Parameterless stopping criteria for density matrix expansions in electronic structure calculations

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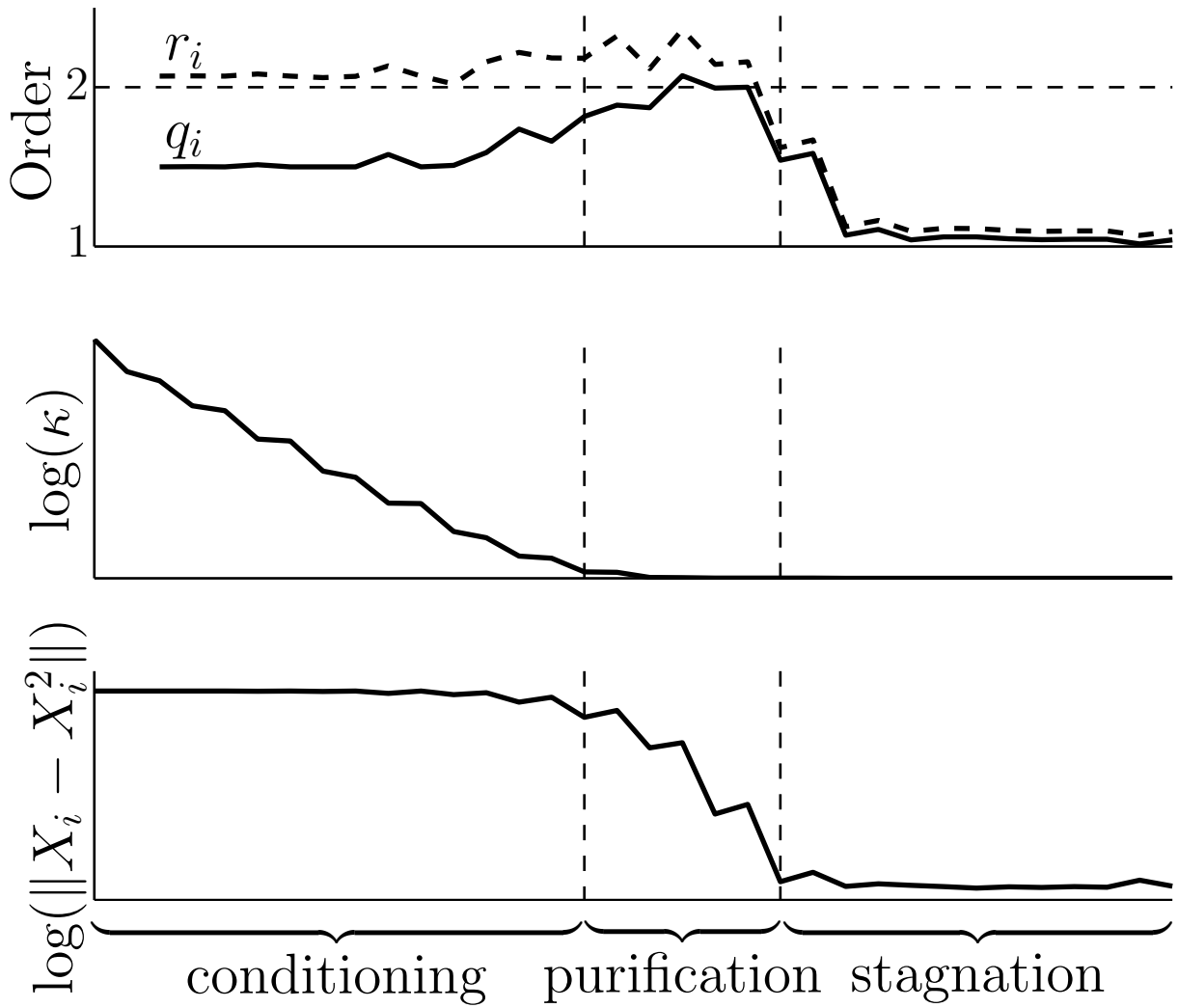
Joint work with Elias Rudberg and Emanuel H. Rubensson

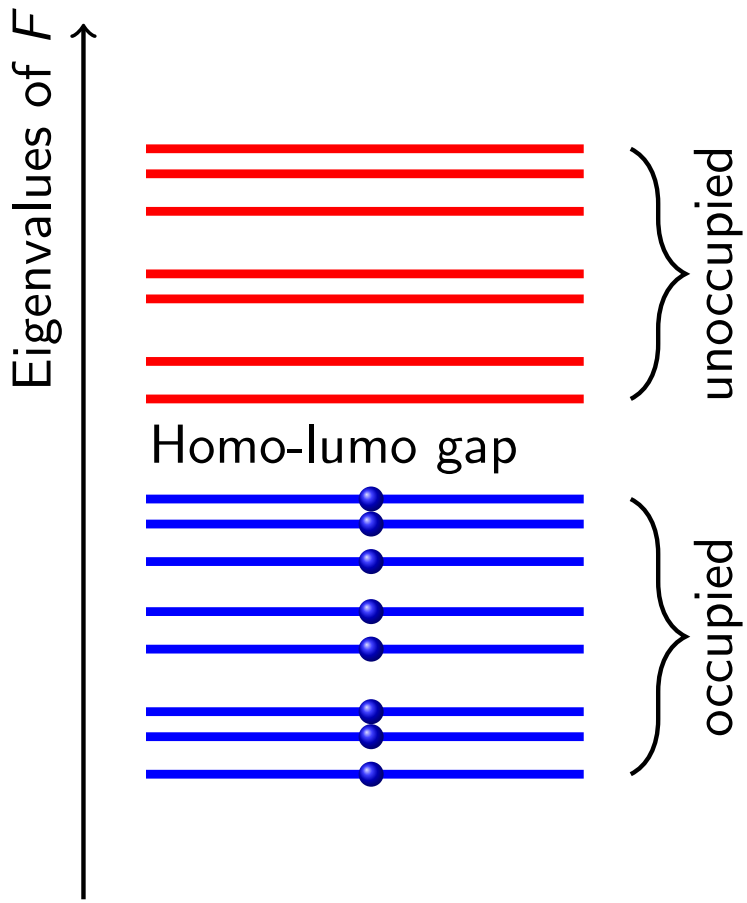
Uppsala University

BIT Circus 2015

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

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

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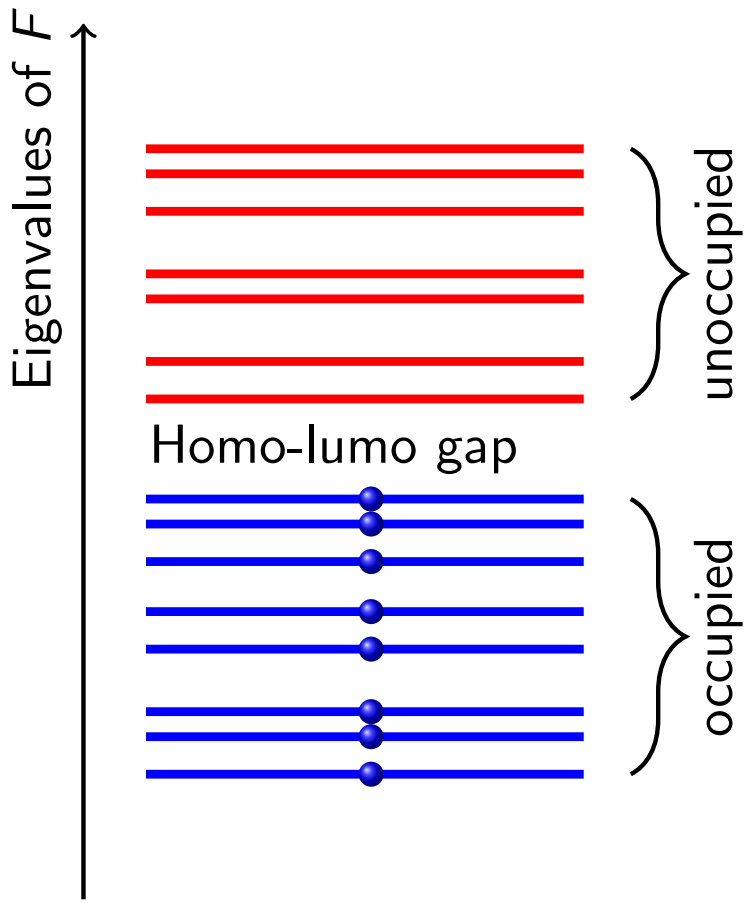

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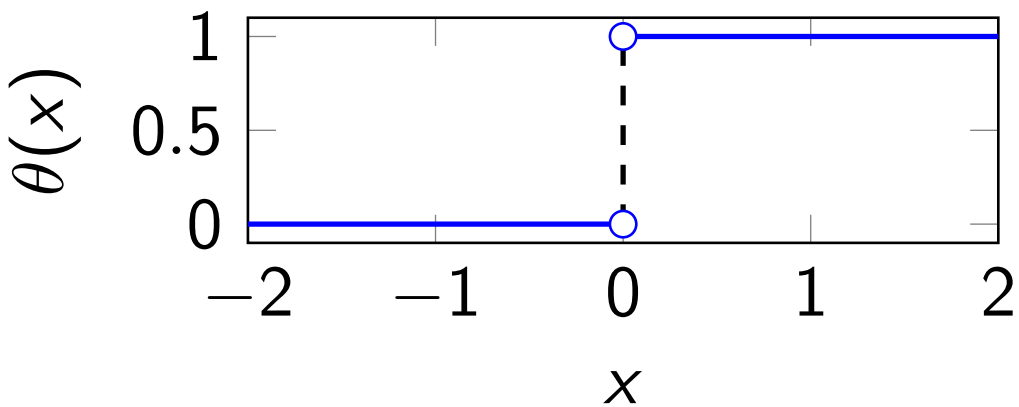
Too expensive!

Large–scale electronic structure calculations
Density matrix construction

Linear scaling computations:

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



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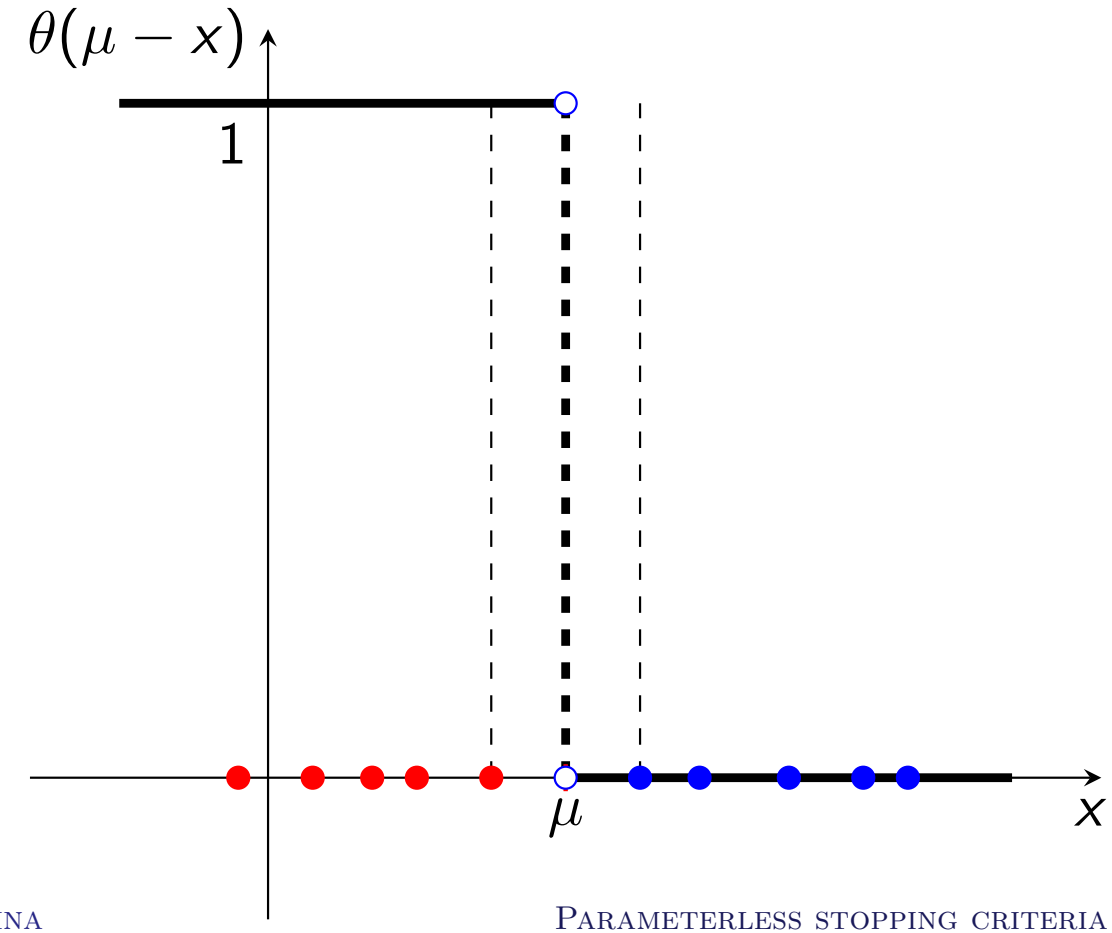

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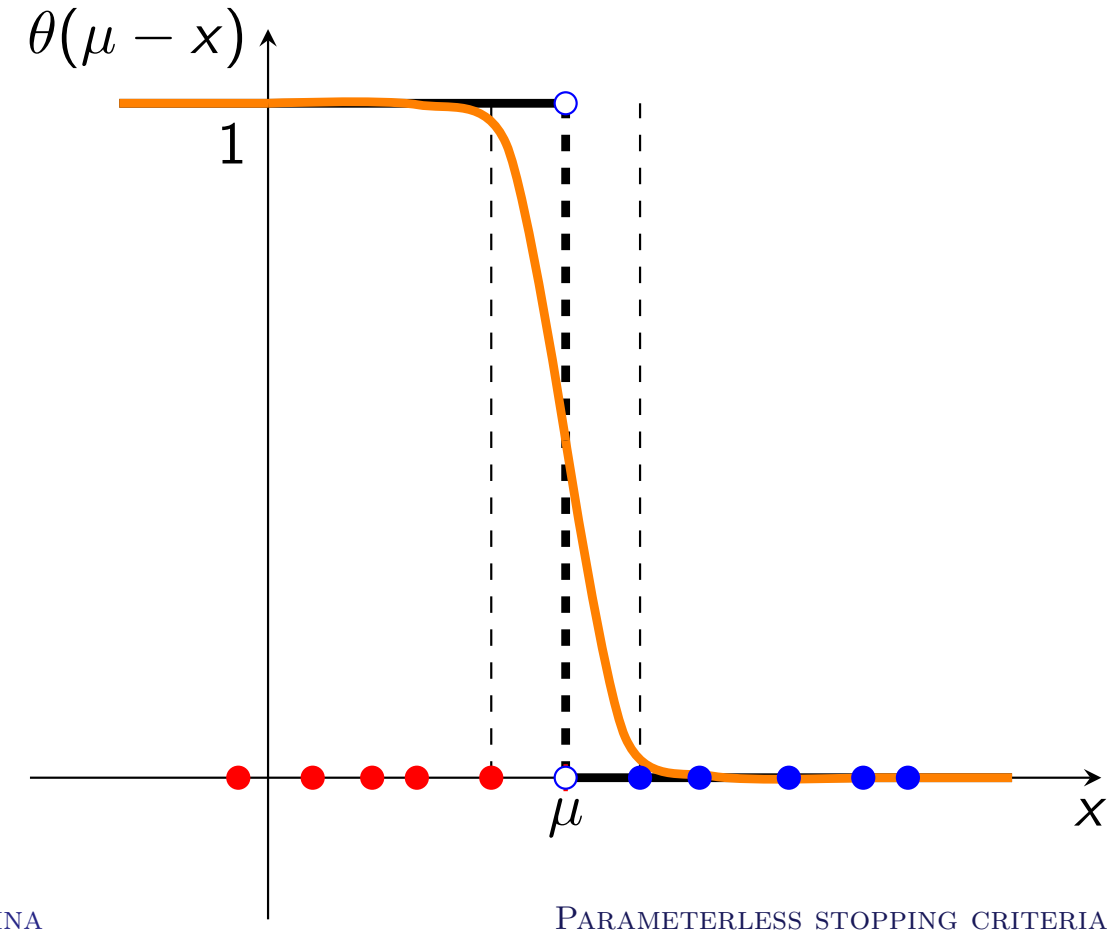

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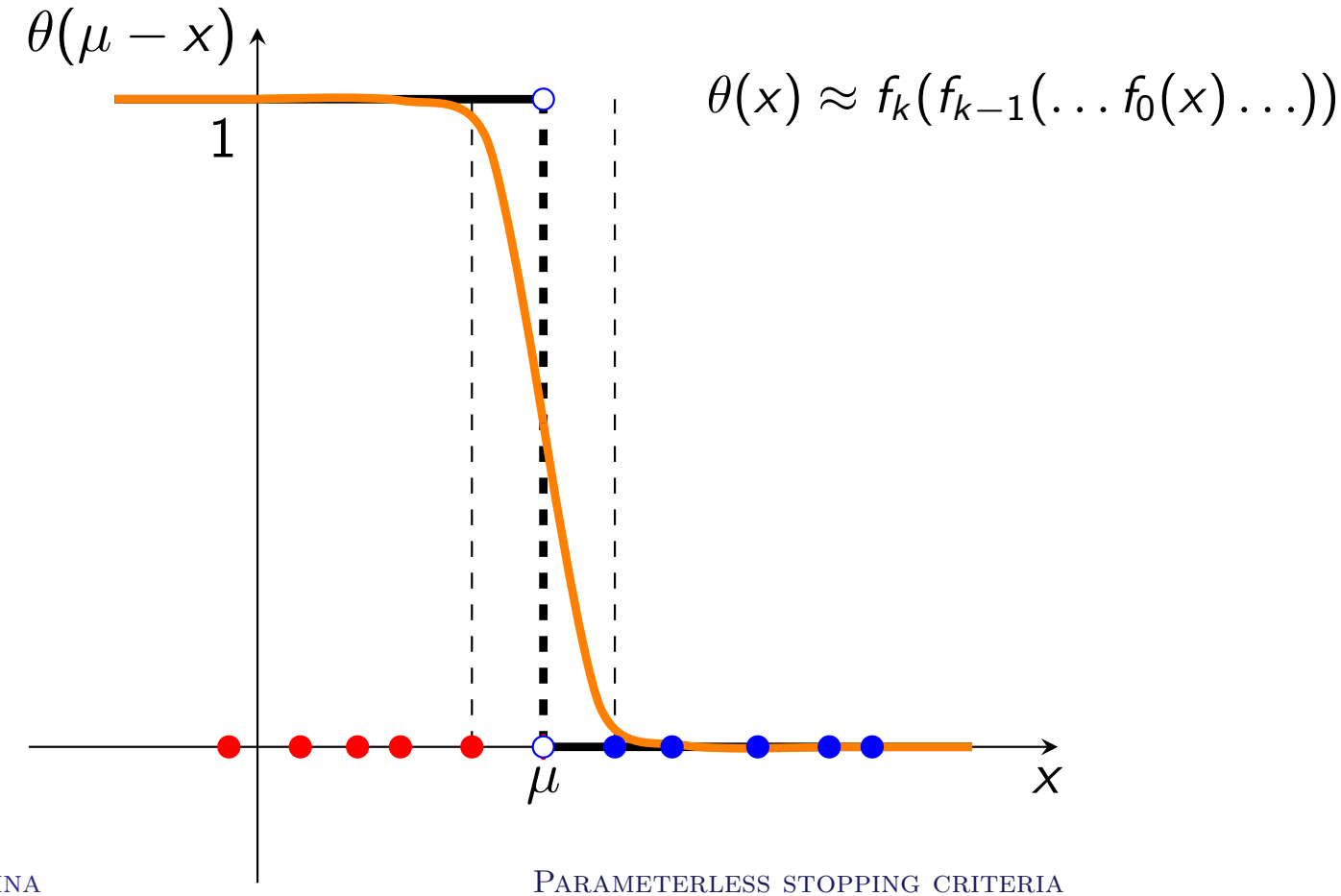

Recursive polynomial expansion (general form)

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

1: $X_0 = f_0(F)$
2: $\widetilde{X}_0 = X_0 + E_0$
3: **while** stopping criterion not fulfilled, for $i = 1, 2, \ldots$ **do**
4: $\quad X_i = f_i(\widetilde{X}_{i-1})$
5: $\quad \widetilde{X}_i = X_i + E_i$
6: **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 expension when eigenvalues are enough close to 0 and 1.

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

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

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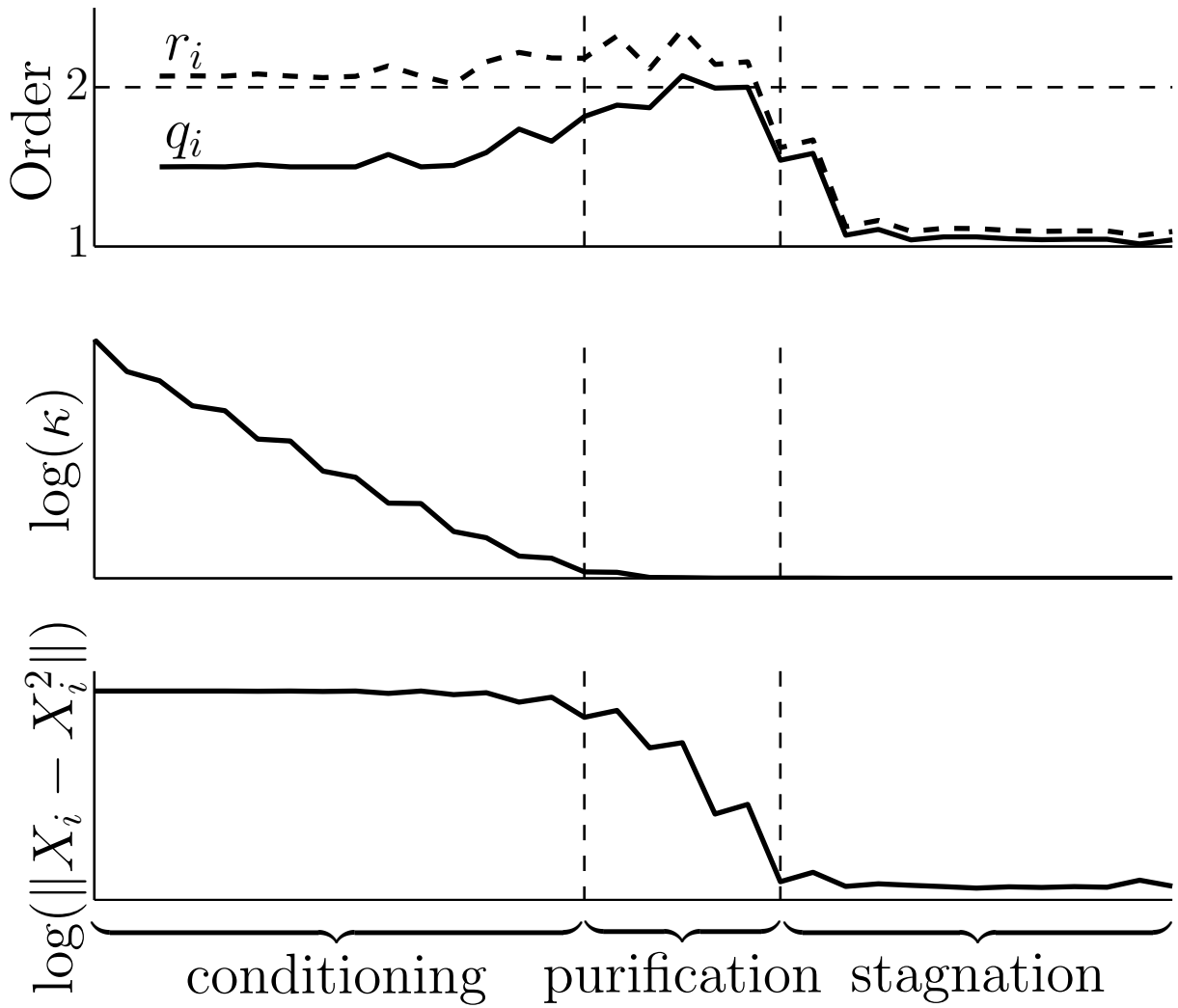
Stop expension when eigenvalues are enough close to 0 and 1.

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:

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

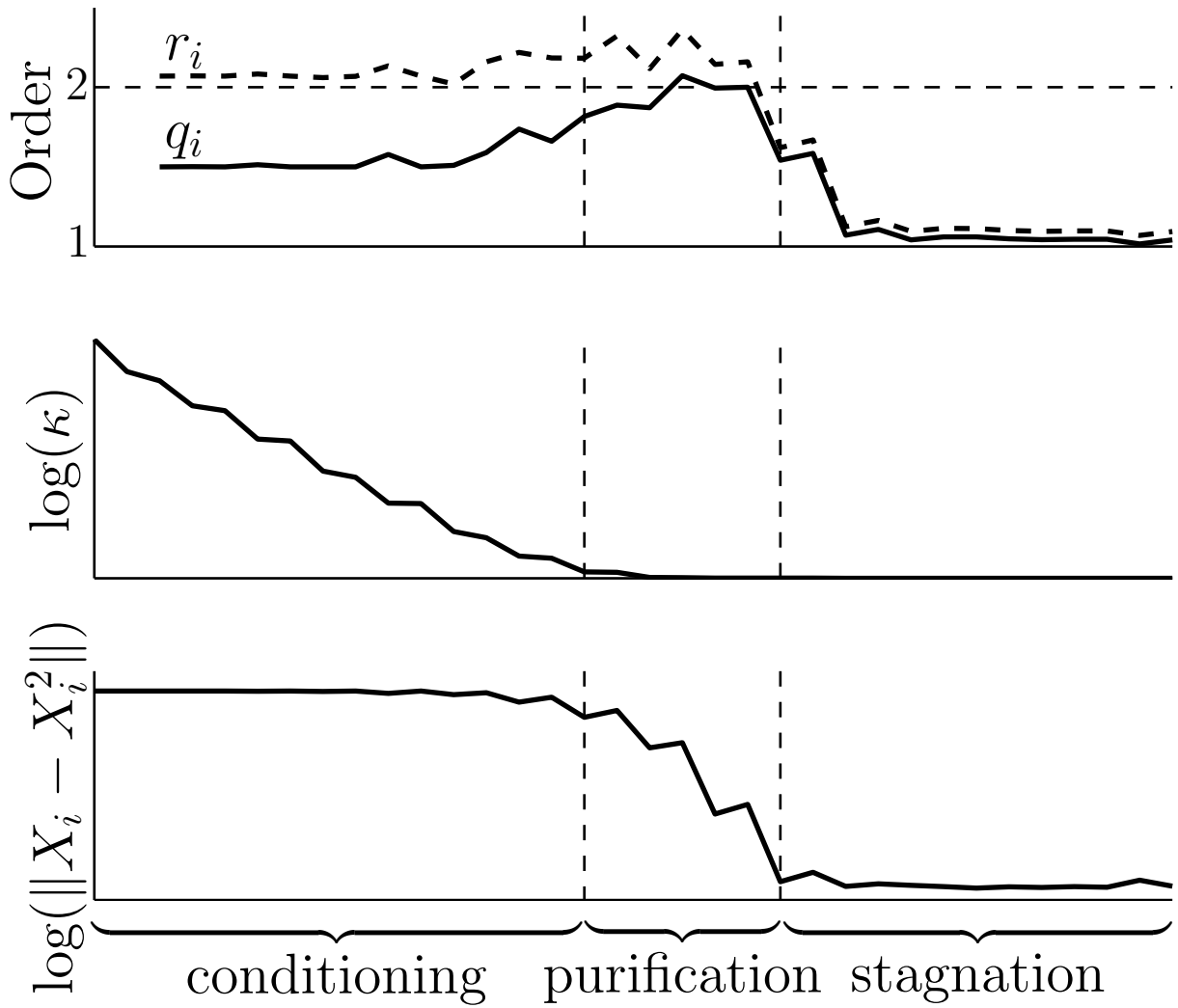
Observed order of convergence in iteration i:

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

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).

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

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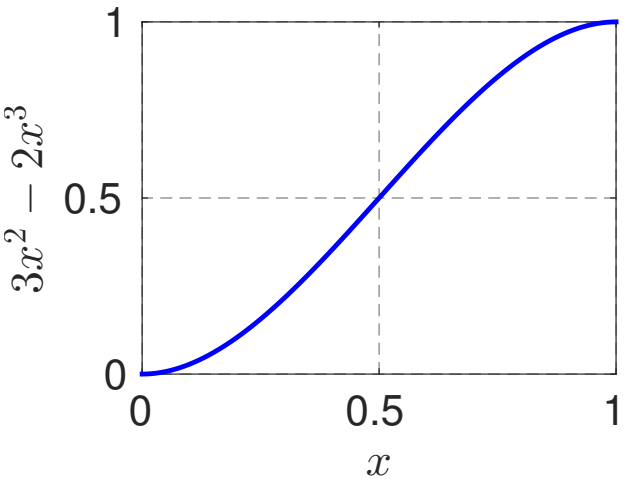
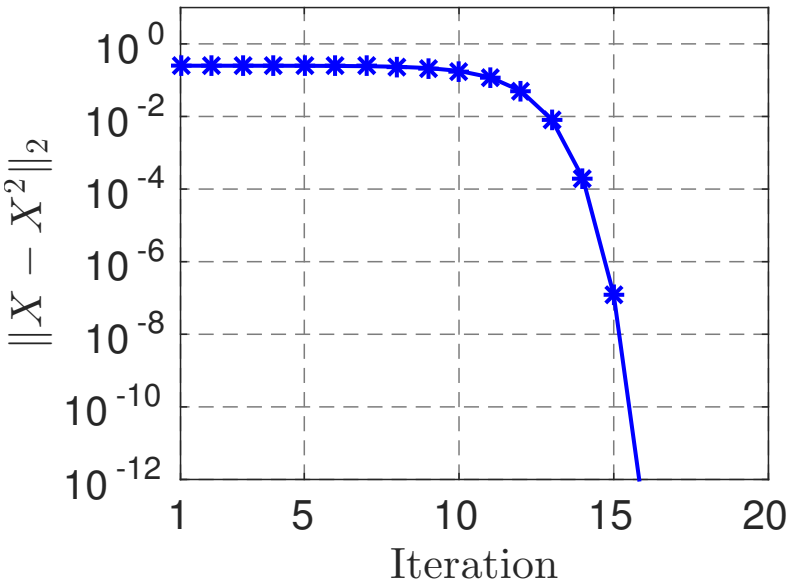
OK if $\max_{x\in[0,1]} \frac{f_i(x)-f_i(x)^2}{(x-x^2)^q}$ does not exist, requires some knowledge of the location of eigenvalues

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





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

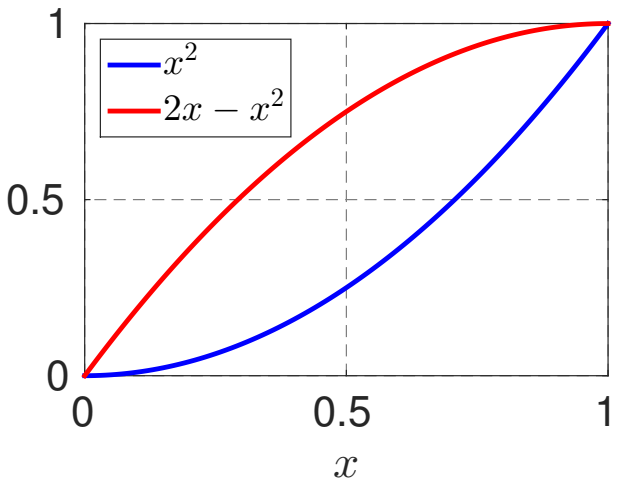
(equiv. to the Newton–Schulz iteration for sign matrix evaluation)

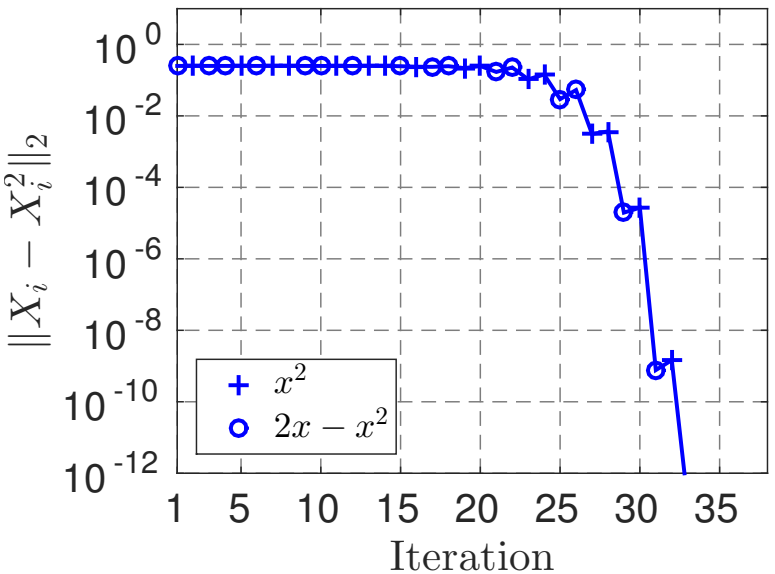
McWeeny polynomial: $3x^2 - 2x^3$

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:

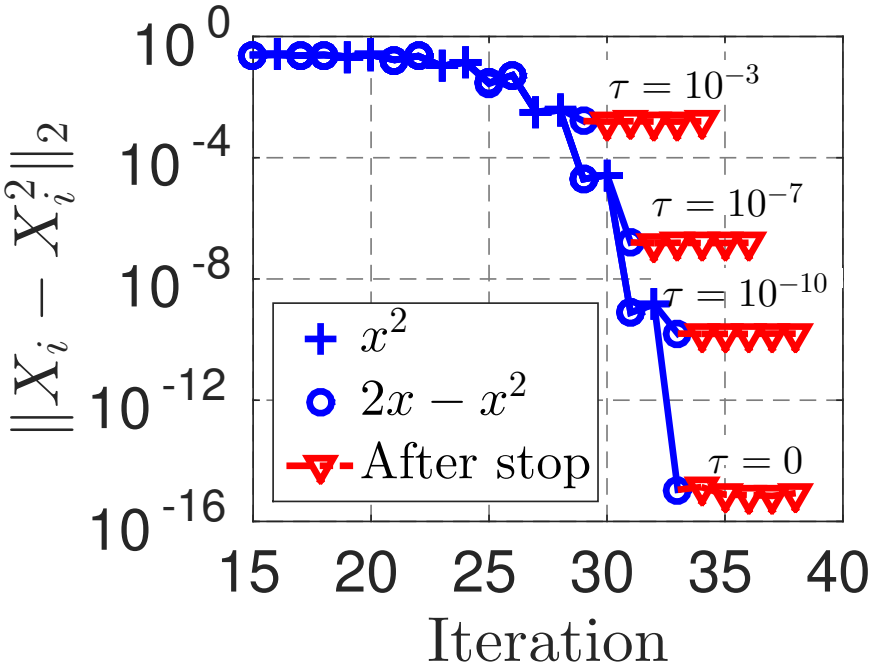
$$\frac{\log(e_i/4.409)}{\log(e_{i-2})} < 1.8$$

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

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).

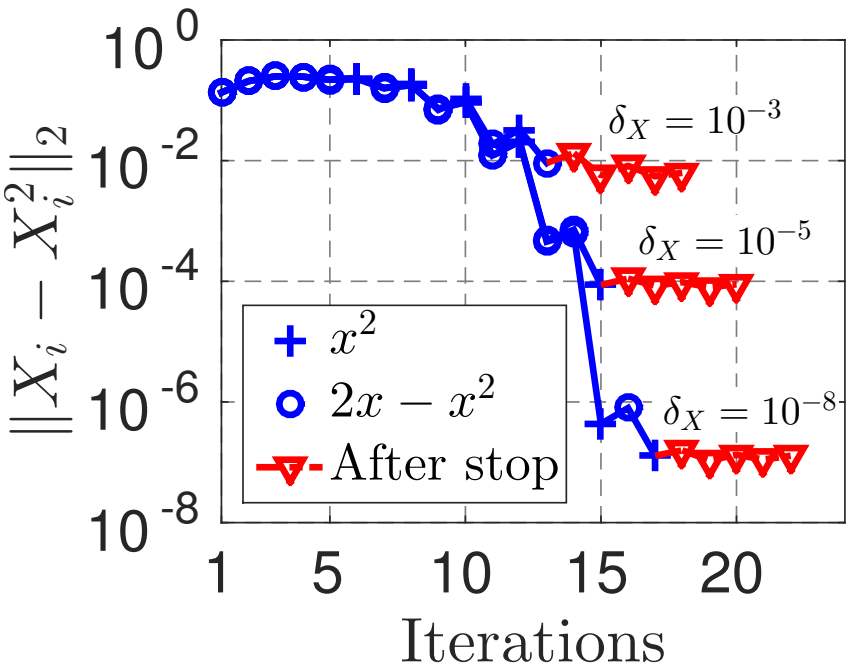
Numerical examples - Dense matrices



$\|E_i\|_2 = \tau$ 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:

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

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

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