

# Extending Monte Carlo Methods to Factor Graphs with Negative and Complex Factors

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**Abstract**—The partition function of a factor graph can sometimes be accurately estimated by Monte Carlo methods. In this paper, such methods are extended to factor graphs with negative and complex factors.

## I. INTRODUCTION

Let  $\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_N$  be finite sets, let  $\mathcal{X}$  be the Cartesian product  $\mathcal{X} \triangleq \mathcal{X}_1 \times \mathcal{X}_2 \times \dots \times \mathcal{X}_N$ , and let  $f$  be a function  $f: \mathcal{X} \rightarrow \mathbb{C}$ . We are interested in numerically computing the partition function

$$Z_f \triangleq \sum_{x \in \mathcal{X}} f(x) \quad (1)$$

for cases where  $N$  is large and  $f$  has some useful factorization.

If  $f$  has a cycle-free factor graph [1], the sum (1) can be computed directly by sum-product message passing. In this paper, however, we are interested in cases where no such factor graph is available (e.g., when the factor graph of  $f$  is a rectangular grid as in Fig. 7).

In the important special case where  $f$  is real-valued and nonnegative (i.e.,  $f(x) \geq 0$  for all  $x \in \mathcal{X}$ ), the probability mass function

$$p(x) \triangleq \frac{f(x)}{Z_f} \quad (2)$$

is the basis of a variety of Monte Carlo methods for estimating (1), see [2], [3]. Such Monte Carlo algorithms have successfully been used, e.g., for the computation of information rates of source/channel models with 2-D memory [4], [5]. Note that  $p$  inherits factorizations (and thus factor graphs) from  $f$ .

In this paper, we extend these Monte Carlo methods to the case where  $f$  is real-valued (but not nonnegative) or complex. The motivation for this extension is twofold. First, the Fourier transform of a function  $f$  preserves the topology of the factor graph, but generally results in complex factors [6], [7]. Second, factor graphs of probability mass functions in quantum mechanics naturally involve complex functions [8]. In both cases, computing quantities of the form (1) is of supreme interest.

In full generality, the computation of (1) is, of course, intractable (already in the nonnegative real case), but good Monte Carlo algorithms may nonetheless work well for many cases of interest (as in the nonnegative real case).

The paper is structured as follows. After introducing some notations in Section II, the proposed algorithms are described in Sections III and IV. The description focuses on the real case; the generalization to the complex case is outlined in Section V. The proposed methods are illustrated by some numerical experiments in Section VI.

## II. PROBABILITIES AND PARTIAL PARTITION FUNCTIONS

We begin the proposed generalization by defining

$$Z_{|f|} \triangleq \sum_{x \in \mathcal{X}} |f(x)| \quad (3)$$

and the probability mass function

$$p_{|f|}(x) \triangleq \frac{|f(x)|}{Z_{|f|}} \quad (4)$$

which will replace (2) in the Monte Carlo algorithms. Note that  $p_{|f|}$  also inherits factorizations (and thus factor graphs) from  $f$ .

In the following, we restrict ourselves to the case where  $f$  is real (but not nonnegative); the generalization to the complex case is indicated in Section V.

Let

$$\mathcal{X}^+ \triangleq \{x \in \mathcal{X} : f(x) > 0\} \quad (5)$$

$$\mathcal{X}^- \triangleq \{x \in \mathcal{X} : f(x) < 0\} \quad (6)$$

$$\mathcal{X}^0 \triangleq \{x \in \mathcal{X} : f(x) = 0\} \quad (7)$$

and thus

$$|\mathcal{X}| = |\mathcal{X}^+| + |\mathcal{X}^-| + |\mathcal{X}^0|. \quad (8)$$

We then define the partial partition functions

$$Z_f^+ \triangleq \sum_{x \in \mathcal{X}^+} f(x) \quad (9)$$

$$Z_f^- \triangleq \sum_{x \in \mathcal{X}^-} f(x) \quad (10)$$

and thus

$$Z_f = Z_f^+ + Z_f^- \quad (11)$$

$$Z_{|f|} = Z_f^+ - Z_f^-. \quad (12)$$

Finally, we define probability mass functions on  $\mathcal{X}^+$  and  $\mathcal{X}^-$  as follows:

$$p_f^+ : \mathcal{X}^+ \rightarrow \mathbb{R} : x \mapsto p_f^+(x) \triangleq \frac{f(x)}{Z_f^+} \quad (13)$$

and

$$p_f^- : \mathcal{X}^- \rightarrow \mathbb{R} : x \mapsto p_f^-(x) \triangleq \frac{f(x)}{Z_f^-} \quad (14)$$

A simple, but key, insight is that sampling from  $p_f^+$  or from  $p_f^-$  can be reduced to sampling from  $p_{|f|}$ : since  $p_{|f|}$  coincides with  $p_f^+$  on  $\mathcal{X}^+$  (up to a scale factor), and with  $p_f^-$  on  $\mathcal{X}^-$  (up to a scale factor), samples  $x^{(1)}, x^{(2)}, \dots$  from  $p_{|f|}$  can be partitioned into samples from  $p_f^+$  and from  $p_f^-$  according to the sign of  $f(x^{(\ell)})$ . For example, samples from  $p_{|f|}$ , and thus both from  $p_f^+$  and from  $p_f^-$ , may be drawn using tree-based Gibbs sampling as in [4], [5], [9].

In this paper, we will now focus on the computation/estimation of the partial partition functions  $Z_f^+$  and  $Z_f^-$  separately. If these estimates are sufficiently accurate,  $Z_f$  can then be computed from (11). This approach is bound to fail, of course, if both  $Z_f^+$  and  $|Z_f^-|$  are large and their difference is small. However, this cancellation problem (which is well-known in quantum mechanics [10]) is beyond the scope of the present paper.

### III. ESTIMATING $Z_f^+$ AND $Z_f^-$

We will now propose two different Monte Carlo methods to estimate the partial partition functions  $Z_f^+$  and  $Z_f^-$ . The first method uses uniform sampling and the second method uses samples from  $p_f^+(x)$  and  $p_f^-(x)$ . Both methods need the value of  $|\mathcal{X}^+|$  and  $|\mathcal{X}^-|$ , the computation of which is addressed in Section IV.

#### A. Uniform Sampling

- 1) Draw samples  $x^{(1)}, x^{(2)}, \dots, x^{(k)}, \dots, x^{(K)}$  uniformly from  $\mathcal{X}^+$ , and samples  $x^{(1)}, x^{(2)}, \dots, x^{(\ell)}, \dots, x^{(L)}$  uniformly from  $\mathcal{X}^-$ .
- 2) Compute

$$\hat{Z}^+ = \frac{|\mathcal{X}^+|}{K} \sum_{k=1}^K f(x^{(k)}) \quad (15)$$

$$\hat{Z}^- = \frac{|\mathcal{X}^-|}{L} \sum_{\ell=1}^L f(x^{(\ell)}) \quad (16)$$

□

It is easily verified that  $E[\hat{Z}^+] = Z_f^+$  and  $E[\hat{Z}^-] = Z_f^-$ .

One way to draw samples uniformly from  $\mathcal{X}^+$  and/or  $\mathcal{X}^-$  is by drawing samples  $x^{(1)}, x^{(2)}, \dots$ , uniformly from  $\mathcal{X}$  and partitioning them according to the sign of  $f(x^{(\ell)})$ .

#### B. Ogata-Tanemura Method [11], [12]

- 1) Draw samples  $x^{(1)}, x^{(2)}, \dots, x^{(k)}, \dots, x^{(K)}$  from  $\mathcal{X}^+$  according to  $p_f^+(x)$ , as in (13), and samples  $x^{(1)}, x^{(2)}, \dots, x^{(\ell)}, \dots, x^{(L)}$  from  $\mathcal{X}^-$  according to  $p_f^-(x)$ , as in (14).

- 2) Compute

$$\hat{\Gamma}^+ = \frac{1}{K|\mathcal{X}^+|} \sum_{k=1}^K \frac{1}{f(x^{(k)})} \quad (17)$$

$$\hat{\Gamma}^- = \frac{1}{L|\mathcal{X}^-|} \sum_{\ell=1}^L \frac{1}{f(x^{(\ell)})} \quad (18)$$

□

It is easy to prove (see Appendix A) that  $E[\hat{\Gamma}^+] = \frac{1}{Z_f^+}$  and  $E[\hat{\Gamma}^-] = \frac{1}{Z_f^-}$ .

### IV. ESTIMATING $|\mathcal{X}^+|$ , $|\mathcal{X}^-|$ , AND $|\mathcal{X}^0|$

Again, we propose two different methods, one for uniform sampling and another for sampling from  $p_{|f|}$ . In each case, the same samples as in Section III can be used.

#### A. Uniform Sampling

- 1) Draw samples  $x^{(1)}, x^{(2)}, \dots, x^{(k)}, \dots, x^{(K)}$  uniformly from  $\mathcal{X}$ .
- 2) Compute

$$\xi^+ = \frac{|\mathcal{X}|}{K} \sum_{k=1}^K [f(x^{(k)}) > 0] \quad (19)$$

$$\xi^- = \frac{|\mathcal{X}|}{K} \sum_{k=1}^K [f(x^{(k)}) < 0] \quad (20)$$

$$\xi^0 = \frac{|\mathcal{X}|}{K} \sum_{k=1}^K [f(x^{(k)}) = 0] \quad (21)$$

□

In these equations,  $[\cdot]$  denotes the Iverson bracket [13, p. 24], which evaluates to one if the condition in the bracket is satisfied and to zero otherwise. It is easy to prove that  $E[\xi^+] = |\mathcal{X}^+|$ ,  $E[\xi^-] = |\mathcal{X}^-|$ , and  $E[\xi^0] = |\mathcal{X}^0|$ .

#### B. Sampling from $p_{|f|}$

We assume  $|\mathcal{X}^0| = 0$ .

- 1) Draw samples  $x^{(1)}, x^{(2)}, \dots, x^{(k)}, \dots, x^{(K)}$  from  $\mathcal{X}$  according to  $p_{|f|}$ , as in (4).
- 2) Compute

$$\hat{\Lambda} = \frac{1}{K} \sum_{k=1}^K \frac{1}{f(x^{(k)})} \quad (22)$$

$$\hat{\Gamma} = \frac{1}{K} \sum_{k=1}^K \frac{1}{|f(x^{(k)})|} \quad (23)$$

□

It is not hard to prove (see Appendix B) that  $E[\hat{\Lambda}] = \frac{|\mathcal{X}^+| - |\mathcal{X}^-|}{Z_{|f|}}$  and  $E[\hat{\Gamma}] = \frac{|\mathcal{X}|}{Z_{|f|}}$ .

Using (8), we can then obtain estimates of  $|\mathcal{X}^+|$  and  $|\mathcal{X}^-|$  from

$$|\mathcal{X}^+| + |\mathcal{X}^-| = |\mathcal{X}| \quad (24)$$

$$|\mathcal{X}^+| - |\mathcal{X}^-| \approx \frac{\hat{\Lambda}}{\hat{\Gamma}} |\mathcal{X}| \quad (25)$$

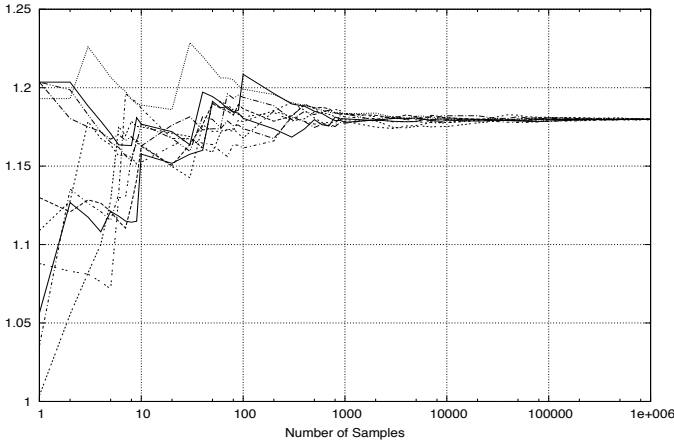


Fig. 1. Estimated  $\frac{1}{N} \log_2(Z_f^+)$  vs. the number of samples, for  $K = 10^5$ ,  $N = 6 \times 6$ , and with factors as in (27). The plot shows 10 sample paths each computed with estimator (15).

## V. EXTENSION TO THE COMPLEX CASE

In (5)–(10), we partitioned  $\mathcal{X}$  and  $Z_f$  according to the sign of  $f(x)$ . In the complex case, we allow more such bins, one for each possible argument (phase) of  $f(x)$ , as illustrated by the example in Section VI-B. The algorithms of Sections III and IV are easily generalized to this setting.

However, the computation of probabilities in factor graphs for quantum probabilities as in [8], can actually be reduced to the real case as in Sections II and III (as will be detailed elsewhere).

## VI. NUMERICAL EXPERIMENTS

In our numerical experiments, we consider two-dimensional factor graphs of size  $N = m \times m$ , with binary variables  $x_1, x_2, \dots, x_N$ , i.e.,  $\mathcal{X}_1 = \mathcal{X}_2 = \dots = \mathcal{X}_N = \{0, 1\}$ .

We suppose  $f : \{0, 1\}^N \rightarrow \mathbb{C}$ , and  $f$  factors into

$$f(x_1, \dots, x_N) = \prod_{k, \ell \text{ adjacent}} \kappa(x_k, x_\ell) \quad (26)$$

where the product runs over all adjacent pairs  $(k, \ell)$ .

The corresponding Forney factor graph with factors as in (26) is shown in Fig. 7, where the boxes labeled “=” are equality constraints [1].

### A. Two-Dimensional Model with Negative Factors

Let us consider a factor graph with factors as

$$\kappa(x_k, x_\ell) = \begin{cases} 1.3, & \text{if } x_k = x_\ell = 0 \\ 1, & \text{if } x_k = x_\ell = 1 \\ -1, & \text{otherwise} \end{cases} \quad (27)$$

For this particular case, we prove in Appendix C that  $|\mathcal{X}^+|$  and  $|\mathcal{X}^-|$  are analytically available as

$$|\mathcal{X}^+| = |\mathcal{X}^-| = 2^{N-1} \quad (28)$$

We estimate  $Z_f^+$  using uniform sampling with estimator (15) of Section III-A, and the Ogata-Tanemura method with estimator (17) of Section III-B.

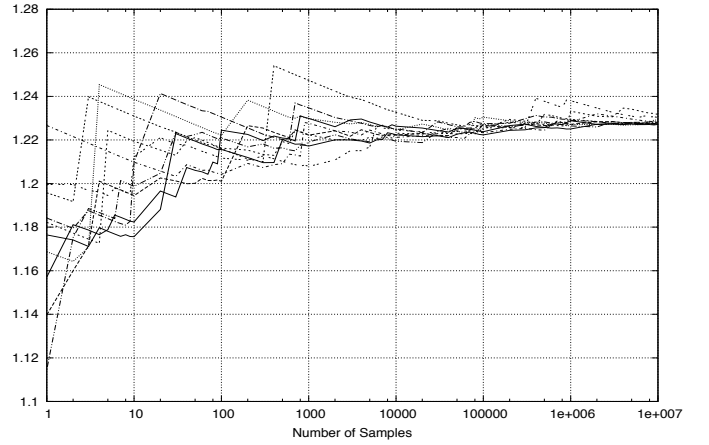


Fig. 2. Same conditions as in Fig. 1, but with  $K = 10^7$  and  $N = 14 \times 14$ .

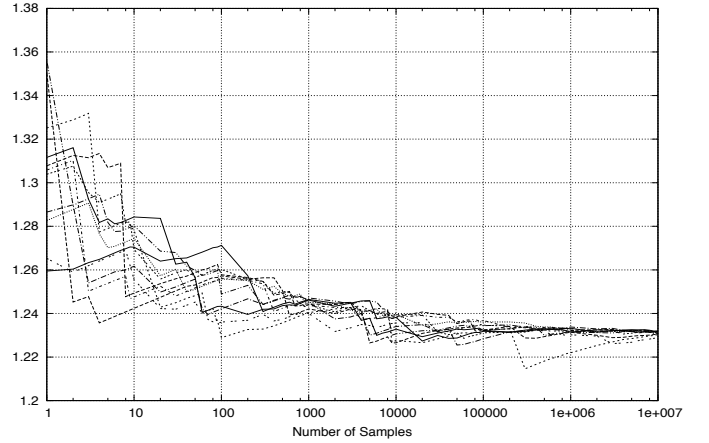


Fig. 3. Estimated  $\frac{1}{N} \log_2(Z_f^+)$  vs. the number of samples, for  $K = 10^7$ ,  $N = 14 \times 14$ , and with factors as in (27). The plot shows 10 sample paths each computed with estimator (17).

Some experimental results are shown in Figs. 1 through 3. All figures refer to  $f$  with factors as in (27), and show the quantity  $\frac{1}{N} \log_2(Z_f^+)$  vs. the number of samples  $K$ .

Figs. 1 and 2 show simulation results using uniform sampling and Fig. 3 using the Ogata-Tanemura method.

For  $N = 6 \times 6$ , the estimated  $\frac{1}{N} \log_2(Z_f^+)$  is about 1.18, and for  $N = 14 \times 14$ , it is about 1.23. As discussed in Section III,  $\frac{1}{N} \log_2(|Z_f^-|)$  can be computed analogously.

### B. Two-Dimensional Model with Complex Factors

We extend our numerical experiments to factor graphs with complex factors as

$$\kappa(x_k, x_\ell) = \begin{cases} 1.5, & \text{if } x_k = x_\ell = 0 \\ i, & \text{if } x_k = x_\ell = 1 \\ 1, & \text{otherwise} \end{cases} \quad (29)$$

where  $i$  is the unit imaginary number.

We define

$$\mathcal{X}^{(+i)} \triangleq \{x \in \mathcal{X} : f(x) \in i\mathbb{R}_{>0}\} \quad (30)$$

$$\mathcal{X}^{(-i)} \triangleq \{x \in \mathcal{X} : f(x) \in -i\mathbb{R}_{>0}\} \quad (31)$$

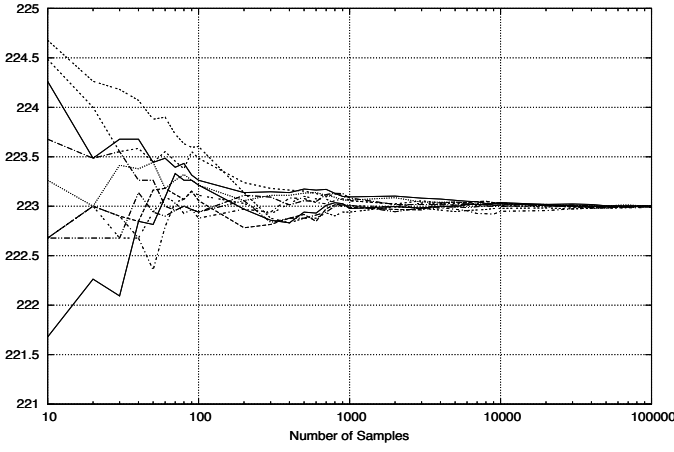


Fig. 4. Estimated  $\log_2(|\mathcal{X}^+|)$  vs. the number of samples, for  $K = 10^5$ ,  $N = 15 \times 15$ , and with factors as in (29). The plot shows 10 sample paths each computed with estimator (19).

where  $\mathbb{R}_{>0} \triangleq \{x \in \mathbb{R} : x > 0\}$ .

To estimate  $|\mathcal{X}^+|$ ,  $|\mathcal{X}^-|$ ,  $|\mathcal{X}^{(i)}|$ , and  $|\mathcal{X}^{(-i)}|$ , we can apply uniform sampling of Section IV-A by first drawing samples  $x^{(1)}, x^{(2)}, \dots$  uniformly from  $\mathcal{X}$ , and then using the samples in the relevant estimators according to the value of  $f(x^{(k)})$ , e.g., in (19) if  $f(x^{(k)})$  is a real positive number.

For a factor graph of size  $N = 15 \times 15$ , Fig. 4 shows the estimated  $\log_2(|\mathcal{X}^+|)$  vs. the number of samples  $K$ . We obtain  $\log_2(|\mathcal{X}^+|) \approx 223$ .

We again apply uniform sampling to estimate  $Z_f^+$ , see Section III-A. Some experimental results are shown in Figs. 5 and 6. All figures refer to  $f$  with factors as in (29), and show the quantity  $\frac{1}{N} \log_2(Z_f^+)$  vs. the number of samples  $K$ .

In Fig. 5, we have  $N = 6 \times 6$  and the estimated  $\frac{1}{N} \log_2(Z_f^+)$  is about 1.26. In Fig. 6, the estimated  $\frac{1}{N} \log_2(Z_f^+)$  is about 1.38 for a factor graph of size  $N = 15 \times 15$ .

## VII. CONCLUSION

We have shown that Monte Carlo methods as in [5] can be extended to estimate the partition function of factor graphs with negative and complex factors. However, the cancellation problem of partial partition functions as in (11) has not been addressed.

### APPENDIX A

Suppose samples  $x^{(1)}, x^{(2)}, \dots, x^{(K)}$  are drawn from  $\mathcal{X}^+$  according to  $p_f^+(x)$ , as in (13). We have

$$\mathbb{E}[\hat{\Gamma}^+] = \frac{1}{K|\mathcal{X}^+|} \sum_{k=1}^K \mathbb{E} \left[ \frac{1}{f(X^{(k)})} \right] \quad (32)$$

$$= \frac{1}{K|\mathcal{X}^+|} \sum_{k=1}^K \sum_{x \in \mathcal{X}^+} \frac{p_f^+(x)}{f(x)} \quad (33)$$

$$= \frac{1}{K|\mathcal{X}^+|} \sum_{k=1}^K \frac{|\mathcal{X}^+|}{Z_f^+} \quad (34)$$

$$= \frac{1}{Z_f^+} \quad (35)$$

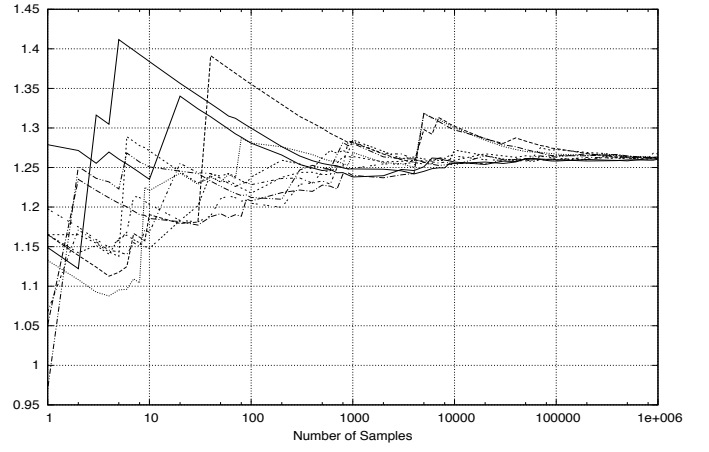


Fig. 5. Estimated  $\frac{1}{N} \log_2(Z_f^+)$  vs. the number of samples, for  $K = 10^6$ ,  $N = 6 \times 6$ , and with factors as in (29). The plot shows 10 sample paths each computed with estimator (15).

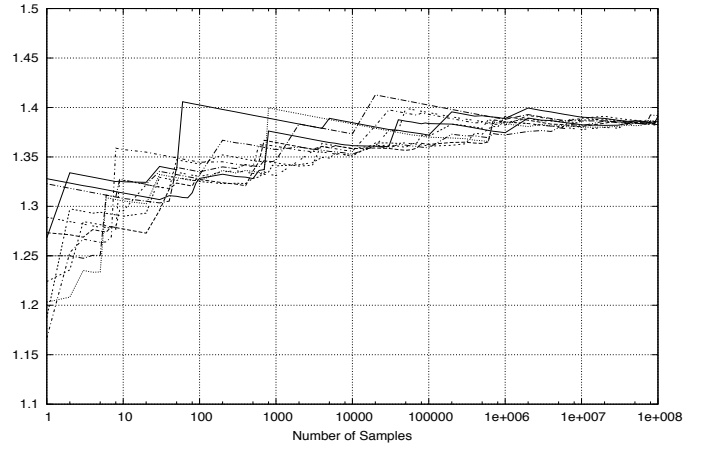


Fig. 6. Estimated  $\frac{1}{N} \log_2(Z_f^+)$  vs. the number of samples, for  $K = 10^8$ ,  $N = 15 \times 15$ , and with factors as in (29). The plot shows 10 sample paths each computed with estimator (17).

The proof of  $\mathbb{E}[\hat{\Gamma}^-] = \frac{1}{Z_f^-}$  follows along the same lines.  $\square$

### APPENDIX B

Suppose samples  $x^{(1)}, x^{(2)}, \dots, x^{(K)}$  are drawn from  $\mathcal{X}$  according to  $p_{|f|}$ , as in (4). We have

$$\mathbb{E}[\hat{\Lambda}] = \frac{1}{K} \sum_{k=1}^K \mathbb{E} \left[ \frac{1}{f(X^{(k)})} \right] \quad (36)$$

$$= \frac{1}{K} \sum_{k=1}^K \sum_{x \in \mathcal{X}} \frac{p_{|f|}(x)}{f(x)} \quad (37)$$

$$= \frac{1}{Z_{|f|}} \sum_{x \in \mathcal{X}} \frac{|f(x)|}{f(x)} \quad (38)$$

$$= \frac{|\mathcal{X}^+| - |\mathcal{X}^-|}{Z_{|f|}} \quad (39)$$

The proof of  $\mathbb{E}[\hat{\Gamma}] = \frac{|\mathcal{X}|}{Z_{|f|}}$  follows along the same lines.  $\square$

## APPENDIX C

We consider a two-dimensional factor graph of size  $N = m \times m$ , where  $m$  is finite and  $m > 2$ , with factors

$$\kappa(x_k, x_\ell) = \begin{cases} a, & \text{if } x_k = x_\ell \\ -a, & \text{otherwise} \end{cases} \quad (40)$$

where  $a \in \mathbb{R}$  and  $a \neq 0$ .

We use the normal factor graph duality theorem [6] to show that for this choice of factors,  $Z_f$ , as defined in (1), is zero.

Consider the dual of the Forney factor graph with factors as in (40). In the dual graph, the equality constraints are replaced by XOR factors, and each factor (40) by its two-dimensional Fourier transform which has the following form

$$\nu(\omega_k, \omega_\ell) = \begin{cases} 4a, & \text{if } \omega_k = \omega_\ell = 1 \\ 0, & \text{otherwise} \end{cases} \quad (41)$$

The corresponding Forney factor graph of the dual graph is shown in Fig. 8, where the unlabeled boxes represent factors as in (41).

Let us denote the partition function of the dual graph by  $Z_d$ . Note that, each factor  $\nu(\omega_k, \omega_\ell)$  is non-zero if  $\omega_k = \omega_\ell = 1$ . Therefore, only the all-ones pattern might have a non-zero contribution to  $Z_d$ . But this pattern does not satisfy the XOR factors of degree three in the dual graph, therefore  $Z_d = 0$ . Using the normal factor graph duality theorem [6, Theorem 2], [7], we conclude that  $Z_f = 0$ . Therefore, using (11) and (12), we obtain

$$Z_f^+ = -Z_f^- = \frac{Z_f}{2} \quad (42)$$

Putting  $a = 1$  (or  $a = -1$ ), we have

$$Z_f^+ = -Z_f^- = 2^{N-1} \quad (43)$$

and hence the following

$$Z_f^+ = |\mathcal{X}^+| \quad (44)$$

$$-Z_f^- = |\mathcal{X}^-| \quad (45)$$

Thus

$$|\mathcal{X}^+| = |\mathcal{X}^-| = 2^{N-1}. \quad (46)$$

Note that for  $m = 2$ , we have  $|\mathcal{X}^+| = |\mathcal{X}|$ ,  $Z_f^+ = Z_f$ , and  $Z_f^- = 0$ . Finally, note that, we can still show  $Z_f = 0$  if  $a \in \mathbb{C}$ .

## ACKNOWLEDGEMENT

The first author would like to thank Radford Neal, Ruslan Salakhutdinov, and Neal Madras for helpful discussions. The authors would also like to thank Pascal Vontobel for his helpful comments on an earlier draft of this paper.

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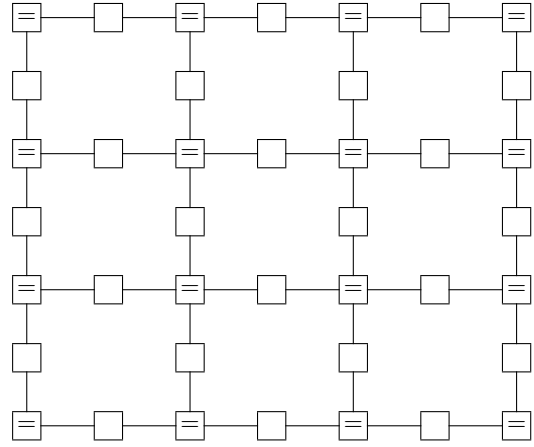


Fig. 7. Forney factor graph with factors as in (40).

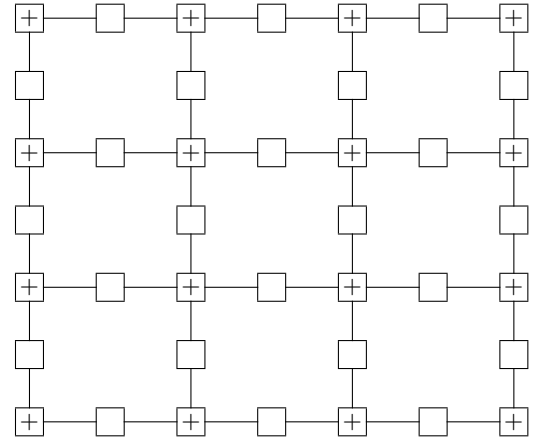


Fig. 8. The dual Forney factor graph where unlabeled boxes represent factors as in (41).

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