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COUNTING WITH COMBINED SPLITTING AND CAPTURE–RECAPTURE METHODS

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We apply the splitting method to three well-known counting problems, namely 3-SAT, random graphs with prescribed degrees, and binary contingency tables. We present an enhanced version of the splitting method based on the capture-recapture technique, and show by experiments the superiority of this technique for SAT problems in terms of variance of the associated estimators, and speed of the algorithms.

Keywords Capture–Recapture; Counting; Gibbs Sampler; Splitting.

Mathematics Subject Classification Primary 65C05, 65C35; Secondary 68W20, 60C05.

1. INTRODUCTION

In this article we apply the splitting method introduced in Botev and Kroese\(^{[4]}\) to a variety of counting problems in the class #P-complete. The classes #P and #P-complete have been introduced by Valiant\(^{[19]}\) in the following way. Given any decision problem in the class NP, one can formulate the corresponding counting problem which asks for the total number of solutions for a given instance of the problem. The set of all these counting problems determines the complexity class #P. Clearly, a #P problem is at least as hard as its corresponding NP problem. In this paper we consider #P-complete problems. Completeness is defined similarly as for the decision problems: a problem is #P-complete if it is in #P, and if every #P problem can be reduced to it in polynomial counting reduction.

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This means that exact solutions to these problems cannot be obtained in polynomial time, and accordingly, our study focuses on approximation algorithms.

As an example, the satisfiability problem—commonly abbreviated to SAT—is well-known to be NP-complete. Its associated counting problem is denoted by #SAT for which is proved that it is #P-complete\(^{[19]}\). For more background on the complexity theory of decision and counting problems we refer to Papadimitriou\(^{[15]}\).

The proposed splitting algorithm for approximate counting is a randomized one. It is based on designing a sequential sampling plan, with a view to decomposing a “difficult” counting problem defined on some set \(\mathcal{X}\) into a number of “easy” ones associated with a sequence of related sets \(\mathcal{X}_0, \mathcal{X}_1, \ldots, \mathcal{X}_m\) and such that \(\mathcal{X}_m = \mathcal{X}\). Splitting algorithms explore the connection between counting and sampling problems, in particular the reduction from approximate counting of a discrete set to approximate sampling of elements of this set, with the sampling performed, typically, by some Markov chain Monte Carlo method.

Recently, counting problems have attracted research interest, notably #SAT which is also called model counting in Gomes and colleagues\(^{[12]}\). Although it has been shown that many solution techniques for SAT problems can be adapted for these problems, yet due to the exponential increase in memory usage and running times of these methods, their application area in counting is limited. This drawback motivated the approximative approach mentioned earlier. There are two main heuristic algorithms for approximate counting methods in #SAT. The first one, called Approx Count, is introduced by Wei and Selman\(^{[20]}\). It is a local search method that uses Markov Chain Monte Carlo (MCMC) sampling to compute an approximation of the true model count of a given formula. It is fast and has been shown to provide good estimates for feasible solution counts, but, in contrast with our proposed splitting method, there are no guarantees as to the uniformity of the MCMC samples. Gogate and Dechter\(^{[11]}\) recently proposed a second model counting technique called Sample Minisat, which is based on sampling from the so-called backtrack-free search space of a Boolean formula through Sample Search. An approximation of the search tree thus found is used as the importance sampling density instead of the uniform distribution over all solutions. Experiments with Sample Minisat show that it is very fast and typically it provides very good estimates.

The splitting method discussed in this work for counting in deterministic problems is based on its classic counterpart for efficient estimation of rare-event probabilities in stochastic problems. The relation between rare-event simulation methods and approximate counting methods have also been discussed, for instance, by Blanchet and Rudoy\(^{[1]}\),

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As said, we propose to apply the sequential sampling method presented in Botev and Kroese\cite{botev2009efficient} which yields a product estimator for counting the number of solutions $|\mathcal{X}^*|$, where the product is taken over the estimators of the consecutive conditional probabilities, each of which represents an “easy” problem. In addition, we shall consider an alternative version, in which we use the generated samples after the last iteration of the splitting algorithm as a sample for the capture-recapture method. This method gives us an alternative estimate of the counting problem. Furthermore, we shall study an extended version of the capture-recapture method when the problem size is too large for the splitting method to give reliable estimates. The idea is to decrease artificially the problem size and then apply a backwards estimation. Whenever applicable, the estimators associated with our proposed enhancements outperform the splitting estimators in terms of variance normalized by computational effort.

The article is organized as follows. We first start with describing the splitting method in detail in Section 2. Section 3 deals with the combination of the classic capture-recapture method with the splitting algorithm. Finally, numerical results and concluding remarks are presented in Sections 4 and 5, respectively.

2. SPLITTING ALGORITHMS FOR COUNTING

The splitting method is one of the main techniques for the efficient estimation of rare-event probabilities in stochastic problems. The method is based on the idea of restarting the simulation in certain states of the system in order to obtain more occurrences of the rare event. Although the method originated as a rare event simulation technique (see Cérou and Guyader\cite{cerou2007particle}, L’Ecuyer and coauthors\cite{lecuyer2007multiple}, Garvels\cite{garvels2005algorithm}, Glasserman and colleagues\cite{glasserman2003monte}, Lagnoux\cite{lagnoux2005restarted}, Melas\cite{melas2007splitting}), it has been modified in Blanchet and Rudoy\cite{blanchet2010stopping}, Botev and Kroese\cite{botev2009efficient}, and Rubinstein\cite{rubinstein2016simulation}, for counting and combinatorial optimization problems.

Consider a NP decision problem with solution set $\mathcal{X}^*$, i.e., the set containing all solutions to the problem. We are interested in computing the size $|\mathcal{X}^*|$ of the solution set. Suppose that there is a larger set $\mathcal{X} \supset \mathcal{X}^*$ which can be represented by a simple description or formula; specifically, its size $|\mathcal{X}|$ is known and easy to compute. We call $\mathcal{X}$ the state space of the problem. Let $p = |\mathcal{X}^*| / |\mathcal{X}|$ denote the fraction (or “probability”) of the solution set w.r.t. the state space. Since $|\mathcal{X}|$ is known, it suffices to compute $p$. In most cases $p$ is extremely small, in other words we deal
with a rare-event probability. However, assuming we can estimate \( p \) by \( \hat{p} \), we obtain automatically

\[
|\mathcal{E}^*| = |\mathcal{E}| \hat{p}
\]

as an estimator of \(|\mathcal{E}^*|\). Note that straightforward simulation based on generation of i.i.d. uniform samples \( X \in \mathcal{E} \) and delivering the Monte Carlo estimator 
\[
\hat{p}_{MC} = \frac{1}{N} \sum_{i=1}^{N} I\{X \in \mathcal{E}^*\}
\]
as an unbiased estimator of \(|\mathcal{E}^*|/|\mathcal{E}|\) fails when \( p \) is a rare-event probability. To be more specific, assume a parametrization of the decision problem. The size of the state space \(|\mathcal{E}|\) is parameterized by \( n \), such that \(|\mathcal{E}| \to \infty \) as \( n \to \infty \). For instance, in SAT \( n \) represents the number of variables. Furthermore we assume that the fraction of the solution set \( p \to 0 \) as \( n \to \infty \). The required sample size \( N \) to obtain a relative accuracy \( \epsilon \) of the 95\% confidence interval by the Monte Carlo estimation method is (see Section 1.13 in Ref.\cite{17})

\[
N \approx \frac{1.96^2}{\epsilon^2 p},
\]

which increases like \( p^{-1} \) as \( n \to \infty \).

The purpose of the splitting method is to estimate \( p \) more efficiently via the following steps:

1. Find a sequence of sets \( \mathcal{E} = \mathcal{E}_0, \mathcal{E}_1, \ldots, \mathcal{E}_m \) such that \( \mathcal{E}_0 \supset \mathcal{E}_1 \supset \cdots \supset \mathcal{E}_m = \mathcal{E}^* \).
2. Write \(|\mathcal{E}^*| = |\mathcal{E}_m|\) as the telescoping product

\[
|\mathcal{E}^*| = |\mathcal{E}_0| \prod_{t=1}^{m} \frac{|\mathcal{E}_t|}{|\mathcal{E}_{t-1}|}, \quad (1)
\]

thus the target probability becomes a product \( p = \prod_{t=1}^{m} c_t \), with ratio factors

\[
c_t = \frac{|\mathcal{E}_t|}{|\mathcal{E}_{t-1}|}. \quad (2)
\]

3. Develop an efficient estimator \( \hat{c}_t \) for each \( c_t \) and estimate \(|\mathcal{E}^*|\) by

\[
\hat{\ell} = |\mathcal{E}^*| = |\mathcal{E}_0| \hat{p} = |\mathcal{E}_0| \prod_{t=1}^{m} \hat{c}_t. \quad (3)
\]

It is readily seen that in order to obtain a meaningful estimator of \(|\mathcal{E}^*|\), we have to solve the following two major problems:
(i) Put the counting problem into the framework (1) by making sure that

$$\mathcal{X}_0 \supset \mathcal{X}_1 \supset \cdots \supset \mathcal{X}_m = \mathcal{X}^*, \quad (4)$$

such that each \( c_t \) is not a rare-event probability.

(ii) Obtain a low-variance estimator \( \hat{c}_t \) of each ratio \( c_t \).

To deal with both problems, we propose an adaptive version of the splitting method. As a demonstration, consider a specific family of decision problems, namely those whose solution set is finite and given by linear integer constraints. In other words, \( \mathcal{X}^* \subset \mathbb{Z}_M^{m} \) is given by

$$\begin{cases} 
\sum_{j=1}^{n} a_{ij} x_j = b_i, & i = 1, \ldots, m_1; \\
\sum_{j=1}^{n} a_{ij} x_j \geq b_i, & i = m_1 + 1, \ldots, m_1 + m_2 = m; \\
x_j \in \{0, 1, \ldots, d\}, & \forall j = 1, \ldots, n. 
\end{cases} \quad (5)$$

Our goal is to count the number of feasible solutions (or points) to the set (5). Note that we assume that we know, or can compute easily, the bounding finite set \( \mathcal{X} = \{0, 1, \ldots, d\}^n \), with points \( x = (x_1, \ldots, x_n) \) (in this case \( |\mathcal{X}| = (d+1)^n \)) as well for other counting problems.

Below we follow Rubinstein\cite{16}. Define the Boolean functions \( C_i : \mathcal{X} \rightarrow \{0, 1\} \) \((i = 1, \ldots, m)\) by

$$C_i(x) = \begin{cases} 
I_{\sum_{j=1}^{n} a_{ij} x_j = b_i}, & i = 1, \ldots, m_1; \\
I_{\sum_{j=1}^{n} a_{ij} x_j \geq b_i}, & i = m_1 + 1, \ldots, m_1 + m_2. 
\end{cases} \quad (6)$$

Furthermore, define the function \( S : \mathcal{X} \rightarrow \mathbb{Z}_+ \) by counting how many constraints are satisfied by a point \( x \in \mathcal{X} \), i.e., \( S(x) = \sum_{i=1}^{m} C_i(x) \). Now we can formulate the counting problem as a probabilistic problem of evaluating

$$p = \mathbb{E}_f \left[ I_{\{S(X) = m\}} \right], \quad (7)$$

where \( X \) is a random point on \( \mathcal{X} \), uniformly distributed with probability density function (pdf) \( f(x) \), denoted by \( X \overset{d}{\sim} f = \mathcal{U}(\mathcal{X}) \). Consider an increasing sequence of thresholds \( 0 = m_0 < m_1 < \cdots < m_{T-1} < m_T = m \), and define the sequence of decreasing sets (4) by

$$\mathcal{X}_i = \{ x \in \mathcal{X} : S(x) \geq m_i \}.$$
Note that in this way
\[ X_t = \{ x \in X_{t-1} : S(x) \geq m_t \}, \]
for \( t = 1, 2, \ldots, T \). The latter representation is most useful since it shows that the ratio factor \( c_t \) in (2) can be considered as a conditional expectation:
\[ c_t = \frac{|X_t|}{|X_{t-1}|} = \mathbb{E}_{g_{t-1}}[I_{S(x) \geq m_t}], \tag{8} \]
where \( X \sim g_{t-1} = \mathcal{U}(X_{t-1}) \). Note that \( g_{t-1}(x) \) is also obtained as a conditional pdf by
\[ g_{t-1}(x) = f(x|X_{t-1}) = \begin{cases} \frac{f(x)}{f(X_{t-1})}, & x \in X_{t-1}; \\ 0, & x \notin X_{t-1}. \end{cases} \tag{9} \]

To draw samples from the uniform pdf \( g_{t-1} = \mathcal{U}(X_{t-1}) \) on a complex set given implicitly, one applies typically MCMC methods. For further details we refer to Rubinstein\(^\text{[16]}\).

### 2.1. The Basic Adaptive Splitting Algorithm

We describe here the adaptive splitting algorithm from Botev and Kroese\(^\text{[4]}\). The thresholds \((m_t)\) are not given in advance, but determined adaptively via a simulation process. Hence, the number \( T \) of thresholds becomes a random variable. In fact, the \((m_t)\)-thresholds should satisfy the requirements\( c_t = |X_t|/|X_{t-1}| \approx \rho_t \), where the parameters \( \rho_t \in (0, 1) \) are not too small, say \( \rho_t \geq 0.01 \), and set in advance. We call these the splitting control parameters. In most applications we choose these all equal, that is \( \rho_t \equiv \rho \).

Consider a sample set \([X]_{t-1} = \{X_1, \ldots, X_N\}\) of \( N \) random points in \( X_{t-1} \). That is, all these points are uniformly distributed on \( X_{t-1} \). Let \( m_t \) be the \((1 - \rho_{t-1})\)-th quantile of the ordered statistics values of the scores \( S(X_1), \ldots, S(X_N) \). The elite set \([X]_{t-1}^{(e)} \subseteq [X]_{t-1} \) consists of those points of the sample set for which \( S(X) \geq m_t \). Let \( N_t \) be the size of the elite set. If all scores \( S(X) \) are distinct, it follows that the number of elites \( N_t = \lceil N \rho_{t-1} \rceil \), where \( \lceil \cdot \rceil \) denotes rounding to the largest integer. However, dealing with a discrete space, typically we will find more samples with \( S(X) \geq m_t \). All these are added to the elite set. Finally we remark that from (9) it easily follows that the elite points are distributed uniformly on \( X_t \).

Regarding the elite set based in \( X_{t-1} \) as a subset of \( X_t \), we do two things. First, we screen out (delete) duplicates, so that we end up with
a set of size $N^{(s)}_t$ of distinct elites. Secondly, each screened elite is the starting point of an independent Markov chain simulation (MCMC method) in $\mathcal{X}_t$ using a transition probability matrix $P_t$ with $g_t = \mathcal{U}(\mathcal{X}_t)$ as its stationary distribution. Because the starting point is uniformly distributed, all consecutive points on the sample path are uniformly distributed on $\mathcal{X}_t$. Therefore, we may use all these points in the next iteration.

Thus, we simulate $N^{(s)}_t$ independent trajectories, each trajectory for $b_t = \lfloor N/N^{(s)}_t \rfloor$ steps. This produces a total of $N^{(s)}_t b_t \leq N$ uniform points in $\mathcal{X}_t$. To continue with the next iteration again with a sample set of size $N$, we choose randomly $N - N^{(s)}_t b_t$ of these sample paths and extend them by one point. Denote the new sample set by $[X]$, and repeat the same procedure as above. The algorithm iterates until we find $m_t = m$, say at iteration $T$, at which stage we stop and deliver

$$|\hat{\mathcal{X}}^*| = |\mathcal{X}| \prod_{t=1}^T \hat{c}_t$$

as an estimator of $|\mathcal{X}^*|$, where $\hat{c}_t = N_t / N$ at iteration $t$.

In our experiments we applied a Gibbs sampler to implement the MCMC simulation for obtaining uniformly distributed samples. To summarize, we give the algorithm.

**Algorithm 2.1** (Basic Splitting Algorithm for Counting).

- **Input:** the counting problem (5); the bounding set $\mathcal{X}_0$; sample size $N$; splitting control parameters $(\rho_t)_t$.
- **Output:** counting estimator (10).

1. Set a counter $t = 1$. Generate a sample set $[X]_0$ of $N$ points uniformly distributed in $\mathcal{X}_0$. Compute the threshold $m_1$, and determine the size $N_1$ of the elite set. Set $\hat{c}_1 = N_1 / N$ as an estimator of $c_1 = |\mathcal{X}_1| / |\mathcal{X}_0|$.  
2. Screen out the elite set to obtain $N^{(s)}_1$ distinct points uniformly distributed in $\mathcal{X}_1$. 
3. Let $b_t = \lfloor N/N^{(s)}_i \rfloor$. For all $i = 1, 2, \ldots, N^{(s)}_t$, starting at the $i$th screened elite point run a Markov chain of length $b_t$ in $\mathcal{X}_t$ with $g_t = \mathcal{U}(\mathcal{X}_t)$ as its stationary distribution. Extend $N - N^{(s)}_t b_t$ randomly chosen sample paths with one point. Denote the new sample set of size $N$ by $[X]_t$. 
4. Increase the counter $t = t + 1$. Compute the threshold $m_t$, and determine the size $N_t$ of the elite set. Set $\hat{c}_t = N_t / N$ as an estimator of $c_t = |\mathcal{X}_t| / |\mathcal{X}_{t-1}|$. 
5. If $m_t = m$ deliver the estimator (10); otherwise repeat from step 2.

**Remark 1.** Note that the goal of our algorithm 2.1 is to produce points uniformly distributed on each subregion $\mathcal{X}_t$. At the first iteration (due to the acceptance-rejection technique) the samples are indeed uniformly distributed.
distributed on the entire space $\mathcal{X}_0$. In the subsequent iterations we generate in parallel a substantial number of independent sequences of uniform points. We also make sure that they have sufficient lengths. By doing so we guarantee that the generated points at each $\mathcal{X}_t$ are distributed approximately uniform, see the discussion in Gelman and Rubin\cite{gelman1992}. We found numerically that this is obtained by choosing the sample size about $10$–$100$ times larger than dimension $n$ and the splitting parameters $\rho_i$ not too small, say $10^{-1} \geq \rho_i \geq 10^{-3}$.

The graphs in Figure 1 support these rapid mixing properties. We applied the splitting algorithm to a 3-SAT problem from the SATLIB benchmark problems, consisting of $n = 75$ literals and $m = 375$ clauses, see Section 4.1 for further details. In each iteration we chose arbitrarily one of the screened elite points as a starting point of the Gibbs sampler of length $N = 1000$. From this sequence of points $X_1, \ldots, X_N$ in the subset $\mathcal{X}_t$ we constructed the time series $y_1, \ldots, y_N$ of their partial sums $y_i = \sum_{j=1}^{n} X_{i,j}$, and computed the autocorrelation function of the times series. The graphs in Figure 1 show these autocorrelation functions of the first four iterations, up to lag 20.

3. COMBINING SPLITTING AND CAPTURE–RECAPTURE

In this section we discuss how to combine the well known capture-recapture (CAP–RECAP) method with the basic splitting Algorithm 2.1. First we present the classical capture–recapture algorithm in the literature.
3.1. The Classic Capture–Recapture in the Literature

Originally the capture–recapture method was used to estimate the size, say \( M \), of an unknown population on the basis of two independent samples, each taken without replacement from it. To see how the CAP-RECAP method works, consider an urn model with a total of \( M \) identical balls. Denote by \( N_1 \) and \( N_2 \) the sample sizes taken at the first and second draws, respectively. Assume, in addition, that

- The second draw takes place after all \( N_1 \) balls have been returned to the urn.
- Before returning the \( N_1 \) balls, each is marked, say we painted them a different color.

Denote by \( R \) the number of balls from the first draw that reappear in the second. Then a biased estimate \( \tilde{M} \) of \( M \) is

\[
\tilde{M} = \frac{N_1 N_2}{R}. \tag{11}
\]

This is based on the observation that \( N_2/M \approx R/N_1 \). Note that the name capture–recapture was borrowed from a problem of estimating the animal population size in a particular area on the basis of two visits. In this case \( R \) denotes the number of animals captured on the first visit and recaptured on the second.

A slightly less biased estimator of \( M \) is

\[
\hat{M} = \frac{(N_1 + 1)(N_2 + 1)}{(R + 1)} - 1. \tag{12}
\]

See Seber\cite{18} for an analysis of its bias. Furthermore, defining the statistic

\[
V = \frac{(N_1 + 1)(N_2 + 1)(N_1 - R)(N_2 - R)}{(R + 1)^2(R + 2)},
\]

Seber\cite{18} shows that

\[
\mathbb{E}[V] \sim Var[\hat{M}] \left( 1 + \mu^2 e^{-\mu} \right),
\]

where

\[
\mu = \mathbb{E}[R] = N_1 N_2 / M,
\]

so that \( V \) is an approximately unbiased estimator of the variance of \( \hat{M} \).
3.2. Splitting Algorithm Combined with Capture–Recapture

Application of the CAP-RECAP to counting problems is trivial. The target is to estimate size $M = |X^*|$. Consider the basic splitting Algorithm 2.1 at the last iteration $T$, when we have found a set of elite points that satisfy all $m$ constraints; i.e., points in the target set $X^*$. For the capture-recapture method we screen out duplicates which gives us a set $[X]_T^{(s)} \subseteq X^*$ of $N_T^{(s)}$ distinct points.

Then (i) we execute step 3 of Algorithm 2.1 (the MCMC simulation) with sample size $N_1^{(cap)}$; (ii) we screen out duplicates; and (iii) we record the resulting set of $N_1$ distinct points. Independently, we execute (i)–(iii) a second time, starting from the points $[X]_T^{(s)}$, now with sample size $N_2^{(recap)}$. After screening out we record a set of $N_2$ distinct points. Finally, we count the number $R$ of distinct points that occur in both recordings and deliver either estimator (11) or (12).

To summarize, we give the algorithm.

**Algorithm 3.1** (Splitting with Capture–Recapture Algorithm for Counting).

- **Input:** the counting problem (5); the bounding set $X_0$; sample sizes $N, N_1^{(cap)}, N_2^{(recap)}$; splitting control parameters $(\rho_i)$.
- **Output:** counting estimator (11) or (12).

1. Set a counter $t = 1$. Generate a sample set $[X]_0$ of $N$ points uniformly distributed in $X_0$. Compute the threshold $m_1$, and determine the elite set of points satisfying $m_1$ constraints.
2. Screen out the elite set to obtain $N_1^{(s)}$ distinct points uniformly distributed in $X_1$.
3. Let $b_i = \lceil N/N_1^{(s)} \rceil$. For all $i = 1, 2, \ldots, N_1^{(s)}$, starting at the $i$th screened elite point run a Markov chain of length $b_i$ in $X_i$ with $g_i = \mathcal{U}(X_i)$ as its stationary distribution. Extend $X_1 - N_1^{(s)} b_i$ randomly chosen sample paths with one point. Denote the new sample set of size $N_1$ by $[X]_i$.
4. Increase the counter $t = t + 1$. Compute the threshold $m_t$, and determine the elite set of points satisfying $m_t$ constraints.
5. If $m_t < m$ repeat from step 2 otherwise, set $T = t$ and go to step 6.
6. Screen out the elite set to obtain $N_T^{(s)}$ distinct points uniformly distributed in $X_T = X^*$.
7. Let $b_T(1) = \lceil N_1^{(cap)}/N_T^{(s)} \rceil$. For all $i = 1, 2, \ldots, N_T^{(s)}$, starting at the $i$th screened elite point run a Markov chain of length $b_T(1)$ in $X_T$ with $g_T = \mathcal{U}(X_T)$ as its stationary distribution. Extend $N_1^{(cap)} - N_T^{(s)} b_T(1)$ randomly chosen sample paths with one point. Screen out duplicates to obtain a set $[X]_T^{(cap)}$ of $N_1$ distinct points in $X^*$. 


8. Repeat step 7 with \( b_T(2) = \lfloor N_2^{\text{recap}} / N_T^{(s)} \rfloor \). After screening out, the remaining set is \([X]_2^{\text{recap}}\) of \( N \) distinct points in \( \mathcal{X}^* \).

9. Compute the number \( R \) of points in \([X]_1^{\text{cap}} \) ∩ \([X]_2^{\text{recap}}\).

10. Deliver estimator (11) or (12).

In Section 4 we report numerical results of simulation experiments executed by the splitting Algorithm 2.1 and by the capture-recapture Algorithm 3.1. As a general observation we found that the performances of the corresponding counting estimators depend on the choice of sample size \( N \) in the two algorithms, and on the size of the target set \( \mathcal{X}^* \). When we keep the sample \( N \) limited to 10000, then for \(|\mathcal{X}^*|\) sizes up to \(10^6\), the CAP-RECAP estimator (12) is more accurate than the product estimator (10), that is

\[
\text{Var}[\hat{\mathcal{X}}^{\text{cap}}] \leq \text{Var}[\hat{\mathcal{X}}^{\text{product}}].
\]

However, if \(10^6 < |\mathcal{X}^*| \leq 10^9\), we propose to apply an extended version of the capture-recapture method, as we will describe in the next section; and for larger target sets (\(|\mathcal{X}^*| > 10^9\)), we propose to execute just the splitting algorithm because the capture-recapture method performs poorly.

### 3.3. Extended Capture–Recapture Method for SAT

Recall that the regular CAP-RECAP method

1. Is implemented at the last iteration \( T \) of the splitting algorithm, that is when some configurations have already reached the desired set \( \mathcal{X}^* \).
2. It provides reliable estimators of \(|\mathcal{X}^*|\) if it is not too large, say \(|\mathcal{X}^*| \leq 10^6\). (We assume sample sizes \( N \leq 10000 \).)

In rare events counting problems, \(|\mathcal{X}^*|\) is indeed \( \leq 10^6\), nevertheless we present below an extended CAP-RECAP version, which extends the original CAP-RECAP for 2-3 orders more, that is, it provides reliable counting estimators for \(10^6 < |\mathcal{X}^*| \leq 10^9\). The enhancement is based on adding a random number \( \tau \) of random constraints to the original solution set \( \mathcal{X}^* \) that was given in Eq. 5. For reasons of exposition we consider the SAT problem only, since it is easy to generate a random clause involving \( n \) literals.

**Algorithm 3.2** (Extended CAP-RECAP for SAT).

* Input: the counting problem (5); the bounding set \( \mathcal{X}_0 \); sample sizes \( N, N_1^{\text{cap}}, N_2^{\text{recap}}, N_m \), where \( N \leq 10000 \); splitting control parameters \((\rho_1)\); \( c^* \) a relatively small number, say \(10^{-2} \leq c^* \leq 10^{-3}\).
• Output: estimator of $|\mathcal{X}^*|$.

1. Execute Algorithm 2.1 and compute estimator $|\mathcal{X}|$ given in (10).

2. If $|\mathcal{X}| > 10^9$, stop; else, if $|\mathcal{X}| \leq 10^6$, execute steps 6–10 of Algorithm 3.1; else continue with step 3.

3. Recall that Algorithm 2.1 stops at iteration $T$ with an elite sample set
\[ \{X_1, \ldots, X_N\} \subset \mathcal{X}_T = \mathcal{X}^* \]. Execute step 2 and step 3 of Algorithm 2.1; i.e., screen out duplicates and run the MCMC simulations (target sample size $N_m$) to obtain a sample set \([X]_T \subset \mathcal{X}_T\) of size $N_m$. Set auxiliary counter $j = 1$.

4. Add one arbitrary (random) auxiliary clause to the model. Let $N_T + j$ be the number of points in \([X]_T\) that satisfy all $m + j$ clauses.

5. If $N_T + j/N_m > c^*$, increase auxiliary counter $j = j + 1$ and repeat from step 4. Else, set $\tau = j$; denote $\mathcal{X}_{T+\tau}$ for the extended model with these new $\tau$ auxiliary clauses; and define
\[ \hat{c}_{T+\tau} = \frac{N_T + j}{N_m} \leq c^*. \] (13)

6. Execute steps 6–10 of the capture-recapture Algorithm 3.1 for the CAP-RECAP estimator $|\mathcal{X}_{T+\tau}|_{\text{cap}}$ of the size of the extended model.

7. Deliver estimator
\[ |\mathcal{X}|_{\text{ecap}} = \hat{c}_{T+\tau}^{-1} \cdot |\mathcal{X}_{T+\tau}|_{\text{cap}}. \] (14)

We call $|\mathcal{X}|_{\text{ecap}}$ the extended CAP-RECAP estimator. It is essential to bear in mind that

• $|\mathcal{X}_{T+\tau}|_{\text{cap}}$ is a CAP-RECAP estimator rather than a splitting (product) one.

• $|\mathcal{X}|_{\text{ecap}}$ does not contain the original estimators $\hat{c}_1, \ldots, \hat{c}_T$ generated by the splitting method.

• Since we only need here the uniformity of the samples at $\mathcal{X}_T$, we can run the splitting method of Section 2.1 all the way with relatively small values of sample size $N$ and splitting control parameter $\rho$ until it reaches the vicinity of $\mathcal{X}^*$ (meaning that the points of the elite set satisfy $m - r$ constraints, where $r = 1$ or $r = 2$; and then switch to larger $N$ and $\rho$.

• In contrast to the splitting estimator which employs a product of $T$ terms, formula (14) employs only a single $c$ factor. Recall that this additional $\hat{c}_{T+\tau}^{-1}$ factor allows to enlarge the CAP-RECAP estimators of $|\mathcal{X}|$ for about two-three additional orders, namely from $|\mathcal{X}| \approx 10^6$ to $|\mathcal{X}| \approx 10^9$.

4. NUMERICAL RESULTS

Below we present numerical results for the splitting algorithm for counting. In particular we consider the following problems:
1. The 3-satisfiability problem (3-SAT).
2. Graphs with prescribed degrees.
3. Contingency tables.

For the 3-SAT problem we shall also use the CAP-RECAP method when appropriate. We shall show that typically CAP-RECAP outperforms the splitting algorithm. The other two problems typically have too large solution sets to be applied by CAP–RECAP. Clearly, if we would make artificially the associated matrix of the restriction coefficients (see Eq. 5) very sparse, the number of solutions could be made < \(10^9\) and CAP-RECAP would be applicable again. However, in this paper we did not follow such untypical situation.

We shall use the following notations.

**Notation A.** For iteration \(t = 1, 2, \ldots\)

- \(N_t\) and \(N_t^{(s)}\) denote the actual number of elites and the number after screening, respectively;
- \(m_t^*\) and \(m_{t'}\) denote the upper and the lower elite levels reached, respectively (the \(m_t\) levels are the same as the \(m_t\) levels in the description of the algorithm);
- \(\rho_t\) is the splitting control parameter (we chose \(\rho_t \equiv \rho\));
- \(\hat{c}_t = N_t/N\) is the estimator of the \(t\)th conditional probability;
- product estimator \(|\mathcal{X}_t^*| = |\mathcal{X}| \prod_{i=1}^t \hat{c}_t\) after \(t\) iterations.

### 4.1. The 3-Satisfiability Problem (3-SAT)

There are \(m\) clauses of length 3 taken from \(n\) boolean (or binary) variables \(x_1, \ldots, x_n\). A literal of the \(j\)th variable is either TRUE \((x_j = 1)\) or FALSE \((x_j = 0 \iff \bar{x}_j = 1, \text{where } \bar{x}_j = \text{NOT}(x_j))\). A clause is a disjunction of literals. We assume that all clauses consist of 3 literals. The 3-SAT problem consists of determining if the variables \(x = (x_1, \ldots, x_n)\) can be assigned in a such way as to make all clauses TRUE. More formally, let \(\mathcal{X} = \{0, 1\}^n\) be the set of all configurations of the \(n\) variables, and let \(C_i : \mathcal{X} \to \{0, 1\}\) be the \(m\) clauses. Then define \(\phi : \mathcal{X} \to \{0, 1\}\) by

\[
\phi(x) = \bigwedge_{i=1}^m C_i(x).
\]

The original 3-SAT problem is to find a configuration of the \(x_j\) variables for which \(\phi(x) = 1\). In this work we are interested in the total number of such configurations (or feasible solutions). Then as discussed in Section 2, \(|\mathcal{X}|\) denotes the set of feasible solutions. Trivially, there are \(|\mathcal{X}| = 2^n\) configurations.
The 3-SAT problems can also be converted into the family of decision problems (5) given in Section 2. Define the \( m \times n \) matrix \( A \) with entries \( a_{ij} \in \{-1, 0, 1\} \) by

\[
a_{ij} = \begin{cases} 
-1 & \text{if } \bar{x}_j \in C_i, \\
0 & \text{if } x_j \notin C_i \text{ and } \bar{x}_j \notin C_i, \\
1 & \text{if } x_j \in C_i.
\end{cases}
\]

Furthermore, let \( b \) be the \( m \)-column vector with entries \( b_i = 1 - |\{j : a_{ij} = -1\}|. \) Then it is easy to see that for any configuration \( x \in \{0, 1\}^n \)

\[
x \in \mathcal{X}^* \iff \phi(x) = 1 \iff Ax \geq b.
\]

Below we compare the efficiencies of the classic, the CAP-RECAP, and the extended CAP-RECAP algorithms. Efficiency is measured by the reciprocal of the product of the variance and the computational effort (see, e.g., Ref.\(^7\)).

As an example we consider the estimation of \( |\mathcal{X}^*| \) for the 3-SAT problem with an instance matrix \( A \) of dimension \((122 \times 515)\), meaning \( n = 122, m = 515 \). In particular Table 1 presents the the performance of the splitting Algorithm 2.1 based on 10 independent runs using \( N = 25,000 \) and \( \rho = 0.1 \), while Table 2 shows the dynamics of a run of the Algorithm 2.1 for the same data.

The relative error, denoted by RE is \( 1.815E - 01 \). Notice that the relative error of a random variable \( Z \) is calculated by the standard formula, namely

\[
RE = \frac{S}{\ell},
\]

| Table 1: Performance of splitting algorithm for the 3-SAT \((122 \times 515)\) model with \( N = 25,000 \) and \( \rho = 0.1 \). |
| Run | nr. of its. | \( |\mathcal{X}^*| \) | CPU |
|------|-------------|----------------|-----|
| 1    | 33          | 1.41E+06       | 212.32 |
| 2    | 33          | 1.10E+06       | 213.21 |
| 3    | 33          | 1.68E+06       | 214.05 |
| 4    | 33          | 1.21E+06       | 215.6 |
| 5    | 33          | 1.21E+06       | 214.15 |
| 6    | 33          | 1.47E+06       | 216.05 |
| 7    | 33          | 1.50E+06       | 252.25 |
| 8    | 33          | 1.73E+06       | 243.26 |
| 9    | 33          | 1.21E+06       | 238.63 |
| 10   | 33          | 1.88E+06       | 224.36 |
| Average | 33  | 1.44E+06       | 224.38 |
where

\[ \hat{\ell} = \frac{1}{N} \sum_{i=1}^{N} Z_i, \quad S^2 = \frac{1}{N-1} \sum_{i=1}^{N} (Z_i - \hat{\ell})^2. \]

We increased the sample size at the last two iterations from \( N = 25,000 \) to \( N = 100,000 \) to get a more accurate estimator.

As can be seen from Table 1, the estimator \( |\hat{X}^*|_{\text{product}} > 10^6 \), hence for this instance the extended CAP-RECAP Algorithm 3.2 can also be used. We shall show that the relative error (RE) of the extended CAP-RECAP estimator \( |\hat{X}^*|_{\text{ecap}} \) is less than that of \( |\hat{X}^*|_{\text{product}} \). Before doing so we need to find the extended 3-SAT instance matrix \((122 \times 515 + \tau)\),

TABLE 2 Dynamics of a run of the splitting algorithm for the 3-SAT \((122 \times 515)\) model using \( N = 25,000 \) and \( \rho = 0.1 \).  

| \( t \) | \( |\hat{X}_t^*| \) | \( N_t \) | \( N_{t-1} \) | \( m_t^* \) | \( m_t \) | \( \hat{\ell}_t \) |
|---|---|---|---|---|---|---|
| 1 | 6.53E+35 | 3069 | 3069 | 480 | 460 | 1.23E-01 |
| 2 | 8.78E+34 | 3364 | 3364 | 483 | 467 | 1.35E-01 |
| 3 | 1.15E+34 | 3270 | 3270 | 484 | 472 | 1.31E-01 |
| 4 | 1.50E+33 | 3269 | 3269 | 489 | 476 | 1.31E-01 |
| 5 | 2.49E+32 | 4151 | 4151 | 490 | 479 | 1.66E-01 |
| 6 | 3.37E+31 | 3379 | 3379 | 492 | 482 | 1.35E-01 |
| 7 | 3.41E+30 | 2527 | 2527 | 494 | 485 | 1.01E-01 |
| 8 | 6.19E+29 | 4538 | 4538 | 495 | 487 | 1.82E-01 |
| 9 | 9.85E+28 | 3981 | 3981 | 497 | 489 | 1.59E-01 |
| 10 | 1.31E+28 | 3316 | 3316 | 498 | 491 | 1.33E-01 |
| 11 | 1.46E+27 | 2797 | 2797 | 501 | 493 | 1.12E-01 |
| 12 | 4.61E+26 | 7884 | 7884 | 501 | 494 | 3.15E-01 |
| 13 | 1.36E+26 | 7380 | 7380 | 501 | 495 | 2.95E-01 |
| 14 | 3.89E+25 | 7150 | 7150 | 502 | 496 | 2.86E-01 |
| 15 | 1.06E+25 | 6782 | 6782 | 503 | 497 | 2.71E-01 |
| 16 | 2.69E+24 | 6364 | 6364 | 503 | 498 | 2.55E-01 |
| 17 | 6.42E+23 | 5969 | 5969 | 504 | 499 | 2.39E-01 |
| 18 | 1.42E+23 | 5525 | 5525 | 506 | 500 | 2.21E-01 |
| 19 | 3.03E+22 | 5333 | 5333 | 506 | 501 | 2.13E-01 |
| 20 | 5.87E+21 | 5061 | 5061 | 507 | 502 | 1.94E-01 |
| 21 | 1.06E+21 | 4850 | 4850 | 507 | 503 | 1.80E-01 |
| 22 | 1.71E+20 | 4611 | 4611 | 507 | 504 | 1.62E-01 |
| 23 | 2.50E+19 | 4347 | 4347 | 509 | 505 | 1.46E-01 |
| 24 | 3.26E+18 | 3960 | 3960 | 510 | 506 | 1.30E-01 |
| 25 | 3.62E+17 | 3578 | 3578 | 510 | 507 | 1.11E-01 |
| 26 | 3.69E+16 | 3239 | 3239 | 510 | 508 | 1.02E-01 |
| 27 | 3.05E+15 | 2870 | 2870 | 511 | 509 | 8.28E-02 |
| 28 | 2.17E+14 | 2527 | 2527 | 512 | 510 | 7.13E-02 |
| 29 | 1.21E+13 | 2182 | 2182 | 513 | 511 | 5.59E-02 |
| 30 | 5.00E+11 | 1730 | 1730 | 513 | 512 | 4.12E-02 |
| 31 | 1.49E+10 | 1300 | 1300 | 514 | 513 | 2.97E-02 |
| 32 | 2.39E+08 | 802 | 802 | 515 | 514 | 1.61E-02 |
| 33 | 1.43E+06 | 402 | 402 | 515 | 515 | 6.00E-03 |
TABLE 3 Performance of the regular CAP-RECAP for the extended $(122 \times 520)$ model with $N = 1,000$ (up to iteration 28), $N = 100,000$ (from iteration 29), $N = 70,000$ (for the two capture-recapture draws), and $\rho = 0.1$.

| Run | nr. of its. | $|\mathcal{X}|_{\text{cap}}$ | CPU |
|-----|-------------|-----------------|-----|
| 1   | 34          | 5.53E+04        | 159.65 |
| 2   | 35          | 5.49E+04        | 174.46 |
| 3   | 35          | 5.51E+04        | 178.08 |
| 4   | 34          | 5.51E+04        | 166.36 |
| 5   | 34          | 5.52E+04        | 159.36 |
| 6   | 33          | 5.52E+04        | 152.38 |
| 7   | 33          | 5.54E+04        | 137.96 |
| 8   | 34          | 5.50E+04        | 137.37 |
| 9   | 35          | 5.51E+04        | 179.08 |
| 10  | 34          | 5.51E+04        | 163.7 |
| Average | 34.1       | 5.51E+04        | 162.78 |

The relative error of $|\mathcal{X}|_{\text{cap}}$ over 10 runs is $2.600E - 03$.

where $\tau$ is the number of auxiliary clauses. Applying the extended CAP-RECAP Algorithm 3.2 with $c^* = 0.05$, we found that $\tau = 5$ and thus the extended instance matrix is $(122 \times 520)$. Recall that the cardinality $|\mathcal{X}_{T^*}|$ of the extended $(122 \times 520)$ model should be manageable by the regular CAP-RECAP algorithm 3.1, that is, we assumed that $|\mathcal{X}_{T^*}| < 10^6$. Indeed, Table 3 presents the performance of the regular CAP-RECAP algorithm for that extended $(122 \times 520)$ model. Here we used again $\rho = 0.1$. As for the sample size, we took $N = 1,000$ until iteration 28 and then switched to $N = 100,000$. The final CAP-RECAP estimator is obtained by taking two equal samples, each of size $N = 70,000$ at the final subset $\mathcal{X}_{T^*}$.

Next we compare the efficiency of the regular CAP-RECAP Algorithm 3.1 for the extended $(122 \times 520)$ model (as per Table 3) with that of the splitting algorithm 2.1 for this model. Table 4 presents the performance of the splitting algorithm for $\rho = 0.1$ and $N = 100,000$.

It readily follows that the relative error of the regular CAP-RECAP is about 30 times less than that of splitting. Notice in addition that the CPU time of CAP-RECAP is about 6 times less than that of splitting. This is so since the total sample size of the former is about 6 time less than of the latter. Using that the relative error involves the square root of the variance, the efficiency improvement by CAP-RECAP is about 5,400.

With these results at hand we can proceed with the extended CAP-RECAP and compare its efficiency with splitting (as per Table 1) for the instance matrix $(122 \times 515)$. Table 5 presents the performance of the extended CAP-RECAP estimator $|\mathcal{X}|_{\text{cap}}$ for the $(122 \times 515)$ model. We set again $\rho = 0.1$. Regarding the sample size we took $N = 1,000$ for the first 31 iterations and then switched to $N = 100,000$ until reaching the level
TABLE 4 Performance of splitting algorithm for the 3-SAT (122 × 520) model with \(N = 100,000\) and \(\rho = 0.1\).

| Run | nr. of its. | \(|\hat{x}^*|\) | CPU |
|-----|-------------|-----------------|-----|
| 1   | 34          | 6.03E+04        | 900.28 |
| 2   | 34          | 7.48E+04        | 904.23 |
| 3   | 34          | 4.50E+04        | 913.31 |
| 4   | 34          | 5.99E+04        | 912.27 |
| 5   | 34          | 6.03E+04        | 910.44 |
| 6   | 33          | 4.94E+04        | 898.91 |
| 7   | 34          | 5.22E+04        | 931.88 |
| 8   | 34          | 5.74E+04        | 916.8 |
| 9   | 34          | 5.85E+04        | 919.63 |
| 10  | 34          | 5.72E+04        | 927.7 |
| Average | 33.9         | 5.75E+04        | 913.54 |

The relative error of \(|\hat{x}^*|\) over 10 runs is \(1.315E - 01\).

\(m = 515\). Recall that the level \(m + \tau = 520\) and the corresponding CAP-RECAP estimator \(|\hat{x}^*|_{\text{cap}}\) was obtained from the set \(\mathcal{X} = \mathcal{X}_{515}\) by adding \(\tau = 5\) more auxiliary clauses. In this case we used for \(|\hat{x}^*|_{\text{cap}}\) two equal samples each of length \(N = 100,000\).

Comparing the results of Table 1 with that of Table 5 it is readily seen that the extended CAP-RECAP estimator \(|\hat{x}^*|_{\text{ecap}}\) outperforms the splitting estimator \(|\hat{x}^*|_{\text{product}}\) in terms of efficiency. In particular, we have that both \(\text{RE}\) and \(\text{CPU}\) times of the former are about 1.6 times less than of the latter. This means that the overall efficiency improvement obtained by \(|\hat{x}^*|_{\text{ecap}}\) versus \(|\hat{x}^*|_{\text{product}}\) is about \(1.6^2 \times 1.6 \approx 4\). Note finally that the total number of samples used in the extended CAP-RECAP estimator \(|\hat{x}^*|_{\text{ecap}}\) is about

TABLE 5 Performance of the extended CAP-RECAP estimator \(|\hat{x}^*|_{\text{ecap}}\) for the (122 × 515) with \(N = 1,000\) (up to iteration 31), \(N = 100,000\) (from iteration 31 and the two capture-recapture draws), \(c^* = 0.05\), and \(\rho = 0.1\).

| Run | nr. its. | \(|\hat{x}^*|_{\text{ecap}}\) | CPU |
|-----|----------|----------------|-----|
| 1   | 33       | 1.73E+06      | 138.99 |
| 2   | 34       | 1.59E+06      | 154.64 |
| 3   | 34       | 1.55E+06      | 161.78 |
| 4   | 33       | 1.20E+06      | 163.53 |
| 5   | 34       | 1.69E+06      | 143.84 |
| 6   | 34       | 1.81E+06      | 151.1 |
| 7   | 34       | 1.29E+06      | 174.08 |
| 8   | 34       | 1.40E+06      | 143.27 |
| 9   | 33       | 1.66E+06      | 171.07 |
| 10  | 34       | 1.30E+06      | 154.71 |
| Average | 33.7       | 1.52E+06      | 155.70 |

The relative error of \(|\hat{x}^*|_{\text{ecap}}\) over 10 runs is \(1.315E - 01\).
\[ N = 31 \times 1,000 + 5 \times 100,000 = 531,000, \]
while in its counterpart - the splitting estimator \( \hat{N} \) product is about \( N = 33 \times 25,000 = 825,000. \)

### 4.2. Random Graphs with Prescribed Degrees

Random graphs with given vertex degrees have attained attention as a model for real-world complex networks, including World Wide Web, social networks and biological networks. The problem is basically finding a graph \( G = (V, E) \) with \( n \) vertices, given the degree sequence \( d = (d_1, \ldots, d_n) \) formed of nonnegative integers. Following Blitzstein and Diaconis\(^2\), a finite sequence \( (d_1, \ldots, d_n) \) of nonnegative integers is called graphical if there is a labeled simple graph with vertex set \( \{1, \ldots, n\} \) in which vertex \( i \) has degree \( d_i \). Such a graph is called a realization of the degree sequence \( (d_1, \ldots, d_n) \). We are interested in the total number of realizations for a given degree sequence, hence \( \mathcal{X}^* \) denotes the set of all graphs \( G = (V, E) \) with the degree sequence \( (d_1, \ldots, d_n) \).

Similar to Eq. 5 for SAT we convert the problem into a counting problem. To proceed consider the complete graph \( K_n \) of \( n \) vertices, in which each vertex is connected with all other vertices. Thus the total number of edges in \( K_n \) is \( m = n(n - 1)/2 \), labeled \( e_1, \ldots, e_m \). The random graph problem with prescribed degrees is translated to the problem of choosing those edges of \( K_n \) such that the resulting graph \( G \) matches the given sequence \( d \). Set \( x_i = 1 \) when \( e_i \) is chosen, and \( x_i = 0 \) otherwise, \( i = 1, \ldots, m \). In order that such an assignment \( x \in \{0, 1\}^m \) matches the given degree sequence \( (d_1, \ldots, d_n) \), it holds necessarily that \( \sum_{j=1}^{m} x_j = \frac{1}{2} \sum_{i=1}^{n} d_i \), since this is the total number of edges. In other words, the configuration space is

\[
\mathcal{X} = \left\{ x \in \{0, 1\}^m : \sum_{j=1}^{m} x_j = \frac{1}{2} \sum_{i=1}^{n} d_i \right\}.
\]

Let \( A \) be the incidence matrix of \( K_n \) with entries

\[
d_{ij} = \begin{cases} 0 & \text{if } v_i \not\in e_j \\ 1 & \text{if } v_i \in e_j. \end{cases}
\]

It is easy to see that whenever a configuration \( x \in \{0, 1\}^m \) satisfies \( Ax = d \), the associated graph has degree sequence \( (d_1, \ldots, d_n) \). We conclude that the problem set is represented by

\[
\mathcal{X}^* = \{ x \in \mathcal{X} : Ax = d \}.
\]
We first present a small example as illustration. Let \( d = (2, 2, 2, 1, 3) \) with \( n = 5 \), and \( m = 10 \). After ordering the edges of \( K_5 \) lexicographically, the corresponding incidence matrix is given as

\[
A = \begin{pmatrix}
1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 1
\end{pmatrix}
\]

It is readily seen that \( x = (0, 0, 1, 1, 0, 1, 0, 1, 0, 1)^T \) and \( x = (1, 0, 0, 1, 1, 0, 0, 0, 1, 1)^T \) present two solutions of this example.

For the random graph problem we define the score function \( S : \mathcal{X} \rightarrow \mathbb{Z}_{\geq 0} \) by

\[
S(x) = -\sum_{i=1}^{n} |\deg(v_i) - d_i|,
\]

where \( \deg(v_i) \) is the degree of vertex \( i \) under the configuration \( x \). Each configuration that satisfies the degree sequence will have a performance function equal to 0.

The implementation of the Gibbs sampler for this problem is slightly different than for the 3-SAT problem, since we keep the number of edges in each realization fixed to \( \sum d_i/2 \). Our first algorithm takes care of this requirement and generates a random \( x \in \mathcal{X} \).

**Algorithm 4.1.**

- **Input:** the prescribed degrees sequence \( (d_1, \ldots, d_n) \).
- **Output:** a random \( x \in \mathcal{X} \).

1. Generate a random permutation of \( 1, \ldots, m \).
2. Choose the first \( \sum d_i/2 \) places in this permutation and deliver a vector \( x \) having ones in those places.

The adaptive thresholds in the basic splitting algorithm are negative, increasing to 0:

\[
m_1 \leq m_2 \leq \cdots \leq m_{T-1} \leq m_T = 0.
\]

The resulting Gibbs sampler (in Step 3 of the basic splitting algorithm starting with a configuration \( x \in \mathcal{X} \) for which \( S(x) \geq m_t \)) can be written as follows.
Algorithm 4.2 (Gibbs Algorithm for Random Graph Sampling).

- **Input:** a configuration $x \in \mathcal{X}$ with $S(x) \geq m_t$.
- **Output:** a uniformly chosen random neighbor with the same property.

For each edge $x_i = 1$, while keeping all other edges fixed, do:

1. Remove $x_i$ from $x$, i.e., make $x_i = 0$.
2. Check all possible placements for the edge resulting a new vector $\tilde{x}$ conditioning on the performance function $S(\tilde{x}) \geq m_t$.
3. With uniform probability choose one of the valid realizations.

We will apply the splitting algorithm to two problems taken from Ref. [2].

### 4.2.1. A Small Problem

For this small problem we have the degree sequence

$$d = (5, 6, 1, \ldots, 1).$$

The solution can be obtained analytically and already given in Ref. [2]:

“To count the number of labeled graphs with this degree sequence, note that there are $\binom{11}{5} = 462$ such graphs with vertex 1 not joined to vertex 2 by an edge (these graphs look like two separate stars), and there are $\binom{11}{4} \binom{7}{5} = 6930$ such graphs with an edge between vertices 1 and 2 (these look like two joined stars with an isolated edge left over). Thus, the total number of realizations of $d$ is 7392.”

As we can see from Table 6, the algorithm easily handles the problem. Table 7 presents the typical dynamics.

### 4.2.2. A Large Problem

A much harder instance (see Ref. [2]) is defined by

$$d = (7, 8, 5, 1, 1, 2, 8, 10, 4, 2, 4, 5, 3, 6, 7, 3, 2, 7, 6, 1, 2, 9, 6, 1, 3, 4, 6, 3, 3, 3, 2, 4, 4).$$

In Ref. [2] the number of such graphs is estimated to be about $1.533 \times 10^{57}$.

Table 8 presents 10 runs using the splitting algorithm.
TABLE 6 Performance of the splitting algorithm for a small problem using \( N = 50,000 \) and \( \rho = 0.5 \).

<table>
<thead>
<tr>
<th>Run</th>
<th>nr. of its.</th>
<th>( \hat{\mid X^* \mid} )</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>7146.2</td>
<td>15.723</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>7169.2</td>
<td>15.251</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>7468.7</td>
<td>15.664</td>
</tr>
<tr>
<td>4</td>
<td>10</td>
<td>7145.9</td>
<td>15.453</td>
</tr>
<tr>
<td>5</td>
<td>10</td>
<td>7583</td>
<td>15.555</td>
</tr>
<tr>
<td>6</td>
<td>10</td>
<td>7206.4</td>
<td>15.454</td>
</tr>
<tr>
<td>7</td>
<td>10</td>
<td>7079.3</td>
<td>15.495</td>
</tr>
<tr>
<td>8</td>
<td>10</td>
<td>7545.1</td>
<td>15.347</td>
</tr>
<tr>
<td>9</td>
<td>10</td>
<td>7597.2</td>
<td>15.836</td>
</tr>
<tr>
<td>10</td>
<td>10</td>
<td>7181.2</td>
<td>15.612</td>
</tr>
<tr>
<td>Average</td>
<td></td>
<td>7312.2</td>
<td>15.539</td>
</tr>
</tbody>
</table>

The relative error of \( \hat{\mid X^* \mid} \) over 10 runs is 2.710E \(-02\).

TABLE 7 Typical dynamics of the splitting algorithm for a small problem using \( N = 50,000 \) and \( \rho = 0.5 \) (recall Notation A at the beginning of Section 4).

<table>
<thead>
<tr>
<th>( t )</th>
<th>( \hat{\mid X^* \mid} )</th>
<th>( N_t )</th>
<th>( N_t^{(c)} )</th>
<th>( m_t )</th>
<th>( m_c )</th>
<th>( \hat{\alpha}_t )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.55E+12</td>
<td>29227</td>
<td>29227</td>
<td>-4</td>
<td>-30</td>
<td>0.5845</td>
</tr>
<tr>
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<td>28144</td>
<td>-4</td>
<td>-18</td>
<td>0.5629</td>
</tr>
<tr>
<td>3</td>
<td>1.09E+12</td>
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<td>21227</td>
<td>-6</td>
<td>-16</td>
<td>0.4245</td>
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<tr>
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<td>3.38E+11</td>
<td>15565</td>
<td>15565</td>
<td>-4</td>
<td>-14</td>
<td>0.3113</td>
</tr>
<tr>
<td>5</td>
<td>7.51E+10</td>
<td>11104</td>
<td>11104</td>
<td>-4</td>
<td>-12</td>
<td>0.2221</td>
</tr>
<tr>
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<td>1.11E+10</td>
<td>7408</td>
<td>7408</td>
<td>-2</td>
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<td>0.1482</td>
</tr>
<tr>
<td>7</td>
<td>1.03E+09</td>
<td>4628</td>
<td>4628</td>
<td>-2</td>
<td>-8</td>
<td>0.0926</td>
</tr>
<tr>
<td>8</td>
<td>3.37E+07</td>
<td>2608</td>
<td>2608</td>
<td>-2</td>
<td>-6</td>
<td>0.0522</td>
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<tr>
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<td>0.0235</td>
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<tr>
<td>10</td>
<td>7223.9</td>
<td>286</td>
<td>280</td>
<td>0</td>
<td>-2</td>
<td>0.0057</td>
</tr>
</tbody>
</table>

TABLE 8 Performance of the splitting algorithm for a large problem using \( N = 100,000 \) and \( \rho = 0.5 \).

<table>
<thead>
<tr>
<th>Run</th>
<th>nr. its.</th>
<th>( \hat{\mid X^* \mid} )</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>39</td>
<td>1.66E+57</td>
<td>4295</td>
</tr>
<tr>
<td>2</td>
<td>39</td>
<td>1.58E+57</td>
<td>4223</td>
</tr>
<tr>
<td>3</td>
<td>39</td>
<td>1.58E+57</td>
<td>4116</td>
</tr>
<tr>
<td>4</td>
<td>39</td>
<td>1.53E+57</td>
<td>4281</td>
</tr>
<tr>
<td>5</td>
<td>39</td>
<td>1.76E+57</td>
<td>4301</td>
</tr>
<tr>
<td>6</td>
<td>39</td>
<td>1.75E+57</td>
<td>4094</td>
</tr>
<tr>
<td>7</td>
<td>39</td>
<td>1.46E+57</td>
<td>4512</td>
</tr>
<tr>
<td>8</td>
<td>39</td>
<td>1.71E+57</td>
<td>4287</td>
</tr>
<tr>
<td>9</td>
<td>39</td>
<td>1.39E+57</td>
<td>4158</td>
</tr>
<tr>
<td>10</td>
<td>39</td>
<td>1.38E+57</td>
<td>4264</td>
</tr>
<tr>
<td>Average</td>
<td></td>
<td>1.58E+57</td>
<td>4253</td>
</tr>
</tbody>
</table>

The relative error of \( \hat{\mid X^* \mid} \) over 10 runs is 8.430E \(-02\).
4.3. Binary Contingency Tables

Given are two vectors of positive integers \( r = (r_1, \ldots, r_m) \) and \( c = (c_1, \ldots, c_n) \) such that \( r_i \leq n \) for all \( i \), \( c_j \leq n \) for all \( j \), and \( \sum_{i=1}^{m} r_i = \sum_{j=1}^{n} c_j \).

A binary contingency table with row sums \( r \) and column sums \( c \) is a \( m \times n \) matrix \( X \) of zero-one entries \( x_{ij} \) satisfying \( \sum_{j=1}^{n} x_{ij} = r_i \) for every row \( i \) and \( \sum_{i=1}^{m} x_{ij} = c_j \) for every column \( j \). The problem is to count all contingency tables.

The extension of the proposed Gibbs sampler for counting the contingency tables is straightforward. We define the configuration space \( \mathcal{X} = \mathcal{X}^{(c)} \cup \mathcal{X}^{(r)} \) as the space where all column or row sums are satisfied:

\[
\mathcal{X}^{(c)} = \left\{ X \in \{0, 1\}^{m+n} : \sum_{i=1}^{m} x_{ij} = c_j \ \forall j \right\},
\]

\[
\mathcal{X}^{(r)} = \left\{ X \in \{0, 1\}^{m+n} : \sum_{j=1}^{n} x_{ij} = r_i \ \forall i \right\}.
\]

Clearly we can sample uniformly at random from \( \mathcal{X} \) without any problem. The score function \( S : \mathcal{X} \rightarrow \mathbb{Z}_- \) is defined by

\[
S(X) = \begin{cases} 
- \sum_{i=1}^{m} \left| \sum_{j=1}^{n} x_{ij} - r_i \right|, & \text{for } X \in \mathcal{X}^{(c)}, \\
- \sum_{j=1}^{n} \left| \sum_{i=1}^{m} x_{ij} - c_j \right|, & \text{for } X \in \mathcal{X}^{(r)},
\end{cases}
\]

that is, the difference of the row sums \( \sum_{j=1}^{n} x_{ij} \) with the target \( r_i \) if the column sums are right, and vice versa.

The Gibbs sampler is very similar to the one in the previous section concerning random graphs with prescribed degrees.

**Algorithm 4.3.** (Gibbs Algorithm for Random Contingency Tables Sampling)

- **Input:** a matrix realization \( X \in \mathcal{X}^{(c)} \) with score \( S(X) \geq m_t \).
- **Output:** a uniformly chosen random neighbour with the same property.

**For each column \( j \) and for each 1-entry in this column \( (x_{ij} = 1) \) do:**

1. Remove this 1, i.e. set \( x'_{ij} = 0 \).
2. Check all possible placements for this 1 in the given column \( j \) conditioning on the performance function \( S(X') \geq m_t \) (\( X' \) is the matrix resulting by setting \( x'_{ij} = 0 \), \( x'_{i'j} = 1 \) for some \( x_{i'j} = 0 \), and all other entries remain unchanged).
3. Suppose that the set of valid realizations is \( \mathcal{A} = \{X' | S(X') \geq m_t\} \). (Please note that this set also contains the original realization \( X \)). Then, with probability \( \frac{1}{|\mathcal{A}|} \) pick any realization at random and continue with step 1.

Note that in this way we keep the column sums correct. Similarly, when we started with a matrix configuration with all row sums correct, we execute these steps for each row and swap 1 and 0 per row.

### 4.3.1. Model 1

The date are \( m = 12, n = 12 \) with row and column sums

\[
 r = (2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2), \quad c = (2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2).
\]

The true count value is known to be 21,959,547,410,077,200 (reported in Chen et al.\[6\]). Table 9 presents 10 runs using the splitting algorithm. Table 10 presents a typical dynamics.

#### Table 9

Performance of the splitting algorithm for Model 1 using \( N = 50,000 \) and \( \rho = 0.5 \).

| Run | nr.its. | \( |\tilde{X}^*| \) | CPU |
|-----|---------|----------------|-----|
| 1   | 7       | 2.15E+16       | 4.54 |
| 2   | 7       | 2.32E+16       | 4.55 |
| 3   | 7       | 2.29E+16       | 4.54 |
| 4   | 7       | 2.11E+16       | 4.58 |
| 5   | 7       | 2.05E+16       | 4.57 |
| 6   | 7       | 2.23E+16       | 4.54 |
| 7   | 7       | 2.02E+16       | 4.55 |
| 8   | 7       | 2.38E+16       | 4.58 |
| 9   | 7       | 2.06E+16       | 4.57 |
| 10  | 7       | 2.14E+16       | 4.55 |
| Average | 7 | 2.17E+16 | 4.56 |

The relative error of \( |\tilde{X}^*| \) over 10 runs is 5.210E - 02.

#### Table 10

Typical dynamics of the splitting algorithm for Model 1 using \( N = 50,000 \) and \( \rho = 0.5 \).

| \( t \) | \( |\tilde{X}^*| \) | \( \hat{N}_t \) | \( \hat{N}^{(s)}_t \) | \( m_t^* \) | \( m_{at} \) | \( \hat{c}_t \) |
|--------|----------------|----------------|----------------|-------|-------|-------|
| 1      | 4.56E+21       | 13361          | 13361          | -2    | -24   | 0.6681 |
| 2      | 2.68E+21       | 11747          | 11747          | -2    | -12   | 0.3874 |
| 3      | 1.10E+21       | 8234           | 8234           | -2    | -10   | 0.4117 |
| 4      | 2.76E+20       | 5003           | 5003           | -2    | -8    | 0.2502 |
| 5      | 3.45E+19       | 2497           | 2497           | 0     | -6    | 0.1249 |
| 6      | 1.92E+18       | 1112           | 1112           | 0     | -4    | 0.0556 |
| 7      | 2.08E+16       | 217            | 217            | 0     | -2    | 0.0109 |
TABLE 11 Performance of the splitting algorithm for Model 2 using $N = 200,000$ and $\rho = 0.5$.

| Run | nr. is. | $|\hat{X}|$ | CPU   |
|-----|---------|------------|-------|
| 1   | 24      | 6.16E+16   | 246.83|
| 2   | 24      | 6.50E+16   | 244.42|
| 3   | 24      | 7.07E+16   | 252.71|
| 4   | 24      | 7.91E+16   | 247.36|
| 5   | 24      | 6.61E+16   | 260.99|
| 6   | 24      | 6.77E+16   | 264.07|
| 7   | 24      | 6.59E+16   | 269.86|
| 8   | 24      | 6.51E+16   | 273.51|
| 9   | 24      | 7.10E+16   | 272.49|
| 10  | 24      | 5.91E+16   | 267.23|
| Average | 24 | 6.71E+16 | 259.95|

The relative error of $|\hat{X}|$ over 10 runs is $7.850E-02$.

4.3.2. Model 2
Consider the problem of counting tables with Darwin’s finch data as marginal sums, e.g., given in Chen and colleagues\[6\]. The data are $m = 12$, $n = 17$ with row and columns sums

$$r = (14, 13, 14, 10, 12, 2, 10, 1, 10, 11, 6, 2),$$

$$c = (3, 3, 10, 9, 9, 7, 8, 9, 7, 8, 2, 9, 3, 6, 8, 2, 2).$$

The true count value is known to be $67, 149, 106, 137, 567, 626$. Table 11 presents 10 runs using the splitting algorithm.

5. CONCLUDING REMARKS
In this article we applied the splitting method to several well-known counting problems, like 3-SAT, random graphs with prescribed degrees and binary contingency tables. While implementing the splitting algorithm, we discussed several MCMC algorithms and in particular the Gibbs sampler. We show how to incorporate the classic capture-recapture method in the splitting algorithm in order to obtain a low variance estimator for the desired counting quantity. Furthermore, we presented an extended version of the capture-recapture algorithm, which is suitable for problems with a larger number of feasible solutions. We finally presented numerical results with the splitting and capture-recapture estimators, and showed the superiority of the latter.
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REFERENCES