Eigenvector continuation in nuclear physics

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SK, A. Ekström, K. Hebeler, A. Sarkar, D. Lee, A. Schwenk, arXiv:1909.08446

P. Demol, T. Duguet, A. Ekström, M. Frosini, K. Hebeler, SK, D. Lee, A. Schwenk, V. Somà, A. Tichai, arXiv:1911.12578

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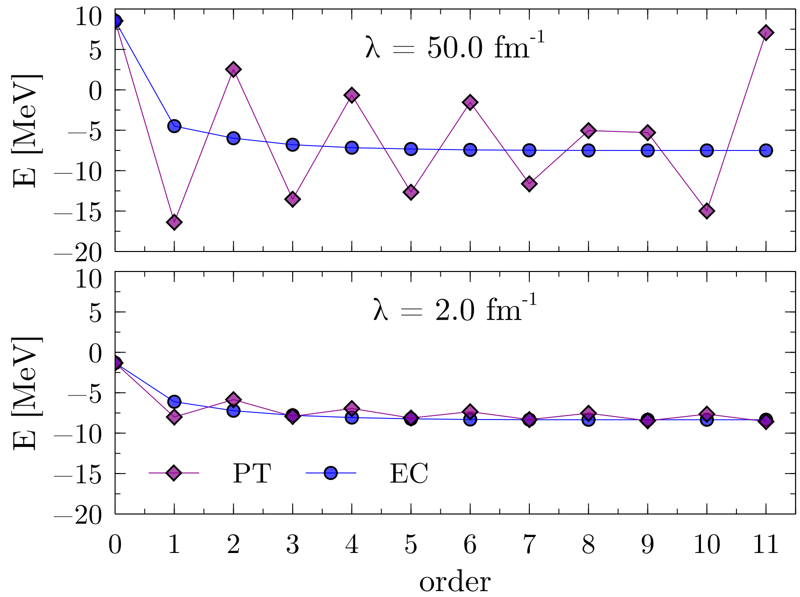
Previously on Eigenvector Continuation

Perturbation theory

- span space by the wavefunction corrections $|\psi_1^{(n)}\rangle \to x_j^{(n)}$, $n = 0, \cdots \mathrm{order}$
- evaluate Hamiltonian between these states
- interpretation: $H = H_{\rm diag} + c\, H_{\rm off\text{-}diag}$, EC-extrapolate to $c = 1$

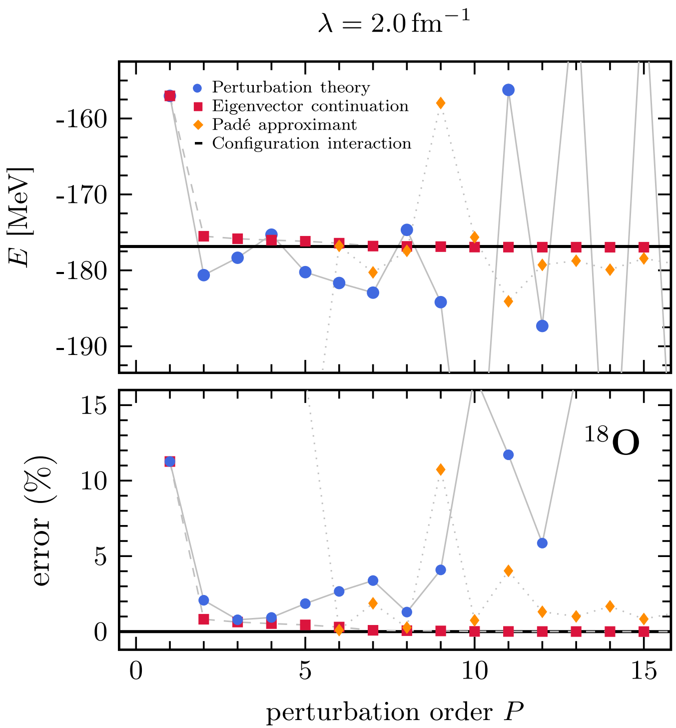


- **same input as PT, but now things converge (to the correct result!)**

New episode

Many-body perturbation theory

- see talk and poster by M. Frosini!
- consider ^{18}O in BMBPT
  - PT under constraint
  - here: limited space
  - realistic: $P \leq 3$
- EM500 interaction
  - SRG evolved to $\lambda = 2.0\text{fm}^{-1}$
- full CI as reference
- **compare EC to simple PT and Padé**



- direct perturbation theory clearly diverges
- **EC is accurate and reliable, Padé becomes erratic at high orders**

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This talk

EC as efficient emulator

Need for emulators

1. Fitting of LECs to few- and many-body observables

- common practice now to use $A > 3$ to constrain nuclear forces, e.g.:
  - JISP16, NNLO_{sat}, α-α scattering

Shirokov et al., PLB **644** 33 (2007); Ekström et al., PRC **91** 051301 (2015); Elhatisari et al., PRL **117** 132501 (2016)

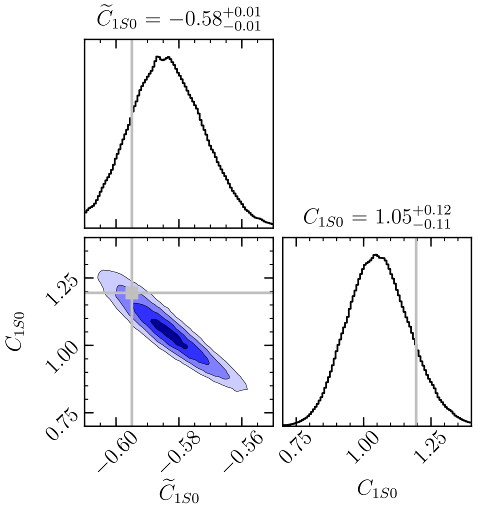
- **fitting needs many calculations with different parameters**
- Kostas' talk this morning!

2. Propagation of uncertainties

- statistical fitting gives posteriors for LECs
- LEC posteriors propagate to observables

Wesolowski et al., JPG **46** 045102 (2019)

- **need to sample a large number of calculations**
- see Dick's colloquium talk!



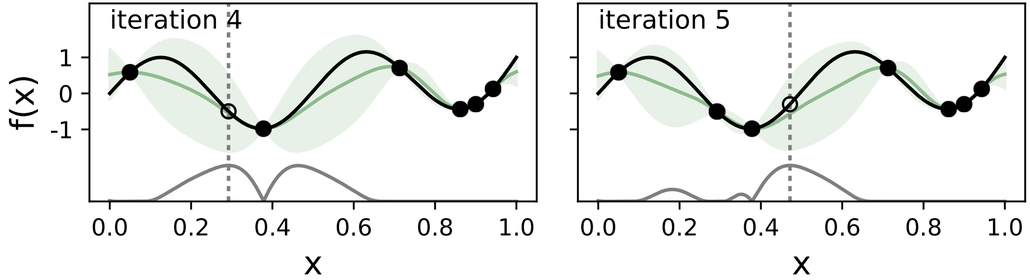
Emulators

Exact calculations can be prohibitively expensive!

Options

- **multi-dimensional polynomial interpolation**
  - simplest possible choice
  - typically too simple, no way to assess uncertainty

- **Gaussian process**



  - statistical modeling, iteratively improvable
  - interpolation with inherent uncertainty estimate

Ekström et al., arXiv:1902.00941

Recall

Eigenvector continuation can interpolate and extrapolate!

Hamiltonian parameter spaces

- original EC: single parameter, $H = H(c)$ — Frame et al., PRL **121** 032501 (2018)
- **consider a Hamiltonian depending on several parameters:**

$$H = H_0 + V = H_0 + \sum_{k=1}^{d} c_k V_k \tag{1}$$

- in particular, V can be a chiral potential with LECs c_k
- Hamiltonian is element of d-dimensional parameter space
- typical for $\mathcal{O}(Q^3)$ calculation: 14 two-body LECs + 2 three-body LECs
- convenient notation: $\vec{c} = \{c_k\}_{k=1}^{d}$

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Generalized EC

- **EC construction is straightforward to generalize to this case:**
- simply replace $c_i \to \vec{c}_i$ in construction
  - $|\psi_i\rangle = |\psi(\vec{c}_i)\rangle$ for $i = 1, \cdots N_{\mathrm{EC}}$
  - $H_{ij} = \langle\psi_i|H(\vec{c}_{\mathrm{target}})|\psi_j\rangle$, $N_{ij} = \langle\psi_i|\psi_j\rangle$

Note: sum in Eq. (1) can be carried out in small (dimension = N_{EC}) space!

Interpolation and extrapolation

Hypercubic sampling

- **want to cover parameter space efficiently with training set $S = \{\vec{c}_i\}$**
- Latin Hypercube Sampling can generate near random sample
- for examples that follow:
  - sample each component $c_k \in [-2, 2]$
  - vary d LECs, fix the rest at $\mathrm{NNLO}_{\mathrm{sat}}$ point

Ekström et al., PRC **91** 051301 (2015)

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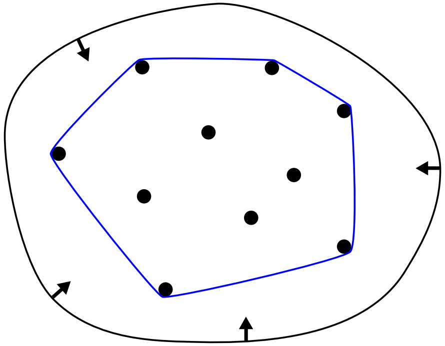
Convex combinations

- **distinguish interpolation and extrapolation target points**
- interpolation region is convex hull of the $\{\vec{c}_i\}$
  - $\text{conv}(S) = \sum_i \alpha_i \vec{c}_i$ with $\alpha_i \geq 0$ and $\sum_i \alpha_i = 1$
- extrapolation for $\vec{c}_{\text{target}} \notin \text{conv}(S)$
- **EC can handle both!**

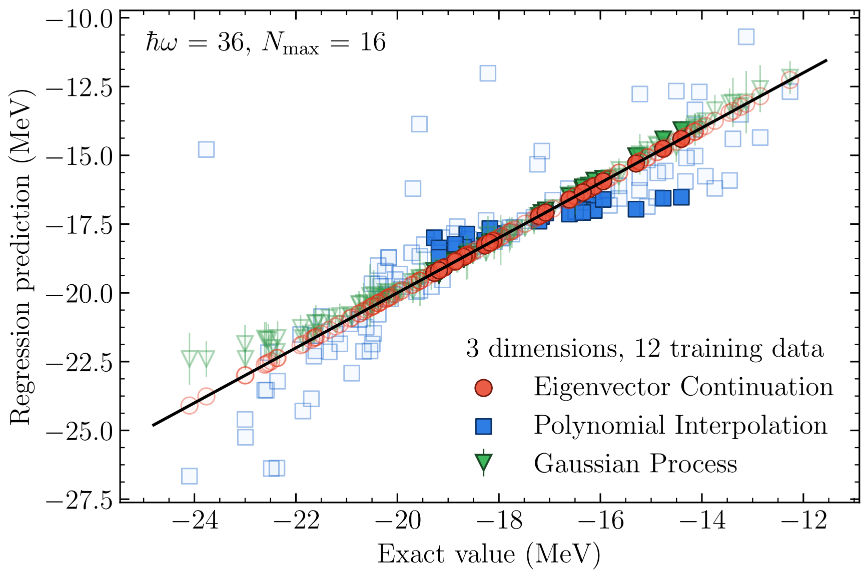


Pbroks13, Wikimedia Commons

Performance comparison: energy

Cross validation

- **compare emulation prediction agains exact result for set** $\{\vec{c}_{\mathrm{target},j}\}_{j=1}^{N}$
- underlying calculation: Jacobi NCSM Ekström implementation of Navratil et al., PRC **61** 044001 (2000)
- observable: ^{4}He ground-state energy
- transparent symbols indicate extrapolation targets



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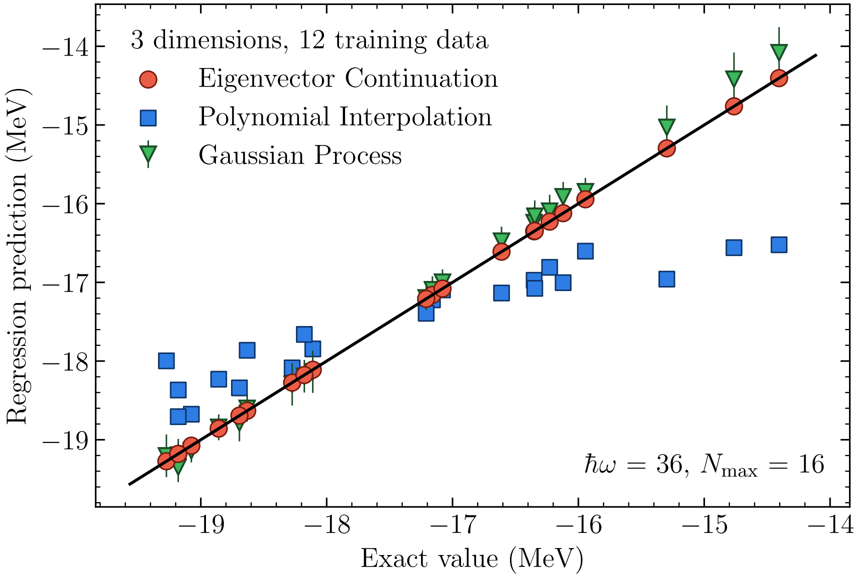

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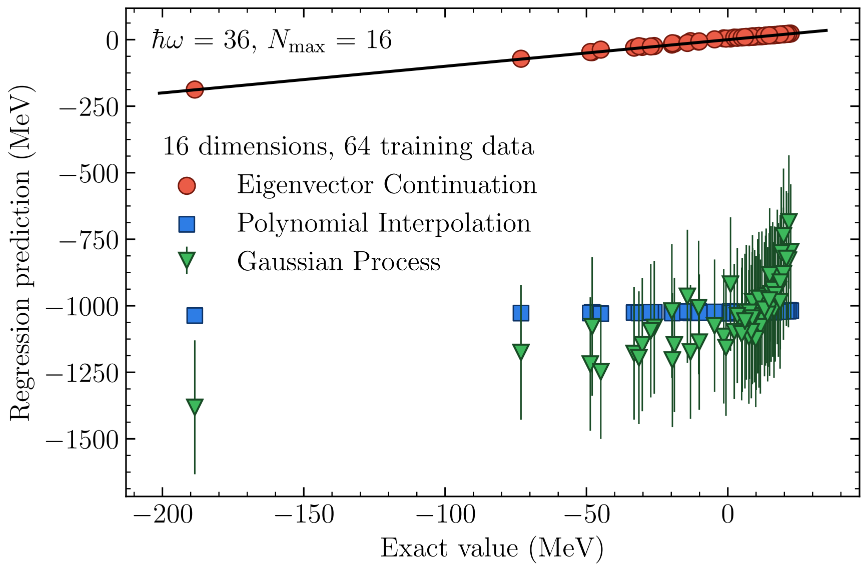

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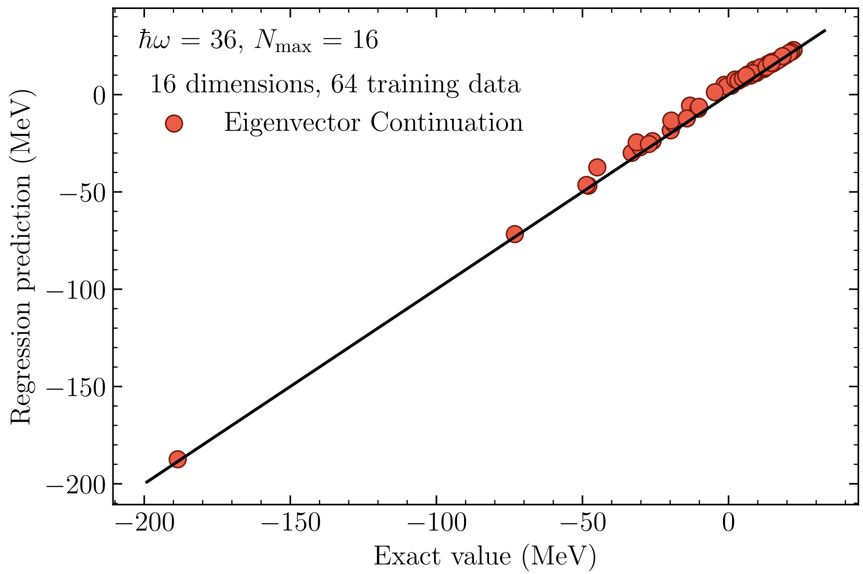
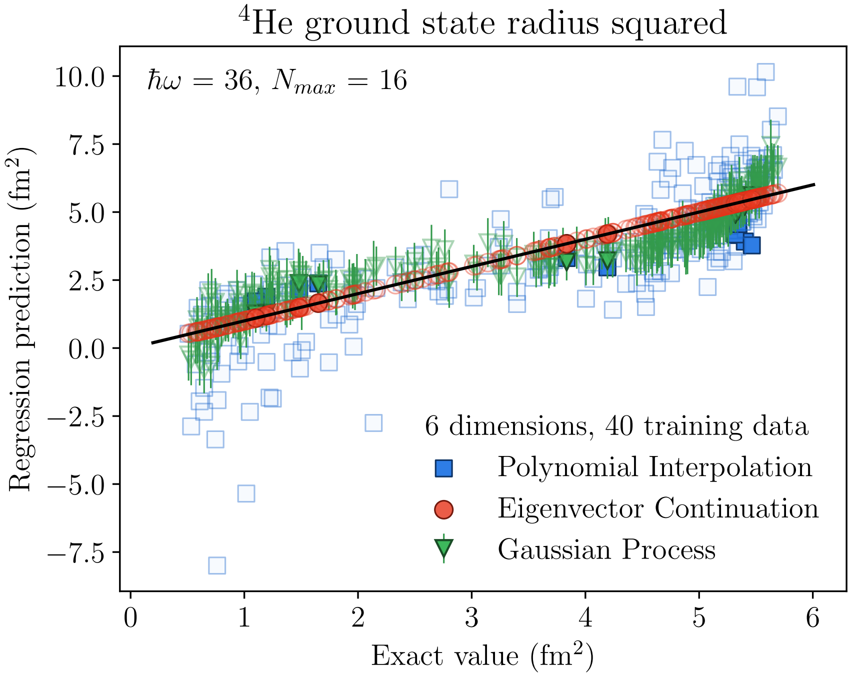


Performance comparison: radius

Operator evaluation

- generalized eigenvalue problem
- EC gives not only energy, but also a continued wavefunction
- **straightforward (and inexpensive) to evaluate arbitrary operators**



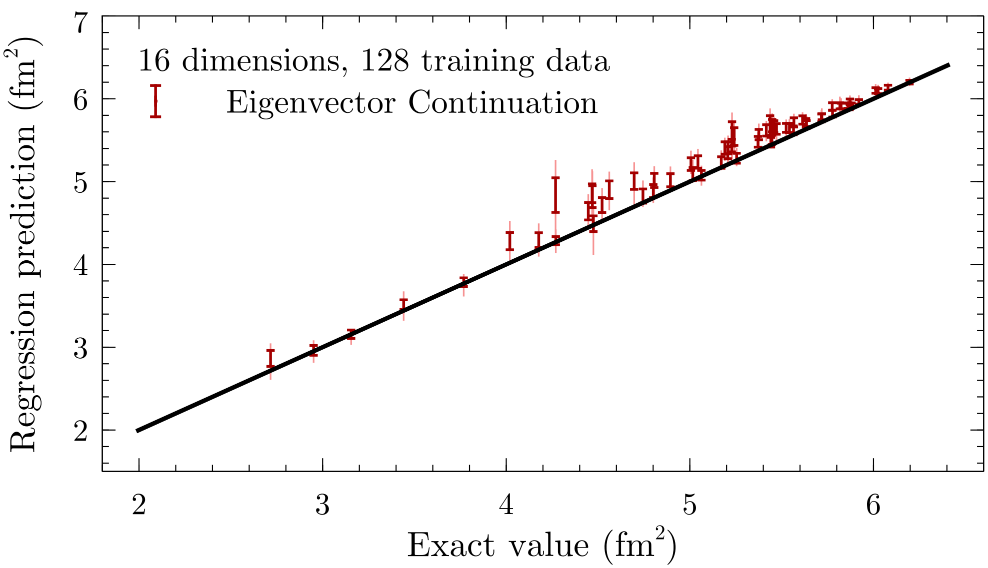
EC uncertainty estimate

- **EC is a variational method**
  - projection of Hamiltonian onto a subspace
  - dimension of this subspace determines the accuracy
  - rate of convergence currently being analyzed

D. Lee + A. Sarkar, work in progress

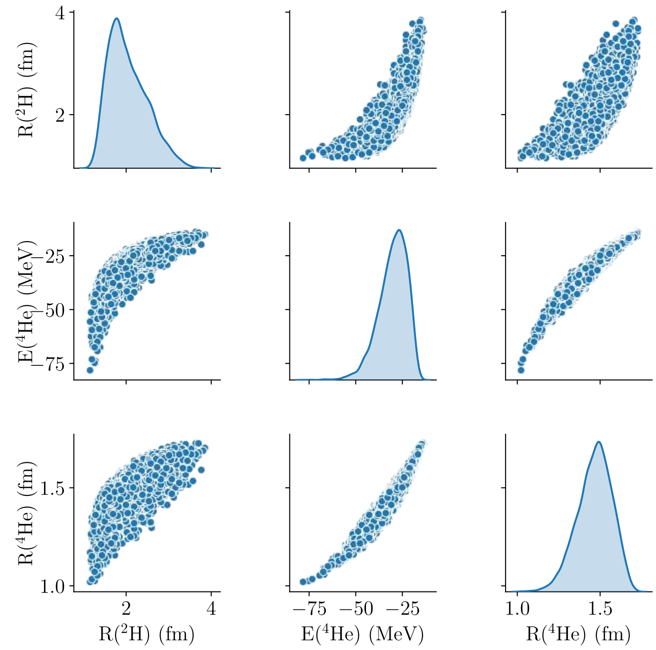
Bootstrap approach

- **leave out sets of basis vectors, take mean and standard deviation**



Application: correlation analysis

- consider 10^4 LEC samples 10% around $\mathrm{NNLO}_{\mathrm{sat}}$ point
- known energy-radius correlation well reflected
- ^{2}H radius only gives lower bound for ^{4}He radius
- this analysis would already be very expensive without EC!



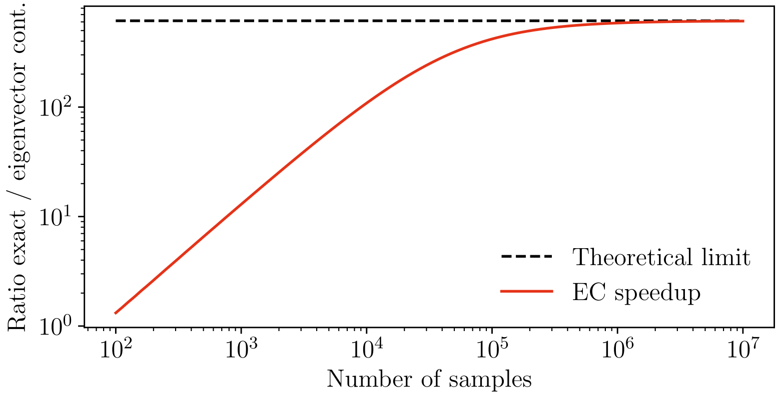
- see talk by Andreas for ^{16}O application!

Computational cost

- **setup of EC subspace basis**
  - combination of Hamiltonian for given $\vec{c}_i$, Lanczos diagonalization
  - total cost $= M^2 \times (2n + N_{\mathrm{mv}})$ flops
- **calculation of norm matrix:** $2n^2 M$ flops
- **reduction of Hamiltonian parts:** $(d+1) \times (2nM^2 + 2n^2 M)$ flops
- **cost per emulated sample point**
  - combination of Hamiltonian parts in small space: $2dn^2$ flops
  - orthogonalization + diagonalization: $26n^3/3 + \mathcal{O}(n^2)$ flops

$M = M(N_{\max})$: model-space dim., n: training data, N: samples, N_{mv}: matrix-vector prod. (Lanczos)

- example for $N_{\max} = 16$, $d = 16$, $N_{\mathrm{EC}} = 64$



Summary and outlook

Eigenvector continuation as efficient emulator

- straightforward setup, reduction to small vector space
- highly competitive, accurate and efficient
- can both interpolate and extrapolate from training set
- provides access to multiple observables
- variational method, upper bound for energies
- provides uncertainty estimates via bootstrap approach

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Future directions

- extrapolate spectra, not just single states
- larger systems, other methods
  - see following talk by A. Ekström
- application for large-scale uncertainty quantification

Thanks...

...to my collaborators:

- A. Schwenk, K. Hebeler, A. Tichai (TU Darmstadt)
- A. Ekström (Chalmers U.)
- D. Lee, A. Sarkar (Michigan State U.)
- T. Duguet, V. Somà, M. Frosini (CEA Saclay)
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