Negative Dependence, Stable Polynomials etc in ML

Part 1

STEFANIE JEGELKA & SUVRIT SRA

Dept of EECS & CSAIL

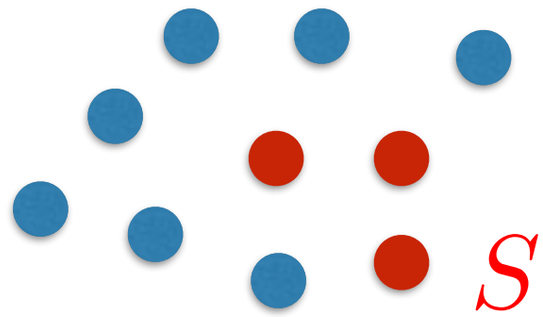
Massachusetts Institute of Technology

Neural information Processing Systems, 2018

ml.mit.edu

Negative Dependence

Discrete probability measure $\mu(S), S \subseteq V$
Equivalently: n binary random variables X_i



negative dependence

0 1 0 1 1 0

$$\mathbb{P}(\in S) \leq \mathbb{P}(\in S)\mathbb{P}(\in S)$$

$$\mathbb{P}(\in S \mid \in S) \leq \mathbb{P}(\in S)$$

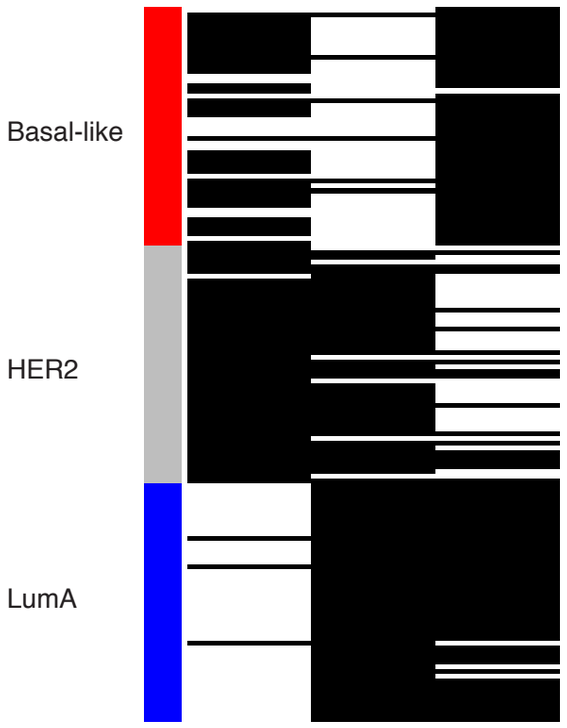
Negative dependence - where?



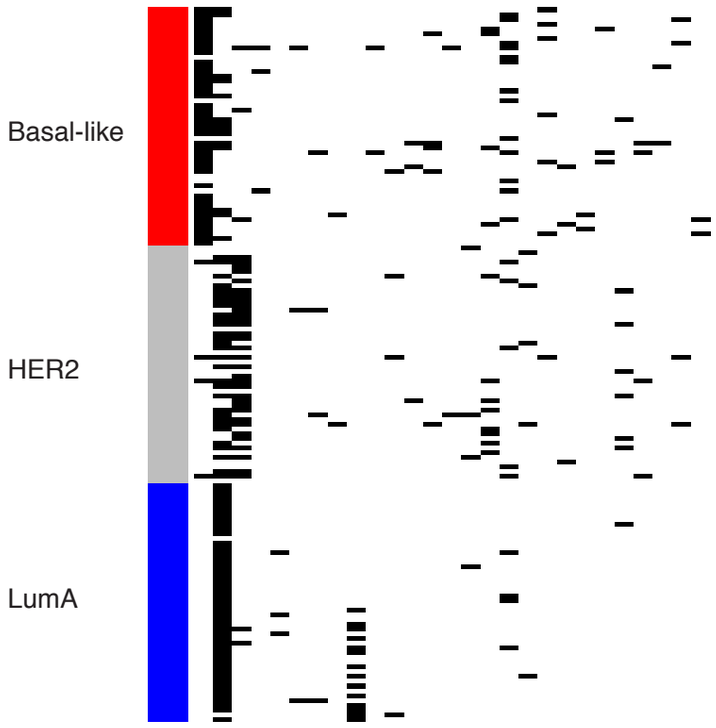



Priors on diversity
Interpretability

Negative Dependence

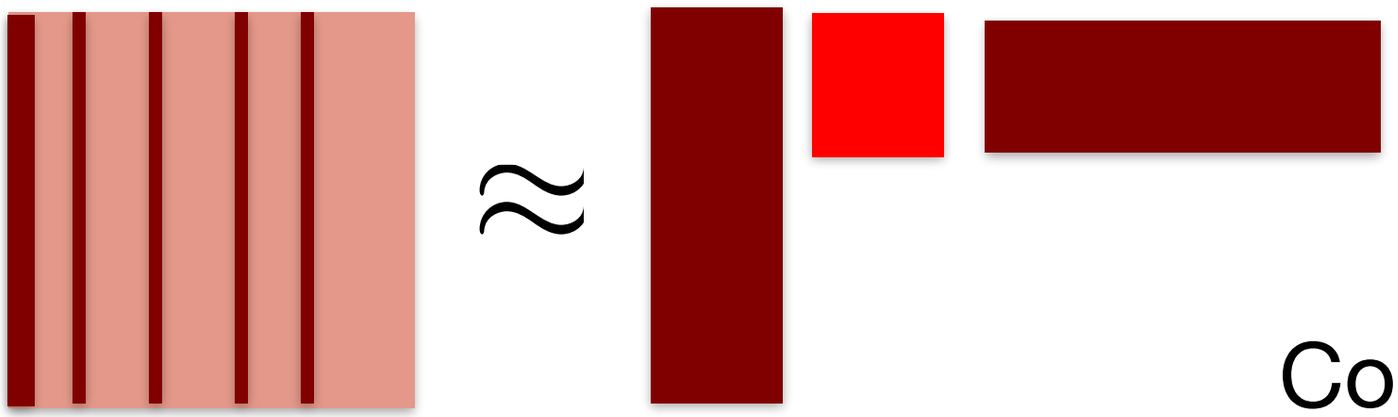


Indian Buffet Process

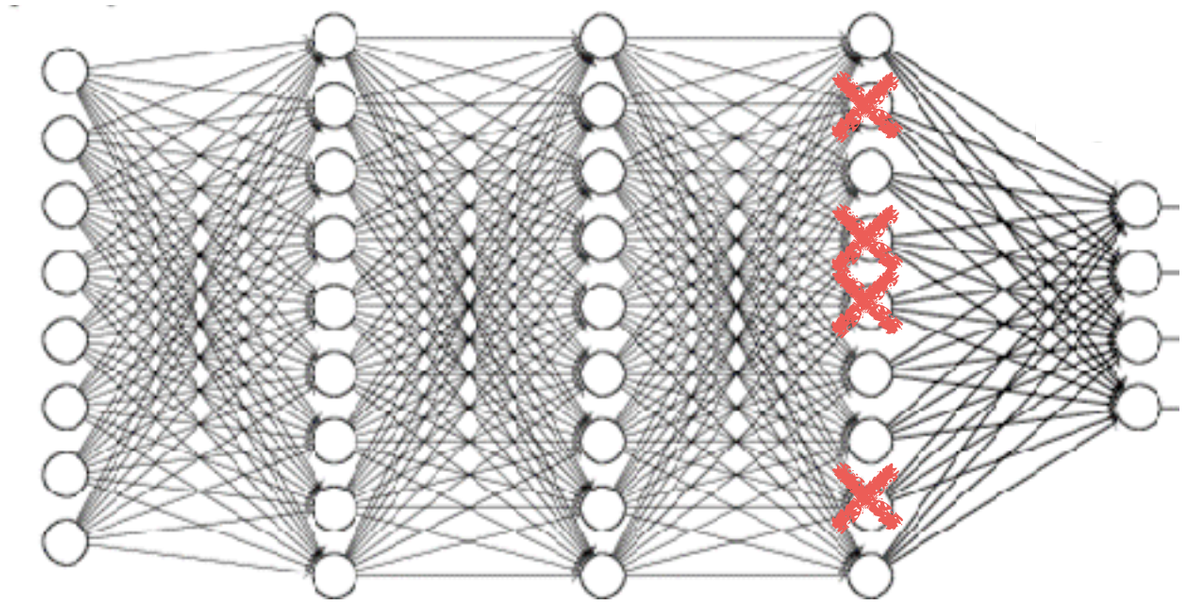


(Xu, Müller, Telesca 2015)

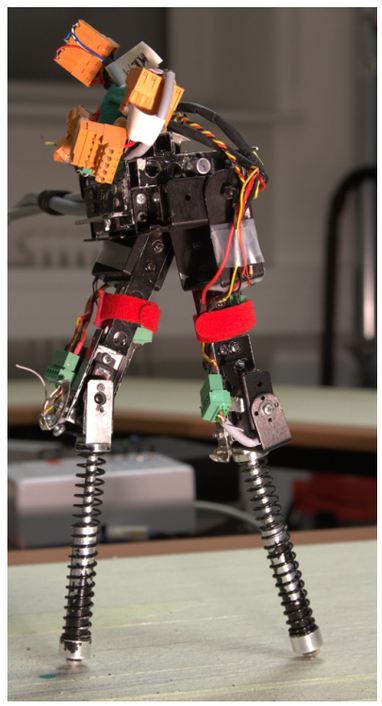
Negative dependence - where?



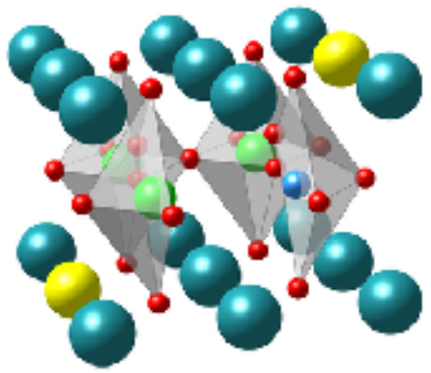
Compressing data
and models



Negative dependence - where?



Exploration,
active learning,
experimental design,
Bayesian Optimization



Outline

1 Intro & Theory

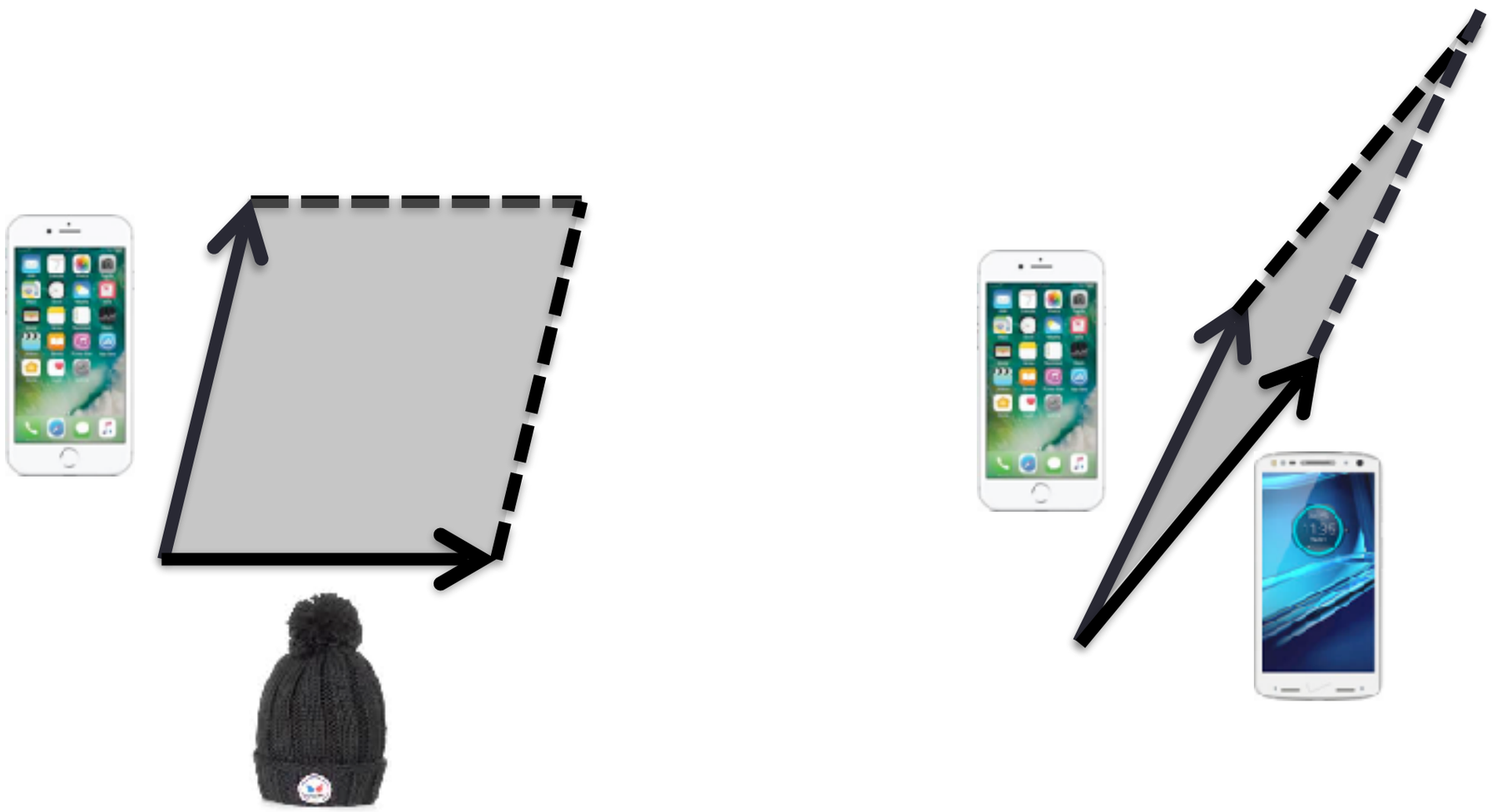
- **Introduction**
  Prominent example: Determinantal Point Processes
- **Stronger notions of negative dependence**
- **Implications: Sampling**

—BREAK—

2 Theory & Applications

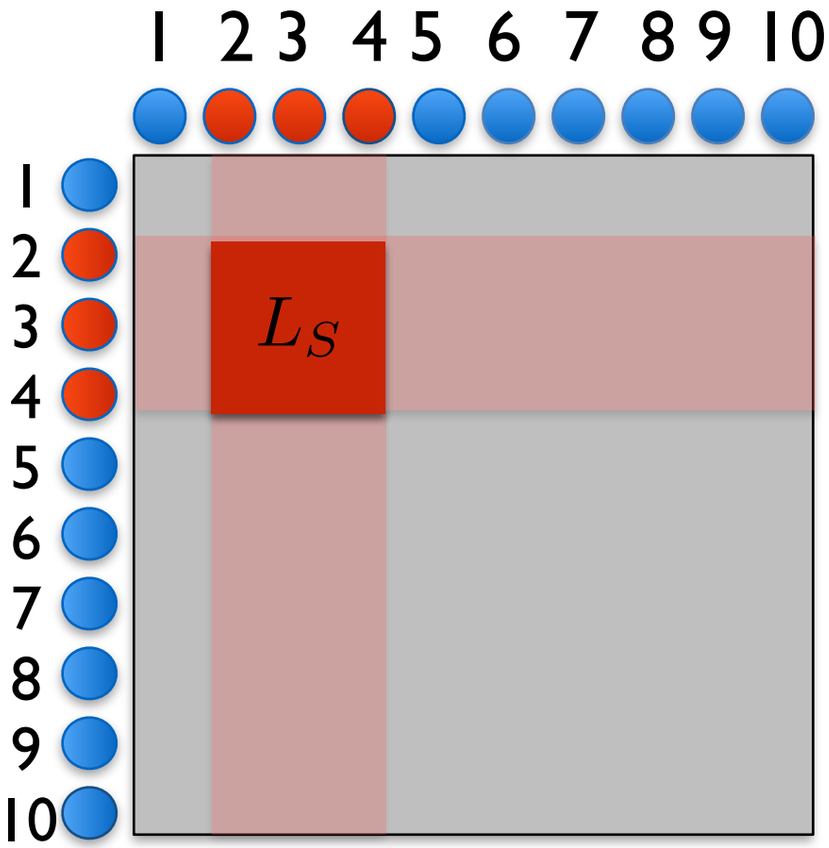
- **Approximating partition functions**
- **Learning a DPP (and some variants)**
- **Applications**
- **Perspectives and wrap-up**

Capturing Diversity: Determinantal Point Processes



$$\mu(S) \propto \mathrm{Vol}^2(\{v_i\}_{i \in S})$$

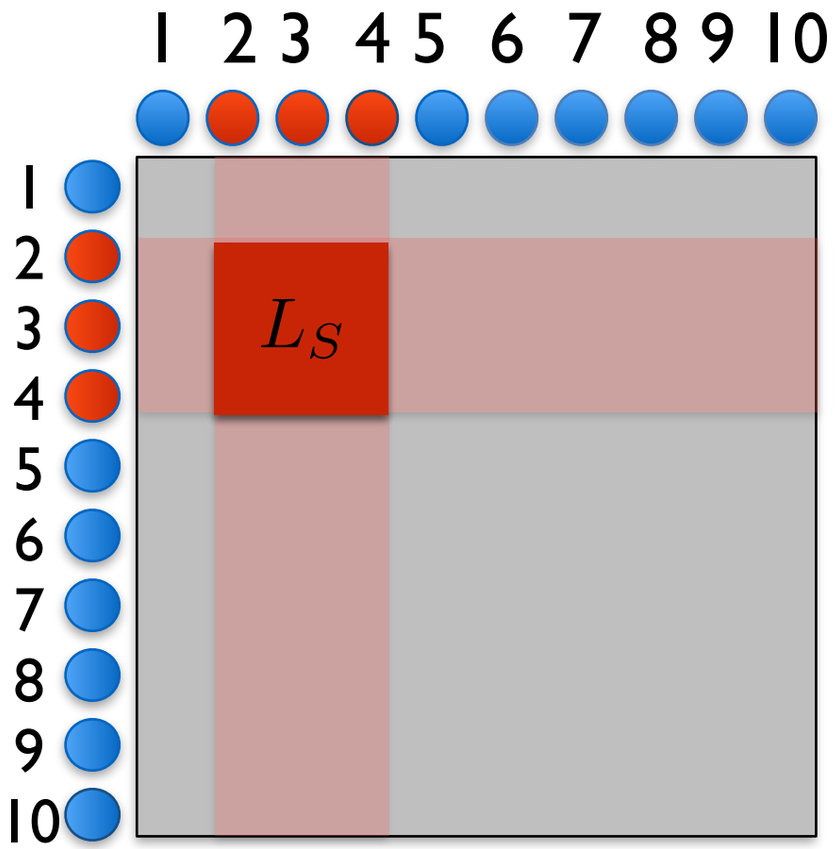
Determinantal Point Processes



PSD similarity matrix L

$$\mu(S) \propto \det(L_S)$$

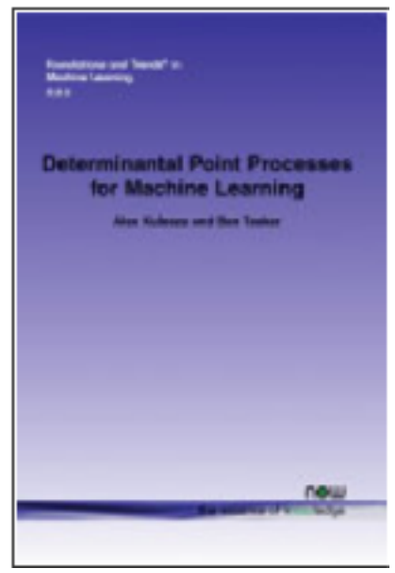
Determinantal Point Processes (DPPs)



PSD similarity matrix L

$$\mu(S) = \frac{\det(L_S)}{\det(L+I)}$$

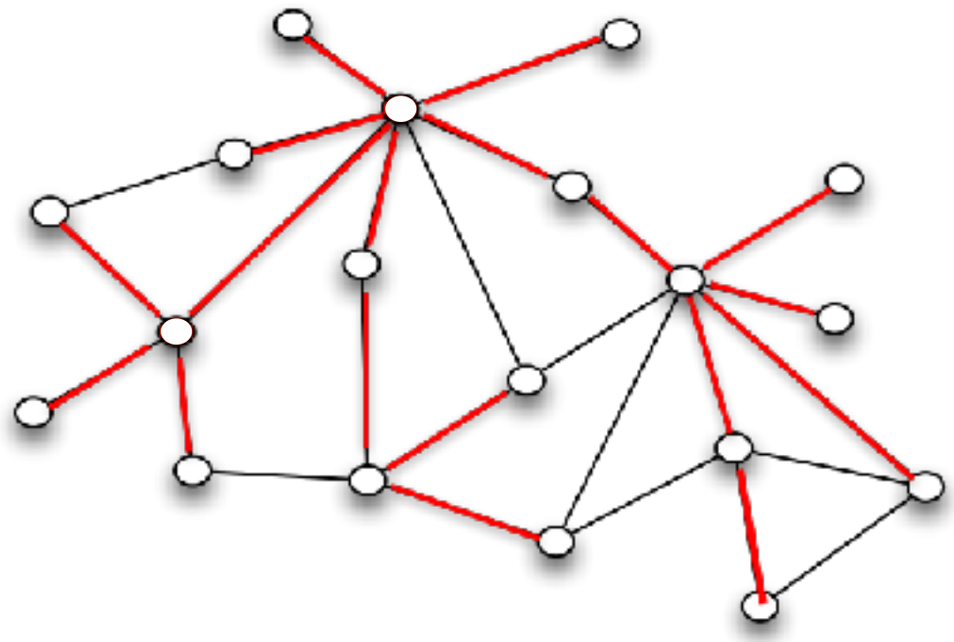
- *Macchi 1975*: “fermion processes”
- *Borodin & Olshanski 2000*: “Determinantal Point Process”
- Introduction to ML: *Kulesza & Taskar*



(Hough, Krishnapur, Peres, Virag 2006; Lyons 2014; Lyons & Peres 2016; Pemantle 2000)

Combinatorial Examples

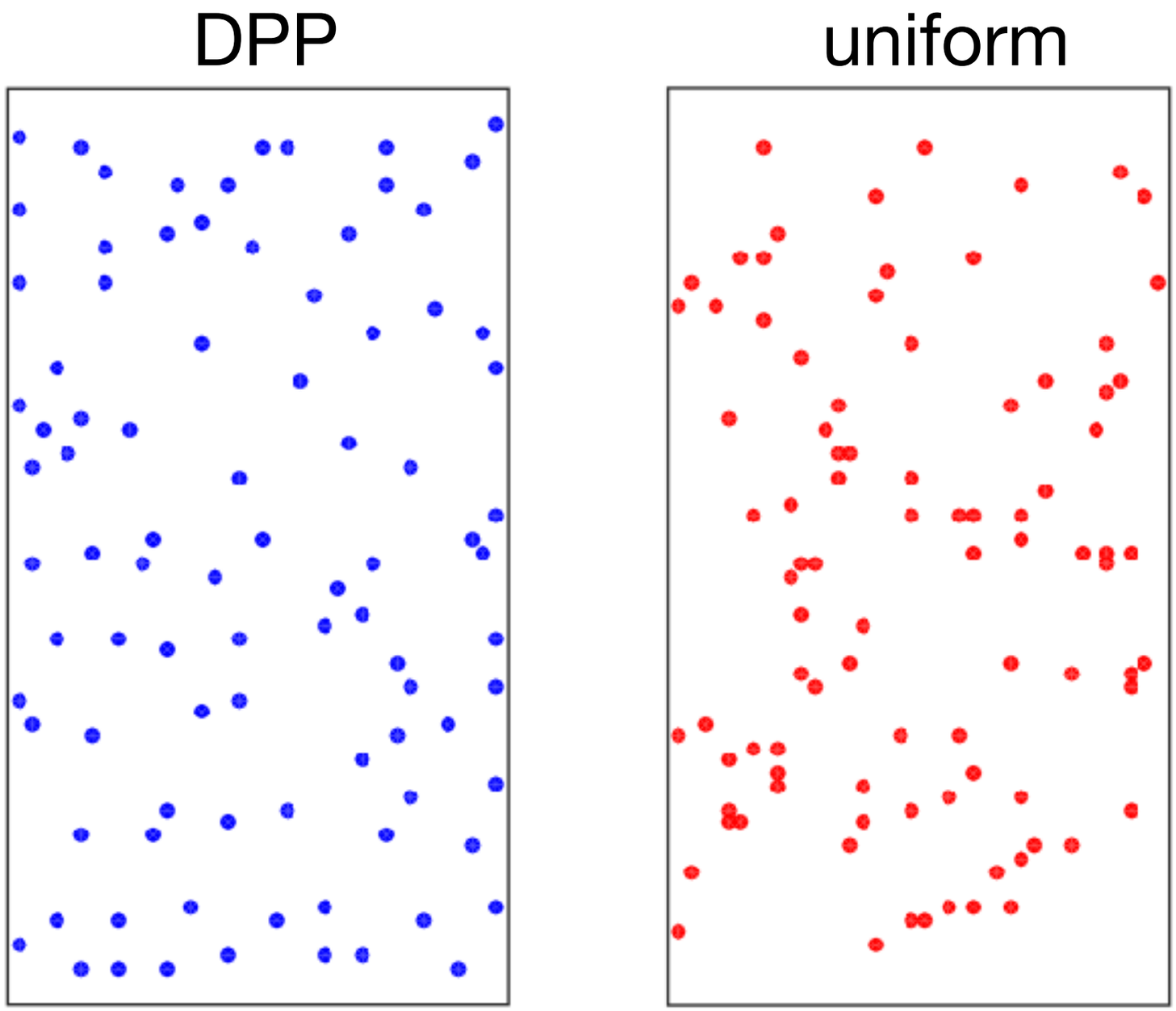
random spanning trees



ascents in random sequences

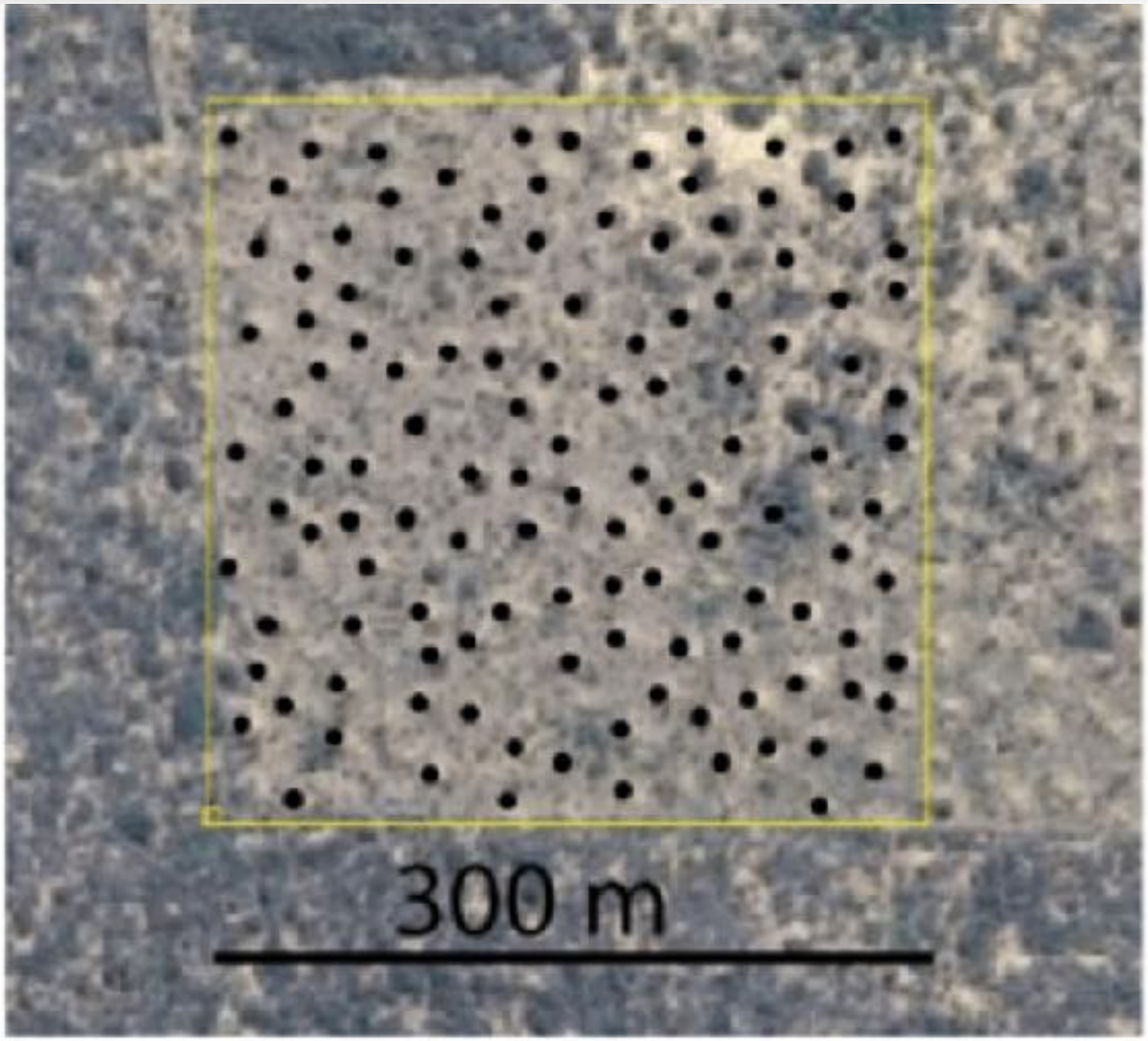
0 2 8 0 9 7 4 5 2 4 9 5 5 2 4

DPP samples



$$l_{ij} = \exp(-\frac{1}{2\sigma^2}\|x_i - x_j\|^2)$$

Repulsion in nature



termite mounds in Brazil

(Martin, Funch, Hanson, Yoo, Current Biology 2018,
http://djalil.chafai.net/blog/2018/11/23/yet-another-determinantal-point-process-in-nature/,)

Outline

Introduction

Examples

Determinantal Point Processes

1

Intro & Theory

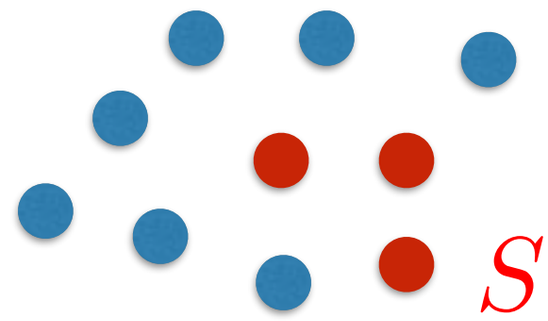
Stronger notions of negative dependence

Relations to polynomials

Implications: Sampling

Negative Dependence

Discrete probability measure $\mu(S), S \subseteq V$
Equivalently: n binary random variables X_i



negative dependence

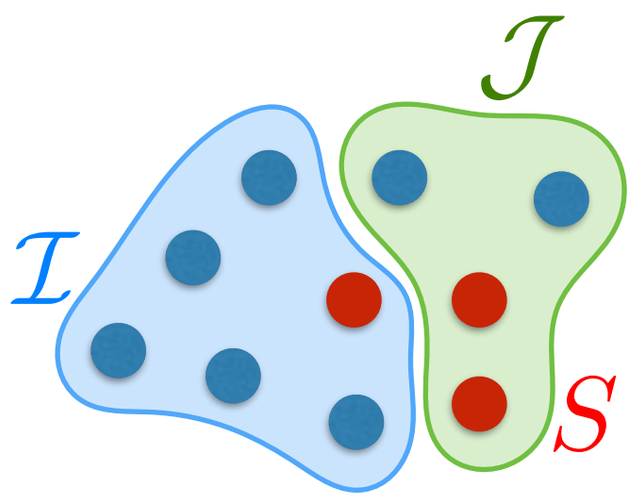
0 1 0 1 1 0

$$\mathbb{P}(\text{📱}\,\text{📱} \in S) \leq \mathbb{P}(\text{📱} \in S)\mathbb{P}(\text{📱} \in S)$$

Stronger Notions

$$\mathbb{P}(\text{[phone]} \in S) \leq \mathbb{P}(\text{[phone]} \in S)\mathbb{P}(\text{[phone]} \in S)$$

equivalently: $\mathbb{E}X_iX_j \leq \mathbb{E}X_i\,\mathbb{E}X_j$

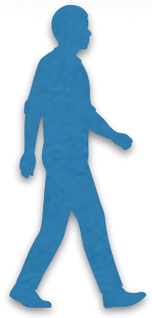


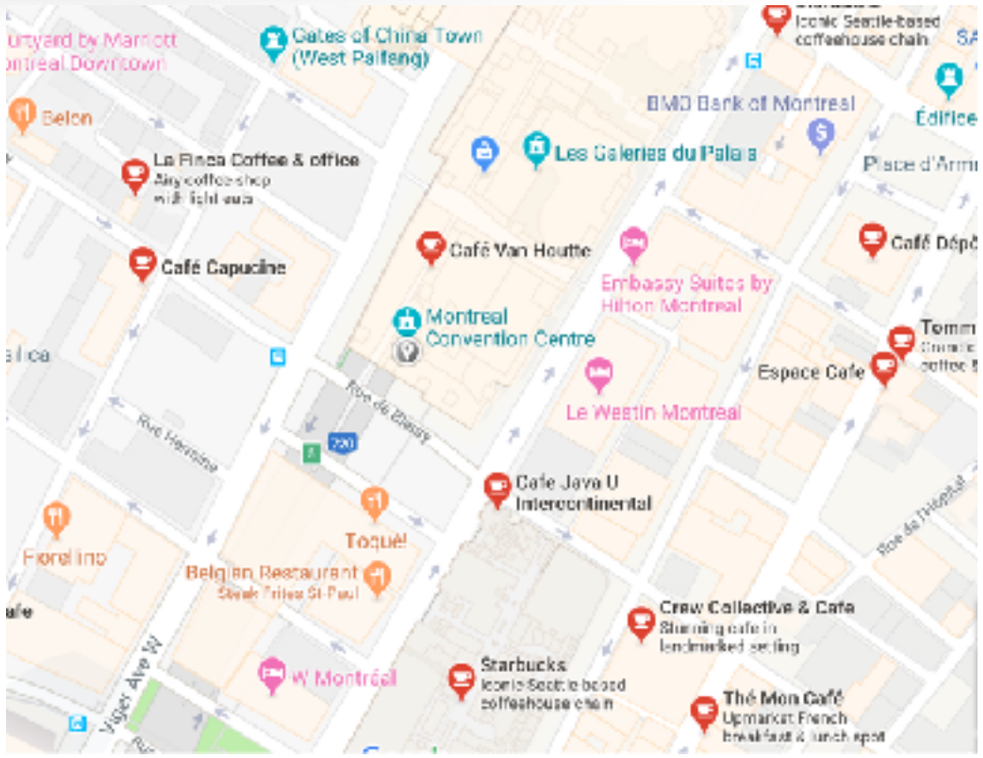
Negative Association

For all monotone increasing functions $G(S), H(S)$

$$\mathbb{E}[G(S \cap \mathcal{I})H(S \cap \mathcal{J})] \leq \mathbb{E}G(S \cap \mathcal{I})\,\mathbb{E}H(S \cap \mathcal{J})$$

Example





$$B_i = \begin{cases} 1 & \text{if thirsty researcher goes to coffee shop } i \\ 0 & \text{otherwise} \end{cases}$$

Detour: Positive Dependence

Positive Association:

For all monotone increasing functions $G(S), H(S)$

$$\mathbb{E}[G(S)H(S)] \quad \geq \quad \mathbb{E}G(S)\,\mathbb{E}H(S)$$

FKG Lattice Condition, Multivariate Totally Positive:

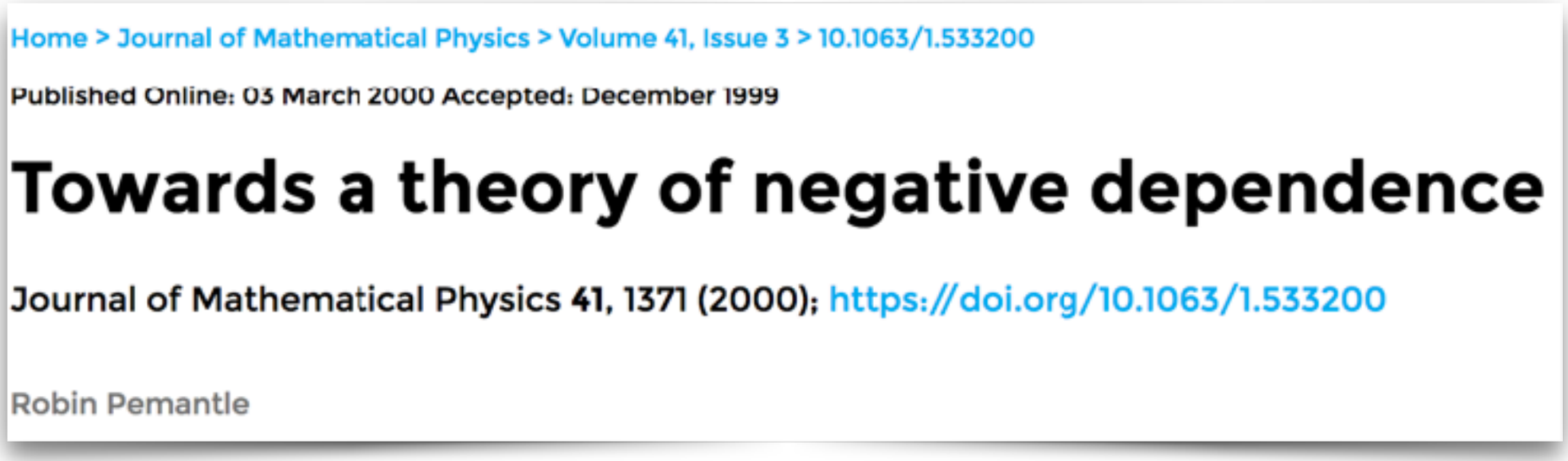
log-supermodularity

$$\mu(S)\mu(T) \;\leq\; \mu(S \cup T)\mu(S \cap T) \quad \forall S, T \subseteq V$$

implies positive association *(Fortuin,Kasteleyn,Ginibre 1971)*

Analog does not hold for negative dependence!

negative association implies log-submodularity, but not conversely


Home > Journal of Mathematical Physics > Volume 41, Issue 3 > 10.1063/1.533200

Published Online: 03 March 2000 Accepted: December 1999

Towards a theory of negative dependence

Journal of Mathematical Physics 41, 1371 (2000); https://doi.org/10.1063/1.533200

Robin Pemantle

The “right notion” should imply:

- Negative Association
- Stochastic Covering
- Log-concave rank sequences $a_k = \mathbb{P}(|S| = k)$
- Closed under “natural” operations
  - conditioning
  - marginalization
  - products …

Generating Polynomial

$$q_\mu(z) = \sum_{S \subseteq V} \mu(S) \prod_{i \in S} z_i, \quad z \in \mathbb{C}^n$$

Example:
2 items

$$q_\mu(z) = \mu_\emptyset + \mu_1 z_1 + \mu_2 z_2 + \mu_{1,2} z_1 z_2$$

Operations on polynomial = operations on distribution

Obtain coefficient $\mu_1 = \mu(\{1\})$

1. differentiate wrt z_1: $\dfrac{\partial}{\partial z_1} q_\mu(z) = \mu_1 + \mu_{1,2} z_2$

2. set $z = 0$

$$\left.\frac{\partial}{\partial z_1} q_\mu(z)\right|_{z=0}$$

Generating Polynomial

$$q_\mu(z) = \sum_{S \subseteq V} \mu(S) \prod_{i \in S} z_i, \quad z \in \mathbb{C}^n$$

Example:
2 items

$$q_\mu(z) = \mu_\emptyset + \mu_1 z_1 + \mu_2 z_2 + \mu_{1,2} z_1 z_2$$

Marginalization: $\pi(\{1\}) = \mathbb{P}(1 \in S)$

Set $z_2 = 1$

$$q_\mu(z_1, 1) = [\mu_\emptyset + \mu_2] + [\mu_1 + \mu_{1,2}] z_1 \qquad = q_\pi(z_1)$$

$\mathbb{P}(1 \notin S)$ $\qquad$ $\mathbb{P}(1 \in S)$

Properties of polynomial $\Leftrightarrow$ Properties of distribution

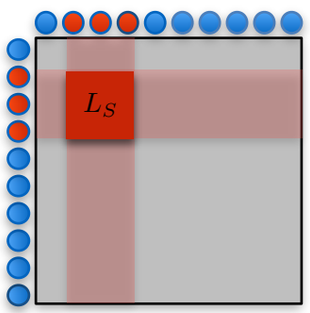
Strongly Rayleigh Measures

$$q_\mu(z) = \sum_{S \subseteq V} \mu(S) \prod_{i \in S} z_i, \quad z \in \mathbb{C}^n$$

$\mu(S)$ is **Strongly Rayleigh (SR)** if $q_\mu(z)$ is *real stable:*

$$\mathrm{Im}(z_i) > 0 \ \forall i \quad \Rightarrow \quad q_\mu(z) \neq 0$$

SR implies almost all conditions laid out by Pemantle!
(Borcea, Bränden, Liggett 2009)



Determinantal Point Process: $q_\mu(z)$ essentially multivariate variant of the characteristic polynomial $\det(z_i I - L)$

Operations on polynomial $\Leftrightarrow$ Operations on distribution

Real Stable Polynomials

$$\mathrm{Im}(z_i) > 0 \ \forall i \quad \Rightarrow \quad q_\mu(z) \neq 0$$

- ✦ Deep mathematical connections
- ✦ Univariate case goes back to Newton (at least)
- ✦ Powerful class of closure properties

Generating polynomial $q(z)$ is SR is equivalent to

$$\frac{\partial q(x)}{\partial z_i}\frac{\partial q(x)}{\partial z_j} \geq q(x)\frac{\partial^2 q(x)}{\partial z_i \partial z_j}, \quad x \in \mathbb{R}^n \ \ \forall i,j$$

$$\Rightarrow \quad \mu(S)\mu(T) \ \geq \ \mu(S \cup T)\mu(S \cap T) \quad \forall S, T \subseteq V$$

Nice properties of SR

- **Closed** under marginalization,
  conditioning on $|S| = k, X_i = 1, X_i = 0$
  ...

- Implies many other types of **negative dependence**,
  e.g. negative association and $\mathbb{E} \prod_i X_i \leq \prod_i \mathbb{E} X_i$

- **Concentration of measure**: X_i behave like independent random variables
  sum $\sum_{i=1}^{n} X_i$, Lipschitz functions $F(S)$, matrices
  (Panconesi,Srinivasan 1997, Dubhashi,Ranjan 1998, Farcomeni 2008, Pemantle,Peres 2011, Kyng,Song 2018, Garbe,Vondrak 2018,…)

Algorithmic Implications

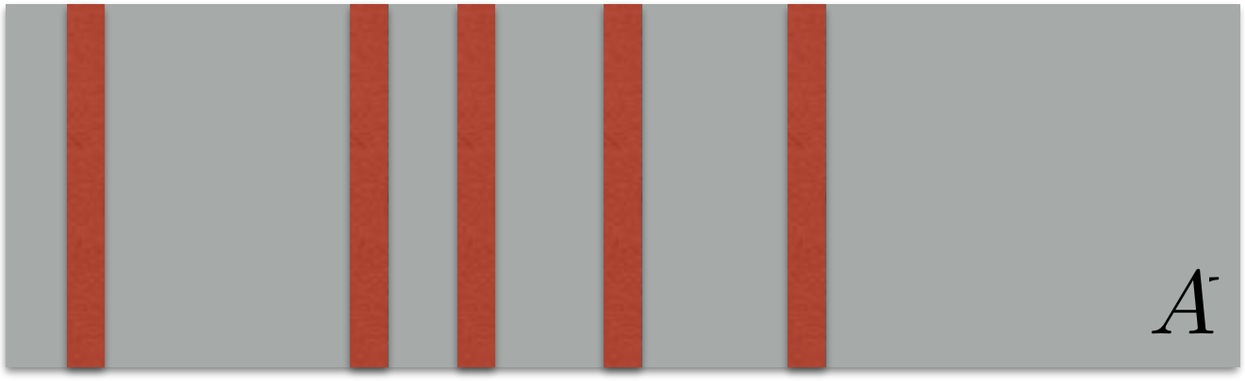
- Sampling
  (Féder,Mihail 1992, Jerrum,Son 2002, Jerrum,Son,Tetali,Vigoda 2004, Anari,Gharan,Rezaei 2016, Li,Jegelka,Sra 2016)

- Approximate partition functions, permanents, volumes, counting
  (Gurvits 2006, Nikolov-Singh 2016, Straszak-Vishnoi 2016, Anari,Gharan, Saberi,Singh 2016, Anari,Gharan 2017…)

- Approximation Algorithms
  (Panconesi,Srinivasan 1997, Hayes 2003, Considine,Byers,Mitzenmacher 2004, Asadpour,Goemans,Madry,Oveis-Gharan,Saberi 2010, Gharan, Saberi,Singh 2011, Spielman,Srivastava 2011, …)

Other SR measures

Dual Volume Sampling



$$P(S) \propto \det(A_S A_S^\top)$$

NOT a DPP … but **Strongly Rayleigh!**

proof: closeness properties of polynomials

(Avron,Boutsidis 2013, Li,Jegelka,Sra 2017, Derezinski,Warmuth 2017)

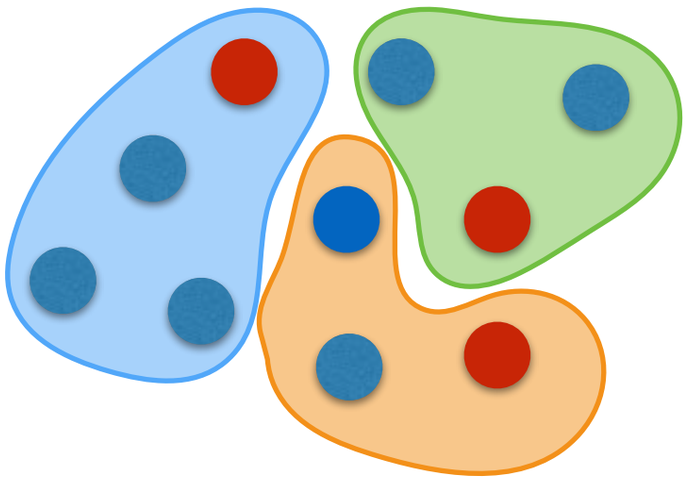
… and limits

$\mu(S)$ is SR. What about $\mu(S)^p$? In general not SR!

(Kulesza,Taskar 2012, Zou,Adams 2012, Gillenwater 2014, Anari, Gharan 2017, Mariet,Sra,Jegelka 2018)

Conditioning on combinatorial constraints: at most one item per group. In general not SR!

(Celis,Deshpande,Kathuria,Straszak,Vishnoi 2017, Celis,Keswani, Straszak,Deshpande,Kathuria,Vishnoi 2018)



Outline

Introduction

Examples

Determinantal Point Processes

1 **Intro & Theory**

Stronger notions of negative dependence

Relations to polynomials

Strongly Rayleigh measures

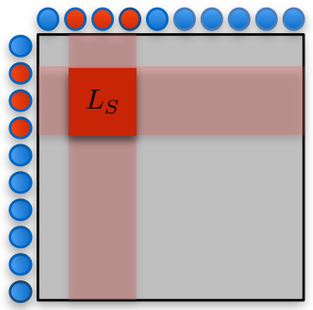
→ **Implications: Sampling**

Sampling for Determinantal Point Processes

EVD/SVD *(Hough, Krishnapur, Peres, Virág 2006)* $O(n^3)$

- ✦ sample subspace via eigenvalues
- ✦ sequentially sample items

Faster via *A*: "dual" sampling *(Kulesza, Taskar 2010)*



$$L = A^\top A$$

$n \times d$

Acceleration: approximate L or A

volume-preserving sketching *(Magen, Zouzias 2008; Deshpande, Rademacher 2010, Gillenwater, Kulesza, Taskar 2012)*
Nyström *(Affandi, Kulesza, Fox, Taskar 2013)*
MCMC *(Bardenet, Hardy 2016)*
Coresets *(Li, Jegelka, Sra 2016)*
R-DPP *(Derezinski 2018)*

Other approaches *(Derezinski, Warmuth 2018, Derezinski, Warmuth, Hsu 2018, Mariet, Sra 2016,…)*

Sampling for general SR measures

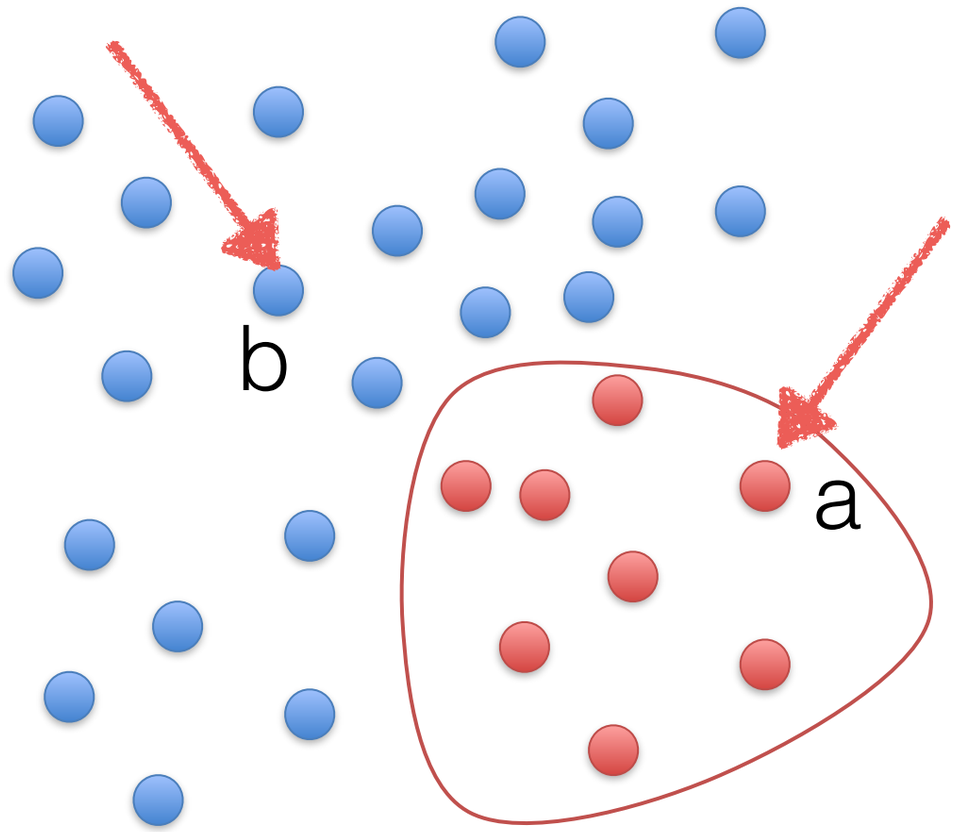
Markov Chain Monte Carlo (MCMC)

in iteration t:

sample $a \in S_{t-1}, b \notin S_{t-1}$ uniformly at random

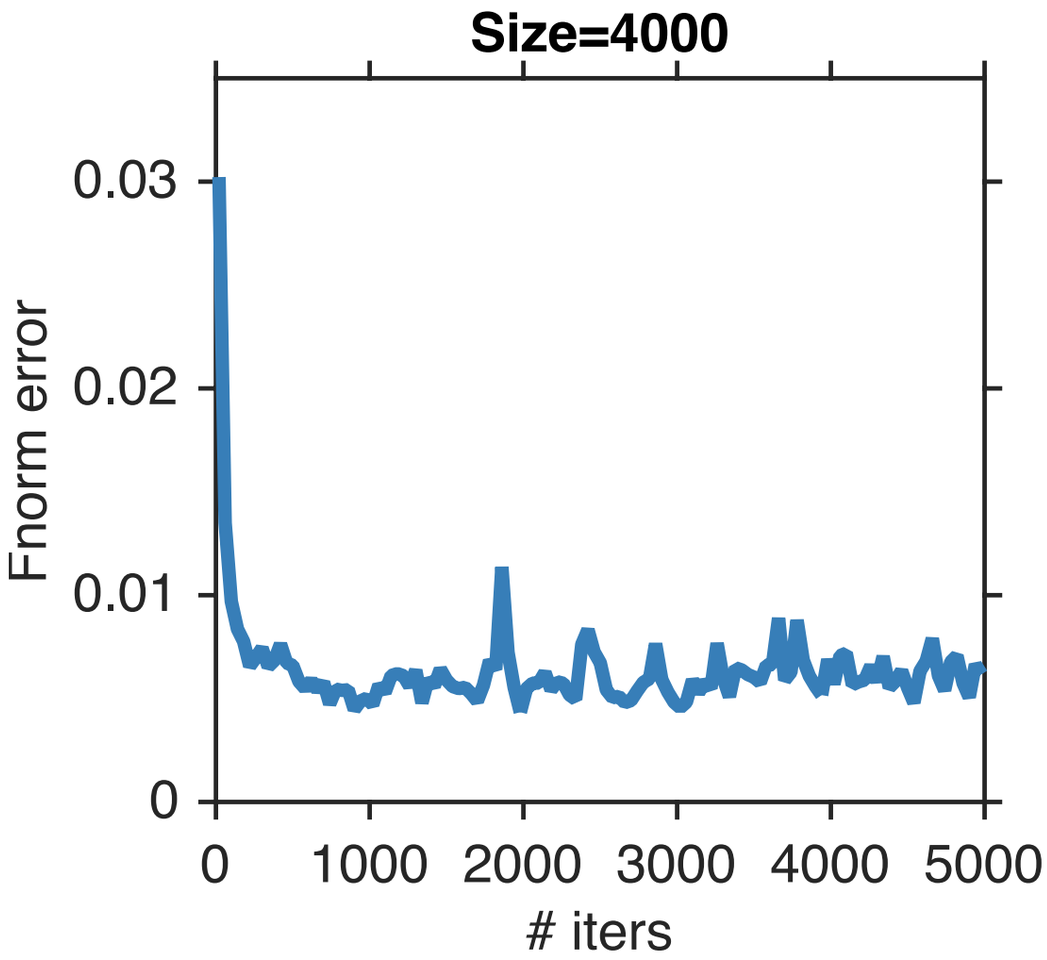
randomly do one of

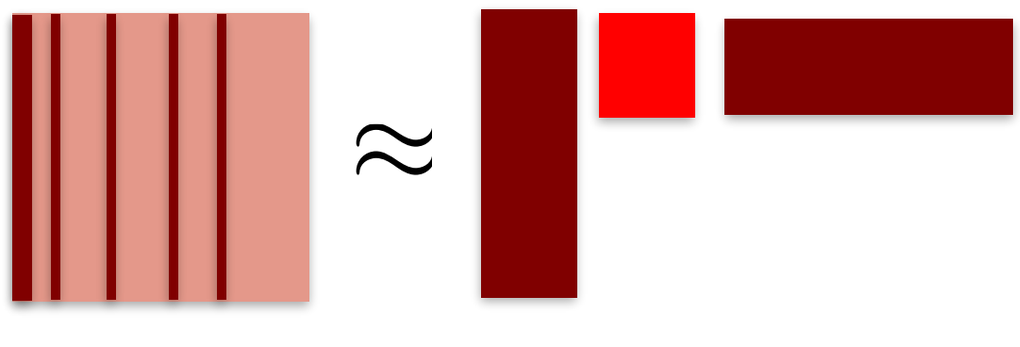
- swap: remove b, add a
- add b
- remove a
- retain $S_t = S_{t-1}$



if conditioning on $|S| = k$: only swaps

Sampling empirically





How many iterations?

Mixing time: #iterations until $\|\mu^t - \mu\|_{\mathrm{TV}} \leq \epsilon$

balanced matroids:

(Féder,Mihail 1992, Jerrum,Son 2002
Jerrum,Son,Tetali,Vigoda, 2004)

$$O\big(nk \log(\tfrac{1}{\epsilon \mu(S_0)})\big) \quad \Big\} |S| = k$$

fixed-cardinality SR:

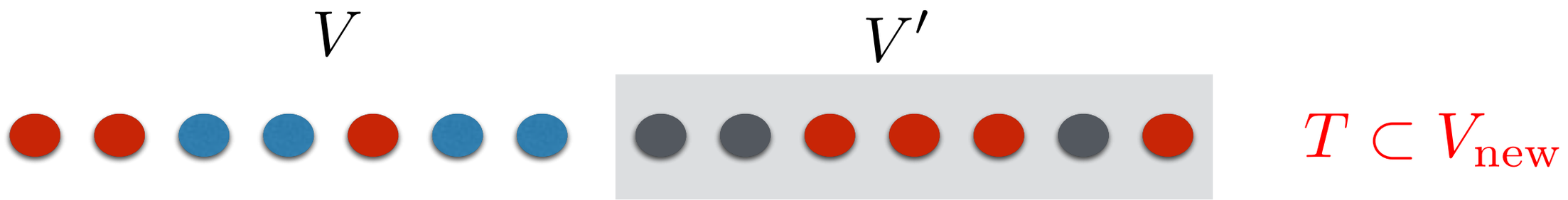
(Anari,Oveis-Gharan,Rezaei 2016)

arbitrary SR:

(Li,Jegelka,Sra 2016)

$$O\big(n^2 \log(\tfrac{1}{\epsilon \mu(S_0)})\big)$$

Sampling: from fixed-cardinality to general SR



$$V_{\text{new}} = V \cup V'$$

- sample n out of 2n, but use only $T \cap V$
- extend measure to “shadow set”
- ***Key:*** measure on 2n is Strongly Rayleigh by closedness properties of real stable polynomials (“symmetric homogenization”)

(Li, Jegelka, Sra 2016)

Sampling

- generic method: MCMC;
  different algorithms for special cases (DPP, dual volume)
- Accelerating each iteration of DPP-MCMC: lazy computations with Gauss quadrature *(Li,Sra,Jegelka 2016)*
- Continuous DPP sampling
  (Affandi,Fox,Taskar 2013, Gharan,Rezaei 2018, …)
- SR sufficient for fast mixing but not necessary: e.g., complete log concavity *(Anari,Liu,Gharan,Vinzant 2018)*
- Sampling log-submodular distributions (negative lattice condition) *(Rebeschini,Karbasi 2015, Gotovos,Hassani, Krause 2018, Gotovos,Hassani,Krause,Jegelka 2018)*

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Stronger notions of negative dependence

Strongly Rayleigh measures and real stable polynomials

Implications: Sampling

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2 **Theory & Applications**

Approximating partition functions

Learning a DPP (and some variants)

Applications

Perspectives and wrap-up