

A Generalization of a Subspace Method for the Symmetric Eigenvalue Problem

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We present a method for computing the eigenvalues of a symmetric matrix A . This method consists in expressing A in the form $A = QXQ^T$, where Q is an orthonormal matrix and X has nonzero components only on main and cross diagonals. The convergence analysis, a comparison with the subspace method and a numerical experiments on a parallel machine are set out.

1. INTRODUCTION

The numerical solutions of the eigenvalues and the corresponding eigenvectors of a large matrix arise in numerous scientific applications. The most popular methods developed to solve this problem are the Jacobi algorithm, the QR algorithm, the Givens method, the Householder transformation [8,9] and the methods based on projection techniques on appropriate subspaces such as Lanczos and Davidson methods [6,10]. An other way to solve this problem is to factorize the matrix A in the form $A = WZW^{-1}$ where W and Z have the form of the matrices introduced by Evans et al. [4,5] for the WZ factorization. This method and its parallel implementation are presented in [1,2].

Let A be a symmetric matrix of order n with n real eigenvalues $\lambda_1, \dots, \lambda_n$. We assume that the multiplicity of each λ_i is ≤ 2 and that $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$. The method, presented in this paper, consists in expressing A in the form $A = QXQ^T$, where Q is an orthonormal matrix and the matrix X having nonzero components only on main and cross diagonals. We will say that X is a *crosswise* matrix. Such matrices and those introduced by the WZ factorization, present similar characteristics with diagonal matrices. Indeed, for solving a linear system $Xy = b$ or for computing the eigenvalues of X they require

$O(n)$ time steps. On the other hand, the associated sequence of computational operations is suitable for the parallel systems [5,9].

Our method consists in computing $m = \lfloor \frac{n-1}{2} \rfloor$ orthonormal matrices Q_i , $1 \leq i \leq m$, such that $X = (Q_1 Q_2 \dots Q_m)^T A (Q_1 Q_2 \dots Q_m)$ is a crosswise matrix. At each step k , we solve a nonlinear system, by using a subspace method, in order to find the matrix Q_k . As corollary of this method, we prove that any symmetric matrix having n real eigenvalues each of multiplicity ≤ 2 is similar to a crosswise one.

The paper is organized as follows. First, we present an algorithm for computing the two dominant eigenelements of A . We expose its characteristics and we show why it leads into the factorization $A = QX^TQ$. Next, we prove the convergence of the algorithm. Finally, we show, via numerical tests on a parallel machine, that our algorithm is faster than the subspace method.

2. THE METHOD

The method consists in computing an orthonormal matrix Q and a crosswise matrix X such that A can be expressed as $A = QXQ^T$. It requires $m = \lfloor \frac{n-1}{2} \rfloor$ steps. At step 1, we compute an orthonormal matrix Q_1 such that $A^{(1)} = Q_1^T A Q_1$ is symmetric and of the form below

$$A^{(1)} = \begin{pmatrix} a_{11}^{(1)} & 0 & \dots & 0 & a_{1n}^{(1)} \\ 0 & a_{22}^{(1)} & \dots & a_{2n-1}^{(1)} & 0 \\ \vdots & & a_{ij}^{(1)} & & \vdots \\ 0 & a_{n-12}^{(1)} & \dots & a_{n-1,n-1}^{(1)} & 0 \\ a_{1n}^{(1)} & 0 & \dots & 0 & a_{nn}^{(1)} \end{pmatrix}. \quad (1)$$

That is, $a_{1j}^{(1)} = a_{j1}^{(1)} = a_{nj}^{(1)} = a_{jn}^{(1)} = 0$ for $2 \leq j \leq n-1$. Let $Q_1 = (q_1, \dots, q_n)$, here $q_i \in \mathbb{R}^n$, $1 \leq i \leq n$, is the i -th column of Q_1 . Let $\langle u, v \rangle$ denotes the scalar product of u and v and $\|u\|$ the Euclidian norm of u . Then $A = Q_1 A^{(1)} Q_1^T$ with Q_1 orthonormal and $A^{(1)}$ of the form (1) imply the following two systems

$$(S_1) \begin{cases} Aq_1 & = a_{11}^{(1)} q_1 + a_{1n}^{(1)} q_n \\ Aq_n & = a_{1n}^{(1)} q_1 + a_{nn}^{(1)} q_n \\ \langle q_1, q_n \rangle & = 0 \\ \|q_1\| & = 1 \\ \|q_n\| & = 1 \end{cases}, \quad (S_2) \begin{cases} Aq_j = \sum_{k=2}^{n-1} a_{kj}^{(1)} q_k \\ \forall 2 \leq j \leq n-1 \end{cases}.$$

Note that (S_1) is a nonlinear system of $2n+3$ equations and $2n+3$ unknowns ($a_{11}^{(1)}, a_{1n}^{(1)} = a_{n1}^{(1)}, a_{nn}^{(1)}$ and the $2n$ components of q_1 and q_n). (S_1) has no unique solution. Indeed, if q_1, q_n are solutions of (S_1) then any rotation of these two

vectors is also a solution of (S_1) . Moreover any algorithm that computes a linear combination of two eigenvectors can be used for solving (S_1) . The following algorithm, used for computing the solutions q_1 and q_n , is a generalization of the subspace method. Further we show how to deduce λ_1, λ_2 and the corresponding eigenvectors from q_1 and q_n and how to factorize A in the form $A = QXQ^T$.

2.1. Algorithm for solving S_1

Let $u^0 \in \mathbb{R}^n$ and $v^0 \in \mathbb{R}^n$ with $\|u^0\| = \|v^0\| = 1$ and $\langle u^0, v^0 \rangle = 0$;
 $p = 0, 1, 2, \dots$ until convergence

$$\gamma_{1,p} = \|Au^p\|; \gamma_{2,p} = \|Av^p\|; \gamma_{3,p} = \langle Au^p, Av^p \rangle; \gamma_p = \sqrt{\gamma_{1,p}^2 \gamma_{2,p}^2 - \gamma_{3,p}^2};$$

$$\tan \theta_p^s = \frac{\gamma_{3,p}}{\gamma_{1,p}^2 + \gamma_p};$$

$$\begin{pmatrix} u^{p+1} \\ v^{p+1} \end{pmatrix} = \begin{pmatrix} \cos \theta_p^s & -\sin \theta_p^s \\ \sin \theta_p^s & \cos \theta_p^s \end{pmatrix} \begin{pmatrix} \frac{1}{\gamma_{1,p}} & 0 \\ -\frac{\gamma_{3,p}}{\gamma_{1,p} \gamma_p} & \frac{\gamma_{1,p}}{\gamma_p} \end{pmatrix} \begin{pmatrix} Au^p \\ Av^p \end{pmatrix}.$$

2.2. Characteristics of the algorithm

We present, without proving them, the most important characteristics of the algorithm. The complete proof of the convergence is given in Section 3.

At each iteration step p , the vectors u^p and v^p verify $\langle u^p, v^p \rangle = 0$ and $\|u^p\| = \|v^p\| = 1$.

According to the definition of θ_p^s the matrix

$$B_p = \begin{pmatrix} \cos \theta_p^s & -\sin \theta_p^s \\ \sin \theta_p^s & \cos \theta_p^s \end{pmatrix} \begin{pmatrix} \frac{1}{\gamma_{1,p}} & 0 \\ -\frac{\gamma_{3,p}}{\gamma_{1,p} \gamma_p} & \frac{\gamma_{1,p}}{\gamma_p} \end{pmatrix}$$

is symmetric. Moreover, if $n > 3$ and u^0, v^0 are carefully chosen (see Section 3) then B_p is invertible and B_p^{-1} converges towards the matrix

$$B^{-1} = \begin{pmatrix} a_{11}^{(1)} & a_{1n}^{(1)} \\ a_{1n}^{(1)} & a_{nn}^{(1)} \end{pmatrix},$$

whose eigenvalues are λ_1 and λ_2 . Furthermore, $u = \lim_{p \rightarrow \infty} u^p, v = \lim_{p \rightarrow \infty} v^p$ are the solution of S_1 ; i.e. $q_1 = u, q_n = v$, and

$$e_1 = \frac{u + r_1 v}{\sqrt{1 + r_1^2}},$$

$$e_2 = \frac{u + r_2 v}{\sqrt{1 + r_2^2}},$$

where

$$r_1 = \frac{a_{nn}^{(1)} - a_{11}^{(1)} + (\lambda_1 - \lambda_2)}{2a_{1n}^{(1)}},$$

$$r_2 = \frac{a_{nn}^{(1)} - a_{11}^{(1)} - (\lambda_1 - \lambda_2)}{2a_{1n}^{(1)}},$$

are two orthonormal eigenvectors associated to λ_1 and λ_2 .

The angle θ_p^s is defined in such a way that the B_p matrix is symmetric. Nevertheless, to determine this angle other choices are possible. Generally speaking, we denote θ_p this angle. If we take $\theta_p = 0$, $\forall p \geq 0$ in the algorithm then we find the subspace method for computing the two dominant eigenvalues of A . The novelty, in our algorithm, is the introduction of the rotation

$$\begin{pmatrix} \cos \theta_p & -\sin \theta_p \\ \sin \theta_p & \cos \theta_p \end{pmatrix},$$

which is, as it was, a relaxation factor of the subspace method. Thus, it allows an acceleration of the algorithm convergence. Formally, if we define the error

$$E(\theta_p) = \sqrt{\|u^{p+1} - u^p\|^2 + \|v^{p+1} - v^p\|^2},$$

here the sequences (u^p) and (v^p) being obtained with a rotation angle equal to $\theta_p, \forall p$ then we show in Section 3 that

$$\forall p \geq 1, E(0) \geq E(\theta_p^s).$$

$E(0)$ is the error at the p -th iteration when applying the subspace method. This shows that our algorithm converges more rapidly than the subspace method. On the other hand, it is possible to compute an angle θ_p^{opt} for which the algorithm is the faster. However, this choice has many disadvantages.

Finally, when θ_p is defined as in the algorithm, i.e. equal to θ_p^s , it permits to construct an orthogonal matrix Q such that $A = QXQ^T$ with X a crosswise matrix.

PROPOSITION 1. *Let A be a symmetric matrix having n real eigenvalues each of multiplicity ≤ 2 . Then A can be factorized in the form $A = QX^TQ$ where Q is an orthonormal matrix and X a crosswise matrix.*

PROOF. First, we compute an orthonormal matrix Q_1 and a symmetric matrix A_1 of order $n - 2$ such that $A = Q_1A^{(1)}Q_1^T$ with

$$A^{(1)} = \begin{pmatrix} a_{11}^{(1)} & 0 & \dots & 0 & a_{1n}^{(1)} \\ 0 & & & & 0 \\ \vdots & & A_1 & & \vdots \\ 0 & & & & 0 \\ a_{1n}^{(1)} & 0 & \dots & 0 & a_{nn}^{(1)} \end{pmatrix},$$

where $(a_{ij}^{(1)})_{1 \leq i, j \leq n}$ be the elements of $A^{(1)}$ and $Q_1 = (q_1, \dots, q_n)$. In that way, $A = Q_1 A^{(1)} Q_1^T$ is equivalent to the two systems S_1 and S_2 .

The previous algorithm gives the solution of the nonlinear system (S_1). Having computed $(q_1, q_n, a_{11}^{(1)}, a_{1n}^{(1)}, a_{nn}^{(1)})$, we determine the vectors $q_j, 2 \leq j \leq n - 1$ by the Gram-Schmidt method [6,8]. From (S_2) we get

$$a_{kj}^{(1)} = \langle q_k, Aq_j \rangle, \quad 2 \leq j, k \leq n - 1.$$

Similarly we decompose the symmetric matrix A_1 of order $n - 2$ in the form $A_1 = Q_2 A^{(2)} Q_2^T$ with

$$A^{(2)} = \begin{pmatrix} a_{22}^{(2)} & 0 & \dots & 0 & a_{2,n-1}^{(2)} \\ 0 & & & & 0 \\ \vdots & & A_2 & & \vdots \\ 0 & & & & 0 \\ a_{2,n-1}^{(2)} & 0 & \dots & 0 & a_{n-1,n-1}^{(2)} \end{pmatrix},$$

where A_2 is a symmetric matrix of order $n - 4$ and so on. Clearly, the method is recursive and results after $m = \lfloor \frac{n-1}{2} \rfloor$ steps in

$$Q = Q_1 \begin{pmatrix} I_1 & 0 & 0 \\ 0 & Q_2 & 0 \\ 0 & 0 & I_1 \end{pmatrix} \dots \begin{pmatrix} I_{p-1} & 0 & 0 \\ 0 & Q_p & 0 \\ 0 & 0 & I_{p-1} \end{pmatrix}$$

and

$$X = \begin{pmatrix} a_{11}^{(1)} & & & a_{1n}^{(1)} \\ & a_{22}^{(2)} & & a_{2,n-1}^{(2)} \\ & & \ddots & \\ & a_{2,n-1}^{(2)} & & a_{n-1,n-1}^{(2)} \\ a_{1n}^{(1)} & & & a_{nn}^{(1)} \end{pmatrix};$$

here I_k denotes the identity matrix of order k .

Note that a decomposition $A = JXJ^{-1}$ can be achieved using the Jacobi method [9]. In this case, the problem size remains unchanged, i.e. equal to n , at each step.

3. CONVERGENCE ANALYSIS

In this section, we show that the method previously described converges. The proof consists in demonstrating that the sequences $(u^p), (v^p)$ and the matrix B_p converge and that λ_1, λ_2 and the eigenvectors can be expressed as a function of $u = \lim_{p \rightarrow \infty} u^p, v = \lim_{p \rightarrow \infty} v^p$ and of $\lim_{p \rightarrow \infty} B_p$.

LEMMA 1. $\forall p \geq 0, \langle u^p, v^p \rangle = 0$ and $\|u^p\| = \|v^p\| = 1$.

PROOF. According to the algorithm, $\|u^0\| = \|v^0\| = 1$ and $\langle u^0, v^0 \rangle = 0$. Now we show by induction that $\forall p \geq 0, \langle u^{p+1}, v^{p+1} \rangle = 0$, and $\|u^{p+1}\| = \|v^{p+1}\| = 1$. By definition

$$\begin{pmatrix} u^{p+1} \\ v^{p+1} \end{pmatrix} = \begin{pmatrix} \cos \theta_p^s & -\sin \theta_p^s \\ \sin \theta_p^s & \cos \theta_p^s \end{pmatrix} \begin{pmatrix} \frac{1}{\gamma_{1,p}} & 0 \\ -\frac{\gamma_{3,p}}{\gamma_{1,p}\gamma_p} & \frac{\gamma_{1,p}}{\gamma_p} \end{pmatrix} \begin{pmatrix} Au^p \\ Av^p \end{pmatrix}.$$

Let

$$\begin{pmatrix} w_1^p \\ w_2^p \end{pmatrix} = \begin{pmatrix} \frac{1}{\gamma_{1,p}} & 0 \\ -\frac{\gamma_{3,p}}{\gamma_{1,p}\gamma_p} & \frac{\gamma_{1,p}}{\gamma_p} \end{pmatrix} \begin{pmatrix} Au^p \\ Av^p \end{pmatrix}.$$

Therefore,

$$\begin{pmatrix} u^{p+1} \\ v^{p+1} \end{pmatrix} = \begin{pmatrix} \cos \theta_p^s & -\sin \theta_p^s \\ \sin \theta_p^s & \cos \theta_p^s \end{pmatrix} \begin{pmatrix} w_1^p \\ w_2^p \end{pmatrix}.$$

So,

$$\|w_1^p\| = \frac{\gamma_{1,p}}{\|Au^p\|} = 1$$

and

$$\begin{aligned} \|w_2^p\|^2 &= \frac{1}{\gamma_p^2} (\gamma_{1,p}^2 \|Av^p\|^2 + \gamma_{3,p}^2 - 2\gamma_{3,p} \langle Au^p, Av^p \rangle) \\ &= \frac{1}{\gamma_p^2} (\gamma_{1,p}^2 \gamma_{2,p}^2 - \gamma_p^2) = 1. \end{aligned}$$

On the other hand,

$$\langle w_1^p, w_2^p \rangle = \frac{1}{\gamma_{1,p}\gamma_p} (\gamma_{1,p}\gamma_{3,p} - \gamma_{3,p}\gamma_{1,p}) = 0.$$

Since

$$\begin{pmatrix} \cos \theta_p^s & -\sin \theta_p^s \\ \sin \theta_p^s & \cos \theta_p^s \end{pmatrix}$$

is a rotation, we deduce that $\langle u^{p+1}, v^{p+1} \rangle = 0$ and $\|u^{p+1}\| = \|v^{p+1}\| = 1$.

LEMMA 2. *The matrix B_p is symmetric.*

PROOF.

$$\begin{aligned} B_p &= \begin{pmatrix} \cos \theta_p^s & -\sin \theta_p^s \\ \sin \theta_p^s & \cos \theta_p^s \end{pmatrix} \begin{pmatrix} \frac{1}{\gamma_{1,p}} & 0 \\ -\frac{\gamma_{3,p}}{\gamma_{1,p}\gamma_p} & \frac{\gamma_{1,p}}{\gamma_p} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\cos \theta_p^s}{\gamma_{1,p}} + \frac{\gamma_{3,p} \sin \theta_p^s}{\gamma_p \gamma_{1,p}} & -\frac{\gamma_{1,p} \sin \theta_p^s}{\gamma_p} \\ \frac{\sin \theta_p^s}{\gamma_{1,p}} - \frac{\gamma_{3,p} \cos \theta_p^s}{\gamma_p \gamma_{1,p}} & \frac{\gamma_p \cos \theta_p^s}{\gamma_{1,p}} \end{pmatrix}. \end{aligned}$$

$$B_p \text{ symmetric} \iff -\frac{\gamma_{1,p} \sin \theta_p^s}{\gamma_p} = \frac{\sin \theta_p^s}{\gamma_{1,p}} - \frac{\gamma_{3,p} \cos \theta_p^s}{\gamma_p \gamma_{1,p}}$$

$$\iff \tan \theta_p^s = \frac{\gamma_{3,p}}{\gamma_{1,p}^2 + \gamma_p},$$

Let (e_1, \dots, e_n) denotes an orthonormal basis composed of the eigenvectors of A . Let $u^p = \sum_{i=1}^n \alpha_{p,i} e_i$ and $v^p = \sum_{i=1}^n \beta_{p,i} e_i$ be the decompositions of the vectors u^p and v^p in this basis. Let

$$\delta_{i,j}^p = \alpha_{p,i} \beta_{p,j} - \alpha_{p,j} \beta_{p,i}.$$

LEMMA 3. $\delta_{i,j}^{p+1} = \frac{\lambda_i \lambda_j}{\gamma_p} \delta_{i,j}^p$.

PROOF. According to the definition of u^{p+1} and v^{p+1} we get

$$u^{p+1} = \sum_{i=1}^n \left(\alpha_{p,i} \left(\frac{\cos \theta_p^s}{\gamma_{1,p}} + \frac{\gamma_{3,p} \sin \theta_p^s}{\gamma_{1,p} \gamma_p} \right) - \beta_{p,i} \frac{\gamma_{1,p} \sin \theta_p^s}{\gamma_p} \right) \lambda_i e_i,$$

$$v^{p+1} = \sum_{i=1}^n \left(\alpha_{p,i} \left(\frac{\sin \theta_p^s}{\gamma_{1,p}} - \frac{\gamma_{3,p} \cos \theta_p^s}{\gamma_{1,p} \gamma_p} \right) + \beta_{p,i} \frac{\gamma_{1,p} \cos \theta_p^s}{\gamma_p} \right) \lambda_i e_i.$$

Consequently,

$$\alpha_{p+1,i} = \left(\alpha_{p,i} \left(\frac{\cos \theta_p^s}{\gamma_{1,p}} + \frac{\gamma_{3,p} \sin \theta_p^s}{\gamma_{1,p} \gamma_p} \right) - \beta_{p,i} \frac{\gamma_{1,p} \sin \theta_p^s}{\gamma_p} \right) \lambda_i,$$

$$\beta_{p+1,i} = \left(\alpha_{p,i} \left(\frac{\sin \theta_p^s}{\gamma_{1,p}} - \frac{\gamma_{3,p} \cos \theta_p^s}{\gamma_{1,p} \gamma_p} \right) + \beta_{p,i} \frac{\gamma_{1,p} \cos \theta_p^s}{\gamma_p} \right) \lambda_i.$$

Let

$$x_p = \frac{\cos \theta_p^s}{\gamma_{1,p}} + \frac{\gamma_{3,p} \sin \theta_p^s}{\gamma_{1,p} \gamma_p}; \quad y_p = -\frac{\gamma_{1,p} \sin \theta_p^s}{\gamma_p},$$

$$z_p = \frac{\sin \theta_p^s}{\gamma_{1,p}} - \frac{\gamma_{3,p} \cos \theta_p^s}{\gamma_{1,p} \gamma_p}; \quad t_p = \frac{\gamma_{1,p} \cos \theta_p^s}{\gamma_p}.$$

Then for $1 \leq i, j \leq n$:

$$\begin{aligned} \delta_{i,j}^{p+1} &= \lambda_i \lambda_j \left((x_p \alpha_{p,i} + y_p \beta_{p,i})(z_p \alpha_{p,j} + t_p \beta_{p,j}) \right. \\ &\quad \left. - (x_p \alpha_{p,j} + y_p \beta_{p,j})(z_p \alpha_{p,i} + t_p \beta_{p,i}) \right) \\ &= \lambda_i \lambda_j (x_p t_p - y_p z_p) \delta_{i,j}^p \\ &= \frac{\lambda_i \lambda_j}{\gamma_p} \delta_{i,j}^p. \end{aligned}$$

LEMMA 4. Let (e_1, \dots, e_n) be an orthonormal basis of \mathbb{R}^n , $x = \sum_{i=1}^n x_i e_i$ and

$$y = \sum_{i=1}^n y_i e_i. \text{ Then } \|x\|^2 \|y\|^2 - \langle x, y \rangle^2 = \sum_{j < i} (x_i y_j - x_j y_i)^2.$$

PROOF. A direct computation shows this lemma.

$$\text{LEMMA 5. } \gamma_p^2 = \frac{\sum_{j < i} (\lambda_i \lambda_j)^{2(p+1)} (\delta_{i,j}^0)^2}{\sum_{j < i} (\lambda_i \lambda_j)^{2p} (\delta_{i,j}^0)^2}, \quad \forall p \geq 1.$$

PROOF. We show this lemma by induction.

$$\gamma_0^2 = \|Au^0\|^2 \|Av^0\|^2 - \langle Au^0, Av^0 \rangle^2.$$

On the other hand,

$$Au^0 = \sum_{i=1}^n \lambda_i \alpha_{0,i} e_i,$$

$$Av^0 = \sum_{i=1}^n \lambda_i \beta_{0,i} e_i.$$

According to Lemma 4, we get

$$\gamma_0^2 = \sum_{j < i} \lambda_i^2 \lambda_j^2 (\delta_{i,j}^0)^2.$$

Since $\|u^0\|^2 = \|v^0\|^2 = 1$ and $\langle u^0, v^0 \rangle = 0$, we deduce that $\sum_{j < i} (\delta_{i,j}^0)^2 = 1$.

Now we assume that the lemma is true for an order p . Then

$$\gamma_{p+1}^2 = \|Au^{p+1}\|^2 \|Av^{p+1}\|^2 - \langle Au^{p+1}, Av^{p+1} \rangle^2 = \sum_{j < i} \lambda_i^2 \lambda_j^2 (\delta_{i,j}^{p+1})^2.$$

On the other hand, following Lemma 3

$$(\delta_{i,j}^{p+1})^2 = \frac{(\lambda_i \lambda_j)^2}{\gamma_p^2} (\delta_{i,j}^p)^2 = (\lambda_i \lambda_j)^{2(p+1)} (\delta_{i,j}^0)^2 \frac{1}{\prod_{k=0}^p \gamma_k^2}.$$

Following the induction assumptions,

$$\gamma_k^2 = \frac{u_{k+1}}{u_k},$$

with

$$u_k = \sum_{j < i} (\lambda_i \lambda_j)^{2k} (\delta_{i,j}^0)^2.$$

So,

$$\prod_{k=0}^p \gamma_k^2 = \frac{u_{p+1}}{u_0} = \sum_{j < i} (\lambda_i \lambda_j)^{2(p+1)} (\delta_{i,j}^0)^2.$$

Finally,

$$(\delta_{i,j}^{p+1})^2 = \frac{(\lambda_i \lambda_j)^{2(p+1)} (\delta_{i,j}^0)^2}{\sum_{j < i} (\lambda_i \lambda_j)^{2(p+1)} (\delta_{i,j}^0)^2}.$$

Consequently,

$$\gamma_{p+1}^2 = \frac{\sum_{j < i} (\lambda_i \lambda_j)^{2(p+2)} (\delta_{i,j}^0)^2}{\sum_{j < i} (\lambda_i \lambda_j)^{2(p+1)} (\delta_{i,j}^0)^2}.$$

COROLLARY 1. *If $\delta_{2,1}^0 \neq 0$ and if $n > 3$ then $\lambda_1 \lambda_2 \neq 0$ and $\gamma_p \neq 0$. Furthermore, B_p is invertible.*

$$\text{LEMMA 6. } H_p = \gamma_{1,p}^2 + \gamma_{2,p}^2 = \frac{\sum_{j < i} (\lambda_i \lambda_j)^{2p} (\lambda_i^2 + \lambda_j^2) (\delta_{i,j}^0)^2}{\sum_{j < i} (\lambda_i \lambda_j)^{2p} (\delta_{i,j}^0)^2}, \forall p \geq 1.$$

PROOF.

$$\gamma_{1,p}^2 = \|Au^p\|^2 = \sum_{i=1}^n \lambda_i \alpha_{p,i}^2,$$

$$\gamma_{2,p}^2 = \|Av^p\|^2 = \sum_{i=1}^n \lambda_i \beta_{p,i}^2.$$

Following Lemma 3 we have,

$$\alpha_{p,i} = \lambda_i (x_{p-1} \alpha_{p-1,i} + y_{p-1} \beta_{p-1,i}),$$

$$\beta_{p,i} = \lambda_i (z_{p-1} \alpha_{p-1,i} + t_{p-1} \beta_{p-1,i}).$$

So,

$$\begin{aligned} H_p &= \sum_{i=1}^n \lambda_i^4 (\alpha_{p-1,i}^2 (x_{p-1}^2 + z_{p-1}^2) + \beta_{p-1,i}^2 (y_{p-1}^2 + t_{p-1}^2)) \\ &\quad + 2(x_{p-1} y_{p-1} + z_{p-1} t_{p-1}) \alpha_{p-1,i} \beta_{p-1,i}. \end{aligned}$$

On the other hand, it is easy to show that

$$x_{p-1}^2 + y_{p-1}^2 = \frac{\gamma_{1,p-1}^2 \gamma_{p-1}^2}{\gamma_{1,p-1}^2 + \gamma_{3,p-1}^2}.$$

Since $\gamma_{p-1}^2 = \gamma_{1,p-1}^2 \gamma_{2,p-1}^2 - \gamma_{3,p-1}^2$ we deduce that

$$x_{p-1}^2 + z_{p-1}^2 = \frac{\gamma_{2,p-1}^2}{\gamma_{p-1}^2}.$$

In the same way, we show that

$$y_{p-1}^2 + t_{p-1}^2 = \frac{\gamma_{1,p-1}^2}{\gamma_{p-1}^2}$$

and

$$x_{p-1} y_{p-1} + z_{p-1} t_{p-1} = \frac{\gamma_{3,p-1}^2}{\gamma_{p-1}^2}.$$

Finally,

$$\begin{aligned} H_p &= \frac{1}{\gamma_{p-1}^2} (\gamma_{2,p-1}^2 \sum_{i=1}^n \lambda_i^4 \alpha_{p-1,i}^2 + \gamma_{1,p-1}^2 \sum_{i=1}^n \lambda_i^4 \beta_{p-1,i}^2 - 2\gamma_{3,p-1}^2 * \\ &\quad * \sum_{i=1}^n \lambda_i^4 \alpha_{p-1,i} \beta_{p-1,i}). \end{aligned}$$

Let $H_p = \frac{1}{\gamma_{p-1}^2} \bar{H}_p$. A direct computation shows that

$$\bar{H}_p = \sum_{i < j} (\lambda_i \lambda_j)^2 (\lambda_i^2 + \lambda_j^2) (\delta_{i,j}^{p-1})^2.$$

Following Lemma 3 we get,

$$\bar{H}_p = \frac{1}{p-2} \sum_{i < j} (\lambda_i \lambda_j)^{2p} (\lambda_i^2 + \lambda_j^2) (\delta_{i,j}^0)^2.$$

$$\prod_{k=0}^2 \gamma_k^2$$

Following Lemma 5 we get

$$H_p = \frac{1}{\gamma_{p-1}^2} \bar{H}_p = \frac{\sum_{i < j} (\lambda_i \lambda_j)^{2p} (\lambda_i^2 + \lambda_j^2) (\delta_{i,j}^0)^2}{\sum_{i < j} (\lambda_i \lambda_j)^{2p} (\delta_{i,j}^0)^2}.$$

LEMMA 7. Assume that $\delta_{2,1}^0 \neq 0$ and $n > 3$ then

- a) $\lim_{p \rightarrow \infty} \gamma_p = \lambda_1 \lambda_2$,
b) $\lim_{p \rightarrow \infty} H_p = \lambda_1^2 + \lambda_2^2$,
c) $\lim_{p \rightarrow \infty} \delta_{i,j}^p = 0$, $\forall i > j$ and $(i, j) \neq (2, 1)$,
d) $\lim_{p \rightarrow \infty} |\delta_{2,1}^p| = 1$,
e) $\lim_{p \rightarrow \infty} \alpha_{p,i} = \lim_{p \rightarrow \infty} \beta_{p,i} = 0$, $\forall i > 2$.

PROOF. **a)** According to Lemma 5, we have

$$\begin{aligned} \gamma_p^2 &= \frac{\sum_{j < i} (\lambda_i \lambda_j)^{2(p+1)} (\delta_{i,j}^0)^2}{\sum_{j < i} (\lambda_i \lambda_j)^{2p} (\delta_{i,j}^0)^2} \\ &= \lambda_1^2 \lambda_2^2 \frac{\sum_{j < i} \left(\frac{\lambda_i \lambda_j}{\lambda_1 \lambda_2} \right)^{2(p+1)} (\delta_{i,j}^0)^2}{\sum_{j < i} \left(\frac{\lambda_i \lambda_j}{\lambda_1 \lambda_2} \right)^{2p} (\delta_{i,j}^0)^2} . \end{aligned}$$

Since, $|\frac{\lambda_i \lambda_j}{\lambda_1 \lambda_2}| < 1$, for $i > j \geq 3$ or $(j = 1$ and $i > 2)$, we have

$$\lim_{p \rightarrow \infty} \left(\frac{\lambda_i \lambda_j}{\lambda_1 \lambda_2} \right)^{2(p+1)} = 0 .$$

Therefore

$$\lim_{p \rightarrow \infty} \gamma_p^2 = (\lambda_1 \lambda_2)^2 \frac{(\delta_{i,j}^0)^2}{(\delta_{i,j}^0)^2} = (\lambda_1 \lambda_2)^2 .$$

b) The same reasoning shows that

$$\lim_{p \rightarrow \infty} H_p = \lambda_1^2 + \lambda_2^2 ,$$

c) According to Lemma 3, $\delta_{i,j}^{p+1} = \frac{\lambda_i \lambda_j}{\gamma_p} \delta_{i,j}^p$. So

$$\lim_{p \rightarrow \infty} \left| \frac{\delta_{i,j}^{p+1}}{\delta_{i,j}^p} \right| = \left| \frac{\lambda_i \lambda_j}{\lambda_1 \lambda_2} \right| < 1, \quad \forall i > j \quad (i, j) \neq (2, 1) .$$

From d'Alembert's criterion we get

$$\lim_{p \rightarrow \infty} \delta_{i,j}^p = 0 \quad \forall i > j \text{ and } (i, j) \neq (2, 1) .$$

d) Now we show that $\lim_{p \rightarrow \infty} |\delta_{2,1}^p| = 1$. According to Lemmas 4 and 5 we get

$$\delta_{2,1}^p = \frac{\lambda_1 \lambda_2}{\gamma_{p-1}} \delta_{2,1}^{p-1} = \frac{1}{\prod_{k=0}^{p-1} \gamma_k} (\lambda_1 \lambda_2)^p \delta_{2,1}^0.$$

Since

$$\prod_{k=0}^{p-1} \gamma_k = \sqrt{\sum_{j < i} (\lambda_i \lambda_j)^{2p} (\delta_{i,j}^0)^2},$$

we deduce that

$$\lim_{p \rightarrow \infty} |\delta_{2,1}^p| = 1.$$

e) A direct computation shows that, $\forall i > 2$

$$\delta_{2,1}^p \alpha_{p,i} = \delta_{i,2}^p \alpha_{p,1} - \delta_{i,1}^p \alpha_{p,2}$$

and

$$\delta_{p,2} \beta_{p,i} = \delta_{i,2}^p \beta_{p,1} - \delta_{i,1}^p \beta_{p,2}.$$

Since $\alpha_{p,1}, \alpha_{p,2}, \beta_{p,1}$ and $\beta_{p,2}$ are bounded, we deduce that

$$\lim_{p \rightarrow \infty} \alpha_{p,i} = \lim_{p \rightarrow \infty} \beta_{p,i} = 0 \quad \forall i > 2.$$

Now we show that B_p^{-1} converges towards a matrix B^{-1} whose eigenvalues are λ_1 and λ_2 . The B_p^{-1} matrix is such that

$$B_p^{-1} \begin{pmatrix} u^{p+1} \\ v^{p+1} \end{pmatrix} = \begin{pmatrix} Au^p \\ Av^p \end{pmatrix}.$$

So,

$$B_p^{-1} = \begin{pmatrix} \langle Au^p, u^{p+1} \rangle & \langle Au^p, v^{p+1} \rangle \\ \langle Av^p, u^{p+1} \rangle & \langle Av^p, v^{p+1} \rangle \end{pmatrix}.$$

Consequently, if the sequences (u^p) and (v^p) converge, then the matrix B_p^{-1} will converge.

LEMMA 8. $\lim_{p \rightarrow \infty} E(\theta_p^s) = 0$.

PROOF. Recall that

$$\begin{aligned} E(\theta_p^s) &= \sqrt{\|u^{p+1} - u^p\|^2 + \|v^{p+1} - v^p\|^2} = \\ &= \sqrt{4 - 2(\langle u^{p+1}, u^p \rangle + \langle v^{p+1}, v^p \rangle)}. \end{aligned}$$

Let

$$\begin{aligned}\bar{E}(\theta_p^s) &= \langle u^{p+1}, u^p \rangle + \langle v^{p+1}, v^p \rangle \\ &= \sum_{i=1, n} \alpha_{p,i} \alpha_{p+1,i} + \sum_{i=1, n} \beta_{p,i} \beta_{p+1,i}.\end{aligned}$$

A direct computation using Lemma 3 shows that

$$\bar{E}(\theta_p^s) = \frac{1}{\sqrt{H_p + 2\gamma_p}} \left(\sum_{i=1}^n \lambda_i (\alpha_{p,i}^2 + \beta_{p,i}^2) + \frac{1}{\gamma_p} \sum_{j < i} \lambda_i \lambda_j (\lambda_i + \lambda_j) \delta_{i,j}^p \right).$$

Following Lemma 6, we get that

$$\lim_{p \rightarrow \infty} \bar{E}(\theta_p^s) = 2.$$

PROPOSITION 2. *The sequences (u^p) and (v^p) converge respectively towards $u = r_{11}e_1 + r_{12}e_2$ and $v = r_{21}e_1 + r_{22}e_2$ with $\begin{pmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{pmatrix}$ an orthonormal matrix.*

PROOF. According to Lemma 7 we have, $\lim_{p \rightarrow \infty} E(\theta_p^s) = 0$. It follows that (u^p) and (v^p) are Cauchy sequences. Therefore, (u^p) and (v^p) converge respectively to u and v . Since

$$u^p = \sum_{i=1}^n \alpha_{p,i} e_i$$

and

$$v^p = \sum_{i=1}^n \beta_{p,i} e_i,$$

with

$$\lim_{p \rightarrow \infty} \alpha_{p,i} = \lim_{p \rightarrow \infty} \beta_{p,i} = 0, \quad \forall i > 2,$$

we deduce that

$$\lim_{p \rightarrow \infty} u^p = u = r_{11}e_1 + r_{12}e_2$$

and

$$\lim_{p \rightarrow \infty} v^p = v = r_{21}e_1 + r_{22}e_2,$$

where

$$r_{1,i} = \lim_{p \rightarrow \infty} \alpha_{p,i},$$

and

$$r_{2,i} = \lim_{p \rightarrow \infty} \beta_{p,i}, \quad i = 1, 2.$$

Therefore, $q_1 = u$ and $q_n = v$ are a solutions of the system S_1 . Since, $\|u\| = \|v\| = 1$ and $\langle u, v \rangle = 0$ the matrix $\begin{pmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{pmatrix}$ is orthonormal.

PROPOSITION 3. B_p^{-1} converges towards a matrix B^{-1} whose eigenvalues are λ_1 and λ_2 .

PROOF. Since the sequences (u^p) and (v^p) converge towards u and v , the matrix B_p^{-1} converges towards the matrix

$$\begin{pmatrix} \langle Au, u \rangle & \langle Au, v \rangle \\ \langle Av, u \rangle & \langle Av, v \rangle \end{pmatrix} = \begin{pmatrix} x & y \\ y & z \end{pmatrix}.$$

Now, we show that the eigenvalues of B^{-1} are λ_1 and λ_2 . Recall that

$$B_p^{-1} = \begin{pmatrix} \gamma_{1,p} \cos \theta_p^s & \gamma_{1,p} \sin \theta_p^s \\ -\frac{\gamma_p \sin \theta_p^s}{\gamma_{1,p}} + \frac{\gamma_{3,p} \cos \theta_p^s}{\gamma_{1,p}} & \frac{\gamma_p \cos \theta_p^s}{\gamma_{1,p}} + \frac{\gamma_{3,p} \sin \theta_p^s}{\gamma_{1,p}} \end{pmatrix}.$$

Following the algorithm, we have

$$\cos \theta_p^s = \frac{\gamma_{1,p}^2 + \gamma_p}{\gamma_{1,p} \sqrt{H_p + 2\gamma_p}}, \quad (2)$$

and

$$\sin \theta_p^s = \frac{\gamma_{3,p}}{\gamma_{1,p} \sqrt{H_p + 2\gamma_p}}. \quad (3)$$

Substituting $\cos \theta_p^s$ by (2) and $\sin \theta_p^s$ by (3) gives the trace S_p of B_p^{-1}

$$S_p = \gamma_p \frac{\cos \theta_p^s}{\gamma_{1,p}} + \frac{\gamma_{3,p} \sin \theta_p^s}{\gamma_{1,p}} + \gamma_{1,p} \cos \theta_p^s = \sqrt{H_p + 2\gamma_p}$$

and the determining $\det(B_p^{-1}) = \gamma_p$. The eigenvalues of B_p^{-1} are solutions of the equation

$$\lambda^2 - S_p \lambda + \det(B_p^{-1}) = 0. \quad (4)$$

The discriminant of eq (4) is $\Delta = H_p - 2\gamma_p \geq 0$ because B_p^{-1} is symmetric. The solutions of equation (4) are

$$\lambda_{1,p} = \frac{1}{2}(\sqrt{H_p + 2\gamma_p} + \sqrt{H_p - 2\gamma_p})$$

and

$$\lambda_{2,p} = \frac{1}{2}(\sqrt{H_p + 2\gamma_p} - \sqrt{H_p - 2\gamma_p}).$$

According to Lemma 7 a-b)

$$\lim_{p \rightarrow \infty} \lambda_{1,p} = \lambda_1$$

and

$$\lim_{p \rightarrow \infty} \lambda_{2,p} = \lambda_2.$$

PROPOSITION 4. Let $r_1 = \frac{z-x+\sqrt{\Delta}}{2y}$ and $r_2 = \frac{z-x-\sqrt{\Delta}}{2y}$. Then the vectors $e_1 = \frac{u+r_1v}{\sqrt{1+r_1^2}}$ and $e_2 = \frac{u+r_2v}{\sqrt{1+r_2^2}}$ are two orthonormal eigenvectors associated respectively to the eigenvalues λ_1 and λ_2 .

PROOF. The matrix B_p^{-1} converges towards the matrix $B^{-1} = \begin{pmatrix} x & y \\ y & z \end{pmatrix}$ verifying

$$B^{-1} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} Au \\ Av \end{pmatrix}. \quad (5)$$

Now, we compute the scalar r for which $w = u + rv$ is an eigenvector of A i.e. $Aw = \lambda w$. From the eq (6) it follows that

$$(S_3) \begin{cases} Au = xu + yv \\ Av = yu + zv \end{cases}.$$

Therefore,

$$Aw = \lambda w \Leftrightarrow xu + yv + r(yu + zv) = \lambda(u + rv).$$

So, we deduce the system

$$(S_4) \begin{cases} x + ry = \lambda \\ y + rz = r\lambda \end{cases}.$$

Hence, r is such that

$$r^2y + (x-z)r - y = 0. \quad (6)$$

The discriminant of eq (6) is $\Delta = (x-z)^2 + 4(y)^2 \geq 0$. If $\Delta = 0$ then $x = z$ and $y = 0$. In this case, x is an eigenvalue of a multiplicity at least equal to 2 and u and v are two eigenvectors associated to the eigenvalue $\lambda = x$. Now, if $\Delta > 0$ then

$$r_1 = \frac{z-x+\sqrt{\Delta}}{2y}, \quad r_2 = \frac{z-x-\sqrt{\Delta}}{2y},$$

are the solutions of the equation. Finally $e_1 = \frac{u+r_1v}{\sqrt{1+r_1^2}}$ (resp. $e_2 = \frac{u+r_2v}{\sqrt{1+r_2^2}}$) is an eigenvector associated to an eigenvalue noted μ_1 (resp. μ_2). According to the system S_4 and Proposition 3, $\mu_1 = x + r_1y = \lambda_1$ and $\mu_2 = x + r_2y = \lambda_2$.

Furthermore, it is easy to verify that $\|e_1\| = \|e_2\| = 1$ and that $\langle e_1, e_2 \rangle = 0$.

3.1. Choice of θ_p

Recall that the error $E(\theta_p)$ is defined by

$$\begin{aligned} E^2(\theta_p) &= \|u^{p+1} - u^p\|^2 + \|v^{p+1} - v^p\|^2 = \\ &= 4 - 2(\langle u^{p+1}, u^p \rangle + \langle v^{p+1}, v^p \rangle). \end{aligned}$$

According to Lemma 6 we have

$$\begin{aligned} \bar{E}(\theta_p) &= \langle u^{p+1}, u^p \rangle + \langle v^{p+1}, v^p \rangle \\ &= \left\langle \sum_{i=1}^n \lambda_i (x_p \alpha_{p,i} + z_p \beta_{p,i}) e_i, \sum_{i=1}^n \alpha_{p,i} e_i \right\rangle \\ &\quad + \left\langle \sum_{i=1}^n \lambda_i (y_p \alpha_{p,i} + t_p \beta_{p,i}) e_i, \sum_{i=1}^n \beta_{p,i} e_i \right\rangle \\ &= x_p \langle Au^p, u^p \rangle + z_p \langle Av^p, u^p \rangle \\ &\quad + y_p \langle Au^p, v^p \rangle + t_p \langle Av^p, v^p \rangle \\ &= \cos \theta_p \left(\frac{\tau_{1,p}}{\gamma_{1,p}} - \frac{\tau_{3,p} \gamma_{3,p}}{\gamma_p \gamma_{1,p}} + \frac{\gamma_{1,p} \tau_{2,p}}{\gamma_p} \right) \\ &\quad + \sin \theta_p \left(\frac{\tau_{1,p} \gamma_{3,p}}{\gamma_p \gamma_{1,p}} - \frac{\tau_{3,p} \gamma_{1,p}}{\gamma_p} + \frac{\tau_{3,p}}{\gamma_{1,p}} \right), \end{aligned}$$

where

$$\tau_{1,p} = \langle Au^p, u^p \rangle, \quad \tau_{2,p} = \langle Av^p, v^p \rangle, \quad \tau_{3,p} = \langle Au^p, v^p \rangle,$$

Let

$$X_p = \frac{\tau_{1,p}}{\gamma_{1,p}} - \frac{\tau_{3,p} \gamma_{3,p}}{\gamma_p \gamma_{1,p}} + \frac{\gamma_{1,p} \tau_{2,p}}{\gamma_p}, \quad Y_p = \frac{\tau_{1,p} \gamma_{3,p}}{\gamma_p \gamma_{1,p}} - \frac{\tau_{3,p} \gamma_{1,p}}{\gamma_p} + \frac{\tau_{3,p}}{\gamma_{1,p}}.$$

Then $E(\theta_p^*)$ is optimal for θ_p verifying

$$\frac{\partial \bar{E}(\theta_p)}{\partial \theta_p} = -X_p \sin \theta_p + Y_p \cos \theta_p = 0.$$

So

$$\tan \theta_p^{opt} = \frac{Y_p}{X_p}.$$

We deduce that

$$\bar{E}(\theta_p^{opt}) = \sqrt{\tau_{1,p}^2 + \tau_{2,p}^2} \leq E(\theta_p),$$

for all choice of θ_p .

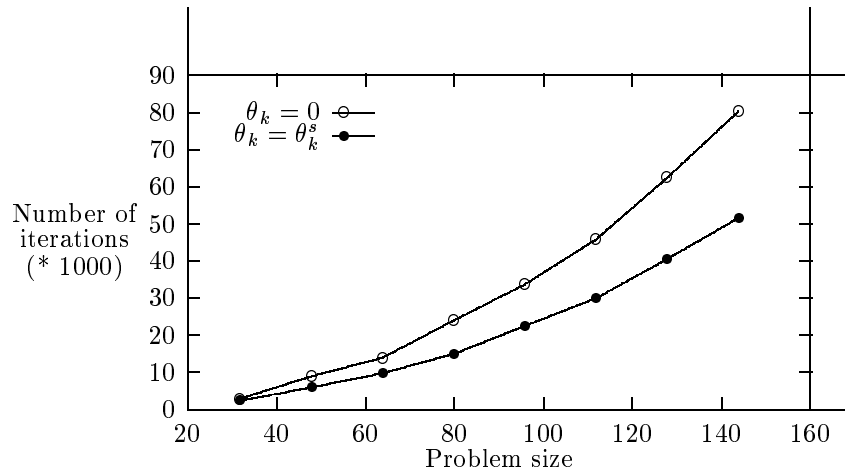


FIGURE 1. Number of iterations for $\theta_p = 0$ and for $\theta_p = \theta_p^s$

4. NUMERICAL TESTS AND CONCLUDING REMARKS

In this section, we report numerical experiments for $\theta_p = \theta_p^s$ and $\theta_p = 0$, on a 16 Transputers SuperNode machine with the C-net programming environment [1,2]. Because of the memory limitation (1 Mo per processor) n is limited to 256.

We call iteration the calculation of u^{p+1}, v^{p+1} from u^p, v^p . From different tests on various matrices [7] we have noted that

- The case $\theta_p = 0$ requires, for n large, approximatively the double number of iterations and the double execution time than the case $\theta_p = \theta_p^s$ as reported in figures 1 and 2. We don't know theoretically the relation between the convergence factors in the two cases.
- The case $\theta_p = 0$, requires a very fine accuracy ϵ . For instance, for $n = 64, n = 96, \dots$ only superior precisions to 10^{-6} allow to give correct results. On the contrary, for $\theta_p = \theta_p^s$, $\epsilon = 10^{-1}$ is sufficient. Also in this case, the problem of the numerical stability of the algorithm has to be studied.

These numeric tests show that the method is more stable and converges more rapidly than the subspace method. The analysis of the factor convergence, the numeric stability and other variants of the algorithm are on the way.

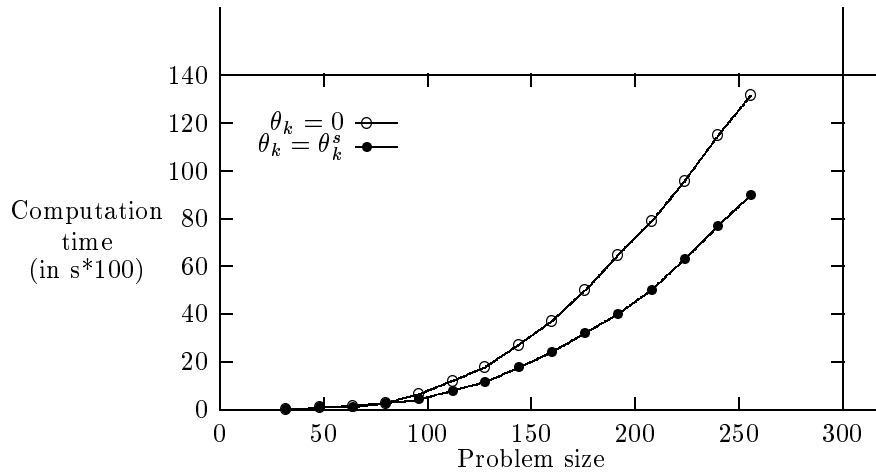


FIGURE 2. Computation time (in s*100) for $\theta_p = 0$ and for $\theta_p = \theta_p^s, \epsilon = 10^{-8}$

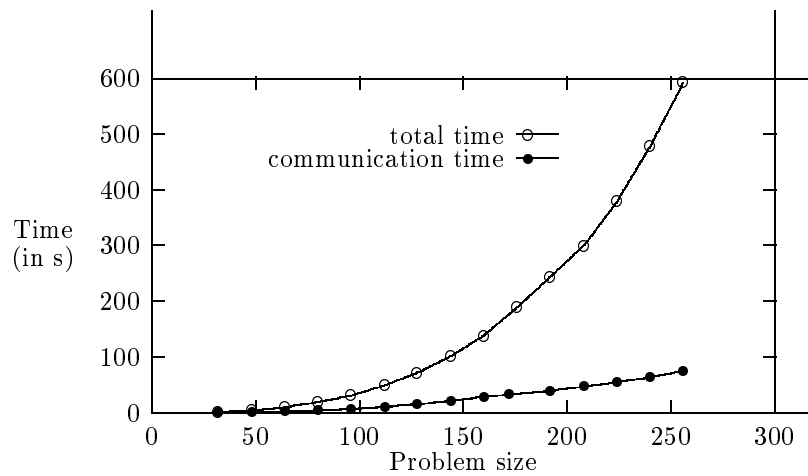


FIGURE 3. Time (in sec) for $\theta_p = \theta_p^s, \epsilon = 10^{-3}$

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