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Scaling matrices and counting the perfect matchings in graphs

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Abstract: We investigate efficient randomized methods for approximating the number of perfect matchings in bipartite graphs and general graphs. Our approach is based on assigning probabilities to edges.

Key-words: Permanent approximation, doubly stochastic matrices, Sinkhorn-Knopp scaling, randomized algorithms.

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Normalisation de matrice et dénombrement des couplages parfaits dans les graphes

Résumé : Nous étudions des méthodes randomisées efficaces pour approximer le nombre de couplages parfaits dans des graphes bipartis et des graphes généraux. Notre approche se base sur l'assignation de probabilités aux arêtes

Mots-clés : matrices bistochastiques, permanent, algorithmes randomisés

1 Introduction

We investigate efficient randomized methods for approximating the number of perfect matchings in bipartite graphs and general graphs. Our main tool is a sparse matrix scaling algorithm which we apply to the adjacency matrix of the given graph (bipartite or general) to assign probabilities to the edges and base random choices to these probabilities. For the bipartite case, a given bipartite graph with n vertices on both sides corresponds to an $n \times n$ unsymmetric adjacency matrix \mathbf{A} , where $a_{ij} = 1$ if the vertex i on the first part and the vertex j on the second part are connected, and $a_{ij} = 0$ otherwise. For the general (undirected) case, given a graph with n vertices, the adjacency matrix is considered to be a symmetric matrix where $a_{ij} = a_{ji} = 1$ if there is an edge between vertices i and j . Previously, we have shown that such scaling algorithms are useful in approximating the maximum cardinality of matchings in bipartite graphs [5] and general graphs [6].

Counting perfect matchings in a bipartite graph is equivalent to computing the permanent of its adjacency matrix, which is defined as $Per(\mathbf{A}) = \sum_{\sigma} \prod a_{i,\sigma(i)}$, where the summation runs over all permutations σ of $1, \dots, n$. While we focus on the case where \mathbf{A} is a 0-1 matrix, our techniques are applicable to the weighted case. Approximating the permanent is a well-studied problem. Valiant [21] showed the problem to be \sharp P-Complete. Jerrum et al. [12] discuss an approach using Markov Chains which can provide an $(1 + \epsilon)$ -approximation for the Permanent in fully polynomial time. The complexity required however restricts the algorithm for being useful in practice. Their Markov Chain Monte Carlo (MCMC) approach makes use of the underlying graph being bipartite and the techniques do not generalize easily to the general graph case. Štefankovic et al. [20] take the MCMC approach and highlight the difficulties that arise. They also propose a Markov Chain efficiently estimating the number of perfect matchings in a special graph class. Gurvits and Samorodnitsky [10] and Linial et al. [16] have used matrix scaling and proposed deterministic approximations with exponential guarantees (2^n and e^n respectively).

Our contribution is more on the practical side, as we describe an algorithm with significantly reduced complexity. We propose an alternative selection mechanism to the original algorithm due to Rasmussen [18]. The same approach has also been studied by Beichl and Sullivan [2], but we offer some new insights as well as a more detailed experimental analysis.

The rest of the report is organized as follows: Section 2 introduces the notation and the background on scaling and the permanent, and Section 3 introduces our idea and the pseudocode of the main approach for bipartite graphs. The extension to the general, undirected case is presented in Section 4. Section 5 presents the experimental results, and Section 4.2 briefly discusses related work. Section 6 concludes the report.

2 Notation and background

Matrices are shown in bold upper case letters, e.g., \mathbf{A} . With \mathbf{A}_{ij} we denote the submatrix of matrix \mathbf{A} obtained by deleting the i th row and the j th column. The entries in the matrix are shown with lower-case letters and subscripts, e.g., $a_{i,j}$ denotes the entry of the matrix \mathbf{A} at the i th row and j th column. The column ids of the nonzeros in the i th row of \mathbf{A} is represented as $\mathbf{A}(i, :)$. Vectors are shown with bold, lower-case roman letters, e.g., \mathbf{v} . Components of a vector are shown with the same letter and subscripts, e.g., v_i . For a random variable X , we use $\mathbb{E}[X]$ to denote its expectation. The base of the natural logarithm is shown with e .

Consider a certain quantity P that we are trying to measure. In our situation, P is equivalent

to the permanent. Assume that we have created an unbiased randomized procedure (or estimator as it is more formally referred to) X such that $\mathbb{E}[X] = P$. A technique for measuring P based on X is achieved by combining the output of N copies of X . More specifically, assuming X_i denotes the outcome of the i th estimator, $X' = \sum_{i=1}^N \frac{X_i}{N}$ is the returned estimate for P .

We say that X' for a quantity P achieves (ϵ, δ) -approximation whenever $\Pr(|X' - P| \leq \epsilon P) \geq 1 - \delta$. In general, an (ϵ, δ) approximation can be achieved by simulating $O\left(\frac{\mathbb{E}[X^2]}{\mathbb{E}[X]^2} \cdot \frac{1}{\epsilon^2} \cdot \log\left(\frac{1}{\delta}\right)\right)$ trials. For this reason, the fraction $\frac{\mathbb{E}[X^2]}{\mathbb{E}[X]^2}$ is called the critical ratio as it essentially decides whether the approximation scheme runs in polynomial time or not.

2.1 Scaling to doubly stochastic form

An $n \times n$ matrix $\mathbf{A} \neq 0$ is said to have *support* if there is a perfect matching in the associated bipartite graph. Furthermore, if all the non-zeros belong to at least one perfect matching then the matrix has *total support*.

Any nonnegative matrix \mathbf{A} with total support can be scaled with two (unique) positive diagonal matrices \mathbf{R} and \mathbf{C} such that \mathbf{RAC} is doubly stochastic (that is, the sum of entries in any row and in any column is one) The Sinkhorn-Knopp algorithm [19] is a well-known method for scaling matrices to doubly stochastic form. This algorithm generates a sequence of matrices (whose limit is doubly stochastic) by normalizing the columns and the rows of the sequence of matrices alternately. If \mathbf{A} is symmetric and scalable, then $\mathbf{S} = \mathbf{RAR}$ is doubly stochastic. While the Sinkhorn-Knopp algorithm obtains this symmetric, doubly stochastic matrix in the limit, there are other iterative algorithms that maintain symmetry all along the way [14, 15].

If an $n \times n$ nonnegative matrix \mathbf{A} is scalable to a doubly stochastic matrix $\mathbf{S} = \mathbf{RAC}$ with positive diagonal matrices \mathbf{R} and \mathbf{C} then the function

$$g_{\mathbf{A}}(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{A} \mathbf{y} - \sum_{i=1}^n \ln x_i - \sum_{j=1}^n \ln y_j \quad (1)$$

attains its minimum value for positive x_i and y_i at $\mathbf{x} = \text{diag}(\mathbf{R})$ and $\mathbf{y} = \text{diag}(\mathbf{C})$ [13, Proposition 2]. In particular, an $n \times n$ 0-1 matrix \mathbf{A} has $n \leq g_{\mathbf{A}}(\mathbf{x}, \mathbf{y}) \leq n + n \ln n$, where the lower bound is met by a permutation matrix and the upper bound is met by the matrix of ones, in both cases $\mathbf{x}^T \mathbf{A} \mathbf{y} = n$.

Idel [11] gives a comprehensive survey of known results for computing doubly stochastic scalings. Recently, tighter analysis of the Sinkhorn-Knopp algorithm [3] has been carried out, and other efficient algorithms based on methods for convex optimization have been proposed [1, 4].

We have the following lemma, highlighting a close connection with the scaling factors and the permanents of a matrix and its minors.

Lemma 1. *Let \mathbf{A} be an $n \times n$ 0-1 matrix with total support. Consider \mathbf{R}, \mathbf{C} diagonal scaling matrices such that $\mathbf{S} = \mathbf{RAC}$ is a double stochastic matrix Then,*

$$\text{Per}(\mathbf{S}) = \text{Per}(\mathbf{A}) \cdot \prod_{i=1}^n r_i \cdot c_i.$$

In addition,

$$r_i \cdot c_j = \frac{\text{Per}(\mathbf{A}_{ij})}{\text{Per}(\mathbf{A})} \cdot \frac{\text{Per}(\mathbf{S})}{\text{Per}(\mathbf{S}_{ij})}.$$

Proof. Since \mathbf{R} and \mathbf{C} are diagonal matrices, we have $\text{Per}(\mathbf{S}) = \text{Per}(\mathbf{A}) \prod r_i \prod c_j$. The equality $\text{Per}(\mathbf{S}_{ij}) = \text{Per}(\mathbf{A}_{ij}) \prod_{k \neq i} r_k \prod_{\ell \neq j} c_\ell$ holds, as all diagonal products in \mathbf{S}_{ij} have the same value $\prod_{k \neq i} r_k \prod_{\ell \neq j} c_\ell$. Dividing the two equalities side by side yields the second result. \square

3 Algorithm and its Analysis

The proposed algorithm to estimate the permanent is shown in Algorithm 1. The algorithm takes an $n \times n$, 0-1 matrix \mathbf{A} with a nonzero permanent, and produces a random variable denoted as $X_{\mathbf{A}}$. Initially $X_{\mathbf{A}}$ is equal to one. The algorithm proceeds in n steps. At every step, the algorithm adds a nonzero entry to a matching, thereby obtaining a perfect matching at the end. At step i , a nonzero entry in the i th row of \mathbf{A} is chosen among those columns \mathbf{A} which have not been matched yet. The nonzero entry chosen at row i defines the matching edge for the i th row. The nonzeros are selected according to the values of the entries in a doubly stochastically scaled version of the remaining matrix. The random variable $X_{\mathbf{A}}$ is multiplied by the reciprocal of the chosen nonzero. For the algorithm to work, we discard the nonzeros in $\mathbf{A}^{(i)}$ that cannot be put into a perfect matching. This is achieved by applying the Dulmage-Mendelsohn [7, 17] decomposition, and filtering out the entries that fall into the off-diagonal blocks in a fine decomposition [17].

Algorithm 1 PERMANENT ESTIMATION

Input $n \times n$, 0-1 matrix \mathbf{A}

Output Permanent estimate $X_{\mathbf{A}}$

- 1: $X_{\mathbf{A}} \leftarrow 1$
- 2: $\mathbf{A}^{(1)} \leftarrow \mathbf{A}$
- 3: **for** $i = 1$ **to** n **do**
- 4: Filter out those entries of $\mathbf{A}^{(i)}$ that cannot be put into a perfect matching
- 5: $[\mathbf{R}^{(\sigma,i)}, \mathbf{C}^{(\sigma,i)}] \leftarrow \text{SCALE}(\mathbf{A}^{(i)})$
- 6: Pick a random nonzero column $j \in \mathbf{A}^{(i)}(1, :)$ by using the probability density function

$$p_j = \frac{s_{1,j}}{\sum_{k \in \mathbf{A}^{(i)}(1, :)} s_{1,k}} \text{ for all nonzeros } a_{1,j}^{(i)}$$

- where $s_{t,k} = r_t^{(\sigma,i)} \cdot c_k^{(\sigma,i)}$ is the corresponding entry in the scaled matrix $\mathbf{S} = \mathbf{R}^{(\sigma,i)} \mathbf{A}^{(i)} \mathbf{C}^{(\sigma,i)}$
- 7: $X_{\mathbf{A}} \leftarrow X_{\mathbf{A}} / p_j$
 - 8: $\mathbf{A}^{(i+1)} \leftarrow \mathbf{A}_{1j}^{(i)} \quad \blacktriangleright$ delete the first row and the j th column of $\mathbf{A}^{(i)}$
-

We first comment on the run time complexity of the algorithm. There are n steps, and each step requires computing a Dulmage-Mendelsohn decomposition of a matrix, and scaling a matrix. This can be achieved by $O(\sqrt{nm})$ time on an $n \times n$ matrix with m nonzeros [17]. There are different algorithms for scaling; see the survey by Idel [11], and more recent papers [1, 3, 4]. The most recent methods based on convex optimization techniques [1, 4] have the smallest run time complexity $\tilde{O}(mn + n^{7/3})$ and $\tilde{O}(m^3/2)$ —where the terms involving the deviation from the required row/column sums and $\log n$ are discarded. The Sinkhorn-Knopp algorithm, which is the easiest to implement, has been shown to have $O(\frac{n^2 \ln n}{\varepsilon^2})$ iterations, each iteration costing $O(m)$ time where ε is the allowable deviation from one. Other easy to implement variants are given elsewhere [14, 15]. To the best of our knowledge these algorithms are not yet shown to be of fully polynomial time—there

are results using the second singular value of the final matrix; and there are no run time analysis with respect to ε . In our experience [5, 6], Sinkhorn-Knopp kind of algorithms work well for scaling 0-1 matrices for all computational (or practical) purposes; usually a few iterations suffice to obtain practically all behaving algorithms. In summary, the worst case time complexity of Algorithm 1 is $\tilde{O}(n(\sqrt{nm} + mn^2 \ln n))$ when the Sinkhorn-Knopp algorithm is used for scaling.

The algorithm identifies a perfect matching at the end. Let $\mathbf{R}^{(\sigma,i)}$ and $\mathbf{C}^{(\sigma,i)}$ denote the scaling matrices at the i th step of the algorithm, where the perfect matching σ is returned. Let also $\sigma_1^{(i)}$ denote the column chosen for the first row at the i th step. With this notation, we can write

$$X_{\mathbf{A}} = \frac{1}{\prod_{i=1}^n r_1^{(\sigma,i)} \cdot c_{\sigma_1^{(i)}}^{(\sigma,i)}}.$$

Theorem 2. *Let $X_{\mathbf{A}}$ be a random variable returned by Algorithm 1 for the estimate of the permanent of an $n \times n$, 0-1 matrix \mathbf{A} . Then $\mathbb{E}[X_{\mathbf{A}}] = \text{Per}(\mathbf{A})$.*

Proof. We prove this by induction; As the base case, for $n = 1$, the argument holds. As the inductive hypothesis, assume that the argument holds for $(n-1) \times (n-1)$ matrices. We have the following:

$$\begin{aligned} \mathbb{E}[X_{\mathbf{A}}] &= \sum_{j:a_{1,j} \neq 0} p_j \cdot \frac{1}{p_j} \cdot \mathbb{E}[X_{\mathbf{A}_{1j}}] \\ &= \sum_{j:a_{1,j} \neq 0} \mathbb{E}[X_{\mathbf{A}_{1j}}] \\ &= \sum_{j:a_{1,j} \neq 0} \text{Per}(X_{\mathbf{A}_{1j}}) \text{ by the inductive hypothesis} \\ &= \text{Per}(\mathbf{A}) \end{aligned}$$

□

Lemma 3. *Let \mathbf{A} be $n \times n$ matrix such that $a_{1,j} = 1$, \mathbf{B} be the $(n-1) \times (n-1)$ submatrix \mathbf{A}_{1j} obtained by deleting the 1st row and the j th column of \mathbf{A} , and by discarding entries that cannot be put in a perfect matching. Let \mathbf{R} , \mathbf{C} , \mathbf{D} , and \mathbf{F} be the positive diagonal matrices scaling \mathbf{A} and \mathbf{B} to the doubly stochastic form (\mathbf{RAC} and \mathbf{DBF} are doubly stochastic). Then,*

$$\prod_{i=2}^n r_i \cdot \prod_{i=1, i \neq j}^n c_i \leq e^{r_1 \cdot c_j - 1} \prod_{i=1}^{n-1} d_i \cdot f_i.$$

Proof. Let \mathbf{r}' and \mathbf{c}' be the vectors $\mathbf{r}' = [r_2, \dots, r_n]^T$ and $\mathbf{c}' = [c_1, \dots, c_{j-1}, c_{j+1}, \dots, c_n]^T$. Observe that for the function (1),

$$g_{\mathbf{B}}(\mathbf{d}, \mathbf{f}) \leq g_{\mathbf{B}}(\mathbf{r}', \mathbf{c}')$$

should hold, since \mathbf{D} and \mathbf{F} scale \mathbf{B} to a doubly stochastic form. Therefore,

$$\mathbf{d}^T \mathbf{B} \mathbf{f} - \sum_{i=1}^{n-1} \ln d_i - \sum_{i=1}^{n-1} \ln f_i \leq \mathbf{r}'^T \mathbf{B} \mathbf{c}' - \sum_{i=1}^{n-1} \ln r'_i - \sum_{i=1}^{n-1} \ln c'_i,$$

which we arrange as

$$\mathbf{d}^T \mathbf{B} \mathbf{f} - \mathbf{r}'^T \mathbf{B} \mathbf{c}' \leq \sum_{i=1}^{n-1} \ln d_i + \sum_{i=1}^{n-1} \ln f_i - \sum_{i=1}^{n-1} \ln r'_i - \sum_{i=1}^{n-1} \ln c'_i. \quad (2)$$

The left hand side can be bounded below; since \mathbf{D} and \mathbf{F} scale \mathbf{B} to a doubly stochastic form,

$$\mathbf{d}^T \mathbf{B} \mathbf{f} = n - 1. \quad (3)$$

Since \mathbf{B} is obtained by discarding some (positive) entries in \mathbf{A}_{1j} we have

$$\mathbf{r}'^T \mathbf{B} \mathbf{c}' \leq \mathbf{r}'^T \mathbf{A}_{1j} \mathbf{c}' = n - 2 + r_1 \cdot c_j. \quad (4)$$

Hence, $\mathbf{d}^T \mathbf{B} \mathbf{f} - \mathbf{r}'^T \mathbf{B} \mathbf{c}' \geq 1 - r_1 \cdot c_j$. Note that this last inequality will be tight, if we do not get rid of any entries from \mathbf{A}_{1j} , in which case $\mathbf{B} = \mathbf{A}_{1j}$. Furthermore, since $0 < r_1 \cdot c_j \leq 1$, we see that

$$0 \leq 1 - r_1 \cdot c_1 \leq \mathbf{d}^T \mathbf{B} \mathbf{f} - \mathbf{r}'^T \mathbf{B} \mathbf{c}'.$$

Combining this with (2) and taking exp of all parts, we have

$$1 \leq e^{1-r_1 \cdot c_j} \leq e^{\mathbf{d}^T \mathbf{B} \mathbf{f} - \mathbf{r}'^T \mathbf{B} \mathbf{c}'} \leq \frac{\prod_{i=1}^{n-1} d_i \cdot f_i}{\prod_{i=1}^{n-1} r'_i \cdot c'_i}, \quad (5)$$

and this concludes the proof. \square

Corollary 4. *Let \mathbf{A} be a symmetric $n \times n$ doubly stochastically scalable matrix with $\alpha_{1j} = \alpha_{j1} = 1$ with all diagonal values zero and \mathbf{R} be its scaling matrix. Assume we remove from \mathbf{A} the rows and columns 1, j , and discard entries that are not in support to obtain \mathbf{B} , a symmetric scalable matrix of size $n - 2$, where \mathbf{D} is its scaling matrix. Then*

$$\prod_{k=1, k \neq 1, j}^n r_k \leq e^{r_1 r_j - 1} \prod_{z=1}^{n-2} d_z$$

Proof. The result is obtained as above by applying function g on matrix B . Let \mathbf{r}' be the vector $\mathbf{r}' = [r_2, \dots, r_{j-1}, r_j, \dots, r_n]^T$.

$$\begin{aligned} g_{\mathbf{B}}(\mathbf{d}, \mathbf{d}) &\leq g_{\mathbf{B}}(\mathbf{r}', \mathbf{r}') \\ \mathbf{d}^T \mathbf{B} \mathbf{d} - \sum_{z=1}^{n-2} \ln d_z &\leq \mathbf{r}'^T \mathbf{B} \mathbf{r}' - \sum_{z=1}^{n-2} \ln r'_z - \sum_{z=1}^{n-2} \ln r'_z, \end{aligned}$$

We have

$$\mathbf{d}^T \mathbf{B} \mathbf{d} = n - 2. \quad (6)$$

and

$$\mathbf{r}'^T \mathbf{B} \mathbf{r}' \leq n - 2 + r_1 \cdot r_j. \quad (7)$$

$$n - 2 - 2 \cdot \sum_{z=1}^{n-2} \ln d_z \leq n - 2 - 2 + 2 \cdot (r_1 \cdot r_j) - 2 \cdot \sum_{z=1}^{n-2} \ln r'_z$$

$$-\sum_{z=1}^{n-2} \ln d_z \leq -1 + r_1 \cdot r_j - \sum_{z=1}^{n-2} \ln r'_z$$

The result then follows by taking the exponent in either side. \square

Theorem 5. Let \mathbf{A} be $n \times n$ matrix with total support, and \mathbf{RAC} be its doubly stochastic scaling. Then $\mathbb{E}[X_{\mathbf{A}}^2] \leq \frac{1}{\prod_i r_i \cdot c_i} \cdot \text{Per}(\mathbf{A})$.

Proof. We prove the theorem by induction. The base case $n = 1$ holds trivially. Assume that the theorem holds for $(n - 1) \times (n - 1)$ matrices. We then have

$$\begin{aligned} \mathbb{E}[X_{\mathbf{A}}^2] &= \sum_{a_{1,j} \neq 0} r_1 \cdot c_j \cdot \left(\frac{1}{r_1^2 \cdot c_j^2} \cdot \mathbb{E}[X_{\mathbf{A}_{1j}}^2] \right) \\ \mathbb{E}[X_{\mathbf{A}}^2] &= \sum_{a_{1,j} \neq 0} \frac{1}{r_1 \cdot c_j} \cdot \mathbb{E}[X_{\mathbf{A}_{1j}}^2] \\ \mathbb{E}[X_{\mathbf{A}}^2] &\leq \sum_{a_{1,j} \neq 0} \frac{1}{r_1 \cdot c_j} \cdot \frac{1}{\prod_z d_z \cdot e_z} \cdot \text{Per}(\mathbf{A}_{1j}) \\ &\quad \text{by the inductive hypothesis, where } \mathbf{D} \text{ and } \mathbf{E} \text{ scale } \mathbf{A}_{1j} \\ \mathbb{E}[X_{\mathbf{A}}^2] &\leq \sum_{a_{1,j} \neq 0} \frac{1}{r_1 \cdot c_j} \cdot \frac{1}{\prod_{z=2}^n r_z \cdot \prod_{z=1, z \neq j}^n c_z} \cdot \text{Per}(\mathbf{A}_{1j}) \quad \text{by Lemma 3,} \\ \mathbb{E}[X_{\mathbf{A}}^2] &\leq \frac{1}{\prod_i r_i \cdot c_i} \cdot \sum_{a_{1,j} \neq 0} \text{Per}(\mathbf{A}_{1j}) \\ \mathbb{E}[X_{\mathbf{A}}^2] &\leq \frac{1}{\prod_i r_i \cdot c_i} \cdot \text{Per}(\mathbf{A}) \end{aligned}$$

\square

We can also propose a theorem which uses mean values to provide with an upper bound

Theorem 6. $\mathbb{E}[X_{\mathbf{A}}^2] \leq \text{Per}(\mathbf{A}) \cdot \text{mean}(\sum_{\sigma} e^{\sum_j r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}}) \cdot \frac{e^{-n}}{\prod_i r_i \cdot c_i}$.

Proof. Consider any perfect matching σ of \mathbf{A} . Let $X_{\mathbf{A}_{\sigma}}^2 = \frac{1}{\prod_{i=1}^n r_1^{(\sigma,i)} c_{\sigma_1^{(i)}}^{(\sigma,i)}}$ be its contribution to the $\mathbb{E}[X_{\mathbf{A}}^2]$ value, which is equivalent to the value of the random variable $X_{\mathbf{A}}$ should this matching be returned.

We use a bottom-up induction to prove the following: Let $1 \leq i \leq n$. Then

$$\prod_{j=i}^n \frac{1}{r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}} \leq \frac{e^{\left(\sum_{j=i}^n r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)} \right) - n - 1 + i}}{\prod_{j=i}^n r_{j-i+1}^{(\sigma,i)} c_{\sigma_1^{(j)}}^{(\sigma,i)}}. \quad (8)$$

That is we provide a relation for the scaling matrices $\mathbf{R}^{(\sigma,i)}$ and $\mathbf{C}^{(\sigma,i)}$ of the i th step and the multiplication of all $r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}$ where $j \geq i$. We use the index $j - i + 1$ to refer to rows with index greater than $i \geq 1$ because in the reshaped matrix of the i th step, row i occupies the position 1. The idea resembles the proof of Theorem 5 except that here a tighter upper bound is provided by having the numerator less than one.

For $i = n$ it holds. Assume it holds until i where $i > 1$. Then, for $i - 1$

$$\prod_{j=i-1}^n \frac{1}{r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}} \leq \frac{e^{\left(\sum_{j=i}^n r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}\right) - n - 1 + i}}{\prod_{j=i}^n r_{j-i+1}^{(\sigma,i)} c_{\sigma_1^{(j)}}^{(\sigma,i)}} \cdot \frac{1}{r_1^{(\sigma,i-1)} c_{\sigma_1^{(i-1)}}^{(\sigma,i-1)}}$$

by the induction hypothesis holding for value i .

Note that $\prod_{j=i}^n r_{j-i+1}^{(\sigma,i)} c_{\sigma_1^{(j)}}^{(\sigma,i)}$ is the product of the scaling factors at the i th step, and that $\prod_{j=i}^n r_{j-(i-1)+1}^{(\sigma,i-1)} c_{\sigma_1^{(j)}}^{(\sigma,i-1)}$ is the product of the scaling factors at the $(i - 1)$ st step excluding the row scaling entry $r_1^{(\sigma,i-1)}$ and the associated column scaling. Therefore, we can replace $\frac{1}{\prod_{j=i}^n r_{j-i+1}^{(\sigma,i)} c_{\sigma_1^{(j)}}^{(\sigma,i)}}$

with $\frac{e^{\left(r_1^{(\sigma,i-1)} c_{\sigma_1^{(i-1)}}^{(\sigma,i-1)}\right) - 1}}{\prod_{j=i}^n r_{j-(i-1)+1}^{(\sigma,i-1)} c_{\sigma_1^{(j)}}^{(\sigma,i-1)}}$ using Lemma 3 to obtain an upper bound. That is

$$\prod_{j=i-1}^n \frac{1}{r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}} \leq \frac{e^{\sum_{j=i}^n r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)} - n - 1 + i} \cdot e^{r_1^{(\sigma,i-1)} c_{\sigma_1^{(i-1)}}^{(\sigma,i-1)} - 1}}{\prod_{j=i}^n r_{j-i+2}^{(\sigma,i-1)} c_{\sigma_1^{(j)}}^{(\sigma,i-1)}} \cdot \frac{1}{r_1^{(\sigma,i-1)} c_{\sigma_1^{(i-1)}}^{(\sigma,i-1)}}.$$

We see that in both terms of the fraction we can include $r_1^{(\sigma,i-1)} c_{\sigma_1^{(i-1)}}^{(\sigma,i-1)}$ to its respective aggregator

$$\prod_{j=i-1}^n \frac{1}{r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}} \leq \frac{e^{\sum_{j=i-1}^n r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)} - n - 1 + (i-1)}}{\prod_{j=i-1}^n r_{j-i+2}^{(\sigma,i-1)} c_{\sigma_1^{(j)}}^{(\sigma,i-1)}}$$

which concludes the proof of (8), as for $j = i - 1$, we have $j - i + 2 = 1$.

Thus for $i = 1$ we get the following:

$$X_{\mathbf{A}_\sigma}^2 \leq \frac{e^{\sum_j r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}}}{\prod_i r_i \cdot c_i} \cdot e^{-n}$$

Since

$$\mathbb{E}[X_{\mathbf{A}}^2] = \sum_{\sigma} X_{\mathbf{A}_\sigma}^2, \quad \text{we get that}$$

$$\mathbb{E}[X_{\mathbf{A}}^2] \leq \sum_{\sigma} \frac{e^{\sum_j r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}}}{\prod_i r_i \cdot c_i} \cdot e^{-n},$$

as we have $Per(\mathbf{A})$ permutations each with each own value. Replacing with the mean multiplied by $Per(\mathbf{A})$ concludes the theorem. \square

Theorem 7. *Let \mathbf{A} be $n \times n$ matrix with total support, and \mathbf{RAC} be its doubly stochastic scaling. There exists a positive vector \mathbf{k} such that $\mathbb{E}[X_{\mathbf{A}}^2] \leq \frac{e^{v-n}}{\prod_i r_i \cdot c_i} \cdot Per(\mathbf{A})$, where $v = \sum_i k_i = \|\mathbf{k}\|_1 \leq n$.*

Proof. We will repeat the proof of Theorem 5 and precise how we can build \mathbf{k} . The base case $n = 1$ holds trivially with $k_1 = 1$. We then have

$$\mathbb{E}[X_{\mathbf{A}}^2] = \sum_{a_{1,j} \neq 0} r_1 \cdot c_j \cdot \left(\frac{1}{r_1^2 \cdot c_j^2} \cdot \mathbb{E}[X_{\mathbf{A}_{1j}}^2] \right)$$

$$\mathbb{E}[X_{\mathbf{A}}^2] = \sum_{a_{1,j} \neq 0} \frac{1}{r_1 \cdot c_j} \cdot \mathbb{E}[X_{\mathbf{A}_{1j}}^2]$$

$$\mathbb{E}[X_{\mathbf{A}}^2] \leq \sum_{a_{1,j} \neq 0} \frac{1}{r_1 \cdot c_j} \cdot \frac{e^{v^{(j)}-(n-1)}}{\prod_z d_z \cdot e_z} \cdot Per(\mathbf{A}_{1j})$$

by the inductive hypothesis, where \mathbf{D} and \mathbf{E} scale \mathbf{A}_{1j} ,

$\mathbf{k}^{(j)}$ is the vector associated with \mathbf{A}_{1j} , and $v^{(j)} = \|\mathbf{k}^{(j)}\|$

$$\mathbb{E}[X_{\mathbf{A}}^2] \leq \sum_{a_{1,j} \neq 0} \frac{1}{r_1 \cdot c_j} e^{r_1 c_j - 1} \cdot \frac{e^{v^{(j)}-(n-1)}}{\prod_{z=2}^n r_z \cdot \prod_{z=1, z \neq j}^n c_z} \cdot Per(\mathbf{A}_{1j}) \quad \text{by Lemma 3,}$$

let $k_1 = \max_j r_1 c_j$ and $k_\ell = \max_j \mathbf{k}_{\ell-1}^{(j)}$ for $\ell = 2, \dots, n$ to define \mathbf{k}

$$\mathbb{E}[X_{\mathbf{A}}^2] \leq \frac{e^{v-n}}{\prod_i r_i \cdot c_i} \cdot \sum_{a_{1,j} \neq 0} Per(\mathbf{A}_{1j})$$

$$\mathbb{E}[X_{\mathbf{A}}^2] \leq \frac{e^{v-n}}{\prod_i r_i \cdot c_i} \cdot Per(\mathbf{A}).$$

Since each entry added to \mathbf{k} is no larger than one, $v = \sum_i k_i = \|\mathbf{k}\|_1 \leq n$ holds, hence the proof. \square

Note that Theorem 7 implies Theorem 5 if we set $k_i = 1$. The theorem is constructive but does not yield a polynomial algorithm. Algorithm 1 can be made to construct a \mathbf{k} associated with a perfect matching σ obtained at the end, to show how much $\frac{1}{\prod_{i=1}^n r_1^{(\sigma,i)} \cdot c_{\sigma_1^{(i)}}^{(\sigma,i)}}$ deviates from a potential

bound that can be obtained by $mean(\sum_{\sigma} e^{\sum_j r_1^{(\sigma,j)} c_{\sigma_1^{(j)}}^{(\sigma,j)}}) \cdot \frac{e^{-n}}{\prod_i r_i \cdot c_i}$ from the previous theorem.

3.1 Related work

Similar algorithms exist in the literature: Rasmussen [18] investigates a simpler approach in which the selection probabilities are uniform (no scaling), and no edges are discarded (so that the estimator returns zero in many cases). He shows that the estimator X_S is unbiased and also obtains the bound $\mathbb{E}[X_S]^2 \leq Per(\mathbf{A})^2 n!$, although $Per(\mathbf{A})^2$ can be reduced to $Per(\mathbf{A})$. Beichl and Sullivan [2]

proposed the same algorithm and performed some analysis, where the $\mathbb{E}[X_{\mathbf{A}}^2]$ is bound using a notation to denote the average value of

$$\frac{1}{\prod_{i=1}^n r_1^{(\sigma,i)} \cdot c_{\sigma_1}^{(\sigma,i)}}$$

over all perfect matchings. This analysis is valuable in the sense to show that scaling helps, but it does not yield computable bounds. On the other hand, our analysis in Theorem 5 gives efficiently computable bounds which are loose and we believe can be extended.

4 An estimator for undirected graphs

Having applied the doubly stochastic sampling on bipartite graphs in the previous section, here we investigate how to extend our approach for the general case. Our aim is to count the number of perfect matchings in undirected graphs. This variant of the algorithm has similar properties with the algorithm for the bipartite case. In particular with X_G showing the random variable and $M(G)$ showing the number of perfect matchings in G , it can be shown that

$$\mathbb{E}[X_G^2] \leq M(G) \frac{1}{\prod_i r_{i,i}},$$

where $r_{i,i}$ s are the diagonal entries of the scaling factor \mathbf{R} of the adjacency matrix of G . Note that since the adjacency matrix \mathbf{A} is symmetric, its scaling is in the form $\mathbf{S} = \mathbf{R}\mathbf{A}\mathbf{R}$, i.e., we do not need separate scaling values for rows and columns. Algorithm 2 shows the pseudocode of the proposed approach.

Algorithm 2 PERMANENT ESTIMATION

Input $G = (V, E)$ is an undirected graph with $n = |V|$ vertices, having a perfect matching

Output An estimate X_G of the number of perfect matchings in G

- 1: $X_G \leftarrow 1$
- 2: $G^{(1)} \leftarrow G$
- 3: **for** $i = 1$ **to** n **by** increments of two **do**
- 4: Let $\mathbf{A}^{(i)}$ be the adjacency matrix of $G^{(i)}$.
- 5: Filter out those entries of $\mathbf{A}^{(i)}$ that cannot be put into a perfect matching in the bipartite graph corresponding to $\mathbf{A}^{(i)}$, and let $G^{(i)}$ correspond to the graph of $\mathbf{A}^{(i)}$
- 6: $[\mathbf{R}^{(i)}] \leftarrow \text{scale}(\mathbf{A}^{(i)})$
- 7: Let $\mathcal{T} = \{j : a_{1,j}^{(i)} \neq 0 \text{ and } G^{(i)} - \{v_1, v_j\} \text{ has a perfect matching}\}$
- 8: Pick a random nonzero column j from \mathcal{T} by using the probability density function

$$p_k = \frac{s_{1,k}}{\sum_{t \in \mathcal{T}} s_{1,t}}, \text{ for all nonzero } a_{1,k}^{(i)} \text{ with } k \in \mathcal{T}$$

where $s_{t,k} = r_t^{(i)} \cdot r_k^{(i)}$ is the corresponding entry in the scaled matrix $\mathbf{S} = \mathbf{R}^{(i)} \mathbf{A}^{(i)} \mathbf{R}^{(i)}$

- 9: $X_G \leftarrow X_G / p_j$
 - 10: $G^{(i+1)} \leftarrow G^{(i)} - \{v_1, v_j\}$ ► delete the vertices v_1 and v_j from $G^{(i)}$ to obtain $G^{(i+1)}$
-

At the beginning of an iteration i , we have a graph $G^{(i)}$ having at least one perfect matching. We then get the adjacency matrix $\mathbf{A}^{(i)}$ of this graph, which is symmetric. We then check if all entries in $\mathbf{A}^{(i)}$ can put into a traversal; that is we look at the Dulmage-Mendelsohn decomposition of the bipartite graph associated with $\mathbf{A}^{(i)}$, and discard edges that cannot be in a perfect matching. We discard those entries (symmetrically) and obtain a sparser matrix $\mathbf{A}^{(i)}$ and scale the resulting matrix. This also translates to an updated $G^{(i)}$. Then, for each edge incident on the first vertex of $G^{(i)}$, we test if there is a perfect matching in $G^{(i)}$ containing that edge. Among all the edges that are inside at least one perfect matching, we choose an edge from a probability distribution where the probabilities are proportional to the scaling entries of the allowed edges. Notice that

$$p_k = \frac{s_{1,k}}{\sum_{t \in \mathcal{T}} s_{1,t}}$$

where $\mathcal{T} = \{j : a_{1,j}^{(i)} \neq 0 \text{ and } G^{(i)} - \{v_1, v_j\} \text{ has a perfect matching}\}$, $s_{1,t} = r_1^{(i)} \cdot r_t^{(i)}$, and $0 < \sum_{t \in \mathcal{T}} s_{1,t} \leq 1$. Therefore, $p_k \geq r_1^{(i)} \cdot r_k^{(i)}$ at Line 8 of Algorithm 2.

By using a proof similar to that of Theorem 2, we can show the following about the expected value of Algorithm 2.

Theorem 8. *Let X_G be a random variable returned by Algorithm 2. Then $\mathbb{E}[X_G] = M(G)$, where $M(G)$ represents the number of perfect matchings in the graph G .*

Proof. We prove the claim via induction. As the base-case, we consider $n = 2$ and the argument holds where the adjacency matrix is $\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Assume that the inductive hypothesis holds for $n - 2$. Let G_{ij} be obtained by removing vertices v_i and v_j from G , which corresponds to deleting the rows and the columns i, j of the adjacency matrix of G to form the $(n - 2) \times (n - 2)$ adjacency matrix \mathbf{A}_{ij} of G_{ij} . We have the following:

$$\begin{aligned} \mathbb{E}[X_G] &= \sum_{j: a_{1,j} \neq 0} p_j \cdot \frac{1}{p_j} \cdot \mathbb{E}[X_{G_{ij}}] \\ &= \sum_{j: a_{1,j} \neq 0} \mathbb{E}[X_{G_{ij}}] \\ &= \sum_{j: a_{1,j} \neq 0} M(G_{ij}) \text{ by the inductive hypothesis} \\ &= M(G) \end{aligned}$$

□

Next, we show a theorem bounding $\mathbb{E}[X_G^2]$.

Theorem 9. *Let G be an undirected graph, \mathbf{A} be the $n \times n$ adjacency matrix of G with all supported nonzeros, and \mathbf{R} be the diagonal matrix which scales \mathbf{A} into the doubly stochastic form, e.g., $\mathbf{R}\mathbf{A}\mathbf{R}$ is doubly stochastic. Then $\mathbb{E}[X_G^2] \leq M(G) \cdot \frac{1}{\prod_i r_i}$.*

Proof. We prove the theorem by induction. The base case $n = 2$ holds trivially. Let the inductive hypothesis be that the argument holds for graphs with $n - 2$ vertices.

$$\mathbb{E}[X_G^2] = \sum_{a_{i,j} \neq 0} p_j \cdot \left(\frac{1}{p_j^2} \cdot \mathbb{E}[X_{G_{ij}}^2] \right)$$

$$\mathbb{E}[X_G^2] = \sum_{a_{i,j} \neq 0} \frac{1}{p_j} \cdot \mathbb{E}[X_{G_{ij}}^2]$$

$$\mathbb{E}[X_G^2] \leq \sum_{a_{i,j} \neq 0} \frac{1}{r_i \cdot r_j} \cdot \mathbb{E}[X_{G_{ij}}^2]$$

because $p_j \geq r_i \cdot r_j$ by the definition p_j at Line 8 of Algorithm 2,

$$\mathbb{E}[X_G^2] \leq \sum_{a_{i,j} \neq 0} \frac{1}{r_i \cdot r_j} \cdot \frac{1}{\prod_z d_z} \cdot M(G_{ij})$$

by the inductive hypothesis, where $\mathbf{R}_{ij} \mathbf{A}_{ij} \mathbf{R}_{ij}$ is doubly stochastic

$$\mathbb{E}[X_G^2] \leq \sum_{a_{i,j} \neq 0} \frac{1}{r_i \cdot r_j} \cdot \frac{1}{\prod_{z \neq i, z \neq j} r_z} \cdot M(G_{ij}) \quad \text{by Corollary 4,}$$

$$\mathbb{E}[X_G^2] \leq \frac{1}{\prod_z r_z} \cdot \sum_{a_{i,j} \neq 0} M(G_{ij})$$

$$\mathbb{E}[X_G^2] \leq \frac{1}{\prod_z r_z} \cdot M(G)$$

□

Note that as in the bipartite case, we have the product of the inverse of the scaling entries for each vertex in the formula.

4.1 Filtering out redundant edges

A complication for the undirected case is that eliminating the edges that are not in any perfect matching no longer works. We demonstrate this by using the fact below:

Fact 10. *Let G be an undirected graph, \mathbf{A} be the $n \times n$ adjacency matrix of G with all supported nonzeros. Let G' be the bipartite graph with $2n$ vertices obtained from \mathbf{A} . Then $Per(\mathbf{A})$ is larger than or equal to the number of perfect matchings in G .*

Proof. For each perfect matching in $G = (V, E)$, there is a corresponding perfect matching in $G' = (V', E')$: Let $\{(u_1, u_2), \dots, (u_{n-1}, u_n)\}$ be a matching in G where $u_i \in V$ for $i \in \{1, \dots, n\}$. Let the vertices in the first and the second part of the bipartite graph G' are denoted as v_i s and w_i s, respectively, where $v_i \in V'$ and $w_i \in V'$ for $i \in \{1, \dots, n\}$.

Since the edge (u_i, u_{i+1}) is in the matching for $i \in \{1, \dots, n\}$, it is in G . Therefore $a_{i,i+1} = a_{i+1,i+1} = 1$ are nonzeros in \mathbf{A} . Therefore in the bipartite graph G' , we have the edges $(v_i, w_{i+1}) \in E'$ and $(v_{i+1}, w_i) \in E'$. From these edges a perfect matching can be constructed in G' .

Therefore for each matching in G , one can construct a perfect matching in G' and the number of the perfect matchings in G' is equal to $Per(\mathbf{A})$. Hence, $Per(\mathbf{A})$ is larger than or equal to the number of perfect matchings in G .

□

Although the above fact ensures that any off-diagonal edge in the Dulmage-Mendehlson decomposition of \mathbf{A} cannot belong to a perfect matching in G , it does not help us eliminate edges that do not belong to such symmetrical matchings (v_i, w_j) and (w_j, v_i) .

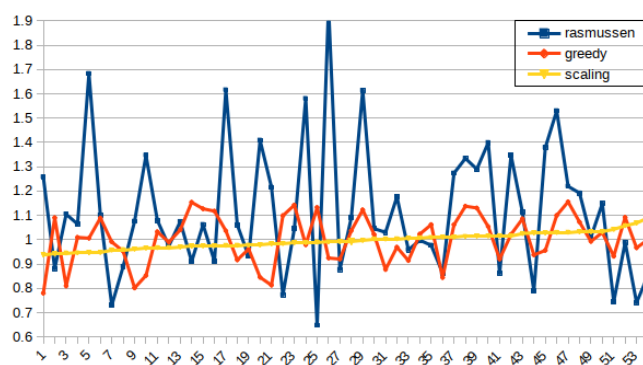
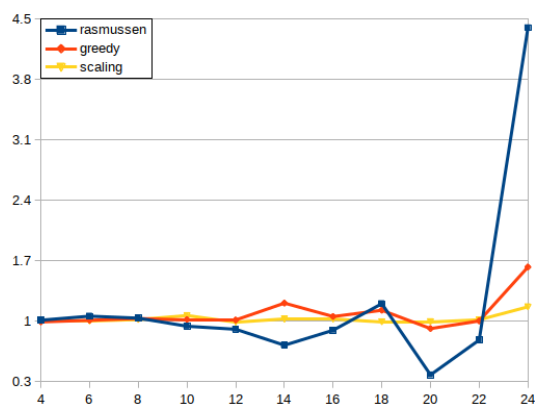
4.2 Related work

Fürer and Kasiviswanathan [9] discuss three randomized algorithms (Simple, REP, and Greedy) similar to ours. The one called Simple is a direct adaptation of Rasmussen's for graphs, and selects neighbours with uniform probability. REP extends Simple such that at certain points during the execution, it creates k copies where each copy selects its own neighbor and the procedure continues in a similar way in each copy. The results of each copy are later combined. They have also proposed a similar algorithm for the bipartite case [8]. Greedy attempts to assign probabilities in a better way by selecting each node with probability inversely proportional to its degree. They conclude that Simple is easy to analyze but has with high worst case bound; Greedy looks good on many graphs but difficult to analyze; and REP is the fastest for random (Erdős-Renyi) graphs with again a high worst case bound. If Greedy were to chose a random neighbor with probability equal to the degree of the neighbor, then it would have been equivalent to applying a single step of Sinkhorn-Knopp. Our approach can be seen as more complicated variant of this approach, yet its analysis seems simpler thanks to the minimization properties of the scaling factors of the function $g_{\mathbf{A}}(x, y)$ shown in (1).

5 Experiments

To see how the proposed heuristic fares in practice, we compare it against the original estimator of Rasmussen as well as Greedy. We used an improved version of Rasmussen's in which edges that do not participate in perfect matchings are discarded. Additionally for all three variants in this paper use a small heuristic and select at each step the row with the least nonzeros remaining. For each test, we take 1000 samples and report their mean. Initially we consider random matrices of size 40 and sparsity $\frac{4}{n}$. Such matrices can have large permanents (e.g., around 10^7) and are among the largest an exact algorithm can handle. The results which are summarized in Figure 1(a) showcase that our approach always has good performance. In contrast, Rasmussen's estimator often reports results that are a lot worse than the other two approaches (even if modified to avoid returning zeros). Greedy exhibits better performance than Rasmussen's, while our approach has better performance than Greedy (it has smaller and less frequent deviation from the value of the permanent).

To provide results with larger n , we focus on the class of matrices which represent grids and for which an exact formula for the permanent is known. The results presented in Figure 1(b) concur with the previous test, suggesting that the assignment of probabilities via scaling makes the overall procedure more reliable.

(a) sparse 40×40 matrices

(b) grid graphs

Figure 1: The approximation ratio for the three approaches in 54 random graphs with $n = 40$ and $4/n$ sparsity factor (in increasing order of the approximation ratio of our estimator), and on square grids of even length as the length increases.

6 Conclusion

We have proposed a technique for approximating the permanent based on matrix scaling. We manage to prove loose yet computable upper bounds for $\mathbb{E}[X_A^2]$. The experimental analysis suggests that an improvement over previous similar methodologies is possible. Future work involves bounding the estimated factors for special graph classes.

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