Tensor network compression for high dimensional integration and its application to Feynman diagrams

Olivier Parcollet

FLATIRON INSTITUTE
Center for Computational Quantum Physics

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Collaborators : X. Waintal, Y. Nuñez-Fernandez, Ph. Dumitrescu, J. Kaye…




DE LA RECHERCHE À L'INDUSTRIE
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High dimensional integrals

- High dimensional integral or sum ($n \geq 5$)

$$\int dx_1 \ldots dx_n \; f(x_1, \ldots, x_n) \qquad \sum_{i_1=1}^{d} \cdots \sum_{i_n=1}^{d} f_{i_1,\ldots,i_n}$$

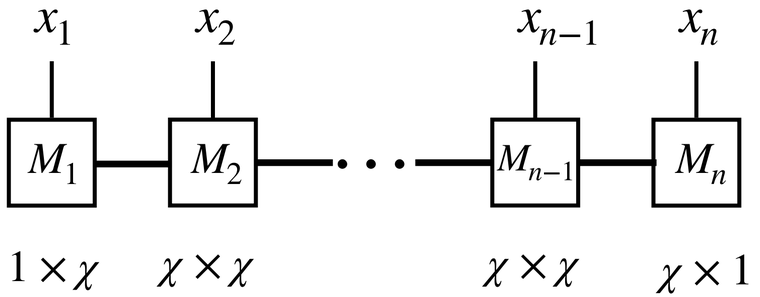
- Discretize the integral (e.g. Legendre grid) with d points : discrete x_i
- Curse of dimensionality : a priori $O(d^n)$

Main idea : compress to integrate

$$\int dx_1 \ldots dx_n \; f(x_1, \ldots, x_n)$$

- If *f* can be written as a Matrix Product State (MPS) …

$$f(x_1, \ldots, x_n) \approx M_1(x_1) \ldots M_n(x_n) \qquad =$$

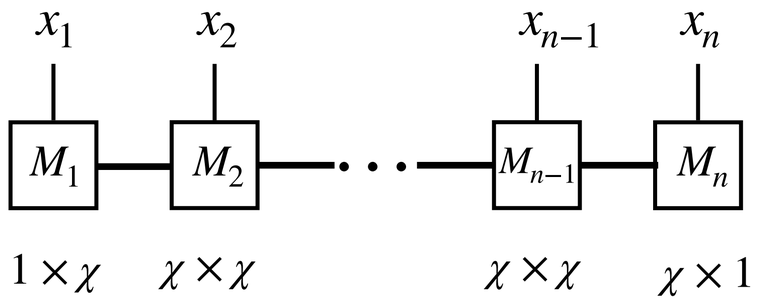


- with an error ε decreasing quickly with the bond dimension χ (*ε-factorizable*) …
- then integration is reduced to 1d integrals. Almost separated variables.

$$\int dx_1 \ldots dx_n \; f(x_1, \ldots, x_n) \approx \left(\int dx_1 M_1(x_1) \right) \ldots \left(\int dx_n M_n(x_n) \right)$$

MPS compression

$$f(x_1, \ldots, x_n) \approx M_1(x_1) \ldots M_n(x_n) \quad =$$



- Key question : are physical integrals compressible in this way ?

- We need a decomposition technique with :
  - Minimal number of evaluations of f
  - A reliable error estimate

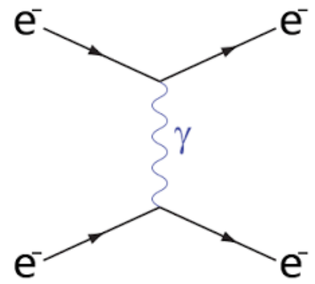
Physics context

Perturbation theory in the quantum many-body problem

- Quantum particles in interaction
- Expand physical quantities in power of the coupling constant U

$$Q = \sum_{n \geq 0} Q_n U^n$$

Feynman diagrams



- Weak coupling: a few orders are enough, e.g. Quantum Electrodynamics
- But our systems of interest at CCQ are at strong coupling/non perturbative !

Perturbation theory : beyond weak coupling

- High order expansion, e.g. $n = 10 - 20$. Typically exponentially hard $O(2^n)$

$$Q = \sum_{n \geq 0} Q_n U^n$$

- Many results, including in strong coupling (i.e. beyond radius of convergence of the series)

Equilibrium : *(diagrammatic QMC) Prokofiev/Svistunov 98, many recent works*
Non equilibrium: *Profumo, Messio, Parcollet, Waintal (2015)*

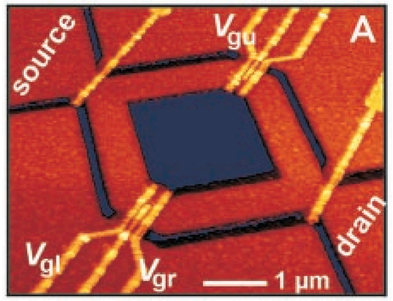
- Q_n = n-dimensional integral (position x_i /time u_i of the Feynman vertices).

$$Q_n(t) = \int du_1 \ldots du_n \sum_{x_1, \ldots, x_n} q_n(u_1, x_1, \ldots, u_n, x_n)$$

- Until now : Monte Carlo. We need better ways to compute Q_n: faster, more precision.

A concrete example : quantum impurity model

- A few interacting quantum degrees of freedom (atom, a single spin 1/2, …) coupled to Fermi sea (an infinite bath of non interacting electrons).

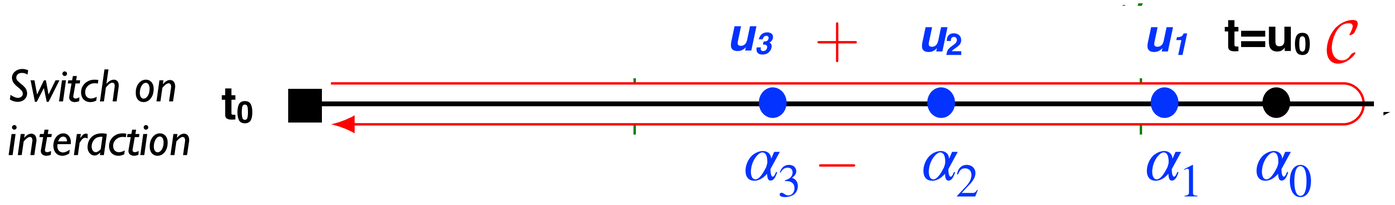


"Quantum dot"

- A central model in the quantum many-body problem.
  - Strong correlation physics: Kondo effect = screening of a spin by a Fermi sea
  - Benchmark: in some specific cases, analytic solution by Bethe Ansatz.
  - "Quantum embeddings", nanophysics, …

$Q_n(t)$: a n-dimensional integral

- Q : number of electrons in the atom.



- Schwinger-Keldysh formalism

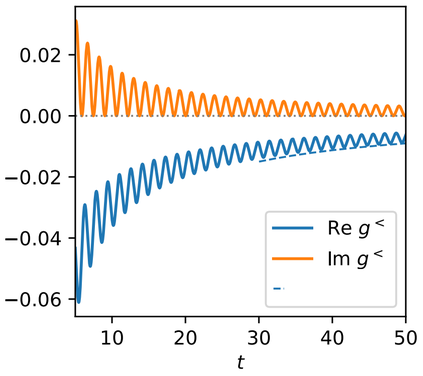
$$Q_n(t) = \frac{1}{n!}\int_{t_0}^{\infty} du_1 \ldots du_n \left(\sum_{\substack{\alpha_1 = \pm 1 \\ \ldots \\ \alpha_n = \pm 1}} \left(\prod_{i=1}^{n} \alpha_i \right) \det_{0 \le i,j \le n} \left[g_{\alpha_i \alpha_j}(u_i - u_j) \right] \right)$$

$$\equiv q_n(t, u_1, \ldots, u_n)$$

Times u_i
Keldysh indices $\alpha_i = \pm 1$

Green function in the non interacting case $U = 0$

- Feynman diagrams explicitly summed by the determinants (Wick theorem).
- Equilibrium/steady state = long time limit $t \to \infty$
- NB : q_n costs $O(2^n)$ to evaluate.



q_n is ε-factorizable !

- q_n is ε-factorizable, in the *time differences* v_i (using a time-ordered domain in u_i)

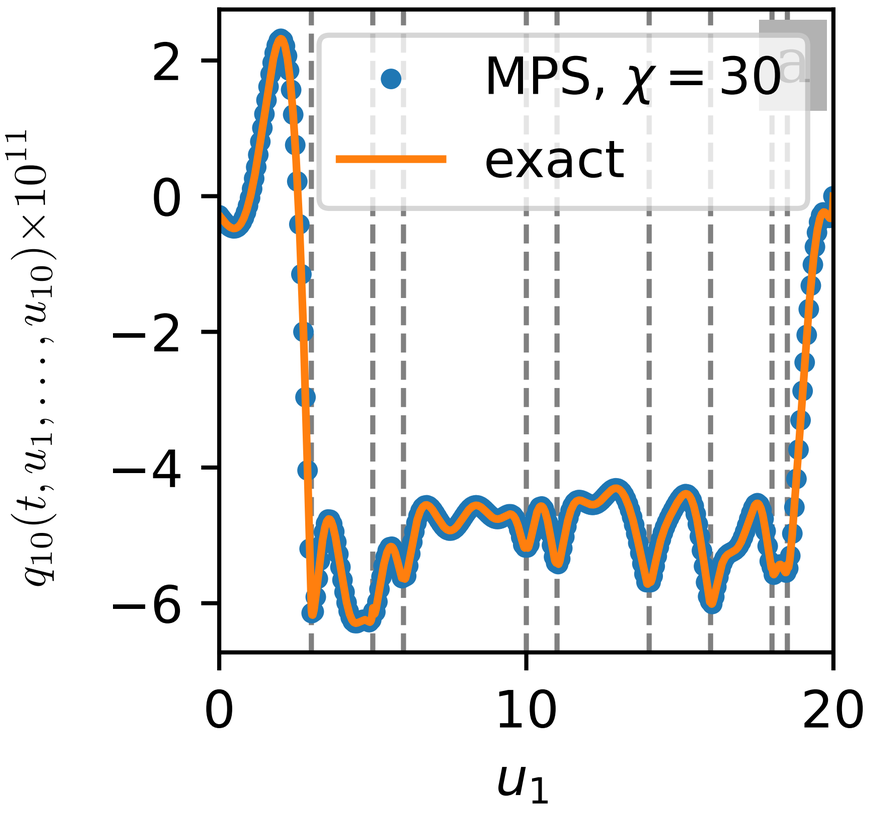
$$v_1 = t - u_1$$
$$v_i = u_{i-1} - u_i \qquad \text{for } 2 \leq i \leq n.$$

$$q_n(t, u_1, \ldots, u_n) \approx M_1(v_1) \ldots M_n(v_n)$$

- Bond dimension χ
- How to reveal the MPS factorization ?

Tensor Cross Interpolation algorithm

q_{10} vs its MPS interpolation



Tensor Cross Interpolation

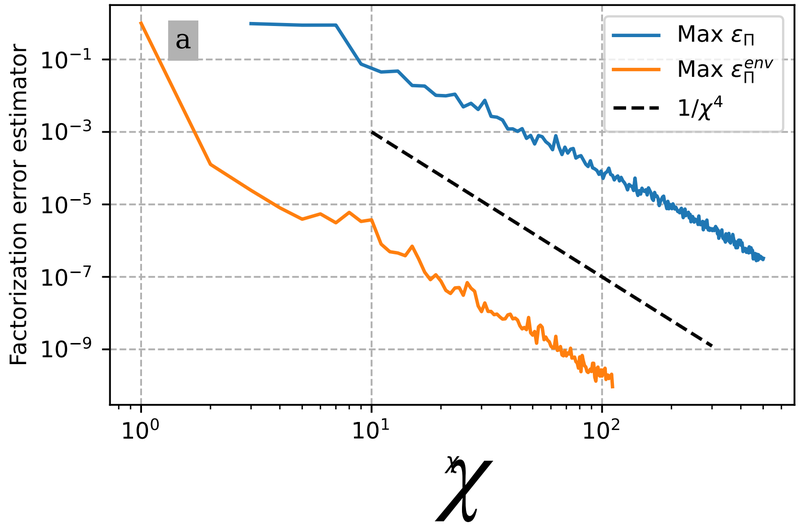
*I. **Oseledets and E. Tyrtyshnikov**, Linear Algebra and its Applications 432, 70 (2010).*
***I. V. Oseledets,** SIAM Journal on Scientific Computing 33, 2295 (2011).*
***D. V. Savostyanov,** Linear Algebra and its Applications 458, 217 (2014)*

***S. Dolgov and D. Savostyanov**, Computer Physics Communications 246, 106869 (2020)*

TCI : summary

- Given a n-dimensional tensor $A(u_1, u_2, \ldots, u_n)$ [u_i are discrete indices with d values]
- It builds a MPS approximation A_χ^{TCI} of A of bond dimension χ, progressively increasing χ
- From the evaluation of A on N points with $N \sim nd\chi^2 \ll d^n$
- With an error estimator $\epsilon(\chi)$, decreasing with χ when the algorithm is successful

$\epsilon(\chi)$



Error estimators

q_{10}, $\epsilon_d = 0$

Cross interpolation formula for a matrix

A low rank decomposition from a small submatrix

- If A is a M x N matrix
- Pivots : subset of rows/columns indices $I = \{i_1, i_2, \ldots, i_\chi\}, J = \{j_1, j_2, \ldots, j_\chi\}$

Cross interpolation formula

$$\mathbb{I} = \{1, 2, \ldots, M\}$$
$$\mathbb{J} = \{1, 2, \ldots, N\}$$

Slices

$$A = A(\mathbb{I}, \mathbb{J}) \approx A(\mathbb{I}, J)A(I, J)^{-1}A(I, \mathbb{J})$$

Pivots

Submatrix of A of size $\chi \times \chi$

Properties

1. Interpolation : exact on the pivots indices
2. If A is of rank χ, it is exact

Exactness for finite rank χ

- Schur complement for a square matrix A

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \qquad \det A = \det[A_{11}]\ \det[A_{22} - A_{21}A_{11}^{-1}A_{12}]$$

- $A(I,J)$ is invertible $\qquad I = \{i_1, i_2, \ldots, i_\chi\} \qquad J = \{j_1, j_2, \ldots, j_\chi\}$
- Rank = χ, so $\forall (x,y)$

$$\begin{vmatrix} A(I,J) & A(I,y) \\ A(x,J) & A(x,y) \end{vmatrix} = 0 = \Big|A(I,J)\Big| \left(A(x,y) - A(x,J)A(I,J)^{-1}A(I,y)\right)$$

$$A(\mathbb{I},\mathbb{J}) = A(\mathbb{I},J)A(I,J)^{-1}A(I,\mathbb{J})$$

$$\mathbb{I} = \{1,2,\ldots,M\}$$
$$\mathbb{J} = \{1,2,\ldots,N\}$$

- Generalization to ϵ-rank …

How to choose pivots ? MaxVol principle

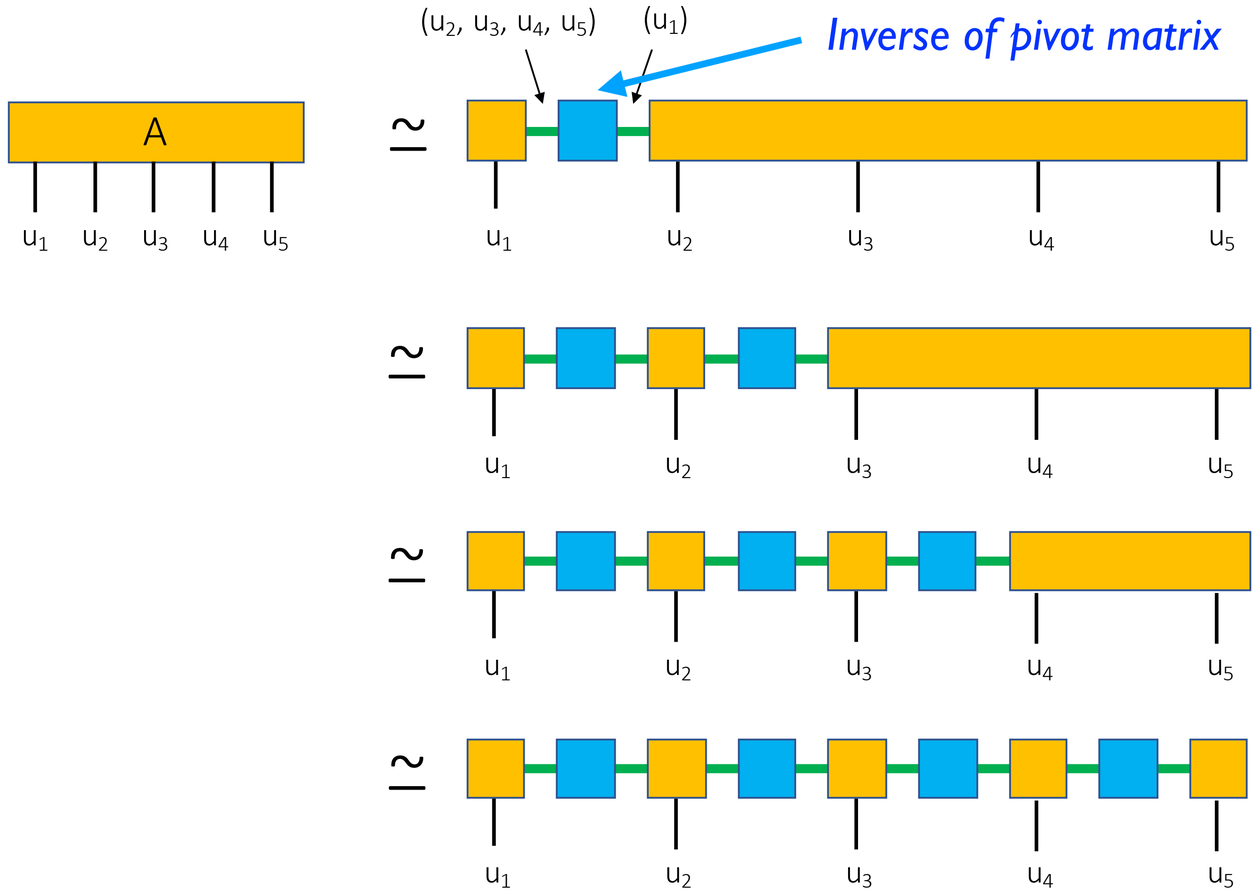
- We have partial $I' \subset I, J' \subset J$ and we want to choose new pivots x, y
  - Maximize the determinant of the pivot matrix [*MaxVol*]
  - Equivalent to maximize the error of the Cross Interpolation

$$\chi' < \chi \qquad I' = \{i_1, i_2, \ldots, i_{\chi'}\} \qquad J' = \{j_1, j_2, \ldots, j_{\chi'}\}$$

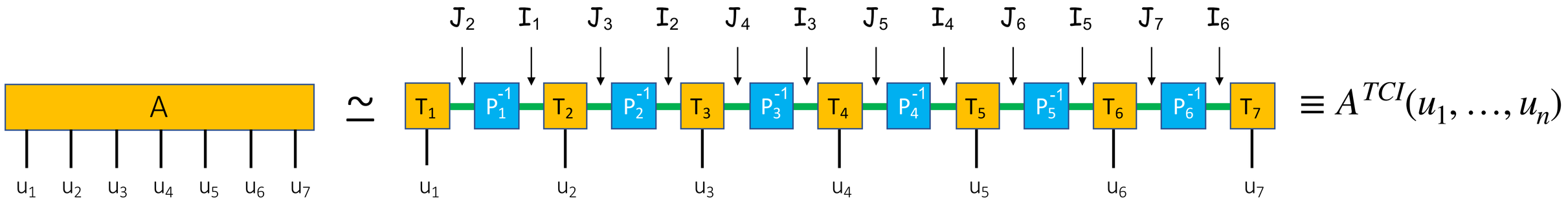
$$\begin{vmatrix} A(I', J') & A(I', y) \\ A(x, J') & A(x, y) \end{vmatrix} = \left|A(I', J')\right| \left(A(x, y) - A(x, J')A(I', J')^{-1}A(I', y)\right)$$

TCI: a naive approach

- $n-$dimensional tensor $A(u_1, u_2, \ldots, u_n)$ [u_i are discrete or continuous indices]
- Naive approach: repeated application of the matrix case (grouping indices)



TCI formula : notations

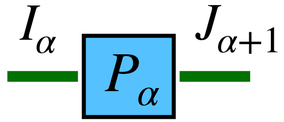


$\equiv A^{TCI}(u_1, \ldots, u_n)$

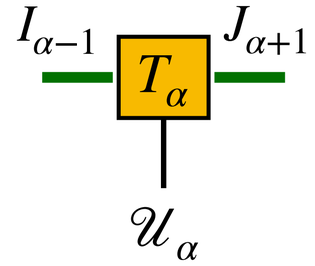
Notations

- Multi-indices $(1 \leq \alpha \leq n)$
  $i = (u_1, u_2, \ldots, u_\alpha)$ and $j = (u_\alpha, u_{\alpha+1}, \ldots, u_n)$
- Pivots (set of multi-indices)
  $I_\alpha = \{i_1, i_2, \ldots, i_\chi\}$ and $J_\alpha = \{j_1, j_2, \ldots, j_\chi\}$
- $\mathcal{U}_\alpha \equiv \{(u_\alpha)\}$ (set of all d values of index u_α)
- Concatenation
  $(u_1, u_2, \ldots, u_{\alpha-1}) \oplus (u_\alpha, \ldots, u_n) \equiv (u_1, \ldots, u_n)$
  $I \oplus J \equiv \{i \oplus j \,|\, i \in I, j \in J\}$

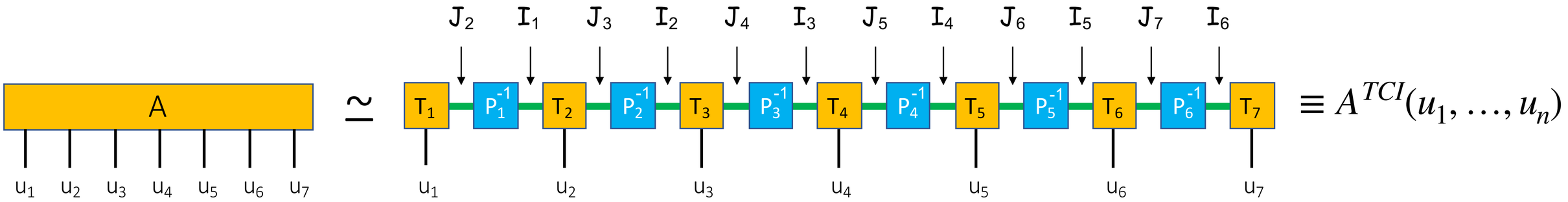
- T, P are subarrays of A
- *Pivots matrices*
  $P_\alpha \equiv A(I_\alpha \oplus J_{\alpha+1})$



- *1d slices*
  $T_\alpha \equiv A(I_{\alpha-1} \oplus \mathcal{U}_\alpha \oplus J_{\alpha+1})$



TCI : nesting property



- Pivot nesting property.

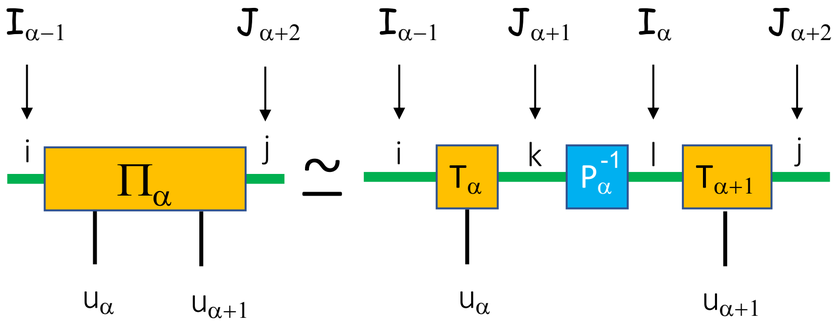
$$I_\alpha \subset I_{\alpha-1} \oplus \mathcal{U}_\alpha$$
$$J_\alpha \subset \mathcal{U}_\alpha \oplus J_{\alpha+1}$$

- Implies that A^{TCI} is an interpolation.
  It is exact on the 1d slice, i.e $T_\alpha \equiv A(I_{\alpha-1} \oplus \mathcal{U}_\alpha \oplus J_{\alpha+1}) = A^{TCI}(I_{\alpha-1} \oplus \mathcal{U}_\alpha \oplus J_{\alpha+1})$

TCI : 2d slices

- Definition : $\Pi_\alpha \equiv A(I_{\alpha-1} \oplus \mathcal{U}_\alpha \oplus \mathcal{U}_{\alpha+1} \oplus J_{\alpha+2})\,.$
- Approximated in TCI by

$$\Pi_\alpha(i, u_\alpha, u_{\alpha+1}, j) \approx \Pi_\alpha^{TCI}(i, u_\alpha, u_{\alpha+1}, j) \equiv \sum_{kl} T_\alpha(i, u_\alpha, k) P_\alpha^{-1}(k, l) T_{\alpha+1}(l, u_{\alpha+1}, j)$$



- Error

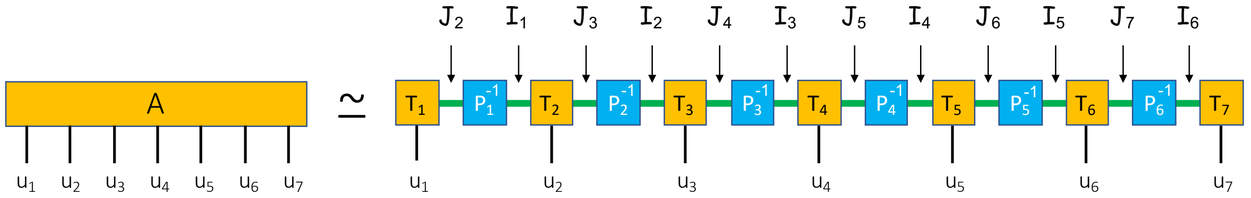
$$\epsilon_\Pi(i, u_\alpha, u_{\alpha+1}, j) \equiv \left|\Pi_\alpha - \Pi_\alpha^{TCI}\right|(i, u_\alpha, u_{\alpha+1}, j) \quad \text{for } i \in I_{\alpha-1}, j \in J_{\alpha+2}$$

$$= |A - A^{TCI}|\,(i, u_\alpha, u_{\alpha+1}, j) \quad \text{(from the nesting condition)}$$

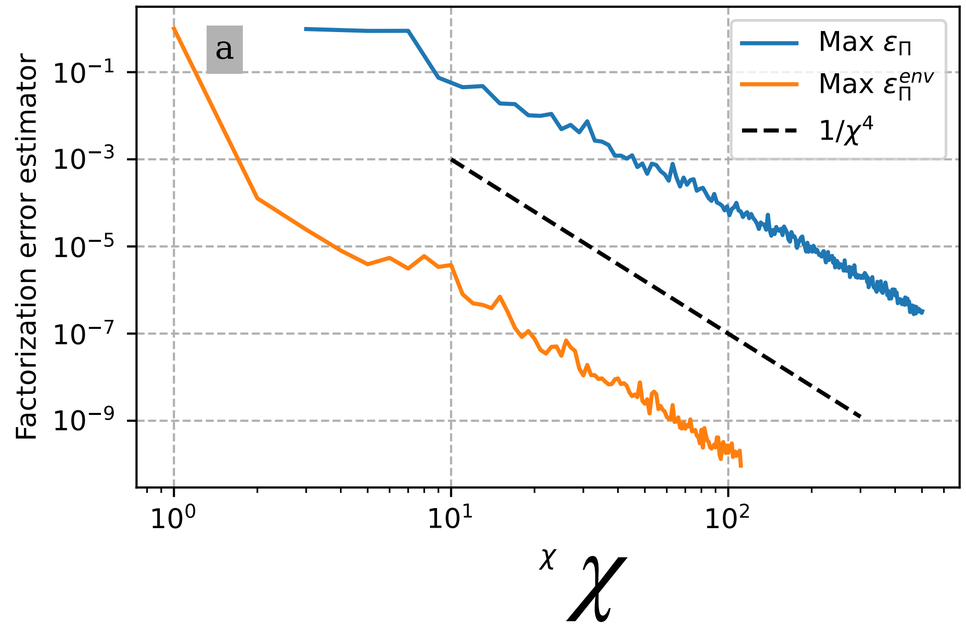
TCI : algorithm in a nutshell

- Add new pivots to reduce the interpolation error <u>on 2d slices</u>

$$\epsilon(\chi) = \max_{\alpha} \max_{\substack{i \in I_{\alpha-1} \\ j \in J_{\alpha+2} \\ u_\alpha, u_{\alpha+1}}} |A - A^{TCI}|(i, u_\alpha, u_{\alpha+1}, j)$$



$\epsilon(\chi)$

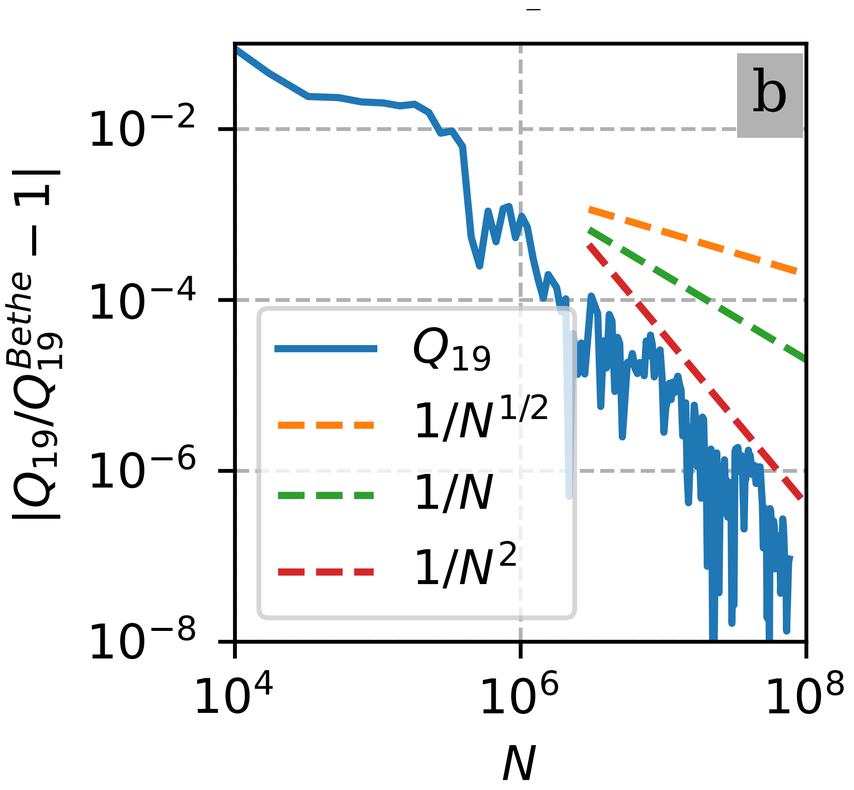


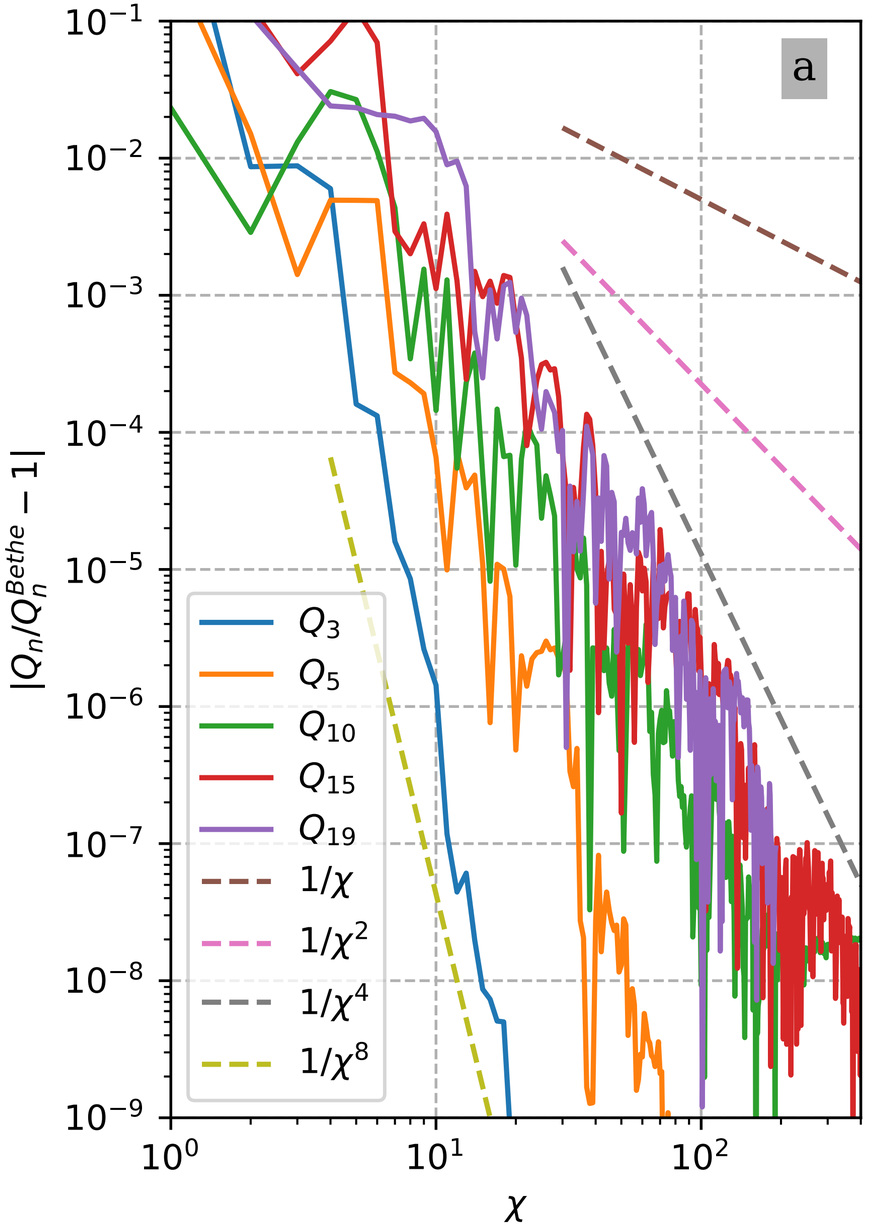
χ

Quantum dot
Benchmarks in equilibrium

Tensor Train Diagrammatics

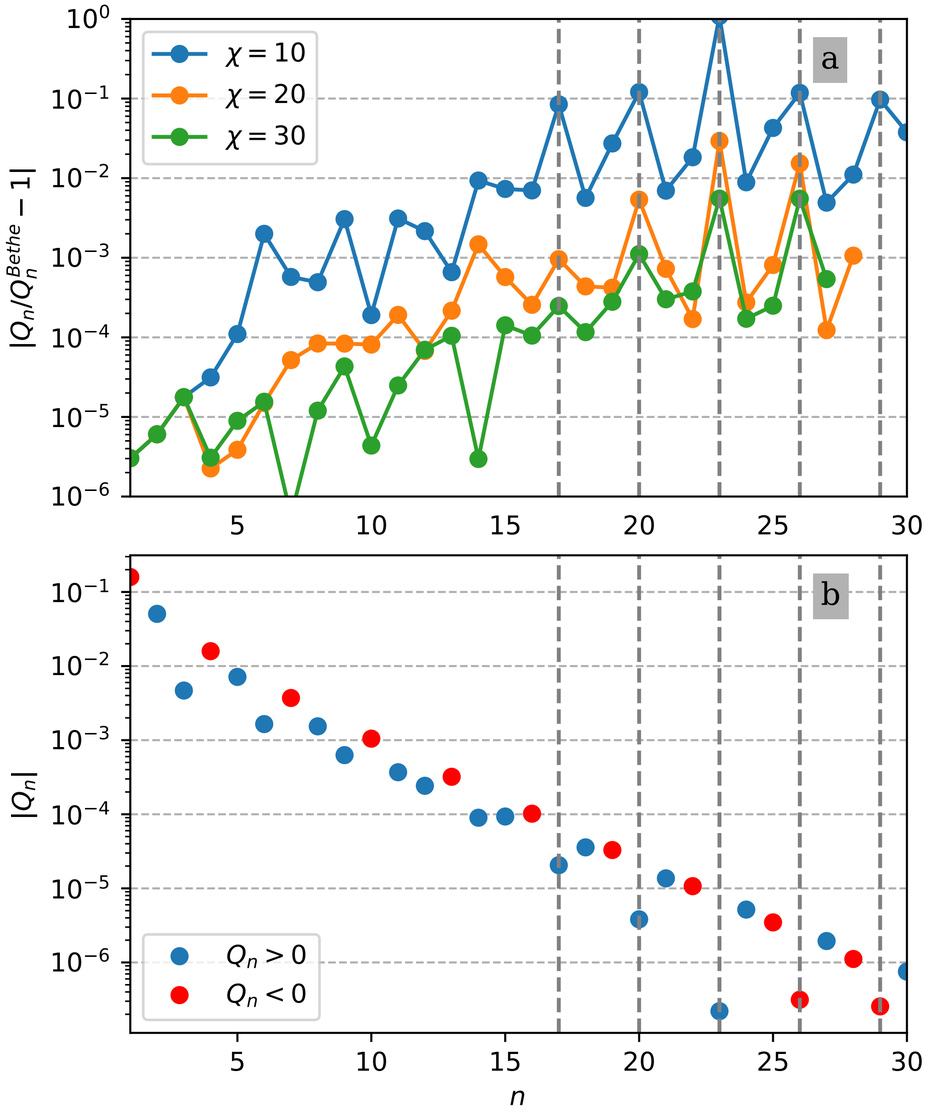
- Factorize q_n with TCI and integrate
- High precision (9 digits) benchmark vs Bethe Ansatz.
- N (number of evaluations of q_n) : $N \sim nd\chi^2$
- Error $\sim 1/N^2$





Bond dimension χ does not grow with dimension n

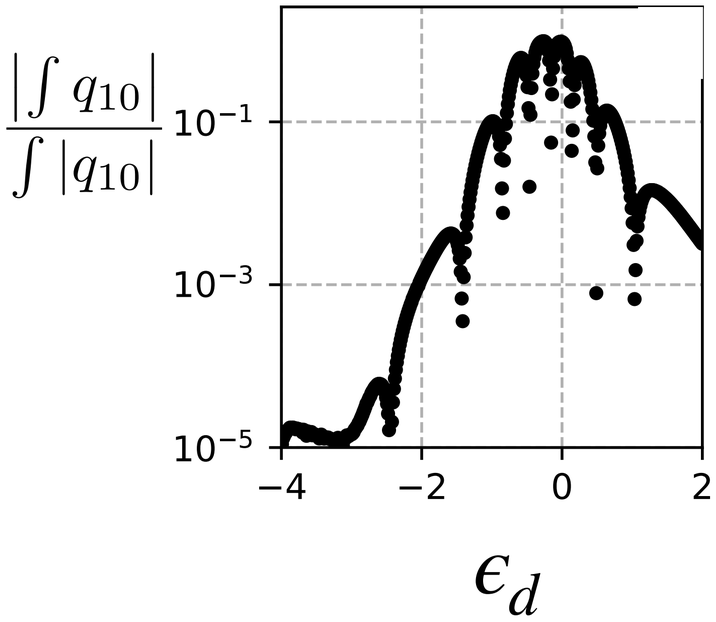
- Compute Q_n up to n = 30



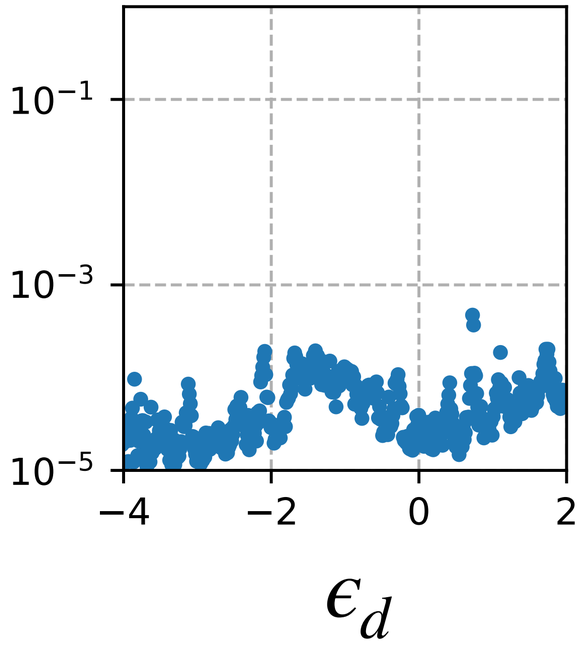
Factorize the sign problem

- The factorization is insensitive to the average sign of the function.
- Reduced to a 1d oscillating integral.
- Example: vary dot energy level ϵ_d (induces oscillating terms $e^{i\epsilon_d t}$)

Average sign of the Q_{10} integral



Factorization error of q_{10} for fixed bond dimension χ



Conclusion

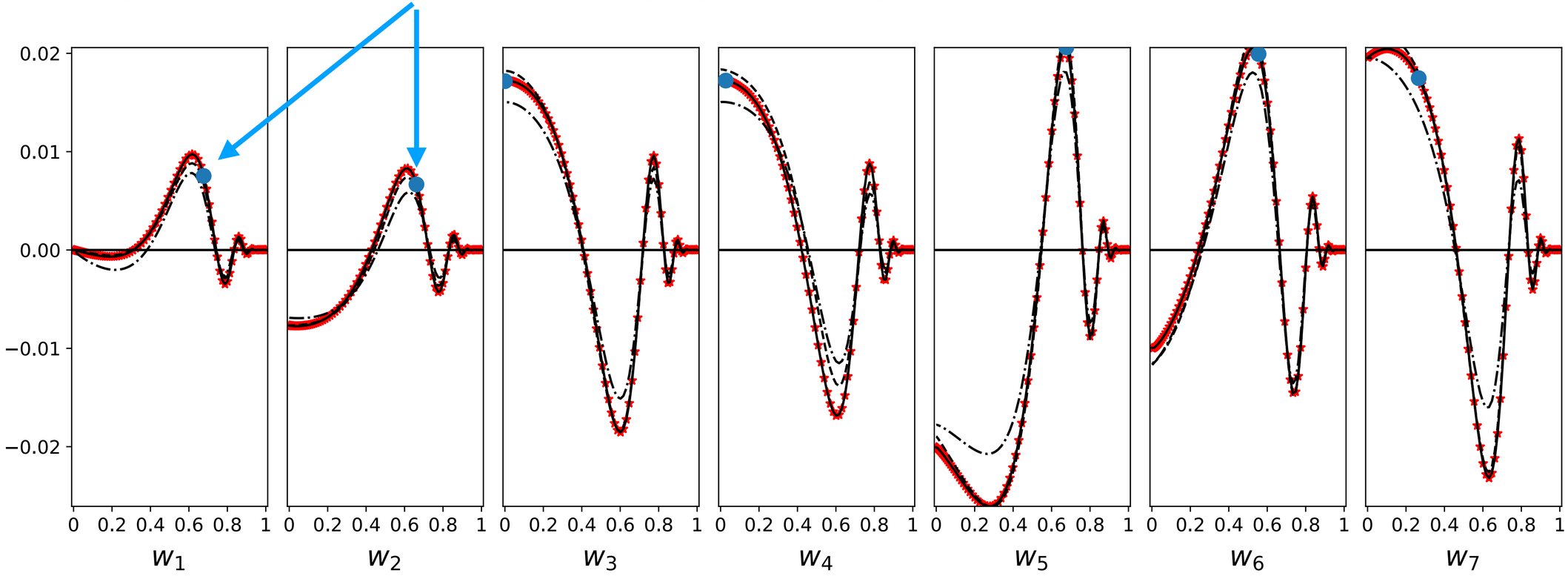
- Tensor Cross Interpolation to integrate in high dimension
- Based on a parsimonious MPS representation of correlation functions.
- Superior to Monte-Carlo (no sign problem, even with very oscillatory functions).

- Research directions:
  - Revisit other QMC algorithms
  - Generalize TCI to other tensor networks beyond MPS.

Thank you for your attention!

Check : out of sample error

- Find the point of maximum discrepancy by searching in various directions



★ $q_7(w_1, \ldots, w_n)$

—●— $\chi = 2$

- - - - - $\chi = 4$

——— $\chi = 40$

$\epsilon_d = -2$

$w_i \equiv \dfrac{2v_i}{1 + v_i}$