

SR

In each step, SR solves the following linear system:

$$(J^\dagger J)\Delta\Theta = J^\dagger E_{\text{loc}}$$

with $n_s \times n_p$ matrix J and $n_s \times 1$ matrix E_{loc} .

SR with pivoted QR

Decompose J as $J\Pi = QR$ where Π is an $n_p \times n_p$ permutation matrix, $Q^\dagger Q = I$ and R is upper-trapezoidal. Assume J is rank-deficient with rank $r \leq n$, R has a block structure:

$$R = \begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix}$$

where R_{11} is a $r \times r$ upper-triangular invertible matrix and R_{12} is a $r \times (n_p - r)$ matrix.

Then

$$\begin{aligned} (J^\dagger J)\Delta\Theta &= J^\dagger E_{\text{loc}} \\ \Leftrightarrow R^\dagger R \Pi^\top \Delta\Theta &= R^\dagger Q^\dagger E_{\text{loc}} \end{aligned}$$

which is the normal equation for the least squares problem $\min_{\Delta\Theta} \|R \Pi^\top \Delta\Theta - Q^\dagger E_{\text{loc}}\|_2^2$.

For clarity, let $x \equiv \Pi^\top \Delta\Theta$ and $y \equiv Q^\dagger E_{\text{loc}}$, the squared 2-norm reads

$$\begin{aligned} &\|Rx - y\|_2^2 \\ &= \left\| \begin{pmatrix} R_{11} & R_{12} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} - \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \right\|_2^2 \\ &= \left\| \begin{pmatrix} R_{11}x_1 + R_{12}x_2 - y_1 \\ -y_2 \end{pmatrix} \right\|_2^2 \\ &= \|R_{11}x_1 + R_{12}x_2 - y_1\|_2^2 + \|y_2\|_2^2 \end{aligned}$$

Since R_{11} is invertible, the first term could be zeroed by choosing $x_1 = R_{11}^{-1}(y_1 - R_{12}x_2)$. Note that R_{11} is upper triangular, so this can be efficiently calculated by backward-substitution.

Naive

Choose $x_2 = \vec{0}$, then $x_1 = R_{11}^{-1}y_1$.

$$\Delta\Theta = \Pi \begin{pmatrix} R_{11}^{-1}y_1 \\ 0 \end{pmatrix}$$

In this case, most of the parameters remain unchanged, only a few parameters are updated.

Note that this choice does not necessarily minimize the norm of x and is just one solution of the underdetermined system.

Least squares

If we take into account the norm of x , the problem is reduced to a full-rank least squares problem for x_2 :

$$\begin{aligned}
& \min_{x_2} \|x\|_2^2 \\
& \Leftrightarrow \min_{x_2} \|R_{11}^{-1}(y_1 - R_{12}x_2)\|_2^2 + \|x_2\|_2^2 \\
& \Leftrightarrow \min_{x_2} \left\| \begin{pmatrix} R_{11}^{-1}R_{12} \\ I \end{pmatrix} x_2 - \begin{pmatrix} R_{11}^{-1}y_1 \\ 0 \end{pmatrix} \right\|_2^2
\end{aligned}$$

Since $\begin{pmatrix} R_{11}^{-1}R_{12} \\ I \end{pmatrix}$ has full column rank, the system is well-posed:

$$\begin{aligned}
x_2^* &= \begin{pmatrix} R_{11}^{-1}R_{12} \\ I \end{pmatrix}^{-1} \begin{pmatrix} R_{11}^{-1}y_1 \\ 0 \end{pmatrix} \\
\Delta\Theta &= \Pi \begin{pmatrix} R_{11}^{-1}(y_1 - R_{12}x_2^*) \\ x_2^* \end{pmatrix}
\end{aligned}$$

MinSR

Note that

$$(J^\dagger J)^{-1} J^\dagger = J^\dagger (J J^\dagger)^{-1}$$

where LHS is the left pseudo-inverse of J and RHS is the right pseudo-inverse of J , one have

$$\Delta\Theta = J^\dagger (J J^\dagger)^{-1} E_{\text{loc}}$$

which only requires the pseudo-inverse of a $n_s \times n_s$ matrix $J J^\dagger$.