



A Heuristic Independent Particle Approximation to Determinantal Point Processes

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Abstract

A determinantal point process is a stochastic point process that is commonly used to capture negative correlations. It has become increasingly popular in machine learning in recent years. Sampling a determinantal point process however remains a computationally intensive task. This note introduces a heuristic independent particle approximation to determinantal point processes. The approximation is based on the physical intuition of fermions and is implemented using standard numerical linear algebra routines. Sampling from this independent particle approximation can be performed at a negligible cost. Numerical results are provided to demonstrate the performance of the proposed algorithm.

Keywords Determinantal point process · Fermions · Localized orbitals

Mathematics Subject Classification 60G55 · 65C50

1 Introduction

A determinantal point process is a stochastic point process that is commonly used to capture negative correlations [13]. Let S be a set of points. A point process A is a determinantal point process with a symmetric kernel $K : S \times S \rightarrow \mathbb{R}$ if for distinct x_1, \dots, x_k one has

$$P(\{x_1, \dots, x_k\} \subset A) = \det(K(x_i, x_j))_{1 \leq i, j \leq k}.$$

To simplify the discussion, we assume for simplicity that S is a discrete set of size N and A has a fixed size k . Such a DPP is called elementary and

$$P(A = \{x_1, \dots, x_k\}) = \det(K(x_i, x_j))_{1 \leq i, j \leq k}. \quad (1)$$

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Being the kernel of an elementary DPP imposes important conditions on K such as $K(\cdot, \cdot)$ is positive semi-definite and $\sum_{x \in S} K(x, x) = k$. In what follows, we shall also refer to the diagonal $K(x, x)$ of K as density $\rho(x)$ and it satisfies the normalizing condition $\sum_{x \in S} \rho(x) = k$.

Many natural point processes can be modeled by DPPs. Examples include distribution of non-interacting Fermions, descent subsequences in random sequences, non-intersecting random walks, edge distributions of spanning trees, and eigenvalue of random matrices [3,4,9,17,18]. More recently, DPP has played a significant role in improving diversity and fairness of sampling algorithms in machine learning, such as in information retrieval [5,20], online learning [15], and support vector machines [19]. For a tutorial on the applications of DPP in machine learning, we refer the readers to [11].

However, sampling from DPP remains to be a challenging computational problem. In [8] Hough et al proposed the standard DPP sampling algorithm with $O(Nk^3)$ complexity. Though various improvements (e.g. [10]) and approximate algorithms (e.g. [7]) have been proposed, sampling from DPP remains a hard computation problem.

1.1 Problem and Contribution

This note considers the problem of approximating DPP with an independent particle process with disjoint support, i.e., generating the k samples by sampling each from a support disjoint region. More specifically, we introduce a disjoint union $S = S_1 \cup \dots \cup S_k$ and associate with each S_i a probability density $\rho_i(\cdot)$ supported on S_i . Each realization of this approximate process is then generated by sampling one point from each $\rho_i(\cdot)$. Equivalently, this also amounts to approximating the kernel matrix K , after an appropriate reordering, with a block-diagonal matrix, where each diagonal block has rank one and unit trace. The main advantage of this approximation is that sampling from this approximation can be done extremely rapidly.

The main contribution of this note is to introduce a simple heuristic algorithm for constructing such an approximation. The algorithm itself requires no more than standard numerical linear algebra routines and the numerical results are provided to demonstrate its effectiveness.

1.2 Motivation.

It is natural to ask why one could expect such an approximation to be reasonable. This approximation, though crude sometimes, is well-motivated from physics and chemistry consideration. In the work of Macchi [13], DPP is originally named *fermionic point process* and the elementary DPP with k points is exactly the distribution function of k non-interacting electrons. In this language, $K(x, x')$ is the density matrix and $\rho(x)$ is the single-electron density. Here, *non-interacting* means that there is no further interaction between the electrons besides the Pauli's exclusion principle [14]. To see this, note that the matrix K can be decomposed as

$$K(x, x') = \sum_{i=1}^k \phi_i(x) \phi_i(x') \quad (2)$$

where the functions $\{\phi_i(x)\}$ from S to \mathbb{R} are called electron orbitals. The multi-electron wave function $\Phi(x_1, \dots, x_k)$ is given by the *Slater determinant* [12,16]

$$\Phi(x_1, \dots, x_k) = \frac{1}{\sqrt{k!}} \det(\phi_i(x_j))_{1 \leq i, j \leq k}.$$

The multi-electron density is then the square of the wave function,

$$|\Phi(x_1, \dots, x_k)|^2 = \frac{1}{k!} |\det(\phi_i(x_j))_{1 \leq i, j \leq k}|^2 = \frac{1}{k!} \det(K(x_i, x_j))_{1 \leq i, j \leq k}.$$

Since electrons are indistinguishable, the probability of finding the k electrons at the location set $\{x_1, \dots, x_k\}$ is given by

$$P(\{x_1, \dots, x_k\}) = k! \cdot \frac{1}{k!} \det(K(x_i, x_j))_{1 \leq i, j \leq k} = \det(K(x_i, x_j))_{1 \leq i, j \leq k},$$

which matches (1) exactly.

The choice of the orbitals $\{\phi_i(x)\}$ in (2) is not unique: applying an arbitrary $k \times k$ orthogonal matrix to $\{\phi_i(x)\}$ generates an equally valid set of orbitals and keeps K and the DPP unchanged. However, different sets of orbitals do have different physical interpretations and computational implications. It is often preferred to choose a set of localized orbitals, such as the atomic orbitals $1s, 2s, 2p_x, 2p_y, 2p_z, \dots$. With these localized orbitals identified, one often says that a certain electron is in a certain orbital, without actually referring to the actual position of the other electrons. This implies that, up to a reasonable approximation, it makes sense to sample each electron from its own orbital independently due to their locality. However, such a strategy can violate the Pauli's exclusion principle, since the localized orbitals can still overlap. In order to enforce the Pauli's exclusion principle in our DPP approximation, the algorithm needs to construct disjoint supports for each particle.

1.3 Content.

The rest of the note is organized as follows. Section 2 describes the algorithm for approximating DPP with independent particles. Several numerical examples are presented in Section 3 to demonstrate the performance of this heuristic algorithm. Finally, Section 4 includes some discussion for future work.

1.4 Data availability statement.

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

2 Algorithm

This section describes the algorithm for approximating DPP with independent particles. Let us recall that, given a kernel matrix $K \in \mathbb{R}^{N \times N}$ defined on S , the objective is to introduce a disjoint union $S = S_1 \cup \dots \cup S_k$ and associate to each S_i a probability density $\rho_i(\cdot)$ supported within S_i . The algorithm consists of two steps: localization and partitioning.

2.1 Localization

Let us introduce the matrix $\Phi = (\phi_1, \dots, \phi_k) \in \mathbb{R}^{N \times k}$ with columns equal to the orbitals $\{\phi_i(x)\}$ in (2). The task of this first step is to find an equivalent set of orbitals $\{v_i(x)\}$, which are as localized as possible. Similar to the definition of Φ , we also introduce the matrix $V = (v_1, \dots, v_k) \in \mathbb{R}^{N \times k}$.

Here, we follow the method of selected columns of density matrix (SCDM) introduced in [6]. In the matrix form, the task is to find an orthogonal matrix O such that

$$V := \Phi O$$

has columns as localized as possible. Directly optimizing a locality measure/functional for V over all possible orthogonal matrices is a non-trivial optimization problem. Instead, the key idea of SCDM is that the density matrix $K = \Phi \Phi^T$ often has localized columns [1,2]. Therefore, instead of searching O from the infinite set of $k \times k$ orthogonal matrices, one can simply look for the columns of O from the columns of Φ^T . This can be implemented for example by performing a pivoted QR factorization to the matrix $K = \Phi \Phi^T$. However, since Φ is a matrix with orthogonal columns, it is equivalent to perform the pivoted QR factorization to the smaller matrix Φ^T instead:

$$[Q, R, \sigma] = \text{qr}(\Phi^T), \tag{3}$$

where Q is a $k \times k$ orthogonal matrix, R is a $k \times N$ upper-triangular matrix, and σ is a k -dimensional integer vectors that identifies the first k pivoted columns of Φ^T . Given σ , the columns in $(\Phi \Phi^T)(:, \sigma) = K(:, \sigma)$ are all localized since they are selected columns of K . However, they are not orthogonal. To regain orthogonality, one can set

$$V = K(:, \sigma)(K(\sigma, \sigma))^{-1/2}. \tag{4}$$

It is easy to check that V is indeed a matrix with orthonormal columns:

$$\begin{aligned} V^T V &= (K(\sigma, \sigma))^{-1/2} K(\sigma, :) K(:, \sigma) (K(\sigma, \sigma))^{-1/2} \\ &= (K(\sigma, \sigma))^{-1/2} K(\sigma, \sigma) (K(\sigma, \sigma))^{-1/2} = I, \end{aligned}$$

where the second step uses the fact that K is a projection.

Though the definition of V in (4) involves the $N \times N$ matrix K , it is equivalent to write

$$V = (\Phi \Phi^T)(:, \sigma) (\Phi(\sigma, :) \Phi^T(:, \sigma))^{-1/2},$$

where it is clear that the computation of V can be performed without any explicit reference to the full matrix K .

2.2 Partitioning

The task of the second step is to partition S into k disjoint subsets S_1, \dots, S_k . The easiest way is to simply set

$$S_i = \{x \in S | i = \text{argmax}_j |v_j(x)|\}, \tag{5}$$

with random tie-breaking at a point $x \in S$ whenever multiple $v_j(\cdot)$ vectors have the same absolute value at x . Once S_i is identified, one set the density $\rho_i(x)$ within each S_i as

$$\rho_i(x) = \begin{cases} \frac{\rho(x)}{\sum_{x \in S_i} \rho(x)}, & x \in S_i, \\ 0, & x \notin S_i. \end{cases} \tag{6}$$

The main shortcoming of this approach is that the sum $\sum_{x \in S_i} \rho(x)$ can deviate noticeably from 1. Therefore, after the renormalization step in (6), the density $\rho_i(x)$ can differ significantly from the original density $\rho(x)$.

To fix this issue, a heuristic balancing step is introduced. We optimize for a set of scaling factors $\{\alpha_i\}$ close to one such that the sets S_i defined via

$$S_i = \{x \in S | i = \operatorname{argmax}_j |(\alpha_j v_j)(x)|\} \tag{7}$$

satisfy the constraints that for each i

$$\sum_{x \in S_i} \rho(x) = 1. \tag{8}$$

Once $\{\alpha_i\}$ are identified, one simply set

$$\rho_i(x) = \begin{cases} \rho(x), & x \in S_i, \\ 0, & x \notin S_i. \end{cases} \tag{9}$$

2.3 Sampling

Once $\{S_i\}$ and $\{\rho_i\}$ are computed, sampling from this independent particle model is straightforward.

1. For each $i = 1, \dots, k$, sample x_i from S_i following the distribution $\rho_i(x)$.
2. Return the set $\{x_1, \dots, x_k\}$.

$\{x_i\}$ are clearly disjoint since $\{S_i\}$ are disjoint.

Claim 1 The one-marginal density of the independent particle approximation is equal to $\rho(x)$, i.e., the one-marginal density of the DPP defined in (1).

Proof By construction, the one-marginal density of the independent particle approximation is equal to $\sum_{i=1}^k \rho_i(x)$ for any $x \in S$. For a fixed x , let i_x be the index of the set in $\{S_i\}$ that covers x , i.e., $x \in S_{i_x}$. Since $\{S_i\}$ are disjoint, from (9) we can conclude $\sum_{i=1}^k \rho_i(x) = \rho_{i_x}(x) = \rho(x)$. \square

The multi-marginal density of this independent particle approximation in general can be quite different from the one of the DPP (1), except the Pauli’s exclusion principle is strictly enforced.

The cost of this sampling algorithm is extremely low. By adopting a binary search structure for the weights of $\rho_i(x)$, each sample x_i can be generated in $O(\log N)$ steps. Therefore, the overall sampling cost is $O(k \log N)$.

3 Numerical Results

This section considers several geometric sampling problems in two dimensional spaces to illustrate the performance of the proposed heuristic algorithm. In each example, the functions $\{\phi_i(x)\}$ of $K(\cdot, \cdot)$ are given as input.

In the first example (see Figure 1), S is a uniform Cartesian grid of $[0, 1]^2$ with $\sqrt{N} = 128$ points in each dimension. Clearly, $N = 128^2$. We set $k = 61$ and the orbital functions $\{\phi_i(x)\}$ to be the $k = 61$ lowest eigenmodes of the discrete Laplacian $-\Delta$ on S with periodic boundary condition. The kernel $K(x, x')$ is given by (2) and in this case the density $\rho(x)$ is a constant function. Figure 1(a) shows the density $\rho(x)$ on the Cartesian grid. Figure 1(b) plots the supports of different regions $\{S_i\}$ with different colors. This plot demonstrate that $\{S_i\}$ are

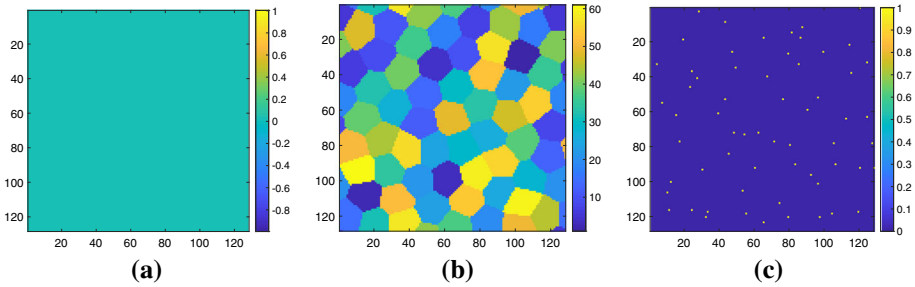


Fig. 1 The first example. **a** density $\rho(x)$. **b** partitioning $\{S_i\}$. **c** a realization of the resulting independent particle process

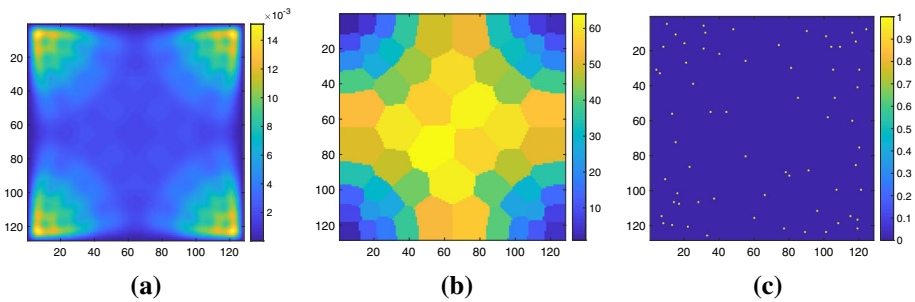


Fig. 2 The second example. **a** Density $\rho(x)$. **b** Partitioning $\{S_i\}$. **c** A realization of the resulting independent particle process

highly localized due to the locality of the new orbitals $\{v_i(x)\}$. Finally, Figure 1(c) shows one realization of the resulting independent particle process.

In the second example (see Figure 2), S is the same uniform Cartesian grid and $N = 128^2$. We set $k = 64$ and choose functions $\{\phi_i(x)\}$ to be the lowest eigenmodes of the differential operator

$$-\Delta + U(x), \quad U(x) \equiv U((x_1, x_2)) = -512 \cdot (\cos(2\pi x_1) + 1) \cdot (\cos(2\pi x_2) + 1),$$

with zero boundary condition. The kernel $K(x, x')$ can again be obtained from (2). In this case the density $\rho(x)$ grows significantly nearly the four corners due to the low potential values there (see Figure 2(a)). Figure 2(b) demonstrates the supports of $\{S_i\}$ with different colors. We see that $\{S_i\}$ are again highly localized with necessary area changes in order to accommodate the density variation across the domain. Finally, Figure 2(c) provides one realization from the resulting independent particle process.

In the third example (see Figure 3), S is still the uniform Cartesian grid with $N = 128^2$. We choose $k = 64$ and let $\{\phi_i(x)\}$ be the lowest eigenmodes of the differential operator

$$-\Delta + U(x), \quad U(x) \equiv U((x_1, x_2)) = +512 \cdot (\cos(2\pi x_1) + 1) \cdot (\cos(2\pi x_2) + 1),$$

with zero boundary condition. The density $\rho(x)$ grows at the domain center due to the low potential $U(x)$ there (see Figure 3(a)). Figure 3(b) demonstrates the supports of $\{S_i\}$ with different colors. $\{S_i\}$ are again highly localized with necessary area changes to accommodate the density variation. Finally, Figure 3(c) gives one realization of the point set from this independent particle process.

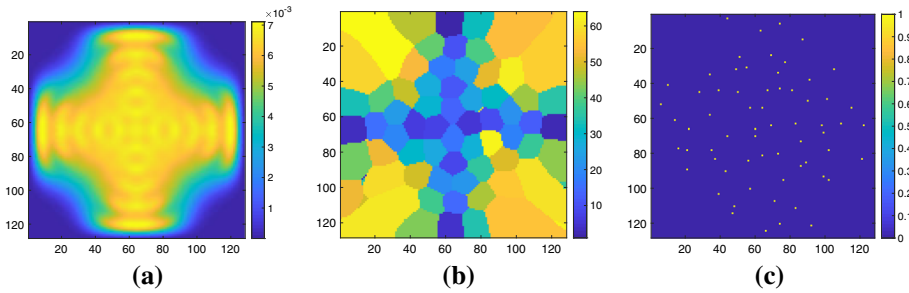


Fig. 3 The third example. **a** Density $\rho(x)$. **b** Partitioning $\{S_i\}$. **c** A realization of the resulting independent particle process

4 Discussions

This note introduces a heuristic independent particle approximation to determinantal point processes. The main benefit of this approximation is that it can be sampled with negligible cost. There are several immediate directions for future work. First, this note only considers the elementary DPP case, and it will be important to generalize this to general DPPs. Second, it will be useful to explore the applications of this algorithm in machine learning applications where the sampling speed of DPP is essential.

Data Availability Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

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