ is $n \times n$ orthogonal matrix, and $\boldsymbol{\Sigma}$ 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 $\boldsymbol{A}$, are usually ordered so that $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$

- Columns $\boldsymbol{u}_i$ of $\boldsymbol{U}$ and $\boldsymbol{v}_i$ of $\boldsymbol{V}$ 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 $\boldsymbol{Ax} \cong \boldsymbol{b}$ is given by

$$\boldsymbol{x} = \sum_{\sigma_i \neq 0} \frac{\boldsymbol{u}_i^T \boldsymbol{b}}{\sigma_i} \boldsymbol{v}_i$$

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

- *Euclidean matrix norm*: $\|\boldsymbol{A}\|_2 = \sigma_{\max}$

- *Euclidean condition number of matrix*: $\text{cond}(\boldsymbol{A}) = \dfrac{\sigma_{\max}}{\sigma_{\min}}$

- *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 $\boldsymbol{A}$ is given by

$$\boldsymbol{A}^+ = \boldsymbol{V}\boldsymbol{\Sigma}^+\boldsymbol{U}^T$$

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

Orthogonal Bases

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

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 $\mathrm{cond}(\boldsymbol{A}) \approx 1/\sqrt{\epsilon_{\mathrm{mach}}}$ 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 $\mathrm{cond}(\boldsymbol{A}) \approx 1/\epsilon_{\mathrm{mach}}$ 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