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COMPARISON OF TWO 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.

Dedicated to the memory of
Alain Largillier (1949-2010).

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1. Projection Methods

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 T 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 $T : X \to X$,

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

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 a finite dimensional subspace X_n spanned by n linear independent elements $(e_{n,j})_{j=1:n}$. 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 $0 =: \tau_{n,0} < \tau_{n,1} < \ldots < \tau_{n,n} := \tau^*$.

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

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

where

$$\langle x, e_{n,j}^* \rangle := \frac{1}{h_{n,j}} \int_{\tau_{n,j-1}}^{\tau_{n,j}} x(\tau)d\tau,$$

$$h_{n,j} := \tau_{n,j} - \tau_{n,j-1}, \quad \pi_n x := \sum_{j=1}^{n} \langle x, e_{n,j}^* \rangle e_{n,j}.$$

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

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

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

$$\underline{T_n} \Phi_n = \Phi_n \Theta_n. \tag{3}$$

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

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

where $\varphi(j) \in X$ for $j = 1 : q$, and $\ell(i) \in X^*$ for $i = 1 : p$.

Proposition 1. *Problem (3) is solved by means of a matrix eigenvalue problem $A_n u_n = u_n \Theta_n$.*

Proof. Take the adjoint evaluation with $\ell_{n,i}$ for each $i = 1 : n$ at both sides of (3), $\langle \underline{T_n} \Phi_n, \ell_{n,i} \rangle = \langle \Phi_n, \ell_{n,i} \rangle \Theta_n$, we get

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

i.e. $A_n u_n = u_n \Theta_n$, where $u_n(i) := \langle \Phi_n, \ell_{n,i} \rangle \in C^{1 \times \mu}$, $i = 1 : n$ 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 (3) as approximation to the solution of (1) is given by the following theorem:

Theorem 1. *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*

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

where

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

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 $0 = \tau_{m,0} < \tau_{m,1} < \ldots < \tau_{m,m} = \tau^*$ 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 (4) 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. (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 (3) and

$$\underline{T_n^*}\Psi_n = \Psi_n\Theta_n^*, \qquad \langle \Phi_n, \Psi_n \rangle = I_\mu. \tag{4}$$

Proposition 2. *The natural extension $\underline{P_n}$ of the spectral projection P_n corresponding to the spectrum of Θ_n is given by*

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

Definition 3. 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

$$\underline{T_n}(\underline{I} - \underline{P_n})x - x\Theta_n = (\underline{I} - \underline{P_n})y. \tag{5}$$

Proposition 3. *The computation of $x = \Sigma_n y \in X^\mu$ for a given $y \in X^\mu$ is represented by*

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

for $x_n := \langle x, \ell_{n,j} \rangle$, $y_n := \langle y, \ell_{n,j} \rangle$ and $p_n := u_n\Theta_n^{-1}v_n^*$ in the basis $\ell_{n,j}$, $j = 1 : n$. The solution of (5) is obtained on an m-dimensional subspace, yielding

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

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

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

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

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

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

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

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 (4). Finally, by equating both sides, we obtain

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

i.e.

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

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 (5):

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

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

$$\begin{aligned} \langle x, \ell_{m,i}\rangle &= (\langle e_{n,j}\langle x, \ell_{n,j}\rangle, \ell_{m,i}\rangle \\ &\quad + \langle \Phi_n\langle y, \Psi_n\rangle, \ell_{m,i}\rangle - \langle y, \ell_{m,i}\rangle)\Theta_n^{-1}, \end{aligned}$$

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

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

$$F(x) := \underline{T}x - x\langle \underline{T}x, \Psi_n\rangle. \tag{6}$$

The iterative refinement formula of the initial solution in (3) is obtained by solving (6) by defect correction ([4] and [6]) 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 $k = 1, 2, ...$

$$
\begin{aligned}
\Theta_n^{(k-1)} &:= \langle \underline{T}\Phi_n^{(k-1)}, \Psi_n^{(0)} \rangle \\
H^{(k)} &:= \underline{T}\Phi_n^{(k-1)}(\Theta_n^{(k-1)})^{-1} \\
\Phi_n^{(k)} &:= H^{(k)} - \Sigma_n(F(H^{(k)})).
\end{aligned}
$$

Theorem 2. *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

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

Proof. Details of the proof can be found in [4]. □

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 entries of matrices A_m and A_n one only needs the kernel g. (See [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. From (3), $\Phi_n = \underline{T_n}\Phi_n\Theta_n^{-1} = \sum_{j=1}^{n} \langle \Phi_n, \ell_{n,j} \rangle e_{n,j}\Theta_n^{-1}$, and taking adjoint evaluation with $\ell_{m,i}$, $i = 1 : m$, $\langle \Phi_n, \ell_{m,i} \rangle = \sum_{j=1}^{n} \langle e_{n,j}, \ell_{m,i} \rangle \langle \Phi_n, \ell_{n,j} \rangle \Theta_n^{-1}$, i.e. $u_m = Du_n\Theta_n^{-1}$.

Proposition 4. *The approximation problem (4) 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 $v_m = C^* v_n(\Theta^*_n)^{-1}$.*

Proof. Let us now consider expression (4). Knowing that, for $f \in X^*$ and $x \in X$,

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

then, from (4), and taking the adjoint evaluation at $e_{n,i}$ for $i = 1 : n$, we have

$$(\underline{T_n^*}\Psi_n)e_{n,i} = \Psi_n(e_{n,i})\Theta_n^*$$

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

i.e. $A_n^* v_n = v_n \Theta_n^*$, where $v_n(i) := \overline{\langle e_{n,i}, \Psi_n\rangle} \in C^{1\times\mu}$, $i = 1 : n$. From (4),

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

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

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

i.e. $v_m = C^* v_n(\Theta_n^*)^{-1}$. □

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 [5] for details). Problem (2) takes the form

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

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 $g(\tau) = \dfrac{\varpi}{2}E_1(\tau)$, where E_1 is the first function of the sequence $(E_\nu)_{\nu\ge1}$ defined by

$$E_\nu(\tau) = \int_1^{\infty} \frac{\exp(-\tau\mu)}{\mu^\nu} d\mu, \quad \tau > 0,\ \nu \ge 1, \tag{7}$$

which satisfies $E'_{\nu+1} = -E_\nu$ and $E_\nu(0) = \dfrac{1}{\nu-1}, \nu > 1$ (see [1]). Note that E_1 has a logarithmic singularity at $\tau = 0$. Take $\varpi = 0.75$. 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 (7). For A_n we obtain (see [2] and [3]), for $i \neq j$:

$$\begin{aligned} A_n(i,j) &= \frac{\varpi}{2h_{n,i}}\Big[-E_3(|\tau_{n,i}-\tau_{n,j}|)+E_3(|\tau_{n,i-1}-\tau_{n,j}|) \\ &\quad +E_3(|\tau_{n,i}-\tau_{n,j-1}|)-E_3(|\tau_{n,i-1}-\tau_{n,j-1}|)\Big], \end{aligned}$$

and

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

The computations were carried out by implementing the series developments given 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 Table 1 with a tolerance of 10^{-6} and in Tables 2 with 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}.

	Number of iterations			CPU time		
eig	e-basis	ℓ-basis	gain	e-basis	ℓ-basis	Gain
1	49	39	26 %	125.8	110.0	14 %
2	43	37	16 %	118.5	107.8	10 %
3	70	57	23 %	151.1	130.3	16 %
4	106	87	22 %	194.6	163.8	18 %

Table 1 Number of iterations and CPU time (in seconds) for a residual tolerance of 10^{-6}.

	Number of iterations			CPU time		
eig	e-basis	ℓ-basis	gain	e-basis	ℓ-basis	Gain
1	348	318	9 %	483.6	422.2	15 %
2	411	375	10 %	557.9	486.5	15 %
3	492	443	11 %	659.2	564.1	17 %
4	628	566	11 %	823.7	700.0	18 %

Table 2 Number of iterations and CPU time (in seconds) for a residual tolerance of 10^{-12}.

4. Conclusions

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 different auxiliary linear system.

References

[1] M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions*, Dover, New York (1960).

[2] M. Ahues, F.D. d'Almeida, A. Largillier, O. Titaud, P. Vasconcelos, An L^1 refined projection approximate solution of the radiation transfer equation in stellar atmospheres, *J. Comput. Appl. Math.*, **140** (2002), 13-26.

[3] M. Ahues, F.D. d'Almeida, A. Largillier, O. Titaud, P. Vasconcelos, Defect correction for spectral computations for a singular integral operator, *Communications on Pure and Applied Analysis*, **5**, No. 2 (2006), 241-250.

[4] M. Ahues, A. Largillier, B.V. Limaye, *Spectral Computations with Bounded Operators*, Chapman and Hall, Boca Raton (2001).

[5] B. Rutily, Multiple scattering theoretical and integral equations, In: *Integral Methods in Science and Engineering: Analytic and Numerical Techniques* (Ed-s: C. Constanda, M. Ahues, A. Largillier), Birkhauser, Boston (2004), 211-231.

[6] H. Stetter, The defect correction principle and discretization methods, *Numer. Math.*, **29** (1978), 425-443.