

Modeling and Simulating Scientific Problems

Fast Summation Algorithms and Tensor Networks Methods

Xuanzhao Gao

2025-1-10

Hong Kong University of Science and Technology

| | |
|---|----|
| A Fast Spectral Sum-of-Gaussians Method for Coulomb Interaction | 2 |
| Automated Discovery of the Optimal Branching Rules | 13 |
| Summary and Outlook | 24 |

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

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

arXiv:2412.04595

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.

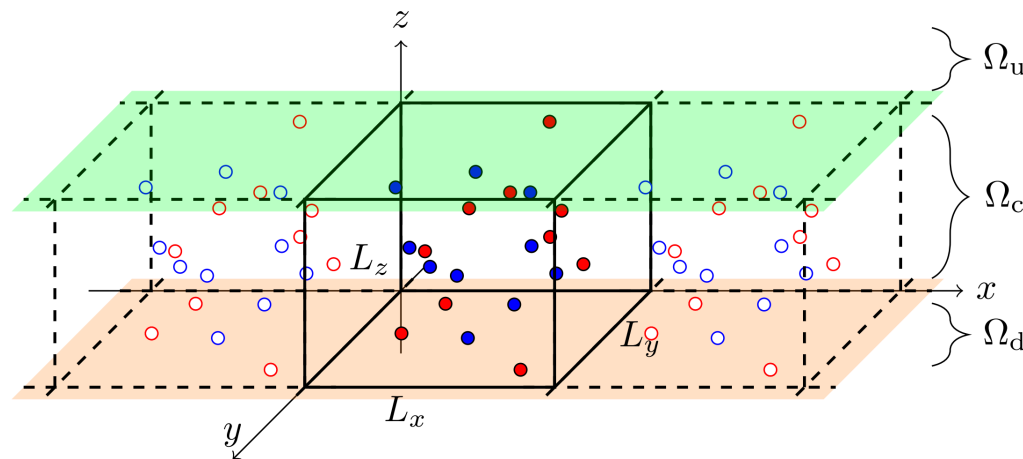


Figure 1: Illustration of a quasi-2D charged system.

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.

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

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).

Some recently developed methods offer potential solutions to this challenge, including:

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

However, these methods have not yet been extended to handle quasi-2D systems.

The sum-of-Gaussians approximation

In our work, we use the bilateral series approximation (Beylkin & Monzón, 2010) of the Coulomb kernel, where

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

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

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

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).

Splitting the far-field potential

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

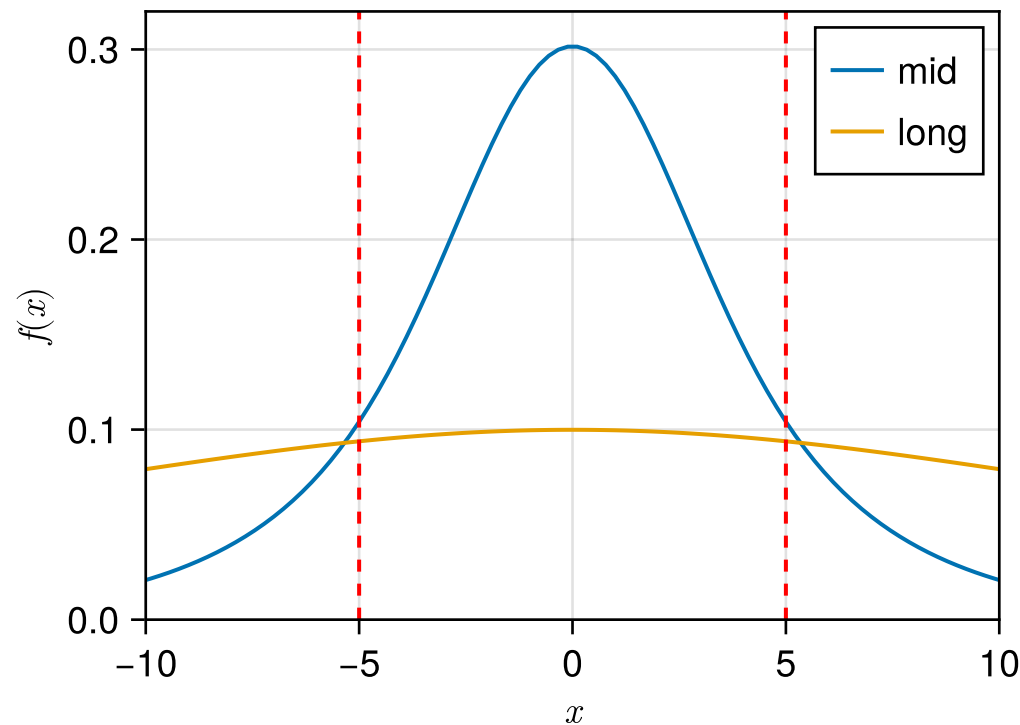


Figure 2: Mid-range part and long-range part of the potential, $L_z = 10$, $\eta \approx 0.6$.

Mid-range potential

The mid-range potential is computed by a standard Fourier spectral solver¹ (type-1 and type-2 NUFFT in 3D (Barnett et al., 2019)) with little zero padding.

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



- 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>

Long-range potential

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

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

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.

Complexity

Using DFT for long-range potential, the complexity is

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

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 $L_z \sim O(\sqrt{L_x L_y})$, the complexity is $O(N \log N)$.

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

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

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

The method¹ 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.

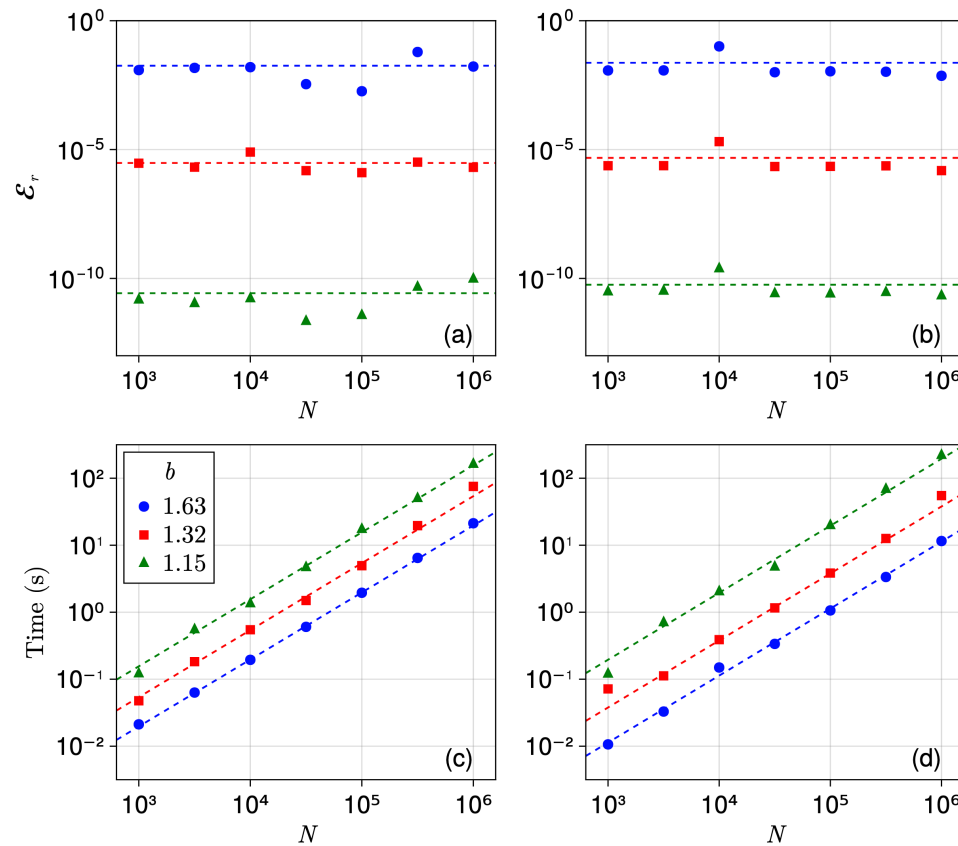


Figure 3: Error and time cost for the SOG method in the (a,c) cubic and (b,d) strongly confined systems.

¹<https://github.com/HPMolSim/FastSpecSOG.jl>

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

It has the following advantages:

- spectrally accurate with rigorous error analysis (Liang et al., 2025)
- 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

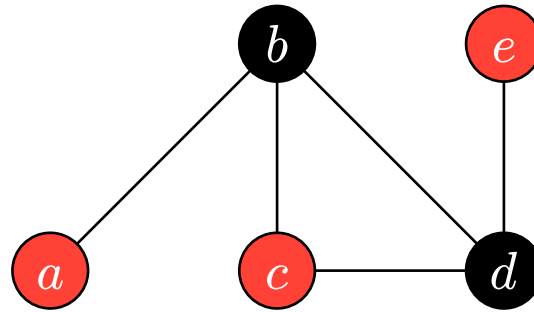
Joint work with Yi-Jia Wang, Pan Zhang, and Jin-Guo Liu

arXiv:2412.07685

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.



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

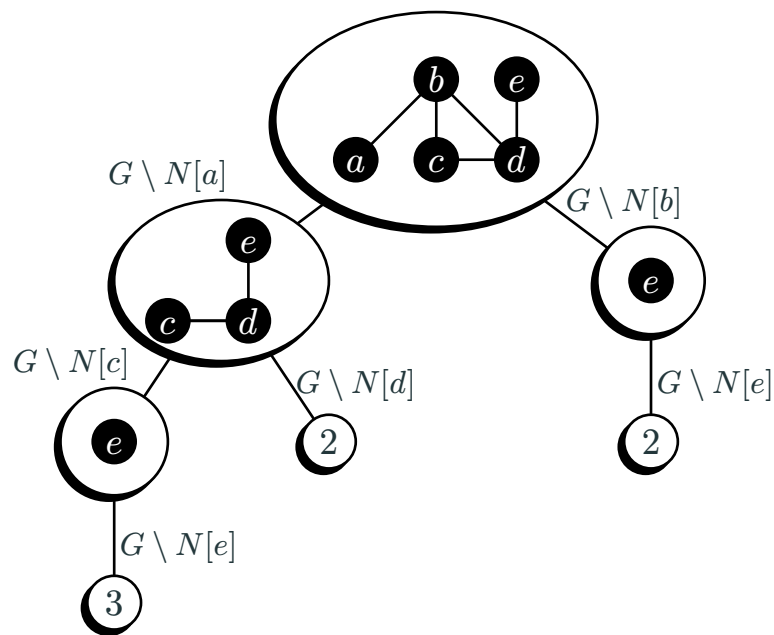
MIS problem has an exponential large solution space and no polynomial-time algorithm is known to solve it exactly.

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

Branching algorithm

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

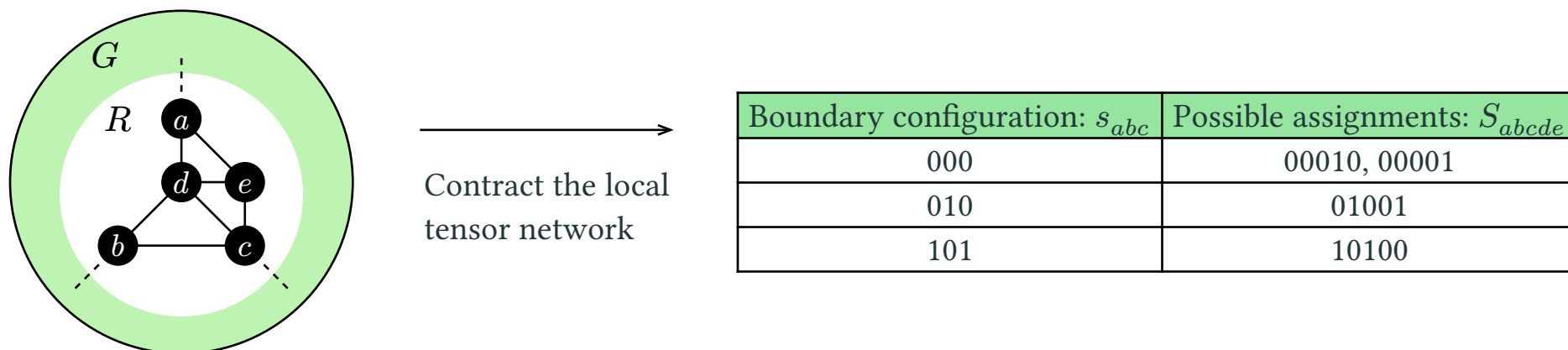
Complexity of a branching algorithm is always described as $O(\gamma^n)$ where γ is the branching factor and n is the size of the problem.



| 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 |

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).



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 ($O^*(1.0836^n)$).

What is the difference?

Tensor network approach

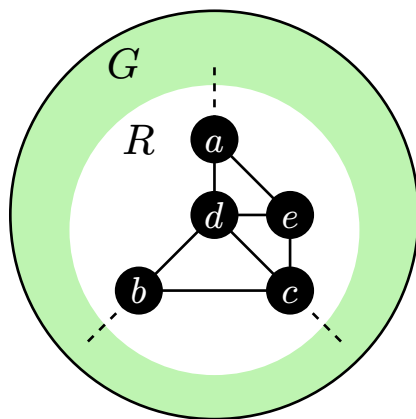
1. Contract the local tensor network for the sub-graph and pick the non-zero elements.
2. For all possible boundaries, fix all the variables and continue the contraction

$$\gamma^n = 3 \times \gamma^{n-5} \rightarrow \gamma \approx 1.2457$$

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

$$\gamma = 1.0$$

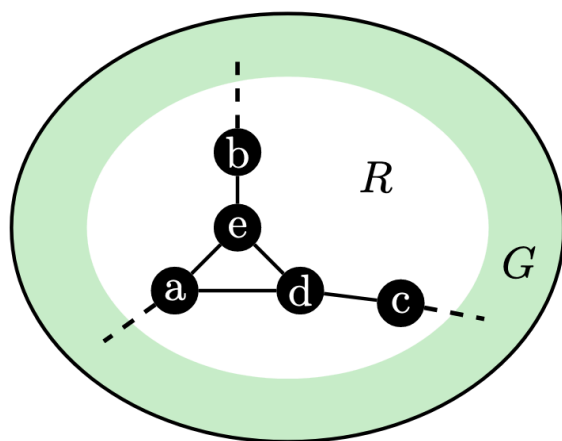


| Boundary configuration: s_{abc} | Possible assignments: S_{abcde} |
|-----------------------------------|-----------------------------------|
| 000 | 00010, 000 0 1 |
| 010 | 010 0 1 |
| 101 | 101 0 0 |

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

The optimal branching algorithm

We use the tensor network to extract the local information, and then automatically search the optimal branching rules¹ (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

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

$$\gamma \approx 1.2671$$

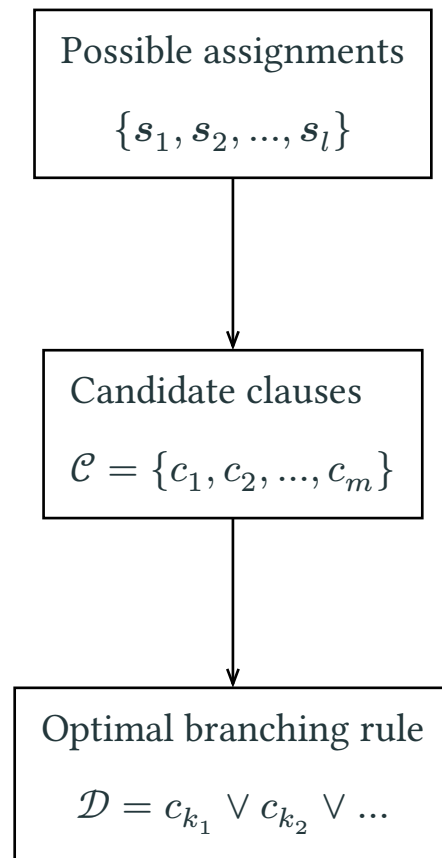
Question: How to solve the rules from the assignments?

¹<https://github.com/OptimalBranching/OptimalBranching.jl>

Finding the optimal branching rule

Bruteforce search? \rightarrow Given l assignments, possible rules: $O(2^{2^l})$.

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



The first step is very direct forward, we generate all possible combination of the assignments (the candidate clauses).

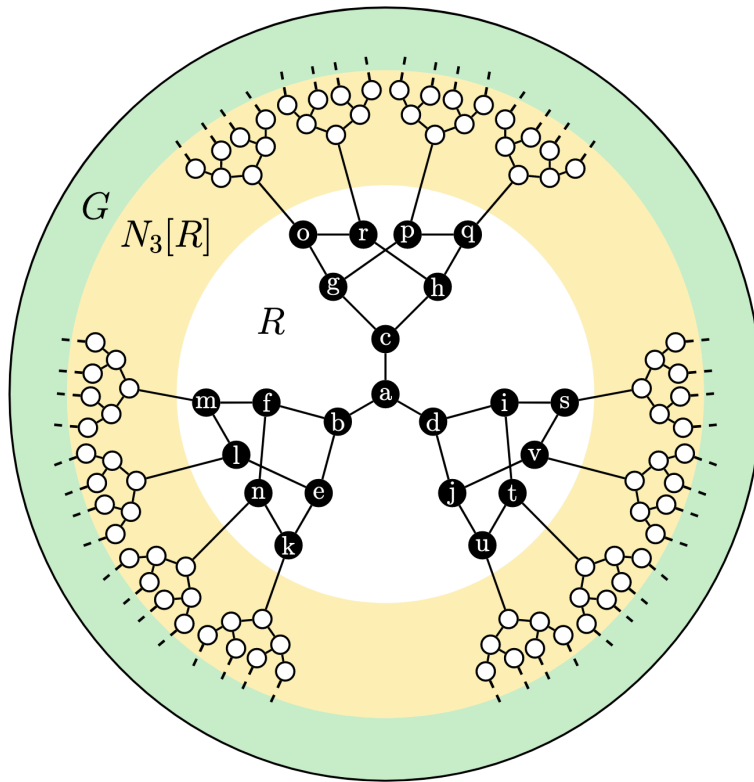
The second step is formulated as a set covering problem, which can be solved by MIP solvers (Achterberg, 2009).

$$\begin{aligned} \min_{\gamma, \mathbf{x}} \gamma \quad \text{s.t.} \quad & \sum_{i=1}^m \gamma^{-\Delta\rho(c_i)} x_i = 1, \\ & \bigcup_{\substack{i=1, \dots, m \\ x_i=1}} J_i = \{1, 2, \dots, l\}, \rightarrow \text{valid branching rule} \\ & x_i \in \{0, 1\} \rightarrow \text{a clause is selected or not} \end{aligned}$$

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

A bottleneck case

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

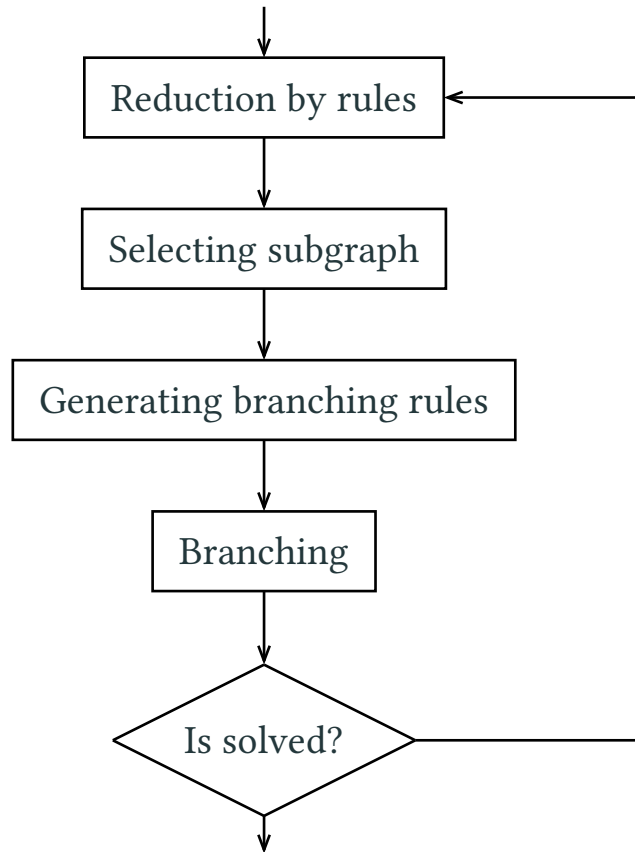


- 71 possible assignments, 15782 candidate clauses.
- 4 branches, size reduced by branches: $[10, 16, 26, 26]$, with $\gamma = 1.0817 < 1.0836$

Numerical results

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 |

23min

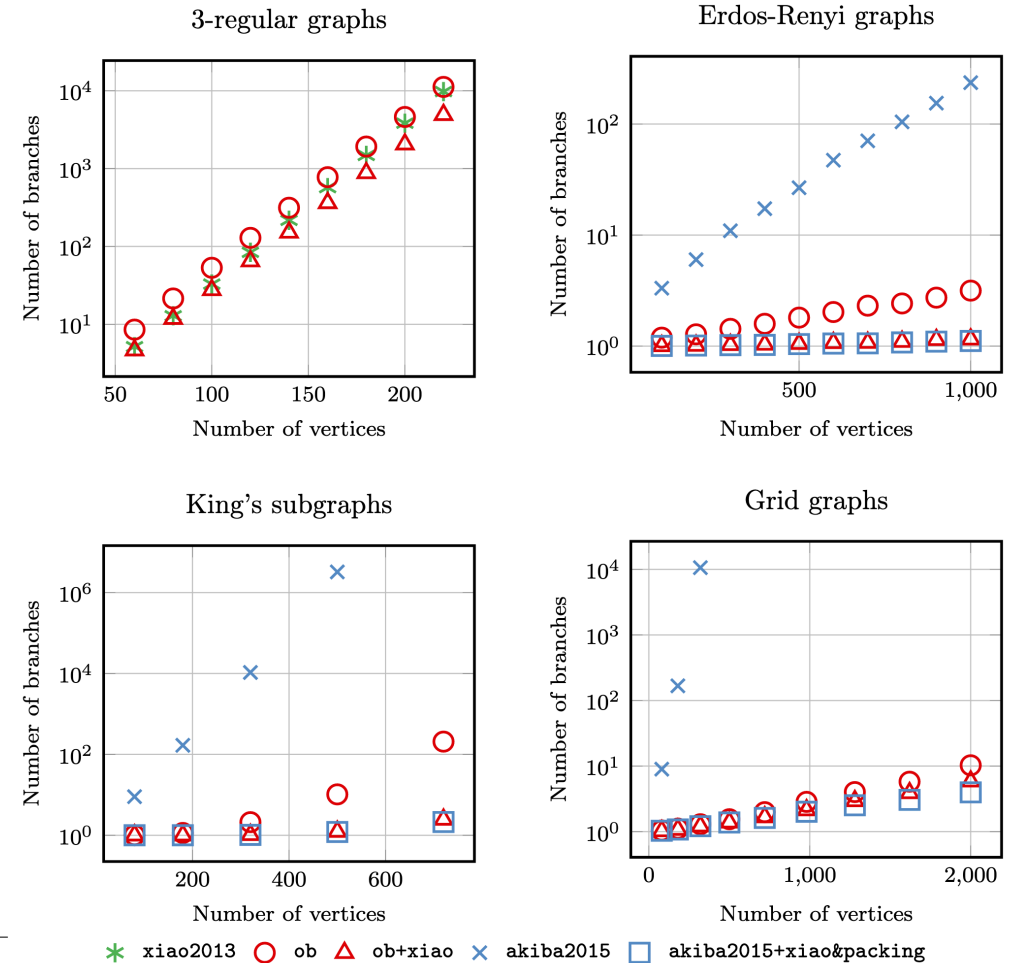
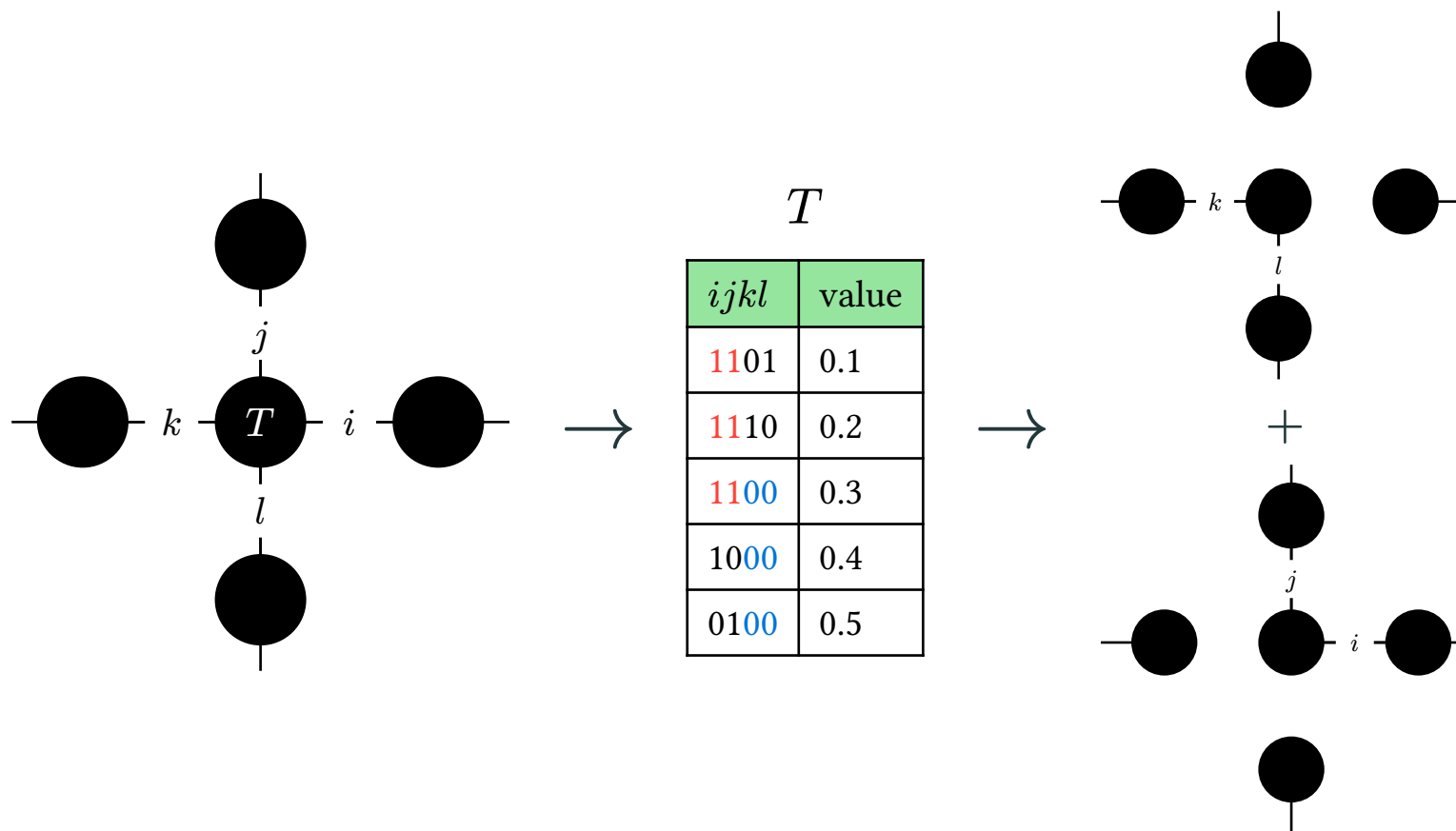


Figure 4: Average number of branches generated by different branching algorithms on 1000 random graphs.

Sparse Tensor Networks Contraction via Optimal Branching

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



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

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 utilize 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

Summary and Outlook

Publications

- **X. Gao**, S. Jiang, J. Liang, Z. Xu, and Q. Zhou, A fast spectral sum-of-Gaussians method for electrostatic summation in quasi-2D systems, Arxiv:2412.04595 (2024)
- Z. Gan, **X. Gao**, J. Liang, and Z. Xu, Fast algorithm for quasi-2D Coulomb systems, Arxiv:2403.01521 (2024)
- Z. Gan, **X. Gao**, J. Liang, and Z. Xu, Random batch Ewald method for dielectrically confined Coulomb systems, Arxiv:2405.06333 (2024)
- **X. Gao** and Z. Gan, Broken symmetries in quasi-2D charged systems via negative dielectric confinement, The Journal of Chemical Physics 161, (2024)

Software packages

- **EwaldSummations.jl**¹: Various Ewald summation methods with parallelization.
- **ChebParticleMesh.jl**²: Toolkits for smooth particle mesh (type-1 and type-2 NUFFT).
- **FastSpecSoG.jl**³: Implementation of the fast spectral SOG method.

¹<https://github.com/HPMolSim/EwaldSummations.jl>

²<https://github.com/HPMolSim/ChebParticleMesh.jl>

³<https://github.com/HPMolSim/FastSpecSoG.jl>

Publications

- **X. Gao**, Y.-J. Wang, P. Zhang, and J.-G. Liu, Automated discovery of branching rules with optimal complexity for the maximum independent set problem, Arxiv:2412.07685 (2024)
- **X. Gao**, X. Li, and J. Liu, Programming guide for solving constraint satisfaction problems with tensor networks, Arxiv:2501.00227 (2024)
- M. Roa-Villescas, **X. Gao**, S. Stuijk, H. Corporaal, and J.-G. Liu, Probabilistic inference in the era of tensor networks and differential programming, Physical Review Research 6, 33261 (2024)

Software packages

- **TreeWidthSolver.jl**¹: Solving the treewidth problem (supported by GSoC 2024).
- **CuTropicalGEMM.jl**²: Custom GPU kernel for tropical matrix multiplication (supported by OSPP 2023).
- **OptimalBranching.jl**³: Implementation of the optimal branching algorithm.

¹<https://github.com/ArrogantGao/TreeWidthSolver.jl>

²<https://github.com/TensorBFS/CuTropicalGEMM.jl>

³<https://github.com/OptimalBranching/OptimalBranching.jl>

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

29min



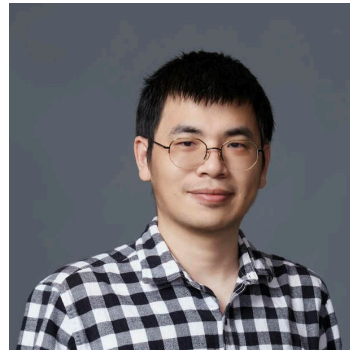
Prof. Zecheng Gan
HKUST(GZ)



Prof. Zhenli Xu
SJTU



Prof. Shidong Jiang
CCM



Prof. Jinguo Liu,
HKUST(GZ)



Prof. Pan Zhang,
ITP, CAS

Also thank Jiuyang Liang (SJTU & CCM), Qi Zhou (SJTU), Martin (TEU), and Yijia Wang (ITP, CAS) for collaboration.

Thank you for your attention!

Appendix

The U-series and its derivative

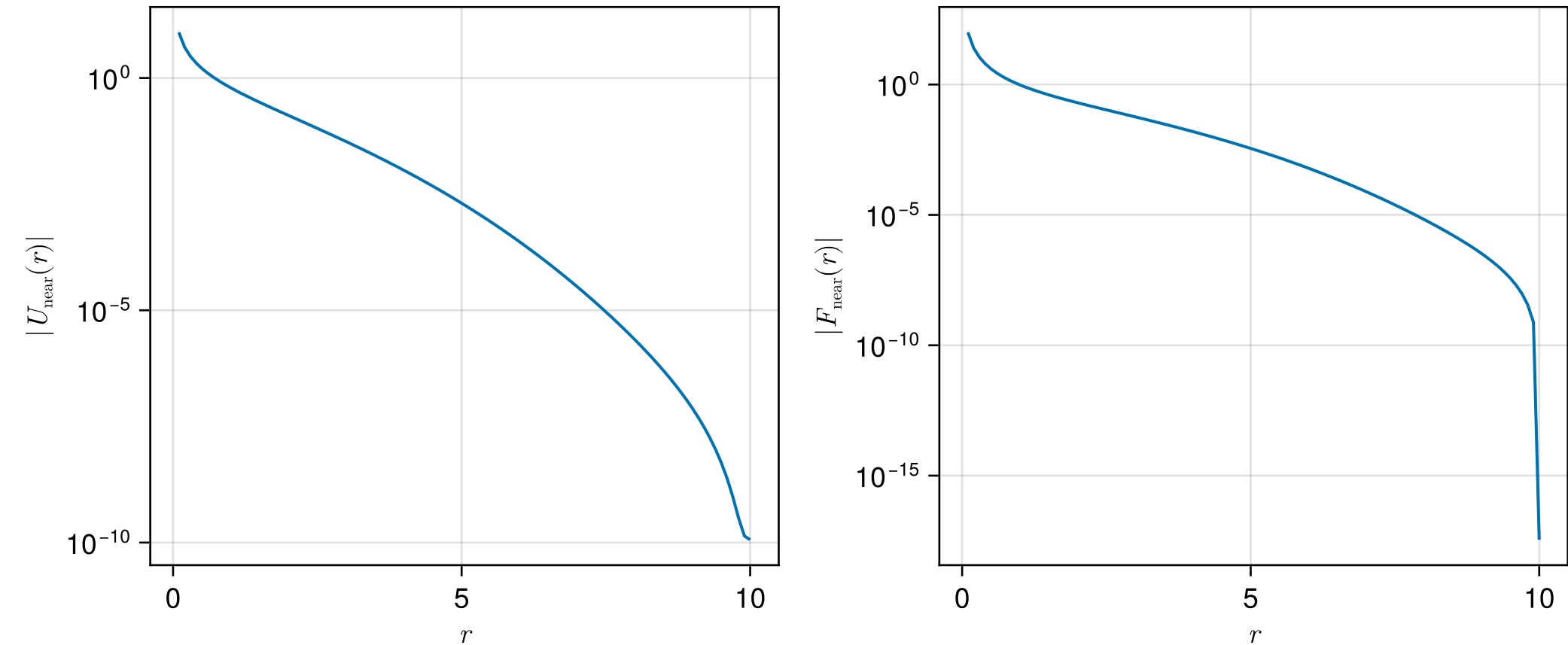


Figure 5: The U-series and its derivative, $r_c = 10.0$.

| 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 |

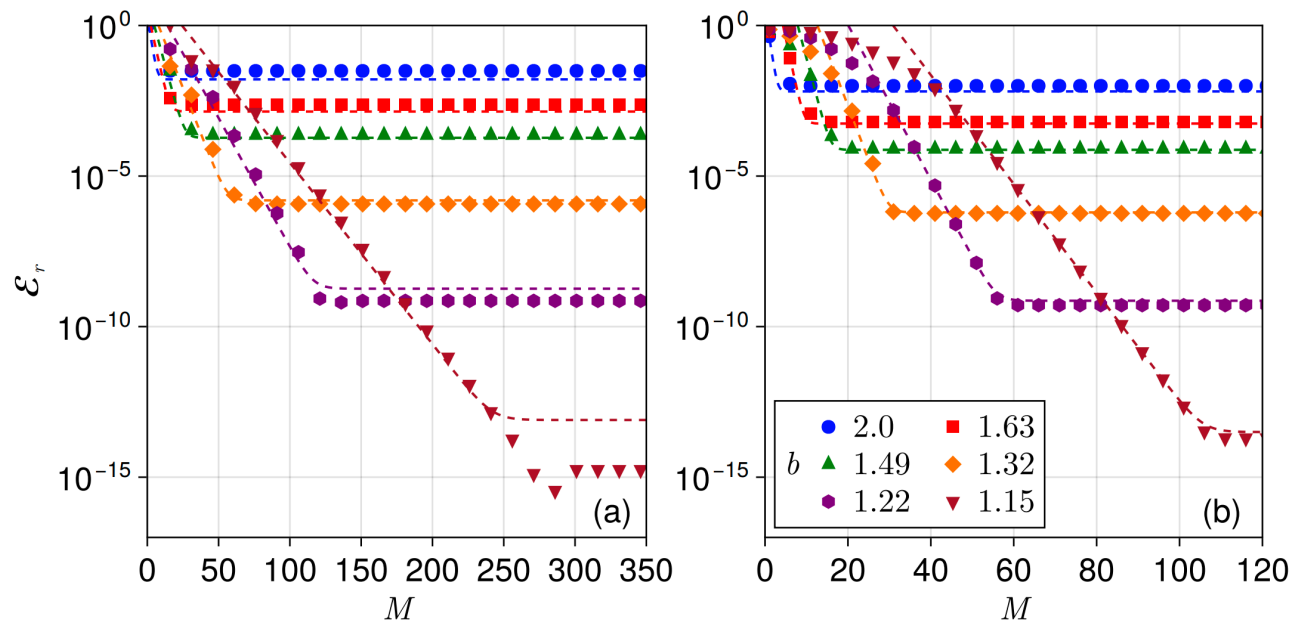


Figure 6: U-series parameters and the error

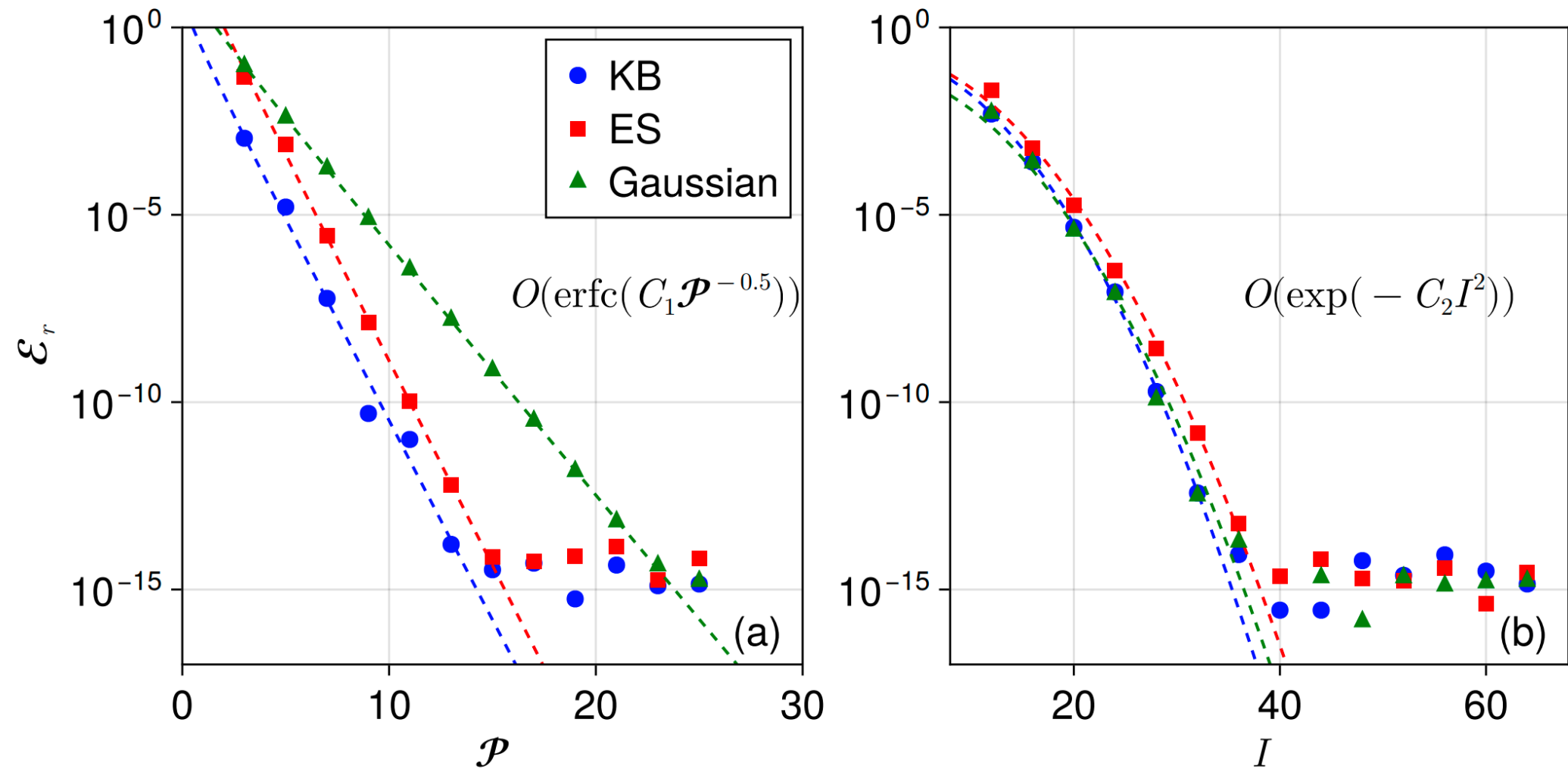


Figure 7: Different window functions.

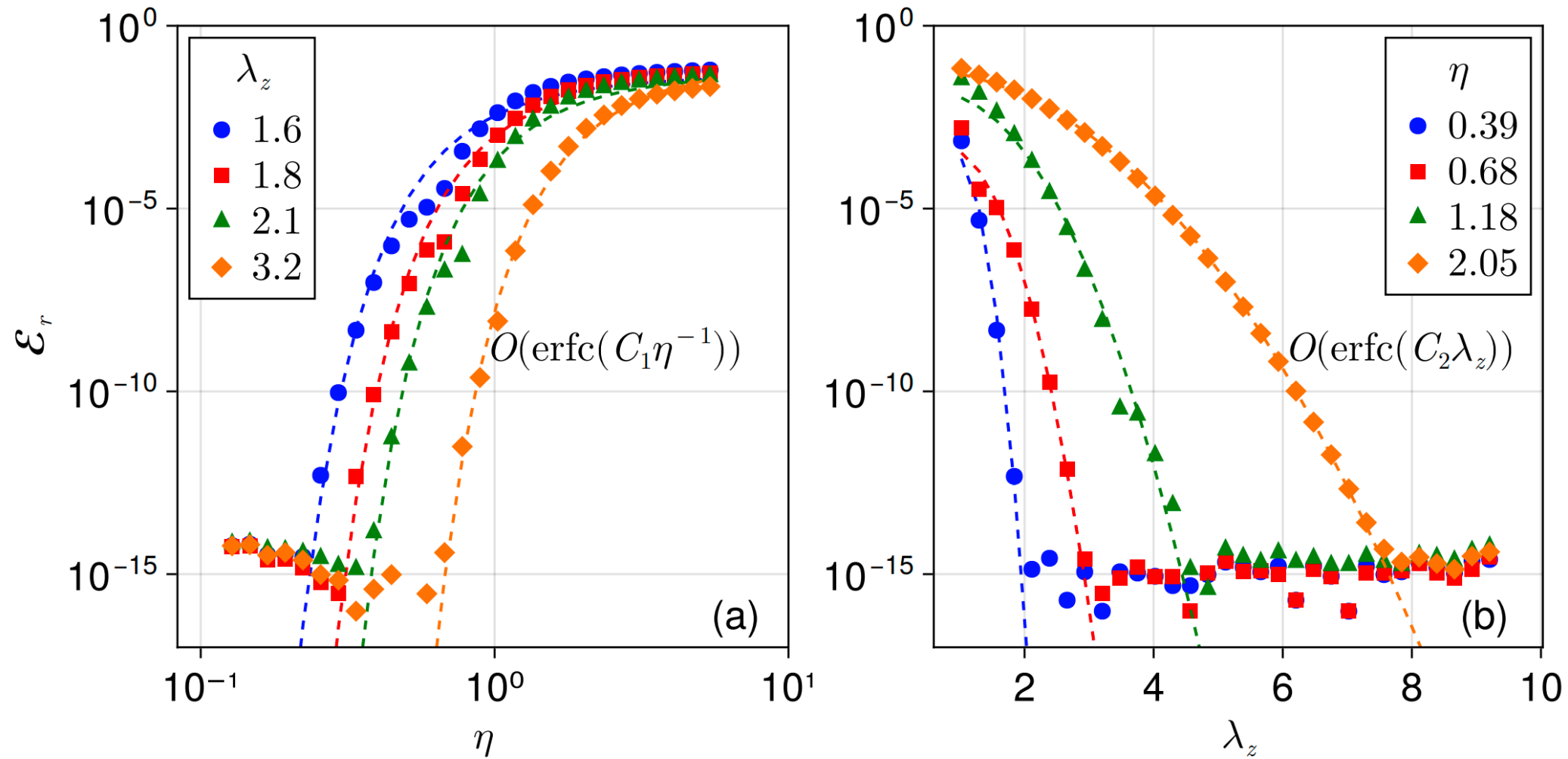


Figure 8: Zero-padding.

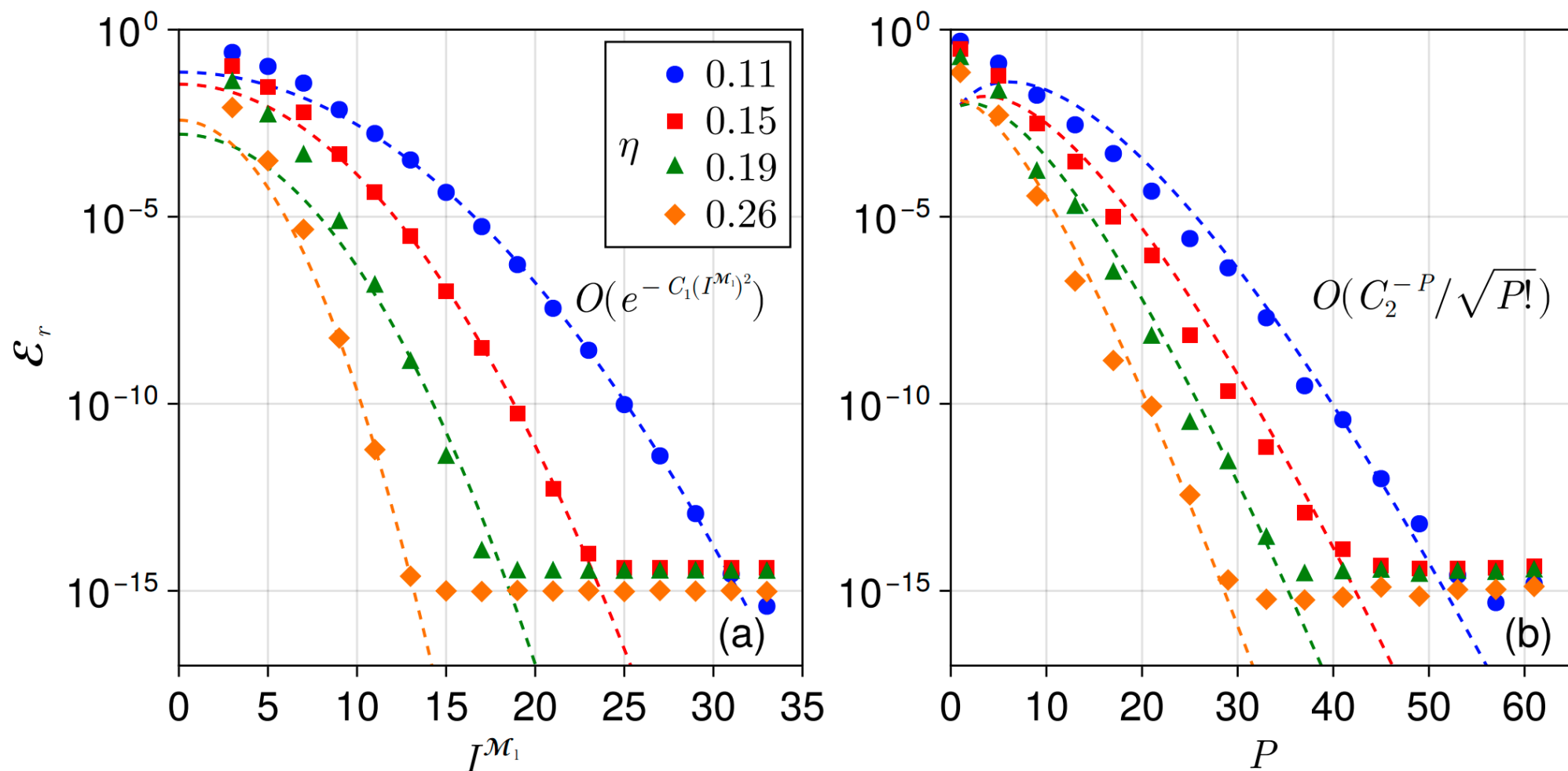


Figure 9: Accuracy of the Fourier-Chebyshev solver.

Strongly confined systems

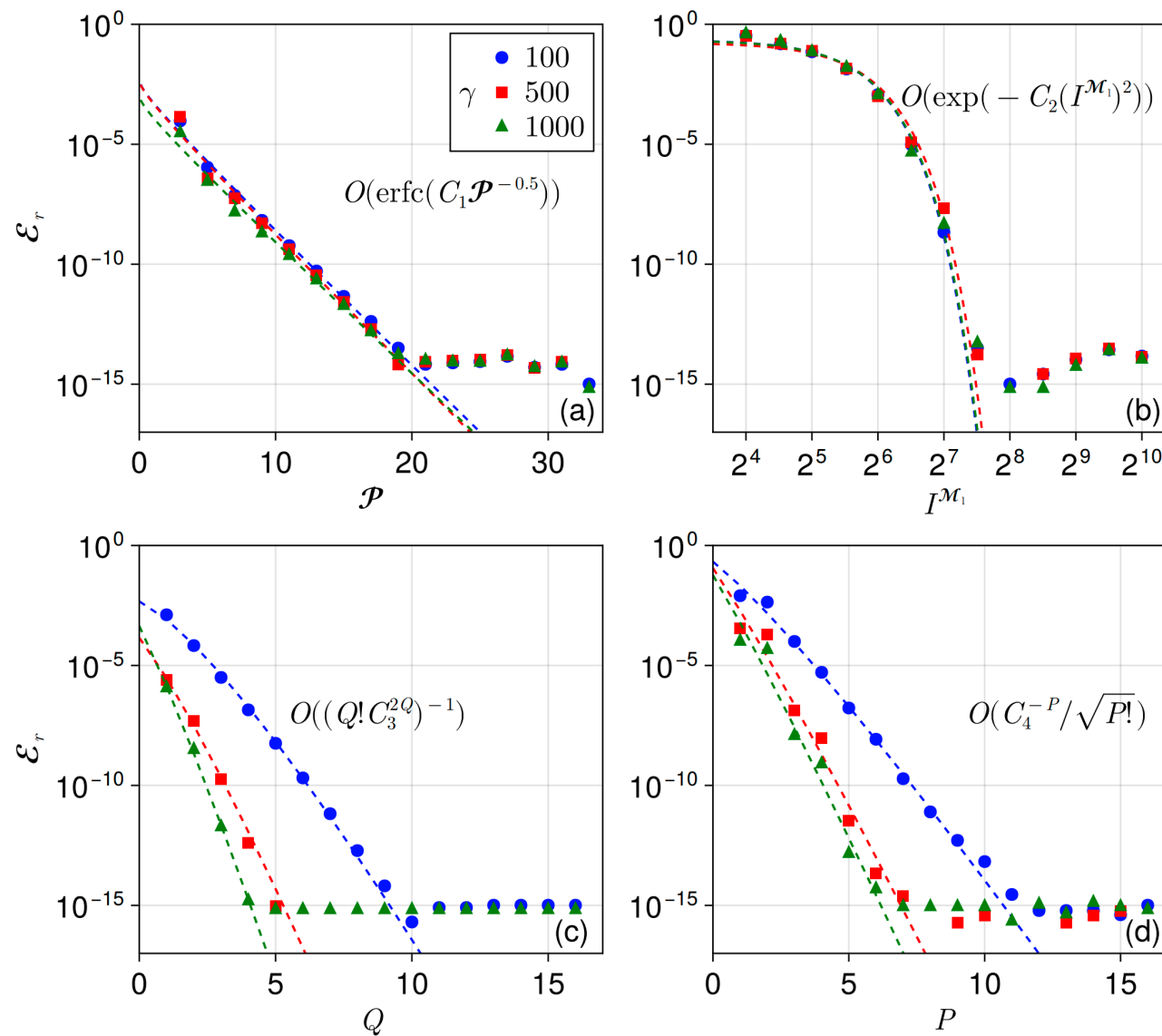
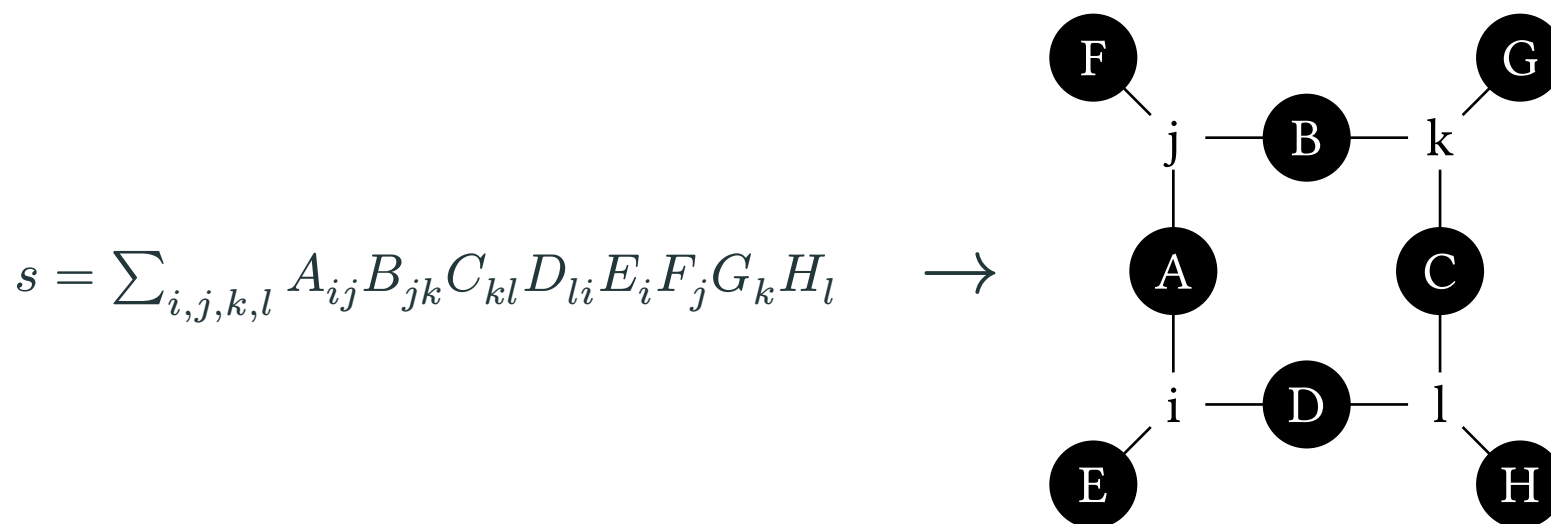


Figure 10: Strongly confined systems.

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

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

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



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

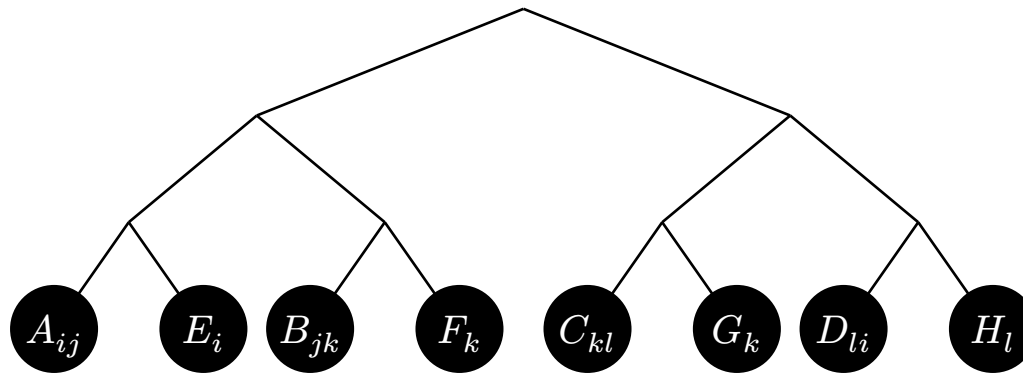


Figure 11: An example of binary contraction tree.

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-hard¹ problem!

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

- OMEinsumContractionOrder.jl² in Julia
- Cotengra³ in Python

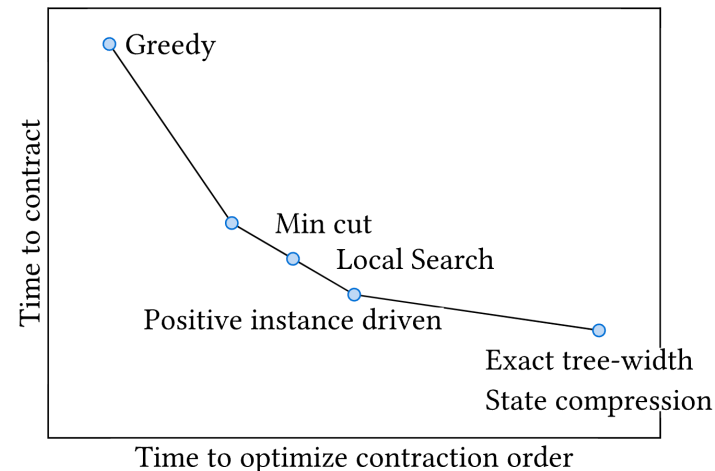


Figure 12: Comparison of different contraction orders.

¹I.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:

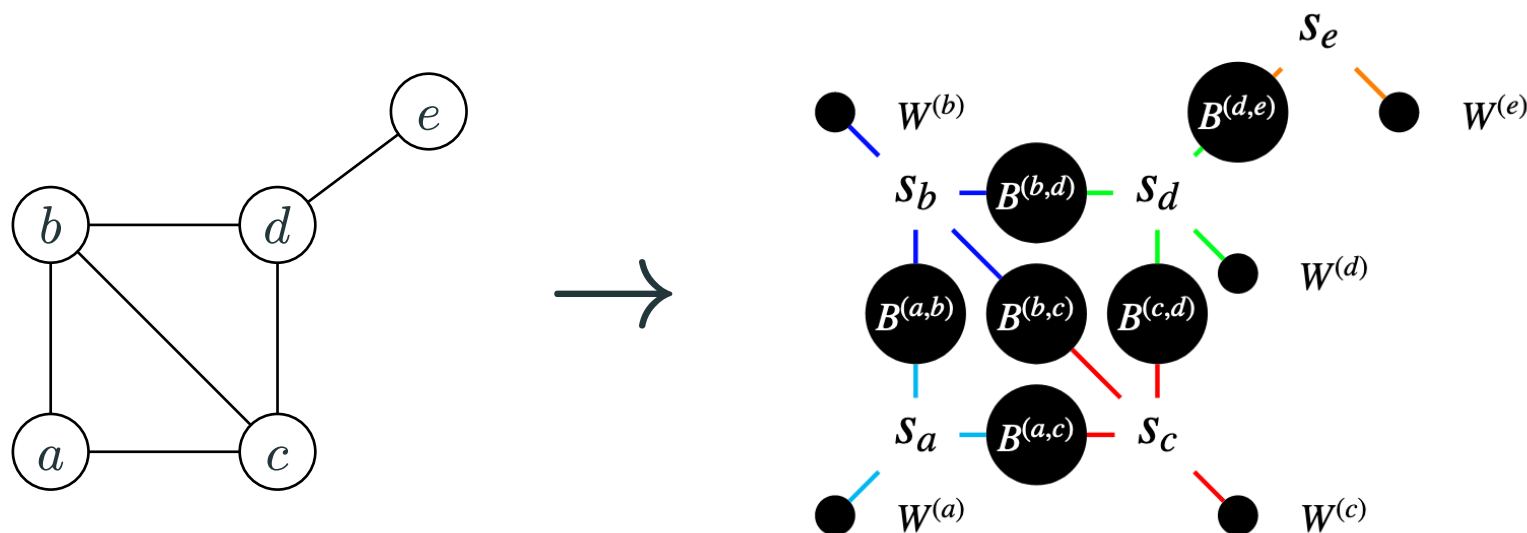
$$T_{i_y \dots} = \max_{i \notin \{i_y \dots\}} \left(A_{i_a \dots} + B_{i_b \dots} + C_{i_c \dots} + \dots \right)$$

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.

Tensor Network for Maximum Independent Set Problem

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.

Solving the set covering problem via Mixed Integer Linear Programming

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:

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

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

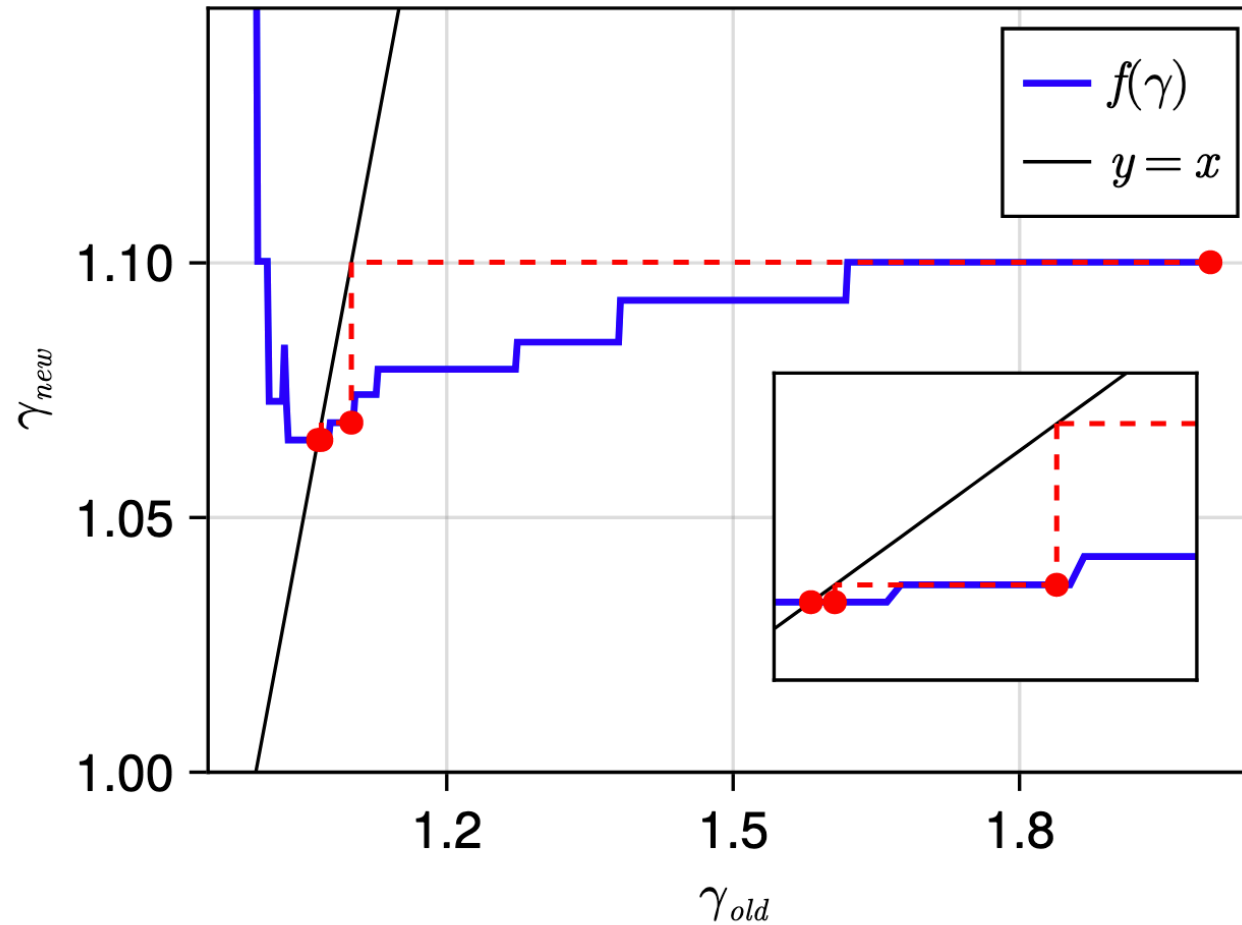


Figure 13: An example of solving the set covering problem via iterative MIP.

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

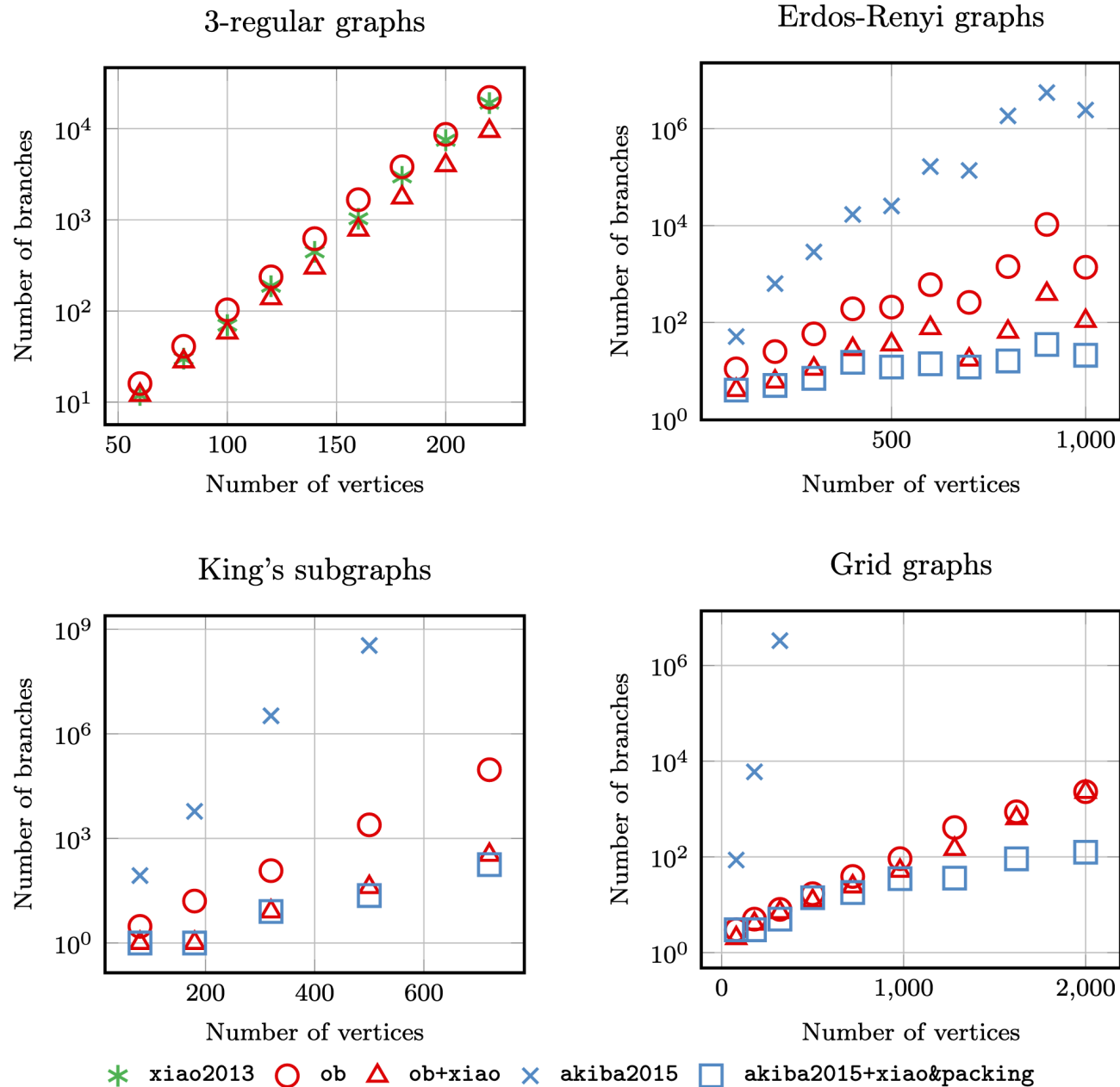


Figure 14: The worst-case complexity of the proposed method on random graphs.

- Achterberg, T. (2009). SCIP: Solving constraint integer programs. *Math. Program. Comput.*, 1(1), 1–41. <https://doi.org/10.1007/s12532-008-0001-1>
- Akiba, T., & Iwata, Y. (2016). Branch-and-reduce exponential/FPT algorithms in practice: A case study of vertex cover. *Theoretical Computer Science*, 609, 211–225. <https://doi.org/10.1016/j.tcs.2015.09.023>
- Barnett, A. H., Magland, J., & Klinteberg, L. af. (2019). A parallel nonuniform fast Fourier transform library based on an ``Exponential of semicircle" kernel. *SIAM J. Sci. Comput.*, 41(5), C479–C504.
- Barros, K., & Luijten, E. (2014). Dielectric Effects in the Self-Assembly of Binary Colloidal Aggregates. *Phys. Rev. Lett.*, 113(1), 17801.
- Beigel, R. (1999). Finding maximum independent sets in sparse and general graphs. *SODA*, 99, 856–857.
- Beylkin, G., & Monzón, L. (2010). Approximation by exponential sums revisited. *Applied and Computational Harmonic Analysis*, 28(2), 131–149.
- Bourgeois, N., Escoffier, B., & Paschos, V. T. (2008). An $O^*(1.0977^n)$ exact algorithm for max independent set in sparse graphs. *Parameterized and Exact Computation: Third*

- International Workshop, IWPEC 2008, Victoria, Canada, May 14-16, 2008. Proceedings 3*, 55–65.
- Chen, J., Kanj, I. A., & Xia, G. (2003). Labeled search trees and amortized analysis: improved upper bounds for NP-hard problems. *Algorithms and Computation: 14th International Symposium, ISAAC 2003, Kyoto, Japan, December 15-17, 2003. Proceedings 14*, 148–157.
- Fomin, F. V., & Høie, K. (2006). Pathwidth of cubic graphs and exact algorithms. *Information Processing Letters*, 97(5), 191–196.
- Fomin, F. V., & Kaski, P. (2013). Exact exponential algorithms. *Communications of the ACM*, 56(3), 80–88.
- Fomin, F. V., Grandoni, F., & Kratsch, D. (2006). Measure and conquer: A simple $O(20.288n)$ independent set algorithm. *SODA*, 6, 18–25.
- Fürer, M. (2006). A faster algorithm for finding maximum independent sets in sparse graphs. *LATIN 2006: Theoretical Informatics: 7th Latin American Symposium, Valdivia, Chile, March 20-24, 2006. Proceedings 7*, 491–501.
- Gao, X., Li, X., & Liu, J. (2024a,). *Programming guide for solving constraint satisfaction problems with tensor networks*. <https://arxiv.org/abs/2501.00227>

- Gao, X., Wang, Y.-J., Zhang, P., & Liu, J.-G. (2024b, December). *Automated Discovery of Branching Rules with Optimal Complexity for the Maximum Independent Set Problem* (Issue arXiv:2412.07685). arXiv. <https://doi.org/10.48550/arXiv.2412.07685>
- Greengard, L., Jiang, S., & Zhang, Y. (2018). The anisotropic truncated kernel method for convolution with free-space Green's functions. *SIAM J. Sci. Comput.*, 40(6), A3733–A3754.
- Jian, T. (1986). An $O(2^{0.304n})$ algorithm for solving maximum independent set problem. *IEEE Transactions on Computers*, 100(9), 847–851.
- Jiang, S., & Greengard, L. (2024). A Dual-space Multilevel Kernel-splitting Framework for Discrete and Continuous Convolution. *Accepted by Commun. Pure Appl. Math.* (2024), Also Available at [\url{Https://arxiv.org/pdf/2308.00292.pdf}](https://arxiv.org/pdf/2308.00292.pdf), 0, .
- Karp, R. M. (1972). *Reducibility among combinatorial problems*. Springer.
- Kneis, J., Langer, A., & Rossmanith, P. (2009,). A fine-grained analysis of a simple independent set algorithm. *IARCS Annual Conference on Foundations of Software Technology and Theoretical Computer Science* (2009).
- Liang, J., Xu, Z., & Zhou, Q. (2025,). *Error estimate of the u-series method for molecular dynamics simulations*. <https://arxiv.org/abs/2305.05369>

- Liu, J.-G., Gao, X., Cain, M., Lukin, M. D., & Wang, S.-T. (2023). Computing solution space properties of combinatorial optimization problems via generic tensor networks. *SIAM Journal on Scientific Computing*, 45(3), A1239–A1270.
- Markov, I. L., & Shi, Y. (2008). Simulating Quantum Computation by Contracting Tensor Networks. *SIAM Journal on Computing*, 38(3), 963–981. <https://doi.org/10.1137/050644756>
- Maxian, O., Peláez, R. P., Greengard, L., & Donev, A. (2021). A fast spectral method for electrostatics in doubly periodic slit channels. *J. Chem. Phys.*, 154(20), 204107.
- Mazars, M. (2011). Long ranged interactions in computer simulations and for quasi-2D systems. *Phys. Rep.*, 500(2–3), 43–116.
- Parry, D. E. (1975). The electrostatic potential in the surface region of an ionic crystal. *Surf. Sci.*, 49(2), 433–440. [https://doi.org/10.1016/0039-6028\(75\)90362-3](https://doi.org/10.1016/0039-6028(75)90362-3)
- Pei, R., Askham, T., Greengard, L., & Jiang, S. (2023). A fast method for imposing periodic boundary conditions on arbitrarily-shaped lattices in two dimensions. *J. Comp. Phys.*, 474, 111792.

- Predescu, C., Lerer, A. K., Lippert, R. A., Towles, B., Grossman, J., Dirks, R. M., & Shaw, D. E. (2020). The u-series: A separable decomposition for electrostatics computation with improved accuracy. *J. Chem. Phys.*, 152(8), 84113.
- Razgon, I. (2006). *A Faster Solving of the Maximum In-dependent Set Problem for Graphs with Maximal Degree 3*.
- Robson, J. M. (2001). *Finding a maximum independent set in time $O(2n/4)$* .
- Robson, J. M. (1986). Algorithms for maximum independent sets. *Journal of Algorithms*, 7(3), 425–440.
- Shamshirgar, D. S., Yokota, R., Tornberg, A.-K., & Hess, B. (2019). Regularizing the fast multipole method for use in molecular simulation. *The Journal of Chemical Physics*, 151(23), 234113.
- Tarjan, R. E., & Trojanowski, A. E. (1977). Finding a maximum independent set. *SIAM Journal on Computing*, 6(3), 537–546.
- Xiao, M.-Y., Chen, J.-E., & Han, X.-L. (2005). Improvement on vertex cover and independent set problem for low-degree graphs. *Jisuanji Xuebao(Chin. J. Comput.)*, 28(2), 153–160.

- Xiao, M. (2009, April). *New Branching Rules: Improvements on Independent Set and Vertex Cover in Sparse Graphs* (Issue arXiv:904.2712). arXiv. <https://doi.org/10.48550/arXiv.0904.2712>
- Xiao, M., & Nagamochi, H. (2013). Confining sets and avoiding bottleneck cases: A simple maximum independent set algorithm in degree-3 graphs. *Theoretical Computer Science*, 469, 92–104. <https://www.sciencedirect.com/science/article/pii/S0304397512008729>
- Xiao, M., & Nagamochi, H. (2017). Exact Algorithms for Maximum Independent Set. *Information and Computation*, 255, 126–146. <https://doi.org/10.1016/j.ic.2017.06.001>
- Yan, W., & Shelley, M. (2018). Flexibly imposing periodicity in kernel independent FMM: A multipole-to-local operator approach. *J. Comput. Phys.*, 355, 214–232.