The *unreasonable effectiveness* of determinantal processes

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- Contends that mathematical concepts have applicability that is often far beyond the context in which they were originally developed.

Unreasonable Effectiveness

- "The miracle of .. the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve. We should be grateful for it and hope that ... it will extend, .. to our pleasure, .. to wide branches of learning."

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- The I.I.D. paradigm has led to ground breaking progress and a vast body of literature, including many ideas and methodologies that have become second nature for applications.
- E.g.s include, but are not limited to, the fundamental theories behind Principal Component Analysis (P.C.A.) and other dimension reduction techniques, Maximum Likelihood based methods (M.L.E.), a wide array of information-theoretic approaches, and so on.

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- In general, lack of independence is largely believed to be an obstacle or a hindrance to overcome, and many approaches involve trying to 'locate' independence or approximate independence in the overall dependency structure.
- In this talk, we will take a different point of view - namely, try to exploit dependence structures in stochastic systems in order to make substantive progress in fundamental learning problems.

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- A DPP is a random set of points that all interact with each other, and where the interaction is encoded by a kernel.
- DPPs are, in a sense, the kernel machine of random point sets.

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- DPP strtucture arises natrually, e.g. as *Slater determinants* in wave-functions for Fermions (following earlier work by Heisenberg and Dirac)
- Connections to a wide interface of physics and mathematics, including random matrices, random polynomials, interacting particle systems ...

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- If $\alpha_1, \ldots, \alpha_m$ are m fixed locations, then the m-point correlation function $\rho_m(\alpha_1, \ldots, \alpha_m)$ is the joint probability (density) of having points at the locations $\alpha_1, \ldots \alpha_m$ in a realization of the random point set.

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- E.g., if the model of random point set is to pick points independently and uniformly at random from a domain, then $\rho_m(\alpha_1, \ldots, \alpha_m) = \rho^m$ where ρ is the mean density of points per unit area.

Determinantal processes

- Determinantal processes are models of random point sets that are parameterised by a kernel function K.
- The m-point correlation functions are given by determinants :

$$\rho_m(\alpha_1, \ldots, \alpha_m) = \mathrm{Det} \begin{bmatrix} K(\alpha_1, \alpha_1), & \ldots & \ldots & K(\alpha_1, \alpha_m) \\ \ldots & \ldots & \ldots & \ldots \\ K(\alpha_m, \alpha_1), & \ldots & \ldots & K(\alpha_m, \alpha_m) \end{bmatrix}$$

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- Clearly, if α_i and α_j are the close to each other (in some feature space) for different i and j, then under mild continuity assumption on the kernel K, the probability density ρ_m is very close to 0.
- Thus, a DPP penalizes points for getting too close to each other, and therefore naturally embodies repulsive interaction between the points, albeit in a highly non-linear and complex manner.

Determinantal Processes

- DPPs are, therefore, effective in modelling situations where the sample points need to be very different from each other.
- E.g., in diversity sampling, the population may be represented by points in some (high dimensional) feature space, and the kernel K incorporates the proximity between these points in the feature space, which in turn encodes the 'similarity' between different points that we want to sample from.

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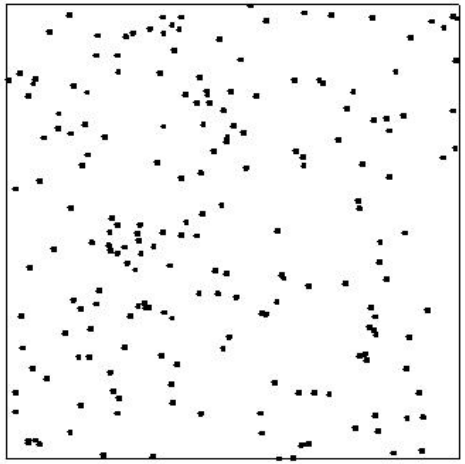
- Recently, DPPs have emerged as a fundamental component of a rapidly developing learning toolbox based on negative dependence that, in many applications, shines over state-of-the-art methods based on statistical independence.

Simulations



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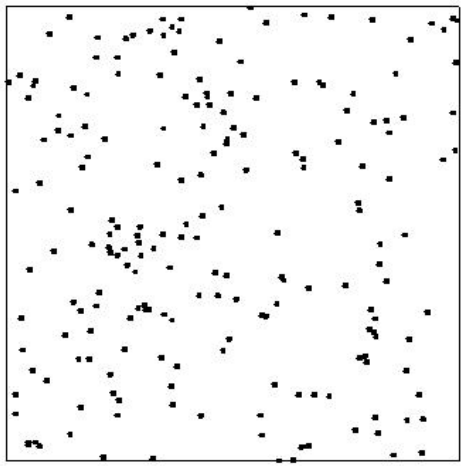

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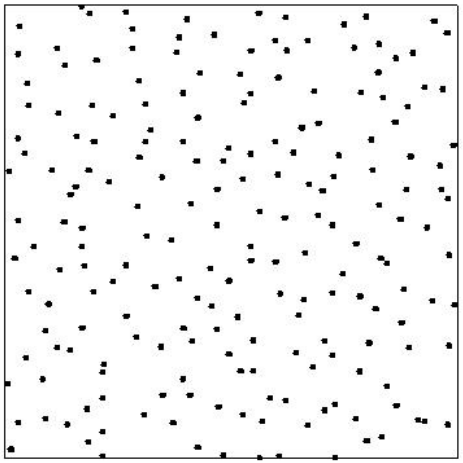

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Gaussian Determinantal Processes

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- Connection to *Spiked Models* of random matrices and *Spiked* PCA.
- Based on joint work with P. Rigollet.

Gaussian Determinantal Processes

- A DPP is specified by the underlying kernel.
- The points of a GDP lives on $\mathbb{R}^d$, and the kernel is simply the d-dimensional Gaussian density with some positive definite covariance matrix Σ (which is the scattering matrix parameterizing the GDP):

$$K(x,y) = \frac{1}{(2\pi)^{d/2}\sqrt{\mathrm{Det}(\Sigma)}} \exp\left(-\frac{1}{2}(x-y)^T\Sigma^{-1}(x-y)\right).$$

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- Our observation consists of the points in a realisation of the GDP inside a ball of large radius R.

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- Note that modulating Σ such that $\mathrm{Det}(\Sigma)$ changes will lead to a change in the mean density of points, and can be detected simply by estimating this average density from the observed points.
- We will therefore focus on parametric modulation that leaves the determinant $\mathrm{Det}(\Sigma)$ invariant - similar to *shear mappings* or *shear transformations*.

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- $\lambda > 0$ corresponds to a spiked model that introduces directional bias in the strength of the dependency structure.

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- The dependence in the directions orthogonal to the spike is much weaker, and decouples to almost independent behaviour at relatively short length scales.

Parameter estimation in GDP

- Let $B(t)$ denotes the Euclidean ball of radius t in $\mathbb{R}^d$, and $|B(t)|$ be its volume. Let $\{X_1, \ldots, X_n\}$ be the observed data points. Let $r > 0$ be a threshold, to be detailed later.

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- Then

$$\hat{\Sigma} = |B(1)| \frac{r^{d+2}}{d+2} I_d - \frac{1}{|B(R-r)|} \sum_{\|X_i - X_j\| < r} (X_i - X_j)(X_i - X_j)^T$$

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  is a consistent estimator of Σ.
- Bias variance tradeoff leads to optimal choice of $r = \Theta(\sqrt{d \log n})$, as $n \to \infty$.

Testing for directionality in GDP

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Based on the test statistic $\|\hat{\Sigma}\|_{\mathrm{op}}$, *we can detect the spike with high probability if the spike size* λ *is above the threshold*

$$\lambda \gtrsim d^2 \log R \left(\frac{c\sqrt{d} \log R}{R} \right)^{d/2}.$$

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The leading eigenvector of $\hat{\Sigma}$ is a consistent estimator of the direction of the spike.

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- It has led to significant methodological progress, e.g. Principal Component Analysis and its derivatives, the entire suite of methods involving the Johnson-Lindenstrauss Lemma and related random projection based techniques, and so on.
- Roughly speaking, dimension reduction involves finding a low-dimensional subspace, or equivalently, a small number of 'significant directions', which contains most of the information about the (high dimensional) data.

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- In P.C.A., we are interested in the directions of maximal variability, which are obtained by taking the principal eigen-directions of the empirical covariance matrix of the data.
- We may view the problem more generally, where dimension reduction will be performed by finding the optimal directions with respect to some other feature (as opposed to variance in the case of P.C.A.). This is going to be one of the directions of focus in our talk.

Dimension Reduction

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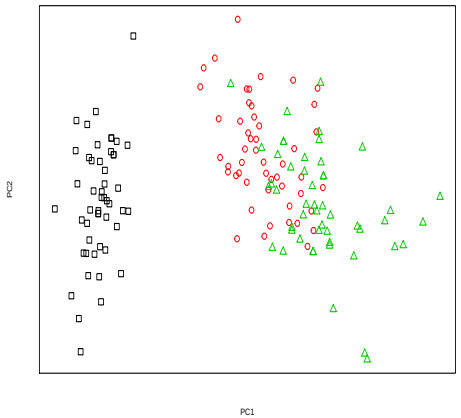
- We may compute the quantity $\hat{\Sigma}$ for any observed data set in $\mathbb{R}^d$. We then perform SVD on $\hat{\Sigma}$ and project the data points on to the principal eigen-directions of $\hat{\Sigma}$ in order to uncover low dimensional directional features in the data.

Dimension Reduction : Fisher's Iris



PCA

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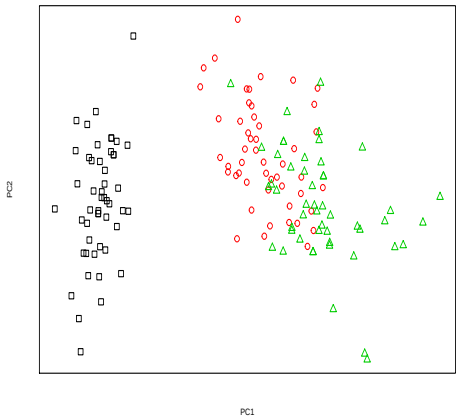

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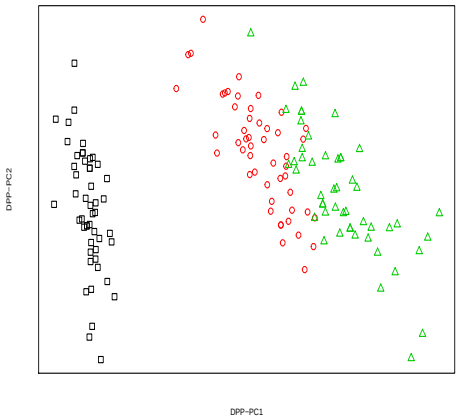
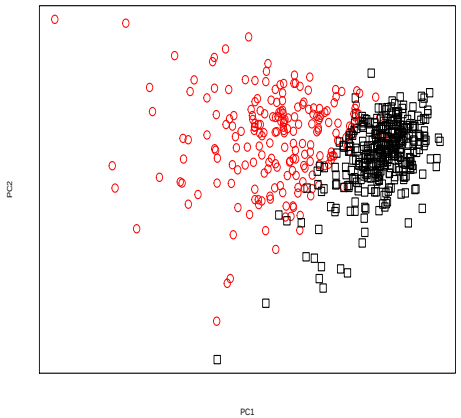


GDP

Dimension Reduction : Wisconsin Breast Cancer



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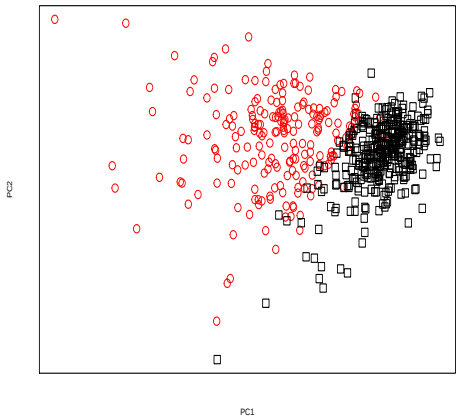

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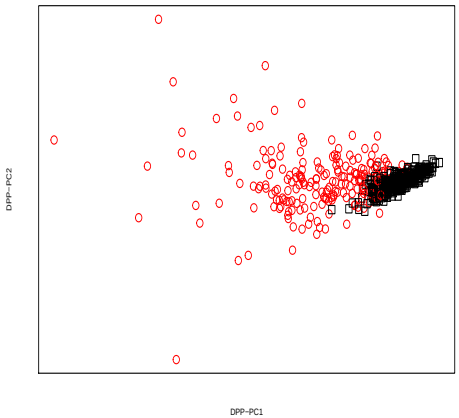

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- In large datasets, SGD relies on constructing an unbiased estimator of the gradient using a small subset of the original dataset, called a minibatch.
- Default minibatch construction involves uniformly sampling a subset of the desired size.

- We contribute an *orthogonal polynomial*-based DPP paradigm for minibatch sampling in SGD, and substantiate it with a robust theoretical foundation.

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- Our approach *leverages the specific data distribution* at hand, which endows it with greater sensitivity and power over existing data-agnostic methods.
- Joint work with R. Bardenet and M. Lin.

- We obtain a detailed theoretical analysis of its convergence properties, *interweaving between the discrete data set and the underlying continuous domain*.
- We propose *gradient estimators* whose *variance decays provably faster with the batchsize* than under uniform sampling.
- For a large enough batchsize and a fixed budget, DPP minibatches lead to a *smaller bound on the mean square approximation error* than uniform minibatches.

The SGD minibatch problem

- Stochastic Gradient Descent (SGD) is the workhorse of modern machine learning
- Useful in a wide array of optimization scenario, ranging from maximum likelihood problems of parametric statistics to back propagation in training deep neural networks, and beyond ....

The SGD minibatch problem

- The fundamental step in a gradient descent approach can be coded as

$$\theta_{t+1} \leftarrow \theta_t - \eta_t \cdot \left[\frac{1}{N} \cdot \sum_{i=1}^{N} \nabla_\theta \mathcal{L}(z_i, \theta) \right],$$

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- However, for large data sets, computing the empirical average at each step can be prohibitively expensive.

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- The fundamental step in stochastic gradient descent can be coded as
$$\theta_{t+1} \leftarrow \theta_t - \gamma_t \widehat{\mathcal{L}(A, \theta_t)}$$
- $\widehat{\mathcal{L}(A, \theta_t)}$ is an estimate of the full data set gradient $\frac{1}{N} \cdot \sum_{i=1}^{N} \nabla_\theta \mathcal{L}(z_i, \theta)$
- $\widehat{\mathcal{L}(A, \theta_t)}$ is *based on a relatively small subsample $A \subset \mathcal{D}$ of the full data set $\mathcal{D}$.*

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- The fundamental step in stochastic gradient descent can be coded as
$$\theta_{t+1} \leftarrow \theta_t - \gamma_t \widehat{\mathcal{L}(A, \theta_t)}$$
- $\widehat{\mathcal{L}(A, \theta_t)}$ is an estimate of the full data set gradient $\frac{1}{N} \cdot \sum_{i=1}^{N} \nabla_\theta \mathcal{L}(z_i, \theta)$
- $\widehat{\mathcal{L}(A, \theta_t)}$ is *based on a relatively small subsample $A \subset \mathcal{D}$ of the full data set $\mathcal{D}$.*
- Such a subsample A is called a minibatch.

The SGD minibatch problem

- A minibatch is a (random) subset $A \subset \mathcal{D}$ of size $|A| = p \ll N$ such that the random variable

$$\Xi_A = \Xi_A(\theta) := \sum_{z_i \in A} w_i \nabla_\theta \mathcal{L}(z_i, \theta), \tag{1}$$

for suitable weights (w_i), provides a good approximation for $\Xi_N = \frac{1}{N} \sum_{z_i \in \mathcal{D}} \nabla_\theta \mathcal{L}(z_i, \theta)$.

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  for suitable weights (w_i), provides a good approximation for $\Xi_N = \frac{1}{N} \sum_{z_i \in \mathcal{D}} \nabla_\theta \mathcal{L}(z_i, \theta)$.
- Natural problem : How to select the *random* subset $A \subset \mathcal{D}$? What is the *nature of randomness* that leads to improved performance of the SGD algorithm ?

The impact of randomness

- The impact of the randomness of A (equivalently, that of Ξ_A) is captured by the following theorem.

Theorem (Moulines-Bach '11)

For smooth and strongly convex expected loss function, compact parameter space, an unbiased estimator Ξ_A for the gradient and step size $\gamma_t \sim t^{-\alpha}$ for some $0 < \alpha < 1$, we have

$$\mathbb{E}\|\theta_t - \theta_\star\|^2 \leq C \cdot \frac{\sigma^2}{t^\alpha} + \mathcal{O}(e^{-t^\alpha}),$$

where $\sigma^2 = \mathbb{E}[\|\Xi_A(\theta_\star)\|^2|\mathcal{D}]$ is the trace of the covariance matrix of the gradient estimator, evaluated at the true optimizer $\theta_\star$.

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- Therefore, the *goal is to make σ^2 small*, as a function of the batch size p.

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- Sampling p data points with / without replacement, Poissonian sampling (select each data point to be in A independently with probability p/N) ...
- Unbiased estimate of the variance

$$\sigma^2(\Xi_{\text{Unif}}) = O_P(p^{-1}).$$

Enter DPPs

- Our approach : select A according to a DPP to effect variance reduction.

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- Our DPP sampler will be tailored to the data distribution, implemented via Orthogonal Polynomials.

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- Multivariate Orthogonal polynomials : consider a reference measure $q(x)dx$ on $[-1,1]^d$.
- Consider the monomial functions $(x_1,\ldots,x_d) \mapsto x_1^{\alpha_1}\cdots x_d^{\alpha_d}$ in the graded lexical order.

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- Then apply the Gram-Schmidt algorithm in $L^2(q(x)\,\mathrm{d}x)$ to these ordered monomials.

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- Then apply the Gram-Schmidt algorithm in $L^2(q(x)\,\mathrm{d}x)$ to these ordered monomials.
- This yields a sequence of orthonormal polynomial functions $(\varphi_k)_{k\in\mathbb{N}}$, the multivariate orthonormal polynomials w.r.t. q.

DPPs based on Multivariate Orthogonal Polynomials

- Construct a DPP with the kernel given by the projection

$$K(x,y) = \sum_{k=0}^{p-1} \varphi_k(x)\varphi_k(y),$$

with respect to the background measure $q(x)dx$.

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- # of sampled points = rank of the projection = p (always !)

An OP based minibatch selector for SGD

- Let $\tilde{\gamma}(z) = \frac{1}{Nh^d} \sum_{i=1}^{N} k\left(\frac{z-z_i}{h}\right)$ be a kernel density estimator of the pdf of the data-generating distribution γ with window size $h > 0$.
- Let $q(x) = q_1(x_1) \dots q_d(x_d)$ be a separable pdf on $[-1, 1]^d$, where each q_i is positive on $[-1, 1]$.

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- Let $K_q^{(p)}$ be the Multivariate OPE kernel with respect to the measure q.

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- Define a new kernel that factors in $\tilde{\gamma}$:

$$K^{(p)}_{q,\tilde{\gamma}}(x,y) := \sqrt{\frac{q(x)}{\tilde{\gamma}(x)}} K^{(p)}_{q}(x,y) \sqrt{\frac{q(y)}{\tilde{\gamma}(y)}}$$

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- However : $K^{(p)}_{q,\tilde{\gamma}}$ is *approximately* a rank-p projection with respect to the uniform distribution on $\mathcal{D}$
- Solution : Spectrally round-off $K^{(p)}_{q,\tilde{\gamma}}$ to a rank-p projection $\widetilde{\mathrm{K}}$.

A DPP based gradient estimator for SGD

- We consider a minibatch $A \sim \mathrm{DPP}(\widetilde{\mathrm{K}}, \hat{\gamma}_N)$, where $\widetilde{\mathrm{K}}$ is the projection as obtained above and the background measure $\hat{\gamma}_N$ is the uniform distribution on $\mathcal{D}$.

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- $\mathbb{E}[\Xi_{A,\mathrm{DPP}}] = \sum_{i=1}^N \left(\frac{\nabla_\theta \mathcal{L}(z_i,\theta)}{\widetilde{\mathsf{K}}(z_i,z_i)} \right) \cdot \widetilde{\mathsf{K}}(z_i, z_i) \cdot \frac{1}{N} = \frac{1}{N} \sum_{i=1}^N \nabla_\theta \mathcal{L}(z_i, \theta)$
- So, $\Xi_{A,\mathrm{DPP}}$ is unbiased, as desired.

Why does $\Xi_{A,\mathrm{DPP}}$ have reduced fluctuations ?

$$\sigma^2(\Xi_{A,\mathrm{DPP}})$$

$$= \frac{1}{N^2} \sum_{i,j} \left\| \frac{\nabla_\theta \mathcal{L}(z_i, \theta)}{\widetilde{K}(z_i, z_i)} - \frac{\nabla_\theta \mathcal{L}(z_j, \theta)}{\widetilde{K}(z_j, z_j)} \right\|_2^2 |\widetilde{K}(z_i, z_j)|^2 \quad \text{[Projection Kernel]}$$

$$\lesssim \mathcal{M}(\theta) \cdot \frac{1}{p^2} \int \int \|z - w\|_2^2 \, |K_q^{(p)}(z, w)|^2 dq(z) dq(w) \quad \text{[under regularity]}$$

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- Use *Christoffel-Darboux formula* to make this control precise

Why does $\Xi_{A,\mathrm{DPP}}$ have reduced fluctuations ?

- Obtain

Theorem (Bardenet-G.-Lin)

$\mathrm{Var}[\Xi_{A,DPP}|\mathcal{D}] = O_P(p^{-(1+1/d)})$.

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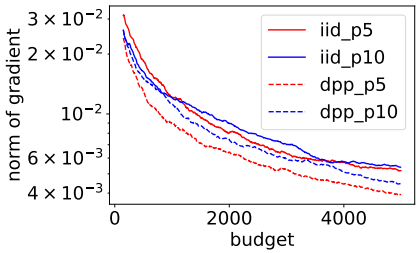
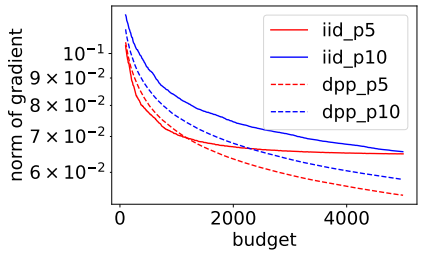
- Improvement in exponent of p compared to uniform random sampling of A !
- Near-completion (with R. Bardenet and M. Lin) : a technique for sampling the gradient estimator *directly*, *without having to sample the DPP* minibatch. Applications to a wide array of DPP based approaches in machine learning (such as coresets), spatial statistics ....

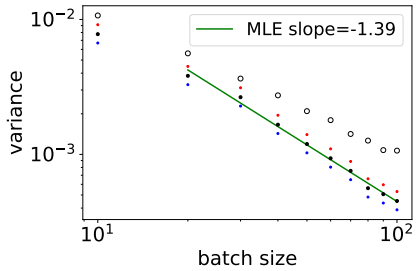
Performance in experiments



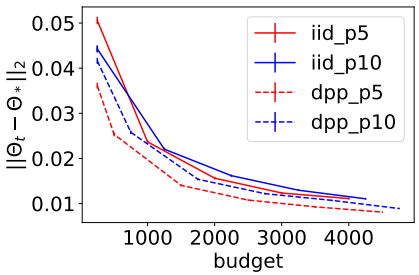
(a) d=3, Lin. Reg.



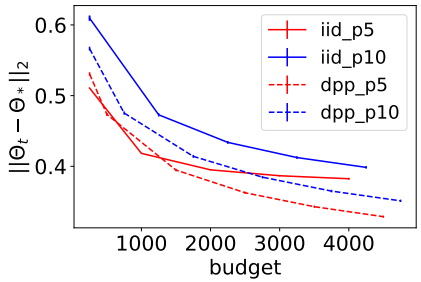
(b) d=11, Log. Reg.



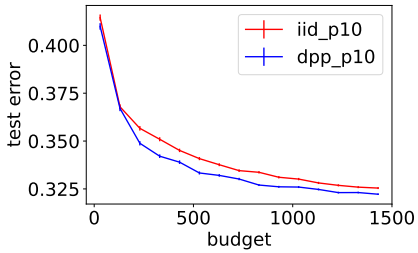
(c) d=3, Var vs log p



(d) d=3, Lin. Reg.



(e) d=11, Log. Reg.



(f) Letter. binary

Figure: Summary of the performance of two sampling strategies in SGD.

References

- Gaussian determinantal processes: A new model for directionality in data, with P. Rigollet,
  Proceedings of the National Academy of Sciences, vol. 117, no. 24 (2020), pp. 13207–13213
  (PNAS Direct Submission)
- Determinantal point processes based on orthogonal polynomials for sampling minibatches in SGD, with R. Bardenet and M. Lin
  Advances in Neural Information Processing Systems 34 (2021)
  (Spotlight at NeurIPS 2021)