

**Problem Set #7**  
**(Due October 22, 2008)**

**ORTHOGONALIZATION METHODS AND LEAST SQUARES**

1. Most orthogonalization methods in numerical analysis form the orthogonal matrix  $Q$  by accumulating elementary transformations (e.g., Householder, Givens, Gram-Schmidt, etc.). As a result, final  $Q$  is not quite orthogonal due to round-off accumulation. Develop an improvement scheme that will such a given, not quite orthogonal,  $Q$  and make it more orthogonal. The orthogonality error should decrease to zero with quadratic convergence.

(Hint: Use  $Q_{n+1} = Q_n + \alpha [I - Q_n Q_n^T] Q_n$ ;  $Q_0 = Q, \alpha = 1/2$ )

2. Suppose you know  $C_1 = [S^T S]^{-1}$ . Then, find  $C = [R^T R]^{-1}$ , where

$$R = \begin{bmatrix} \alpha & y^T \\ 0 & S \end{bmatrix}$$

3. Generate 11 data points by taking  $t_i = (i-1)/10$  and  $b_i = \text{erf}(t_i), i = 1, 2, \dots, 11$ . where:

$$\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+1}}{n!(2n+1)}$$

- (a) Fit the data in a least-squares sense with polynomials of degree from 1 to 10. Compare the fitted polynomial with  $\text{erf}(t)$  for a number of values of  $t$  between the data points, and see how the maximum error depends on  $n$ , the number of coefficients in the polynomial.
- (b) Since  $\text{erf}(t)$  is an odd function of  $t$ , that is,  $\text{erf}(t) = -\text{erf}(-t)$ , it is reasonable to fit the same data by a linear combination of odd powers of  $t$ ,

$$\text{erf}(t) \approx c_1 t + c_2 t^3 + \dots + c_n t^{2n-1}$$

Again, see how the error between data points depends on  $n$ . Since  $t$  varies over  $[0,1]$  in this problem, it is not necessary to consider using basis polynomials.

- (c) Polynomials are not particularly good approximations for  $\text{erf}(t)$  because they are unbounded for large  $t$ . So, using the same data points, fit a model of the form:

$$\text{erf}(t) \approx c_1 + e^{-t^2} (c_2 + c_3 z + c_4 z^2 + c_5 z^3)$$

where  $z = 1/(1+t)$ . How does the error between the data points compare with the polynomial models?

4. The following figures from the U.S. census Bureau give the population of the United states.

<u>Year</u>	<u>Population</u>
1900	75,994,575
1910	91,972,266
1920	105,710,620
1930	122,775,046
1940	131,669,275
1950	150,697,361
1960	179,323,175
1970	203,235,298
1980	226,547,082

5. An outlier can sometimes have a dramatic effect on the parameters in a model, and this is why it is important to check for such points, and determine if they are correct. To illustrate this point, we will consider the following artificial data set:

$$t_i = \begin{cases} i, & i=1,2,\dots,10 \\ 20, & i=11 \end{cases} ; \quad y_i = \begin{cases} 0, & i=1,2,\dots,10 \\ M, & i=11 \end{cases}$$

We will experiment with various values of M. Fit the data to a straight line using least-squares approach for  $M = 0, 5, 10, 15, 20$ . How rapidly do the parameters change as a function of  $M$ ? Using a scaled residual plot (i.e., residual/its standard deviation), is it possible to identify point 11 as a potential outlier?

6. Using weighted least squares, fit the following data by a quadratic polynomial:

$t$	$y$	$\sigma_y$
0.00	20.00	20.00
0.25	51.58	24.13
0.50	68.73	26.50
0.75	75.46	27.13
1.00	74.36	26.00
1.25	67.09	23.13
1.50	54.73	18.50
1.75	37.98	12.13
2.00	17.28	4.00

7. Many cyclic phenomena in nature can be modeled by a sinusoid and its higher harmonics:

$$y(t) = \sum A_i \sin \left[ \frac{2\pi}{(T/i)} (t + \phi_i) \right]$$

The number  $A_i, T$  and  $\phi_i$  are called the amplitude, period, and phase, respectively, of the  $i$ -th harmonic. Given data, fitting to this model in the least squares sense is a nonlinear least-squares problem. However, in many situations, the period  $T$  is known

or can be guessed, leaving only the amplitude and phase as unknowns. However, this still appears to be nonlinear because  $\phi_i$  is inside the sine. Can you find a transformation such that only a linear least squares problem need be solved?

8. Let  $A$  be an  $m$  by  $n$  matrix and define a diagonal matrix  $D = I + \delta \underline{e}_i \underline{e}_i^T$  for  $\delta > -1$ . Define the LS solution to  $\|D(A\underline{x} - \underline{b})\|_2$  by  $\underline{x}(\delta)$  and its residual by  $\underline{r}(\delta) = \underline{b} - A\underline{x}(\delta)$ . Express the  $k^{\text{th}}$  component of  $\underline{r}(\delta)$ , denoted by  $r_k(\delta)$ , in terms of  $r_k(0)$ .