Numerical Analysis
FMN011

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Data Linearization and the QR factorization.

Data linearization: the exponential model

The parameters of

$$y = c_1 e^{c_2 t}$$

are not linear. To apply linear least squares we linearize the model:

$$\ln y = \ln c_1 + c_2 t$$

Let $Y = \ln y$ and $k = \ln c_1$, to get the straight line

$$Y = k + c_2 t$$

To obtain the parameters k and c_2, one needs to modify the data (t, y) to $(t, Y) = (t, \ln y)$. After computing k, c_1 must be calculated as e^k.

Data linearization: the power law

The parameters of

$$y = c_1 t^{c_2}$$

are nonlinear, but we can linearize the model:

$$\ln y = \ln c_1 + c_2 \ln t$$

Let $Y = \ln y$, $k = \ln c_1$ and $T = \ln t$, to get the straight line

$$Y = k + c_2 T$$

The original data must be modified to $(T, Y) = (\ln t, \ln y)$ and to obtain c_1 we compute e^k.

Orthogonal matrices vs Vandermonde

We know that solving the normal equations is ill-conditioned, because A^TA inherits and even worsens the large condition number of the Vandermonde matrix A.

An orthogonal matrix is a matrix with real entries such that $Q^{-1} = Q^T$.

$$\kappa_2(Q) = \|Q\|_2 \, \|Q^{-1}\|_2 = \sqrt{\rho(Q^TQ)}\,\sqrt{\rho(QQ^T)} = \sqrt{\rho(I)}\sqrt{\rho(I)} = 1$$

As orthogonal matrices have 2-norm condition number equal to 1, we will develop a method to solve the least squares problem using orthogonal matrices.

Gram-Schmidt Orthogonalization

Compute an **orthogonal** basis for the space spanned by k given linearly independent vectors, $\{v_1, v_2, \ldots, v_k\}$.

Define the unit vector in the direction of v_1,

$$q_1 = \frac{v_1}{\|v_1\|_2}$$

The projection of v_2 onto q_1 is $(q_1^T v_2)q_1$, so vector $y_2 = v_2 - (q_1^T v_2)q_1$ is perpendicular to v_1 and

$$q_2 = \frac{y_2}{\|y_2\|_2}$$

is a unit vector that is perpendicular to v_1 and such that $\{q_1, q_2\}$ span the same subspace as $\{v_1, v_2\}$.

Gram-Schmidt algorithm

Define

1. $y_1 = v_1, \quad q_1 = \dfrac{v_1}{\|v_1\|_2}$

2. $y_2 = v_2 - q_1(q_1^T v_2), \quad q_2 = \dfrac{y_2}{\|y_2\|_2}$

$\vdots$

k. $y_k = v_k - q_1(q_1^T v_k) - \cdots - q_{k-1}(q_{k-1}^T v_k), \quad q_k = \dfrac{y_k}{\|y_k\|_2}$

Note that $q_j \perp q_i$

Example: Gram-Schmidt on the columns of a matrix

$$A = \begin{pmatrix} -4 & -4 \\ -2 & 7 \\ 4 & -5 \end{pmatrix} = \begin{pmatrix} \mathbf{v_1} & \mathbf{v_2} \end{pmatrix}$$

$$\|y_1\|_2 = \sqrt{(-4)^2 + (-2)^2 + 4^2} = 6 \Rightarrow q_1 = \begin{pmatrix} -4/6 \\ -2/6 \\ 4/6 \end{pmatrix}$$

$$y_2 = \begin{pmatrix} -4 \\ 7 \\ -5 \end{pmatrix} + 3 \begin{pmatrix} -4/6 \\ -2/6 \\ 4/6 \end{pmatrix} = \begin{pmatrix} -6 \\ 6 \\ -3 \end{pmatrix} \Rightarrow q_2 = \begin{pmatrix} -6/9 \\ 6/9 \\ -3/9 \end{pmatrix}$$

$\begin{pmatrix} -4 & -4 \\ -2 & 7 \\ 4 & -5 \end{pmatrix}$ and $\begin{pmatrix} -4/6 & -6/9 \\ -2/6 & 6/9 \\ 4/6 & -3/9 \end{pmatrix}$ span the same plane.

Orthogonalization of a matrix

Let $r_{ii} = \|y_i\|_2$, $r_{ji} = q_j^T v_i$.

We can write $v_i = r_{ii}q_i + r_{1i}q_1 + \cdots + r_{i-1,i}q_{i-1}$, so

$$A = \left(\begin{array}{ccc} \mathbf{q_1} & \cdots & \mathbf{q_k} \end{array} \right) \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1k} \\ & r_{22} & \cdots & r_{2k} \\ & & \ddots & \vdots \\ & & & r_{kk} \end{pmatrix}$$

If $\mathbf{v_1}, \ldots, \mathbf{v_k}$ are linearly independent, all r_{ii} are nonzero.

If $\mathbf{v_i}$ is spanned by $\mathbf{v_1}, \ldots, \mathbf{v_{i-1}}$, then $r_{ii} = 0$ and the Gram-Schmidt method terminates.

The QR-factorization

Once we have the Gram-Schmidt orthogonalization of an $n \times k$ matrix A, we can complete the orthonormal basis by adding vectors $\mathbf{q_{k+1}}, \ldots, \mathbf{q_n}$,

$$A = \begin{pmatrix} \mathbf{q_1} & \cdots & \mathbf{q_k} & \mathbf{q_{k+1}} & \cdots & \mathbf{q_n} \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & \cdots & r_{1k} \\ & r_{22} & \cdots & r_{2k} \\ & & \ddots & \vdots \\ & & & r_{kk} \\ 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{pmatrix}$$

$Q = (\mathbf{q_1} \cdots \mathbf{q_n})$ is an orthogonal $n \times n$ matrix and R is an $n \times k$ upper triangular matrix.

Orthogonal matrices and the QR-factorization

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

A square matrix Q is orthogonal if its columns are pairwise orthogonal unit vectors ($\mathbf{q_i^T q_j} = 0$ and $\|\mathbf{q_i}\|_2 = 1$).

If Q is orthogonal, then $\|Qx\|_2 = \|x\|_2$.

In $A = QR$, Q is an orthogonal matrix and R is upper triangular.

Example: QR-factorization by Gram-Schmidt

To $\begin{pmatrix} -4 \\ -2 \\ 4 \end{pmatrix}$, $\begin{pmatrix} -4 \\ 7 \\ -5 \end{pmatrix}$ we add vector $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ to complete the space $\mathbb{R}^3$.

$$y_3 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \frac{4}{6}\begin{pmatrix} -4/6 \\ -2/6 \\ 4/6 \end{pmatrix} + \frac{6}{9}\begin{pmatrix} -6/9 \\ 6/9 \\ -3/9 \end{pmatrix} = \begin{pmatrix} 1/9 \\ 2/9 \\ 2/9 \end{pmatrix}, q_3 = \begin{pmatrix} 1/3 \\ 2/3 \\ 2/3 \end{pmatrix}$$

$r_{11} = \|y_1\|_2 = 6,\ r_{12} = q_1^T v_2 = -3,\ r_{22} = \|y_2\|_2 = 9$

The QR-factorization of A is

$$\begin{pmatrix} -4 & -4 \\ -2 & 7 \\ 4 & -5 \end{pmatrix} = \begin{pmatrix} -2/3 & -2/3 & 1/3 \\ -1/3 & 2/3 & 2/3 \\ 2/3 & -1/3 & 2/3 \end{pmatrix} \begin{pmatrix} 6 & -3 \\ 0 & 9 \\ 0 & 0 \end{pmatrix}$$

Least Squares and QR-factorization

The least squares solution minimizes

$$\|b - Ax\|_2 = \|b - QRx\|_2 = \|Q^T(b - QRx)\|_2 = \|Q^Tb - Rx\|_2$$

Let $d = Q^Tb$. We can find x so that

$$\left(\begin{array}{c} d_1 \\ \vdots \\ d_k \\ \hline d_{k+1} \\ \vdots \\ d_n \end{array}\right) - \left(\begin{array}{cccc} r_{11} & r_{12} & \cdots & r_{1k} \\ & r_{22} & \cdots & r_{2k} \\ & & \ddots & \vdots \\ & & & r_{kk} \\ \hline 0 & \cdots & \cdots & 0 \\ \vdots & & & \vdots \\ 0 & \cdots & \cdots & 0 \end{array}\right) \begin{pmatrix} x_1 \\ \vdots \\ x_k \end{pmatrix} = \left(\begin{array}{c} 0 \\ \vdots \\ 0 \\ \hline d_{k+1} \\ \vdots \\ d_n \end{array}\right)$$

Steps for least squares solving by QR-factorization

$$A = QR \Rightarrow Ax = QRx = b \Rightarrow Rx = Q^T b$$

Given the $m \times n, m > n$ system $Ax = b$,

1. Find Q and R such that $A = QR$
2. Set $\hat{R} =$ upper $n \times n$ submatrix of R
3. Set $\hat{d} =$ upper n entries of $d = Q^T b$
4. Solve $\hat{R}x = \hat{d}$

Example

Solve the least squares problem $\begin{pmatrix} -4 & -4 \\ -2 & 7 \\ 4 & -5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 9 \\ 0 \end{pmatrix}$

$$\begin{pmatrix} -4 & -4 \\ -2 & 7 \\ 4 & -5 \end{pmatrix} = \begin{pmatrix} -2/3 & -2/3 & 1/9 \\ -1/3 & 2/3 & 2/9 \\ 2/3 & -1/3 & 2/9 \end{pmatrix} \begin{pmatrix} 6 & -3 \\ 0 & 9 \\ 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 6 & -3 \\ 0 & 9 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} -5 \\ 4 \end{pmatrix}$$