Fully guaranteed and computable bounds for eigenvalue problems

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joint work with Eric Cancès, Yvon Maday, Benjamin Stamm, Martin Vohralík

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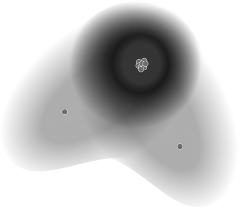
Motivation : Kohn–Sham model (1965)

Compute the **electronic density** of a molecular system.



Mathematical problem : M **nonlinear eigenvalue** equations in 3D

Find M orthonormal eigenfunctions

$$\Phi^0 = (\phi_1^0, \dots, \phi_M^0) \in X = \left\{ \Phi = (\phi_1, \dots, \phi_M) \in \left[H^1(\Omega) \right]^M \middle| \int_\Omega \phi_i \phi_j = 1 \right\}$$

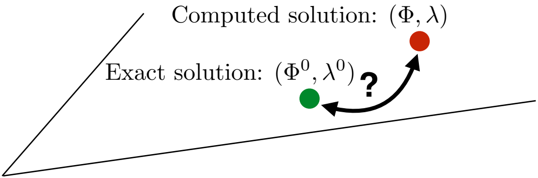
with corresponding lowest eigenvalues $\lambda_1^0, \dots, \lambda_M^0$, such that

$$\left(-\frac{1}{2}\Delta + V^{KS}_{\mathbf{R_k}, \rho_{[\Phi^0]}} \right) \phi_i^0 = \lambda_i^0 \phi_i^0, \quad i = 1, \dots, M, \quad \text{with} \quad \rho_{[\Phi^0]} = 2 \sum_{i=1}^{M} |\phi_i^0|^2.$$

Difficulties : Several eigenvalues to compute, possibly degenerate, nonlinearity.

How to estimate the discretization error ?

Wish-list for a good error bound



The goal is to derive an inequality of the type :

$$\|(\Phi^0, \lambda^0) - (\Phi, \lambda)\|_? \leq \eta(disc., algo., \ldots) = \text{ Error bound}$$

Properties of the error bound :

1. Computable upper bound of the error
2. Valid under checkable assumptions
3. Efficient (close to the error)
4. Cheap to compute
5. Allow adaptivity

Outline

Error estimation for a linear eigenvalue problem

Nonlinear eigenvalue problem

Combining different sources of errors

Towards fully guaranteed error bounds

Add error bars to simulations ?

In that direction, some fully guaranteed bounds for (mostly linear) **eigenvalue problems** appearing in different contexts :

- Vibration problems in mechanics
- Neutronics
- Stability constants in implicit function theorem
- Arises from minimization problems with norm constraint

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Eigenvalue error estimation : Kato 1949, Aronszajn 1951, Bazley-Fox 1966, Weinstein 1972, Beattie-Goerisch 1995...

Eigenvalue and eigenvector estimation : Grubisic and Ovall 2009, Liu and Oishi 2013, Sebestová and Vejchodsky 2014, Carstensen and Gedicke 2014, Liu and Vejchodsky 2019.

Goal : estimation of the error without uncomputable terms, and with checkable conditions.

Cancès, Dusson, Maday, Stamm, and Vohralík, Math. Comput. 89 (2020).

An eigenvalue problem

Setting : A is an operator on a Hilbert space $\mathcal{H}$ with domain $D(A)$

- **self-adjoint**
- **bounded below** (A is a positive definite operator)
- with **compact resolvent**.

There exist $0 < \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_k \to +\infty$ and $(\varphi_k)_{k\geq 1}$ such that

$$\forall k, \quad A\,\varphi_k = \lambda_k \varphi_k,$$

Discretization : Find $(\varphi_{kh}, \lambda_{kh}) \in X_h \times \mathbb{R}$ such that

$$A\,\varphi_{kh} \simeq \lambda_{kh}\varphi_{kh}.$$

Goal : Find guaranteed error bounds for $\|\varphi_{kh} - \varphi_k\|$ and $|\lambda_{kh} - \lambda_k|$.

Examples :

- Laplace operator : $-\Delta$
- Schrödinger operator : $-\Delta + V$, with $V \in L^\infty(\Omega)$.

Approach

Analysis based on the **residual** :

$$\mathrm{Res}(\varphi_{ih}, \lambda_{ih}) = A\varphi_{ih} - \lambda_{ih}\varphi_{ih}$$

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1. **Abstract estimations** : linking the quantities

$$\begin{matrix} \|\varphi_{ih} - \varphi_i\|, \\ \|A^{1/2}(\varphi_{ih} - \varphi_i)\|, \\ |\lambda_{ih} - \lambda_i|, \end{matrix} \quad \text{to} \quad \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1} = \|A^{-1/2}(A\varphi_{ih} - \lambda_{ih}\varphi_{ih})\|.$$

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2. **Estimation of the dual norm of the residual**

   $\|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}$ difficult to compute.

   Reconstruction of a flux $\boldsymbol{\sigma}_{ih}$.

   Link $\|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}$ to $\boldsymbol{\sigma}_{ih}$.

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   Lower and upper bounds in the eigenvalues

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3. **Estimate constants in the estimations**
   Lower and upper bounds in the eigenvalues
4. **Gather all estimates**

How to deal with clusters of eigenvalues

We want to compute eigenvalues $(\lambda_m, \ldots, \lambda_M)$ and corresponding eigenvectors $(\varphi_m, \ldots, \varphi_M)$.

Problem : degenerate/almost degenerate eigenvalues, eigenvectors not uniquely defined

Work with **orthogonal projector** - density matrices :

$$\gamma = \sum_{i=m}^{M} |\varphi_i\rangle\langle\varphi_i|, \qquad \text{orthogonal projector on Span}(\varphi_m, \ldots, \varphi_M)$$

$$\gamma_h = \sum_{i=m}^{M} |\varphi_{ih}\rangle\langle\varphi_{ih}|, \qquad \text{orthogonal projector on Span}(\varphi_{m,h}, \ldots, \varphi_{M,h})$$

Errors measured on the sum of eigenvalues and Hilbert–Schmidt norms of density matrices :

$$\sum_{i=m}^{M} (\lambda_{ih} - \lambda_i), \qquad \|A^{1/2}(\gamma - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}$$

Abstract a posteriori error estimation

- The norm $\|A^{1/2} \bullet \|$ is referred to as the *energy norm*.
  Example : if $A = -\Delta, \quad \|A^{1/2} \bullet \| = \|\nabla \bullet \|$.

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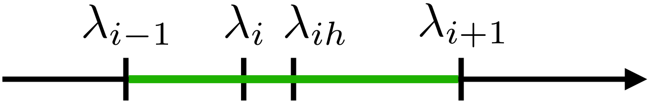
Assumptions : there holds

- λ_i simple eigenvalue,
- **Key assumption :** $\lambda_{i-1} < \lambda_{ih}$ when $i > 1$ and $\lambda_{ih} < \lambda_{i+1}$,



- Conforming approximation : $(\varphi_{ih}, \lambda_{ih}) \in X \times \mathbb{R}^+$, $\|\varphi_{ih}\|_{L^2} = 1$,
  $\|A^{1/2}\varphi_{ih}\|^2_{L^2} = \lambda_{ih}$ (for simplicity of the presentation).

Linking the errors to the residual

Theorem [Eigenvalue bounds and eigenvector bounds]

(Cances, D., Maday, Stamm, Vohralík) : Under the above assumptions,

$$\lambda_{ih} - \lambda_i \leq \|A^{1/2}(\varphi_i - \varphi_{ih})\|^2$$

$$\|A^{1/2}(\varphi_i - \varphi_{ih})\|^2 \leq \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}^2 + (\lambda_{ih} + \lambda_i)\|\varphi_i - \varphi_{ih}\|^2$$

$$\|\varphi_i - \varphi_{ih}\| \leq \sqrt{2}\widetilde{C}_{ih}^{-\frac{1}{2}} \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1},$$

$$\widetilde{C}_{ih} := \min\left\{\lambda_{i-1}\left(1 - \frac{\lambda_{ih}}{\lambda_{i-1}}\right)^2, \lambda_{i+1}\left(1 - \frac{\lambda_{ih}}{\lambda_{i+1}}\right)^2\right\},$$

Valid for any conforming discretization method

What remains to estimate :

- $\|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}$
- $\widetilde{C}_{ih}$: requires **coarse** lower bounds on the eigenvalues

Dual norm of the residual estimation

based on work by Ern and Vohralík

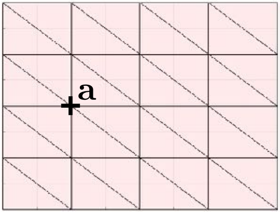
Additional assumptions :

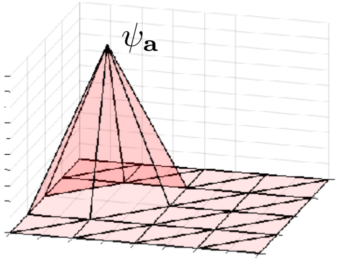
0- Laplace operator : $A = -\Delta$.
1- **Piecewise polynomials**. There holds

$$\varphi_{ih} \in \mathbb{P}_p(\mathcal{T}_h),\ p \geq 1.$$

2- **Galerkin orthogonality of the residual to $\psi_{\mathbf{a}}$.** There holds

$$\lambda_{ih}(\varphi_{ih}, \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} - (\nabla \varphi_{ih}, \nabla \psi_{\mathbf{a}})_{\omega_{\mathbf{a}}} = \langle \mathrm{Res}(\varphi_{ih}, \lambda_{ih}), \psi_{\mathbf{a}} \rangle_{X',X} = 0 \quad \forall \mathbf{a} \in \mathcal{X}_h^{\mathrm{int}}.$$





Reconstruction and residual equivalences

Equilibrated flux reconstruction :

$$\boldsymbol{\sigma}_{ih} \in \mathbf{X}_h \subset \mathbf{H}(\mathrm{div}, \Omega), \quad \nabla\cdot\boldsymbol{\sigma}_{ih} = \lambda_{ih}\varphi_{ih}$$

for each $\mathbf{a} \in \mathcal{X}_h$, define $\boldsymbol{\sigma}_{ih}^{\mathbf{a}}$ solution of a local problem. Then set

$$\boldsymbol{\sigma}_{ih} := \sum_{\mathbf{a}\in\mathcal{X}_h} \boldsymbol{\sigma}_{ih}^{\mathbf{a}} \in \mathbf{H}(\mathrm{div}, \Omega).$$

We obtain

$$\|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1} \leq \|\nabla\varphi_{ih} + \boldsymbol{\sigma}_{ih}\|_{L^2}, \leq (d+1) C_{\mathrm{st}} C_{\mathrm{cont,PF}} \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}.$$

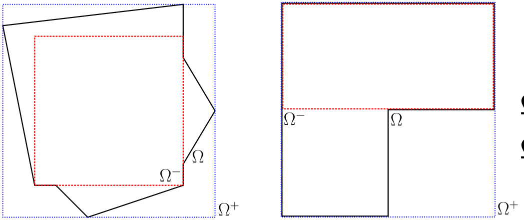
Estimation of the constants

Estimate $$\widetilde{C}_{ih} := \min\left\{\lambda_{i-1}\left(1-\frac{\lambda_{ih}}{\lambda_{i-1}}\right)^2, \lambda_{i+1}\left(1-\frac{\lambda_{ih}}{\lambda_{i+1}}\right)^2\right\}.$$

- upper bounds on λ_{i-1} : $\overline{\lambda}_{i-1}$.
- lower bounds on λ_{i+1} : $\underline{\lambda}_{i+1}$

Different methods to get lower bounds :

- Liu and Oishi (on convex domains for $d = 2$), Carstensen and Gedicke, Liu (non-conforming method) on a **coarse** mesh
- Principle of domain inclusion :



$$\Omega \subset \Omega^+ \Rightarrow \lambda_k \geq \lambda_k(\Omega^+)$$
$$\Omega^- \subset \Omega \Rightarrow \lambda_k \leq \lambda_k(\Omega^-)$$

- Practical strategy : $\underline{\lambda}_{i+1} = \lambda_{(i+1)h}$.

A posteriori estimates

Combination of the different ingredients :

1. Estimations of $\|\varphi_i - \varphi_{ih}\|_{L^2}, \|\nabla(\varphi_i - \varphi_{ih})\|_{L^2}, \lambda_i - \lambda_{ih}$ in terms of $\|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}$

$$\|\nabla(\varphi_i - \varphi_{ih})\|^2 \leq \left[1 + 2(\lambda_{ih} + \lambda_i)\widetilde{C}_{ih}\right] \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}^2$$

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$$
\begin{aligned}
\|\nabla(\varphi_i - \varphi_{ih})\|^2 &\leq \left[1 + 2(\lambda_{ih} + \lambda_i)\widetilde{C}_{ih}\right] \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}^2 \\
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2. Estimation of $\|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}$ in terms of $\|\nabla \varphi_{ih} + \boldsymbol{\sigma}_{ih}\|_{L^2}$
3. Dealing with the constants (coarse lower bounds of eigenvalues)

$$
\begin{aligned}
\|\nabla(\varphi_i - \varphi_{ih})\|^2 &\leq \left[1 + 2(\lambda_{ih} + \lambda_i)\widetilde{C}_{ih}\right] \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}^2 \\
&\leq \left[1 + 2(\lambda_{ih} + \lambda_i)\widetilde{C}_{ih}\right] \|\nabla \varphi_{ih} + \boldsymbol{\sigma}_{ih}\|_{L^2}^2 \\
&\leq m_{ih} \|\nabla \varphi_{ih} + \boldsymbol{\sigma}_{ih}\|_{L^2}^2
\end{aligned}
$$

Final estimations

Theorem (Cances, D., Maday, Stamm, Vohralík) :

$$\tilde{\eta}_i^2 \leq \lambda_{ih} - \lambda_i \leq \eta_i^2 \quad \text{and} \quad \|\nabla(\varphi_{ih} - \varphi_i)\|_{L^2} \leq \eta_i,$$

$$\eta_i = m_{ih}\|\nabla\phi_{ih} + \boldsymbol{\sigma}_{ih}\|_{L^2}, \quad \tilde{\eta}_i = \tilde{\eta}_i(r_{ih}).$$

m_{ih} can be asymptotically brought to 1 under additional regularity assumption.

Possible extensions :

- Nonconforming methods : Nonconforming finite elements, Discontinuous Galerkin method, mixed finite elements
- Inexact solver : error balance between iteration and discretization error

Cancès, Dusson, Maday, Stamm, and Vohralìk, SIAM J. Numer. Anal., 55 (2017), pp. 2228-2254.

Comparison with single eigenvalue case

We want to compute eigenvalues $(\lambda_m, \ldots, \lambda_M)$ and corresponding eigenvectors $(\varphi_m, \ldots, \varphi_M)$.

	One eigenvalue case	Cluster case
Eigenvalue error	$(\lambda_{ih} - \lambda_i)$	$\sum_{i=m}^{M} (\lambda_{ih} - \lambda_i)$
Energy error	$\Vert A^{1/2}(\varphi_i - \varphi_{ih})\Vert$	$\Vert A^{1/2}(\gamma - \gamma_h)\Vert_{\mathfrak{S}_2(\mathcal{H})}$
Residual	$\Vert \mathrm{Res}(\varphi_{ih}, \lambda_{ih})\Vert_{-1}$	$\Vert A^{-1/2}\mathrm{Res}(\gamma_h)\Vert_{\mathfrak{S}_2(\mathcal{H})}$

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Residual	$\|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|_{-1}$	$\|A^{-1/2}\mathrm{Res}(\gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}$

Residual :

$$\mathrm{Res}(\gamma_h) := (1 - \gamma_h)A\gamma_h$$

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Errors measured in **Hilbert–Schmidt norm** : for an operator $B \in \mathcal{L}(\mathcal{H})$, and $(e_k)_{k\geq 1}$ an orthonormal basis of $\mathcal{H}$

$$\lVert B\rVert_{\mathfrak{S}_2(\mathcal{H})} := \mathrm{Tr}(B^\dagger B)^{1/2} = \left(\sum_{k\geq 1} \lVert Be_k\rVert^2\right)^{1/2}.$$

Scalar product : $(B, C)_{\mathfrak{S}_2(\mathcal{H})} = \mathrm{Tr}(B^\dagger C) = \sum_{i\geq 1}(\varphi_i, B^\dagger C\varphi_i).$

Different estimates

Link between cluster and single eigenpair residuals (Cancès, D., Maday, Stamm, Vohralík) There holds

$$\|A^{-1/2}\mathrm{Res}(\gamma_h)\|^2_{\mathfrak{S}_2(\mathcal{H})} = \sum_{i=m}^{M} \|\mathrm{Res}(\varphi_{ih}, \lambda_{ih})\|^2_{-1}.$$

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- Exact eigenvectors : $\Phi^0 = (\varphi_m, \ldots, \varphi_M)$.
- Discrete eigenvectors : $\Phi_h = (\varphi_{mh}, \ldots, \varphi_{Mh})$.
- Rotated discrete eigenvectors : $\Phi^0_h = (\varphi^0_{mh}, \ldots, \varphi^0_{Mh})$ such that

$$\Phi^0_h = (\varphi^0_{mh}, \ldots, \varphi^0_{Mh}) := \mathrm{argmin}_{\mathbf{U}\in O(J)} \|\mathbf{U}\Phi_h - \Phi^0\|,$$

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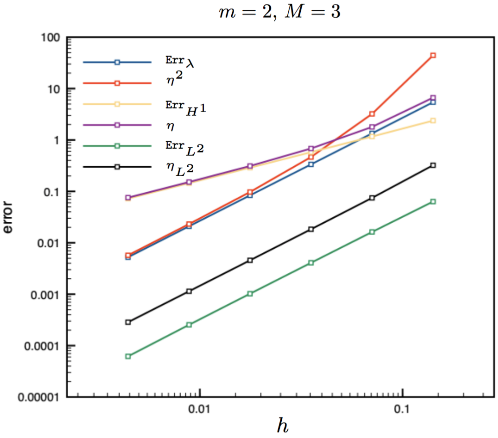
Link between density matrix and eigenvector errors (Cancès, D., Maday, Stamm, Vohralík) There holds

$$\frac{1}{\sqrt{2}}\|\gamma - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})} \le \|\Phi^0 - \Phi_h^0\| \le \|\gamma - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})},$$

$$\frac{1}{\sqrt{2}}\|A^{1/2}(\gamma - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \le \|A^{1/2}(\Phi^0 - \Phi_h^0)\| \le C\|A^{1/2}(\gamma - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})},$$

Laplace operator, Square, finite elements

Cluster with 2 eigenvalues : $m = 2$, $M = 3$.



$$\mathrm{Err}_\lambda := \sum_{i=m}^{M} (\lambda_{ih} - \lambda_i),$$

$$\mathrm{Err}_{H^1} := \| |\nabla| (\gamma - \gamma_h) \|_{\mathfrak{S}_2(\mathcal{H})}$$

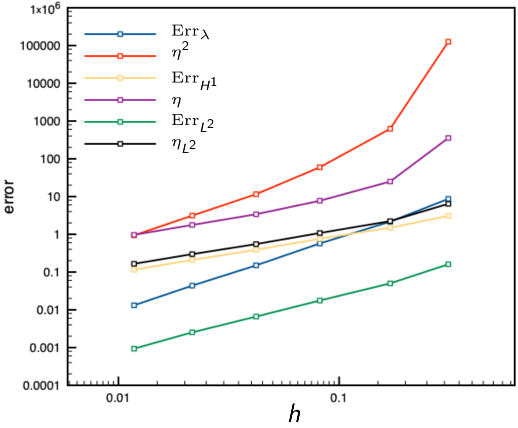
$$\mathrm{Err}_{L^2} := \| \gamma - \gamma_h \|_{\mathfrak{S}_2(\mathcal{H})}$$

$$\mathrm{Err}_\lambda \leq \eta^2, \qquad \mathrm{Err}_{H^1} \leq \eta, \qquad \mathrm{Err}_{L^2} \leq \eta_{L^2}.$$

$$\|A^{1/2}(\gamma - \gamma_h)\|^2_{\mathfrak{S}_2(\mathcal{H})} \leq \|A^{-1/2}\mathrm{Res}(\gamma_h)\|^2_{\mathfrak{S}_2(\mathcal{H})} + (\lambda_M + \lambda_{Mh})\|\gamma - \gamma_h\|^2_{\mathfrak{S}_2(\mathcal{H})}.$$

Laplace operator, L-shape, finite elements

Cluster with 4 eigenvalues : $m = 2$, $M = 5$.



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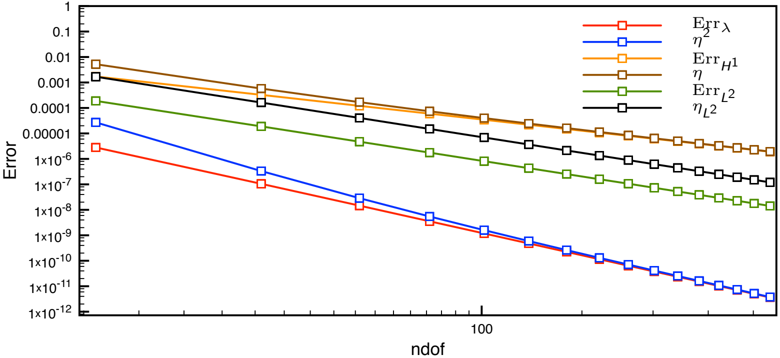
$$\|A^{1/2}(\gamma - \gamma_h)\|^2_{\mathfrak{S}_2(\mathcal{H})} \leq 2{c_h}^2 \|A^{-1/2}\mathrm{Res}(\gamma_h)\|^2_{\mathfrak{S}_2(\mathcal{H})} + \frac{\lambda_M}{2} \|\gamma - \gamma_h\|^4_{\mathfrak{S}_2(\mathcal{H})}.$$

Schrödinger operator, 1D box, planewaves

Operator $A = -\Delta + V, \quad V \in L^\infty(\Omega)$.

Cluster with 2 eigenvalues : $m = 2$, $M = 3$.



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$$\mathrm{Err}_{H^1} \leq \eta,$$

$$\mathrm{Err}_{L^2} \leq \eta_{L^2}.$$

Outline

Error estimation for a linear eigenvalue problem

Nonlinear eigenvalue problem

Combining different sources of errors

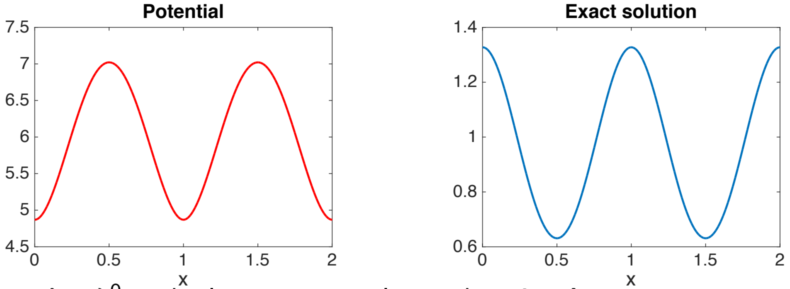
Problem presentation : the Gross-Pitaevskii equation

Physical problem : Ground state of a system of bosons at very low temperature.

Nonlinear eigenvalue problem : Find $(\phi^0, \lambda^0) \in H^1_{\#}(\Omega)$ such that $\|\phi^0\|_{L^2} = 1$ and

$$\Big(-\Delta + V + (\phi^0)^2 \Big)\phi^0 = \lambda^0 \phi^0.$$

Setting : 1-Dimensional, Periodic Setting.



Remark : λ^0 is the lowest eigenvalue and is **simple**.

Exact solution : (ϕ^0, λ^0)

Resolution with planewave discretization and iterative algorithm

A posteriori analysis–Approach

How to find a guaranteed, computable and guaranteed upper bound of the error $\|\phi^0 - \phi_N^k\|_{H^1}$?

Residual-based a posteriori analysis :

$$\mathrm{Res}(\phi_N^k, \lambda_N^k) = (-\Delta + V + (\phi_N^k)^2)\phi_N^k - \lambda_N^k \phi_N^k.$$

First-order development of the residual :

$$0 = \mathrm{Res}(\phi^0, \lambda^0) \simeq \mathrm{Res}(\phi_N^k, \lambda_N^k) + D\mathrm{Res}_{(\phi_N^k, \lambda_N^k)}(\phi^0 - \phi_N^k)$$

$$\phi^0 - \phi_N^k \simeq -D\mathrm{Res}^{-1}_{(\phi_N^k, \lambda_N^k)} \left(\mathrm{Res}(\phi_N^k, \lambda_N^k)\right)$$

- A first **coarse** bound based on **inverse function theorem**, writing
  $$\|\phi^0 - \phi_N^k\|_{H^1} \leq 2\|D\mathrm{Res}^{-1}_{(\phi_N^k, \lambda_N^k)}\|_{H^{-1}, H^1} \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}}.$$
- A second **precise** bound valid only in the asymptotic regime, writing
  $$-D\mathrm{Res}^{-1}_{(\phi_N^k, \lambda_N^k)} \left(\mathrm{Res}(\phi_N^k, \lambda_N^k)\right) = -\Delta^{-1}\mathrm{Res}(\phi_N^k, \lambda_N^k) + \text{ superconvergent terms.}$$

Ref : Dusson, Maday 2017.

Guaranteed bounds

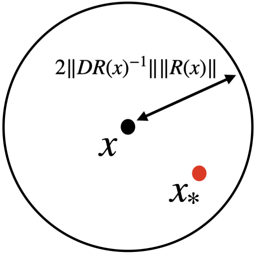
Solve $Res(x) = 0$ with $Res : Y \to Z$.

Inverse function theorem - Newton–Kantorovitch [1]

Two conditions to be satisfied :

- $DRes(x) \in \mathcal{L}(Y; Z)$ is an isomorphism
- $2\|DRes(x)^{-1}\|_{Z,Y'} L(2\|DRes(x)^{-1}\|_{Z,Y'} \|Res(x)\|_{Z'}) \leq 1$

  with $\quad L(\alpha) = \sup_{y \in \bar{B}(x,\alpha)} \|DRes(x) - DRes(y)\|_{Y,Z'}.$



Then the problem $Res(x) = 0$ has a unique solution x_* in the ball $\bar{B}(x, 2\|DRes(x)^{-1}\|_{Z,Y'} \|Res(x)\|_{Z'})$.

Moreover, $\boxed{\|x - x_*\|_Y \leq 2\|DRes(x)^{-1}\|_{Z,Y'} \|Res(x)\|_{Z'}.}$

- Possible to obtain guaranteed bounds
- Requires control over first and second order derivatives
- Result on existence of solution

1. Caloz, Rappaz : Numerical analysis for nonlinear and bifurcation problems. Handb. Numer. Anal. 5, 487-637 (1997).

First a posteriori bound

To characterize the error bound :

- Determine **computable** conditions on N and k s.t. $D\mathrm{Res}_{(\phi_N^k,\lambda_N^k)}$ **is an isomorphism**
- Find a **computable** bound for $\|D\mathrm{Res}^{-1}_{(\phi_N^k,\lambda_N^k)}\|_{H^{-1},H^1}$

Extra-computation : Resolution of a discrete linear eigenvalue problem.

Theorems (D., Maday) :

- **Guaranteed bound :** Under the previous conditions, there exists a unique (ϕ,λ) such that $\mathrm{Res}(\phi,\lambda)=0$ and

$$\|\phi-\phi_N^k\|_{H^1}+|\lambda-\lambda_N^k|\leq 2\gamma\|\mathrm{Res}(\phi_N^k,\lambda_N^k)\|_{H^{-1}} \qquad (1)$$

- **Ground state :** There exists a computable condition depending on $\|\phi-\phi_N^k\|_{H^1}$, $|\lambda-\lambda_N^k|$, ϕ_N^k, $\lambda_N^k,\mu_N^1,\mu_N^2$ guaranteeing that (ϕ,λ) is the ground state (ϕ^0,λ^0) of our problem.

A **coarse** a posteriori error bound valid under computable conditions.

Second a posteriori bound

Theorem [Asymptotic error bound] (D., Maday) :
If $\|\phi^0 - \phi_N^k\|_{H^1}$ and $|\lambda^0 - \lambda_N^k|$ are small enough, then we can show that

$$\left(1 - \varepsilon(\phi^0 - \phi_N^k, \lambda^0 - \lambda_N^k)\right) \|\phi^0 - \phi_N^k\|_{H^1} \leq \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}} + F(\phi_N^k, \lambda_N^k, \mu_N^1, \mu_N^2),$$

where

- $\varepsilon(\phi^0 - \phi_N^k, \lambda^0 - \lambda_N^k) \xrightarrow[\|\phi^0 - \phi_N^k\|_{H^1} \to 0]{} 0$ can be estimated with the first bound
- $F(\phi_N^k, \lambda_N^k, \mu_N^1, \mu_N^2)$ is asymptotically small, and equal to 0 if $\|(V + 3(\phi_N^k)^2 - \lambda_N^k - 1)_-\|_{L^\infty} = 0$.

Asymptotically,

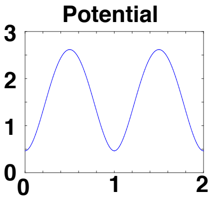
$$\|\phi^0 - \phi_N^k\|_{H^1} \leq \alpha_N^k \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}},$$

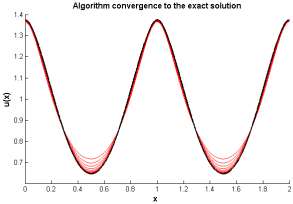
with α_N^k computable and as close to 1 as we wish.

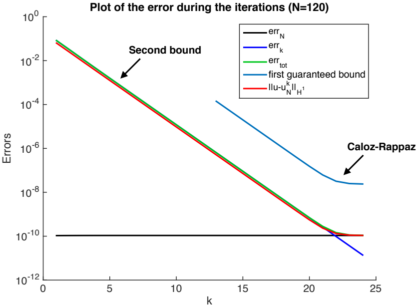
Better bound...but guaranteed only if the error is small enough.

Numerical simulations

- Fourier coefficients of the potential V are given by $\widehat{V}_k = -\frac{1}{\sqrt{2\pi}} \frac{1}{|k|^4 - \frac{1}{4}}$.
- Reference solution computed in a discrete space with N=500.







Outline

Error estimation for a linear eigenvalue problem

Nonlinear eigenvalue problem

Combining different sources of errors

Error balance for efficient simulation

How to perform **efficient simulations** using error bounds ?

Example : Error estimation comes from different sources 1, 2, 3.

$$\mathrm{Err}_{\mathrm{tot}} \simeq \mathrm{Err}_1 + \mathrm{Err}_2 + \mathrm{Err}_3.$$

Efficient scheme : try to **balance the errors**

$$\mathrm{Err}_1 \simeq \mathrm{Err}_2 \simeq \mathrm{Err}_3.$$

In that direction :

- Discretization and SCF iterations [D., Maday, IMA J. Numer. Anal. (2017)]
- Discretization and eigenvalue solver [Cances, D., Maday, Stamm, Vohralik, Numer. Math. (2018)]
- Discretization and arithmetic error [Herbst, Levitt, Cances (2020)]

Example of error balance

D., Maday, IMA J. Numer. Anal. (2017) : **Gross-Pitaevskii**-type eigenvalue problem (in 1d).

Two sources of error : discretization (dimension $2N+1$), iterations (k).

How to get the **best compromise** between the discretization and the number of iterations ?

1. Decompose the residual into **two parts :**

$$H_{\rho_N^k}\phi_N^k - \lambda_N^k\phi_N^k = \mathrm{Res}_{N,k} = \mathrm{Res}_N + \mathrm{Res}_k,$$

   with

$$\mathrm{Res}_N = H_{\rho_N^{k-1}}\phi_N^k - \lambda_N^{k-1}\phi_N^{k-1},$$

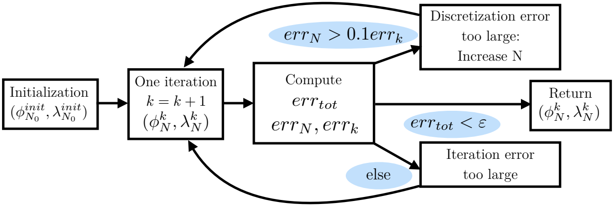
$$\mathrm{Res}_k = H_{\rho_N^k}\phi_N^k - H_{\rho_N^{k-1}}\phi_N^k - \lambda_N^k\phi_N^k + \lambda_N^{k-1}\phi_N^{k-1}.$$

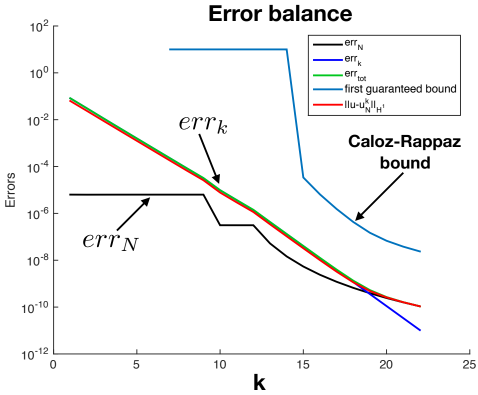
2. Decompose the error bound : essentially,

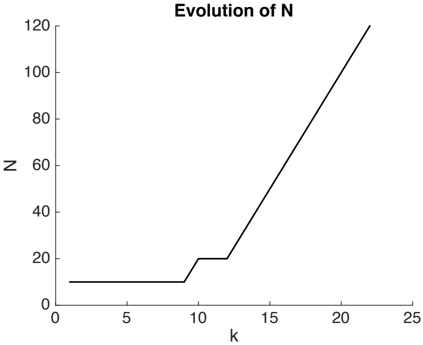
$$\|\phi^0 - \phi_N^k\|_{H^1} \leq \alpha_N^k \|\mathrm{Res}(\phi_N^k, \lambda_N^k)\|_{H^{-1}} \leq \alpha_N^k \left(\|\mathrm{Res}_N\|_{H^{-1}} + \|\mathrm{Res}_k\|_{H^{-1}}\right)$$

3. Compute each of these terms for **adaptative refinement**.

Error balance results







Conclusion

- Guaranteed bounds for **clusters** of eigenvalues
- **Computable bounds** available if dual norms of the residual can be estimated/computed
- Generic framework using density matrices
- Balance to find between computational cost and accuracy of error bound

Perspectives :

- Non self-adjoint eigenvalue problems
- Dealing with more generic nonlinear problems

$$\left(-\frac{1}{2}\Delta + V^{KS}_{\mathbf{R_k},\rho_{[\Phi^0]}}\right)\phi_i^0 = \lambda_i^0\phi_i^0, \quad i = 1,\dots,M, \quad \text{with} \quad \rho_{[\Phi^0]} = 2\sum_{i=1}^{M}|\phi_i^0|^2.$$

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Thank you for your attention.