Parameterless stopping criteria for density matrix expansions in electronic structure calculations

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Joint work with Elias Rudberg and Emanuel H. Rubensson

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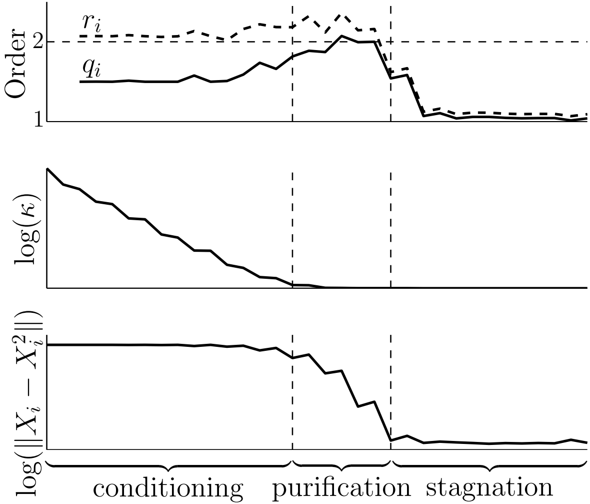
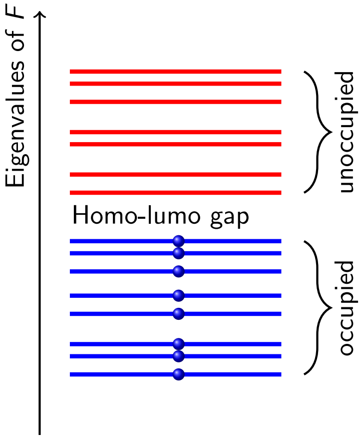
What you can learn from this presentation?



Large–scale electronic structure calculations
Density matrix construction



Eigenvalue problem for effective Hamiltonian F:

$$Fx_i = \lambda_i x_i$$

Density matrix

$$D := \sum_{i=1}^{n_{\mathrm{occ}}} x_i x_i^T$$

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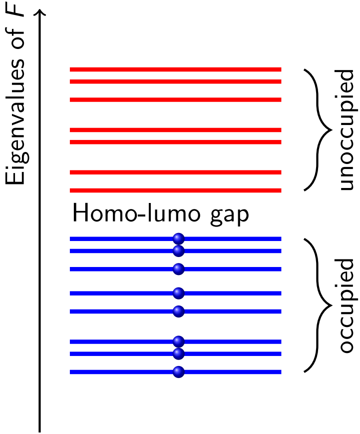

Eigenvalue problem for effective Hamiltonian F:

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$$D := \sum_{i=1}^{n_{\mathrm{occ}}} x_i x_i^T$$

Too expensive!

Large–scale electronic structure calculations
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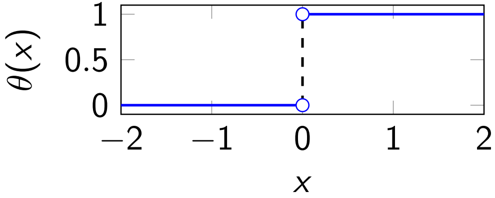
Linear scaling computations:

$$D = \theta(\mu I - F), \quad \mu \text{ is in homo-lumo gap}$$



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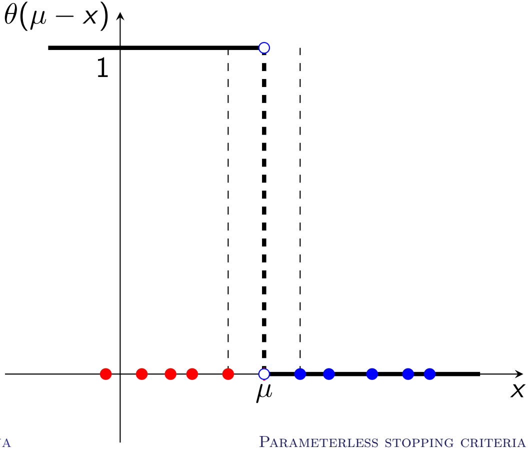

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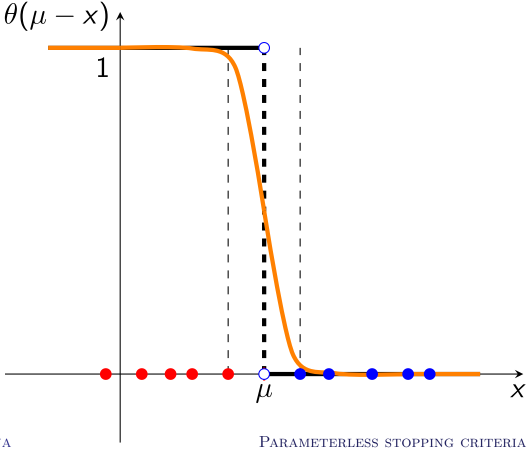

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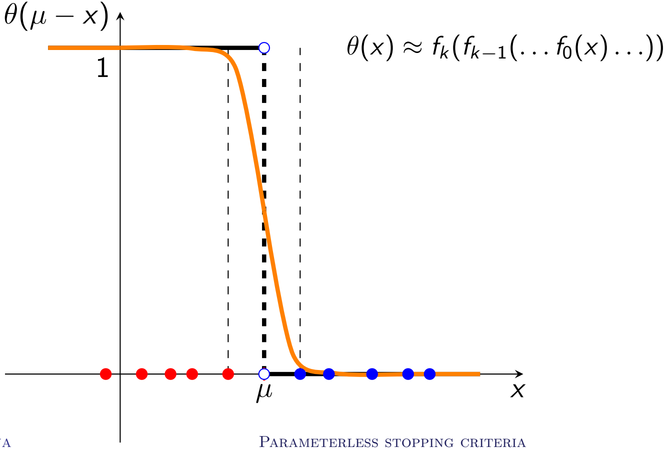

Recursive polynomial expansion (general form)

Build D from F by recursive application of low-order polynomials:

$X_0 = f_0(F)$
$\widetilde{X}_0 = X_0 + E_0$
while stopping criterion not fulfilled, for $i = 1, 2, \ldots$ **do**
    $X_i = f_i(\widetilde{X}_{i-1})$
    $\widetilde{X}_i = X_i + E_i$
end while

Issues:

- How to select polynomials f_i? — consider $f_0 : \lambda(X_i) \subseteq [0, 1]$
- How to perform truncation?
- When to stop expansion?

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When to stop?

Stop expansion when eigenvalues are close enough to 0 and 1.

Measure of closeness to convergence is **idempotency error**:

$$e_i = \|X_i - X_i^2\|_2 < 1$$

When to stop?

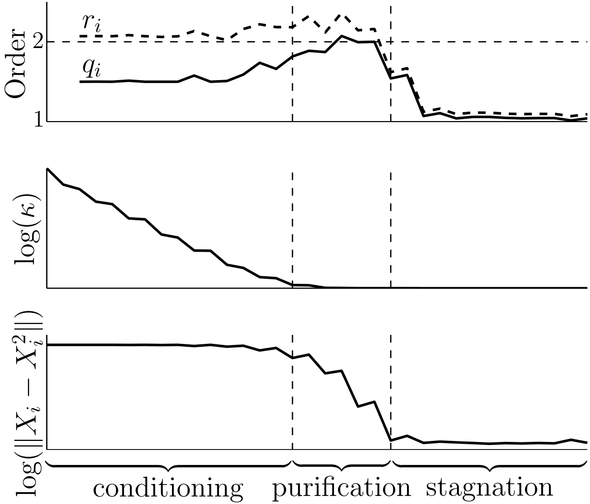
Stop expansion when eigenvalues are close enough to 0 and 1.

Measure of closeness to convergence is **idempotency error**:

$$e_i = \|X_i - X_i^2\|_2 < 1$$

- How to define "enough"?
- How to relate the stopping criterion with truncation?

Phases of the recursive expansion



Development of the stopping criterion

Theoretical order of convergence q satisfies:

$$\lim_{i\to\infty} \frac{e_i}{e_{i-1}^q} = C_\infty$$

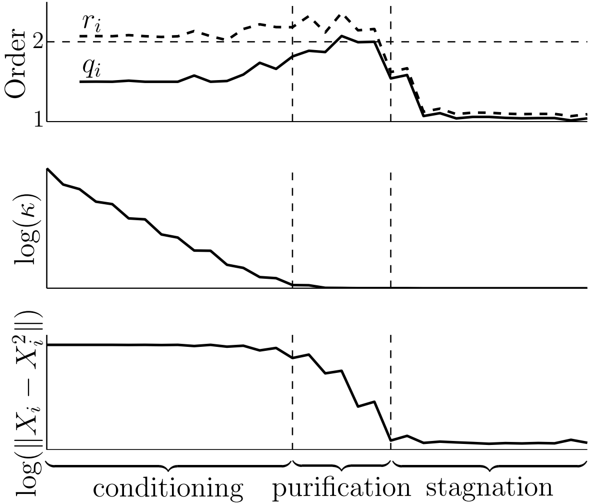
Observed order of convergence in iteration i:

$$q \approx \frac{\log(e_i/C_\infty)}{\log(e_{i-1})} := q_i \quad \Rightarrow \quad r_i := \frac{\log(e_i/C_q)}{\log(e_{i-1})}$$

Our solution: find smallest C_q such that

$$r_i \geq q \quad \Leftrightarrow \quad C_q \geq \frac{e_i}{e_{i-1}^q}$$

Phases of the recursive expansion



Stopping criterion (general form)

Compute r_i in every iteration.
If $r_i < q$, expansion reached stagnation phase
(stop expansion).

Due to possible small perturbations of the order, use $\tilde{q} < q$

How to find $C_q \geq \frac{e_i}{e_{i-1}^q}$*?*

Find

$$\max_{x\in[0,1]} \frac{f_i(x) - f_i(x)^2}{(x - x^2)^q},$$

$q > 1$ is the theoretical order of convergence

How to find $C_q \geq \frac{e_i}{e_{i-1}^q}$ *?*

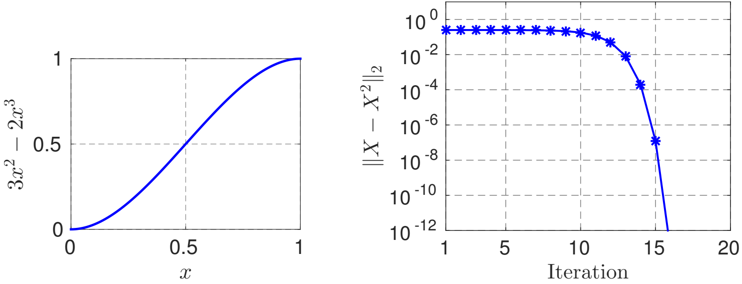
Find

$$\max_{x\in[0,1]} \frac{f_i(x) - f_i(x)^2}{(x - x^2)^q},$$

$q > 1$ is the theoretical order of convergence

OK if $\max_{x\in[0,1]} \frac{f_i(x)-f_i(x)^2}{(x-x^2)^q}$ does not exist, requires some knowledge of the location of eigenvalues

McWeeny polynomial: $3x^2 - 2x^3$



A. H. R. Palser and D. E. Manolopoulos, Phys. Rev. B, 58 (1998)

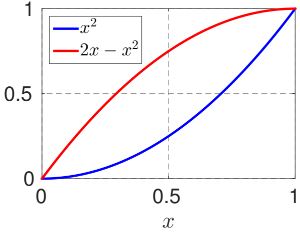
(equiv. to the Newton–Schulz iteration for sign matrix evaluation)

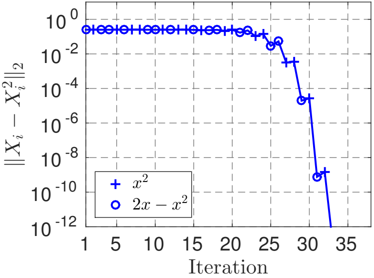
McWeeny polynomial: $3x^2 - 2x^3$

Stop expansion as soon as:

$$\frac{\log(e_i/4)}{\log(e_{i-1})} < 1.8$$

Spectral projection polynomials (SP2): x^2, $2x - x^2$





A. M. N. Niklasson, Phys. Rev. B, 66 (2002)

Spectral projection polynomials (SP2): x^2, $2x - x^2$

Stop expansion as soon as:

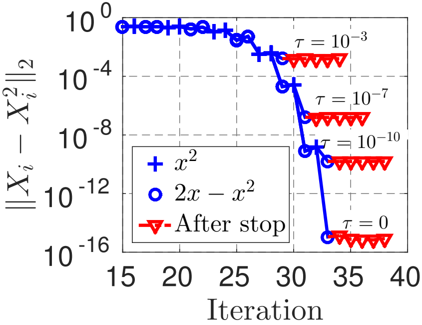
$$\frac{\log(e_i/4.409)}{\log(e_{i-2})} < 1.8$$

$$\text{if} \quad p_i \neq p_{i-1}$$

The get C_q use compositions of x^2 and $2x - x^2$.

If $p_{i-1} = p_i$ then $p_i \neq p_{i+1}$ after an initial phase in the expansion (if homo and lumo bounds are known).

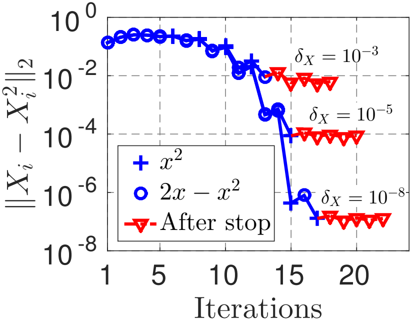
Numerical examples - Dense matrices



$\|E_i\|_2 = \tau$ for $i = 1, 2, \ldots$

Random symmetric matrices, homo-lumo gap 0.01

Numerical examples - Sparse matrices



If $|X_{ij}| < \delta_X$ then set $X_{ij} = 0$.

HF/STO-3G on linear alkane molecule $C_{160}H_{322}$
(1122 basis functions (= matrix size) and 641 occupied orbitals).

Conclusion

Stopping criteria . . .

- automatically and accurately detect when numerical errors start to dominate, i.e. transition between purification and stagnation phases;
- do not require any user defined parameter;
- are general, can be derived for various choices of polynomials;
- can be used for various strategies for removal of small matrix elements;
- can be used for dense and sparse matrices;
- are easy to implement.

If you are interested...

A. Kruchinina, E. Rudberg, and E. H. Rubensson,
"Parameterless stopping criteria for density matrix expansions in electronic structure calculations",
arXiv:1507.02087, July 2015.

Thank you for your attention!

Large–scale electronic structure calculations Congruent transformation

Solve generalized symmetric definite eigenproblem
(non-orthogonal basis set)

$$Fx = \lambda Sx$$

Factorization and congruence tranformation:

$$S \to Z^* S Z = I, \quad \widehat{F} := Z^* F Z$$

Eigenvalue problem (orthogonal basis set)

$$\widehat{F} y = \lambda y, \quad Zy = x$$

Theorem

Let f be a continuous function from $[0,\ 1]$ to $[0,\ 1]$ and assume that the limits

$$\lim_{x\to a^+} \frac{f(x) - f(x)^2}{(x - x^2)^q} \quad \textit{and} \quad \lim_{x\to(1-a)^-} \frac{f(x) - f(x)^2}{(x - x^2)^q}$$

exist for some $q > 0$, where $a \in [0,\ 0.5]$. Let H denote the set of Hermitian matrices with all eigenvalues in $[0,\ 1]$ and at least one eigenvalue in $[a,\ 1-a]$. Then,

$$\max_{X\in H} \frac{\|f(X) - f(X)^2\|_2}{\|X - X^2\|_2^q} = \max_{x\in[0,1]} g(x,a),$$

where

$$g(x,a) := \begin{cases} \frac{f(x)-f(x)^2}{(x-x^2)^q} & \textit{if } a \leq x \leq 1-a, \\ \frac{f(x)-f(x)^2}{(a-a^2)^q} & \textit{otherwise.} \end{cases}$$