Lecture `linalg5`: Least squares and QR–factorization

November 4, 2022

Summary: Supplemental material on QR–factorization. Focus here is on Givens rotations, whereas Sauer employs Householder reflections.

References: T. Sauer's *Numerical Analysis*, Section 4.3, pages 218–229. Material here also taken in part from C. F. Van Loan's *Introduction to Scientific Computing*.

Background

Last time we learned how to solve the least squares problem:

$$\text{minimize } \|A\mathbf{x} - \mathbf{b}\| \text{ over all } \mathbf{x} \in \mathbb{R}^n,$$

where A is m–by–n with $m > n$ and has full column rank. We learned that the unique solution $\mathbf{x}_{LS}$ is obtained by solving the *normal equations*, the square n–by–n system $A^T A\mathbf{x} = A^T\mathbf{b}$. While the formulation of the least squares problem in terms of the normal equations is both elegant and practical for small n, for large n the matrix $A^T A$ tends to have a large condition number κ. If κ is too large, then in solving the normal equations numerically, we will obtain a numerical solution of poor quality. Therefore, we now describe a second, more robust, way to attack the least squares problem: QR–factorization. The idea is quite similar to the LU–factorization $A = LU$, except now $A = QR$, where the m–by–m matrix Q is *orthogonal* rather than lower triangular. R is an m–by–n upper triangular matrix. In this lecture, we'll explain why this new factorization is useful and we'll illustrate one way of implementing it.

Mathematical preliminaries

Consider the 2–by–2 matrix[1]

$$Q(\alpha,\beta) = \frac{1}{\sqrt{\alpha^2+\beta^2}}\begin{pmatrix} \alpha & \beta \\ -\beta & \alpha \end{pmatrix},\ Q^T(\alpha,\beta) = \frac{1}{\sqrt{\alpha^2+\beta^2}}\begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix},\ Q^T Q = QQ^T = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{1}$$

Q is an example of an *orthogonal* matrix: its transpose is its inverse. Actually, Q is slightly more. Indeed, it's a *special orthogonal* matrix in that $\det Q = 1$. Since $1 = \det I = \det(M^T M) = \det M^T \cdot \det M = (\det M)^2$, an orthogonal matrix M must have $\det M = \pm 1$. We've mentioned that permutation matrices are orthogonal, but some have determinant -1, for example the 2–by–2 matrix

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2}$$

[1] Due to the form of Q, we could express it as a rotation matrix

$$Q(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}.$$

Van Loan adopts this point of view, but we'll not need it.

The action of $Q(\alpha,\beta)$ on a 2–vector is

$$Q(\alpha,\beta)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{\sqrt{\alpha^2+\beta^2}}\begin{pmatrix} \alpha x_1 + \beta x_2 \\ -\beta x_1 + \alpha x_2 \end{pmatrix}. \tag{3}$$

The special choices $\alpha = x_1$ and $\beta = x_2$ then ensure that

$$Q(x_1,x_2)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{\sqrt{x_1^2+x_2^2}}\begin{pmatrix} x_1^2 + x_2^2 \\ -x_2 x_1 + x_1 x_2 \end{pmatrix} = \begin{pmatrix} \sqrt{x_1^2+x_2^2} \\ 0 \end{pmatrix}. \tag{4}$$

In other words, $Q(x_1,x_2)$ is tailored to "zero out" the second entry of the 2–vector $\mathbf{x}$. The special choices $\alpha = -x_1$ and $\beta = -x_2$ achieve the same effect,

$$Q(-x_1,-x_2)\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \frac{1}{\sqrt{x_1^2+x_2^2}}\begin{pmatrix} -x_1^2 - x_2^2 \\ x_2 x_1 - x_1 x_2 \end{pmatrix} = \begin{pmatrix} -\sqrt{x_1^2+x_2^2} \\ 0 \end{pmatrix}. \tag{5}$$

Moreover, the vectors

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \text{ and } \begin{pmatrix} \sqrt{x_1^2+x_2^2} \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} -\sqrt{x_1^2+x_2^2} \\ 0 \end{pmatrix} \tag{6}$$

all have the same norm (length), namely $\sqrt{x_1^2+x_2^2}$. So the action of either Q has preserved the length of $\mathbf{x}$. In these notes, for simplicity we only consider the first type of Q in (4).

Norm–preservation is an important feature of any orthogonal matrix M, whether it be 2–by–2 or n–by–n. Here is why this is so. Let's compute the squared norm of $M\mathbf{x}$:

$$\begin{aligned}
\|M\mathbf{x}\|^2 &= (M\mathbf{x})\cdot(M\mathbf{x}) && \text{(relation between 2–norm and dot product)} \\
&= (M\mathbf{x})^T M\mathbf{x} && \text{(another form of dot product)} \\
&= \mathbf{x}^T M^T M\mathbf{x} && \text{(by properties of transpose)} \\
&= \mathbf{x}^T\mathbf{x} && \text{(by orthogonality of } M\text{)} \\
&= \|\mathbf{x}\|^2.
\end{aligned} \tag{7}$$

So, indeed, $\|M\mathbf{x}\| = \|\mathbf{x}\|$, that is the action of M preserves the length of $\mathbf{x}$. Another quintessential point is that the set of n–by–n orthogonal matrices is a group. In fact, this set of matrices is (a representation of) the group $O(n)$. This means, among other things, that $M, P \in O(n) \implies MP \in O(n)$. Now, $MP \in O(n)$ means $(MP)^T$ is the inverse of MP, clearly true since $(MP)^T MP = P^T M^T MP = P^T IP = P^T P = I$. A subgroup of $O(n)$ is $SO(n)$, the set of all orthogonal matrices with determinant $+1$. $SO(n)$ is a group in its own right, and in particular $SO(3)$ is the group of rotations in 3 dimensions.

Basic idea

Let's consider the 4–by–3 overdetermined system $A\mathbf{x} = \mathbf{b}$, where

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix} \qquad \text{(this system is generally not solvable),} \tag{8}$$

assuming we want a solution in the least square sense, that is one that minimizes $\|A\mathbf{x} - \mathbf{b}\|$. However, we will not use the normal equations approach. Rather we shall find a factorization $A = QR$, where Q is a 4–by–4 orthogonal matrix and R is a 4–by–3 upper triangular matrix

$$R = \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ 0 & 0 & 0 \end{pmatrix}. \tag{9}$$

Provided A has full column rank, all diagonal elements $r_{kk} \neq 0$. Why does this help? Because minimizing $\|A\mathbf{x} - \mathbf{b}\|$ is equivalent to minimizing $\|R\mathbf{x} - Q^T\mathbf{b}\|$. This is true because

$$A\mathbf{x} - \mathbf{b} = QR\mathbf{x} - \mathbf{b} \implies Q^T(A\mathbf{x} - \mathbf{b}) = R\mathbf{x} - Q^T\mathbf{b}. \tag{10}$$

Since $R\mathbf{x} - Q^T\mathbf{b}$ is obtained from $A\mathbf{x} - \mathbf{b}$ via the action of the orthogonal matrix Q^T (if Q is orthogonal, then so is Q^T), these two vectors must have the same length. Therefore, we seek to minimize

$$\begin{aligned}\|R\mathbf{x} - Q^T\mathbf{b}\|^2 &= \left\| \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} \right\|^2 \\ &= (r_{11}x_1 + r_{12}x_2 + r_{13}x_3 - w_1)^2 + (r_{22}x_2 + r_{23}x_3 - w_2)^2 + (r_{33}x_3 - w_3)^2 + w_4^2, \end{aligned} \tag{11}$$

where $\mathbf{w} = Q^T\mathbf{b}$. No matter how we choose $\mathbf{x}$, we'll always have $\|R\mathbf{x} - Q^T\mathbf{b}\| \geq |w_4|$. So let's just solve

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix} \tag{12}$$

to get our least squares solution $\mathbf{x}_{LS}$. A nice feature of the QR approach is that we also know the length of the residual, which tells us how close (in the 2–norm) $\mathbf{x}_{LS}$ is to being an exact solution. Indeed, we have

$$\|A\mathbf{x}_{LS} - \mathbf{b}\| = \|R\mathbf{x}_{LS} - Q^T\mathbf{b}\| = \|R\mathbf{x}_{LS} - \mathbf{w}\| = \sqrt{0^2 + 0^2 + 0^2 + w_4^2} = |w_4|. \tag{13}$$

So $|(Q^T\mathbf{b})_4|$ measures closeness to an exact solution. One question remains: **how do we find Q?** We build it up in stages. In lieu of a general discussion, we here provide a concrete example.

4–by–3 example

Consider the example from last time. Namely, the data set $\mathcal{D}_4 = \{(-1,1),(0,1),(1,3),(2,11)\}$ taken from $y = \frac{2}{3}x^3 + x^2 + \frac{1}{3}x + 1$. Let us construct be best quadratic polynomial which fits the data. Using monomials, our modal set is then $\mathcal{B}_3 = \{\phi_1(x), \phi_2(x), \phi_3(x)\} = \{1, x, x^2\}$. We then seek to minimize the length $\|V\mathbf{c} - \mathbf{y}\|$ of the residual vector $V\mathbf{c} - \mathbf{y}$, and in detail the residual vector is

$$\begin{pmatrix} \phi_1(-1) & \phi_2(-1) & \phi_3(-1) \\ \phi_1(0) & \phi_2(0) & \phi_3(0) \\ \phi_1(1) & \phi_2(1) & \phi_3(1) \\ \phi_1(2) & \phi_2(2) & \phi_3(2) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \\ 3 \\ 11 \end{pmatrix}. \tag{14}$$

Using our observation (4) for how to "zero out" the last component of a 2–vector with an orthogonal matrix Q, we'll now start zeroing out those elements of V sitting below the diagonal. First to zero out the $(4,1)$ entry $v_{41} = 1$ in the last equation,[2]

$$\text{apply } G_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \text{ to get } \begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ \sqrt{2} & \frac{3}{\sqrt{2}} & \frac{5}{\sqrt{2}} \\ \boxed{0} & \frac{1}{\sqrt{2}} & \frac{3}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \\ 7\sqrt{2} \\ 4\sqrt{2} \end{pmatrix}, \tag{15}$$

where we have boxed the entry that's been zeroed by G_1. Notice that the matrix G_1 is orthogonal, and has the form

$$G_1 = \begin{pmatrix} I_{2\times 2} & 0_{2\times 2} \\ 0_{2\times 2} & Q(1,1) \end{pmatrix}. \tag{16}$$

[2] We use the G notation here, because such an orthogonal matrix is called a *Givens rotation*.

We shall build up the orthogonal matrix Q^T by successive orthogonal transformations with this structure, that is the 4–by–4 identity $I_{4\times 4}$ with a 2–by–2 $Q(\alpha,\beta)$ overwritten over a 2–by–2 diagonal subblock of $I_{4\times 4}$. Here are the possible types for a G (all are 4–by–4):

$$\begin{pmatrix} Q(\alpha,\beta) & 0_{2\times 2} \\ 0_{2\times 2} & I_{2\times 2} \end{pmatrix}, \qquad \begin{pmatrix} 1 & 0_{1\times 2} & 0 \\ 0_{2\times 1} & Q(\alpha,\beta) & 0_{2\times 1} \\ 0 & 0_{1\times 2} & 1 \end{pmatrix}, \qquad \begin{pmatrix} I_{2\times 2} & 0_{2\times 2} \\ 0_{2\times 2} & Q(\alpha,\beta) \end{pmatrix}. \tag{17}$$

Returning to (15), we now zero out the $(3,1)$ entry of $G_1 V$ (that is, the $\sqrt{2}$). To do so, we

$$\text{apply } G_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \\ 0 & -\sqrt{\frac{2}{3}} & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \text{ to get } \begin{pmatrix} 1 & -1 & 1 \\ \sqrt{3} & \sqrt{3} & \frac{5}{\sqrt{3}} \\ \boxed{0} & \sqrt{\frac{3}{2}} & \frac{5}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{3}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} 1 \\ 5\sqrt{3} \\ 2\sqrt{6} \\ 4\sqrt{2} \end{pmatrix}. \tag{18}$$

From here one, we just list the operations (always performed on the last equation) and their results, hoping that the process underway is clear. Boxes indicate the entry zeroed out by the action of the corresponding G_k.

$$\text{Apply } G_3 = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \text{ to get } \begin{pmatrix} 2 & 1 & 3 \\ \boxed{0} & \sqrt{3} & \frac{1}{\sqrt{3}} \\ 0 & \sqrt{\frac{3}{2}} & \frac{5}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{3}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} 8 \\ 2\sqrt{3} \\ 2\sqrt{6} \\ 4\sqrt{2} \end{pmatrix}. \tag{19}$$

$$\text{Apply } G_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \\ 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} \text{ to get } \begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{3} & \frac{1}{\sqrt{3}} \\ 0 & \sqrt{2} & 2\sqrt{2} \\ 0 & \boxed{0} & \sqrt{\frac{2}{3}} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} 8 \\ 2\sqrt{3} \\ 5\sqrt{2} \\ \sqrt{6} \end{pmatrix}. \tag{20}$$

$$\text{Apply } G_5 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{\frac{3}{5}} & \sqrt{\frac{2}{5}} & 0 \\ 0 & -\sqrt{\frac{2}{5}} & \sqrt{\frac{3}{5}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \text{ to get } \begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{5} & \sqrt{5} \\ 0 & \boxed{0} & \sqrt{\frac{10}{3}} \\ 0 & 0 & \sqrt{\frac{2}{3}} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} 8 \\ \frac{16}{\sqrt{5}} \\ 3\sqrt{\frac{6}{5}} \\ \sqrt{6} \end{pmatrix}. \tag{21}$$

$$\text{Apply } G_6 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sqrt{\frac{5}{6}} & \sqrt{\frac{1}{6}} \\ 0 & 0 & -\sqrt{\frac{1}{6}} & \sqrt{\frac{5}{6}} \end{pmatrix} \text{ to get } \begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{5} & \sqrt{5} \\ 0 & 0 & 2 \\ 0 & 0 & \boxed{0} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} - \begin{pmatrix} 8 \\ \frac{16}{\sqrt{5}} \\ 4 \\ \frac{2}{\sqrt{5}} \end{pmatrix}. \tag{22}$$

Therefore, we get the solution $\mathbf{c}_{LS}$ to the least squares problem by solving

$$\begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{5} & \sqrt{5} \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 8 \\ \frac{16}{\sqrt{5}} \\ 4 \end{pmatrix}, \tag{23}$$

which by backward substitution is $\mathbf{c}_{LS} = (2/5, 6/5, 2)$. Moreover, from (22) we know that the minimum value of $\|V\mathbf{c} - \mathbf{y}\|$ is $\|V\mathbf{c}_{LS} - \mathbf{y}\| = 2/\sqrt{5}$.

To find the Q in this QR–factorization of V, we set

$$Q^T = G_6G_5G_4G_3G_2G_1 = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{3}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{3}{2\sqrt{5}} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2\sqrt{5}} & \frac{3}{2\sqrt{5}} & -\frac{3}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} \end{pmatrix} \implies Q = \begin{pmatrix} \frac{1}{2} & -\frac{3}{2\sqrt{5}} & \frac{1}{2} & -\frac{1}{2\sqrt{5}} \\ \frac{1}{2} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2} & \frac{3}{2\sqrt{5}} \\ \frac{1}{2} & \frac{1}{2\sqrt{5}} & -\frac{1}{2} & -\frac{3}{2\sqrt{5}} \\ \frac{1}{2} & \frac{3}{2\sqrt{5}} & \frac{1}{2} & \frac{1}{2\sqrt{5}} \end{pmatrix}. \tag{24}$$

Since $Q^TV = R$, we have $V = QR$ or

$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -\frac{3}{2\sqrt{5}} & \frac{1}{2} & -\frac{1}{2\sqrt{5}} \\ \frac{1}{2} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2} & \frac{3}{2\sqrt{5}} \\ \frac{1}{2} & \frac{1}{2\sqrt{5}} & -\frac{1}{2} & -\frac{3}{2\sqrt{5}} \\ \frac{1}{2} & \frac{3}{2\sqrt{5}} & \frac{1}{2} & \frac{1}{2\sqrt{5}} \end{pmatrix} \begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{5} & \sqrt{5} \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}. \tag{25}$$

Other QR–factorizations are possible, for example,

$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{3}{2\sqrt{5}} & \frac{1}{2} & \frac{1}{2\sqrt{5}} \\ -\frac{1}{2} & \frac{1}{2\sqrt{5}} & -\frac{1}{2} & -\frac{3}{2\sqrt{5}} \\ -\frac{1}{2} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2} & \frac{3}{2\sqrt{5}} \\ -\frac{1}{2} & -\frac{3}{2\sqrt{5}} & \frac{1}{2} & -\frac{1}{2\sqrt{5}} \end{pmatrix} \begin{pmatrix} -2 & -1 & -3 \\ 0 & -\sqrt{5} & -\sqrt{5} \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}. \tag{26}$$

The latter one is returned by MATLAB's `qr` function.[3]

Afterword: QR versus LU

Note that the QR–method could be applied to an n–by–n square system, to cast $A\mathbf{x} = \mathbf{b}$ into the form $R\mathbf{x} = Q^T\mathbf{x}$, which could then be solved by backward substitution. Why not just use QR in all cases and do away with the LU? The reason is that QR on a square system costs about $2n^3$ flops (using Givens rotations), whereas LU costs about $2n^3/3$. So it's mostly just that LU is cheaper. There is a less expensive way to perform QR (using so–called Householder reflections), but that method is still twice as expensive than LU.

[3] It's different presumably because MATLAB computes the factorization using Householder reflections rather than Givens rotations. See the *Afterword* section.