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Date: 7.2.04
Homeworknumber: 3
Homework Title: 3.24

Problem description:

Verify that the dominant term in the operation count (number of multiplications or number of additions) for solving an $m \times n$ linear least squares problem using the normal equations and Cholesky factorisation is $mn^2/2 + n^3/6$.

Problem solution:

The normal equations method uses the $n \times n$ matrix $A^* := A^T A$ of the $m \times n$ matrix A for solving the linear least squares problem $Ax \cong b$. Solving the linear system works as follows:

$$Ax \cong b, \quad \text{the } m \times n \text{ linear system,} \quad (1)$$

$$A^T Ax \cong A^T b, \quad \text{we get an } n \times n \text{ matrix } A^* := A^T A, \quad (2)$$

$$LL^T x \cong A^T b, \quad \text{Cholesky factorisation of } A^* \text{ gives two} \quad (3)$$

triangular matrices L, L^T ,

$$Lz \cong b^*, \quad \text{solving the system for } z := L^T x \text{ and } b^* := A^T b, \quad (4)$$

$$L^T x \cong z, \quad \text{solving the system gives the solution } x. \quad (5)$$

Algorithm:

1. To get A^* from (2)

for $i = 1 : n$

for $j = i : n$

$$a_{ij}^* = \sum_{k=1}^m a_{ik} a_{jk}$$

$$a_{ji}^* = a_{ij}^*$$

end

$$b_i^* = \sum_{k=1}^m a_{ik} b_k$$

end

2. The Cholesky-Factorisation of A^* in (3)

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for  $j = 1 : n$ 
  for  $k = 1 : (j - i)$ 
    for  $i = j : n$ 
       $a_{ij}^* = a_{ij}^* - a_{ik}^* a_{jk}^*$ 
    end
  end
   $a_{jj}^* = \sqrt{a_{jj}^*}$ 
  for  $k = (j + 1) : n$ 
     $a_{kj}^* = a_{kj}^* / a_{jj}^*$ 
  end
end
end

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3. To step (4)

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for  $i = 1 : n$ 
   $z_i = \frac{b_i^* - \sum_{j=1}^{i-1} a_{ij}^* z_j}{a_{ii}^*}$ 
end

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4. Final solution (5)

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for  $i = 1 : n$ 
   $x_{n+1-i} = \frac{z_{n+1-i}^* - \sum_{j=n+1-i}^n a_{(n+1-i)j}^* z_j}{a_{(n+1-i)(n+1-i)}^*}$ 
end

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The number of multiplications s_m in the algorithm (for the dominant term the third and fourth step of the algorithm can be ignored):

$$\begin{aligned}
s_m &= \sum_{i=1}^n \left(\sum_{j=i}^n \left(\sum_{k=1}^m 1 \right) + \sum_{k=1}^m 1 \right) + \sum_{j=1}^n \left(\left(\sum_{k=1}^{j-1} \sum_{i=j}^n 1 \right) + 1 + \sum_{k=(j+1)}^n 1 \right) \\
&= \sum_{i=1}^n \left((n - i + 1)m + m \right) + \sum_{j=1}^n \left((j - 1)(n - j + 1) + 1 + (n - j) \right) \\
&= nm(n + 2) - m \sum_{i=1}^n i + \sum_{j=1}^n (jn - j^2 + j) \\
&= nm(n + 2) - m \frac{n(n + 1)}{2} + (n + 1) \frac{n(n + 1)}{2} - \frac{n(n + 1)(2n + 1)}{6} \\
&= \frac{mn^2}{2} + \frac{3mn}{2} + \frac{n^3}{6} + \frac{n^2}{2} + \frac{n}{3}
\end{aligned}$$

The number of additions s_a in the algorithm (for the dominant term the

third and fourth step of the algorithm can be ignored):

$$\begin{aligned}
s_a &= \sum_{i=1}^n \left(\sum_{j=i}^n (m-1) + (m-1) \right) + \sum_{j=1}^n \left(\sum_{k=1}^{j-1} \sum_{i=j}^n 1 \right) \\
&= \sum_{i=1}^n \left((n-i+1)(m-1) + (m-1) \right) + \sum_{j=1}^n \left((j-1)(n-j+1) \right) \\
&= n(m-1)(n+2) - (m-1) \frac{n(n+1)}{2} + \sum_{j=1}^n (nj - n - j^2 + 2j - 1) \\
&= \frac{mn^2}{2} + \frac{3mn}{2} - \frac{n^2}{2} - \frac{3n}{2} - \\
&\quad - (n+1)n + (n+2) \frac{n(n+1)}{2} - \frac{n(n+1)(2n+1)}{6} \\
&= \frac{mn^2}{2} + \frac{3mn}{2} + \frac{n^3}{6} - \frac{n^2}{2} - \frac{5n}{3}
\end{aligned}$$

Results:

The dominant term in the operation count is both for additions and for multiplications $mn^2/2 + n^3/6$