Three Approaches to Solving Least Squares Problems

Problem: Given $Z = \{x_1, x_2, x_3, x_4\}$ and the four functions $g_1, g_2, g_3,$ and f described by this table:

	g_1	g_2	g_3	f
x_1	1	1	1	1
x_2	.01	0	0	0
x_3	0	.01	0	0
x_4	0	0	.01	0

Find the best approximation to f from the span of $g_1, g_2,$ and g_3 in the least squares sense. Assume the work is done using three digit rounding floating point arithmetic. (Thus, in particular, $fl(1+.0001)=1$.)

1. Normal Equations:

Since $fl(1+.0001)=1$, we obtain the matrix $A^T A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$, which is singular. We cannot determine a unique solution.

2. Classical Gram-Schmidt:

After performing the orthonormalization, we have

	$\tilde{g}_1$	$\tilde{g}_2$	$\tilde{g}_3$
x_1	1	0	0
x_2	.01	$-.709$	$-.709$
x_3	0	.709	0
x_4	0	0	.709

. For coefficients, we calculate $\begin{bmatrix} a_1^* \\ a_2^* \\ a_3^* \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$. The residual $f - g^*$ on Z is $\begin{bmatrix} 0 \\ .01 \\ 0 \\ 0 \end{bmatrix}$ whose norm is $.01$

3. Modified Gram-Schmidt with coefficients computed directly:

After performing the orthonormalization, we have

	$\tilde{g}_1$	$\tilde{g}_2$	$\tilde{g}_3$
x_1	1	0	0
x_2	.01	−.709	−.407
x_3	0	.709	−.412
x_4	0	0	.82

. For coefficients, we again calculate $\begin{bmatrix} a_1^* \\ a_2^* \\ a_3^* \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$. The residual $f - g^*$ on Z is again $\begin{bmatrix} 0 \\ .01 \\ 0 \\ 0 \end{bmatrix}$ whose norm is $.01$

4. Modified Gram-Schmidt with coefficients computed by modification:

Now we have $\begin{bmatrix} a_1^* \\ a_2^* \\ a_3^* \end{bmatrix} = \begin{bmatrix} .331 \\ .334 \\ .335 \end{bmatrix}$. The residual $f - g^*$ on Z is $\begin{bmatrix} 0 \\ .00331 \\ .00334 \\ .00335 \end{bmatrix}$ whose norm is .005773578...

5. Exact Solution:

The exact solution is $x = \dfrac{10000}{30001}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$. The residual $f - g^*$ on Z is $\begin{bmatrix} 1/30001 \\ 100/30001 \\ 100/30001 \\ 100/30001 \end{bmatrix}$ whose norm is $.005773311\ldots$