On correction equations and domain decomposition for computing invariant subspaces

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Introduction

How to correct bases of invariant subspaces ?

Case of real symmetric matrices (or complex hermitian)

Matrices obtained from discretized operators on partitioned domains (domain decomposition).

Matrices are large, sparse and block structured (for adequate unknown numberings)

We search methods which manipulate the considered matrix as an operator :

$$A : \begin{array}{ccc} \mathbb{R}^n & \longrightarrow & \mathbb{R}^n \\ x & \longrightarrow & Ax. \end{array}$$

Approximate invariant subspace

Let us assume that $U \subset \mathbb{R}^{n\times k}$ is an orthonormal basis of an approximate invariant subspace $\mathcal{U}$ of $\mathbb{R}^n$ of dimension k: $\quad A\mathcal{U} \not\subset \mathcal{U}$.

Projecting onto $\mathcal{U} \oplus \mathcal{U}^{\perp}$:

$$\begin{aligned} AU &= UU^T(AU) + (I - UU^T)(AU) \\ &= UD + R, \end{aligned}$$

where

$$\boxed{A}\;\boxed{U} = \boxed{U}\;\boxed{D} + \boxed{R}$$

- Matrix of the restricted operator : $D = U^T AU$
- Residual :
  $$\begin{aligned} R &= AU - UD \\ &= (I - UU^T)(AU) \end{aligned}$$
  (lack of invariance)

Backward error and residual bounds

Since $AU = UD + R \Rightarrow (A - RU^T)U = UD$:

Theorem : *The subspace $\mathcal{U}$ is invariant by the matrix $\tilde{A} = A - RU^T$. The correction $\Delta = -RU^T$ is minimum (for the 2-norm) within all corrections Δ for which $\mathcal{U}$ is invariant by $(A + \Delta)$.*

Theorem : *A is symmetric with eigenvalues $(\lambda_i)_{i=1,\cdots,n}$. Let $(\mu_i)_{i=1,\cdots,k}$ be the eigenvalues of $D = U^t AU$, then there exist k eigenvalues of A, numbered $(\lambda_{i_j})_{j=1,\cdots,k}$, such that*

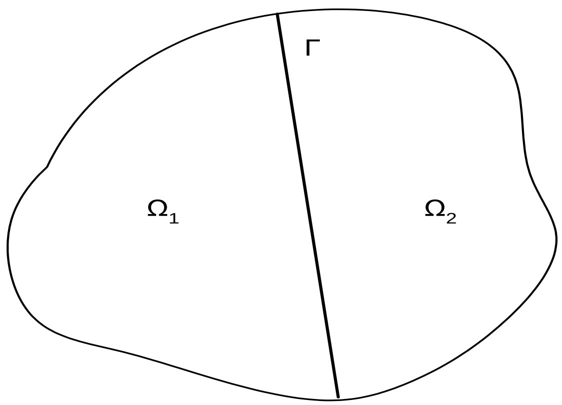
$$|\lambda_{i_j} - \mu_j| \leq \|R\|_2,$$

where $R = AU - UD$.

For $i = 1, \cdots, k$, the eigenvalues μ_i of D are called Ritz values of A obtained from $\mathcal{U}$. The vectors $x_i = Uy_i$, where y_i is the eigenvector of D corresponding to μ_i, is called Ritz vector .

The problem

Let A be an operator defined on a domain $\Omega = \bigcup_{i=1}^{p} \Omega_i$ and A_i the restriction of the operator on Ω_i.



The simplest case of two subdomains Ω_1, Ω_2 and an interface Γ.

How to build an approximation of the spectrum of A from the knowledge of the spectra of $(A_i)_{1,p}$?

General block correction

$U \in \mathbb{R}^{n\times m}$: orthonormal basis of an approximate invariant subspace and $D = U^T AU$.

$$R \;=\; AU - UD = (I - UU^T)AU \Rightarrow U^T R = 0.$$

Goal : Obtain (W, Δ) such that

$$A(U + W) \;=\; (U + W)(D + \Delta). \tag{1}$$

But mn equations and $mn + m^2$ unknowns ; the system is closed by the condition :

$$U^T W = 0. \tag{2}$$

Two possible algorithms:

- Solving (1-2) by Newton.
- Iterating on the first order expression of (1-2).

First order correction

Neglecting second order terms from the system (1-2) yields the equations:

$$\begin{cases} AW - WD - U\Delta = -R \\ U^T W = 0. \end{cases} \quad (3)$$

By multiplying the first equation on the left side by U^T, and using relation $U^T R = 0$: $\Delta = U^T A W$.

Therefore, system (3) is equivalent to computing W in the correction equation

$$(I - UU^T)AW - WD \;=\; -R \quad (4)$$

and then computing $\Delta = U^T A W$. The obtained solution W satisfies $U^T W = 0$ as required.

Equation (4) is a Sylvester equation :
$KW - WD = -R$ with $K \in \mathbb{R}^{n\times n}$, $D \in \mathbb{R}^{m\times m}$ and $W \in \mathbb{R}^{n\times m}$.

Newton method for solving System 1-2

After the change of unknowns $U_{k+1} = U + W_k = U_k + Z_k$:

Algorithm : Newton-Sylvester iteration (Quadratic convergence)

0. Select U_0 s.t. $U_0^T U = I$ (e.g., $U_0 = U$)
1. For $k = 0, \cdots,$ until convergence Do:
2. Compute $D_k = U^T A U_k$, and $R_k = AU_k - U_k D_k$
3. Solve (for Z_k): $(I - U_k U^T) A Z_k - Z_k D_k = -R_k$
4. Set $U_{k+1} = U_k + Z_k$
5. EndDO

Line 2 : matrix multiplications (dense and sparse).

Line 3 : Sylvester equation (diagonalization of D_k, change of basis, m sparse linear $n \times n$-systems.

Non linear correction

At each step, reevaluate D and compute U in (5):

$$(I - UU^T)AW - WD \;=\; -R \quad \text{with} \quad U^T W = 0. \tag{5}$$

Algorithm : Iterative correction (Cubic convergence)

0. Select U_0 (e.g., $U_0 = U$)
1. For $k = 0, \cdots,$ until convergence Do:
2. Compute $D_k = U_k^T A U_k$, and $R_k = AU_k - U_k D_k$
3. Solve (for W_k): $(I - U_k U_k^T)AW_k - W_k D_k = -R_k$
4. Orthogonalize : $[U_{k+1}, S_k] = \text{qr}(U_k + W_k)$.
5. EndDO

Line 4 : Additional computation w.r.t. Newton-Sylvester.

Remark : The correction (5) is used in Jacobi-Davidson and in TRACMIN (Trace Minimization).

Test matrix 1

5-Point discretized Laplacian on a 14×17 mesh : $n = 238$.

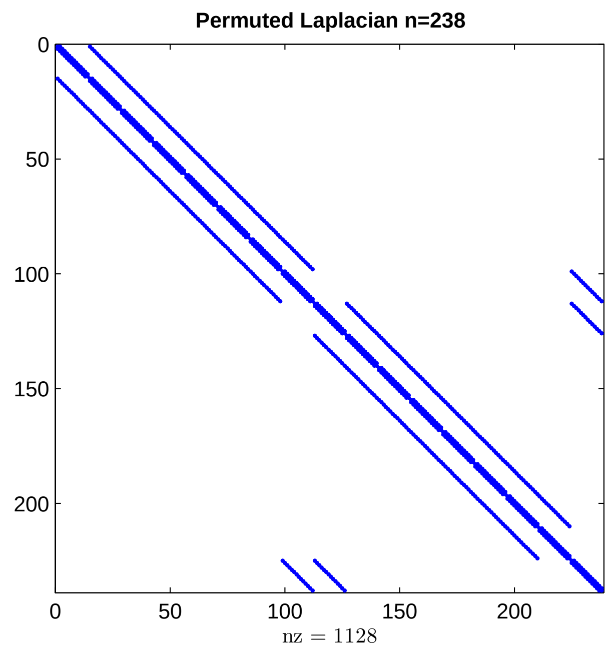
T_1 and T_2 of order 112 and C of order 14 :

$$T = \begin{pmatrix} T_1 & 0 & B_1 \\ 0 & T_2 & B_2 \\ B_1^T & B_2^T & C \end{pmatrix}$$

Initial guess :

$$U_0 = \begin{pmatrix} U^{(1)} & 0 \\ 0 & U^{(2)} \\ 0 & 0 \end{pmatrix}.$$

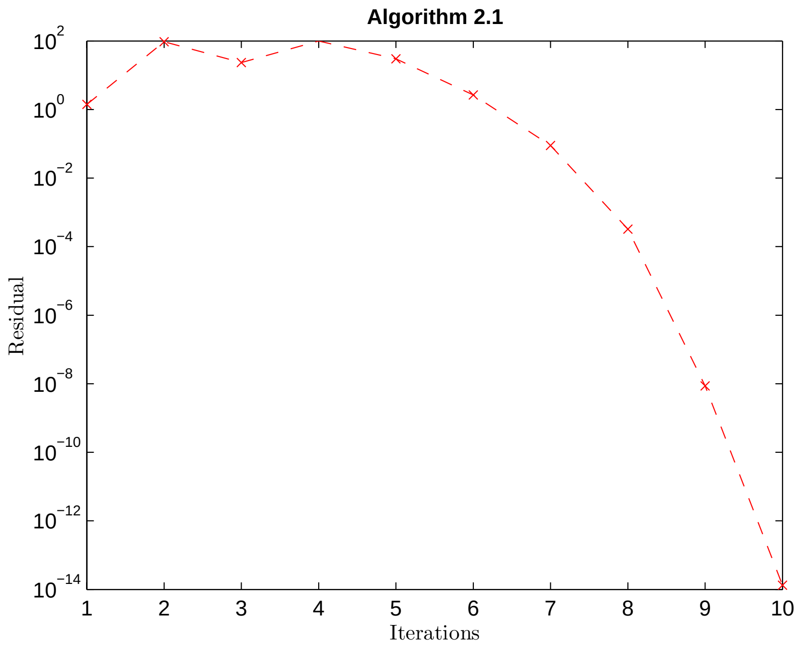
where $U^{(1)} \in \mathbb{R}^{112\times 10}$ are the eigenvectors of the 10 smallest eigenvalues of T_i.



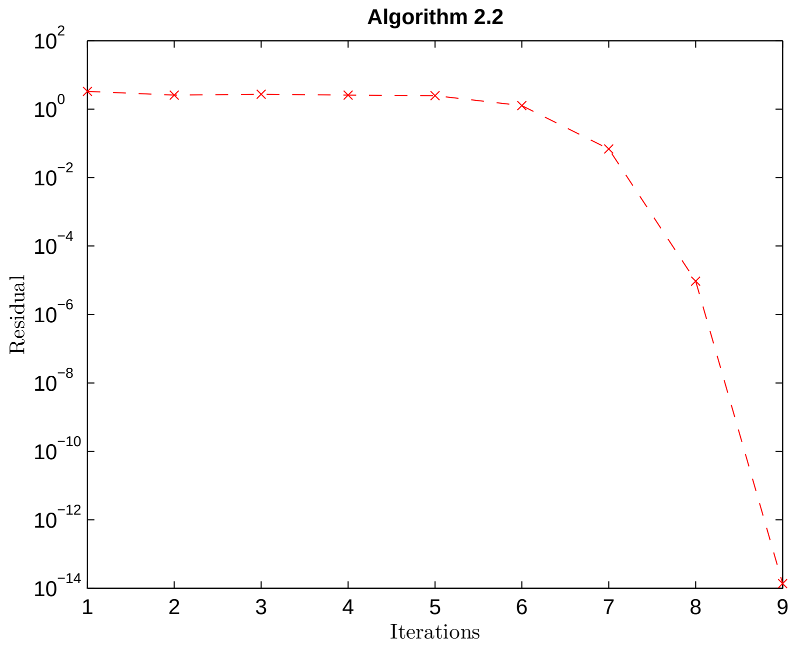
Pattern of the matrix

Convergence

Newton-Sylvester



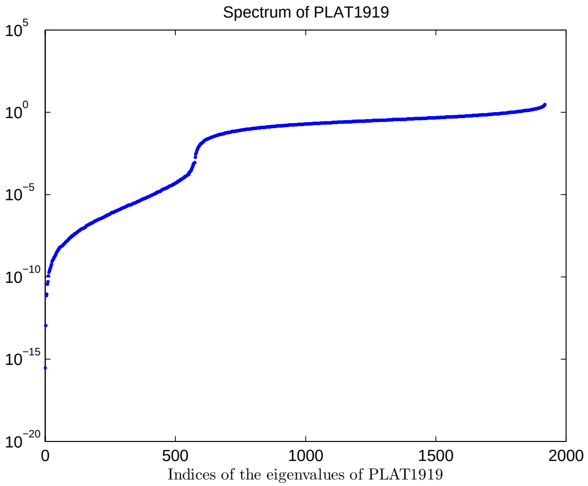
Non Linear Correction



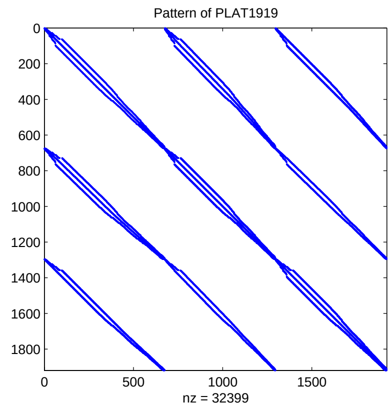
Computing interior eigenvalues

Test matrix 2: `PLAT1919` (From Matrix Market) ; $n = 1919$.

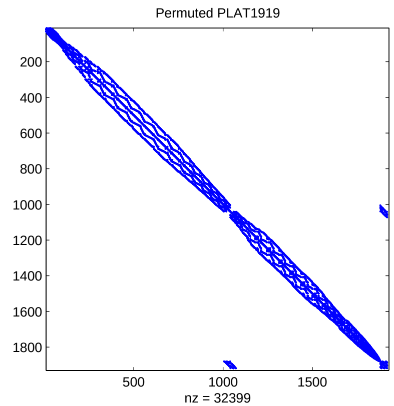
Computing $m = 6$ eigenvalues the closet to $\sigma = 0.995$.



Spectrum



Original matrix



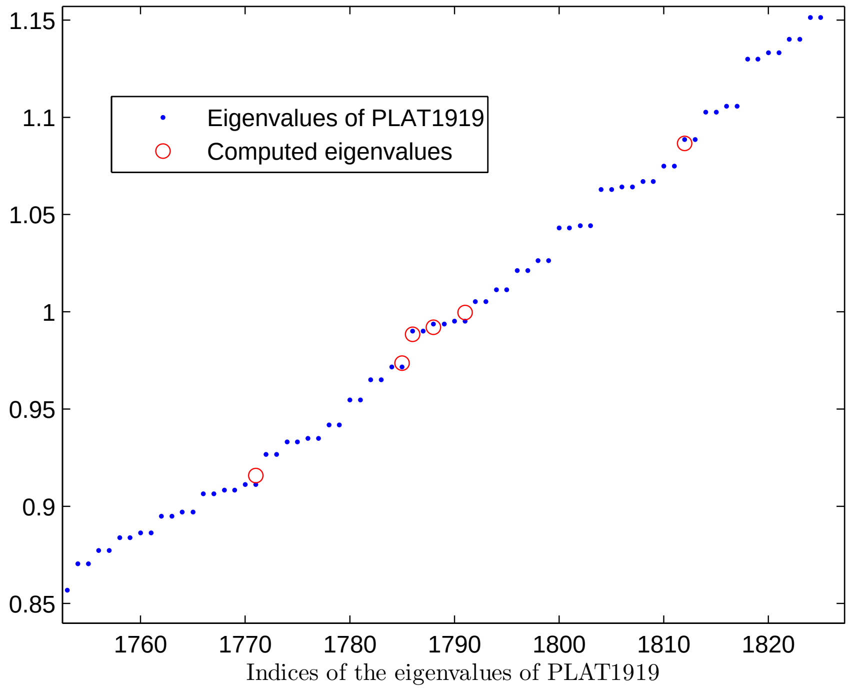
Rearranged matrix

Results

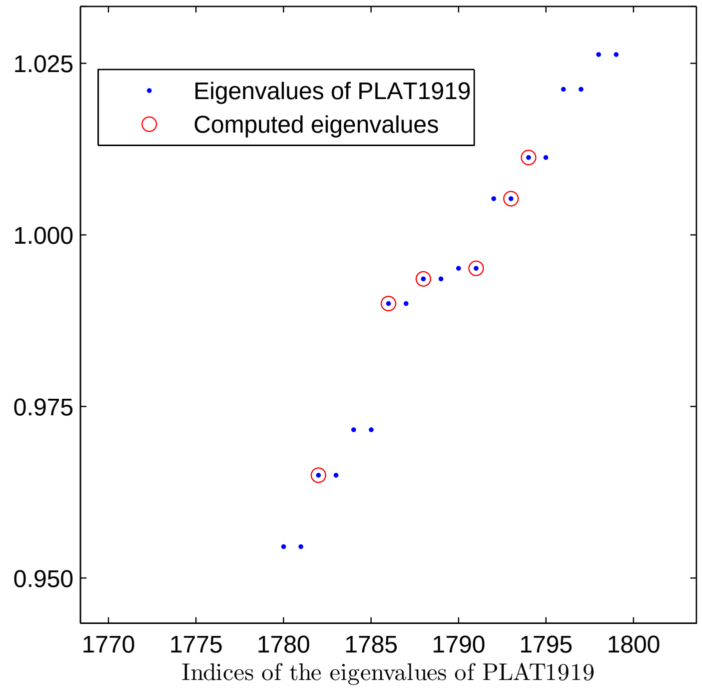
Computed eigenvalues :

Newton-Sylvester After $k = 10$ iterations Residual : 5×10^{-2}			Non Linear Corr. After $k = 6$ iterations Residual : 3×10^{-11}		
eigenvalue	index	error	eigenvalue	index	error
0.91576	1771	4×10^{-3}	0.96497	1782	1×10^{-15}
0.97367	1785	2×10^{-3}	0.99000	1786	1×10^{-15}
0.98842	1786	2×10^{-3}	0.99359	1788	2×10^{-15}
0.99213	1788	1×10^{-3}	0.99515	1791	2×10^{-15}
0.99964	1791	4×10^{-3}	1.0053	1793	4×10^{-15}
1.0866	1812	2×10^{-3}	1.0113	1794	2×10^{-15}

Location in the spectrum



Newton-Sylvester



Non Linear Correction

$\Rightarrow$ There are missing eigenvalues.

Use of Sturm sequences to determine intervals of missing eigenvalues.

Need of pursuing with a deflating technique and Inverse iteration.

Back to Domain Decomposition

$$A = \begin{pmatrix} B & E \\ E^T & C \end{pmatrix},$$

where $B \in \mathbb{R}^{(n-p)\times(n-p)}$. B is a block diagonal matrix corresponding to the inner nodes of each subdomain and E and C correspond to the interactions between the domains.

Let $U = \begin{pmatrix} I & -B^{-1}E \\ 0 & I \end{pmatrix}$; therefore: $U^T A U = \begin{pmatrix} B & 0 \\ 0 & S \end{pmatrix}$

where $S = C - E^T B^{-1} E$ is the Schur complement.

The CMS approximation (one level of AMLS)

The standard initial problem

$$\begin{pmatrix} B & E \\ E^T & C \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix} = \lambda \begin{pmatrix} u \\ y \end{pmatrix},$$

becomes the transformed generalized eigenvalue problem

$$\begin{pmatrix} B & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix} = \lambda \begin{pmatrix} I & -B^{-1}E \\ -E^T B^{-1} & M_S \end{pmatrix} \begin{pmatrix} u \\ y \end{pmatrix},$$

where $M_S = I + E^T B^{-2} E$.

CMS (*) consists of neglecting the coupling matrices and coupling in the RHS. An uncoupled problem is therefore obtained :

$$\begin{aligned} B\ v &= \mu\ v \\ S\ s &= \eta\ M_S\ s, \end{aligned}$$

from which the desired approximations are computed to be used in a Rayleigh-Ritz estimation.

(*) CMS=Component Mode Synthesis = one step of AMLS (Multilevel approach).

Two equivalent approaches

Applying the RR procedure defined by the transformed problem and the basis

$$\left\{ \widehat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix} \quad i = 1, \ldots, m_B; \qquad \widehat{s}_j = \begin{pmatrix} 0 \\ s_j \end{pmatrix} \quad j = 1, \ldots, m_S \right\},$$

is equivalent to apply the RR procedure on the original problem and the basis

$$\left\{ \widehat{v}_i = \begin{pmatrix} v_i \\ 0 \end{pmatrix} \quad i = 1, \ldots, m_B; \qquad \widehat{u}_j = \begin{pmatrix} -B^{-1}Es_j \\ s_j \end{pmatrix} \quad j = 1, \ldots, m_S \right\},$$

where (s_j) are eigenvectors of the pencil (S, M_S).

Drawback of the CMS correction : this is a "one shot" approximation.

Second approach : the Newton-Sylvester iteration

Let $V_1 \in \mathbb{R}^{p \times m}$ $(1 \leq m \leq p < n)$ an orthogonal basis of an invariant subspace of B, so that $BV_1 = V_1 D$, where $D = diag(\mu_1, \cdots, \mu_m)$ and we let $U = \begin{pmatrix} V_1 \\ 0 \end{pmatrix} \in \mathbb{R}^{n \times m}$.

Applying the Newton-Sylvester iteration amounts to solve the Sylvester equation : $(I - UU^T)AZ - ZD = -R$ where $R = AU - UD = \begin{pmatrix} 0 \\ E^T V_1 \end{pmatrix}$.
Since D is diagonal this system decouples into the m distinct linear systems,

$$(I - UU^T)Az_i - \mu_i z_i = -r_i = -\begin{pmatrix} 0 \\ E^T v_i \end{pmatrix} \ .$$

The final expression of the first correction

Let $P_1 = I - V_1 V_1^T$.

In the end, the column-vectors of the new matrix U^{new} are given by

$$u_i^{new} = u_i + z_i = \begin{pmatrix} v_i - P_1 (B - \mu_i I)^\dagger P_1 E s_i \\ s_i \end{pmatrix} \quad \text{with} \quad s_i = -S_*(\mu_i)^{-1} E^T v_i$$

where $S_*(\mu_i) = C - \mu_i I - E^T P_1 (B - \mu_i I)^\dagger P_1 E$ is the projected Schur complement.

The residuals satisfy $(A - \mu_i I) u_i^{new} = \begin{pmatrix} -V_1 V_1^T E s_i \\ 0 \end{pmatrix}$.

It is, of course possible to apply additional steps of this correction process. However, these additional steps will require expensive Sylvester-like equations to be solved at each step with different shifts.

Iterative CMS

To make easier the correction, the following is proposed :

Algorithm : Iterative CMS

0. Select U_0 s.t. $U_0^T U_0 = I$ from eigenvectors in each subdomain.
1. For $k = 0, \cdots,$ until convergence Do:
2. Compute $R_k = AU_k - U_k(U_k^T AU_k)$
3. Solve (for Z_k): $(I - U_k U_k^T)AZ_k = -R_k$
4. Set $V = [U_k, Z_k]$
5. Compute U_{k+1} using RR on A with V.
6. EndDo

Step 3 can be solved by solving

$$\begin{pmatrix} A & -U_k \\ U_k^T A & -I \end{pmatrix} \begin{pmatrix} Z_k \\ T \end{pmatrix} = \begin{pmatrix} -R_k \\ 0 \end{pmatrix} .$$

Numerical tests

Schrödinger operator : $H = -\Delta + V$ on a rectangular domain in 2-D with Dirichlet boundary conditions.

V is the Gaussian $V(x,y) = -\beta e^{-(x-x_c)^2-(y-y_c)^2}$ in which (x_c, y_c) is the center of the domain and $\beta = 100$.

The domain is a rectangle of dimension
$(n_x + 1) \times h = 1$ and $(n_y + 1) \times h$.

The domain is then split in two horizontally , in the middle of the domain.

n_{ev} eigenvalues are sought.

Tested methods :

*** No correction :** RR with W composed of $n_{ev}/2$ eigenvectors of each domain.

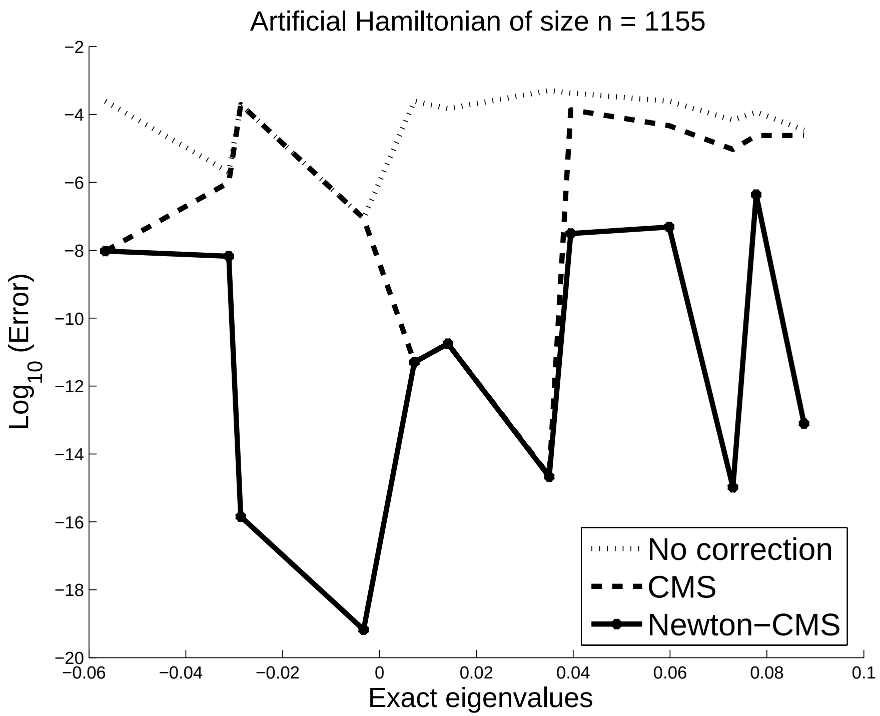
*** CMS :** the previous basis is augmented by $Z = \begin{pmatrix} -B^{-1}G \\ G \end{pmatrix}$ where G is matrix of eigenvectors of S associated with the smallest n_{ev} eigenvalues (dimension of the basis : $2n_{ev}$).

*** Newton-CMS :** as before but $G = S^{-1}E^TW$ (obtained from one inverse iteration with A).

*** Correction :** one iteration of the Iterative CMS.

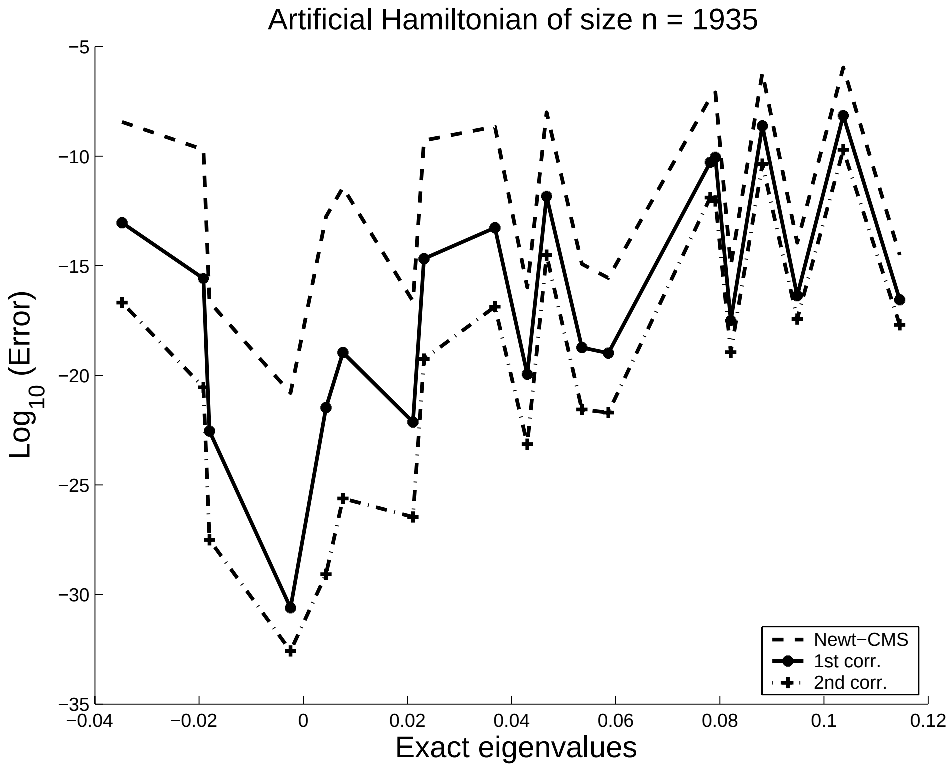
Numerical tests (2)

Test 1



$n_x = 35,\ n_y = 33\ (n = 1155).$
$n_{ev} = 12.$

Test 2



$n_x = 45,\ n_y = 43\ (n = 1935).$
$n_{ev} = 20.$

Conclusion

Block variants of the correction equation were derived by viewing the eigenvalue problem as a system of nonlinear equations.

Resulting algorithms converge cubically or quadratically but they require the solution of a different Sylvester equation at each step.

In the case of CMS, experiments show that it is possible to obtain good improvements by adaptations of these algorithms which do not require to refactor the matrix at each step.

Reference

BP,YS. Comput. Methods Appl. Mech. Engrg. 196 (2007).