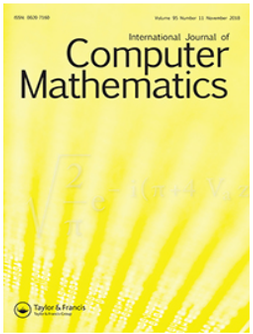

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ARTICLE

Conjugate gradients for symmetric positive semidefinite least-squares problems

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ABSTRACT

The cgSLS (conjugate gradients for symmetric positive semidefinite least-squares) algorithm is presented. The algorithm exploits the cyclic property of invariant Krylov spaces to reduce the least-squares problem with a symmetric positive semidefinite matrix A to the minimization of the related energy function with the Hessian A on the range of A, so that a simple modification of the conjugate gradient (CG) method is applicable. At the same time, the algorithm generates approximations of the projection of the right-hand side to the range of A. The asymptotic rate of convergence of the new algorithm is proved to be the same as that of the CG method for the related consistent problem. An error bound in terms of the square root of the regular condition number of A is also given. The performance of the algorithm is demonstrated by numerical experiments.

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1. Introduction

We are interested in a special linear least-squares problem

$$\min \|x\| \quad \text{s.t.} \quad x \in \arg\min_y \|Ay - b\|, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ denotes a symmetric positive semi-definite (SPS) matrix, $b, x \in \mathbb{R}^n$, and $\|x\|$ denotes the Euclidean norm of x. The problem is equivalent to

$$A^2x = Ab, \quad x \in \mathrm{Im}A, \tag{2}$$

where ImA denotes the range of A. We assume that the problem is large and sparse, so that it is difficult to be solved by direct methods, and that it is reasonably conditioned or preconditioned [16], so that the regular condition number

$$\bar\kappa(A) = \lambda_{\max}/\bar\lambda_{\min},$$

defined by the extreme non-zero eigenvalues $\lambda_{\max}$ and $\bar\lambda_{\min}$ of A, is not too large.

The problems of this type arise, for example, in realizations of the minimum-variance unbiased estimates for linear regression models [1] or in mechanics when the Neumann conditions are obtained from measurements [5]. Our research has been motivated by our effort to adapt the active set-based algorithms (see, e.g. [11] or [10]) to the solution of problems in particle dynamics [15]. In this case,

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the dimension of auxiliary linear problems is proportional to the number of particles; so it is desirable to resolve (1) with millions of variables.

A number of direct or iterative algorithms, most of them being developed for the solution of more general least-squares problems, can be applied to the solution of (1). For a comprehensive overview, see, for example, Björck [4]. Here we are interested in the conjugate gradient (CG)-based algorithms adjusted to the solution of (1). The CG algorithm was proposed by Hestenes and Stiefel in their classical paper on the CG method [14] for the solution of systems with symmetric positive definite (SPD) matrices. The application of CG to the solution of consistent systems like (2) is straightforward, and it is even possible to avoid multiplication by A^2 by using the CGLS algorithm (see, e.g. [21]). However, the analysis of convergence of CGLS reveals that the number iterations that are necessary to get an approximate solution of (1) is proportional to $\bar{\kappa}(A)$, which is much more than $\sqrt{\bar{\kappa}(A)}$ required by the standard CG for non-singular A [3]. The reason is that CGLS is based on the minimization in the Krylov space associated with A^2 rather than with A.

The Krylov space methods that exploit the Krylov spaces associated with A enjoy a similar asymptotic rate of convergence as the standard CG for the related consistent system. They were proposed by Axelsson [2], who considered the application of CG to the non-symmetric systems and to the associated normal equations. The same idea was used by Paige and Saunders [20], who introduced MINRES for the solution of symmetric possibly indefinite systems, or Saad and Schulz [22], who exploited it in their seminal paper on GMRES. Choi, Paige and Sounders proposed a modification of MINRES for the solution of linear least squares problems [9]. For more discussions and empirical comparisons, see Choi and Sounders [8] or Fong and Saunders [12]. See also RRGMRES (range restricted GMRES by Neumann *et al.* [19] and experiments with different Krylov spaces in Calvetti, Lewis, and Reichel [6].

A simple modification of CG for (1) that exploits the Krylov spaces associated with A has been proposed by Calvetti *et al.* [7]. Here we propose a variant of CG which generates a conjugate basis of ImA by means of the standard CG for an associated feasible problem and uses the basis to get the approximations of the solution of (1) and of the orthogonal projection Qb of b to ImA. We also give bounds on the rate of convergence in terms of the regular condition number of A and illustrate the effectivity of the algorithm by numerical experiments.

2. Equivalent formulations and Krylov spaces

First recall that problem (1) is equivalent to the problem to find

$$\min_{x\in \mathrm{Im}A} q(x), \quad q(x) = \frac{1}{2}x^{\mathrm{T}}A^2x - (Ab)^{\mathrm{T}}x. \tag{3}$$

The solution $\hat{x}$ of Equation (3) is a unique vector which satisfies $\hat{x} \in \mathrm{Im}A$ and the KKT conditions (normal equations) (2) (see, e.g. [4]). If we multiply both sides of Equation (2) by the Moore–Penrose inverse $A^{\dagger}$ [13] on the left, we get that the solution $\hat{x}$ of (3) satisfies also

$$Ax = Qb, \tag{4}$$

where Q is the orthogonal projector onto ImA. Since for any $x \in \mathrm{Im}A$

$$b^{\mathrm{T}}x = (Qb)^{\mathrm{T}}x,$$

it follows that $\hat{x}$ is also a unique solution of

$$\min_{x\in \mathrm{Im}A} f(x), \quad f(x) = \frac{1}{2}x^{\mathrm{T}}Ax - b^{\mathrm{T}}x \tag{5}$$

or

$$\min_{x\in \mathrm{Im}A} f_Q(x), \quad f_Q(x) = \frac{1}{2}x^{\mathrm{T}}Ax - (Qb)^{\mathrm{T}}x. \tag{6}$$

It is well known that the solution of (6) can be approximated by the minimizers of f on Krylov spaces $\mathcal{K}^i(A, Qb)$, $1 \le i \le n$, where for any $z \in \mathbb{R}^n$, we denote

$$\mathcal{K}^i(A, z) = \mathrm{Span}(z, Az, \ldots, A^{i-1}z), \quad i = 1, 2, \ldots.$$

Since $\mathcal{K}^i(A, Qb)$ is a subspace of $\mathbb{R}^n$, its dimension cannot exceed n. It follows that there is $d = d(A, Qb) > 0$, the grade of the vector Qb with respect to A, such that

$$\mathcal{K}^{d-1}(A, Qb) \subsetneq \mathcal{K}^d(A, Qb) = \mathcal{K}^{d+1}(A, Qb) = \mathcal{K}^{d+2}(A, Qb) = \cdots.$$

The following lemma recalls the cyclic property [17] of the invariant Krylov space $\mathcal{K}(A, Ab) = \mathcal{K}^d(A, Ab)$ that can be used to generate $\mathcal{K}(A, Qb)$.

Lemma 2.1: *Let A denote an SPS matrix and $b \in \mathbb{R}^n$. Then*

$$Qb \in \mathcal{K}(A, Ab) \quad \text{and} \quad \mathcal{K}(A, Qb) = \mathcal{K}(A, Ab) = A\mathcal{K}(A, Qb). \tag{7}$$

Proof: Let us denote

$$f_A(x) = \tfrac{1}{2}x^{\mathrm{T}}Ax - (Ab)^{\mathrm{T}}x.$$

Since $\mathcal{K}(A, Ab)$ is a subspace of ImA and the restriction $f_A|\mathcal{K}(A, Ab)$ of f_A to $\mathcal{K}(A, Ab)$ is coercive, it follows that there is

$$z = \arg\min f_A(x) \quad \text{s.t.} \quad x \in \mathcal{K}(A, Ab)$$

and z satisfies

$$\nabla f_A(z)^{\mathrm{T}}y = (Az - Ab)^{\mathrm{T}}y = 0 \quad \text{for any} \quad y \in \mathcal{K}(A, Ab).$$

Since $Az, Ab \in \mathcal{K}(A, Ab) = A\mathcal{K}(A, Ab)$, it follows that $y = Az - Ab$ satisfies $y \in \mathcal{K}(A, Ab)$ and thus

$$\|Az - Ab\|^2 = 0.$$

Since $z, Qb \in$ ImA, we have

$$\|z - Qb\| = 0.$$

Thus $Qb \in \mathcal{K}(A, Ab)$. The rest is easy. ■

3. cgSLS algorithm

The CG method has been proposed for the solution of the system

$$Ax = b \tag{8}$$

with SPD A. The CG algorithm for Equation (8) is based on several observations:

- The solution $\hat{x}$ of Equation (8) belongs to $\mathcal{K}(A, b)$.
- It is possible to generate very efficiently a conjugate basis $\{p^1, p^2, \ldots, p^i\}$ of $\mathcal{K}^i(A, b)$, $(p^k)^{\mathrm{T}}Ap^\ell = 0$ for $k \ne \ell$.
- For $x = \xi_1 p^1 + \cdots + \xi_i p^i$ and f defined by Equation (5), it holds

$$f(x) = f(\xi_1 p^1) + \cdots + f(\xi_i p^i)$$

and

$$\min_{x \in \mathbb{R}^n} f(x) = \min_{\xi_1 \in \mathbb{R}} f(\xi_1 p^1) + \cdots + \min_{\xi_i \in \mathbb{R}} f(\xi_i p^i).$$

Table 1. CGs for SPS least-squares problem (cgSLS).

	Given an SPS matrix A of the order n and an n-vector b.
Step 0.	{*Initialization.*} Set $i=0, x^0=o, y^0=o, g^0=-b, g_A^0=-Ab, p^1=g_A$. **while** $\|Ax^i-y^i\|+\|g_A{}^i\|$ is not small
Step 1.	{*Minimization of f and f_A on $\mathcal{K}^i(A,Ab)$.*} $\alpha=(g^i)^{\mathsf{T}}p^{i+1}/(p^{i+1})^{\mathsf{T}}Ap^{i+1}=\arg\min_{\alpha\in\mathbb{R}} f(x^i-\alpha p^{i+1})$ $\alpha_A=(g_A^i)^{\mathsf{T}}p^{i+1}/(p^{i+1})^{\mathsf{T}}Ap^{i+1}=\arg\min_{\alpha\in\mathbb{R}} f_A(x^i-\alpha p^{i+1})$ $x^{i+1}=x^i-\alpha p^{i+1}, y^{i+1}=y^i-\alpha_A p^{i+1}$
Step 2.	{*Update of the gradients of f and f_A.*} $g^{i+1}=g^i-\alpha Ap^{i+1}, g_A^{i+1}=g_A^i-\alpha_A Ap^{i+1}$
Step 3.	{*New conjugate direction.*} $i=i+1$ $\beta=(g_A^i)^{\mathsf{T}}Ap^i/(p^i)^{\mathsf{T}}Ap^i, p^{i+1}=g_A^i-\beta p^i$ **end while**
Step 4.	{*Return (possibly inexact) solutions.*} $\tilde{x}=x^i, \tilde{y}=y^i$

If $b\in \mathrm{Im}A$, then all the above observations remain valid for SPS A. Due to Lemma 2.1, we can thus apply the CG procedure to generate a conjugate basis of $\mathcal{K}(A,Ab)=\mathcal{K}(A,Qb)$ and approximations y^i for the unique solution $\hat{y}=Qb$ of

$$\min_{y\in\mathrm{Im}A} f_A(y).$$

At the same time, we can use the conjugate basis to generate approximations x^k of the minimizer $\hat{x}$ of f on $\mathcal{K}(A,Ab)=\mathcal{K}(A,Qb)$. Since for any $x\in\mathrm{Im}A$, $f(x)=f_Q(x)$, we get the solution of (5) and (6). The resulting algorithm is given in Table 1.

In Step 1, we denote zero vector by o. Notice that y^i are just the standard CG iterates for the solution of (1). Because

$$Ax^i=g^i+b,$$

we can evaluate the test without additional multiplications by A. Thus if we store Ap^{i+1}, the most expensive operation, the multiplication by A, is executed only once in each step. The algorithm requires the storage for one generation of x, y, g, g_A, p, b, and Ap. The cost of the iteration is dominated by one matrix–vector product and six scalar products, which compares favourably with alternative algorithms for the least squares problems (see [8]). Since $\hat{y}=Qb$,

$$\|y^i-\hat{y}\|\le\|A^\dagger\|\|Ay^i-Ab\|=\|A^\dagger\|\|g_A^i\|,$$

and

$$\|Ax^i-Qb\|\le\|Ax^i-y^i\|+\|y^i-\hat{y}\|\le\|Ax^i-y^i\|+\|A^\dagger\|\|g_A^i\|,$$

the test guarantees a small approximation error of both x^i and y^i.

The following theorem guarantees that the algorithm is well defined and finds the solution in a finite number of steps.

Proposition 3.1: *Let x^i, y^i, and p^i be generated by the cgSLS algorithm for the solution of* (1)*; let $g^i=Ax^i-b=\nabla f(x^i)$ and $g_A^i=Ay^i-Ab=\nabla f_A(y^i)$. Then the following statements hold:*

(i) *If $g_A^i\neq o$, then x^i, y^i, and p^{i+1} are well defined and*

$$\|p^{i+1}\|\ge\|g_A^i\|.$$

(ii) *If* $g_A^i = o$, *then* $y^i = \hat{y} = Qb$ *and* $x^i = \hat{x} = A^\dagger b$.
(iii) *cgSLS finds* $\hat{x}$ *and* $\hat{y}$ *in a finite number of steps.*

Proof: (i) The statement is trivial for $i = 0$. If $i \geq 1$, then y^i is a minimizer of f_A on $\mathcal{K}^i(A, Ab)$, so $(g_A^i)^{\mathrm{T}} y = 0$ for any $y \in \mathcal{K}^i(A, Ab)$. Thus $(g_A^i)^{\mathrm{T}} p^i = 0$ and

$$\|p^{i+1}\|^2 = \|g_A^i\|^2 + \|p^i\|^2 \geq \|g_A^i\|^2.$$

Since $p^{i+1} \in \mathcal{K}^{i+1}(A, Ab)$, it follows that $p^{i+1} \in \mathrm{Im}A$ and $(p^{i+1})^{\mathrm{T}} A p^{i+1} > 0$.

(ii) The first part of (ii) is rather trivial. Indeed, if $g_A^i = o$, then $Ay^i = Ab$. Since $y^i \in \mathcal{K}^i(A, Ab)$ it follows that $y^i = \hat{y} = Qb$.

To prove the second part, let us assume that $g_A^i = o$ and notice that $y^i = Qb$ implies

$$Qb \in \mathcal{K}^i(A, Ab) \quad \text{and} \quad \mathcal{K}^i(A, Ab) = \mathcal{K}^{i+1}(A, Qb). \tag{9}$$

Because $g^0 \neq o, \ldots g^{i-1} \neq o$, it follows that

$$\mathcal{K}^1(A, Ab) \subsetneq \cdots \subsetneq \mathcal{K}^i(A, Ab),$$

so $Ab, \ldots, A^i b$ is a basis of $\mathcal{K}^i(A, Ab)$. Observing that the mapping

$$\tau : \mathcal{K}^i(A, Qb) \ni z \mapsto Az \in \mathcal{K}^i(A, Ab)$$

is isomorphism, we get that $Qb, Ab, \ldots, A^{i-1} b$ is a basis of $\mathcal{K}^i(A, Qb)$, so by Equation (9) $A^i b \in \mathcal{K}^i(A, Qb)$ and

$$\mathcal{K}^i(A, Qb) = \mathcal{K}^i(A, Ab) = \mathcal{K}^{i+1}(A, Qb). \tag{10}$$

It follows that i is the grade of Qb with respect to A and

$$\mathcal{K}^i(A, Ab) = \mathcal{K}(A, Qb).$$

To finish the proof, notice that

$$x^i = \arg \min_{x \in \mathcal{K}^i(A, Ab)} f(x) = \arg \min_{x \in \mathcal{K}(A, Qb)} f(x),$$

so that

$$(Ax^i - b)^{\mathrm{T}} z = 0, \quad z \in \mathcal{K}(A, Qb).$$

Taking $z = Ax^i - Qb = Q(Ax^i - b)$, we get

$$(Ax^i - b)^{\mathrm{T}} Q(Ax^i - b) = \|Ax^i - Qb\|^2 = 0,$$

that is, $x^i = \hat{x} = A^\dagger b$.

(iii) Observing that g_A^i is orthogonal to $\mathcal{K}^i(A, Ab)$ and belongs to $\mathcal{K}^{i+1}(A, Ab)$, it follows that that it must generate $g_A^i = o$ in at most n steps. The rest follows by (ii). ■

4. Convergence and error bounds

Let us show that it is possible to give bounds on the error of cgSLS iterations that are similar to the well known ones of the classical CG method. Indeed, the iterates y^i are just the CG iterations on the range of A for the minimal norm solution of (4), so that we can give an error bound [3]

$$\|\mathrm{e}_A^i\|_A \le 2\left(\frac{\sqrt{\bar\kappa}-1}{\sqrt{\bar\kappa}+1}\right)^i \|\mathrm{e}_A^0\|_A, \tag{11}$$

where

$$e_A^i = y^i - \hat y, \quad e_A^0 = y^0 - \hat y = -Qb.$$

The bound on the approximation error of the iterate s x^i and the asymptotic rate of convergence are given by the following theorem.

Theorem 4.1: *Let x^i denote the iterations generated by cgSLS for the least-squares problem* (1) *with the solution $\hat x$ and let $\bar\kappa$ denote the regular condition number of A.*

Then

$$\|\mathrm{e}^{2i-1}\|_A \le 6\left(\frac{\sqrt{\bar\kappa}-1}{\sqrt{\bar\kappa}+1}\right)^i \|\mathrm{e}^0\|_A \tag{12}$$

and

$$\lim_{i\to\infty} \sqrt[i]{\|\mathrm{e}^i\|_A} = \frac{\sqrt{\bar\kappa}-1}{\sqrt{\bar\kappa}+1}, \tag{13}$$

where

$$\mathrm{e}^i = x^i - \hat x \quad \text{and} \quad \mathrm{e}^0 = x^0 - \hat x = -\hat x.$$

***Proof*:** We shall adapt the well established tools of analysis developed for CG. Let us denote

$$e = e(x) = x - \hat x, \quad \mathrm{e}^0 = -\hat x,$$
$$g = g(x) = Ax - Qb = Ae(x), \quad g^k = Ax^k - Qb, \quad e_A^0 = -Qb,$$

and recall that for any $x \in \mathrm{Im}A$

$$f(x) - f(\hat x) = \tfrac12\|x-\hat x\|_A^2 = \tfrac12\|e\|_A^2.$$

Since cgSLS looks for the iterations in $\mathcal{K}^i(A, Ab)$, it follows that they can be written in the form

$$x^i = \xi_1 Ab + \cdots + \xi_i A^i b.$$

Taking into account that $\mathrm{e}^0 = -\hat x$ and $Ab = A^2\hat x = -A^2\,\mathrm{e}^0$, we get

$$\mathrm{e}^i = \xi_1 Ab + \cdots + \xi_i A^i b - \hat x = \mathrm{e}^0 - \xi_1 A^2\,\mathrm{e}^0 - \cdots - \xi_i A^{i+1}\,\mathrm{e}^0 = p_{i+1}(A)\,\mathrm{e}^0,$$

where

$$p_{i+1}(\lambda) = 1 - \xi_1\lambda^2 - \xi_2\lambda^3 - \cdots - \xi_i\lambda^{i+1} = 1 - \lambda^2(\xi_1 + \xi_2\lambda + \cdots + \xi_i\lambda^{i-1}).$$

Since the iterates x^i minimize e^i on the Krylov space $\mathcal{K}^i(A, Ab)$, we get the estimate

$$\|\mathrm{e}^i\|_A \le \min_{p\in\mathcal{P}^{i+1}} \max_{\lambda\in\sigma(A)} |p(\lambda)|\|\mathrm{e}^0\| \le \min_{p\in\mathcal{P}^{i+1}} \max_{\lambda\in[\lambda_{\min},\lambda_{\max}]} |p(\lambda)|\|\mathrm{e}^0\|, \tag{14}$$

where $\mathcal{P}^i$ denotes the set of all polynomials p of the degree i that satisfy $p(0) = 1$ and have zero coefficient of the linear term. Thus to get an estimate for the error bound in ith iteration, it is enough

to find a polynomial $\bar{p} \in \mathcal{P}^{i+1}$ with small values $|\bar{p}(\lambda)|$ for $\lambda \in [\lambda_{\min}, \lambda_{\min}]$. It is useful to observe that if we denote by $\mathcal{Q}^j$ the set of all polynomials of the degree j, $j = 0, 1, 2, \ldots$, then we can express each polynomial $p_{i+1} \in \mathcal{P}^{i+1}$ by means of $q_{i-1} \in \mathcal{Q}^{i-1}$ as

$$p_{i+1}(\lambda) = 1 - \lambda^2 q_{i-1}(\lambda).$$

To find $\bar{p}$, we shall use the extremal properties of the Chebyshev polynomials (see, e.g. [18]). Recall that the transformed (weighted and shifted) Chebyshev polynomial

$$t_i = t_i(\lambda) = t_i(\bar{\lambda}_{\min}, \lambda_{\max}, \lambda)$$

minimizes $\max |1 - \lambda q(\lambda)|$ for $\lambda \in [\bar{\lambda}_{\min}, \lambda_{\max}]$ and $q \in \mathcal{Q}^{i-1}$ [18]. The transformed Chebyshev polynomials are related to the Chebyshev polynomials

$$T_i(\lambda) = \cos(i \arccos \lambda)$$

by

$$t_i = T_i\left(\frac{2\lambda - \lambda_{\max} - \bar{\lambda}_{\min}}{\lambda_{\max} - \bar{\lambda}_{\min}}\right) / T_i\left(-\frac{\lambda_{\max} + \bar{\lambda}_{\min}}{\lambda_{\max} - \bar{\lambda}_{\min}}\right)$$

and satisfy

$$|t_i(\lambda)| \leq 2\left(\frac{\sqrt{\bar{\kappa}} - 1}{\sqrt{\bar{\kappa}} + 1}\right)^i, \quad \lambda \in [\bar{\lambda}_{\min}, \lambda_{\max}]. \tag{15}$$

To prove Equation (12), let us define

$$\bar{p}_{2i}(\lambda) = t_i(\lambda)(2 - t_i(\lambda)), \quad i = 1, 2, \ldots, \tag{16}$$

and notice that $|t_i(\lambda)| \leq 1$, $\lambda \in [\lambda_{\min}$ and $\lambda_{\max}]$ imply

$$|\bar{p}_{2i}(\lambda)| \leq 3|t_i(\lambda)|, \quad \lambda \in [\lambda_{\min}, \lambda_{\max}]. \tag{17}$$

To see that $\bar{p}_{2i} \in \mathcal{P}^{2i}$, recall that $t_i(0) = 1$, so that $\bar{p}_{2i} = 1$. Moreover, t_i can be written in the form

$$t_i(\lambda) = 1 - \lambda q_{i-1}(\lambda), \quad q_{i-1} \in \mathcal{Q}^{i-1},$$

so that

$$\bar{p}_{2i}(\lambda) = (1 - \lambda q_{i-1}(\lambda))(1 + \lambda q_{i-1}(\lambda)) = 1 - \lambda^2 q_{i-1}^2(\lambda)$$

and the linear term of $\bar{p}_{2i}$ is zero. To get Equation (12), it is now enough to substitute Equation (15) into Equation (17).

To prove Equation (13), notice that t_i can be written in the form

$$t_i(\lambda) = 1 + \tau_1\lambda + \tau_2\lambda^2 + \cdots + \tau_i\lambda^i = 1 - \lambda q_{i-1}(\lambda),$$

so that the polynomial

$$\bar{p}_{i+1}(\lambda) = (1 - \tau_1\lambda)t_i(\lambda) \tag{18}$$

satisfies $\bar{p}_{i+1} \in \mathcal{P}^{i+1}$. It follows that

$$\begin{aligned} \|e^i\| &\le \max_{\lambda\in[\bar{\lambda}_{\min},\lambda_{\max}]} |\bar{p}_{i+1}(\lambda)|\|e^0\| \\ &\le \max_{\lambda\in[\bar{\lambda}_{\min},\lambda_{\max}]} |1 - \tau_1\lambda| \max_{\lambda\in[\bar{\lambda}_{\min},\lambda_{\max}]} |t_i(\lambda)|\|e^0\|. \end{aligned} \tag{19}$$

To give a bound on the linear term, notice that τ_1 can be expressed by means of the roots $\sigma_1, \sigma_2, \ldots, \sigma_i$ of t_i as

$$\tau_1 = -1/\sigma_1 - 1/\sigma_2 - \cdots - 1/\sigma_i,$$

so that for $\lambda \in [\bar{\lambda}_{\min}, \lambda_{\max}]$

$$|1 - \tau_1\lambda| \le 1 + \lambda_{\max}/\sigma_1 + \cdots + \lambda_{\max}/\sigma_i \le 1 + i\bar{\kappa}. \tag{20}$$

Combining Equations (19), (20), and (15), we get

$$\|e^i\| \le 2(1 + i\,\bar{\kappa}) \left(\frac{\sqrt{\bar{\kappa}} - 1}{\sqrt{\bar{\kappa}} + 1}\right)^i.$$

Using the standard results of the analysis, we get Equation (13). ■

5. Numerical experiments

We implemented cgSLS in Matlab environment and tested it on the solution of two academic benchmarks whose exact solution was easy to obtain by other means. The performance of cgSLS was compared with CGLS and standard CG applied to the solution of the related feasible problem with the right-hand side equal to $A\hat{x} = Qb$. The latter algorithm was labelled CGQ. The CGQ algorithm is in a sense an optimal basic algorithm for (1) when the orthogonal projector Q on ImA is known.

5.1. Benchmark with uniformly distributed spectrum

At first, we tested our algorithm on the class of problem (1) with a diagonal matrix A and the unit right-hand side vector b defined by

$$\begin{aligned} A &= \operatorname{diag}(\overbrace{0, \ldots, 0}^{n-m}, 1/m, 2/m, \ldots, m/m), \\ b &= \frac{1}{\|b_{\text{rand}}\|} b_{\text{rand}} \in \mathbb{R}^n,\ n = 1000,\ m = 800, \end{aligned}$$

so $\bar{\kappa}(A) = m$. We resolved hundred problems with random right-hand sides by the algorithms cgSLS, CGLS, and CGQ and draw the average relative energetic errors $\|e^i\|_A/\|e^0\|_A$ in Figure 1. The results show not only that cgSLS clearly outperforms CGLS, but also that the performance of cgSLS copies that of CGQ with some delay. We can observe that the asymptotic rate of convergence of cgSLS and CGQ is the same in agreement with the theory.

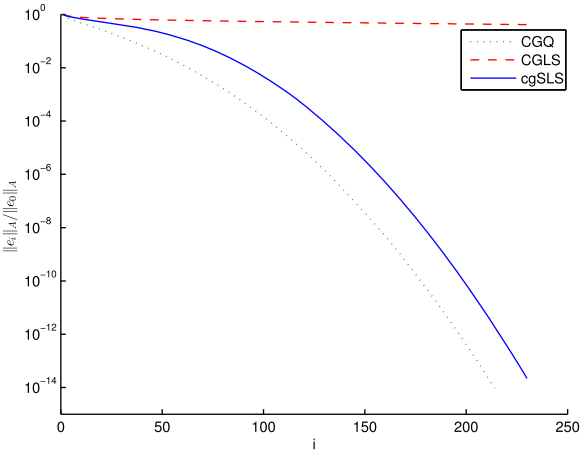

Figure 1. Decrease of average relative error – uniformly distributed spectrum.

5.2. Poisson equation with Neumann boundary condition

We tested our algorithm also on the least-squares solution of the Poisson equation with Neumann boundary condition given by

$$\begin{aligned} -\Delta u &= 0 \quad \text{on } \Omega, \\ \frac{\partial u}{\partial n} &= q \quad \text{on } \Gamma, \end{aligned} \tag{21}$$

where $\Omega = [0,1] \times [0,1]$ and

$$q(x) = \begin{cases} \sin(\pi x_1) & \text{for } x = (x_1, x_2) \in \mathbb{R}^2, \quad 0 \le x_1 \le 1 \text{ and } x_2 = 0, \\ 0 & \text{elsewhere.} \end{cases}$$

The function q is chosen so that it *does not satisfy* the compatibility condition

$$\int_\Gamma q \, \mathrm{d}\Gamma = 0.$$

For the discretization, we used the finite element method with linear elements defined on 100×100 grid. The solution of the problem is in Figure 2.

As above, we resolved the problem with the algorithms cgSLS, CGLS, and CGQ and draw the relative energetic errors in Figure 3. The results confirm that cgSLS clearly outperforms CGLS and that the performance of cgSLS copies that of CGQ with some delay. The latter observation is in agreement with the estimates provided by Theorem 4.1, which give the same bounds on the asymptotic rate of convergence of cgSLS and CGQ but provides larger error bounds for the iterations of cgSLS in the early stage of computations.

6. Comments and conclusions

We have presented a simple modification of the standard CG algorithm which can find the least-squares solution of the inconsistent system of linear equations with an SPS matrix A and the projection of the right-hand side b onto ImA in a number of multiplications which is only slightly greater than that required by the standard CG for the related feasible system. The algorithm requires only one matrix–vector multiplication per iteration. The asymptotic rate of convergence of the algorithm is

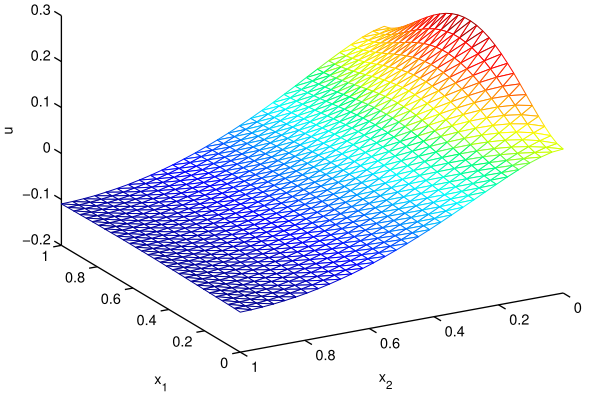

Figure 2. Solution of the Neumann problem.

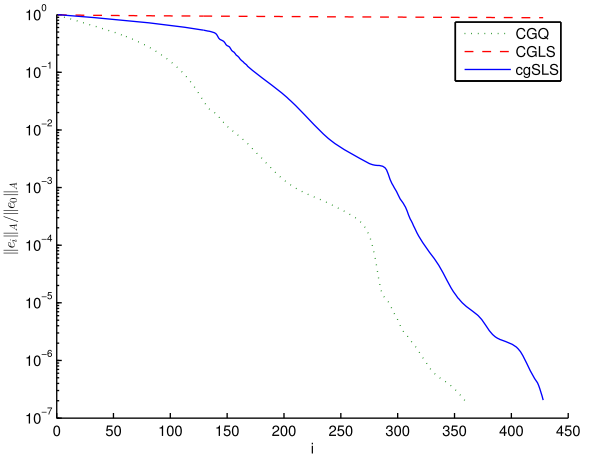

Figure 3. Decrease of relative error – Neumann problem.

proved to be the same as that of the CG method for the related consistent problem. The theoretical results are in agreement with numerical experiments. The performance of the algorithm can be improved by a suitable problem dependent preconditioning [16].

Disclosure statement

No potential conflict of interest was reported by the authors.

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