Lecture # 12
The Proper Use of Classical Gram–Schmidt

This lecture puts together a number of results that have not quite made the textbooks.

Adding a column to a QR decomposition using classical Gram–Schmidt (CGS).

$$X = Q_1 R$$

$X, Q_1 \in \mathbf{R}^{m \times n}$, $m > n$, Q_1 left orthogonal, and R upper triangular. Let

$$Q_1 = (\mathbf{q}_1, \ldots, \mathbf{q}_n).$$

Assume that Q_1 satisfies

$$Q_1^T Q_1 = I + L + L^T$$

where $L = (\ell_{ij})$ is strictly lower triangular. That is,

$$\ell_{ij} = \begin{cases} 0 & i \leq j \\ \mathbf{q}_i^T \mathbf{q}_j & i > j \end{cases}$$

We wish to add a column of X (and to Q_1) to obtain

$$\bar{X} = \begin{pmatrix} X & \mathbf{x}_0 \end{pmatrix} = \begin{pmatrix} Q_1 & \mathbf{q}_0 \end{pmatrix} \begin{pmatrix} R & \mathbf{f} \\ 0 & \beta \end{pmatrix} \tag{1}$$

where $Q_1^T \mathbf{q}_0 = 0$. In fact, we would like to have

$$\|Q_1^T \mathbf{q}_0\|_2 \leq \|L\|_2 \tag{2}$$

In fact, we let

$$E = L + L^T$$

then

$$Q_1^T Q_1 = I + E.$$

Note that

$$\|E\|_2 \leq 2\|L\|_2.$$

Thus the bound (2) is enforced by

$$\|Q_1^T \mathbf{q}_0\|_2 \leq \|L\|_2 \leq 0.5\|E\|_2. \tag{3}$$

We know from (1) that

$$\mathbf{x}_0 = Q_1\mathbf{f} + \beta\mathbf{q}_0.$$

To recover, $\mathbf{f}$, β, and $\mathbf{q}_0$, we compute

$$Q_1^T\mathbf{x}_0 = Q_1^T Q_1\mathbf{f} + \beta Q_1^T\mathbf{q}_0. \tag{4}$$

If $Q_1^T\mathbf{q}_0 = 0$ and $Q_1^T Q_1 = I$, then

$$\mathbf{f} = Q_1^T\mathbf{x}_0.$$

We then compute

$$\begin{aligned} \mathbf{r}_1 &= \mathbf{x}_0 - Q_1\mathbf{f} & (5) \\ \beta &= \|\mathbf{r}_1\|_2 & (6) \\ \mathbf{q}_0 &= \mathbf{r}_1/\beta. & (7) \end{aligned}$$

Equations (4)–(7) describe one step of classical Gram–Schmidt (CGS). So we relabel $\beta_1 = \beta$, $\mathbf{f}_1 = \mathbf{f}$ and $\mathbf{q}_0^{(1)}$ and assess how orthogonal $\mathbf{q}_0^{(1)}$ is to Q_1. Without loss of generality, we assume that

$$\|\mathbf{x}_0\|_2 = 1.$$

Otherwise, $\|\mathbf{x}_0\|_2$ is just factored through this analysis.

Note that

$$\begin{aligned} Q_1^T\mathbf{r}_1 &= Q_1^T\mathbf{x}_0 - Q_1^T Q_1\mathbf{f}_1 \\ &= Q_1^T\mathbf{x}_0 - Q_1^T Q_1\mathbf{f}_1 \\ &= (I - Q_1^T Q_1)\mathbf{f}_1 \\ &= E\mathbf{f}_1 \end{aligned}$$

Thus

$$\|Q_1^T\mathbf{r}_1\|_2 \leq \|E\|_2\|\mathbf{f}_1\|_2.$$

To get a bound on $\|Q_1^T\mathbf{q}_0^{(1)}\|_2$, note that

$$\|Q_1^T\mathbf{q}_0^{(1)}\|_2 \leq \|E\|_2\|Q_1^T\mathbf{x}_0\|_2/\beta_1.$$

Using the factor that

$$\beta_1^2 = \|\mathbf{r}_1\|_2^2 = \|\mathbf{x}_0 - Q_1\mathbf{f}_1\|_2$$

we get

$$
\begin{aligned}
\beta_1^2 &= \mathbf{x}_0^T \mathbf{x}_0 - 2\mathbf{x}_0^T Q_1 \mathbf{f}_1 + \mathbf{f}_1^T Q_1^T Q_1 \mathbf{f}_1 \\
&= 1 - 2\mathbf{f}_1^T \mathbf{f}_1 + \mathbf{f}_1^T (I + E)\mathbf{f}_1 \\
&= 1 - \mathbf{f}_1^T \mathbf{f}_1 + \mathbf{f}_1^T E \mathbf{f}_1 \\
&= 1 - \|\mathbf{f}_1\|_2^2 + \mathbf{f}_1^T E \mathbf{f}_1
\end{aligned}
$$

Thus

$$\|f_1\|_2^2 - \mathbf{f}_1^T E \mathbf{f}_1 = 1 - \beta_1^2$$

which implies (you can prove this)

$$\|f_1\|_2 \leq \sqrt{1 - \beta_1^2} / \sqrt{1 - \|E\|_2}.$$

Thus

$$
\begin{aligned}
\|Q_1^T \mathbf{q}_0^{(1)}\|_2 &\leq \frac{\|E\|_2}{\sqrt{1 - \|E\|_2}} \frac{\sqrt{1 - \beta_1^2}}{\beta_1} \\
&= \|E\|_2 \frac{\sqrt{1 - \beta_1^2}}{\beta_1} + O(\|E\|_2^2).
\end{aligned}
$$

We neglect the higher order term. Thus $\mathbf{q}_0^{(1)}$ satisfies (3) if

$$\frac{\sqrt{1 - \beta_1^2}}{\beta_1} \leq 0.5$$

which happens if and only if

$$\beta_1 \geq \sqrt{4/5}.$$

So, in that case, we accept $\beta = \beta_1$, $\mathbf{f}_1 = \mathbf{f}$, and $\mathbf{q}_0^{(1)} = \mathbf{q}_0$. Otherwise, we can reorthogonalize, by computing

$$
\begin{aligned}
\mathbf{f}_2 &= Q_1^T \mathbf{q}_0^{(1)} \\
\mathbf{r}_2 &= \mathbf{q}_0^{(1)} - Q_1 \mathbf{f}_2 \\
\beta_2 &= \|\mathbf{r}_2\|_2 \\
\mathbf{q}_0^{(2)} &= \mathbf{r}_2 / \beta_2
\end{aligned}
$$

We can again argue that

$$\|Q_1^T \mathbf{q}_0^{(2)}\|_2 \le \frac{\sqrt{1-\beta_2^2}}{\beta_2}\|E\|_2.$$

Thus, we test to see if

$$\beta_2 \ge \sqrt{4/5}.$$

If this is true, we accept $\mathbf{q}_0 = \mathbf{q}_0^{(2)}$ and let

$$\begin{aligned}\mathbf{f} &= \mathbf{f}_1 + \beta_1 \mathbf{f}_2 \\ \beta &= \beta_1 \beta_2\end{aligned}$$

and we have the factorization (1).

If $\beta_2 < \sqrt{4/5}$ there are two possibilities. If either $\beta_1 = 0$ or $\beta_2 = 0$, then we have the rank deficient factorization

$$\bar{X} = \begin{pmatrix} X & \mathbf{x}_0 \end{pmatrix} = Q_1 \begin{pmatrix} R & \mathbf{f} \end{pmatrix} \tag{8}$$

In this case, $\mathbf{q}_0$ is unnecessary!

The other possibility is that $\beta_2 \in (0, \sqrt{4/5})$. In that case, it can be shown that

$$\beta = \beta_1 \beta_2 = O(\|E\|_2)$$

implying that $\mathbf{x}_0$ is nearly dependent upon the columns of Q_1. One way to handle that is to set $\beta = 0$ and have the factorization (8). However, if we insist on a factorization, then there is another route to obtain a $\mathbf{q}_0$ – most any vector that is orthogonal to Q_1 will do.

To get a vector orthogonal to Q_1,we let $\mathbf{e}_k$ be the kth column of the identity matrix and choose k so that

$$\|Q_1^T \mathbf{e}_k\|_2 = \min_{1 \le j \le m} \|Q_1^T \mathbf{e}_j\|_2.$$

We note that since

$$\|Q_1\|_F^2 = \sum_{j=1}^{m} \|Q_1^T \mathbf{e}_j\|_2^2 = n$$

then

$$\|Q_1^T \mathbf{e}_k\|_2 \le \sqrt{n/m}.$$

If we apply two passes of CGS to $\mathbf{e}_k$ (this takes a little work, but you can verify this for yourself), we obtain a vector $\mathbf{q}_0$ such that

$$\|Q_1^T \mathbf{q}_0\|_2 \le \sqrt{n/(m-n)}\|E\|_2^2.$$

To obtain, a value for β, we compute

$$\beta = \beta_1 \mathbf{q}_0^T \mathbf{r}_2 = \mathbf{q}_0^T(\mathbf{x}_0 - Q_1 \mathbf{f}).$$

After an elaborate argument, one can show that

$$\mathbf{x}_0 + \delta \mathbf{x}_0 = \begin{pmatrix} Q_1 & \mathbf{q}_0 \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \beta \end{pmatrix}$$

where

$$\|\delta \mathbf{x}_0\|_2 = O(\|E\|_2).$$

This $\delta \mathbf{x}_0$ is thus small enough to be neglected!

The resulting MATLAB-like algorithm is as follows.

function $[\mathbf{q}_0, \mathbf{f}, \beta] =$ *add_column*$(Q_1, \mathbf{x}_0)$
$\beta_0 = \|\mathbf{x}_0\|_2$; % Take care of $\|\mathbf{x}_0\|_2$
$\mathbf{q}_0 = \mathbf{x}_0/\beta_0$;
$\mathbf{f}_1 = Q_1^T \mathbf{q}_0$;
$\mathbf{r}_1 = \mathbf{q}_0 - Q_1 \mathbf{f}_1$;
$\beta_1 = \|\mathbf{r}_1\|_2$;
if $\beta_1 == 0$
  $\beta = \beta_1$; $\mathbf{q}_0 = 0$; **quit**
end;
$\mathbf{q}_0 = \mathbf{r}_1/\beta_1$;
if $\beta_1 \ge \sqrt{0.8}$
  $\beta = \beta_0\beta_1$; $\mathbf{f} = \mathbf{f}_1$; **else**
  $\mathbf{f}_2 = Q_1^T \mathbf{q}_0$;
  $\mathbf{r}_2 = \mathbf{q}_0 - Q_1 \mathbf{f}_2$;
  $\beta_2 = \|\mathbf{r}_2\|_2$;
  if $\beta_2 \ge \sqrt{0.8}$
    $\mathbf{q}_0 = \mathbf{r}_2/\beta_2$;
    $\mathbf{f} = \mathbf{f}_1 + \beta_1 \mathbf{f}_2$;
    $\beta = \beta_0\beta_1\beta_2$;
  else

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      Find e_k such that
      ||Q_1^T e_k||_2 = min_{1≤j≤n} ||Q_1^T e_j||_2
      h_1 = Q_1^T e_k;
      t_1 = e_k − Q_1 h_1 ;
      q_0 = t_1/||t_1||_2;
      h_2 = Q_1^T q_0;
      t_2 = q_0 − Q_1 h_2;
      q_0 = t_2/||t_2||_2;
      β = β_0 β_1 q_0^T r_2;
   end;
end;
end add_column
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What this says is that if $\mathbf{x}_0$ is not dependent upon Q_1, then two steps of classical Gram–Schmidt will obtain an orthogonal $\mathbf{q}_0$, and a factorization of the form (1).

If $\mathbf{x}_0$ is dependent upon Q_1, we can obtain an acceptable factorization with two more Gram–Schmidt steps. The advantage of this algorithm is that the heavy lifting is done by matrix-vector multiplications rather than dot products. The former are more efficient than the latter on most modern architectures because they reduce memory accesses.

Next time, we will look at two algorithms from the literature that exploit the results above.