Efficient approximate sampling of projection determinantal point processes

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#### **Motivation**

#### Image search/recommendation systems



'bolt' query

#### **Motivation**

Extractive text summarization (Kulesza & Taskar, 2012)



#### Definition

- $\{1, \ldots, N\}$  indices/labels of items
  - images
  - sentences
  - edges of a graph
- DPP(**K**) a measure on subsets of  $\{1, \ldots, N\}$
- ► K a PSD similarity kernel
- $\mathcal{X} \sim \mathsf{DPP}(\mathbf{K})$  if  $\forall S \subseteq \{1, \dots, N\}$ ,

 $\mathbb{P}\left[S\subseteq\mathcal{X}\right]=\det \mathbf{K}_{S}$ 

 $\blacktriangleright$  Existence is guaranteed when  $\mathbf{0}_{\textit{N}} \preceq \textbf{K} \preceq \textbf{I}_{\textit{N}}$ 

- ▶ K is an orthogonal projection matrix
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  - Summaries made of r sentences
  - Bags of r images

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• Gram matrix  

$$\mathbf{K} = \sum_{i=1}^{r} u^{(i)} u^{(i)^{\mathsf{T}}} = \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi}$$
with  $\varphi_n = (u_n^{(1)}, \dots, u_n^{(r)})^{\mathsf{T}}$ 

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with  $\varphi_n = (u_n^{(1)}, \dots, u_n^{(r)})^{\mathsf{T}}$ 

• Geometrical interpretation  $\mathbb{P}[S \subseteq \mathcal{X}] = \det \mathbf{K}_S$   $= \operatorname{Vol}^2 \{\varphi_i; i \in S\}$ 



#### Diversity

Negative association

$$\mathbb{P}\left[\{i,j\} \subseteq \mathcal{X}\right] = \begin{vmatrix} \mathbb{P}\left[i \in \mathcal{X}\right] & \mathbf{K}_{ij} \\ \mathbf{K}_{ij} & \mathbb{P}\left[j \in \mathcal{X}\right] \end{vmatrix}$$
$$= \mathbb{P}\left[i \in \mathcal{X}\right] \mathbb{P}\left[j \in \mathcal{X}\right] - \mathbf{K}_{ij}^{2}$$
$$\leq \mathbb{P}\left[i \in \mathcal{X}\right] \mathbb{P}\left[j \in \mathcal{X}\right]$$

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- The larger  $|\mathbf{K}_{ij}|$  the smaller  $\mathbb{P}\left[\{i, j\} \subseteq \mathcal{X}\right]$ 
  - Diversity/repulsion
  - $|\mathbf{K}_{ij}|$  yields departure from independence

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• Build the  $r \times N$  feature matrix

$$\mathbf{A} = \left(\sqrt{q_1}\phi_1|\ldots|\sqrt{q_N}\phi_N\right)$$

- If  $\|\phi_i\|^2 = 1$ , 'angles' encode diversity
- ► q<sub>i</sub> measures relevance of item i

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- ► If X ~ DPP(K),

• 
$$|\mathcal{X}| \stackrel{a.s.}{=} r$$
  
• For  $B = \{i_1, \dots, i_r\}$ ,

 $\mathbb{P}\left[\mathcal{X}=B
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- If  $\mathcal{X} \sim \mathsf{DPP}(\mathbf{K})$ ,

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$$|\mathcal{X}| \stackrel{\text{a.s.}}{=} r$$
  
• For  $B = \{i_1, \dots, i_r\}$ ,  
 $\mathbb{P}[\mathcal{X} = B] \propto |\det \mathbf{A}_{:B}|^2 = \operatorname{Vol}^2 \{\sqrt{q_i}\phi_i ; i \in B\}$ 

► DPP(K) has support

$$\mathcal{B} \triangleq \{B; |B| = r, \det \mathbf{A}_{:B} \neq 0\}$$

i.e. collection of columns of  $\boldsymbol{\mathsf{A}}$  forming a basis

#### Assumption

Uniform spanning trees (Lyons, 2003)



Vertex-edge incidence matrix

Uniform spanning trees (Lyons, 2003)



e₄

1

 $e_5$ 

Uniform spanning trees (Lyons, 2003)







Uniform spanning trees (Lyons, 2003)





DPP(K) is a measure on the edge set of G
 B = collection of spanning trees of G

$$\blacktriangleright \mathbb{P}[\mathcal{X} = B] = \frac{\left|\det \mathbf{A}_{:B}\right|^{2}}{\det \mathbf{A}\mathbf{A}^{\mathsf{T}}} = \frac{1}{|\mathcal{B}|}\mathbb{1}_{B \in \mathcal{B}}$$

Rk: Unimodularity, transfer current matrix, matrix tree theorem, Laplacian solvers



#### Exact sampling

- From  $r \times N$  feature matrix  $\mathbf{A} = (\phi_1 | \dots | \phi_N)$
- To  $N \times N$  projection kernel  $\mathbf{K} = \mathbf{A}^{\mathsf{T}} [\mathbf{A}\mathbf{A}^{\mathsf{T}}]^{-1} \mathbf{A}$

**Exact sampling** (Hough et al., 2006; Kulesza & Taskar, 2012) Sample  $\mathcal{X} \sim \mathsf{DPP}(\mathbf{K})$ 

Marginals

$$\mathbb{P}\left[\mathcal{X}=B
ight]=\mathsf{det}\,\mathbf{K}_B$$

• Chain rule, 
$$J = \{i_1, \ldots, i_k\}$$

$$\mathbb{P}\left[i_{k+1}=i|J\right]\propto \mathbf{K}_{ii}-\mathbf{K}_{i,J}\mathbf{K}_{J}^{-1}\mathbf{K}_{J,i}$$

• Costly: eigen-decomposition + Gram-Schmidt =  $O(N^3 + Nr^2)$ 

Rk: Uniform spanning trees (Aldous, 1990; Propp & Wilson, 1998), generation of mazes

#### Approximate sampling - 1

From  $r \times N$  feature matrix  $\mathbf{A} = (\phi_1 | \dots | \phi_N)$ 

Approximate sampling (Anari et al., 2016; Li et al., 2016)

Build a Markov chain,  $\mathbf{B} \triangleq \mathbf{A}_{:B}$ 

- State space  $\mathcal{B} \triangleq \{B; \det \mathbf{B} \neq 0\}$
- Stationary distribution

$$\propto \left|\det \mathbf{B}
ight|^2 = \operatorname{Vol}^2\left\{\phi_i \text{ ; } i \in B
ight\} \cdot \mathbb{1}_{B \in \mathcal{B}}$$

- Basis-exchange graph
  - $B \leftrightarrow B' = (B \setminus \{i\}) \cup \{j\}$
  - Full analysis: polynomial mixing time
  - $\blacktriangleright$  Local and correlated moves on  ${\cal B}$

# Approximate sampling - 1

#### Approximate sampling - 2

From  $r \times N$  feature matrix  $\mathbf{A} = (\phi_1 | \dots | \phi_N)$ 

Approximate sampling (G., Bardenet & Valko, 2017)

Build a Markov chain,  $\mathbf{B} \triangleq \mathbf{A}_{:B}$ 

- State space  $\mathcal{B} \triangleq \{B \text{ ; det } \mathbf{B} \neq 0\}$
- Stationary distribution

$$\propto \left|\det \mathbf{B}\right|^2 = \operatorname{Vol}^2\left\{\phi_i \ ; \ i \in B
ight\} \cdot \mathbb{1}_{B \in \mathcal{B}}$$

- Wander in a continuous embedding of B
  - Geometrical representation of B
  - More decorelated moves, empirically faster mixing

# Approximate sampling - 2

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#### Continuous embedding of the state space $\ensuremath{\mathcal{B}}$

Volume spanned by feature vectors

 $\mathcal{Z}(\mathbf{A}) \triangleq \mathbf{A}[0,1]^N$ 



#### Continuous embedding of the state space $\ensuremath{\mathcal{B}}$

Volume spanned by feature vectors



admits a natural tiling (Dyer & Frieze, 1994),  $\mathbf{B} \triangleq \mathbf{A}_{:B}$ 

$$\mathsf{Vol}\,\mathcal{Z}(\mathsf{A}) = \sum_{B\in\mathcal{B}}\mathsf{Vol}\,\mathsf{B} = \sum_{B\in\mathcal{B}}|\mathsf{det}\,\mathsf{B}|$$

#### Random walk on $\mathcal{B}$ i.e. on tiles

- From  $r \times N$  feature matrix  $\mathbf{A} = (\phi_1 | \dots | \phi_N)$
- Limiting distribution,  $\mathbf{B} \triangleq \mathbf{A}_{:B}$

$$\mathbb{P}\left[\mathcal{X}=B\right] \propto \operatorname{Vol}^{2} \mathbf{B} \cdot \mathbb{1}_{B \in \mathcal{B}}$$

• State space 
$$\mathcal{B} \triangleq \{B; \det \mathbf{B} \neq 0\}$$

• Continuous embedding of  $\mathcal{B}$  via tiling of  $\mathcal{Z}(\mathbf{A}) = \mathbf{A}[0,1]^N$ 



#### Random walk on $\ensuremath{\mathcal{B}}$ i.e. on tiles

#### Underlying continuous walk

- $\mathcal{Z}(\mathbf{A})$  is a polytope (convex)
- ▶ Hit-and-run is efficient for convex bodies (Lovász & Vempala, 2003)



#### Random walk on $\mathcal{B}$ i.e. on tiles

#### Continuous random walk on $\mathcal{Z}(A)$



#### Random walk on $\ensuremath{\mathcal{B}}$ i.e. on tiles

# Continuous random walk on $\mathcal{Z}(\mathbf{A})$

Discrete random walk on  $\ensuremath{\mathcal{B}}$ 

Identify the tile in which x lies

► 
$$B_x = \{i; y_i^* \in ]0, 1[\}$$

#### Random walk on $\mathcal{B}$ i.e. on tiles

# Continuous random walk on $\mathcal{Z}(A)$ $x + \alpha_m^+ d$ $x + \alpha_M d$

Continuous target distribution

$$\pi(x)\,\mathrm{d} x = \sum_{B\in\mathcal{B}} C_B \times \mathbb{1}_{\mathbf{B}}(x)\,\mathrm{d} x$$

#### Discrete random walk on $\mathcal{B}$

Identify the tile in which x lies

$$\begin{array}{ll} \min_{y \in \mathbb{R}^N} & c^{\mathsf{T}}y \\ \text{s.t.} & \mathbf{A}y = x \\ & 0 \leq y \leq 1 \end{array}$$

► 
$$B_x = \{i; y_i^* \in ]0, 1[\}$$



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Discrete target distribution

$$\mathbb{P}\left[B_x=B
ight]\propto\int_{\mathbf{B}}\pi(x)\,\mathrm{d}x=\mathit{C}_B imes\mathsf{Vol}\,\mathbf{B}$$

#### Acceptance = 1

Continuous target distribution

$$\pi(x) \, \mathrm{d}x = \mathbb{1}_{\mathcal{Z}(\mathbf{A})}(x) \, \mathrm{d}x = \sum_{B \in \mathcal{B}} 1 \times \mathbb{1}_{\mathbf{B}}(x) \, \mathrm{d}x$$



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Vol  $\mathbf{B}=$ Vol $^{1}\mathbf{B}$ 





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Acceptance = 
$$\frac{\operatorname{Vol} B(\tilde{x})}{\operatorname{Vol} B(x)}$$

Continuous target distribution

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#### Behaviour of our chain

Relative error of the estimation of  $\mathbb{P}[\{i_1, i_2, i_3\} \subseteq \mathcal{X}] = \det \mathbf{K}_{\{i_1, i_2, i_3\}}$ 



- Better mixing
- More decorelated

#### Fast sampling of projection DPPs?

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Sovle LPs

Fast sampling of projection DPPs?

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#### Efficient sampling of projection DPPs!

#### Some experiments

#### Summarizing a news article from Slate

Find Y to maximize (Kulesza & Taskar, 2012)

$$\int \text{Rouge-1F}(Y, Z) \text{DPP}(Z) dZ \approx \frac{1}{N} \sum_{i=1}^{N} \text{Rouge-1F}(Y, Y_i)$$

where  $Y_i$  are samples from our Markov chain



Figure 1: Estimation of the integrated cost

- Provide feature matrix A (full row rank)
  - Build DPP(A<sup>T</sup>(AA<sup>T</sup>)<sup>-1</sup>A)
  - Continuous embedding of the state space
  - New bridge MCMC  $\cap$  Optimization = hit-and-run + LPs
  - Efficient sampling

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- Applications:
  - ML (Kulesza & Taskar, 2012; Kathuria et al., 2016)
  - Graph sampling (Tremblay et al., 2017)
  - Monte Carlo with DPPs (Bardenet & Hardy, 2016)

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- Generalization
  - ▶ *k*-DPPs (Kulesza & Taskar, 2011)
  - Generic and continuous DPPs (Hough et al., 2006)

#### Conclusion

- Provide feature matrix A (full row rank)
  - Build DPP( $\mathbf{A}^{\mathsf{T}}(\mathbf{A}\mathbf{A}^{\mathsf{T}})^{-1}\mathbf{A}$ )
  - Continuous embedding of the state space
  - ▶ New bridge New bridge MCMC  $\cap$  Optimization = hit-and-run + LPs
  - Efficient sampling
- Applications:
  - ML (Kulesza & Taskar, 2012; Kathuria et al., 2016)
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  - Difficult because of LPs
  - Choice of linear objective c in LP (identification of the tile)
- Generalization
  - k-DPPs (Kulesza & Taskar, 2011)
  - Continuous DPPs (Hough et al., 2006)

POSTER #80

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