Capacity estimation of two-dimensional channels using Sequential Monte Carlo

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Abstract—We derive a new Sequential-Monte-Carlo-based algorithm to estimate the capacity of two-dimensional channel models. The focus is on computing the noiseless capacity of the 2-D $(1, \infty)$ run-length limited constrained channel, but the underlying idea is generally applicable. The proposed algorithm is profiled against a state-of-the-art method, yielding more than an order of magnitude improvement in estimation accuracy for a given computation time.

I. INTRODUCTION

With ever increasing demands on storage system capacity and reliability there has been increasing interest in page-oriented storage solutions. For these types of systems variations of two-dimensional constraints can be imposed to help with, amongst other things, timing control and reduced intersymbol interference [1]. This has sparked an interest in analyzing information theoretic properties of two-dimensional channel models for use in e.g. holographic data storage [2].

Our main contribution is a new algorithm, based on sequential Monte Carlo (SMC) methods, for numerically estimating the capacity of two-dimensional channels. We show how we can utilize structure in the model to sample the auxiliary target distributions in the SMC algorithm exactly. The focus in this paper is on computing the noiseless capacity of constrained finite-size two-dimensional models. However, the proposed algorithm works also for various generalizations and noisy channel models.

Recently, several approaches have been proposed to solve the capacity estimation problem in two-dimensional constrained channels. These methods rely either on variational approximations [3] or on Markov chain Monte Carlo [4], [5]. Compared to these methods our algorithm is fundamentally different; samples are drawn sequentially from a sequence of probability distributions of increasing dimensions using SMC coupled with a finite state-space forward-backward procedure. We compare our proposed algorithm to a state-of-the-art Monte Carlo estimation algorithm proposed in [4], [5]. Using SMC algorithms has earlier been proposed to compute the information rate of one-dimensional continuous channel models with memory [6]. Although both approaches are based on SMC, the methods, implementation and goals are very different.

II. TWO-DIMENSIONAL CHANNEL MODELS

As in [5] we consider the 2-D $(1, \infty)$ run-length limited constrained channel. The 2-D $(1, \infty)$ run-length limited con-

straint implies that no two horizontally or vertically adjacent bits on a 2-D lattice may be both be equal to 1. An example is given below:

$$
\begin{array}{ccccc}
\cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & 0 & 1 & 0 & \cdots \\
\cdots & 0 & 0 & 1 & \cdots \\
\cdots & 0 & 1 & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots
\end{array}
$$

This channel can be modelled as a probabilistic graphical model (PGM). A PGM is a probabilistic model which *factorizes* according to the structure of an underlying graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$, with vertex set $\mathcal{V}$ and edge set $\mathcal{E}$. In this article we will focus on square lattice graphical models with pair-wise interactions, see Figure 1. That means that the
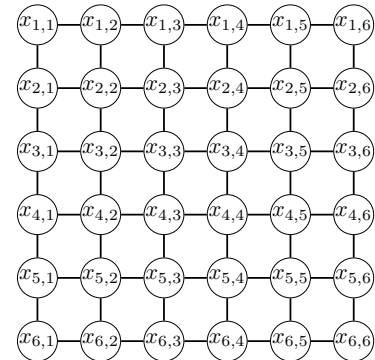

Fig. 1. $M \times M$ square lattice graphical model with pair-wise interactions. The nodes correspond to random variables $x_{\ell,j}$ and the edges encodes the interactions $\psi(x_{\ell,j}, x_{m,n})$.

joint probability mass function (PMF) of the set of random variables, $X := \{x_{1,1}, \ldots, x_{1,M}, x_{2,M}, \ldots, x_{M,M}\}$, can be represented as a product of factors over the pairs of variables in the graph:

$$
p(X) = \frac{1}{Z} \prod_{(\ell j, mn) \in \mathcal{E}} \psi(x_{\ell,j}, x_{m,n}). \tag{1}
$$

Here, Z—the partition function—is given by

$$
Z = \sum_{X} \prod_{(\ell j, mn) \in \mathcal{E}} \psi(x_{\ell,j}, x_{m,n}), \tag{2}
$$

and $\psi(x_{\ell,j}, x_{m,n})$ denotes the so-called potential function encoding the pairwise interaction between $x_{\ell,j}$ and $x_{m,n}$. For a more in-depth exposition of graphical models we refer the reader to [7].

A. Constrained channels and PGM

The noiseless 2-D $(1, \infty)$ run-length limited constrained channel can be described by a square lattice graphical model as in Figure 1, with binary variables $x_{\ell,j} \in \{0,1\}$ and pair-wise interactions between adjacent variables. Defining the factors as

$$\psi(x_{\ell,j}, x_{m,n}) = \begin{cases} 0, & \text{if } x_{\ell,j} = x_{m,n} = 1, \\ 1, & \text{otherwise,} \end{cases} \qquad (3)$$

results in a joint PMF given by

$$p(X) = \frac{1}{Z} \prod_{(\ell j, mn) \in \mathcal{E}} \psi(x_{\ell,j}, x_{m,n}), \qquad (4)$$

where the partition function Z is the number of satisfying configurations or, equivalently, the cardinality of the support of $p(X)$. For a channel of dimension $M \times M$ we can write the finite-size noiseless capacity as

$$C_M = \frac{1}{M^2} \log_2 Z. \qquad (5)$$

Hence, to compute the capacity of the channel we need to compute the partition function Z. Unfortunately, calculating Z exactly is in general computationally intractable. This means that we need a way to approximate the partition function. Note that for this particular model, known upper and lower bounds of the infinite-size noiseless capacity, $M \to \infty$, agree on more than eight decimal digits [8], [9]. However, our proposed method is applicable in the finite-size case, as well as to other models where no tight bounds are known.

B. High-dimensional undirected chains

In the previous section we described how we can calculate the noiseless capacity for 2-D channel models by casting the problem as a partition function estimation problem in the PGM framework. In our running example the corresponding graph is the $M \times M$ square lattice PGM depicted in Figure 1. We now show how we can turn these models into high-dimensional undirected chains by introducing a specific new set of variables. We will see that this idea, although simple, is a key enabler of our proposed algorithm.

We define $\mathbf{x}_k$ to be the M-dimensional variable corresponding to all the original variables in column k, i.e.

$$\mathbf{x}_k = \{x_{1,k}, \ldots, x_{M,k}\}, \qquad k = 1, \ldots, M. \qquad (6)$$

The resulting graphical model in the $\mathbf{x}_k$'s will be an undirected chain with joint PMF given by

$$p(X) = \frac{1}{Z} \prod_{k=1}^{M} \phi(\mathbf{x}_k) \prod_{k=2}^{M} \psi(\mathbf{x}_k, \mathbf{x}_{k-1}), \qquad (7)$$

where the partition function Z is the same as for the original model and the $\phi(\mathbf{x}_k)$'s and $\psi(\mathbf{x}_k, \mathbf{x}_{k-1})$'s are the in-column and between-column interaction potentials, respectively. In terms of the original factors of the 2-D $(1, \infty)$ run-length limited constrained channel model we get

$$\phi(\mathbf{x}_k) = \prod_{j=1}^{M-1} \psi(x_{j+1,k}, x_{j,k}), \qquad (8a)$$

$$\psi(\mathbf{x}_k, \mathbf{x}_{k-1}) = \prod_{j=1}^{M} \psi(x_{j,k}, x_{j,k-1}). \qquad (8b)$$

We illustrate this choice of auxiliary variables and the resulting undirected chain in Figure 2. This transformation of the PGM
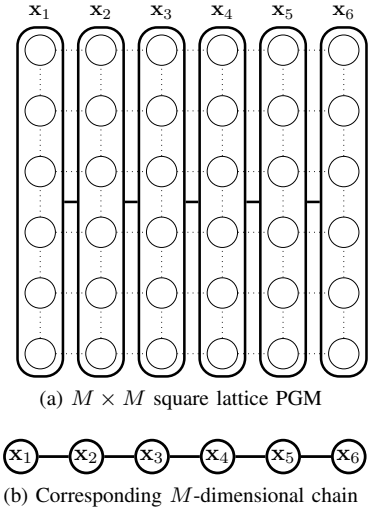

(a) $M \times M$ square lattice PGM

(b) Corresponding M-dimensional chain

Fig. 2. $M \times M$ square lattice graphical model converted to an M-dimensional undirected chain model.

is a key enabler for the partition function estimation algorithm we propose in the subsequent section.

III. SEQUENTIAL MONTE CARLO

Sequential Monte Carlo methods, also known as particle filters, are designed to sample sequentially from some sequence of target distributions: $\bar{\gamma}_k(\mathbf{x}_{1:k})$, $k = 1, 2 \ldots$. While SMC is most commonly used for inference on directed chains, in particular for state-space models, these methods are in fact much more generally applicable. Specifically, as we shall see below, SMC can be used to simulate from the joint PMF specified by an undirected chain. Consequently, by using the representation introduced in Section II it is possible to apply SMC to estimate the partition function of the 2-D $(1, \infty)$ run-length limited constrained channel. We start this section with a short introduction to SMC samplers with some known theoretical results. These results are then used to compute an unbiased estimate of the partition function. We leverage the undirected chain model with the SMC sampler and show how we can perform the necessary steps using *Forward Filtering/Backward Sampling* (FF/BS) [10], [11]. For a more thorough description of SMC methods see e.g. [12], [13].

A. Estimating the partition function using fully adapted SMC

We propose to use a *fully adapted* SMC algorithm [14]. That the sampler is *fully adapted* means that the proposal distributions for the resampling and propagation steps are optimally chosen with respect to minimizing the variance of the importance weights, i.e. the importance weights for a fully adapted sampler are all equal. Using the optimal proposal distributions—which can significantly reduce the variance of estimators derived from the sampler—is not tractable in general. However, as we shall see below, this is in fact possible for the square lattice PGM described above.

For the undirected chain model (see Figure 2b), we let $\bar{\gamma}_k(\mathbf{x}_{1:k})$ be the PMF induced by the sub-graph corresponding

to the first k variables. Specifically, $\bar{\gamma}_k(\mathbf{x}_{1:k}) = \frac{\gamma_k(\mathbf{x}_{1:k})}{Z_k}$, where the unnormalized distributions $\gamma_k(\mathbf{x}_{1:k})$ are given by

$$\gamma_1(\mathbf{x}_1) = \phi(\mathbf{x}_1), \tag{9a}$$
$$\gamma_k(\mathbf{x}_{1:k}) = \gamma_{k-1}(\mathbf{x}_{1:k-1})\phi(\mathbf{x}_k)\psi(\mathbf{x}_k, \mathbf{x}_{k-1}), \tag{9b}$$

with $\phi(\cdot), \psi(\cdot)$ as defined in (8) and Z_k being the normalizing constant for $\gamma_k(\mathbf{x}_{1:k})$. We take the sequence of distributions $\bar{\gamma}_k(\mathbf{x}_{1:k})$ for $k = 1, \ldots, M$ as the target distributions for the SMC sampler. Note that $\bar{\gamma}_k(\mathbf{x}_{1:k})$ for $k < M$ is *not*, in general, a marginal distribution under $p(X)$. This is, however, not an issue since by construction $\bar{\gamma}_M(\mathbf{x}_{1:M}) = p(X)$ (where $\mathbf{x}_{1:M}$ identifies to X), i.e. at iteration $k = M$ we still recover the correct target distribution.

At iteration k, the SMC sampler approximates $\bar{\gamma}_k(\mathbf{x}_{1:k})$ by a collection of particles $\{\mathbf{x}_{1:k}^i\}_{i=1}^N$, where $\mathbf{x}_{1:k} = \{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$ is the set of all variables in column 1 through k of the PGM. These samples define an empirical point-mass approximation of the target distribution,

$$\widehat{\gamma}_k^N(\mathbf{x}_{1:k}) := \frac{1}{N}\sum_{i=1}^N \delta(\mathbf{x}_{1:k} - \mathbf{x}_{1:k}^i),$$

where $\delta(x)$ is the Kronecker delta. The standard SMC algorithm produces a collection of weighted particles. However, as mentioned above, in the fully adapted setting we use a specific choice of proposal distribution and resampling probabilities, resulting in equally weighted particles [14].

Consider first the initialization at iteration $k = 1$. The auxiliary probability distribution $\bar{\gamma}_1(\mathbf{x}_1)$ corresponds to the PGM induced by the first column of the original square lattice model. That is, the graphical model for $\bar{\gamma}_1(\mathbf{x}_1)$ is a chain (the first column of Figure 2a). Consequently, we can sample from this distribution exactly, as well as compute the normalizing constant Z_1, using FF/BS. The details are given in the subsequent section. Simulating N times from $\bar{\gamma}(\mathbf{x}_1)$ results in an *equally weighted* sample $\{\mathbf{x}_1^i\}_{i=1}^N$ approximating this distribution.

We proceed inductively and assume that we have at hand a sample $\{\mathbf{x}_{1:k-1}^i\}_{i=1}^N$, approximating $\bar{\gamma}_{k-1}(\mathbf{x}_{1:k-1})$. This sample is propagated forward by simulating, conditionally independently given the particle generation up to iteration $k-1$, as follows: We decide which particle among $\{\mathbf{x}_{1:k-1}^j\}_{j=1}^N$ that should be used to generate a new particle $\mathbf{x}_{1:k}^i$ (for each $i \in \{1, \ldots, N\}$) by drawing an *ancestor index* a_k^i with probability

$$\mathbb{P}(a_k^i = j) = \frac{\nu_{k-1}^j}{\sum_l \nu_{k-1}^l}, \qquad j \in \{1, \ldots, N\}, \tag{10}$$

where ν_{k-1}^i are resampling weights. The variable a_k^i is the index of the particle at iteration $k-1$ that will be used to construct $\mathbf{x}_{1:k}^i$. Generating the ancestor indices corresponds to a selection—or resampling—process that will put emphasis on the most likely particles. This is a crucial step of the SMC sampler. For the fully adapted sampler, the resampling weights $\nu_{k-1}^i = \nu_{k-1}(\mathbf{x}_{k-1}^i)$ are chosen in order to adapt the resampling to the *consecutive target distribution* $\bar{\gamma}_k$ [14]. Intuitively, a particle $\mathbf{x}_{1:k-1}^i$ that is probable under the marginal distribution $\sum_{\mathbf{x}_k} \bar{\gamma}_k(\mathbf{x}_{1:k})$ will be assigned a large weight.

Specifically, in the fully adapted algorithm we pick the re-sampling weights according to

$$\nu_{k-1}(\mathbf{x}_{k-1}) = \sum_{\mathbf{x}_k} \frac{\gamma_k(\mathbf{x}_{1:k})}{\gamma_{k-1}(\mathbf{x}_{1:k-1})} = \sum_{\mathbf{x}_k} \phi(\mathbf{x}_k)\psi(\mathbf{x}_k, \mathbf{x}_{k-1}). \tag{11}$$

Given the ancestors, we simulate $\mathbf{x}_k^i$ from the optimal proposal distribution: $\mathbf{x}_k^i \sim q(\cdot \mid \mathbf{x}_{k-1}^{a_k^i})$ for $i = 1, \ldots, N$, where

$$q(\mathbf{x}_k \mid \mathbf{x}_{k-1}) = \frac{\phi(\mathbf{x}_k)\psi(\mathbf{x}_k, \mathbf{x}_{k-1})}{\sum_{\mathbf{x}_k'} \phi(\mathbf{x}_k')\psi(\mathbf{x}_k', \mathbf{x}_{k-1})}. \tag{12}$$

Again, simulating from this distribution, as well as computing the resampling weights (11), can be done exactly by running FF/BS on the kth column of the model. Finally, we augment the particles as, $\mathbf{x}_{1:k}^i := (\mathbf{x}_{1:k-1}^{a_k^i}, \mathbf{x}_k^i)$. As pointed out above, with the choices (11) and (12) we obtain a collection of equally weighted particles $\{\mathbf{x}_{1:k}^i\}_{i=1}^N$, approximating $\bar{\gamma}_k(\mathbf{x}_{1:k})$.

At iteration $k = M$, the SMC sampler provides a Monte Carlo approximation of the joint PMF $p(X) = \bar{\gamma}_M(\mathbf{x}_{1:k})$. While this can be of interest on its own, we are primarily interested in the normalizing constant Z (i.e. the partition function). However, it turns out that the SMC algorithm in fact provides an estimator of Z_k as a byproduct, given by

$$\widehat{Z}_k^N := Z_1 \prod_{\ell=1}^{k-1} \left(\frac{1}{N}\sum_{i=1}^N \nu_\ell^i \right). \tag{13}$$

It may not be obvious to see why (13) is a natural estimator of the normalizing constant Z_k. However, it has been shown that this SMC-based estimator is unbiased for any $N \geq 1$ and $k = 1, \ldots, K$. This result is due to [15, Proposition 7.4.1]. Specifically, for our 2-D constrained channel example, it follows that at the last iteration $k = M$ we have an unbiased estimator of the partition function

$$\mathbb{E}[\widehat{Z}_M^N] = Z. \tag{14}$$

Furthermore, under a weak integrability condition the estimator is asymptotically normal with a rate $\sqrt{N}$:

$$\sqrt{N}(\widehat{Z}_M^N - Z) \xrightarrow{d} \mathcal{N}(0, \sigma^2), \tag{15}$$

where an explicit expression for σ^2 is given in [15, Proposition 9.4.1].

B. SMC samplers and Forward Filtering/Backward Sampling

To implement the fully adapted SMC sampler described above we are required to compute the sums involved in equations (11) and (12). By brute force calculation our method would be computationally prohibitive as the complexity is exponential in the dimensionality M of the chain. However, as we show below, it is possible to use FF/BS to efficiently carry out these summations. This development is key to our proposed solution to the problem of estimating the partition function, since the computational complexity of estimating the channel capacity is reduced from $\mathcal{O}(NM2^M)$ (brute force) to $\mathcal{O}(NM^2)$ (FF/BS).

Initially, at $k = 1$, the graph describing the target distribution $\bar{\gamma}_1(\mathbf{x}_1)$ is trivially a chain which can be sampled

from exactly by using FF/BS. Additionally, the normalizing constant Z_1 can be computed in the forward pass of the FF/BS algorithm. However, this is true for any consecutive iteration k as well. Indeed, simulating $\mathbf{x}_k$ under $\bar{\gamma}_k$, conditionally on $\mathbf{x}_{1:k-1}$, again corresponds to doing inference on a chain. This means we can employ FF/BS to compute the resampling weights (11) (corresponding to a conditional normalizing constant computation) and to simulate $\mathbf{x}_k$ from the optimal proposal (12).

Let k be a fixed iteration of the SMC algorithm. The forward filtering step of FF/BS is performed by sending messages

$$m_{j+1}^i(x_{j+1,k}) = \sum_{x_{j,k}} \psi(x_{j+1,k}, x_{j,k})\psi(x_{j,k}, x_{j,k-1}^i)m_j^i(x_{j,k}), \tag{16}$$

for $j = 1, \ldots, M-2$, i.e. from the top to the bottom of column k. The resampling weights are given as a byproduct from the message passing as

$$\nu_{k-1}(\mathbf{x}_{k-1}^i) = \sum_{\mathbf{x}_k} \boldsymbol{\phi}(\mathbf{x}_k)\boldsymbol{\psi}(\mathbf{x}_k, \mathbf{x}_{k-1}^i)$$
$$= \sum_{x_{M,k}} \psi(x_{M,k}, x_{M,k-1}^i)m^i(x_{M-1,k}). \tag{17}$$

After sampling the ancestor indices a_k^i as in (10), we perform backward sampling to sample the full column of variables $\mathbf{x}_k$, one at a time in reverse order $j = M, \ldots, 1$,

$$x_{j,k}^i \sim \frac{\psi(x_{j,k}, x_{j+1,k}^i)\psi(x_{j,k}, x_{j,k-1}^{a_k^i})m^{a_k^i}(x_{j,k})}{\sum_{x'_{j,k}} \psi(x'_{j,k}, x_{j+1,k}^i)\psi(x'_{j,k}, x_{j,k-1}^{a_k^i})m^{a_k^i}(x'_{j,k})}, \tag{18}$$

with straightforward modifications for $j = 1$ and M. This results in a draw $\mathbf{x}_k^i = (x_{1,k}^i, \ldots, x_{M,k}^i)$ from the optimal proposal $q(\cdot \mid \mathbf{x}_{k-1}^{a_k^i})$ defined in (12). A summary of the resulting solution is provided in Algorithm 1. Furthermore, for increased numerical stability we pass normalized messages and compute the resampling weights and the partition function estimate directly in the log-space.

Algorithm 1 Channel capacity estimation

Perform each step for $i = 1, \ldots, N$, except setting $\widehat{Z}_k^N$.
Sample $\mathbf{x}_1^i$ using FF/BS (16), (18).
Set $\widehat{Z}_1^N = Z_1$.
for $k = 2$ **to** M **do**
    Calculate $\nu_{k-1}(\mathbf{x}_{k-1}^i)$ using forward filtering (16)-(17).
    Sample a_k^i according to (10).
    Sample $\mathbf{x}_k^i$ using backward sampling (18).
    Set $\mathbf{x}_{1:k}^i = (\mathbf{x}_{1:k-1}^{a_k^i}, \mathbf{x}_k^i)$.
    Set $\widehat{Z}_k^N = \widehat{Z}_{k-1}^N \left(\frac{1}{N}\sum_{i=1}^N \nu_{k-1}(\mathbf{x}_{k-1}^i)\right)$
end for

IV. EXPERIMENTS

We compare our algorithm to the state-of-the-art Monte Carlo approximation algorithm proposed in [5] on the same example that they consider as explained in Section II. Since

the key enabler to the algorithm proposed in [5] is tree sampling according to [16]—a specific type of blocked Gibbs sampling—we will in the sequel refer to this algorithm as the *tree sampler*. All results are compared versus average wall-clock execution time. We run each algorithm 10 times independently to estimate error bars as well as mean-squared-errors (MSE) compared to the true value (computed using a long run of the tree sampler). For the MCMC-based tree sampler, we use a burn-in of 10% of the generated samples when estimating the capacity. The tree sampler actually gives two estimates of the capacity at each iteration; we use the average of these two when comparing to the SMC algorithm. Code for reproducing the results is available at [17].

Consider first a channel with dimension $M = 10$. We can see the results with error bars from 10 independent runs in Figure 3 of both algorithms. The rightmost data point corresponds to approximately 20k iterations/particles. Both algorithms converge to the value $C_{10} \approx 0.6082$. However, the SMC algorithm is clearly more efficient and with less error per fix computation time. We estimated the true value by running 10 independent tree samplers for 100k iterations, removed burn-in and taking the mean as our estimate.
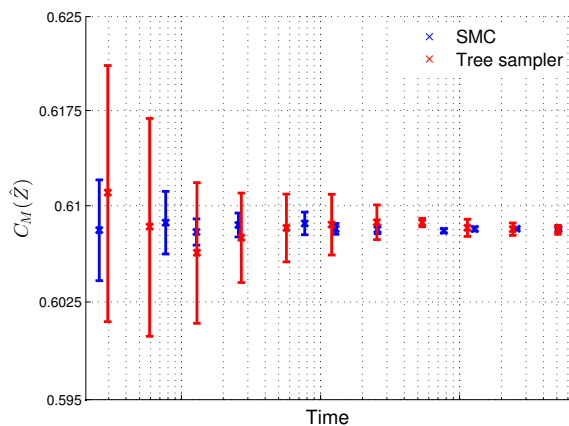

Fig. 3. Estimates of the capacity C_{10}, with error bars, based on 10 independent runs of our proposed SMC-based method and the tree sampler [5]. Plotted versus wall-clock time in log-scale. Note that this is also an upper bound on the infinite-size capacity, i.e. $C_M \geq C_\infty \approx 0.5879$.

The estimated true value was subsequently used to calculate the MSE as displayed in Figure 4. The central limit theorem for the SMC sampler (see (15)) tells us that the error should decrease at a rate of $1/N$ which is supported by this experiment. Furthermore, we can see that the SMC algorithm on average gives an order of magnitude more accurate estimate than the tree sampler per fix computation time. In our second example we scale up the model to $M = 60$, i.e. a total of 3600 nodes as opposed to 100 in the previous example. The basic tree sampler performs poorly on this large model with very slow mixing and convergence. To remedy this problem [5] propose to aggregate every W columns in the tree sampler and sample these exactly by simple enumeration, resulting in further blocking of the underlying Gibbs sampler. However, this results in an algorithm with a computational complexity exponential in W [5]. The same strategy can be applied to our algorithm and we compare the tree sampler and SMC for widths $W = 1$ and 3. There seems to be no gain in increasing the width higher than this for either method. The
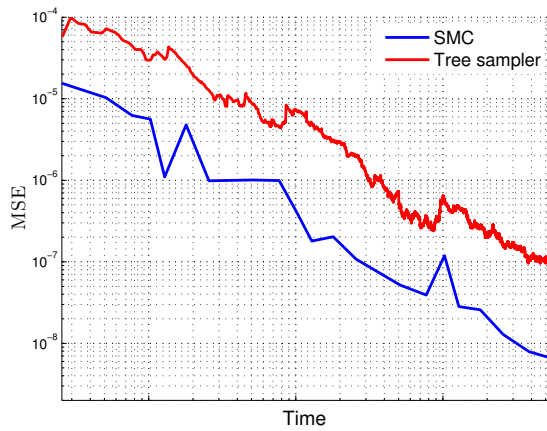
Fig. 4. Mean-squared-error of the capacity C_{10} estimates based on 10 independet runs of our proposed SMC-based method and the tree sampler [5]. Plotted versus wall-clock time in log-log-scale.

resulting MSEs[1] based on 10 independent runs of the tree sampler and the SMC algorithm are presented in Figure 5. As we can see the basic tree sampler converges very slowly,
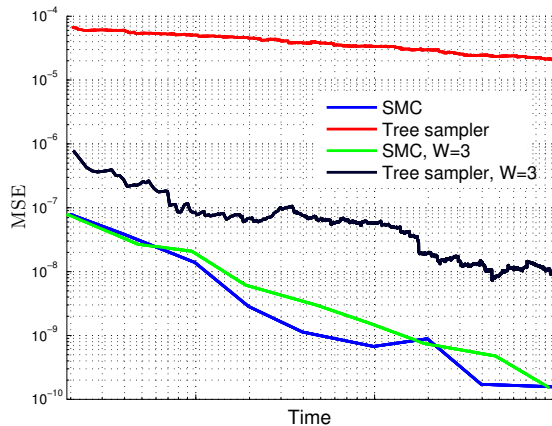

Fig. 5. Mean-squared-error of the capacity C_{60} estimates based on 10 independet runs of our proposed SMC-based method and the tree sampler [5] for strip widths 1 (standard) and 3 respectively. Plotted versus wall-clock time in log-log-scale.

in line with results from [5]. On the other hand, our proposed SMC sampling method performs very well, even with $W = 1$, and on average it has more than an order-of-magnitude smaller error than the tree sampler with $W = 3$. In comparing the two different SMC methods there seems to be no apparent gain in increasing the width of the strips added at each iteration in this case.

V. CONCLUSIONS

We have introduced an SMC method to compute the noiseless capacity of two-dimensional channel models. The proposed algorithm was shown to improve upon a state-of-the-art Monte Carlo estimation method by more than an order-of-magnitude. Furthermore, while this improvement was obtained using a sequential implementation, the SMC method is easily

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[1]For this model the basic tree sampler converges too slowly and the tree sampler with $W = 3$ was too computationally demanding to provide an accurate estimate of the "true" value. For this reason, we estimate the true value by averaging 10 independent runs of SMC with $N = 200k$.

parallelizable over the particles (which is not the case for the MCMC-based tree sampler), offering further improvements by making use of modern computational architectures. This gain is of significant importance because the running time can be on the order of days for realistic scenarios. Extensions to calculate the information rate of noisy 2-D source/channel models by the method proposed in [5] are straightforward.

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