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Numerical Analysis – Lecture 7

5 Linear least squares

5.1 Statement of the problem

Suppose that an $m \times n$ matrix A and a vector $\boldsymbol{b} \in \mathbb{R}^m$ are given. The equation $A\boldsymbol{x} = \boldsymbol{b}$ has in general no solution (if $m > n$) or an infinity of solutions (if $m < n$). 'Equations' of this form occur frequently when we collect m observations (which, typically, are prone to measurement error) and wish to exploit them to form an n-variable linear model, whereby $n \ll m$. (In statistics, this is called *linear regression.*) Bearing in mind the likely presence of errors in A and $\boldsymbol{b}$, we seek $\boldsymbol{x} \in \mathbb{R}^n$ that minimizes the Euclidean length $\|A\boldsymbol{x} - \boldsymbol{b}\|$ – the *least squares problem.*

Theorem $\boldsymbol{x} \in \mathbb{R}^n$ is a solution of the least squares problem iff $A^{\mathrm{T}}(A\boldsymbol{x} - \boldsymbol{b}) = \boldsymbol{0}$.

Proof. If $\boldsymbol{x}$ is a solution then it minimizes

$$f(\boldsymbol{x}) := \|A\boldsymbol{x} - \boldsymbol{b}\|^2 = \langle A\boldsymbol{x} - \boldsymbol{b}, A\boldsymbol{x} - \boldsymbol{b}\rangle = \boldsymbol{x}^{\mathrm{T}} A^{\mathrm{T}} A\boldsymbol{x} - 2\boldsymbol{x}^{\mathrm{T}} A^{\mathrm{T}}\boldsymbol{b} + \boldsymbol{b}^{\mathrm{T}}\boldsymbol{b}.$$

Hence $\nabla f(\boldsymbol{x}) = \boldsymbol{0}$. But $\frac{1}{2}\nabla f(\boldsymbol{x}) = A^{\mathrm{T}}A\boldsymbol{x} - A^{\mathrm{T}}\boldsymbol{b}$, hence $A^{\mathrm{T}}(A\boldsymbol{x} - \boldsymbol{b}) = \boldsymbol{0}$.
Conversely, suppose that $A^{\mathrm{T}}(A\boldsymbol{x} - \boldsymbol{b}) = \boldsymbol{0}$ and let $\boldsymbol{u} \in \mathbb{R}^n$. Hence, letting $\boldsymbol{y} = \boldsymbol{u} - \boldsymbol{x}$,

$$\begin{aligned} \|A\boldsymbol{u} - \boldsymbol{b}\|^2 &= \langle A\boldsymbol{x} + A\boldsymbol{y} - \boldsymbol{b}, A\boldsymbol{x} + A\boldsymbol{y} - \boldsymbol{b}\rangle = \langle A\boldsymbol{x} - \boldsymbol{b}, A\boldsymbol{x} - \boldsymbol{b}\rangle + 2\boldsymbol{y}^{\mathrm{T}} A^{\mathrm{T}}(A\boldsymbol{x} - \boldsymbol{b}) \\ &\quad + \langle A\boldsymbol{y}, A\boldsymbol{y}\rangle = \|A\boldsymbol{x} - \boldsymbol{b}\|^2 + \|A\boldsymbol{y}\|^2 \geq \|A\boldsymbol{x} - \boldsymbol{b}\|^2 \end{aligned}$$

and $\boldsymbol{x}$ is indeed optimal. □

Corollary Optimality of $\boldsymbol{x} \Leftrightarrow A\boldsymbol{x} - \boldsymbol{b}$ is orthogonal to all columns of A.

5.2 Normal equations

One way of finding optimal $\boldsymbol{x}$ is by solving the $n \times n$ linear system $A^{\mathrm{T}}A\boldsymbol{x} = A^{\mathrm{T}}\boldsymbol{b}$ – the *normal equations.* This approach is popular in many applications. However, there are three disadvantages. Firstly, $A^{\mathrm{T}}A$ might be singular, secondly sparse A might be replaced by a dense $A^{\mathrm{T}}A$ and, finally, forming $A^{\mathrm{T}}A$ might lead to loss of accuracy. Thus, suppose that our computer works in the IEEE arithmetic standard (≈ 15 significant digits) and let

$$A = \begin{bmatrix} 10^8 & -10^8 \\ 1 & 1 \end{bmatrix} \qquad \Longrightarrow \qquad A^{\mathrm{T}}A = \begin{bmatrix} 10^{16}+1 & -10^{16}+1 \\ -10^{16}+1 & 10^{16}+1 \end{bmatrix} \approx 10^{16} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.$$

Given $\boldsymbol{b} = [0, 2]^{\mathrm{T}}$ the solution of $A\boldsymbol{x} = \boldsymbol{b}$ is $[1, 1]^{\mathrm{T}}$, as can be easily found by Gaussian elimination. However, our computer 'believes' that $A^{\mathrm{T}}A$ is singular!

5.3 QR and least squares

Lemma Let A be any $m \times n$ matrix and let $\boldsymbol{b} \in \mathbb{R}^m$. The vector $\boldsymbol{x} \in \mathbb{R}^n$ minimizes $\|A\boldsymbol{x} - \boldsymbol{b}\|$ iff it minimizes $\|\Omega A\boldsymbol{x} - \Omega\boldsymbol{b}\|$ for an arbitrary $m \times m$ orthogonal matrix Ω.

Proof. Follows at once from the identity

$$\|\Omega A\boldsymbol{x} - \Omega\boldsymbol{b}\|^2 = (\Omega A\boldsymbol{x} - \Omega\boldsymbol{b})^{\mathrm{T}}(\Omega A\boldsymbol{x} - \Omega\boldsymbol{b}) = (A\boldsymbol{x} - \boldsymbol{b})^{\mathrm{T}}\Omega^{\mathrm{T}}\Omega(A\boldsymbol{x} - \boldsymbol{b}) = \|A\boldsymbol{x} - \boldsymbol{b}\|^2.$$

□

An irrelevant, yet important remark The property that orthogonal matrices leave the Euclidean distance intact is called *isometry* and it has many important ramifications throughout mathematics and mathematical physics.

Method of solution Suppose that $A = QR$, a QR factorization with R in a *standard form.* Because of the lemma, we let $\Omega := Q^{\mathrm{T}}$, hence seek $\boldsymbol{x}$ that minimizes $\|R\boldsymbol{x} - Q^{\mathrm{T}}\boldsymbol{b}\|$. In general $(m > n)$ many rows of R consist of zeros. Suppose for simplicity that $\operatorname{rank} R = \operatorname{rank} A = n$. Then the bottom $m - n$ rows of R are zero. Therefore we find $\boldsymbol{x}$ by solving the (nonsingular) linear system given by the first n equations of $R\boldsymbol{x} = Q^{\mathrm{T}}\boldsymbol{b}$. Similar (although more complicated) algorithm applies when $\operatorname{rank} R \le n - 1$. Note, recalling our former remark, that we don't require Q explicitly and need to evaluate only $Q^{\mathrm{T}}\boldsymbol{b}$.

6 Polynomial interpolation

6.1 The interpolation problem

Given $n + 1$ distinct real points $x_0, x_1, \ldots, x_n$ and real numbers $f_0, f_1, \ldots, f_n$, we seek a function $p : \mathbb{R} \to \mathbb{R}$ such that $p(x_i) = f_i$, $i = 0, 1, \ldots, n$. Such a function is called an *interpolant.*
We denote by $\mathbb{P}_n[x]$ the set of all real polynomials of degree at most n and observe that each $p \in \mathbb{P}_n[x]$ is uniquely defined by its $n + 1$ coefficients. This, intuitively, justifies seeking an interpolant from $\mathbb{P}_n[x]$.

6.2 The Lagrange formula

Although, in principle, we may solve a linear problem with $n + 1$ unknowns to determine a polynomial interpolant, this can be accomplished more easily by using the explicit *Lagrange formula.* We claim that

$$p(x) = \sum_{k=0}^{n} f_k \prod_{\substack{\ell=0\\ \ell\neq k}}^{n} \frac{x - x_\ell}{x_k - x_\ell}, \qquad x \in \mathbb{R}.$$

Note that $p \in \mathbb{P}_n[x]$, as required. We wish to show that it interpolates the data. Define $L_j(x) := \prod_{\ell=0,\, \ell\neq j}^{n} (x - x_\ell)/(x_j - x_\ell)$, $j = 0, 1, \ldots, n$ (*Lagrange cardinal polynomials*). It is trivial to verify that $L_j(x_j) = 1$ and $L_j(x_k) = 0$ for $k \neq j$, hence $p(x_j) = \sum_{k=0}^{n} f_k L_k(x_j) = f_j$, $j = 0, 1, \ldots, n$.

Uniqueness Suppose that both $p \in \mathbb{P}_n[x]$ and $q \in \mathbb{P}_n[x]$ interpolate to the same $n+1$ data. Then the nth degree polynomial $p - q$ vanishes at $n + 1$ distinct points. Hence it is identically zero, $p \equiv q$ and the interpolating polynomial is unique.