

# Approximate inference on planar graphs using Loop Calculus and Belief Propagation

Vicenç Gómez<sup>1</sup>, Hilbert J Kappen<sup>1</sup> and Michael Chertkov<sup>2</sup>

<sup>1</sup>Radboud University Nijmegen, Donders Institute for Brain, Cognition and Behaviour, Nijmegen (The Netherlands), <sup>2</sup>Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos (USA)

## Abstract

- Exact inference on a **binary** graphical model defined on a **planar** graph is easy for graphs **without external fields** [6, 3], otherwise is intractable [1].
- We introduce novel results for **approximate inference on general planar** graphical models using the **loop calculus framework** [2].
- The loop calculus allows to express the exact partition function  $Z$  of a graphical model as a **finite sum of terms** that can be evaluated once the belief propagation (BP) solution is known.
- We develop an algorithm for the approach presented in [2] which represents an efficient truncation scheme on planar graphs and a new representation of the series in terms of Pfaffians of matrices.
- We show that the first term of the Pfaffian series can provide very accurate approximations.
- The algorithm **outperforms previous truncation schemes** of the loop series and is **competitive with other state-of-the-art methods** for approximate inference.

## Belief Propagation and loop Series

We use a Forney graph  $\mathcal{G} := (\mathcal{V}, \mathcal{E})$  representation of a probabilistic model defined on binary variables:

- $\mathcal{V}$  is a set of nodes, where each node  $a \in \mathcal{V}$  represents an interaction.
- Each edge  $(a, b) \in \mathcal{E}$  represents a binary variable  $\sigma_{ab} := \{\pm 1\}$ .

The joint probability distribution of such a model factorizes as:

$$p(\boldsymbol{\sigma}) = Z^{-1} \prod_{a \in \mathcal{V}} f_a(\boldsymbol{\sigma}_a), \quad Z = \sum_{\boldsymbol{\sigma}} \prod_{a \in \mathcal{V}} f_a(\boldsymbol{\sigma}_a),$$

where  $Z$  is the partition function.

- A **generalized loop** or "loop" in a graph  $\mathcal{G}$  is any subgraph  $C$  such that each node in  $C$  has degree 2 or larger.

Given the partition function  $Z^{BP}$  obtained at a fixed point of the BP algorithm, the exact  $Z$  is related with  $Z^{BP}$  via the **loop series expansion**:

$$Z = Z^{BP} \cdot z, \quad z = \left( 1 + \sum_{C \in \mathcal{C}} r_C \right), \quad r_C = \prod_{a \in C} \mu_{a, \bar{a}_C}, \quad (1)$$

where  $\mathcal{C}$  is the set of all the generalized loops within the graph. Each loop term  $r_C$  is a product of terms  $\mu_{a, \bar{a}_C}$  associated with every node  $a$  of the loop:

$$\mu_{a, \bar{a}_C} = \frac{\sum_{\boldsymbol{\sigma}_a} b_a(\boldsymbol{\sigma}_a) \prod_{b \in \bar{a}_C} (\sigma_{ab} - m_{ab})}{\prod_{b \in \bar{a}_C} \sqrt{1 - m_{ab}^2}}, \quad m_{ab} = \sum_{\sigma_{ab}} \sigma_{ab} b_{ab}(\sigma_{ab}).$$

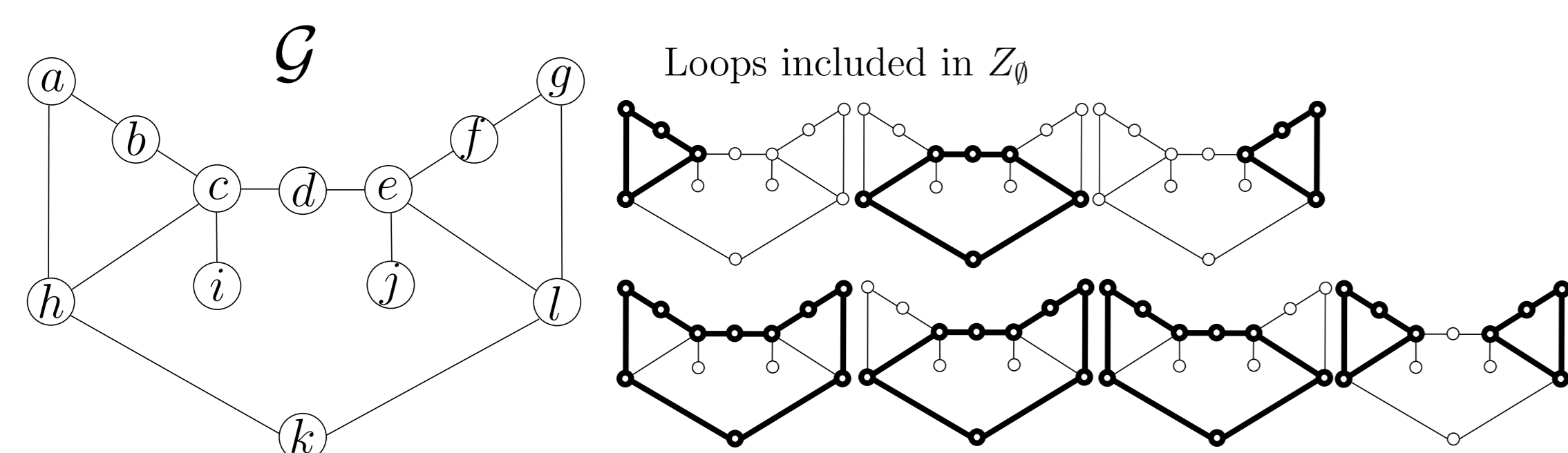
$b_a(\cdot)$  and  $b_{ab}(\cdot)$  denote the BP "beliefs".  $\bar{a}_C$  denotes the set of neighbors of  $a$  within  $C$ .

We consider planar graphs with all nodes of degree not larger than 3 and we denote by **triplet** a node with degree 3 in  $\mathcal{G}$ .

- A **2-regular loop** is a loop in which all nodes have degree exactly 2.
- The **2-regular partition function**  $Z_\emptyset$  is the **truncated form** of (1) which sums all 2-regular loops only:

$$Z_\emptyset = Z^{BP} \cdot z_\emptyset, \quad z_\emptyset = 1 + \sum_{C \in \mathcal{C}, t. |\bar{a}_C|=2, \forall a \in C} r_C.$$

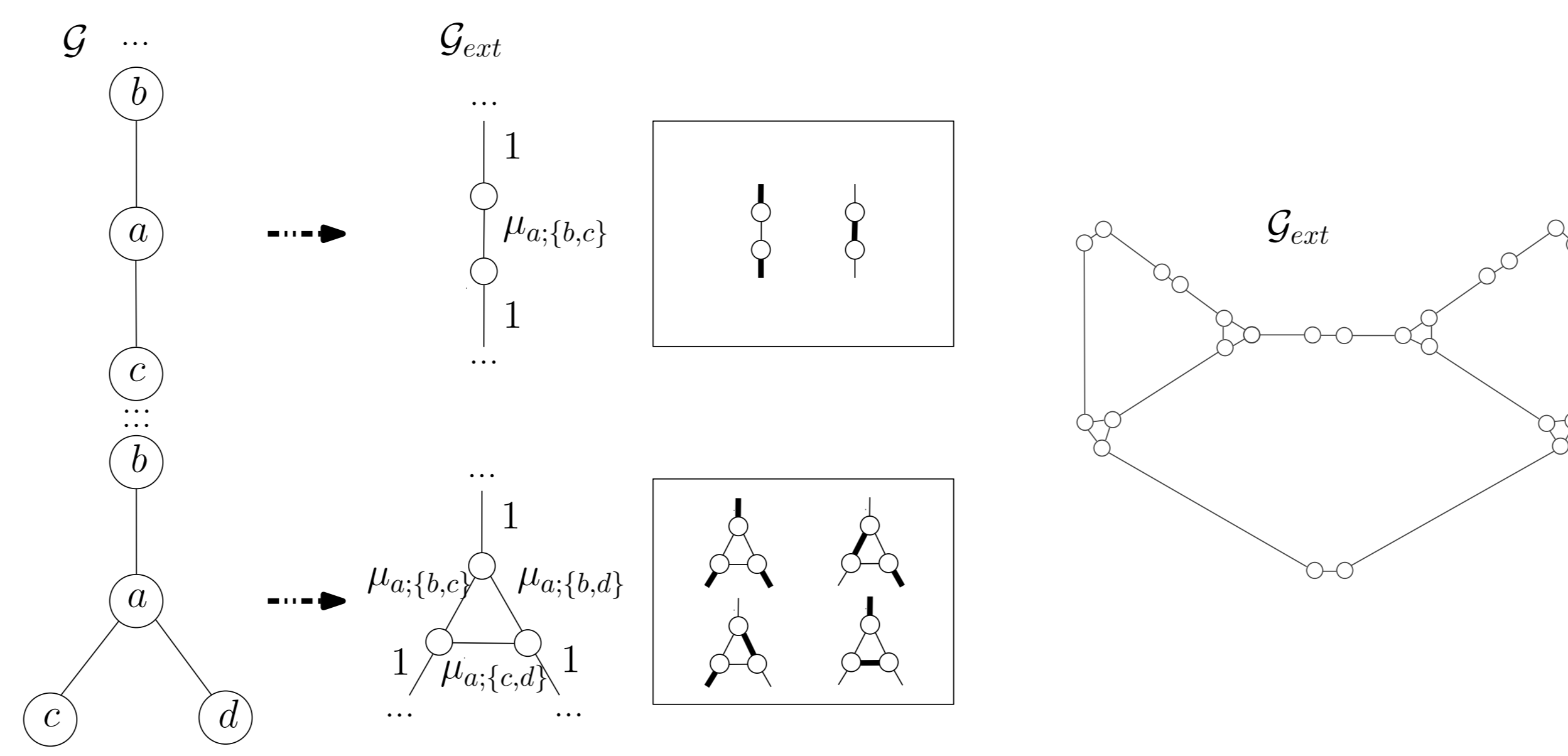
Example:



## Loop series as Pfaffian series

### First term: The 2-regular partition function $Z_\emptyset$ . Efficient computation using perfect matchings

- The original graph  $\mathcal{G}$  is extended  $\mathcal{G}_{ext}$  applying Fisher's rules [3]:



- Perfect matchings** in  $\mathcal{G}_{ext}$  correspond to **2-regular loops** in  $\mathcal{G}$ .
- Therefore  $z_\emptyset = \sum$  weighted perfect matchings in  $\mathcal{G}_{ext}$ . If  $\mathcal{G}$  is **planar**  $\rightarrow z_\emptyset$  can be computed in time  $\mathcal{O}(N_{\mathcal{G}_{ext}}^3)$  using **Kasteleyn algorithm** [6] (requires the evaluation of a Determinant/Pfaffian of a matrix).
- Exact inference for the **zero external field** case:  $Z_\emptyset = Z$ .

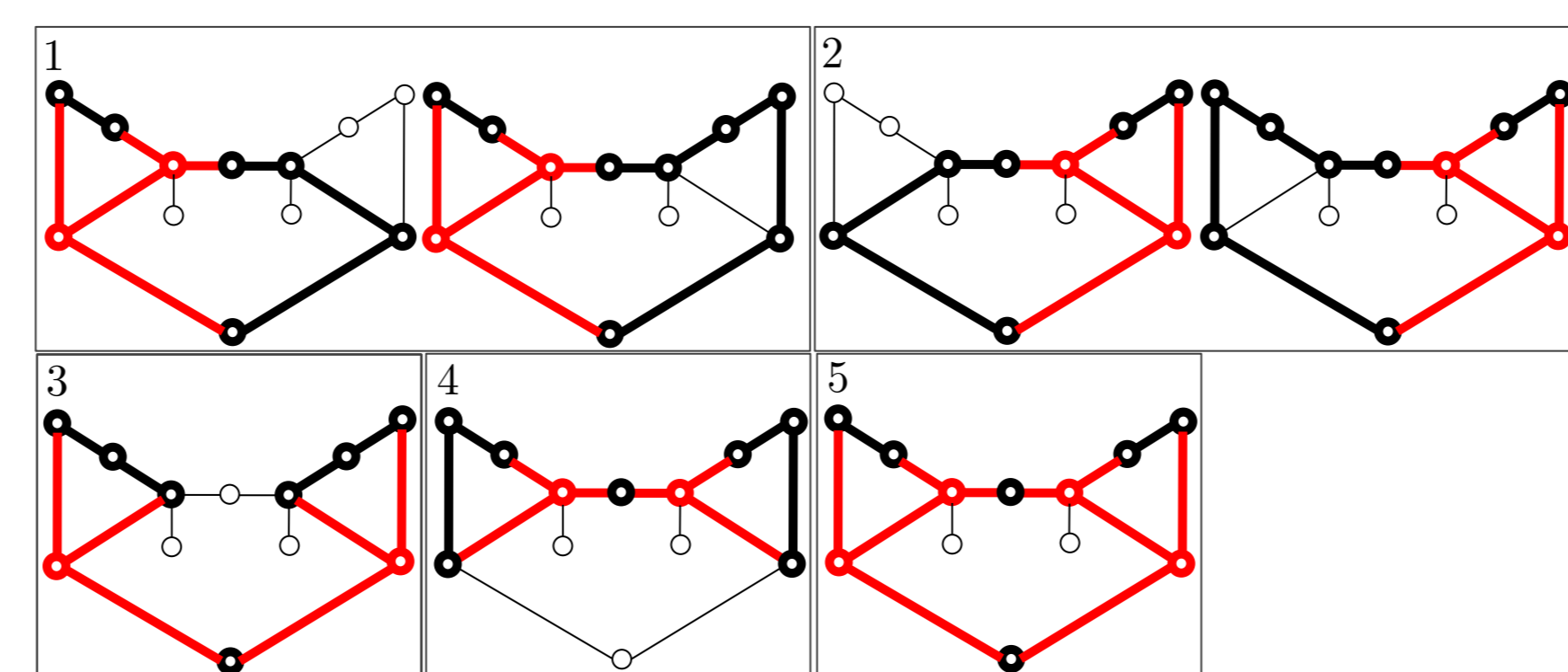
## Higer order terms

- For each possible set  $\Psi$  including an **even number of triplets**, there exists a unique correspondence between **loops** in  $\mathcal{G}$  including the triplets in  $\Psi$  and **perfect matchings** in another extended graph  $\mathcal{G}_{ext\Psi}$  constructed **after removal of the triplets**  $\Psi$  in  $\mathcal{G}$ .
- Full loop series is represented as Pfaffian series and each term  $Z_\Psi$  is tractable (requires the evaluation of a Pfaffian of a matrix):

$$z = \sum_{\Psi} Z_\Psi, \quad Z_\Psi = z_\Psi \prod_{a \in \Psi} \mu_{a, \bar{a}}, \quad |z_\Psi| = \left| \sum \text{weighted perf. matchings } \mathcal{G}_{ext\Psi} \right|$$

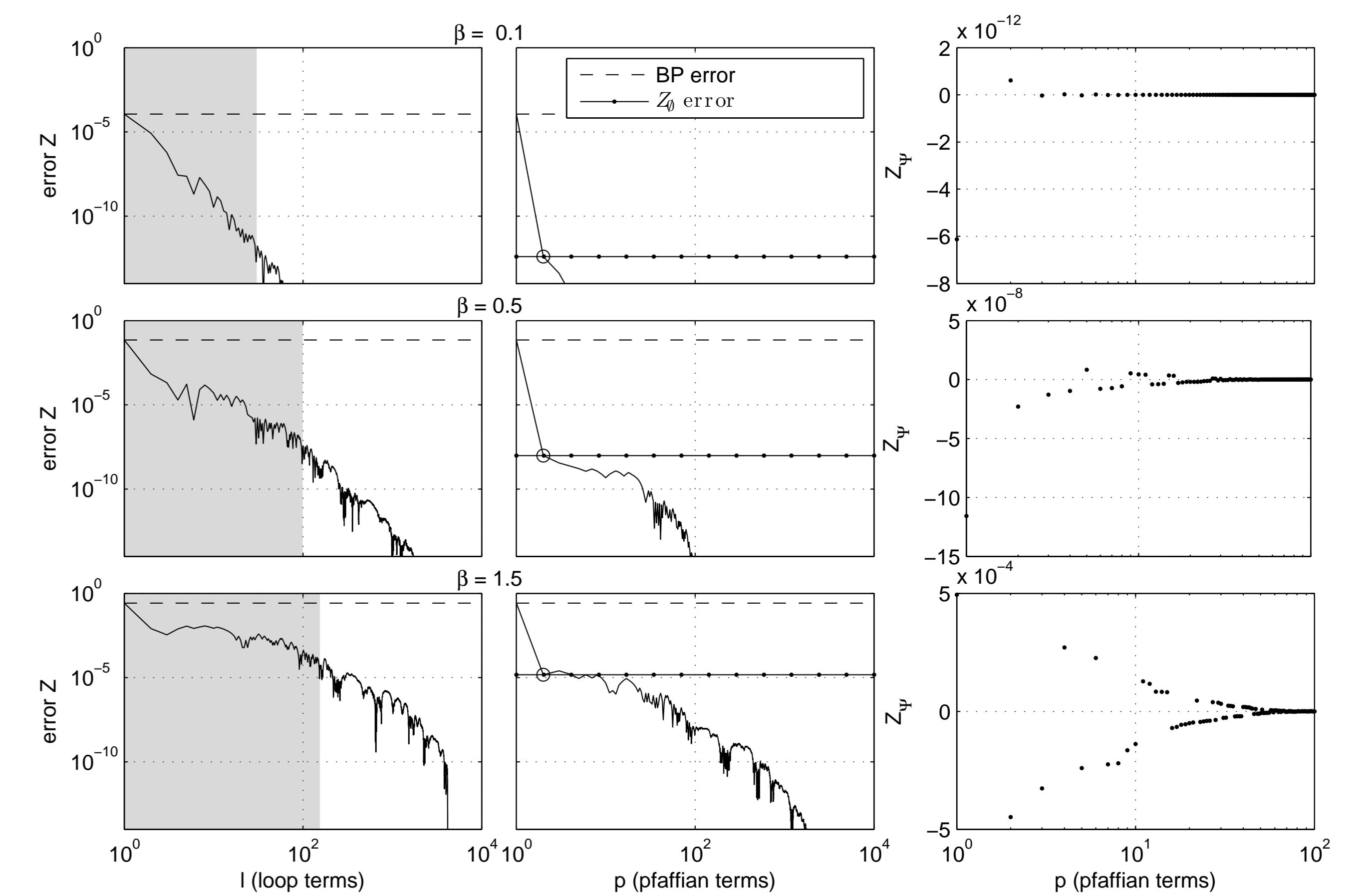
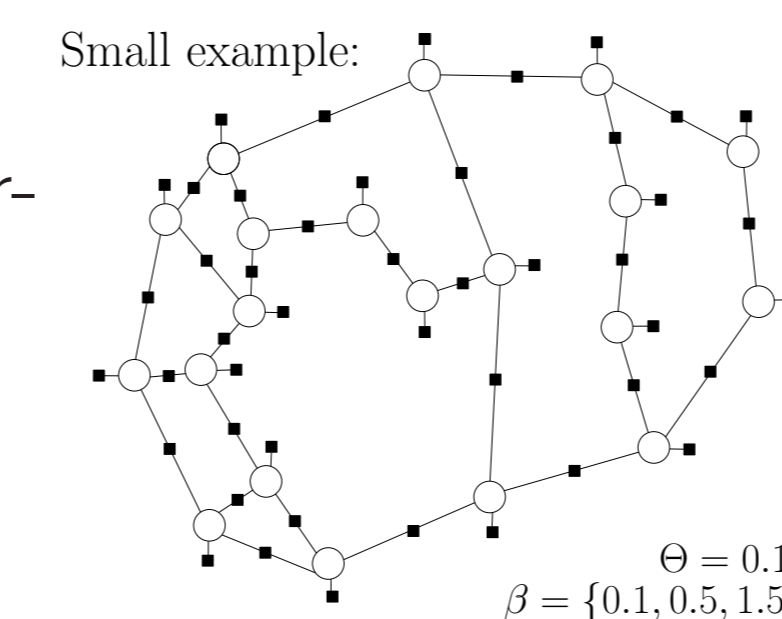
Example:

- $\Psi = \{c, h\}$
- $\Psi = \{e, l\}$
- $\Psi = \{h, l\}$
- $\Psi = \{c, e\}$
- $\Psi = \{c, e, h, l\}$



## Results (Ising model with mixed interactions)

- Loop terms can be **positive or negative**.
- Nonzero external field  $\rightarrow$  The model is planar-intractable
- Pairwise interactions  $\sim \mathcal{N}(0, \beta/2)$ .
- Local fields  $\sim \mathcal{N}(0, \beta\Theta)$ .



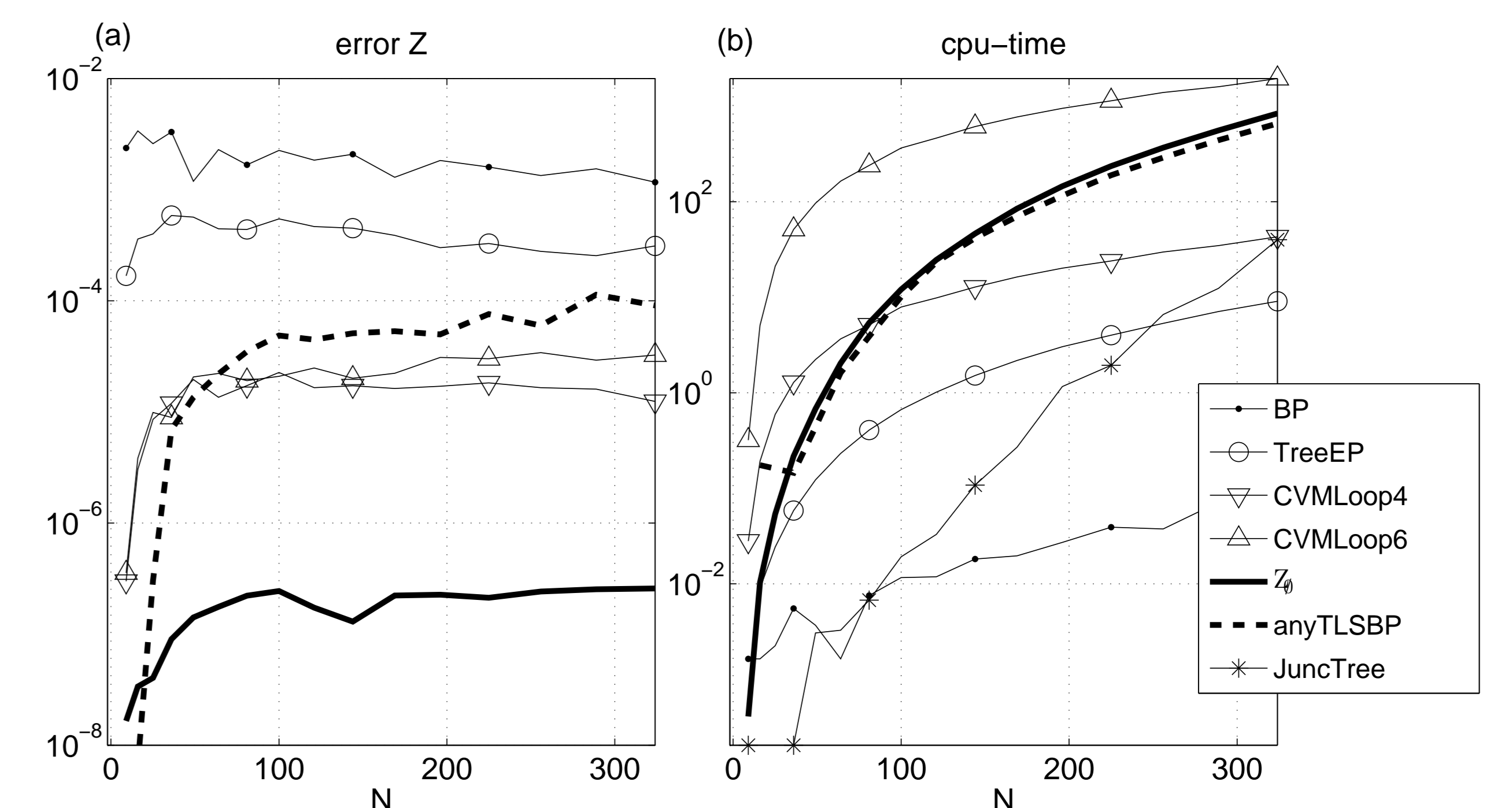
- Without explicit search of loops**, the  $z_\emptyset$  correction can give a **significant improvement** on the BP solution, even in hard problems.

## Scalability on Ising grids with mixed interactions

We compare the  $Z_\emptyset$  approximation with BP and the following algorithms:

- Tree-Structured Expectation Propagation (TreeEP)** [7].
- Cluster Variation Method (CVM-Loopk)** [5].
- anyTLSBP**: Another truncation algorithm for the loop series [4].

Results as a function of the grid size for **strong couplings**  $\beta = 1$  and **very weak local fields**  $\Theta = 0.01$ .



- $Z_\emptyset$  is the best approximate method at the cost of more cpu-time.
- Results are independent of the network size.

- F. Barahona. On the computational complexity of Ising spin glass models. *J. Phys. A-Math. Gen.*, 15(10):3241–3253, 1982.
- M. Chertkov, V. Y. Chernyak, and R. Teodorescu. Belief propagation and loop series on planar graphs. *J. Stat. Mech-Theory E.*, 2008(05):P05003 (19pp), 2008.
- M. Fisher. On the dimer solution of the planar Ising model. *J. Math. Phys.*, 7(10), 1966.
- V. Gómez, J. M. Mooij, and H. J. Kappen. Truncating the loop series expansion for belief propagation. *J. Mach. Learn. Res.*, 8:1987–2016, 2007.
- T. Heskes, K. Albers, and H. J. Kappen. Approximate inference and constrained optimization. In *19th UAI*, pages 313–320, 2003.
- P. W. Kasteleyn. Dimer statistics and phase transitions. *J. Math. Phys.*, 4(2):287–293, 1963.
- T. Minka and Y. Qi. Tree-structured approximations by expectation propagation. In *NIPS*. 04.