Over-determined linear systems

Linear Algebra, Michaelmas Term 2018
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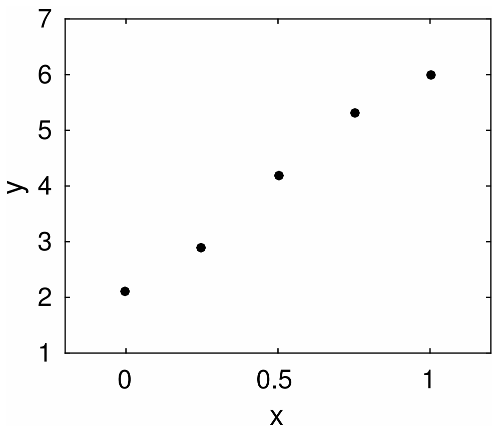
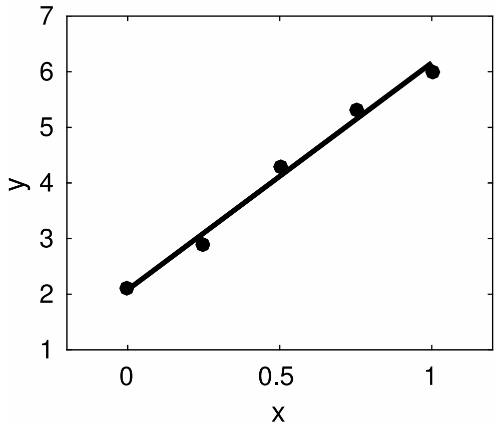
Suppose we have the experimental data relating x and y below



The data suggests a linear relation between x and y



Suppose we want to fit a straight line $y = ax + b$ to the data

Let us suppose we have N data points $(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$

We can write this as the linear system

$$\begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$

Clearly we are unlikely to be able to satisfy every equation

As there are more equations than unknowns this is known as an over-determined system

Instead we can minimise the sum of squares given by

$$\|\mathbf{r}\|^2 = \|A\mathbf{u} - \mathbf{b}\|^2$$

where

$$A = \begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{pmatrix}, \qquad \mathbf{u} = \begin{pmatrix} a \\ b \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$

$\mathbf{u}$ is then known as the least-squares solution to $A\mathbf{u} = \mathbf{b}$

In general, suppose we want to calculate the least squares solution of $A\mathbf{u} = \mathbf{b}$, where:

- A is a $N \times M$ matrix, with $N > M$
- $\mathbf{u}$ is a vector of length M
- $\mathbf{b}$ is a vector of length N

We will need the matrix $B = A^\top A$

B is of size $M \times M$, and is symmetric

We want to minimise

$$\begin{aligned} \|\mathbf{r}\|^2 &= \|A\mathbf{u} - \mathbf{b}\|^2 \\ &= (\mathbf{u}^\top A^\top - \mathbf{b}^\top)(A\mathbf{u} - \mathbf{b}) \\ &= \mathbf{u}^\top A^\top A\mathbf{u} - \mathbf{b}^\top A\mathbf{u} - \mathbf{u}^\top A^\top \mathbf{b} + \mathbf{b}^\top \mathbf{b} \\ &= \mathbf{u}^\top B\mathbf{u} - 2\mathbf{b}^\top A\mathbf{u} + \mathbf{b}^\top \mathbf{b} \\ &= \sum_{i=1}^{M}\sum_{j=1}^{M} u_i B_{ij} u_j - 2\sum_{i=1}^{N}\sum_{j=1}^{M} b_i A_{ij} u_j + \sum_{i=1}^{N} b_i^2 \end{aligned}$$

We are allowed to vary $u_1, u_2, \ldots, u_M$ when minimising the expression above

You will see on the Continuous Mathematics course next term that the minimum is at the point where

$$\frac{\partial}{\partial u_k}\left(\|\mathbf{r}\|^2\right) = 0, \qquad k = 1, 2, \ldots, M$$

Partial differentiation, and partial differentiation of products will also be covered on the Continuous Mathematics course next term

For $k = 1, 2, \dots, M$ we have

$$\begin{aligned}
\frac{\partial}{\partial u_k}\left(\|\mathbf{r}\|^2\right) &= \frac{\partial}{\partial u_k}\left(\sum_{i=1}^{M}\sum_{j=1}^{M} u_i B_{ij} u_j - 2\sum_{i=1}^{N}\sum_{j=1}^{M} b_i A_{ij} u_j + \sum_{i=1}^{N} b_i^2\right) \\
&= \sum_{j=1}^{M} B_{kj} u_j + \sum_{i=1}^{M} u_i B_{ik} - 2\sum_{i=1}^{N} b_i A_{ik} \\
&= \sum_{j=1}^{M} B_{kj} u_j + \sum_{i=1}^{M} B_{ki} u_i - 2\sum_{i=1}^{N} A_{ki}^{\top} b_i \\
&= 2\left(\sum_{i=1}^{M} B_{ki} u_i - \sum_{i=1}^{N} A_{ki}^{\top} b_i\right)
\end{aligned}$$

Setting this quantity to zero gives

$$B\mathbf{u} = A^{\top}\mathbf{b}$$

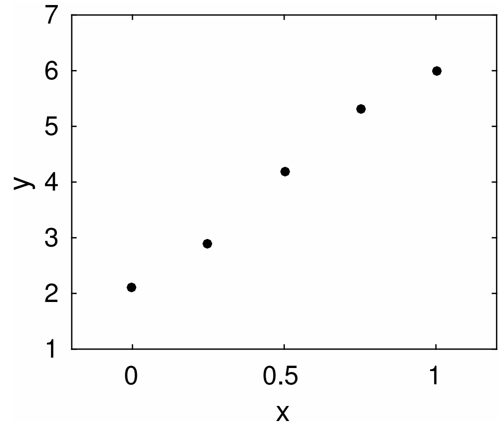
Remembering that $B = A^{\top}A$, the least-squares solution satisfies the normal equations

$$A^{\top}A\mathbf{u} = A^{\top}\mathbf{b}$$

This is a linear system of size $M \times M$

Example

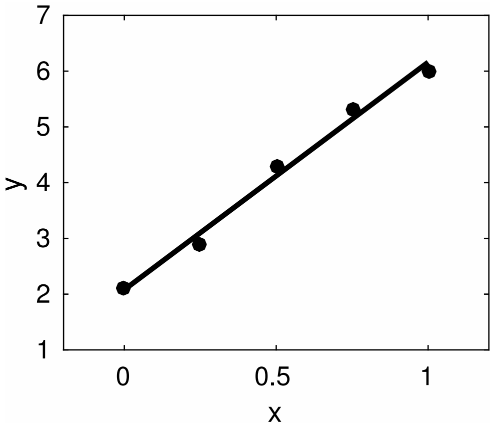
Find the straight line $y = ax + b$ that is the least squares fit to the data points $(0, 2.1), (0.25, 2.9), (0.5, 4.2), (0.75, 5.3), (1, 6)$



The over determined system is $A\mathbf{u} = \mathbf{b}$, where

$$A = \begin{pmatrix} 0 & 1 \\ 0.25 & 1 \\ 0.5 & 1 \\ 0.75 & 1 \\ 1 & 1 \end{pmatrix}, \qquad \mathbf{u} = \begin{pmatrix} a \\ b \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} 2.1 \\ 2.9 \\ 4.2 \\ 5.3 \\ 6 \end{pmatrix}$$

Solving the normal equations, $A^\top A\mathbf{u} = A^\top \mathbf{b}$, gives $\mathbf{u} = \begin{pmatrix} 4.08 \\ 2.08 \end{pmatrix}$, and so the line of best fit is $y = 4.08x + 2.08$



Gram-Schmidt revisited

Let $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_M$ be linearly independent vectors

The Gram-Schmidt procedure then generates M orthonormal vectors $\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_M$ with an identical span to $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_M$

The Gram-Schmidt procedure is summarised below

Set

$$\mathbf{q}_1 = \frac{1}{\|\mathbf{v}_1\|}\mathbf{v}_1$$

Set

$$\mathbf{q}_2 = \frac{\mathbf{v}_2 - (\mathbf{q}_1 \cdot \mathbf{v}_2)\mathbf{q}_1}{\|\mathbf{v}_2 - (\mathbf{q}_1 \cdot \mathbf{v}_2)\mathbf{q}_1\|}$$

Set

$$\mathbf{q}_3 = \frac{\mathbf{v}_3 - (\mathbf{q}_1 \cdot \mathbf{v}_3)\mathbf{q}_1 - (\mathbf{q}_2 \cdot \mathbf{v}_3)\mathbf{q}_2}{\|\mathbf{v}_3 - (\mathbf{q}_1 \cdot \mathbf{v}_3)\mathbf{q}_1 - (\mathbf{q}_2 \cdot \mathbf{v}_3)\mathbf{q}_2\|}$$

At step n set

$$\mathbf{q}_n = \frac{\mathbf{v}_n - \sum_{i=1}^{n-1}(\mathbf{q}_i \cdot \mathbf{v}_n)\mathbf{q}_i}{\|\mathbf{v}_n - \sum_{i=1}^{n-1}(\mathbf{q}_i \cdot \mathbf{v}_n)\mathbf{q}_i\|}$$

It is then straightforward to verify that $\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_M$ are orthonormal, i.e.

$$\mathbf{q}_i \cdot \mathbf{q}_j = \begin{cases} 1, & i = j, \\ 0, & i \neq j \end{cases}$$

We may then write this in matrix form as

$$
\begin{aligned}
A &= \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \mathbf{v}_3 & \dots & \mathbf{v}_M \end{pmatrix} \\
&= \begin{pmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 & \dots & \mathbf{q}_M \end{pmatrix}
\begin{pmatrix}
\mathbf{q}_1 \cdot \mathbf{v}_1 & \mathbf{q}_1 \cdot \mathbf{v}_2 & \mathbf{q}_1 \cdot \mathbf{v}_3 & \dots & \mathbf{q}_1 \cdot \mathbf{v}_M \\
0 & \mathbf{q}_2 \cdot \mathbf{v}_2 & \mathbf{q}_2 \cdot \mathbf{v}_3 & \dots & \mathbf{q}_2 \cdot \mathbf{v}_M \\
0 & 0 & \mathbf{q}_3 \cdot \mathbf{v}_3 & \dots & \mathbf{q}_2 \cdot \mathbf{v}_M \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \dots & \mathbf{q}_M \cdot \mathbf{v}_M
\end{pmatrix} \\
&= QR
\end{aligned}
$$

If each $\mathbf{v}_i$ contains N entries then A and Q are $N \times M$ matrices, and R is a $M \times M$ upper triangular matrix

Note that

$$
\begin{aligned}
Q^\top Q &= \begin{pmatrix} \mathbf{q}_1^\top \\ \mathbf{q}_2^\top \\ \mathbf{q}_3^\top \\ \vdots \\ \mathbf{q}_N^\top \end{pmatrix}
\begin{pmatrix} \mathbf{q}_1 & \mathbf{q}_2 & \mathbf{q}_3 & \dots & \mathbf{q}_N \end{pmatrix} \\
&= \begin{pmatrix}
\mathbf{q}_1 \cdot \mathbf{q}_1 & \mathbf{q}_1 \cdot \mathbf{q}_2 & \mathbf{q}_1 \cdot \mathbf{q}_3 & \dots & \mathbf{q}_1 \cdot \mathbf{q}_N \\
\mathbf{q}_2 \cdot \mathbf{q}_1 & \mathbf{q}_2 \cdot \mathbf{q}_2 & \mathbf{q}_2 \cdot \mathbf{q}_3 & \dots & \mathbf{q}_2 \cdot \mathbf{q}_N \\
\mathbf{q}_3 \cdot \mathbf{q}_1 & \mathbf{q}_3 \cdot \mathbf{q}_2 & \mathbf{q}_3 \cdot \mathbf{q}_3 & \dots & \mathbf{q}_3 \cdot \mathbf{q}_N \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\mathbf{q}_N \cdot \mathbf{q}_1 & \mathbf{q}_N \cdot \mathbf{q}_2 & \mathbf{q}_N \cdot \mathbf{q}_3 & \dots & \mathbf{q}_N \cdot \mathbf{q}_N
\end{pmatrix} \\
&= \mathcal{I}
\end{aligned}
$$

as $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_N$ are orthonormal

This factorisation of A is known as the QR factorisation of A

Using the QR factorisation in the normal equations

Suppose A is a $N \times M$ matrix, with $N > M$

The normal equations for the over-determined linear system $A\mathbf{u} = \mathbf{b}$ are

$$A^\top A\mathbf{u} = A^\top \mathbf{b}$$

Let $A = QR$ be the QR factorisation of A

The matrix Q is of size $N \times M$, and satisfies $Q^\top Q = \mathcal{I}$

The matrix R is of size $M \times M$, and is upper-triangular

We will assume that the diagonal entries of R are non-zero, so that R is invertible

The normal equations now become

$$
\begin{aligned}
(QR)^\top QR\mathbf{u} &= (QR)^\top \mathbf{b} \\
R^\top Q^\top QR\mathbf{u} &= R^\top Q^\top \mathbf{b} \\
R^\top R\mathbf{u} &= R^\top Q^\top \mathbf{b} \\
R\mathbf{u} &= Q^\top \mathbf{b}
\end{aligned}
$$

This is an upper-triangular system that may be solved very easily

Why a QR factorisation should be used when solving the normal equations

When solving the over-determined system $A\mathbf{u} = \mathbf{b}$, the normal equations are

$$A^\top A\mathbf{u} = A^\top \mathbf{b}$$

We have proposed solving this system by first calculating the QR factorisation of A

Having written $A = QR$, where $Q^\top Q = \mathcal{I}$, and R is an upper triangular matrix, we then solve

$$R\mathbf{u} = Q^\top \mathbf{b}$$

We now explain why

Matrix norms

Let A be a non-singular $N \times N$ matrix, and let $\mathbf{v}$ be a vector of length N

We define the norm of A by

$$\|A\| = \max_{\mathbf{v}\neq\mathbf{0}} \frac{\|A\mathbf{v}\|}{\|\mathbf{v}\|}$$

From this definition it is clear that

$$\|A\| \geq \frac{\|A\mathbf{v}\|}{\|\mathbf{v}\|}$$

and so

$$\|A\mathbf{v}\| \leq \|A\|\|\mathbf{v}\|$$

Further, note that for two non-singular matrices A and B,

$$
\begin{aligned}
\|AB\mathbf{v}\| &= \|A(B\mathbf{v})\| \\
&\leq \|A\|\|B\mathbf{v}\| \\
&\leq \|A\|\|B\|\|\mathbf{v}\|
\end{aligned}
$$

and so

$$\frac{\|AB\mathbf{v}\|}{\|\mathbf{v}\|} \leq \|A\|\|B\|$$

Then

$$\|AB\| = \max_{\mathbf{v}\neq\mathbf{0}} \frac{\|AB\mathbf{v}\|}{\|\mathbf{v}\|} \leq \|A\|\|B\|$$

To calculate $\|A\|$ we consider the matrix $A^\top A$

As $A^\top A$ is a symmetric matrix, we may write $A^\top A = P^\top D P$, where $P^\top P = \mathcal{I}$, and D is a diagonal matrix, where the entries on the diagonal are the eigenvalues of $A^\top A$

In a worksheet we derived the following properties:

1. The eigenvalues of $A^\top A$ are positive
2. For all vectors $\mathbf{v}$, we have
$$\lambda_{\min}\|\mathbf{v}\|^2 \leq \mathbf{v}^\top A^\top A\mathbf{v} \leq \lambda_{\max}\|\mathbf{v}\|^2$$
3. There exists a vector $\mathbf{w}$ such that
$$\mathbf{w}^\top A^\top A\mathbf{w} = \lambda_{\max}\|\mathbf{w}\|^2$$
4. There exists a vector $\mathbf{y}$ such that
$$\mathbf{y}^\top A^\top A\mathbf{y} = \lambda_{\min}\|\mathbf{y}\|^2$$

where $\lambda_{\min}, \lambda_{\max}$ are the smallest and largest eigenvalues of $A^\top A$

We then have, for all $\mathbf{v}$:

$$\begin{aligned}\frac{\|A\mathbf{v}\|^2}{\|\mathbf{v}\|^2} &= \frac{\mathbf{v}^\top A^\top A\mathbf{v}}{\|\mathbf{v}\|^2}\\ &\leq \frac{\lambda_{\max}| \mathbf{v}\|^2}{\|\mathbf{v}\|^2}\\ &= \lambda_{\max}\end{aligned}$$

and so

$$\frac{\|A\mathbf{v}\|}{\|\mathbf{v}\|} \leq \sqrt{\lambda_{\max}}$$

We also have, for $\mathbf{w}$:

$$\begin{aligned}\frac{\|A\mathbf{w}\|^2}{\|\mathbf{w}\|^2} &= \frac{\mathbf{w}^\top A^\top A\mathbf{w}}{\|\mathbf{w}\|^2}\\ &= \frac{\lambda_{\max}| \mathbf{w}\|^2}{\|\mathbf{w}\|^2}\\ &= \lambda_{\max}\end{aligned}$$

and so

$$\frac{\|A\mathbf{w}\|}{\|\mathbf{w}\|} = \sqrt{\lambda_{\max}}$$

Therefore

$$\|A\| = \max_{\mathbf{v}\neq\mathbf{0}} \frac{\|A\mathbf{v}\|}{\|\mathbf{v}\|} = \sqrt{\lambda_{\text{max}}}$$

$\|A\|$ is therefore given by the square root of the largest eigenvalue of $A^\top A$.

We may also write the norm of A^{-1} in terms of the eigenvalues of $A^\top A$

We write

$$\begin{aligned}\|A^{-1}\| &= \max_{\mathbf{v}\neq\mathbf{0}} \frac{\|A^{-1}\mathbf{v}\|}{\|\mathbf{v}\|} \\ &= \max_{\mathbf{u}\neq\mathbf{0}} \frac{\|\mathbf{u}\|}{\|A\mathbf{u}\|}, \qquad \text{where } \mathbf{u} = A^{-1}\mathbf{v} \\ &= \left(\min_{\mathbf{u}\neq\mathbf{0}} \frac{\|A\mathbf{u}\|}{\|\mathbf{u}\|}\right)^{-1}\end{aligned}$$

Using a similar argument to earlier we may show that

$$\min_{\mathbf{u}\neq\mathbf{0}} \frac{\|A\mathbf{u}\|}{\|\mathbf{u}\|} = \sqrt{\lambda_{\text{min}}}$$

Therefore

$$\|A^{-1}\| = \left(\min_{\mathbf{u}\neq\mathbf{0}} \frac{\|A\mathbf{u}\|}{\|\mathbf{u}\|}\right)^{-1} = \sqrt{\frac{1}{\lambda_{\text{min}}}}$$

$\|A^{-1}\|$ is therefore given by the reciprocal of the square root of the smallest eigenvalue of $A^\top A$.

The conditioning of a linear system

Suppose we want to solve the linear system $M\mathbf{u} = \mathbf{c}$ where M is a non-singular matrix

The vector $\mathbf{c}$ will contain error due to finite precision arithmetic and experimental error

Let $\mathbf{c}$ be the vector that would be on the right-hand-side if no error existed

Let $\delta\mathbf{c}$ be the (unknown) error

In practice we will have some idea of the relative error in $\mathbf{c}$, i.e. an estimate of $\|\delta\mathbf{c}\|/\|\mathbf{c}\|$

Let $\mathbf{u}$ be the solution of the linear system in the absence of error

$\mathbf{u}$ then satisfies

$$M\mathbf{u} = \mathbf{c}$$

In practice, the right hand side will be $\mathbf{c} + \delta\mathbf{c}$, and we will solve

$$M(\mathbf{u} + \delta\mathbf{u}) = \mathbf{c} + \delta\mathbf{c}$$

where $\delta\mathbf{u}$ is the 'error' on $\mathbf{u}$ caused by the error in $\mathbf{c}$

We now estimate $\delta\mathbf{u}$ in terms of $\|\delta\mathbf{c}\|/\|\mathbf{c}\|$

We may write these two linear systems as

$$\begin{aligned} M\mathbf{u} &= \mathbf{c} \\ M(\delta\mathbf{u}) &= \delta\mathbf{c} \end{aligned}$$

Recall that

$$\|M\mathbf{u}\| \leq \|M\|\|\mathbf{u}\|$$

Using the first linear system

$$\begin{aligned} \|M\mathbf{u}\| &= \|\mathbf{c}\| \\ \|M\|\|\mathbf{u}\| &\geq \|\mathbf{c}\| \\ \|\mathbf{u}\| &\geq \|\mathbf{c}\|\|M\|^{-1} \end{aligned}$$

The second linear system may be written

$$\delta\mathbf{u} = M^{-1}(\delta\mathbf{c})$$

We then have

$$\begin{aligned} \|\delta\mathbf{u}\| &= \|M^{-1}(\delta\mathbf{c})\| \\ &\leq \|M^{-1}\|\|\delta\mathbf{c}\| \end{aligned}$$

Combining the results on the last two slides gives

$$\frac{\|\delta\mathbf{u}\|}{\|\mathbf{u}\|} = k(M)\frac{\|\delta\mathbf{c}\|}{\|\mathbf{c}\|}$$

where $k(M)$ is known as the condition number of M, and is given by

$$\begin{aligned} k(M) &= \|M\|\|M^{-1}\| \\ &= \sqrt{\frac{\lambda_{\max}}{\lambda_{\min}}} \end{aligned}$$

where $\lambda_{\min}, \lambda_{\max}$ are the smallest and largest eigenvalues of $M^\top M$

We now have a bound on $\|\delta\mathbf{u}\|$ in terms of the relative error $\|\delta\mathbf{c}\|/\|\mathbf{c}\|$ and the eigenvalues of $M^\top M$

Note that

$$\begin{aligned} \|\mathcal{I}\| &= \max_{\mathbf{v}\neq\mathbf{0}} \frac{\|\mathcal{I}\mathbf{v}\|}{\|\mathbf{v}\|} \\ &= \max_{\mathbf{v}\neq\mathbf{0}} \frac{\|\mathbf{v}\|}{\|\mathbf{v}\|} \\ &= 1 \end{aligned}$$

As a consequence

$$\begin{aligned} 1 &= \|AA^{-1}\| \\ &\le \|A\|\|A^{-1}\| \\ &= k(A) \end{aligned}$$

and so the condition number of a matrix is always greater than or equal to 1

Recall that we can solve the over-determined system $A\mathbf{u} = \mathbf{b}$ by solving either

- $A^\top A\mathbf{u} = A^\top\mathbf{b}$ or
- $R\mathbf{u} = Q^\top\mathbf{b}$, where $A = QR$ and $Q^\top Q = \mathcal{I}$

Using the first of these methods the error bound is

$$\frac{\|\delta\mathbf{u}\|}{\|\mathbf{u}\|} = k(A^\top A)\frac{\|\delta\mathbf{c}\|}{\|\mathbf{c}\|}, \quad \text{where} \quad \mathbf{c} = A^\top\mathbf{b}$$

Using the second of these methods the error bound is

$$\frac{\|\delta\mathbf{u}\|}{\|\mathbf{u}\|} = k(R)\frac{\|\delta\mathbf{c}\|}{\|\mathbf{c}\|}, \quad \text{where} \quad \mathbf{c} = Q^\top\mathbf{b}$$

We will now assume that

$$\frac{\|\delta\mathbf{c}\|}{\|\mathbf{c}\|}$$

is the same for either method of solving the normal equations

We will start with the second of these linear systems

The condition number of this system depends on the eigenvalues of $R^\top R$

Note that $R^\top R = (Q^\top A)^\top (Q^\top A) = A^\top Q^\top Q A = A^\top A$

We then have $k(R) = \sqrt{\frac{\lambda_{\max}}{\lambda_{\min}}}$, where $\lambda_{\min}, \lambda_{\max}$ are the smallest and largest eigenvalues of $A^\top A$

We now think about the first linear system

The condition number of this system depends on the eigenvalues of $(A^\top A)^\top A^\top A = A^\top A A^\top A = (A^\top A)^2$

We write $A^\top A = P^\top D P$, where $P^\top P = \mathcal{I}$, and D is a diagonal matrix with the eigenvalues of $A^\top A$ on the diagonal

We then have $(A^\top A)^2 = P^\top D^2 P$, and so the eigenvalues of $(A^\top A)^2$ are the squares of the eigenvalues of the eigenvalues of $A^\top A$

Hence,

$$\begin{aligned} k(A^\top A) &= \frac{\lambda_{\max}}{\lambda_{\min}} \\ &= (k(R))^2 \end{aligned}$$

As $k(R) > 1$ we have

$$k(A^\top A) > k(R)$$

and the QR factorisation method will be less affected by error in the right-hand-side vector