18.335 Mid-term Exam (Fall 2009)

Problem 1: Caches and QR (30 pts)

In class, we learned the Gram-Schmidt and modified Gram-Schmidt algorithms to form the (reduced) A=QR factorization of an $m\times n$ matrix A (with independent columns a_1,a_2,\ldots and $n\leq m$). In particular, for simplicity let us consider the computation of the $m\times n$ matrix Q only (whose columns are the orthonormal basis for the column space of A), not worrying about keeping track of R, and for simplicity consider classical (not modified) Gram-Schmidt:

$$\begin{array}{l} q_1 = a_1/\|a_1\| \\ \text{for } j = 2, 3, \dots, n \\ v_j = a_j - \sum_{i=1}^{j-1} q_i(q_i^*a_j) \\ q_j = v_j/\|v_j\| \end{array}$$

In this question, you will consider the cache complexity of this algorithm with an ideal cache of size Z (no cache lines). If the algorithm is implemented directly as written above, there is little temporal locality and $\Theta(mn^2)$ misses are required, independent of Z. You are also **given** that you can multiply an $m \times n$ matrix with an $n \times p$ matrix using $\Theta(mn + np + mp + mnp/\sqrt{Z})$ misses, and can add two $m \times n$ matrices using $\Theta(mn)$ misses.

- 1. Suppose that n is even and we have performed QR factorization (by some algorithm) on the first-half n/2 columns of A to obtain an $m \times (n/2)$ matrix Q_1 , and also on the second-half n/2 columns separately to obtain an $m \times (n/2)$ matrix Q_2 . Using Q_1 and Q_2 , describe how to (efficiently) find the $m \times n$ matrix Q from the QR factorization of A, and give the number of cache misses (in Θ notation, ignoring constant factors).
- 2. Describe an algorithm to compute the Q from the QR factorization of A that has fewer than $\Theta(mn^2)$ misses asymptotically, and give the number of cache misses (in Θ notation, ignoring constant factors). (You can describe either a cache-oblivious or blocked algorithm, but I find a recursive cache-oblivious algorithm easier.) You can assume that n is a power-of-2 size, for convenience.

Problem 2: Lanczos (30 pts)

Let A be a Hermitian $m \times m$ matrix with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_m$ and corresponding orthonormal eigenvectors $\hat{q}_1, \hat{q}_2, \dots, \hat{q}_m$. Consider the Lanczos algorithm applied to A:

$$\begin{array}{l} \beta_0=0\text{, }q_0=0\text{, }b=\text{arbitrary, }q_1=b/\|b\|\\ \text{for }n=1,2,3,\dots\\ v=Aq_n\\ \alpha_n=q_n^Tv\\ v\leftarrow v-\beta_{n-1}q_{n-1}-\alpha_nq_n\\ \beta_n=\|v\|\\ q_{n+1}=v/\beta_n \end{array}$$

After m steps, recall that this gives a unitary matrix $Q = (q_1q_2\cdots q_m)$ and a

tridiagonal matrix
$$T = \begin{pmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \ddots \\ & & \ddots & \ddots \end{pmatrix}$$
 such that $AQ = QT$.

Suppose that the initial b is orthogonal to one of the eigenvectors \hat{q}_i corresponding to a simple (not repeated) eigenvalue λ_i . Explain why the Lanczos process must break down ($\beta_n = 0$ for some n) if it is carried out in exact arithmetic (no rounding), and the T_n matrix (the $n \times n$ upper-left corner of T) at the n-th step (where breakdown occurs) cannot have an eigenvalue λ_i .

Problem 3: Backwards stability (30 pts)

Let A be any invertible $m \times m$ matrix and b be any vector in \mathbb{C}^n , and consider the function $f(A,b) = A^{-1}b$: that is, the function returning the solution to Ax = b. Now, consider the analogous function $\tilde{f}(A,b)$ implemented in floating-point arithmetic by a **backwards-stable** algorithm, e.g. Gaussian elimination with partial pivoting, or Householder QR factorization. That is, if we let f(A,b) = x (the solution: x is the *output* in this case) and $\tilde{f}(A,b) - f(A,b) = \delta x$ (the rounding error in the solution), then there is some δA and δb where $(A+\delta A)(x+\delta x) = b + \delta b$ and δA and δb are (yadda yadda...you should know the precise definition by now).

Show that if $\tilde{f}(A,b)$ is backwards stable with respect to the inputs A and b, then it must be backwards stable with respect to A alone. That is, find a small $\delta A' = \|A\| O(\varepsilon_{\text{machine}})$ such that $(A + \delta A')(x + \delta x) = b$.

(Hint: if you need to construct a matrix to turn one vector into another, you can always use a unitary rotation followed by a rescaling. And, of course, you can pick any convenient norm that you want, by the equivalence of norms.)

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