Comparison of two Different Discretizations for Spectral Computations for Integral Operators *

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Abstract

Let us consider a Fredholm integral operator and the corresponding invariant subspace basis problem. The spectral elements of the integral operator will be computed by a projection method on a subspace of dimension n followed by an iterative refinement method based on defect correction. The test problem to be used is the integral formulation of the transfer problem that represents the restriction of a strongly coupled system of nonlinear equations dealing with radiative transfer in stellar atmospheres. This restriction comes from considering that the temperature and the pressure are given and makes the problem a linear one. We will describe and compare two versions for the matrix implementation of the iterative refinement method based on projection methods and defect correction. These versions differ in the basis functions considered in the discretization of the problem.

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1 Projection methods for integral problems.

Let us consider the invariant subspace basis problem

$$\underline{T}\Phi = \Phi\Theta \tag{1}$$

where $\Phi \in X^\mu$, the product space having μ factors equal to X,

$$\Phi\Theta = \left[\sum_{j=1}^{\mu}\Theta(j,1)\Phi(j), \ldots, \sum_{j=1}^{\mu}\Theta(j,\mu)\Phi(j)\right]$$

for $\Phi = [\Phi(1), \ldots, \Phi(\mu)]$ and Θ a complex matrix of order μ. $\underline{T}$ denotes the operator that applies to each element of an ordered family of μ elements of X, the operator T. The Fredholm integral operator will be treated in $X = L^1(I)$ and is given by $T : X \to X$,

$$(Tx)(\tau) = \int_I g(|\tau - \tau'|)x(\tau')d\tau', \quad \tau \in I. \tag{2}$$

Integral operators of this type are usually discretized, for instance, by projection methods, onto a finite dimensional subspace. The operator T is thus approximated by its projection onto the finite dimensional subspace $X_n = \text{span}\{e_{n,j},\ j = 1..n\}$ and this approximation is denoted by T_n. In this case we will consider in X_n the basis of piecewise constant functions on each subinterval of I determined by a grid of $n+1$ points $\tau_{n,0} < \tau_{n,1} < \ldots < \tau_{n,n}$.

Definition 1. *(see [2]) For $x \in X$ the projection approximation T_n is defined by*

$$T_n x = \pi_n T x = \sum_{j=1}^{n}\langle Tx, e^*_{n,j}\rangle e_{n,j}, \tag{3}$$

where $\langle x, e^*_{n,j}\rangle = \frac{1}{h_{n,j}}\int_{\tau_{n,j-1}}^{\tau_{n,j}} x(\tau)d\tau$, $h_{n,j} = \tau_{n,j} - \tau_{n,j-1}$ and $\pi_n x = \sum_{j=1}^{n}\langle x, e^*_{n,j}\rangle e_{n,j}$.

Hence T_n is a bounded finite rank operator in X such that for all $x \in X$,

$$T_n x = \sum_{j=1}^{n}\langle x, \ell_{n,j}\rangle e_{n,j}, \tag{4}$$

where $\ell_{n,j} = T_n^* e^*_{n,j}$ is a basis of X^* the Hilbert-adjoint space of the Banach space X.

The projection approximation to problem (1) is

$$\underline{T_n}\Phi_n = \Phi_n\Theta_n. \tag{5}$$

Definition 2. *The adjoint evaluation $\langle\varphi, \ell\rangle = \overline{\ell(\varphi)}$, $\varphi \in X, \ell \in X^*$ is extended to the notion of a Gram matrix with p rows and q columns :*

$$G = \langle[\varphi(1), \ldots, \varphi(q)], [\ell(1), \ldots, \ell(p)]\rangle,$$

defined by

$$G(i,j) := \langle \varphi(j), \ell(i) \rangle = \overline{\ell(i)(\varphi(j))},$$

where $\varphi(j) \in X$ *for each* j *and* $\ell(i) \in X^*$ *for each* i.

Proposition 3. *The approximation problem (5) is solved by means of the matrix eigenvalue problem* $A_n u_n = u_n \Theta_n$.

Proof. If we take the adjoint evaluation of $\ell_{n,i}$ for all $i = 1, ..., n$ at both sides of (5)

$$\langle \underline{T_n} \Phi_n, \ell_{n,i} \rangle = \langle \Phi_n, \ell_{n,i} \rangle \Theta_n$$

$$\sum_{j=1}^{n} \langle e_{n,j}, \ell_{n,i} \rangle \langle \Phi_n, \ell_{n,j} \rangle = \langle \Phi_n, \ell_{n,i} \rangle \Theta_n$$

$$A_n u_n = u_n \Theta_n,$$

with $u_n(i) = \langle \Phi_n, \ell_{n,i} \rangle \in C^{1 \times \mu}$, $i = 1, ..., n$ and $A_n(i,j) = \langle e_{n,j}, \ell_{n,i} \rangle$. □

The eigenvalues of Θ_n are considered here as approximations to those of Θ. The accuracy of the solution of (5) as approximation to the solution of (1) is given by the following theorem :

Theorem 4. *For* n *large enough, there exists a basis* $\Phi^{(n)}$ *of the maximal invariant subspace of* T *associated to the spectrum of* Θ *such that*

$$\left| \widehat{\lambda}_n - \widehat{\lambda} \right| + \left\| \Phi_n - \Phi^{(n)} \right\| \leq \left\| (I - \pi_n) T^2 \right\|,$$

where

$$\widehat{\lambda}_n = \frac{1}{\mu} tr(\Theta_n), \qquad \widehat{\lambda} = \frac{1}{\mu} tr(\Theta),$$

and Φ_n *contains* μ *elements of* X *which form a basis of the maximal invariant subspace of* T_n *associated to the spectrum of* Θ_n.

Proof. see [4]. □

If, for a given n, the accuracy of the approximate Φ_n and Θ_n is not sufficient we apply iterative refinement to improve it.

A finer grid of $m + 1$ points $0 = \tau_{m,0} < \tau_{m,1} < \ldots < \tau_{m,m} = \tau^*$ is set to obtain a projection operator T_m which is only used to replace the operator T in the refinement scheme (and not to solve the corresponding approximate equation (6) with dimension m). The accuracy of the refined solution is the same that would be obtained by applying the projection method directly to this fine grid operator (for instance, see [4]).

2 Iterative refinement.

Let Ψ_n be a basis of the invariant subspace of T_n^* corresponding to the spectrum of Θ_n^*. In other words, the initial data satisfies (5) and

$$\underline{T_n^*}\Psi_n = \Psi_n\Theta_n^*, \qquad \langle \Phi_n, \Psi_n \rangle = I_\mu. \tag{6}$$

Definition 5. *The natural extension $\underline{P_n}$ of the spectral projection P_n corresponding to the spectrum of Θ_n is*

$$\forall x \in X^\mu, \quad \underline{P_n}(x) = \Phi_n \langle x, \Psi_n \rangle .$$

Definition 6. *The block reduced resolvent Σ_n of $\underline{T_n}$ corresponding to the spectrum of Θ_n is defined by :*

For all $y \in X^\mu$, $x = \Sigma_n y \in X^\mu$ is the solution of the Sylvester equation

$$\underline{T_n}(\underline{I} - \underline{P_n})x - x\Theta_n = (\underline{I} - \underline{P_n})y. \tag{7}$$

Proposition 7. *The computation of $x = \Sigma_n y \in X^\mu$ for a given $y \in X^\mu$ is represented by*

$$A_n (I_n - p_n) x_n - x_n\Theta_n = (I_n - p_n) y_n \tag{8}$$

for $x_n = \langle x, \ell_{n,j} \rangle$, $y_n = \langle y, \ell_{n,j} \rangle$ and the projection $p_n = u_n\Theta_n^{-1}v_n^*$ in the basis $\ell_{n,j}, j = 1, ..., n$.

The solution of (7) can be done on a subspace of dimension m, yielding

$$x_m = \left(Dx_n + u_m\Theta_n^{-1}v_n^*y_n - y_m\right)\Theta_n^{-1}. \tag{9}$$

Proof. $\underline{T_n}(\underline{I} - \underline{P_n})x - x\Theta_n = (\underline{I} - \underline{P_n})y$ is equivalent to

$$e_{n,j} \langle x, \ell_{n,j} \rangle - e_{n,j} \left\langle \underline{P_n}x, \ell_{n,j} \right\rangle - x\Theta_n = y - \Phi_n \langle x, \Psi_n \rangle$$

$$e_{n,j} \langle x, \ell_{n,j} \rangle - e_{n,j} \langle \Phi_n \langle x, \Psi_n \rangle , \ell_{n,j} \rangle - x\Theta_n = y - \Phi_n \langle x, \Psi_n \rangle ,$$

by the definitions of T_n and P_n.

We get for the l.h.s., by applying $\langle \cdot, \ell_{n,i} \rangle$, $j = 1, ..., n$,

$$\langle e_{n,j} \langle x, \ell_{n,j} \rangle , \ell_{n,i} \rangle - \left\langle e_{n,j} \langle \Phi_n \langle x, \Psi_n \rangle , \ell_{n,j} \rangle , \ell_{_{n,i}} \right\rangle - \langle x\Theta_n, \ell_{n,i} \rangle =$$

$$= \langle e_{n,j}, \ell_{n,i} \rangle \langle x, \ell_{n,j} \rangle - \langle e_{n,j}, \ell_{n,i} \rangle \langle \Phi_n, \ell_{n,j} \rangle \langle x, \Psi_n \rangle - \langle x, \ell_{n,i} \rangle \Theta_n$$

and for the r.h.s.

$$\langle y, \ell_{n,i} \rangle - \langle \Phi_n \langle y, \Psi_n \rangle , \ell_{n,i} \rangle = \langle y, \ell_{n,i} \rangle - \langle \Phi_n, \ell_{n,i} \rangle \langle y, \Psi_n \rangle =$$

$$= \langle y, \ell_{n,i} \rangle - \langle \Phi_n, \ell_{n,i} \rangle \Theta_n^{-1} \langle e_{n,j}, \Psi_n \rangle \langle y, \ell_{n,j} \rangle$$

because $\langle y, \Psi_n \rangle = \Theta_n^{-1} \langle e_{n,j}, \Psi_n \rangle \langle y, \ell_{n,j} \rangle$ (as we can see from (6)).

Finally, by equating both sides, we obtain

$$A_n x_n - A_n u_n \Theta_n^{-1} v_n^* x_n - x_n\Theta_n = y_n - u_n\Theta_n^{-1}v_n^*y_n$$

$$A_n\left(I_n - p_n\right)x_n - x_n\Theta_n = \left(I_n - p_n\right)y_n$$

for $x_n = \langle x, \ell_{n,j}\rangle$, $y_n = \langle y, \ell_{n,j}\rangle$ and $p_n = u_n\Theta_n^{-1}v_n^*$.

To obtain x_m we need to apply $\langle\cdot, \ell_{m,i}\rangle$, $i = 1, ..., m$, to (7) :

$$e_{n,j}\left\langle x, \ell_{n,j}\right\rangle - x\Theta_n = y - \Phi_n\left\langle y, \Psi_n\right\rangle$$

$$x = \left(e_{n,j}\left\langle x, \ell_{n,j}\right\rangle + \Phi_n\left\langle y, \Psi_n\right\rangle - y\right)\Theta_n^{-1}$$

$$\langle x, \ell_{m,i}\rangle = \left(\left\langle e_{n,j}\left\langle x, \ell_{n,j}\right\rangle, \ell_{m,i}\right\rangle + \left\langle \Phi_n\left\langle y, \Psi_n\right\rangle, \ell_{m,i}\right\rangle - \langle y, \ell_{m,i}\rangle\right)\Theta_n^{-1}$$

$$x_m = \left(Dx_n + u_m\Theta_n^{-1}v_n^*y_n - y_m\right)\Theta_n^{-1}. \qquad \square$$

Let $F : X^\mu \to X^\mu$ defined by

$$F(x) = \underline{T}x - x\langle\underline{T}x, \Psi_n\rangle. \tag{10}$$

The iterative refinement formula of the initial solution in (5) is obtained by solving (10) by defect correction ([5], [4] and [9]) where we use operator Σ_n as local approximate inverse of F.

Algorithm 1: $\Phi_n^{(0)} = \Phi_n$
for $k = 1, 2, ...$
$\Phi_n^{(k)} = \Phi_n^{(k-1)} - \Sigma_n(F(\Phi_n^{(k-1)}))$.

To improve the rate of convergence at each iteration an intermediate step of fixed point iteration is added.

Algorithm 2: $\Phi_n^{(0)} = \Phi_n$
for $k = 1, 2, ...$
$\Theta_n^{(k-1)} = \langle\underline{T}\Phi_n^{(k-1)}, \Psi_n^{(0)}\rangle$
$H^{(k)} = \underline{T}\Phi_n^{(k-1)}\left(\Theta_n^{(k-1)}\right)^{-1}$
$\Phi_n^{(k)} = H^{(k)} - \Sigma_n(F(H^{(k)}))$.

Theorem 8. *There is a positive integer n_1 such that for each fixed $n \geq n_1$, all the iterates of Algorithm 2 are well defined; and for all $k = 0, 1, 2, \ldots$*

$$\max\{|\widehat{\lambda}_n^{(k)} - \widehat{\lambda}|,\ \|\Phi_n^{(k)} - \Phi^{(n)}\|\} \leq (\beta\|(I - \pi_n)T^2\|)^{k+1},$$

where β is a constant, independent of n and k and

$$\widehat{\lambda}_n^{(k)} = \frac{1}{\mu}tr(\langle\underline{T}\Phi_n^{(k-1)}, \Psi_n^{(0)}\rangle).$$

Proof. Details of the proof can be found in [5] and [4]. $\square$

The iterative refinement method requires two operators T_n and T_m corresponding to the projections onto X_n and X_m respectively. The functional basis in X_n is $\{e_{n,j}\}_{j=1,...,n}$ and in X_m it is $\{e_{m,j}\}_{j=1,...,m}$, and the matrices representing the operators T_n and T_m restricted to X_n and X_m are respectively A_n and A_m. The matrix that represents T_m in X_n will be denoted by C and the representation of T_n in X_m will be D. To compute the coefficient elements of matrices A_m and A_n one needs to define first the kernel g. After it is easy to obtain the coefficient elements of matrices C and D (see for instance [2]).

In [3] we developed the matrix relationships and expressions used in this algorithm by using the canonical basis $(e_{n,j}), j = 1, ..., n$ in X_n and $(e^*_{n,j}), j = 1, ..., n$ in X^*_n. Now we will consider the basis $(e_{n,j}), j = 1, ..., n$ in X_n and $(\ell^*_{n,j}), j = 1, ..., n$ in X^*_n.

In order to implement the algorithms we need to relate u_n with u_m using $u_m = Du_n\Theta_n^{-1}$.

From (5)

$$\Phi_n = \underline{T_n}\Phi_n\Theta_n^{-1} = \sum_{j=1}^{n} \langle \Phi_n, \ell_{n,j}\rangle\, e_{n,j}\Theta_n^{-1},$$

and taking adjoint evaluation by $\ell_{m,i}$, $i = 1, ..., m$ yields

$$\langle \Phi_n, \ell_{m,i}\rangle = \sum_{j=1}^{n} \langle e_{n,j}, \ell_{m,i}\rangle \langle \Phi_n, \ell_{n,j}\rangle \Theta_n^{-1}$$

$$u_m = Du_n\Theta_n^{-1}.$$

Proposition 9. *The approximation problem (6) is solved by means of the matrix eigenvalue problem $A^*_n v_n = v_n\Theta^*_n$. It can be done also on the subspace of dimension m, yielding $v_m = C^* v_n \left(\Theta^*_n\right)^{-1}$.*

Proof. Let us now consider expression (6). Knowing that for $f \in X^*$ and for $x \in X$

$$\left(\underline{T^*_n} f\right) x = f\left(\underline{T_n} x\right) =$$

$$= f\left(\sum_{j=1}^{n} \langle x, \ell_{n,j}\rangle\, e_{n,j}\right) =$$

$$= \sum_{j=1}^{n} \overline{\langle x, \ell_{n,j}\rangle} f\left(e_{n,j}\right) =$$

$$= \sum_{j=1}^{n} \overline{\langle x, \ell_{n,j}\rangle \langle e_{n,j}, f\rangle},$$

then from (6) and by taking the adjoint evaluation at $e_{n,i}$, $i = 1, ..., n$ we have

$$\left(\underline{T^*_n}\Psi_n\right) e_{n,i} = \Psi_n\left(e_{n,i}\right)\Theta^*_n$$

$$\sum_{j=1}^{n} \overline{\langle e_{n,i}, \ell_{n,j}\rangle\langle e_{n,j}, \Psi_n\rangle} = \overline{\langle e_{n,i}, \Psi_n\rangle}\Theta_n^*$$

$$A_n^* v_n = v_n \Theta_n^*,$$

with $v_n(i) = \overline{\langle e_{n,i}, \Psi_n\rangle} \in C^{1\times\mu}$, $i = 1, ..., n$.

From (6)

$$\Psi_n = \underline{T_n^*}\Psi_n \left(\Theta_n^*\right)^{-1},$$

and taking the adjoint evaluation by $e_{m,i}$, $i = 1, ..., m$ yields

$$\Psi_n \left(e_{m,i}\right) = \underline{T_n^*}\Psi_n \left(e_{m,i}\right) \left(\Theta_n^*\right)^{-1}$$

$$\overline{\langle e_{m,i}, \Psi_n\rangle} = \sum_{j=1}^{n} \overline{\langle e_{m,i}, \ell_{n,j}\rangle\langle e_{n,j}, \Psi_n\rangle} \left(\Theta_n^*\right)^{-1}$$

$$v_m = C^* v_n \left(\Theta_n^*\right)^{-1}. \qquad \square$$

3 Numerical results.

To test the previous approaches, we consider an integral formulation of a transfer problem that represents the restriction of a strongly coupled system of nonlinear equations modeling the radiative transfer in stellar atmospheres. This restriction comes from considering that the temperature and the pressure are given (see [2] and [8] for details). Problem (2) takes the form

$$(Tx)(\tau) = \int_0^{\tau_*} g(|\tau - \tau'|)x(\tau')d\tau', \quad 0 \le \tau \le \tau^*, \tag{11}$$

where $I = [0, \tau^*]$, $\tau^\star$ is the optical depth of the stellar atmosphere, $\varpi \in]0, 1[$ is the albedo (assumed to be constant). The kernel g is defined by $g(\tau) = \frac{\varpi}{2}E_1(\tau)$, where $E_1(\tau) = \int_1^\infty \frac{\exp(-\tau\mu)}{\mu}d\mu, \tau > 0$. This is the first of the sequence of functions

$$E_\nu(\tau) = \int_1^\infty \frac{\exp(-\tau\mu)}{\mu^\nu}d\mu, \tau > 0, \nu \ge 1, \tag{12}$$

which has the following property: $E_{\nu+1}^{'} = -E_\nu$ and $E_\nu(0) = \frac{1}{\nu-1}, \nu > 1$ (see [1]). E_1 has a logarithmic singularity at $\tau = 0$.

We consider for the equation modeling the radiative transfer problem of the absorption of photons due to internal sources in the stellar atmospheres the albedo to be $\varpi = 0.75$. The interval $I = [0, \tau^*]$ is divided into four zones where we consider different regular grids. In our tests, τ^* is taken as 4000. The computations were done on a personal computer.

The coefficient elements of matrices A_m and A_n can be obtained, using the properties of the family of exponential-integrals (12). For A_n we obtain (see [2] and [3]) (similarly for A_m):

Table 1: Number of iterations for a residual tolerance of $1e-6$.

eig	e-basis	ℓ-basis	gain
1	49	39	26 %
2	43	37	16 %
3	70	57	23 %
4	106	87	22 %

Table 2: CPU time (seconds) for a residual tolerance of $1e-6$.

eig	e-basis	ℓ-basis	gain
1	125.8	110.0	14 %
2	118.5	107.8	10 %
3	151.1	130.3	16 %
4	194.0	163.8	18 %

$$A_n(i,j) = \frac{\varpi}{2h_{n,i}}(-E_3(|\tau_{n,i}-\tau_{n,j}|) + E_3(|\tau_{n,i-1}-\tau_{n,j}|)+$$
$$+E_3(|\tau_{n,i}-\tau_{n,j-1}|) - E_3(|\tau_{n,i-1}-\tau_{n,j-1}|))$$

if $i \neq j$ and

$$A_n(i,i) = \varpi[1 + \frac{1}{2h_{n,i}}(2E_3\left(h_{n,i}\right) - 1)].$$

The computations were carried out by implementing the series developments in [1].

The number of iterations and CPU time in seconds, for the computation of the largests eigenpairs of the problem for $\tau^* = 4000$, are shown in Tables 1 and 2 respectively, for a tolerance of 10^{-6} and in Tables 3 and 4 for a tolerance of 10^{-12}.

We can see that the method shows a good performance for both tolerances and both basis. As expected, the number of iterations grows with the required precision and it is larger for lower order eigenpairs. The method can profit by computing a set of the largest eigenpairs since the computation of the initial approximate eigenpairs can be reused for the refinement process.

In terms of CPU time, the ℓ-basis approach allows a gain between 10 and 18% for a tolerance of 10^{-6} and a gain between 15 and 18% for a tolerance of 10^{-12}. In regard to the number of iterations, the use of ℓ-basis carries out a reduction of about 16-23% for a tolerance of 10^{-6} and of about 10% for 10^{-12}.

Table 3: Number of iterations for a residual tolerance of $1e-12$.

eig	e-basis	ℓ-basis	gain
1	348	318	9 %
2	411	375	10 %
3	492	443	11 %
4	628	566	11 %

Table 4: CPU time (seconds) for a residual tolerance of $1e-12$.

eig	e-basis	ℓ-basis	gain
1	483.6	422.2	15 %
2	557.9	486.5	15 %
3	659.2	564.1	17 %
4	823.7	700.0	18 %

In conclusion, solving the eigenvalue problem in a low dimensional discretization space and then refining iteratively the previous approximation to the spectral elements of T is an effective approach to solve integral eigenvalue problems. We developed an alternative approach to the discretization of the refinement method by using the ℓ-basis and we proved, in this paper, that it is better in number of iterations and CPU time than the one that uses basis (e_n) (developed in [3]). Those valuable gains were achieved without changing the way data is generated and by only taking into account a new basis where the finite dimensional approximate solutions are projected.

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