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REDUCING THE NUMBER OF FLOATING POINT OPERATIONS IN THE JACOBI METHOD

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ABSTRACT – We present a strategy for reducing the number of floating point operations required by the Jacobi method for finding eigenvalues of symmetric matrices. Experiments show that our strategy can reduce the execution time of this method in practice.

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Reducing the number of floating point operations in the Jacobi method

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Abstract

We present a strategy for reducing the number of floating point operations required by the Jacobi method for finding eigenvalues of symmetric matrices. Experiments show that our strategy can reduce the execution time of this method in practice.

key words. Jacobi method for eigenvalues.

1. Introduction

This paper presents a strategy for reducing the number of floating point operations (flops) required by the classical Jacobi method for finding eigenvalues of symmetric matrices. Similar ideas can be applied to one sided Jacobi methods. We assume that the reader is familiar with the Jacobi method. [P]. This paper is based on the observation that, for matrices of the same size, one sweep of the Jacobi method requires twice as many flops as matrix multiplication. In order to describe our strategy we need the concept of *principal submatrix*. We say that a $k \times k$ matrix B is principal submatrix of a $n \times n$ matrix A if B can be obtained by choosing a set $D \in \{1, \ldots, n\}$ with $n-k$ indices and deleting the rows and columns of A with index in D. Our strategy consists in roughly halfing the operation count for the Jacobi method by decomposing the matrix in principal submatrices, accumulating the rotations with pivots in these submatrices and using matrix multiplication to apply these rotations to the rest of the matrix. By analogy with the traditional block Jacobi methods, we call such strategy a *submatrix Jacobi method.*

Recursive submatrix Jacobi methods lead to orderings for which one sweep can be applied using only $O(n^{\frac{3+\alpha}{2}})$ flops, where $\alpha < 2.37$ is the smallest exponent for which we can multiply $n \times n$ matrices in $O(n^\alpha)$ flops, instead of the usual $O(n^3)$ flops. As expected, the constants hidden in the $O(n^\alpha)$ make them useless. We will not pursue this kind of result. More realistically, we can still save a factor ranging from $\frac{3}{2}$ to 2, depending on how our machine performs $ax + b$. If we count $ax + b$ as one operation, or count only multiplies and neglect adds, then the proposed strategy reduces the number of operations in one sweep from $2n^3 + O(n^2)$ to $n^3 + o(n^3)$. If we count $ax + b$ as two operations, then the strategy leads to a reduction of the number of operations in one sweep from $3n^3 + O(n^2)$ to $2n^3 + o(n^3)$.

The rest of the paper is organized as follows. In the next section we present our basic idea. In section 3 we present some suggestions on how to implement it and in section 4 we show experiments comparing its performance and accuracy with a traditional Jacobi method on an IRIX station.

A note of caution: doubling the performance is well within reach of usual optimizing techniques. The experiments in section 4 show that our idea may win or loose, depending for example on how the compiler optimizes. The purpose of this paper is to present a simple idea, not to discuss the myriad of factors involved in practical implementations.

2. The basic idea

We restrict ourselves to machines that perform $ax + b$ as the basic floating point operation. Let us count the number of flops in one rotation of the Jacobi method. We first compute the angle, which requires $\alpha = O(1)$ flops. Next we update $2n$ entries (because of symmetry) using the expression

$$\tilde{a}_{rs} = \cos a_{rs} \pm \sin a_{uv} = \cos(a_{rs} \pm \tan a_{uv}),$$

requiring 2 flops per entry. Thus, one rotation requires $4n + \alpha$ flops. Since one sweep corresponds to $\frac{n(n-1)}{2}$ rotations, it requires $2n^3 + \alpha\frac{n(n-1)}{2}$ flops. Therefore, in the case when $\alpha \ll n$, one sweep is roughly equivalent to two matrix multiplications.

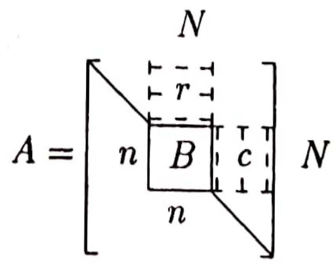

Figure 1. Entries affected by rotations in B.

Let us now analyze what happens when we perform all the rotations in the diagonal block B, of size n, of the matrix A, which has size N, accumulate these rotations in the $n \times n$ matrix J_B, and then apply all the rotations to A at once, using multiplication by J_B. One sweep for B takes $2n^3 + \alpha\frac{n(n-1)}{2}$ flops and forming J_B

requires an extra $2n^3$ flops. We need then to update the other entries of A. Entries above B (see Figure 1), are updated via $\tilde{r} = r \cdot J_B^T$, and entries to the right of B, are updated using the formula $\hat{c} = J_B.c$. Thus, updating either r or c requires n^2 flops and, since the total number of vectors r's and c's is equal to $N - n$, the overall work, in flops, is

$$4n^3 + (N-n)n^2 + \alpha\frac{n(n-1)}{2} = Nn^2 + 3n^3 + \alpha\frac{n(n-1)}{2}. \tag{2.1}$$

On the other hand, applying one Jacobi rotation at a time to A would require

$$2n(n-1)N + \alpha\frac{n(n-1)}{2} \tag{2.2}$$

flops. Thus the ratio of the work performed when accumulating the rotations to the work performed by applying one rotation at a time is

$$\rho = \frac{Nn^2 + 3n^3 + \alpha\frac{n(n-1)}{2}}{2n(n-1)N + \alpha\frac{n(n-1)}{2}}. \tag{2.3}$$

In the case $\alpha \ll N$ we have

$$\rho \approx \frac{1 + 3\frac{n}{N}}{2(1 - \frac{1}{n})},$$

and if $1 \ll n \ll N$ then $\rho \approx 1/2$. As a conclusion, in the case $\alpha \ll n \ll N$ we can save roughly half of the flops by accumulating the rotations.

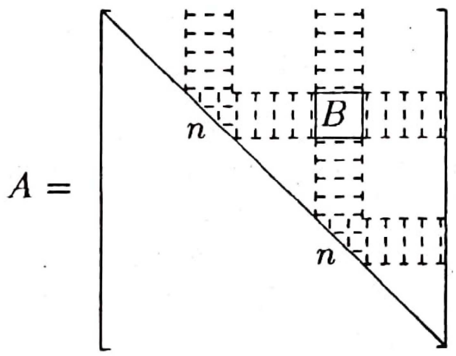

Figure 2. Entries affected by rotations in B.

It is important to have a diagonal block in the argument above, because if B is not diagonal (Figure 2) then the rotations in B act upon $2n$ rows and columns of A, whereas one sweep on a diagonal block acts only in n rows and columns of A. Accumulating the rotations is not as efficient in this case. However, the same analysis holds if B is a principal submatrix of A, because principal submatrices are nothing but diagonal blocks disguised by a permutation of rows and columns.

Here our approach diverges from usual block Jacobi methods:

We decompose the matrix as a union of principal submatrices S_k, of size n_k, with $1 \ll n_k \ll N$, and apply the rotations in each submatrix by first accumulating them and then using matrix vector multiplication to update the rest of the matrix.

In order to apply this idea efficiently, we need a simple scheme to decompose the off-diagonal part of A in principal submatrices S_k, i.e., finding $D_k = \{\, i \mid (i,i) \in S_k \,\}$ such that for every pair (i,j), $i \neq j$, there exists exactly one D_k containing i and j. It turns out that this can be easily done if $N = p^2$, where p is a prime number, and we describe now a simple method to achieve that. The method is based on the so called *finite plane geometries* $EG(2,p^2)$ (see [BM].) We think of the p^2 diagonal entries as being points in a "plane mod p", associating d_i with $(i - p\left\lfloor \frac{i}{p} \right\rfloor, \left\lfloor \frac{i}{p} \right\rfloor)$. ($\lfloor x \rfloor$ is the biggest integer less than or equal to x). In other words, the first coordinate of the point associated with d_i is the remainder in the division of i by p and the second coordinate is the quocient.

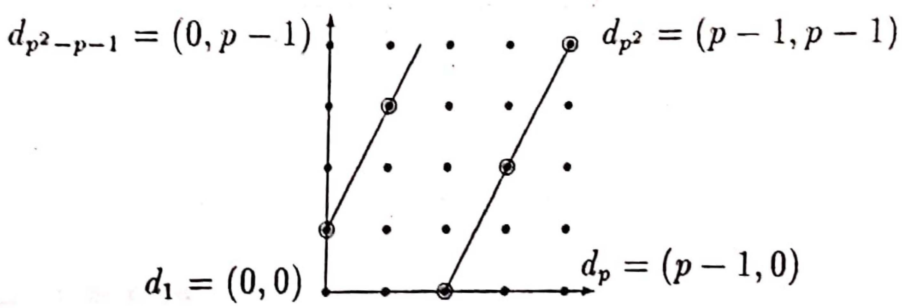

Figure 3: $EG(2,p^2)$, i.e., $\mathbb{Z} \times \mathbb{Z}$ with coordinates taken mod p, and a (single) straight line, with inclination 2.

The D_k's can be taken to be the straight lines in this finite plane. There are two kinds of straight lines: vertical and inclined. The vertical lines are determined by their intersection with the x axis. The vertical line that contains $(k,0)$ is formed by the points (k, pi) for $i = 0, \ldots, p-1$. (Keep in mind that we are thinking mod p.) Each inclined straight line is determined by its intersection with the y axis and by its inclination λ, which is between 0 and $p-1$ (inclusive). The inclined straight line with inclination λ that contains $(0,k)$ is formed by the points $(i, k + \lambda i)$, for $i = 0, \ldots, p-1$. There are p vertical and p^2 inclined straight lines, given a total of $p^2 + p$ straight lines. As for the usual Euclidean geometry, two distinct straight lines in $EG(2,p^2)$ can have at most one point in common, which implies that the off-diagonal of the S_k's are disjoint. Any two points are connected by some straight line, which implies that the union of the S_k's is indeed A. (see [BM] for proofs of these results.)

The natural question is then what to do if $N \neq p^2$. We propose the following: find the smallest prime p for which $N < p^2$, which we call p_N, and consider only the N points in $EG(2, p_N^2)$ forming a region R as in the Figure 4.

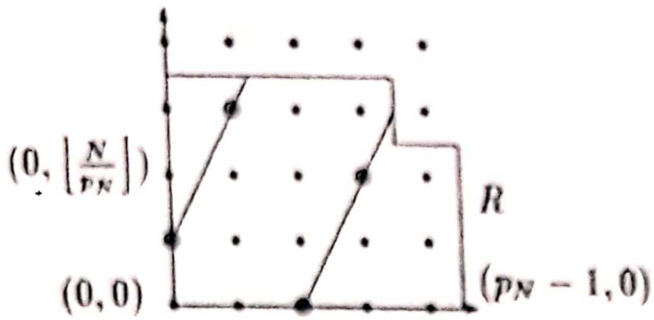

Figure 4: $EG(2, p_N^2)$ and a truncated straight line with inclination 2.

The D_k's are now built as truncated straight lines, containing only the points in R. To be more precise, we exclude from the straight lines points in the set

$$X = \{ (x, y) \mid y > \left\lfloor \frac{N}{p_N} \right\rfloor \} \bigcup \{ (x, \left\lfloor \frac{N}{p_N} \right\rfloor + 1) \mid x > p_N - p_N \left\lfloor \frac{N}{p_N} \right\rfloor \}. \qquad (2.4)$$

This method works because p_N is not much bigger than $\sqrt{N}$. To be more precise,

Lemma 1. *If* $N < 10^8$, *then* $p_N < 1.6\sqrt{N}$.

proof: The proof is by brute force: we wrote a computer program that verified the lemma above for all $1 \leq N \leq 10^8$.

The restriction $N < 10^8$ in Lemma 1 is superfluous. However, to prove lemma 1 without it would require some Analytic Number theory. Since the Jacobi method is used for dense matrices, 10^8 suffices for practical applications and we decided to state the lemma 1 as above. The interested reader can use the results in [A] to prove Lemma 1 for N arbitrary and to show that

$$\lim_{N \to \infty} \frac{\sqrt{N}}{p_N} = 1. \qquad (2.5)$$

Let us now analyze, for $N < 10^8$, what happens when we remove the points in X from the straight lines in $EG(2, p_N^2)$. The top $p_N - \lfloor N/p_N \rfloor - 1$ horizontal straight lines will become empty. The horizontal line passing through $(0, \lfloor N/p_N \rfloor)$ can also be significantly reduced. However, the other truncated straight lines will have on the order of $\sqrt{N}$ points. In fact, let r be one of these straight lines and let n_r be the number of points left in r after deleting the points in X. Since r is a straight line in $EG(2, p_N^2)$, it has p_N points. Therefore $n_r < 1.6\sqrt{N}$. On the other hand, r intercepts each of the $p_N - \lfloor \frac{N}{p_N} \rfloor$ top horizontal straight lines in at most one point. Therefore, the intersection of X and r has at most $p_N - \lfloor \frac{N}{p_N} \rfloor$ points. Since r has p_N points,

$$n_r \geq p_N - (p_N - \left\lfloor \frac{N}{p_N} \right\rfloor) = \left\lfloor \frac{N}{p_N} \right\rfloor \geq \left\lfloor \frac{N}{1.6\sqrt{N}} \right\rfloor > 0.62\sqrt{N} - 1.$$

Summarizing, $p_N - \left\lfloor \frac{N}{p_N} \right\rfloor$ lines will be completely removed, the horizontal line through $(0, \left\lfloor \frac{N}{p_N} \right\rfloor)$ may be truncated to any size, and the other truncated lines will have on the order of $\sqrt{N}$ points. In fact, using (2.5), it can be shown that asymptotically, as $N \to \infty$, they will have $\sqrt{N}$ points. Therefore, $1 \ll n_r \ll N$ for all the remaining straight lines but one and the analysis of the case $N = p^2$ is valid for all N.

Most of the work in pivoting the entries in S_k according to our strategy is performed when applying the rotation to the rest of A. We could apply several sweeps to S_k, accumulate the rotations, apply them to A at once, and still pay roughly the same number of flops. Since we are performing more rotations, we would expect faster convergence. Unfortunately, experiments show that the resulting improvement in convergence is not worth the extra work.

3. Implementation

In this section we describe how we implemented the algorithm. As before, N denotes the dimension of the matrix and p_N is the smallest prime bigger than or equal to $\sqrt{N}$. The diagonal entry d_i is associated to $(i - p_N \left\lfloor \frac{i}{p_N} \right\rfloor, \left\lfloor \frac{i}{p_N} \right\rfloor) \in EG(2, p_N^2)$. The algorithm loops over all the straight lines in $EG(2, p_N^2)$. For each straight line, it creates a vector of diagonals, DIAG, by associating to each point $(x, y) \in EG(2, p_N^2)$, with $0 \leq x, y < p_N$, the diagonal $x + yp_N$ and discarding the diagonals bigger than or equal to N.

Each instance of the vector DIAG may have a different number of entries, n, with $n \leq p_N$. If $n \geq 2$, then we move the submatrix corresponding to the rows and columns of M with indices in DIAG to a $n \times n$ auxiliary matrix MAUX. We then apply one sweep of the usal Jacobi method to MAUX, accumulating the rotations in a $n \times n$ matrix ROT. In other to apply the rotations to the remaining entries of M, we perform a loop in which we gather n of them in a vector VAUX at a time, make VAUX = ROT $\times$ VAUX and scatter the entries of VAUX back to the original matrix. Since $p_N = O(\sqrt{N})$, the size of the work space is $O(p_N^2) = O(N)$ and is negligible compared to the size of M (N^2 .)

4. Experiments

In this section we present experimental results that give a fair view of the performance of our idea: it can work but it is sensitive, for example, to the way the compiler optimizes. The experiments also show that, at least for random matrices, our strategy is as accurate as the usual ones. Our test matrices were obtained by adding random matrices, with entries taken from a uniform distribution in $[0, 1]$, to their transpose. For the matrices with size up to 200 we used 200 samples and for the matrices of size 400 we used 20 samples. The routines were coded in $C{+}{+}$, in double precision, and executed on an IRIX station. We stopped iterating when the Frobenius norm of the off-diagonal dropped below 10^{-15}.

Average Performance						
n	time in seconds				Number of Sweeps	
	Default optimization		Level 2 optimization			
	row	submatrix	row	submatrix	row	submatrix
50	0.61	2.13	0.61	1.02	8.01	7.96
100	4.98	17.0	4.97	5.07	8.96	8.39
200	46.8	99.3	46.5	37.8	9.32	9.02
400	603	885	563	313	10	10

In the performance experiments, we compared our strategy with the traditional ordering by rows. The column with the number of sweeps indicates that submatrix Jacobi methods converge slightly faster than the usual strategies, but we do not have an explanation for this fact and we do not believe it is significant. "optimization" indicates the level of optimization used when compiling both routines. Notice how optimization affects the relative costs of the row and submatrix Jacobi methods. With level 2 optimization it pays to use the submatrix Jacobi method for dimension $n \geq 200$. In comparison, with default optimization $n = 400$ is not big enough to amortize the overhead associated with the submatrix Jacobi method. This happens because optimization changes the relative costs of the crucial operations in the usual and submatrix Jacobi methods. Most of the time in usual methods is spent evaluating the expression

$$a_{ij} = \cos *(a_{ij} \pm \tan *a_{is}), \tag{4.6}$$

whereas in submatrix Jacobi methods

$$r = r + x * y \tag{4.7}$$

accounts for most of the work. The optimized version of (4.6) costs about three times more than the optimized version of (4.7). However, the default version of (4.6) is only 1.27 times more expensive than the default version of (4.7).

Accuracy				
n	Maximum Absolute difference		Maximum Relative difference	
	column	submatrix	column	submatrix
50	-13.7	-13.4	-11.8	-11.9
100	-13.3	-13.1	-11.6	-11.7
200	-12.8	-12.8	-11.2	-11.3
400	-12.6	-12.5	-11.9	-11.8

In the accuracy experiments we compared

$$\delta_c = \max_{i=1,n} \log_{10} |\lambda_i^{(c)} - \lambda_i^{(r)}| \quad \text{and} \quad \delta_m = \max_{i=1,n} \log_{10} |\lambda_i^{(m)} - \lambda_i^{(r)}|,$$

where $\lambda_i^{(\theta)}$ is the ith eigenvalue computed using ordering θ, which can be the ordering by rows (r), by columns (c) or come from a submatrix Jacobi method (m). In the first column of the accuracy table, we have the maximum value attained by δ_c. In the second column, we list the maximum value of δ_m. The third and fourth columns present the maximum of

$$\rho_c = \max_{i=1,n} \log_{10} \frac{|\lambda_i^{(c)} - \lambda_i^{(r)}|}{|\lambda_i^{(r)}|} \quad \text{and} \quad \rho_m = \max_{i=1,n} \log_{10} \frac{|\lambda_i^{(m)} - \lambda_i^{(r)}|}{|\lambda_i^{(r)}|}.$$

Since the ordering by columns is as accurate as the ordering by rows. and the experiments show that $\delta_c \approx \delta_m$ and $\rho_c \approx \rho_m$, we conclude that submatrix Jacobi methods do not sacrifice accuracy for this class of matrices.

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