NLA 2021-2022
Least squares problem

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Rank deficient LSP

Let A be an $m \times n$ matrix and set $r = \text{rank}(A)$

It is *rank deficient* when

$$\boxed{r < n}$$

Typical in data analysis, when the variables have not been chosen wisely

If $r < n$ then the solution of the LSP is not unique: for all $x \in \text{Ker}(A) \simeq \mathbb{R}^{n-r}$ we have that

$$A\,(x_{\text{min}} + x) = A\,x_{\text{min}} + A\,x = A\,x_{\text{min}}$$

also solves the LSP

Example

For some medical research on the effect of a drug on sugar levels in blood, we take the following data from patients:

- initial blood level (sugar)
- amount of drug
- weight on day i, $i = 1, \ldots, 7$
- final blood level

To correlate the final sugar level in terms of the rest of the data, we consider the LSP

$$\begin{array}{c} \text{patient}_1 \\ \vdots \\ \vdots \\ \text{patient}_m \end{array} \begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_9 \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ \vdots \\ b_9 \end{bmatrix}$$

Example (cont.)

The solution x_{min} would be the used as the predictor, since

$$b_i \approx \text{ patient}_i \cdot x_{\text{min}}$$

The matrix A is probably close to rank 3: the experiment is not well-designed, and columns $3, \ldots, 9$ should be identified from our knowledge of the problem

Otherwise, we might take x_{min} very large, and a patient changing weight during the week would receive an irrealistic prediction

Rank deficient LSP via QR factorization

Suppose that $r < n$ and set

$$A = Q\,R = Q \begin{array}{cc} & \begin{array}{cc} \scriptstyle r & \scriptstyle n-r \end{array} \\ & \left[\begin{array}{cc} R_{1,1} & R_{1,2} \\ 0 & 0 \end{array}\right] \begin{array}{l} \scriptstyle r \\ \scriptstyle n-r \end{array} \end{array}$$

With round off, we hope to compute

$$R = \begin{bmatrix} R_{1,1} & R_{1,2} \\ 0 & R_{2,2} \end{bmatrix}$$

with $R_{2,2}$ small (e.g. of size $\approx \varepsilon \, \|A\|_2$)

$\rightsquigarrow$ we set $R_{2,2} = \mathbb{0}$ and then minimize $\|A\,x - b\|_2$ as follows:

complete Q to an orthogonal $m \times m$ matrix $[Q\ \widetilde{Q}]$, so that

$$\|A\,x - b\|_2^2 = \left\| \begin{bmatrix} Q^T \\ \widetilde{Q}^T \end{bmatrix} (A\,x - b) \right\|_2^2 = \|R\,x - Q^T b\|_2^2 + \|\widetilde{Q}^T b\|_2^2$$

(multiplying by an orthogonal $m \times m$ matrix does not change the 2-norm)

Rank deficient LSP via QR factorization (cont.)

Write $Q = \begin{array}{cc} r & n-r \\ \left[Q_1\right. & \left.Q_2\right] \end{array}$ and $x = \begin{array}{cc} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} & \begin{array}{l} r \\ n-r \end{array} \end{array}$. Then

$$\|A\,x - b\|_2^2 = \|R_{1,1}\,x_1 + R_{1,2}\,x_2 - Q_1^T b\|_2^2 + \|Q_2^T b\|_2^2 + \|\widetilde{Q}^T b\|_2^2$$

This expression is minimized by

$$x = \begin{bmatrix} R_{1,1}^{-1}(Q_1^T b - R_{1,2}\,x_2) \\ x_2 \end{bmatrix}$$

for any $(n-r)$-vector x_2

The typical choice is

$$x_2 = \mathbb{0}$$

Rank deficient LSP via QR factorization (cont.)

In general, this method is *not completely reliable* because R might be close to rank deficient even if $R_{2,2}$ is not small

Instead we apply QR factorization with pivoting

$$A\,P = Q\,R$$

with P is a permutation $m \times m$ matrix:

at step i, choose the largest column j of A with $i \leqslant j \leqslant n$ and compute the Householder reflection that zeroes the entries $i+1, \ldots, m$ in the i-th column

$\rightsquigarrow$ attempts to keep $R_{1,1}$ well-conditionned and $R_{2,2}$ small