Numerical Algorithms for Visual Computing III 2011
Example Solutions for Assignment 8

Problem 1 (Gram-Schmidt Sucks Reloaded)
The goal of this exercise is to show at hand of two simple examples that the method of Gram and Schmidt may be subject to strong numerical errors, which may appear for large vectors or small machine accuracy.

1. Let us begin our analysis by considering both matrices first analytically and then numerically, we will then compare these results. Beginning with matrix A_1:

$$A_1 \quad := \quad \begin{pmatrix} 1 & 0 \\ 1 & 2 \\ 0 & 1 \\ 0 & 1 \end{pmatrix}$$

we have

$$w_1 := \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad w_2 := \begin{pmatrix} 0 \\ 2 \\ 1 \\ 1 \end{pmatrix}$$

Then we can compute the orthogonal vectors q_1, q_2 as follows:

$$\begin{aligned}
q_1 \quad &:= \quad \frac{w_1}{\|w_1\|} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\
q_2' \quad &:= \quad w_2 - \langle w_2, q_1 \rangle q_1 \\
&= \begin{pmatrix} 0 \\ 2 \\ 1 \\ 1 \end{pmatrix} - \left\langle \begin{pmatrix} 0 \\ 2 \\ 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right\rangle \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ 2 \\ 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \\ 1 \\ 1 \end{pmatrix} \\
q_2 \quad &:= \quad \frac{q_2'}{\|q_2'\|} = \frac{1}{2} \begin{pmatrix} -1 \\ 1 \\ 1 \\ 1 \end{pmatrix}
\end{aligned}$$

Computing numerically with 4-digit precision gives us:

$$\begin{aligned}
q_1 &:= \frac{w_1}{\|w_1\|} = 0.7071 \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\
q_2' &:= w_2 - \langle w_2, q_1 \rangle q_1 \\
&= \begin{pmatrix} 0 \\ 2 \\ 1 \\ 1 \end{pmatrix} - \left\langle \begin{pmatrix} 0 \\ 2 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0.7071 \\ 0.7071 \\ 0 \\ 0 \end{pmatrix} \right\rangle \begin{pmatrix} 0.7071 \\ 0.7071 \\ 0 \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ 2 \\ 1 \\ 1 \end{pmatrix} - 1.4142 \begin{pmatrix} 0.7071 \\ 0.7071 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -0.9999 \\ 1.0001 \\ 1 \\ 1 \end{pmatrix} \\
q_2 &:= \frac{q_2'}{\|q_2'\|} = \begin{pmatrix} -0.4999 \\ 0.5001 \\ 0.5 \\ 0.5 \end{pmatrix}
\end{aligned}$$

For our second matrix we can compute analytically

$$A_2 := \begin{pmatrix} 8 & 21 \\ 13 & 34 \\ 21 & 55 \\ 34 & 89 \end{pmatrix}$$

we have

$$w_1 := \begin{pmatrix} 8 \\ 13 \\ 21 \\ 34 \end{pmatrix} \qquad w_2 := \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix}$$

Then we can compute the orthogonal vectors q_1, q_2 as follows:

$$
\begin{aligned}
q_1 &:= \frac{w_1}{\|w_1\|} = \frac{1}{\sqrt{1830}} \begin{pmatrix} 8 \\ 13 \\ 21 \\ 34 \end{pmatrix} \\
q_2' &:= w_2 - \langle w_2, q_1 \rangle q_1 \\
&= \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix} - \left\langle \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix}, \frac{1}{\sqrt{1830}} \begin{pmatrix} 8 \\ 13 \\ 21 \\ 34 \end{pmatrix} \right\rangle \frac{1}{\sqrt{1830}} \begin{pmatrix} 8 \\ 13 \\ 21 \\ 34 \end{pmatrix} \\
&= \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix} - \frac{4791}{1830} \begin{pmatrix} 8 \\ 13 \\ 21 \\ 34 \end{pmatrix} = \frac{1}{1830} \begin{pmatrix} 102 \\ -63 \\ 39 \\ -24 \end{pmatrix} \\
q_2 &:= \frac{q_2'}{\|q_2'\|} = \frac{1}{\sqrt{16470}} \begin{pmatrix} 102 \\ -63 \\ 39 \\ -24 \end{pmatrix}
\end{aligned}
$$

Computing with 4-digit accuracy, this looks as follows

$$
\begin{aligned}
q_1 &:= \frac{w_1}{\|w_1\|} = 0.0234 \begin{pmatrix} 8 \\ 13 \\ 21 \\ 34 \end{pmatrix} = \begin{pmatrix} 0.1872 \\ 0.3042 \\ 0.4914 \\ 0.7956 \end{pmatrix} \\
q_2' &:= w_2 - \langle w_2, q_1 \rangle q_1 \\
&= \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix} - \left\langle \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix}, \begin{pmatrix} 0.1872 \\ 0.3042 \\ 0.4914 \\ 0.7956 \end{pmatrix} \right\rangle \begin{pmatrix} 0.1872 \\ 0.3042 \\ 0.4914 \\ 0.7956 \end{pmatrix} \\
&= \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix} - 112.1094 \begin{pmatrix} 0.1872 \\ 0.3042 \\ 0.4914 \\ 0.7956 \end{pmatrix} = \begin{pmatrix} 21 \\ 34 \\ 55 \\ 89 \end{pmatrix} - \begin{pmatrix} 20.9869 \\ 34.1037 \\ 55.0906 \\ 89.1942 \end{pmatrix} = \begin{pmatrix} 0.0131 \\ -0.1037 \\ -0.0906 \\ -0.1942 \end{pmatrix} \\
q_2 &:= \frac{q_2'}{\|q_2'\|} = 4.1942 \begin{pmatrix} 0.0131 \\ -0.1037 \\ -0.0906 \\ -0.1942 \end{pmatrix} = \begin{pmatrix} 0.0550 \\ -0.4349 \\ -0.3800 \\ -0.8145 \end{pmatrix}
\end{aligned}
$$

2. Now let us compare the analytical results with the numerical results. Obviously we would expect that the two vectors that we get by the Gram-Schmidt method to be orthogonal, i.e. it should hold

$$\cos(\alpha) \quad = \quad \frac{\langle q_1, q_2 \rangle}{\|q_1\| \cdot \|q_2\|}$$

and $\alpha = 90^\circ$ for orthogonal vectors. Computing for the analytical solution for the orthogonal vectors of matrix A_1, we get

$$\cos^{-1}(\langle q_1, q_2 \rangle) \quad = \quad \cos^{-1}(\frac{1}{2\sqrt{2}} - \frac{1}{2\sqrt{2}}) = \cos^{-1}(0) = 90^\circ$$

so this is the desired result. However, for the numerical solution, we get

$$\cos^{-1}(\langle q_1, q_2 \rangle) \quad = \quad \cos^{-1}(0.0001) =\approx 89.9943^\circ$$

which is nearly orthogonal, but shows that already significant numerical issues may arise. Coming to matrix A_2, we get for the analytical computed vectors

$$\cos^{-1}(\langle q_1, q_2 \rangle) \quad = \quad \cos^{-1}(0) = \cos^{-1}(0) = 90^\circ$$

but for the numerical solution

$$\cos^{-1}(\langle q_1, q_2 \rangle) \quad = \quad \cos^{-1}(-0.9569) = \cos^{-1}(0) = 163.1170^\circ$$

we can see quite a devastating effect, i.e. the resulting vectors are not orthogonal to each other.

3. We neglect for part three the vectors q_1 and q_2 of matrix A_1 and only consider the results from matrix A_2. As vector $w_1 = q_1 = \tilde{q}_1$ is already normalized, we only need to find a vector $\tilde{q}_2$ with the Gram-Schmidt algorithm:

$$\begin{aligned}
\tilde{q}_2 &= w_2 - \langle w_2, \tilde{q}_1 \rangle q_1 \\
&= \begin{pmatrix} 0.0550 \\ -0.4349 \\ -0.3800 \\ -0.8145 \end{pmatrix} - \langle \begin{pmatrix} 0.0550 \\ -0.4349 \\ -0.3800 \\ -0.8145 \end{pmatrix}, \begin{pmatrix} 0.1872 \\ 0.3042 \\ 0.4914 \\ 0.7956 \end{pmatrix} \rangle \begin{pmatrix} 0.1872 \\ 0.3042 \\ 0.4914 \\ 0.7956 \end{pmatrix} \\
&= \begin{pmatrix} 0.0550 \\ -0.4349 \\ -0.3800 \\ -0.8145 \end{pmatrix} + 0.9569 \begin{pmatrix} 0.1872 \\ 0.3042 \\ 0.4914 \\ 0.7956 \end{pmatrix} \\
&= \begin{pmatrix} 0.0550 \\ -0.4349 \\ -0.3800 \\ -0.8145 \end{pmatrix} + \begin{pmatrix} 0.1796 \\ 0.2919 \\ 0.4715 \\ 0.7635 \end{pmatrix} = \begin{pmatrix} 0.2346 \\ -0.1430 \\ 0.0915 \\ -0.0510 \end{pmatrix}
\end{aligned}$$

Then the scalar product between $\tilde{q}_1$ and $\tilde{q}_2$ is 0.0048 which results in an angle of 89.7250°. So a successive application may help orthogonalising vectors that have not been orthogonal in the first hand, however one should always consider numerical issues arising due to small machine accuracy.

Problem 2 (Gram-Schmidt Sucks Revolutions)

$$A := \begin{pmatrix} 1 & 2 & 1 \\ 0 & 1 & 2 \\ 1 & 2 & 0 \end{pmatrix}$$

Algorithm of the modified Gram-Schmidt:

$$
\begin{aligned}
&\text{for } k = 1...n \\
&\quad r_{kk} = ||a_k||_2 \\
&\quad q_k = 1/r_{kk} \cdot a_k \\
&\quad \text{for } j = (k+1)...n \\
&\qquad r_{kj} = q_k^\top a_j \\
&\qquad a_j := a_j - r_{kj} q_k \\
&\quad \text{end} \\
&\text{end}
\end{aligned}
$$

Solution:

In this exercise, we have: $a_1 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$, $a_2 = \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix}$ and $a_3 = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}$.

Now, we use the algorithm from above for $k = 1, 2, 3$:

For $k = 1$ and $j = 2, 3$, we get:

$$
\begin{aligned}
r_{11} &= ||a_1||_2 = \sqrt{2} \\
q_1 &= \frac{1}{r_{11}} \cdot a_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} \\
r_{12} &= q_1^\top a_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}^\top \cdot \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix} = 2\sqrt{2} \\
a_2 &:= a_2 - r_{12} q_1 = \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix} - 2\sqrt{2} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\
r_{13} &= q_1^\top a_3 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix}^\top \cdot \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \\
a_3 &:= a_3 - r_{13} q_1 = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} - \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 2 \\ -\frac{1}{2} \end{pmatrix}
\end{aligned}
$$

For $k = 2$ and $j = 3$, we get:

$$
\begin{aligned}
r_{22} &= ||a_2||_2 = \sqrt{0^2 + 1^2 + 0^2} = 1 \\
q_2 &= \frac{1}{r_{22}} \cdot a_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\
r_{23} &= q_2^\top a_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}^\top \cdot \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} = 2 \\
a_3 &:= a_3 - r_{23} q_2 = \begin{pmatrix} \frac{1}{2} \\ 2 \\ -\frac{1}{2} \end{pmatrix} - 2 \cdot \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ -\frac{1}{2} \end{pmatrix}
\end{aligned}
$$

For $k = 3$, we get:

$$r_{33} = ||a_3||_2 = \sqrt{\frac{1}{4} + 0 + \frac{1}{4}} = \frac{1}{\sqrt{2}}$$

$$q_3 = \frac{1}{r_{33}} \cdot a_3 = \frac{1}{\frac{1}{\sqrt{2}}} \cdot \begin{pmatrix} \frac{1}{2} \\ 0 \\ -\frac{1}{2} \end{pmatrix} = \sqrt{2} \cdot \begin{pmatrix} \frac{1}{2} \\ 0 \\ -\frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

This leads to the 2 matrix Q and R:

$$Q = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix} \qquad \text{and} \qquad R = \begin{pmatrix} \sqrt{2} & 2\sqrt{2} & \frac{1}{\sqrt{2}} \\ 0 & 1 & 2 \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}$$
