Modeling and Simulating Scientific Problems

Fast Summation Algorithms and Tensor Networks Methods

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Outline

A Fast Spectral Sum-of-Gaussians Method for Coulomb Interaction

Joint work with Qi Zhou, Jiuyang Liang, Zhenli Xu, and Shidong Jiang

arXiv:2412.04595

1min

Quasi-2D charged systems

Quasi-2D systems (Mazars, 2011) are at the macroscopic scale in xy, but microscopic in z, so that are always modeled as doubly periodic in simulations.

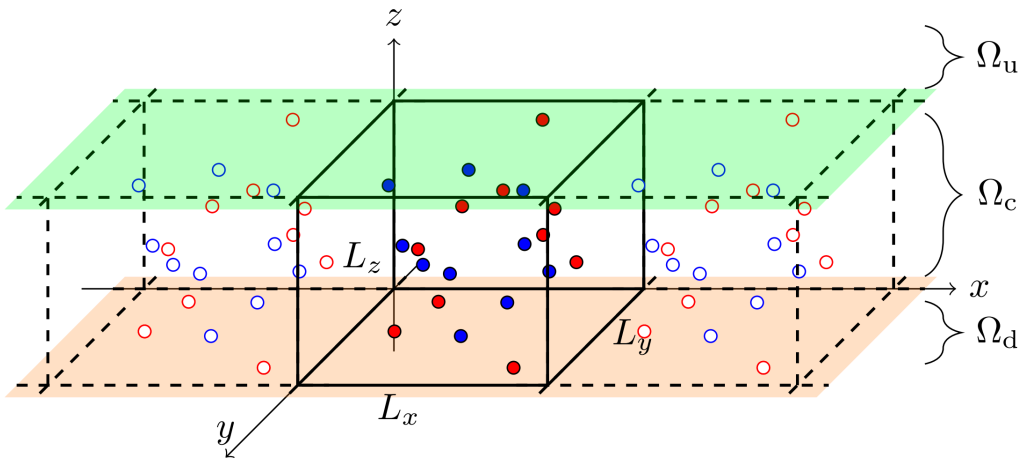


Figure 1: Illustration of a quasi-2D charged system.

Coulomb interaction plays a key role in nature, leading to effect such as ion transportation and self-assembly (Barros & Luijten, 2014).

However, the Coulomb interaction decays as r^{-1} in 3D, so that it is long ranged and singular at $r = 0$, which make such simulation computationally expensive.

2min

Algorithms for Q2D charged systems

Methods have been developed to accelerate the Coulomb interaction in Q2D systems.

The very first method is the Ewald2D (Parry, 1975) method based on the Ewald splitting of the Coulomb kernel. It is accurate but with $O(N^2)$ complexity.

To reduce the complexity, most methods rely on the following three strategies:

- **Fourier spectral method** (Lindbo & Tornberg, 2011; 2012; Maxian et al., 2021; Nestler et al., 2015; Shamshirgar et al., 2021; Shamshirgar & Tornberg, 2017): based on Ewald splitting and fast Fourier transform (FFT), with $O(N \log N)$ complexity.
- **Fast multipole methods** (Greengard & Rokhlin, 1987; Liang et al., 2020; 2022; Pei et al., 2023; Yan & Shelley, 2018): accelerated by hierarchical low-rank compression, adaptive and with $O(N)$ complexity.
- **Random batch Ewald** (Gan et al., 2024a; 2024b; Jin et al., 2021): based on Ewald splitting and random batch sampling, stochastic and with $O(N)$ complexity.

3min

Algorithms for Q2D charged systems

For doubly periodic systems, one major challenge is the large prefactor in $O(N)$ or $O(N \log N)$ compared to 3D-PBC solvers (Mazars, 2011), especially when the system is strongly confined in the z direction, i.e., $L_z \ll L_x, L_y$.

- For the FFT based methods, huge zero-padding in z is required (Maxian et al., 2021).
- For the FMM based methods, more near field contributions is included (Yan & Shelley, 2018).

The recently developed methods including

- Anisotropic truncation kernel method (Greengard et al., 2018)
- Periodic FMM (Pei et al., 2023)
- Dual-space multilevel kernel-splitting method (Jiang & Greengard, 2024)

offer potential solutions to this challenge, but these methods have not yet been extended to handle quasi-2D systems.

4min

The sum-of-Gaussians approximation

In our work, we use a sum-of-Gaussians (SOG) approximation (Beylkin & Monzón, 2010) of the Coulomb kernel, where

$$\frac{1}{r} \approx \frac{2\log b}{\sqrt{2\pi\sigma^2}} \sum_{l=-\infty}^{\infty} \frac{1}{b^l} e^{-\frac{r^2}{\left(\sqrt{2}b^l\sigma\right)^2}}, \text{ with } \mathcal{E}_r < 2\sqrt{2}e^{-\frac{\pi^2}{2\log b}}$$

Based on that, the u-series decomposition (Predescu et al., 2020) splits the potential into three parts:

$$\frac{1}{r} \approx \underbrace{\left(\frac{1}{r} - \sum_{l=0}^{M} w_l e^{-\frac{r^2}{s_l^2}}\right) \mathbb{1}_{r<r_c}}_{\text{near-field}} + \underbrace{\sum_{l=0}^{m} w_l e^{-\frac{r^2}{s_l^2}}}_{\text{mid-range}} + \underbrace{\sum_{l=m+1}^{M} w_l e^{-\frac{r^2}{s_l^2}}}_{\text{long-range}}$$

The weight of the narrowest Gaussian is modified to be

$$w_0 = \omega \frac{2\log b}{\sqrt{2\pi\sigma^2}}$$

to enforce the C^0 and C^1 continuity of the near-field potential at $r = r_c$, which is important for MD simulations (Shamshirgar et al., 2019).

5min

Splitting the far-field potential

Selecting m so that $s_m < \eta L_z < s_{m+1}$, where η is $O(1)$ constant.

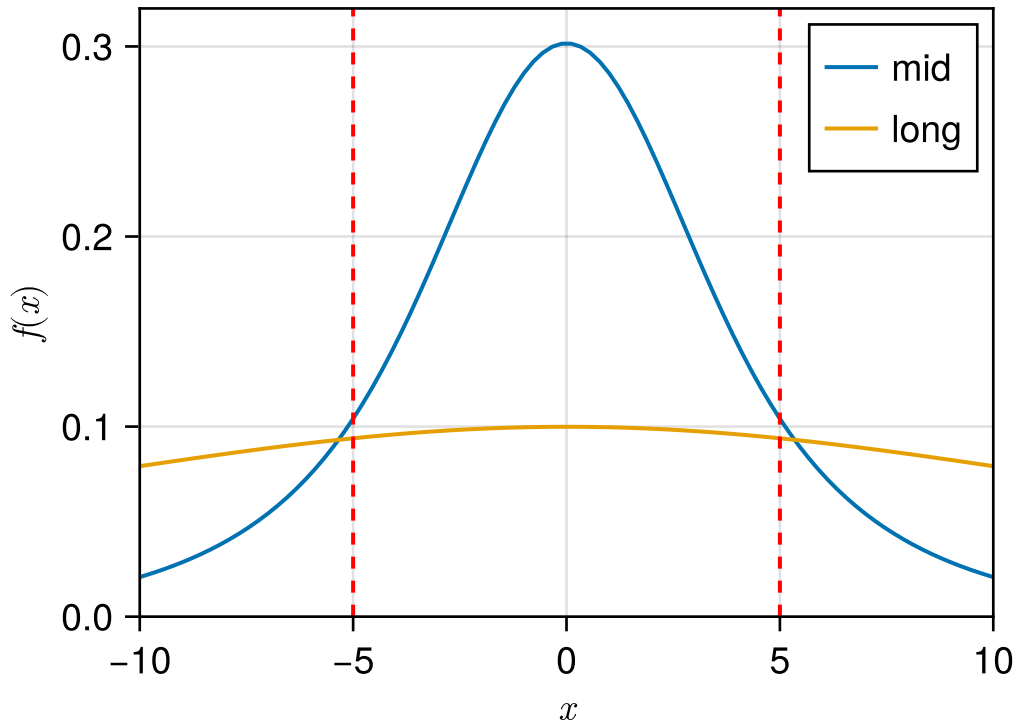


Figure 2: Mid-range part and long-range part of the potential, $L_z = 10$, $\eta \approx 0.6$.

6min

Mid-range potential

The mid-range potential is computed by a standard Fourier spectral solver[1] (type-1 and type-2 NUFFT in 3D (Barnett et al., 2019)) with little zero padding.

$$\Phi^l_{\text{mid}}(\vec{r}) = \sum_{\vec{n}} \sum_{j=1}^{N} q_j w_l e^{-\frac{\left(\vec{r}-\vec{r}_j+\vec{n}\circ\vec{L}\right)^2}{s_l^2}}, \quad s_l < \eta L_z$$

- The smoothness and separability of the Gaussian removes the need of the kernel truncation in the free direction.
- No upsampling is needed since the Fourier transform of the Gaussian decays quickly and it compensates the loss of accuracy in calculating the Fourier transform of the data.

[1] https://github.com/HPMolSim/ChebParticleMesh.jl

7min

Long-range potential

The long-range potential is computed by a Fourier-Chebyshev solver.

$$\Phi^l_{\text{long}}(\vec{r}) = \sum_{\vec{n}} \sum_{j=1}^{N} q_j w_l e^{-\frac{\left(\vec{r}-\vec{r}_j+\vec{n}\circ\vec{L}\right)^2}{s_l^2}}, \quad s_l > \eta L_z$$

The extremely smooth long-range Gaussians are interpolated on the Chebyshev proxy points in z, similar to that of the periodic FMM (Pei et al., 2023), and only $O(1)$ number of Chebyshev points are required.

Then 2D NUFFT can be used to evaluate the potential on a tensor-product grid.

In cubic systems, $L_x \sim L_y \sim L_z$, $O(1)$ Fourier modes in xy and $O(1)$ Chebyshev points in z, no need for NUFFT.

8min

Complexity

Using DFT for long-range potential, the complexity is

$$O(\underbrace{4\pi r_c^3 \rho_r N}_{\text{near-field}} + \underbrace{\mathcal{P}_x \mathcal{P}_y \mathcal{P}_z N + \frac{\lambda_z\left(1+\frac{\delta}{L_z}\right)}{r_c^3 \rho_r} N \log N}_{\text{mid-range by 3D-NUFFT}} + \underbrace{\frac{P L_x L_y}{\eta^2 L_z^2} N}_{\text{long-range by DFT}})$$

where $\mathcal{P}_x, \mathcal{P}_y, \mathcal{P}_z$ are the window supports, λ_z is the padding ratio, δ is the extended length of the box in the free direction to accommodate the support of the window function, P is the number of Chebyshev points. By taking $r_c \sim O(1)$ and assume $L_z \sim O\left(\sqrt{L_x L_y}\right)$, the complexity is $O(N \log N)$.

Using 2D-NUFFT for long-range potential, the complexity is

$$O(\underbrace{4\pi r_c^3 \rho_r N}_{\text{near-field}} + \underbrace{\mathcal{P}_x \mathcal{P}_y \mathcal{P}_z N + \frac{\lambda_z\left(1+\frac{\delta}{L_z}\right)}{r_c^3 \rho_r} N \log N}_{\text{mid-range by 3D-NUFFT}} + \underbrace{\mathcal{P}_x \mathcal{P}_y P N + \frac{P L_x L_y}{s_{m+1}^2} N \log N}_{\text{long-range by 2D-NUFFT}})$$

which is needed when $L_z \ll L_x, L_y$, the total complexity is also $O(N \log N)$.

10min

The method[1] is benchmarked on the following systems:

- Cubic systems with fixed aspect ratio and volume density.
- Strongly confined systems with fixed L_z and surface density.

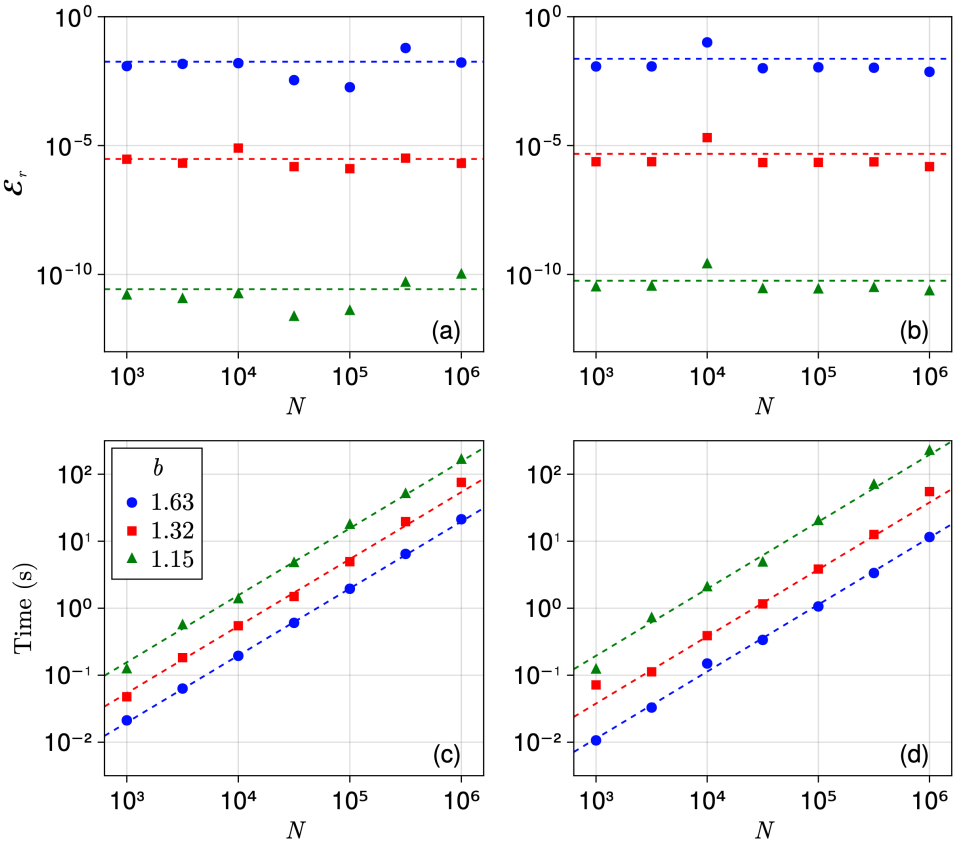


Figure 3: Error and time cost for the SOG method in the (a,c) cubic and (b,d) strongly confined systems.

[1] https://github.com/HPMolSim/FastSpecSoG.jl

Summary

11min

A fast and accurate solver for Q2D charged systems is developed based on the sum-of-Gaussian approximation of the Coulomb kernel and kernel splitting, which can be regarded as a 2-level DMK method (Jiang & Greengard, 2024).

It has the following advantages:

- spectrally accurate with rigorous error analysis
- need little/no zero-padding for systems that are confined in a rectangular box of high aspect ratio
- does not require any upsampling in the gridding step
- all calculations are carried out in the fundamental cell itself
- easy to be implemented and parallelized for large-scale MD simulations

Currently, the major shortcoming of this method is its non-adaptive nature, and has a complexity of $O(N \log N)$ rather than $O(N)$.

Automated Discovery of the Optimal Branching Rules

Joint work with Yi-Jia Wang, Pan Zhang, and Jin-Guo Liu

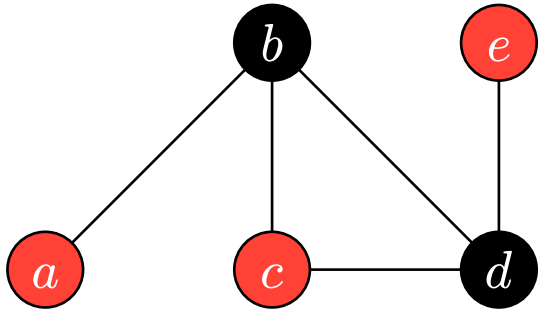
arXiv:2412.07685

12min

The maximum independent set problem

One of the first batch of 21 NP-hard problems proved by (Karp, 1972).

An independent set is a set of vertices in a graph, no two of which are adjacent.



$G = (V, E)$, MIS = $\{a, c, e\}$, size $\alpha(G) = 3$

MIS problem has an exponential large solution space and no polynomial-time algorithm is known to solve it exactly.

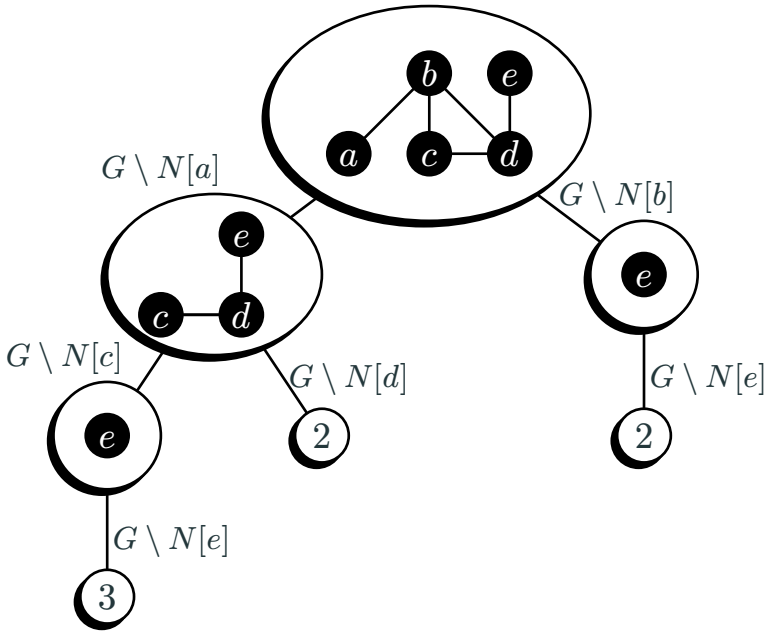
The branching algorithms (Fomin & Kaski, 2013) is the most widely used method to solve this problem.

14min

Branching algorithm

Branching algorithm rely on predesigned rules to search the solution space in a tree-like structure.

Complexity of a branching algorithm is always described as $O(\gamma^n)$ where γ is the branching factor and n is the size of the problem.

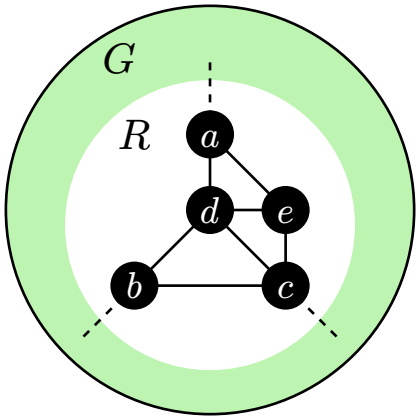


Year	Running times	References	Notes
1977	$O^*(1.2600^n)$	(Tarjan & Trojanowski, 1977)	
1986	$O^*(1.2346^n)$	(Jian, 1986)	
1986	$O^*(1.2109^n)$	(Robson, 1986)	
1999	$O^*(1.0823^m)$	(Beigel, 1999)	num of edges
2001	$O^*(1.1893^n)$	(Robson, 2001)	
2003	$O^*(1.1254^n)$ for 3-MIS	(Chen et al., 2003)	
2005	$O^*(1.1034^n)$ for 3-MIS	(Xiao et al., 2005)	
2006	$O^*(1.2210^n)$	(Fomin et al., 2006)	
2006	$O^*(1.1225^n)$ for 3-MIS	(Fomin & Høie, 2006)	
2006	$O^*(1.1120^n)$ for 3-MIS	(Fürer, 2006)	
2006	$O^*(1.1034^n)$ for 3-MIS	(Razgon, 2006)	
2008	$O^*(1.0977^n)$ for 3-MIS	(Bourgeois et al., 2008)	
2009	$O^*(1.0919^n)$ for 3-MIS	(Xiao, 2009)	
2009	$O^*(1.2132^n)$	(Kneis et al., 2009)	
2013	$O^*(1.0836^n)$ for 3-MIS	(Xiao & Nagamochi, 2013)	SOTA
2016	$O^*(1.2210^n)$	(Akiba & Iwata, 2016)	PACE winner
2017	$O^*(1.1996^n)$	(Xiao & Nagamochi, 2017)	SOTA

16min

Tensor networks for the MIS problem

Tensor networks can be used to extract the local information of the sub-graph (Gao et al., 2024a; Liu et al., 2023).



Contract the local tensor network

Boundary configuration: s_{abc}	Possible assignments: s_{abcde}
000	00010, 00001
100	10000
010	01001
001	00100
110	11000
101	10100

However, a pure tensor network method does not work well for non-geometric graphs. Its complexity on 3-regular graphs is about $O(1.1224^n)$, far from the SOTA ($O^*(1.0836^n)$).

17min

What is the difference?

Tensor network approach

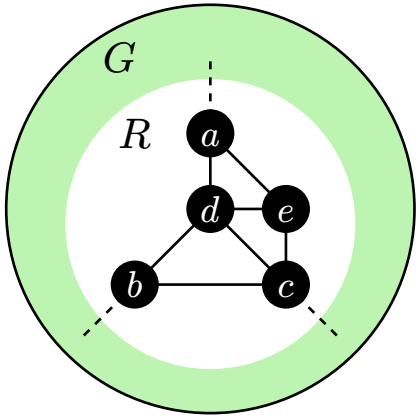
1. Contract the local tensor network for the sub-graph and pick the non-zero elements.
2. For all possible boundaries, fix all the variables and continue the contraction

$$\gamma^n = 6 \times \gamma^{n-5} \to \gamma \approx 1.4310$$

Branching algorithm

1. Search for structures in the sub-graph.
2. Find d and e are connected and $N[e] \subset N[d]$, satisfying the domination rule, fix $d = 0$, i.e., not in the MIS

$$\gamma = 1.0$$



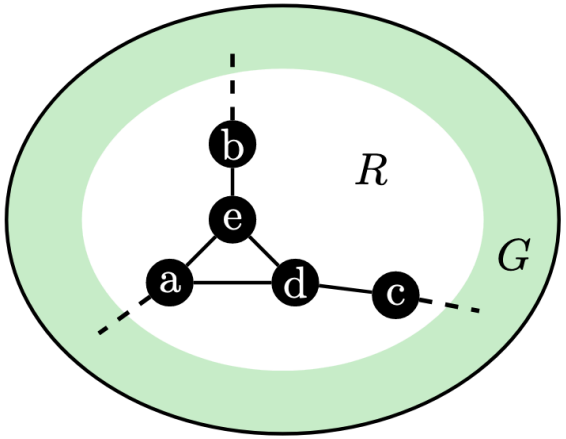
Boundary configuration: s_{abc}	Possible assignments: s_{abcde}
000	00010, 00001
100	10000
010	01001
001	00100
110	11000
101	10100

Key point: No need to use all results, find the *correct pattern*!

18min

The optimal branching algorithm

We use the tensor network to extract the local information, and then automatically search the optimal branching rules[1] (Gao et al., 2024b).



s_{abcde}	clauses in $\mathcal{D}$
$S_{000} = \{00001, 00010\}$	$\neg a \wedge \neg b \wedge \neg d \wedge e$
$S_{001} = \{00101\}$	
$S_{010} = \{01010\}$	$\neg a \wedge b \wedge \neg c \wedge d \wedge \neg e$
$S_{111} = \{11100\}$	$a \wedge b \wedge c \wedge \neg d \wedge \neg e$

Naive branching

4 branches, each fix 5 variables

$\gamma^n = 4 \times \gamma^{n-5}$

$\gamma \approx 1.3195$

Optimal branching

3 branches, fix [4, 5, 5] variables

$\gamma^n = \gamma^{n-4} + 2 \times \gamma^{n-5}$

$\gamma \approx 1.2671$

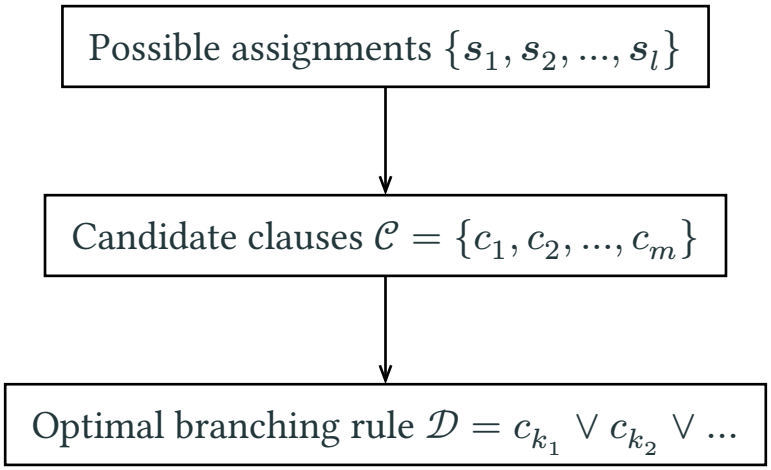
Question: How to solve the rules from the assignments?

[1] https://github.com/OptimalBranching/OptimalBranching.jl

19min

Finding the optimal branching rule

The process of finding the optimal branching rules is as the following:



The candidate clauses are the combinations of the possible assignments, for example, a combination of the 3rd and 4th assignments is given by:

$$\text{combine}(\neg a \wedge b \wedge \neg c \wedge d \wedge \neg e, a \wedge b \wedge c \wedge \neg d \wedge \neg e) = b \wedge \neg e$$

we say $b \wedge \neg e$ covers $\{3, 4\}$. The clauses are generated iteratively.

20min

Set covering via mixed integer programming

Then we solve a set covering problem by formulating it as a mixed integer programming problem, which can be solved by MIP solvers (Achterberg, 2009).

$$\min_{\gamma, \boldsymbol{x}} \gamma \quad \text{s.t.} \sum_{i=1}^{m} \gamma^{-\Delta\rho(c_i)} x_i = 1,$$

$$\bigcup_{\substack{i=1,\ldots,m \\ x_i=1}} J_i = \{1, 2, \ldots, n\}, \qquad \rightarrow \text{valid branching rule}$$

$$x_i \in \{0, 1\} \qquad \rightarrow \text{a clause is selected or not}$$

where $\rho(c_i)$ is the size reduced by the clause c_i of the problem.

The chosen clauses form the optimal branching rule:

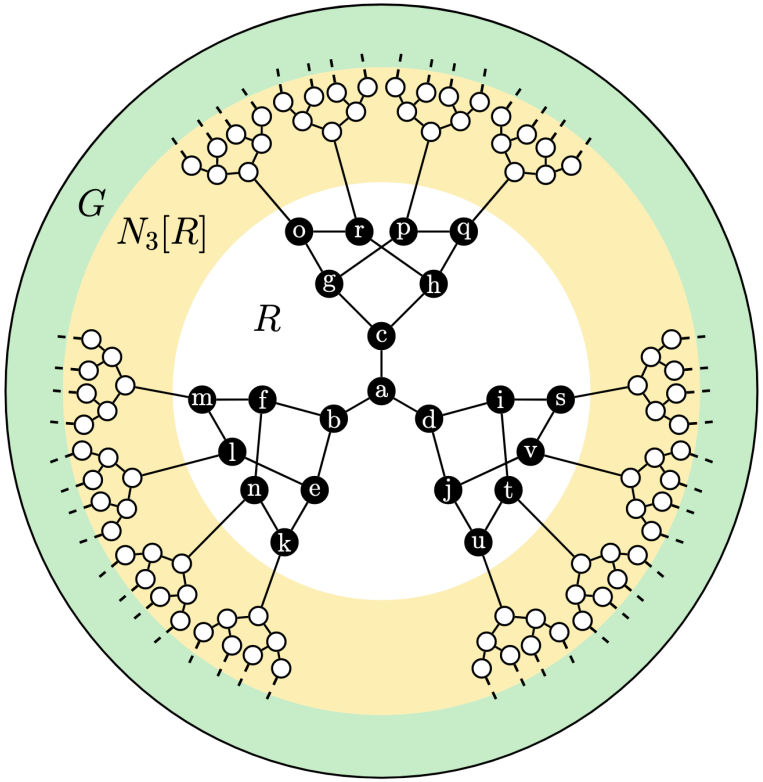
$$\mathcal{D} = c_{k_1} \vee c_{k_2} \vee \ldots \vee c_{k_m}$$

with the minimum γ among all the possible branching rules.

21min

A bottleneck case

A bottle neck case has been reported in Xiao's work (Xiao & Nagamochi, 2013), with a branching factor of 1.0836.

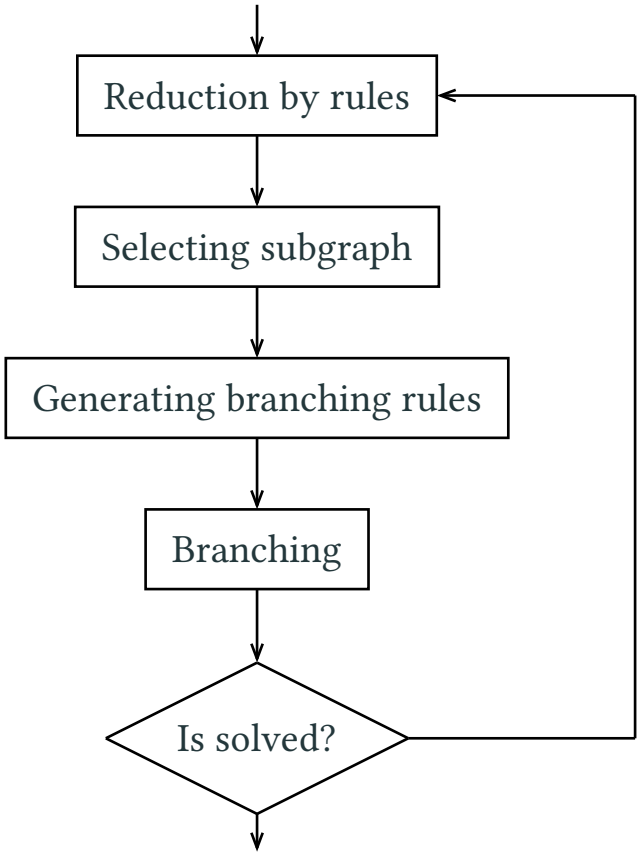


- 71 possible assignments, 15782 candidate clauses.
- 4 branches, size reduced by branches: $[10, 16, 26, 26]$, with $\gamma = 1.0817 < 1.0836$

22min

Benchmarks on random graphs

On-the-fly branching algorithm:



	ob	ob+ xiao	xiao2013	akiba2015	akiba2015+ xiao&packing
3-regular graphs	1.0457	1.0441	1.0487	-	-
Erdos-Renyi graphs	1.0011	1.0002	-	1.0044	1.0001
King's sub-graphs	1.0116	1.0022	-	1.0313	1.0019
Grid graphs	1.0012	1.0009	-	1.0294	1.0007

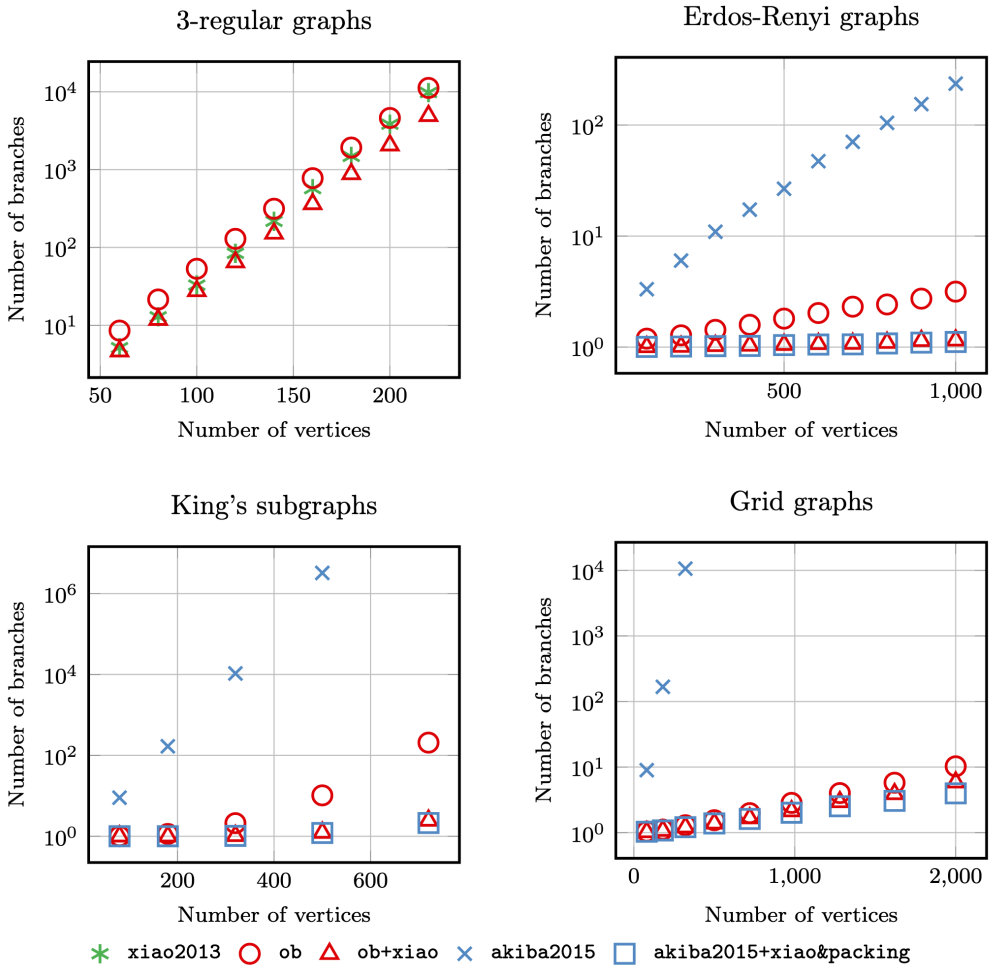
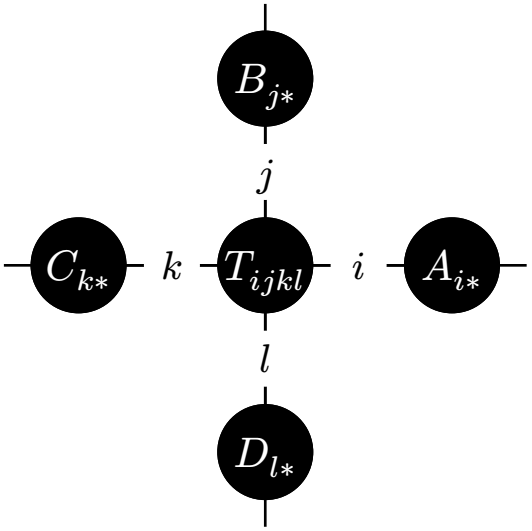


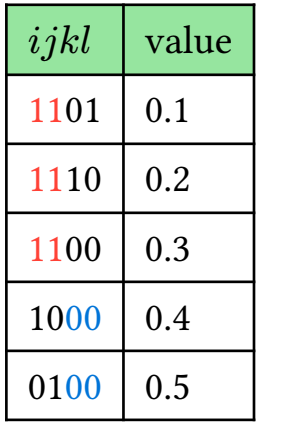
Figure 4: Average number of branches generated by different branching algorithms on 1000 random graphs.

24min

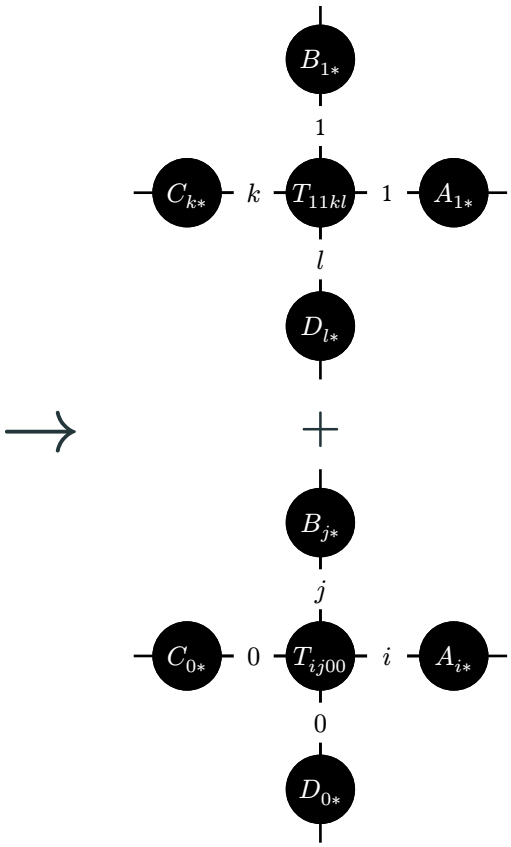
Sparse Tensor Networks Contraction via Optimal Branching

The optimal branching algorithm can be applied to contract the sparse tensor networks.





$ijkl$	value
1101	0.1
1110	0.2
1100	0.3
1000	0.4
0100	0.5



Such sparsity is common in many problems, including probabilistic inference, combinatorial optimization, and quantum circuit simulations (Markov & Shi, 2008).

Summary

25min

A new method to automatically discover the optimal branching rules is proposed, by combining the tensor network method and the branching algorithm.

With this method, we achieved an average complexity of $O(1.0441^n)$ on random 3-regular graphs, which outperforms the SOTA ($O(1.0487^n)$).

Advantages:

- generate the branching rules automatically without human effort
- fully utlize the information of the sub-graph
- the sub-graph can be selected flexibly
- can be applied to different problems, not only the MIS problem

Disadvantages:

- solving the rule can be computationally expensive
- cannot capture the rules need graph rewriting

Conclusion and Outlook

Software packages

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Fast Summation Algorithms

- **EwaldSummations.jl**: Various Ewald summation methods with parallelization.
- **ChebParticleMesh.jl**: Toolkits for smooth particle mesh (type-1 and type-2 NUFFT).
- **FastSpecSoG.jl**: Implementation of the fast spectral SOG method.

Tensor Network Algorithms

- **TreeWidthSolver.jl**: Solving the treewidth problem (supported by GSoC 2024).
- **CuTropicalGEMM.jl**: Custom GPU kernel for tropical matrix multiplication (supported by OSPP 2023).
- **OMEinsumContractionOrders.jl**: Optimizing the tensor network contraction order.
- **OptimalBranching.jl**: Implementation of the optimal branching algorithm.

Future Research Plans

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Fast Summation Algorithms

- efficient methods based on the DMK framework (Jiang & Greengard, 2024)

Tensor Network Algorithms

- branching based sparse tensor network contraction
- more flexible quantum many-body ansatz

Acknowledgements

30min

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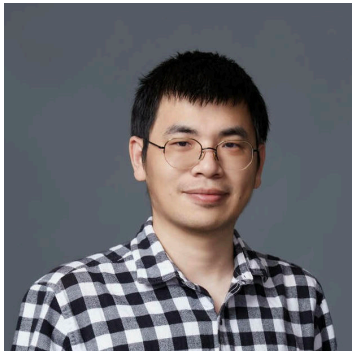

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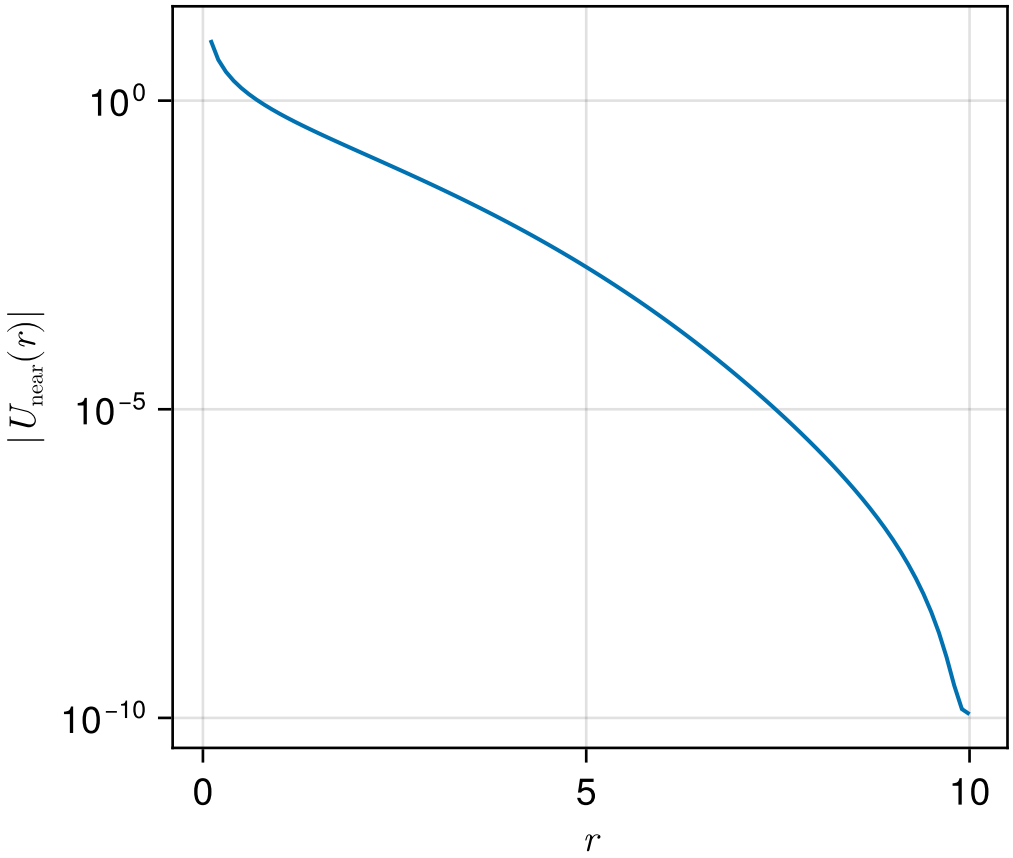
Thank you for your attention!

Appendix

The U-series and its derivative



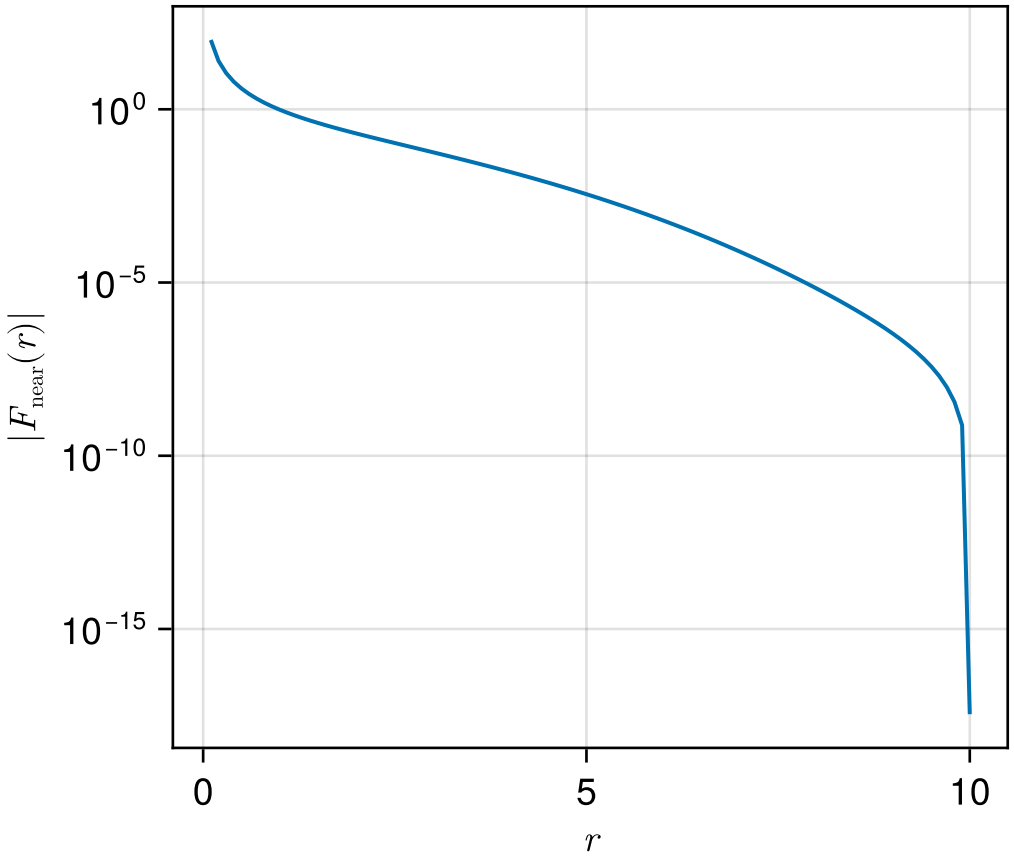


Figure 5: The U-series and its derivative, $r_c = 10.0$.

b	r_0	ω	Energy		Force	
			Error	M	Error	M
2	1.9892536839080267	0.9944464927622323	3.12×10^{-2}	16	9.93×10^{-3}	11
1.62976708826776469	2.7520026668023417	1.0078069793438068	2.33×10^{-3}	31	6.21×10^{-4}	16
1.48783512395703226	3.7554672283554990	0.9919117057598183	2.29×10^{-4}	46	7.98×10^{-5}	26
1.32070036405934420	4.3914554711638349	1.0018891411481198	1.18×10^{-6}	76	5.76×10^{-7}	41
1.21812525709410644	5.6355288151271085	1.0009014615603334	7.14×10^{-10}	166	5.14×10^{-10}	71
1.14878150173321925	7.2956245490719404	1.0000368348358225	1.30×10^{-15}	271	1.98×10^{-14}	116

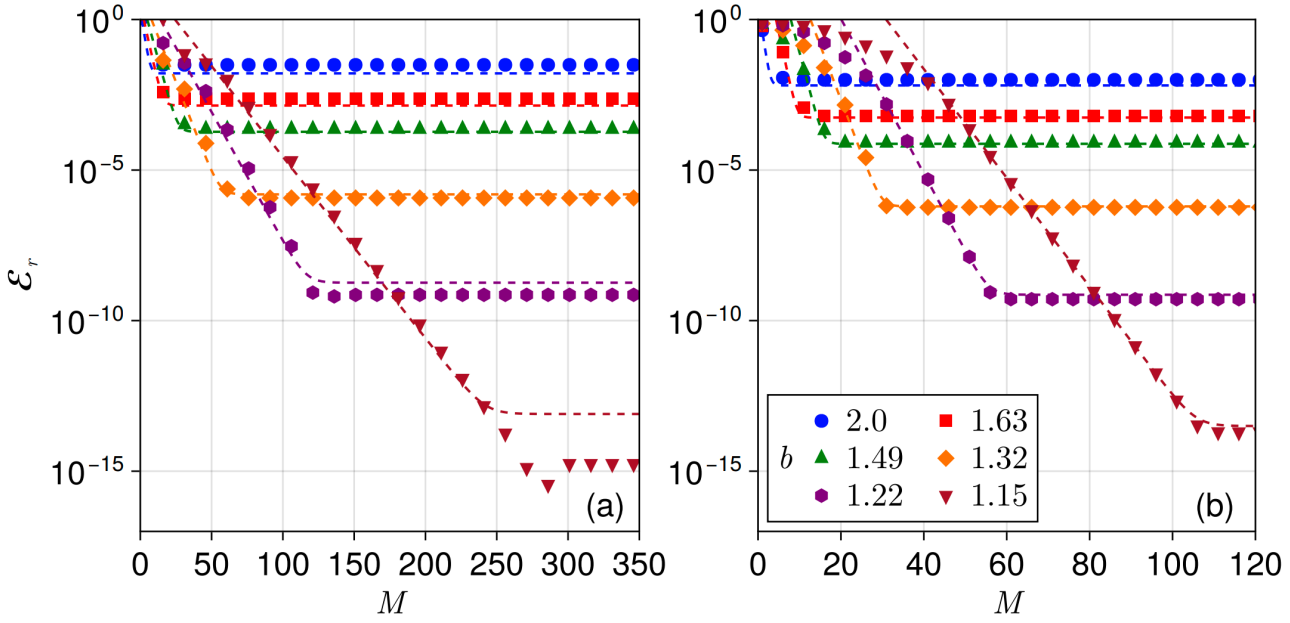


Figure 6: U-series parameters and the error

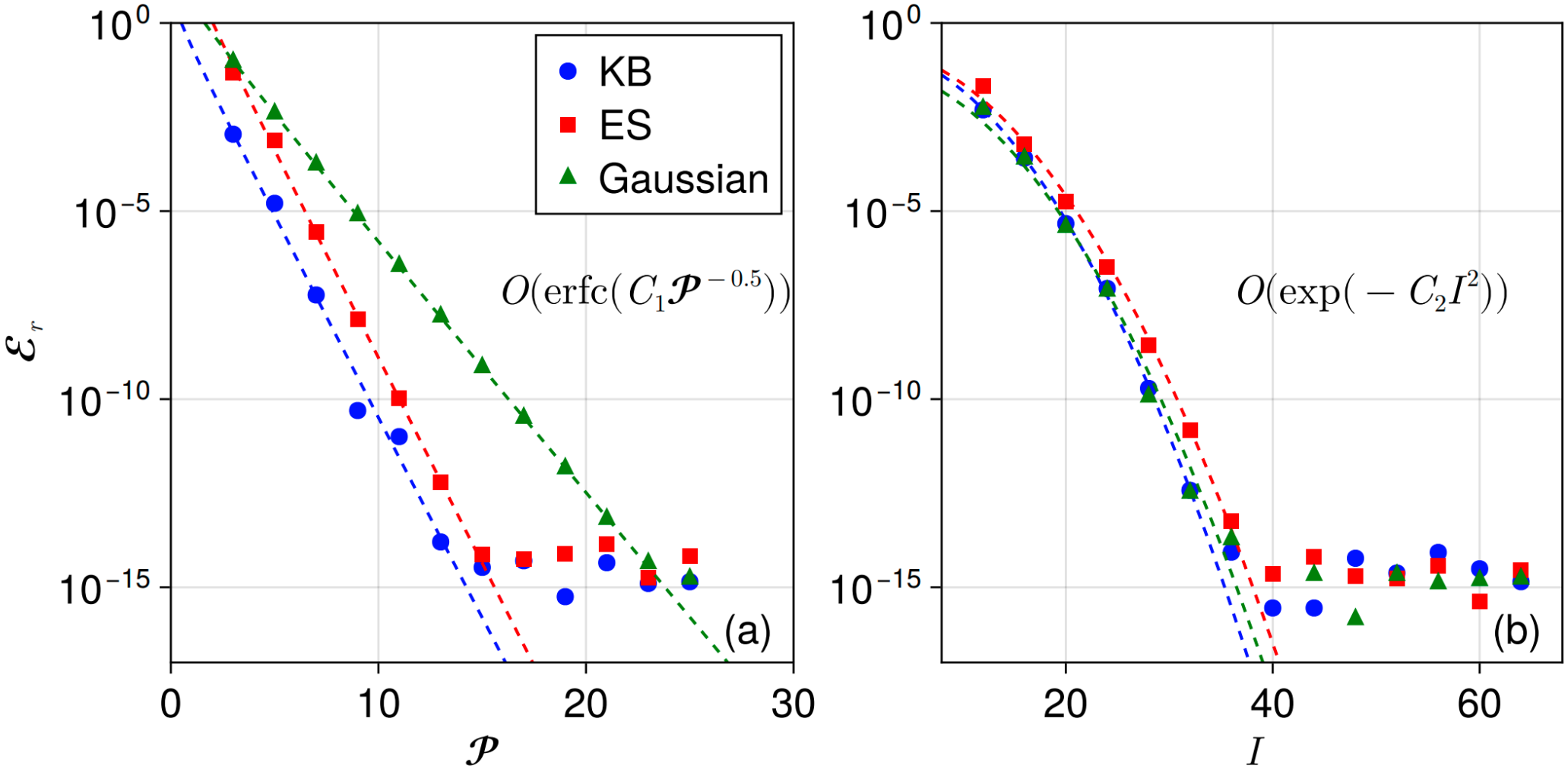


Figure 7: Different window functions.

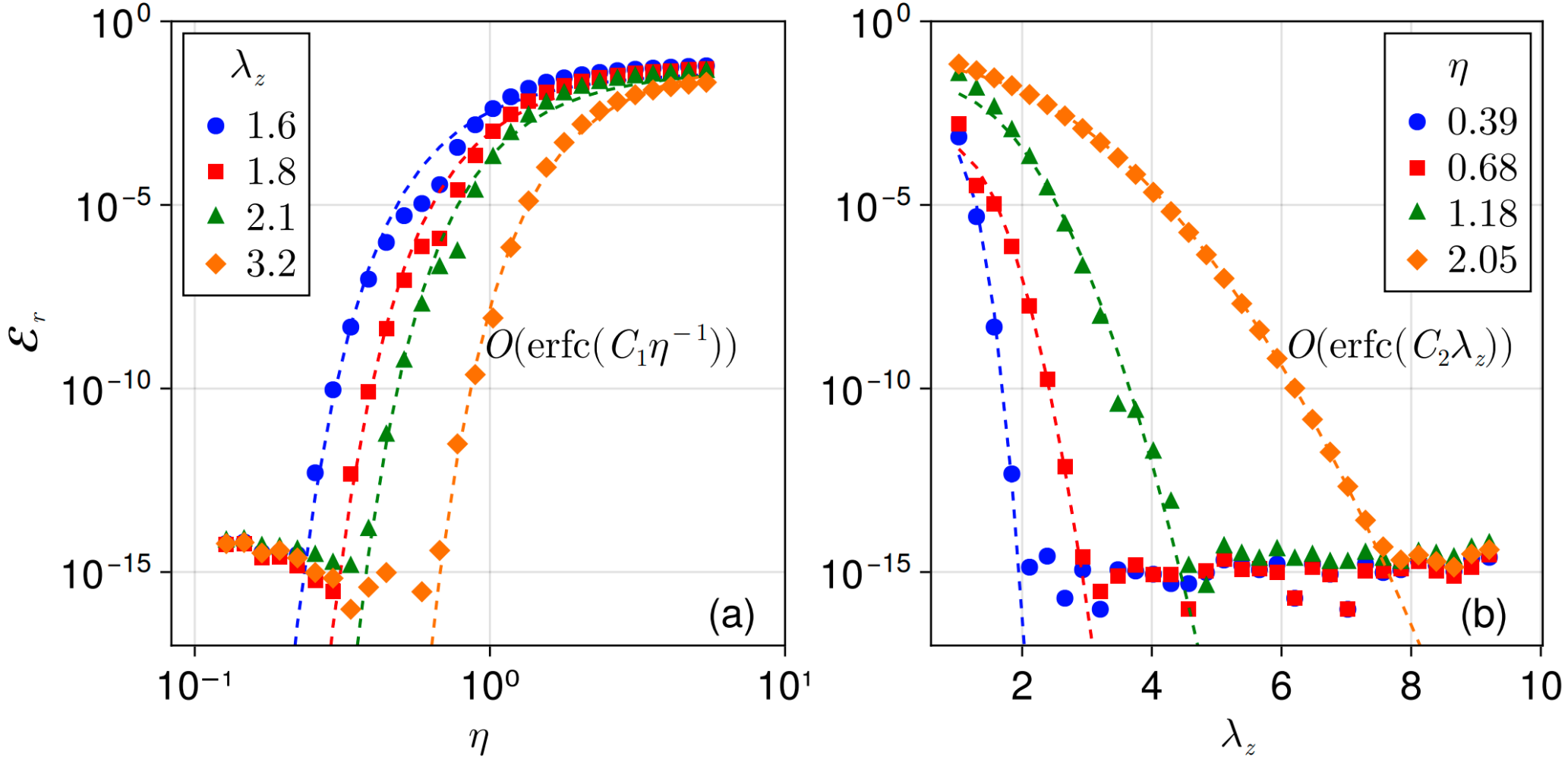


Figure 8: Zero-padding.

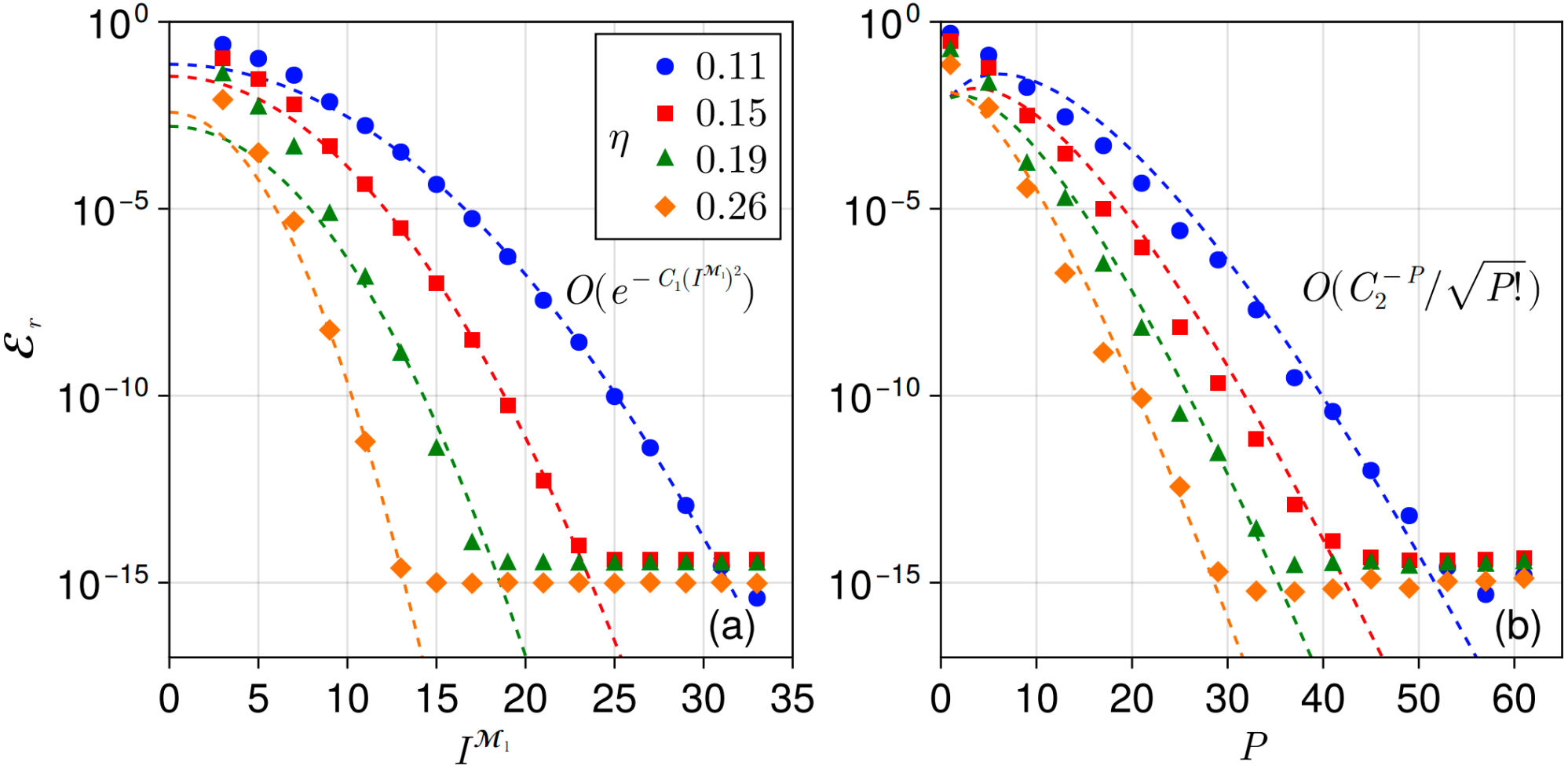


Figure 9: Accuracy of the Fourier-Chebyshev solver.

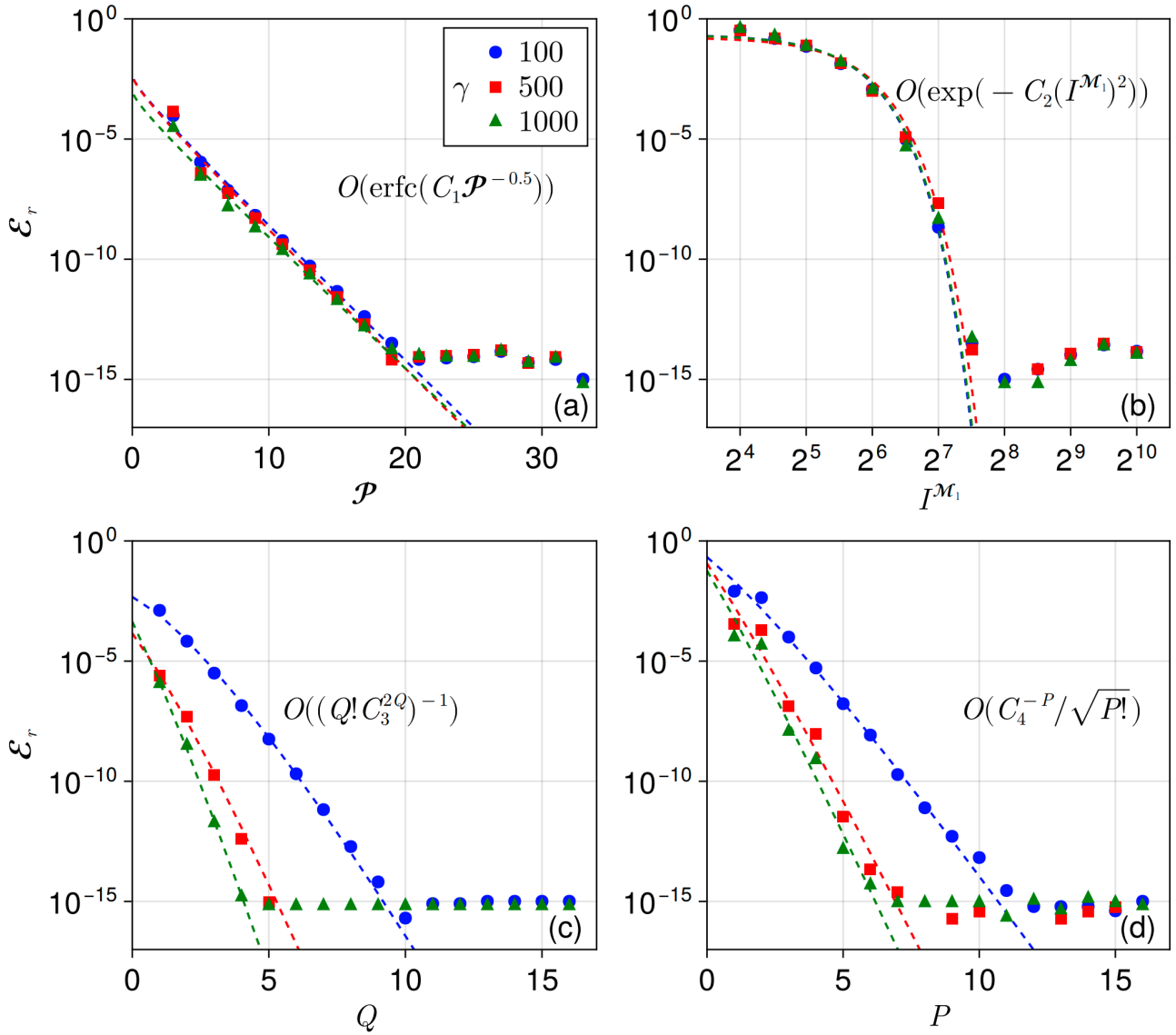


Figure 10: Strongly confined systems.

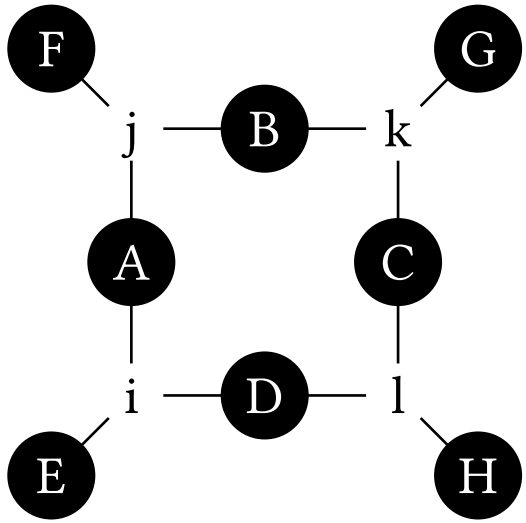
Einsum notation

Tensor networks can be represented as the so called Einsum notation:

$$Y_{i_y \ldots} = \sum_{i \notin \{i_y \ldots\}} A_{i_a \ldots} B_{i_b \ldots} C_{i_c \ldots} \ldots$$

It also has a hyper-graph representation, where each node is a tensor and each edge is an index:

$$s = \sum_{i,j,k,l} A_{ij} B_{jk} C_{kl} D_{li} E_i F_j G_k H_l \quad \longrightarrow$$



A contraction order can be represented as a rooted (binary) tree:

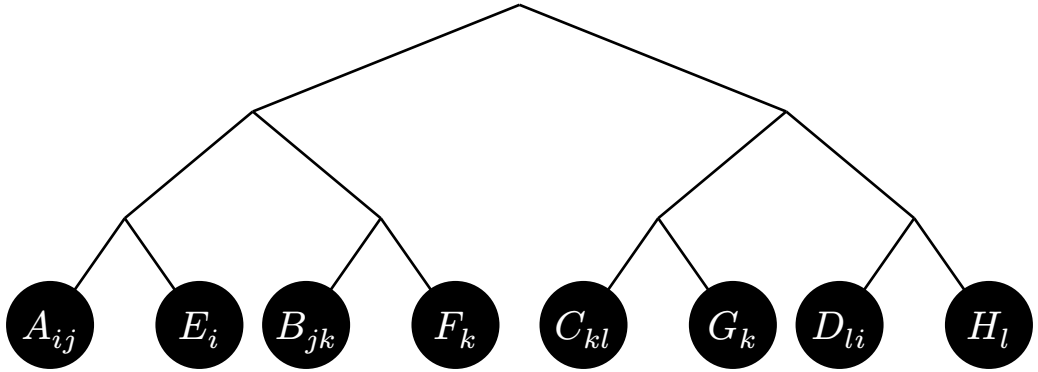


Figure 11: An example of binary contraction tree.

Different contraction orders can lead to different complexities, the order with the minimum complexity is called the optimal contraction order.

Optimizing the contraction order

Finding the optimal contraction order is a NP-hard[1] problem!

In the past few years, tools have been developed to optimize the contraction order:

- OMEinsumContractionOrder.jl[2] in Julia
- Cotengra[3] in Python

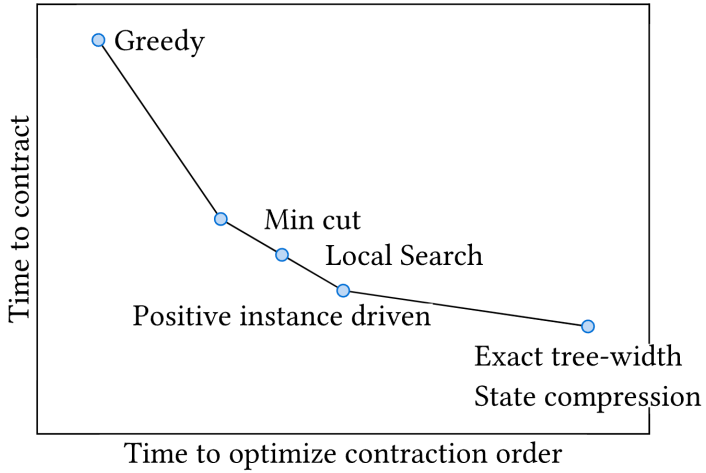


Figure 12: Comparison of different contraction orders.

[1] I.L. Markov, Y. Shi, SIAM J. Comput. 38, 963–981 (2008).

[2] https://github.com/TensorBFS/OMEinsumContractionOrder.jl

[3] https://github.com/jcmgray/cotengra

In tropical semiring, the multiplication and addition are defined as:

$$a \otimes b = a + b$$
$$a \oplus b = \max(a, b)$$

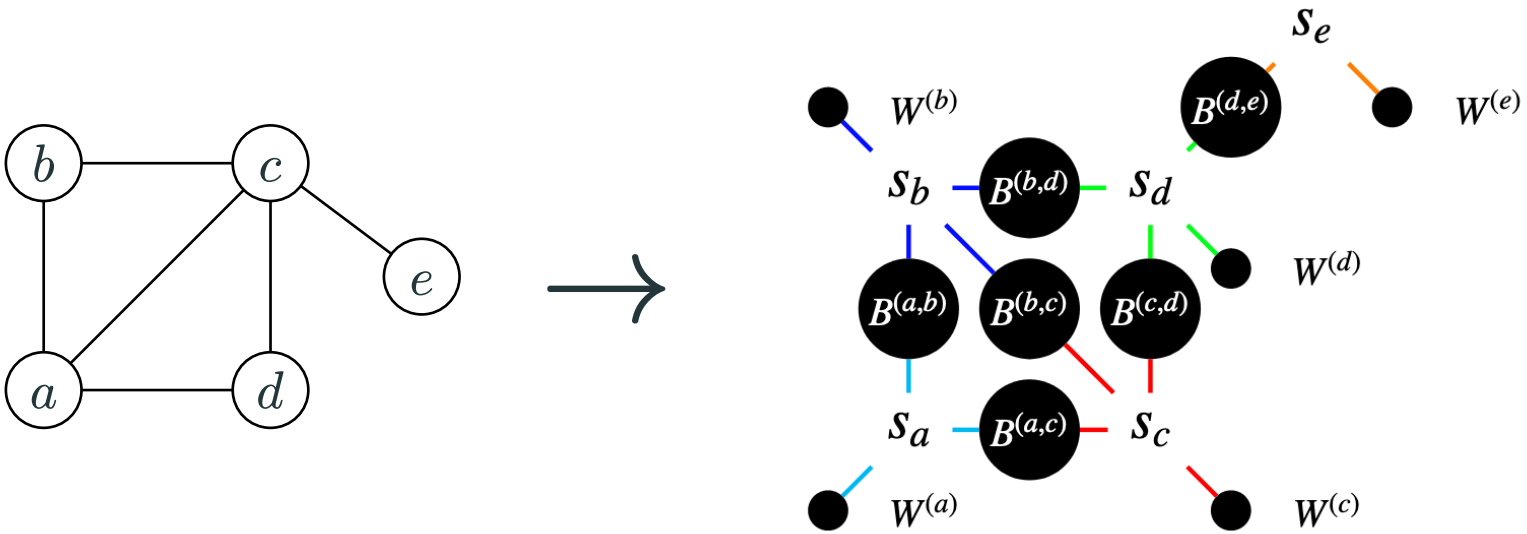
By replacing the matrix multiplication with the tropical matrix multiplication, we get the tropical TN, where the contraction results:

$$T_{i_y \ldots} = \max_{i \notin \{i_y \ldots\}} \left(A_{i_a \ldots} + B_{i_b \ldots} + C_{i_c \ldots} + \ldots \right)$$

which is the maximum of the sum of the elements among all the possible assignments.

Very useful in combinatorial optimization problems and ground state search.

A tropical TN can be used to solve the MIS problem, a simple example is shown below:



with

$$B = \begin{pmatrix} 0 & 0 \\ 0 & -\infty \end{pmatrix}, \text{ and } W = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

under a tropical semiring.

In the original set covering problem, the function to be optimized is not linear. We solve it iteratively.

Fixed the branching complexity γ, find a solution to x that satisfies

$$\min_x \sum_{i=1}^{|\mathcal{C}|} \gamma^{-\Delta\rho(c_i)} x_i, \text{ s.t. } \bigcup_{\substack{i=1,\dots,|\mathcal{D}|,\\ x_i=1}} J_i = \{1, 2, \dots, |\mathcal{S}_R|\}$$

It corresponds to the following WMSC problem:

$$\begin{cases} \text{Alphabet: } \{1, 2, \dots, |\mathcal{S}_R|\} \\ \text{Sets: } \left\{J_1, J_2, \dots, J_{|\mathcal{C}|}\right\} \\ \text{Weights: } i \mapsto \gamma^{-\Delta\rho(c_i)} \end{cases}$$

After each iteration, the branching complexity γ is updated, coverge in a few iterations.

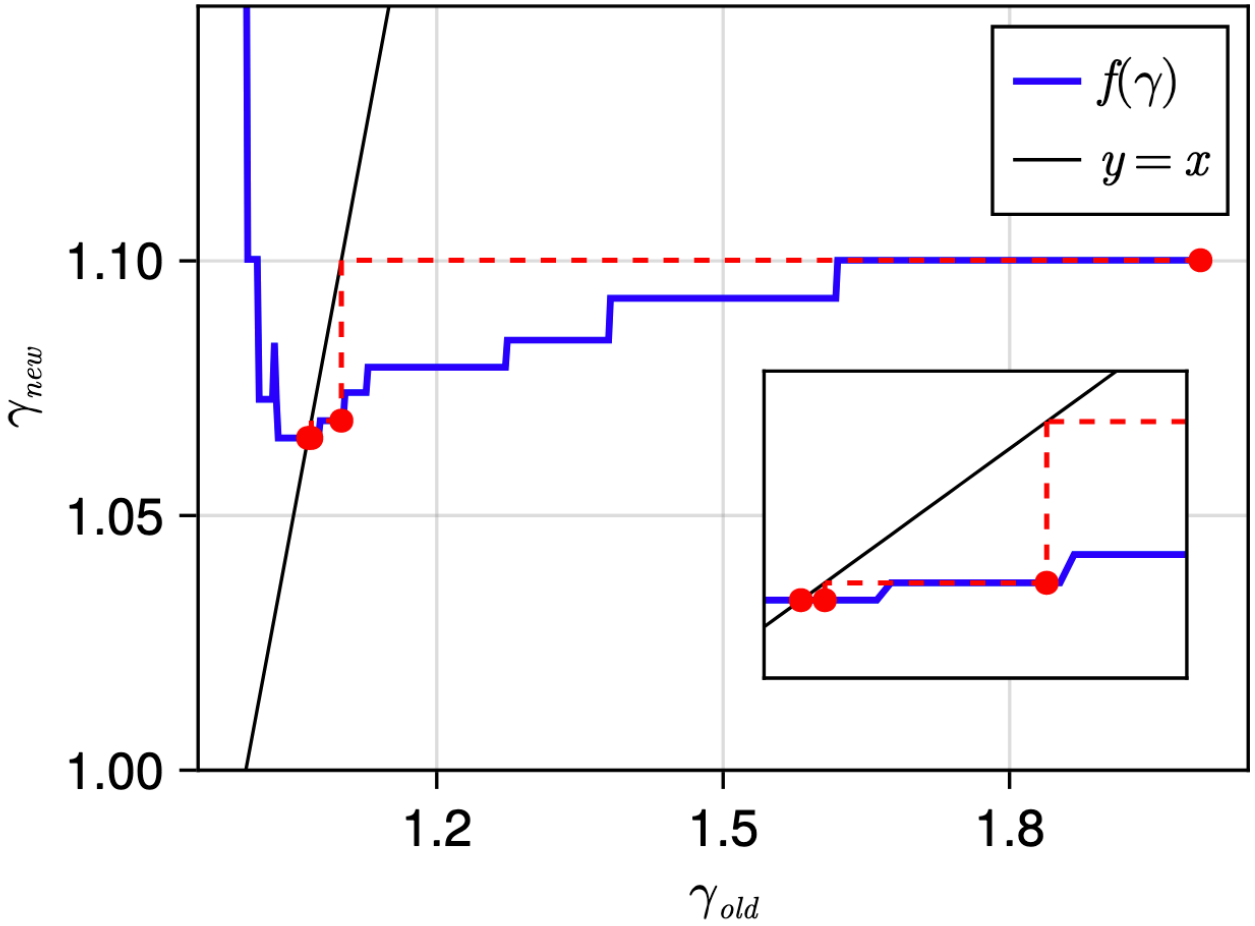


Figure 13: An example of solving the set covering problem via iterative MIP.

The branching algorithm used in benchmark

Branching / Reduction	Optimal Branching (this work)	Xiao 2013	Akiba 2015
d1/d2 reduction	ob	-	akiba2015
d1/d2 reduction Xiao's rules	ob+xiao	xiao2013	-
d1/d2 reduction Xiao's rules packing rule	-	-	akiba2015+xiao&packing

Benchmarks for the worst-case complexity

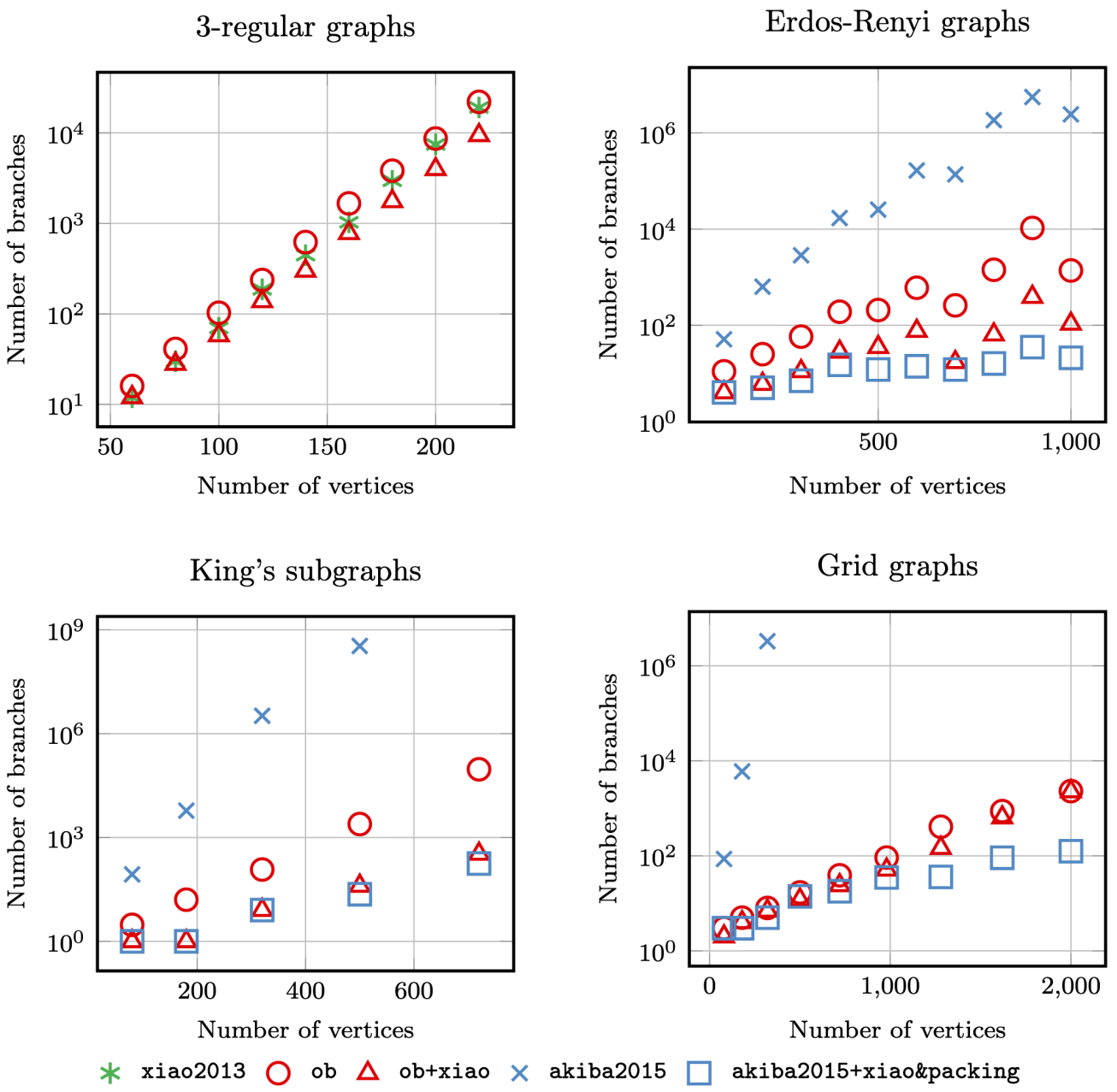


Figure 14: The worst-case complexity of the proposed method on random graphs.

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