MEMe: An Accurate Maximum Entropy Method for Efficient Approximations in Large-Scale Machine Learning

Diego Granziol, Binxin Ru, Stefan Zohren, Xiaowen Dong, Michael Osborbe, Stephen Roberts
Oxford University
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Address line

Abstract

We develop a novel robust Maximum Entropy algorithm, capable of dealing with hundreds of moments, allowing for computationally efficient approximations which are shown to be significantly better than existing approaches. The usefulness of the approach is showcased across a set of applications. In particular we highlight its effectiveness in: Determinantal Point Processes; spectral decompositions of large sparse graphs; as well as information-theoretic Bayesian Optimisation.

Introduction

Algorithmic scalability is a keystone in the realm of modern machine learning. Making high quality inference, on large, feature rich datasets under a constrained computational budget is arguably the primary goal of the learning community. We develop a novel, robust Maximum Entropy algorithm using Newton conjugate gradient and Hessian information with a Legendre/Chebyshev basis, as opposed to power moments. Our algorithm is stable for a large number of moments, surpassing the $m \approx 8$ limit of previous MaxEnt algorithms Granziol and Roberts (2017b); Bandyopadhyay et al. (2005); Mead and Papanicolaou (1984). We show that the ability to handle more moment information, which can be calculated cheaply either analytically or with the use of stochastic trace estimation, explained in section leads to significantly enhanced performance. We showcase the utility of the algorithm by applying it to improve the scalability of Determinantal Point Processes, Learning the number of clusters in large graphs and active approximations in Bayesian Optimisation. We further derive bounds on the error of the estimated underlying densities and establish a link between Maximum Entropy methods and constrained variational inference.

The Method of Maximum Entropy

The method of maximum entropy, hereafter referred to as *MaxEnt* (Pressé et al., 2013) is a procedure for generating the most conservative estimate[1] of a probability distribution possible with the given information, the most non-committal with regard to missing information (Jaynes, 1957a). Intuitively, on a bounded domain, the most conservative distribution, the distribution of maximum entropy, is the one that assigns equal probability to all the accessible states. Hence, the method of maximum entropy can be thought of choosing the flattest, or most equiprobable distribution, satisfying the given constraints. To determine the maximially entropic density $p(x)$,we maximise the entropic functional

$$S = -\int p(x)\log p(x)dx - \sum_i \alpha_i \left[\int p(x)\lambda^i dx - \mu_i\right] \tag{1}$$

with respect to $p(\lambda)$, where $\mathbb{E}_p[\lambda^i] = \mu_i$ are the power moment constraints on the spectral density. The first term in Equation (1) is referred to as the Boltzmann-Shannon-Gibbs (BSG) entropy, which has been applied in multiple fields, ranging from condensed matter physics (Giffin, Cafaro, and Ali, 2016) to finance (Neri and Schneider, 2012), under the axioms of consistency, uniqueness, invariance under coordinate transformations, sub-set and system independence, it can be proved that for constraints in the form of expected values, drawing self-consistent inferences requires maximising the entropy (Shore and Johnson, 1980; Pressé et al., 2013).

Variational Inference

Variational Methods Fox and Roberts (2012) in machine learning pose the problem of intractable density estimation from the application of Bayes' rule as a functional optimization problem,

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)} \approx q(z), \tag{2}$$

and seek to find the appropriate $q(z)$. Typically, whilst the functional form of $p(x|z)$ is known, calculating $p(x) = \int p(x|z)p(z)dz$ is intractable. Using Jensen's inequality we can show that,

$$\log p(x) \geq \mathbb{E}_q[\log p(x,z)] - \mathbb{E}_q[\log q(z)].^2 \tag{3}$$

Further the reverse KL divergence between the posterior and the variational distribution, $\mathbb{D}_{kl}(q|p)$, can be written as,

$$\log p(x) = \mathbb{E}_q[\log p(x,z)] - \mathbb{E}_q[\log q(z)] + \mathbb{D}_{kl}(q|p). \tag{4}$$

[1] With respect to the uniform distribution.

[2] Where the R.H.S is known as the evidence lower bound (ELBO).

Hence maximising the evidence lower bound is equivalent to minimising the reverse KL divergence between p and q.

MaxEnt as Constrained Variational Inference

We consider minimising the reverse KL divergence between our surrogate posterior $q(x)$ and our prior $p_0(x)$

$$\mathcal{D}_{kl}(q|p_0) = -H(q) - \int_0^1 q(\lambda) \log p_0(\lambda) d\lambda, \quad (5)$$

such that the normalization and moment constraints are satisfied. Here $H(q)$ denotes the differential entropy of the density q.

By the theory of Lagrangian duality, the convexity of the KL divergence and the affine nature of the moment constraints, we maximise the dual Boyd and Vandenberghe (2009),

$$-H(q) - \int q(x) \log p_0(x) d\lambda - \sum_{i=0}^{m} \alpha_i \left(\int_0^1 q(x) \lambda^i dx - \mu_i \right), \quad (6)$$

or alternatively we minimise

$$H(q) + \int q(x) \log p_0(x) d\lambda - \sum_{i=0}^{m} \alpha_i \left(\int_0^1 q(x) \lambda^i dx - \mu_i \right). \quad (7)$$

Link to Information Physics

In the field of information physics the minimization of Equation (7) is known as the method of relative entropy Caticha (2012). It can be derived as the unique functional satisfying the axioms of,

1. **Locality:** local information has local effects.
2. **Co-ordinate invariance:** the co-ordinate set carries no information.
3. **Sub-System Independence:** for two independent subsystem it should not matter if we treat the inference separately or jointly.
4. **Objectivity:** Under no new information, our inference should not change. Hence under no constraints, our posterior should coincide with our prior.

The justification for restricting ourselves to a functional is derived from considering the set of all distributions $q_j(x)$ compatible with the constraints and devising a transitive ranking scheme. It can be shown, further, that Newton's laws, non-relativistic quantum mechanics and Bayes' rule can all be derived under this formalism. In the case of a flat prior over the spectral domain, we reduce to the method of maximum entropy with moment constraints Jaynes (1982, 1957b).

Algorithm

The generalised dual objective function which we minimise is,

$$\mathcal{S}(q, q_0) = \int_0^1 q_0(x) \exp(-[1 + \sum_i \alpha_i x^i]) dx + \sum_i \alpha_i \mu_i, \quad (8)$$

which can be shown to have gradient

$$\frac{\partial \mathcal{S}(q, q_0)}{\partial \alpha_j} = \mu_j - \int_0^1 q_0(x) x^j \exp(-[1 + \sum_i \alpha_i x^i]) dx, \quad (9)$$

and Hessian

$$\frac{\partial^2 \mathcal{S}(q, q_0)}{\partial \alpha_j \partial \alpha_k} = \int_0^1 q_0(x) x^{j+k} \exp(-[1 + \sum_i \alpha_i x^i]) dx. \quad (10)$$

Log Determinant

A common hindrance, appearing in Gaussian graphical models, Gaussian Processes Rue and Held (2005); Rasmussen (2006), sampling, variational inference MacKay (2003), metric/kernel learning Davis et al. (2007); Van Aelst and Rousseeuw (2009), Markov random fields Wainwright and Jordan (2006), Determinantal Point Processes (DPP's) and Bayesian Neural networks MacKay (1992), is the calculation of the log determinant of a large positive definite matrix. For a large positive definite matrix $K \in \mathcal{R}^{n \times n}$, the canonical solution involves the Cholesky decomposition, $K = LL^T$. The log determinant is then trivial to calculate as $\log \mathrm{Det}(K) = 2 \sum_{i=1}^{n} \log L_{ii}$. This computation invokes a computational complexity $\mathcal{O}(n^3)$ and storage complexity $\mathcal{O}(n^2)$ and is thus unfit for purpose for $n > 10^4$, i.e. even a small sample set in the age of big data.

Related Work

Recent work in machine learning combined stochastic trace estimation with Taylor approximations for Gaussian process parameter learning Zhang and Leithead (2007); Boutsidis et al. (2017), Further developments included improved performance using Chebyshev polynomials Han, Malioutov, and Shin (2015) and Lanczos techniques with structured kernel interpolation (SKI) in order to accelerate matrix vector multiplications (MVM's) to $\mathcal{O}(n + i \log i)$, where i is the number of inducing points Dong et al. (2017). SKI relies on an extension of Kronecker and Toeplitz methods, which are limited to low dimensional (typically $D \leq 5$) data, which cannot be assumed in general. Secondly, whilst Lanczos methods have a convergence rate of double that of the Chebyshev approaches, the derived bounds require $\mathcal{O}(\sqrt{\kappa})$ Lanczos steps Ubaru, Chen, and Saad (2016), where κ is the matrix condition number. In many practical cases of interest $\kappa > 10^{10}$ and thus the large number of m matrix vector multiplications becomes prohibitive. We restrict ourselves to the high-dimensional, high-condition number, big data limit.

Log Determinants as a Spectral Estimation Problem

Any symmetric positive definite (PD) matrix K, is diagonalizable by a unitary transformation U, i.e $K = U^t D U$, where D is the matrix with the eigenvalues of K along the diagonal. Hence we can write the log determinant as:

$$\log \mathrm{Det} K = \log \prod_i \lambda_i = \sum_{i=1}^{n} \log \lambda_i = n \mathbb{E}_\mu(\log \lambda). \quad (11)$$

Here we have used the cyclicity of the determinant and $\mathbb{E}_\mu$ denotes the expectation under the spectral measure. The latter can be written as:

$$\int_{\lambda_{min}}^{\lambda_{max}} d\mu(\lambda) \log \lambda = \int_{\lambda_{min}}^{\lambda_{max}} \sum_{i=1}^{n} \frac{1}{n} \delta(\lambda - \lambda_i) \log \lambda d\lambda. \tag{12}$$

Where $\lambda_{max,min}$ correspond to the largest and smallest eigenvalues respectively. Given that the matrix is PD, we know that $\lambda_{min} > 0$ and we can divide the matrix by an upper bound, $\lambda_u \geq \lambda_{max}$, via the Gershgorin circle theorem Gershgorin (1931) such that,

$$\begin{aligned} &\log \text{Det} \frac{K}{\lambda_u} = n\mathbb{E}_\mu(\log \lambda') = n\mathbb{E}_\mu(\log \lambda) - n\lambda_u \\ &\therefore \log \text{Det} K = n\mathbb{E}_\mu(\log \lambda') + n\lambda_u. \end{aligned} \tag{13}$$

Where $\lambda' = \lambda/\lambda_u$ and $\lambda_u = \arg\max_i(\sum_{j=1}^{n} |K_{ij}|)$, i.e the max sum of the rows of the absolute of the matrix K. Hence we can comfortably work with the transformed measure,

$$\int_{\lambda_{min}/\lambda_u}^{\lambda_{max}/\lambda_u} p(\lambda') \log \lambda' d\lambda' = \int_0^1 p(\lambda') \log \lambda' d\lambda', \tag{14}$$

as the spectral density $p(\lambda)$ is 0 outside of its bounds, which are bounded by $[0, 1]$ respectively.

Stochastic Trace Estimation

Using the expectation of quadratic forms, for any multivariate random variable v with mean m and variance Σ, we can write

$$\mathbb{E}(zz^t) = mm^t + \Sigma \xrightarrow[m=0]{\Sigma=I} I, \tag{15}$$

where in the last equality we have assumed that the variable possesses zero mean and unit variance. By the linearity of trace and expectation for any $m \geq 0$ we can write

$$\sum_{i=1}^{n} \lambda^m = n\mathbb{E}_\mu(\lambda^m) = \text{Tr}(IK^m) = \mathbb{E}(zK^m z^t). \tag{16}$$

In practice we approximate the expectation over all random vectors with a simple Monte Carlo average. i.e for d random vectors ,

$$\mathbb{E}(zK^m z^t) \approx \frac{1}{d} \left(\sum_{j=1}^{j=d} z_j K^m z_j^t \right), \tag{17}$$

where we take the product of the matrix K with the vector z_j, m times, so as to avoid costly $\mathcal{O}(n^3)$ matrix matrix multiplication. This allows us to calculate the non central moment expectations in $\mathcal{O}(dmn^2)$ for dense matrices, or $\mathcal{O}(dm \times nnz)$ for sparse matrices, where $d \times m << n$. The random unit vector z_j can be drawn from any distribution, such as a Gaussian. The algorithm is outlined in Algorithm 4.

Experiments

For simplicity we have kept all the formulas in terms of power moments, however we find vastly improved performance and conditioning when we switch to orthogonal Polynomial bases (so that the errors between moment estimations are uncorrelated). We implement both Chebyshev and Legendre moments in our Lagrangian and find similar performance for both. The use of Chebyshev moments in Machine Learning and Computer Vision has been reported to be of practical siginifcance previously Yap, Raveendran, and Ong (2001). We use Python's SciPy minimize standard newton-conjugate gradient algorithm to solve the objective, given the gradient and hessian to within a gradient tolerance $gtol$. To make the Hessian better conditioned so as to achieve convergence we add jitter 10^{-8} along the diagonal. We use a grid size of 10^{-4} for the quadrature. The pseudo code is given in Algorithm 2. The log eterminant is then calculated using Algorithm 1.

Algorithm 1 Computing Log Determinant using Constrained Variational Inference

Input: PD Symmetric Matrix A, Order of stochastic trace estimation k, Tolerance ϵ
Output: Log Determinant Approximation $\log |K|$
$B = K/\lambda_u$
μ (moments)$\leftarrow$ StochasticTraceEstimation(B, k)
α (coefficients) $\leftarrow$ MaxEnt(μ, ϵ)
$q(\lambda) \leftarrow q(\lambda|\alpha)$
$\log |A| \leftarrow n \int \log(\lambda) q(\lambda) d\lambda + n \log(\lambda_u)$

Comparison to Previous MaxEnt algorithm

In Granziol and Roberts (2017a) it was proven that the addition of an extra constraint cannot increase the entropy of the MaxEnt solution. For the problem of log determinants, this signifies that the entropy of the spectral approximation should decrease with the addition of every moment constraint. We implement the Maximum Entropy algorithm Bandyopadhyay et al. (2005) in the same manner as applied for log determinant estimation in Fitzsimons et al. (2017). We show results for the Themomech UFL SuiteSparse dataset, with $n = 80,900$, for which the true log determinant can be calculated. We see that for the MaxEnt algorithm Bandyopadhyay et al. (2005) implementation used inFitzsimons et al. (2017) that for $m > 8$ moments, the error (Figure **??**) and the entropy (Figure**??**) begin to increase. For our algorithm, beyond seeing that the performance is vastly increased (Figure **??**), the error continually decreases with increasing moment information and the Entropy (Figure **??**) decreases smoothly.

Synthetic Kernel Data

We simulate the kernel matrices from a Gaussian/Determinental Point Process Rasmussen and Williams (2006), by generating a typical squared exponential kernel matrix $K \in \mathbb{R}^{n \times n}$ using the Python GPy package with 6 dimensional, Gaussian inputs. We then add noise of variance 10^{-8} along the diagonals. We employ a variety of realistic uniform length-scales. We use $m = 30$ Moments, $d = 50$ Hutchinson probe vectors and compare our novel MaxEnt algorithm against the Taylor approximation, Chebyshev Han, Malioutov, and Shin (2015) and Lanczos Ubaru, Chen, and Saad (2017) in Table . We see that for

Figure 1: Comparison of Classical and Novel MaxEnt algorithms

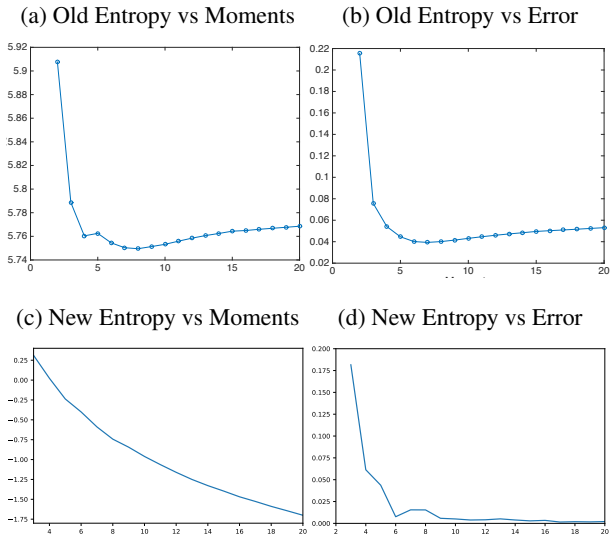


Table 1: Absolute relative error for MaxEnt, Chebyshev & Lanczos methodson varying length-scale l, with varying condition number κ on squared exponential kernel matrices $K \in \mathbb{R}^{1000\times1000}$.

κ	l	MaxEnt	Chebyshev	Lanczos
3×10^1	0.05	**0.0014**	0.0037	0.0024
1.1×10^3	0.15	0.0522	**0.0104**	0.0024
1.0×10^5	0.25	0.0387	0.0795	**0.0072**
2.4×10^6	0.35	0.0263	0.2302	**0.0196**
8.3×10^7	0.45	**0.0284**	0.3439	0.0502
4.2×10^8	0.55	**0.0256**	0.4089	0.0646
4.3×10^9	0.65	**0.00048**	0.5049	0.0838
1.4×10^{10}	0.75	**0.0086**	0.5049	0.1050
4.2×10^{10}	0.85	**0.0177**	0.5358	0.1199

low condition numbers (Figure 3) The benefit of framing the log determinant as an optimization problem is marginal, whereas for large condition numbers (Figures 4) the benefits are substantial, with orders of magnitude better results than competing methods. We also provide the number of Chebyshev and Lanczos steps required to achieve similar performance.

Machine Learning Application 1: DPPs

Determinantal point processes (DPPs) Macchi (1975) are probabilistic models capturing global negative correlations. In machine learning their natural selection of diversity has found applications in the field of summarization Gong et al. (2014), human pose detection Kulesza (2012), clustering Kang (2013), Low rank kernel matrix approximations Li, Jegelka, and Sra (2016) and Manifold learning Wachinger and Golland (2015). Formally, it defines a distribution on 2^y, where $y = [n]$ is the finite ground set. For a random variable $X \subseteq Y$ drawn from a given DPP we have

$$P(X = x) \propto \det(K_X) = \frac{\det(K_x)}{\det(K + I)}, \tag{18}$$

where $K \in R^{d\times d}$ is a positive definite matrix referred to as the L-ensemble kernel. Greedy algorithms that find the most diverse set Y of y that achieves the highest probability, i.e $\operatorname{argmax}_{X\subseteq y}\det(K_Y)$ require the calculation of the marginal gain,

$$\log\det K_{X\cup\{i\}} - \log\det L_X. \tag{19}$$

ADD DPP EXPERIMENT HERE

Machine Learning Application 2: Learning Cluster Number

For many clustering algorithms, the number of clusters is taken as a given input Liu et al. (2013),Cucuringu et al. (2016) The estimation of the cluster number is a challenging problem, (Von Luxburg, 2007), with likelihood, ad-hoc, information theoretic, stability and spectral approaches advocated. In the latter, one analyses the spectral gap in the eigenvalue spectrum, which we refer to as *eigengap* for short. The Lancsoz algorithm, which exploits matrix sparsity by working with matrix vector multiplications, has computational complexity $\mathcal{O}(n_{\text{nz}} \times m + nm^2) \times d$, where for very large sparse matrices, the second term becomes dominant. Given that empirically many social, biological and technical communities are sparse and that all we need for detecting cluster count is an estimation of the eigenvalues and not the eigenvectors, we look for an alternative computationally more effective method of estimating the spectral density. We use the method of maximum entropy, with computational complexity equivalent to Lancsoz without the second term.

CLUSTERING USING THE EIGENSPECTRA

It is well known Von Luxburg (2007), that the multiplicity of the 0 eigenvalues is equal to the number of disconnected components in the graph. Hence were we to define a community as a completely disconnected component, we could simply count the number of 0 eigenvalues. However given that real world networks are rarely completely disconnected, this procedure would be of little practical utility. We hence consider groups of nodes containing far greater intra-group connections than inter-group connections as well defined clusters. If the graph is connected, but consists of k subgraphs which are "weakly" linked to each other, the graph Laplacian has one zero eigenvalue and all the other eigenvalues positive. This is easily seen by looking at

$$\mathbf{u}^T L\mathbf{u} = \sum_{i,j=1}^{n} w_{ij}(u_i - u_j)^2 \tag{20}$$

which is positive, as $w_{ij} > 0$ and given a connected graph G has a single 0 eigenvalue, all other eigenvalues are thus positive. For small changes in the Laplacian, we expect from matrix perturbation theory (Bhatia, 2013) that the next $k - 1$ smallest eigenvalues will be close to 0. Hence, given the spectral decomposition, the number of eigenvalues very close to 0 corresponds to the number of clusters.

Algorithm 2 MaxEnt Algorithm

Input: Moments $\{\mu_i\}$, Tolerance ϵ, Hessian noise η
Output: Coefficients $\{\alpha_i\}$
Initialize $\alpha_i = 0$.
Minimize $\int_0^1 p_\alpha(\lambda)d\lambda + \sum_i \alpha_i \mu_i$
Gradient $\mu_j - \int_0^1 p_\alpha(\lambda)\lambda^j d\lambda$
Hessian $= \int_0^1 p_\alpha(\lambda)\lambda^{j+k} d\lambda$
Hessian $= (H + H')/2 + \eta$
Until $\forall j$ Gradient$_j < \epsilon$

Algorithm 3 Cluster Estimator Algorithm

Input: Lagrange Multipliers α_i, Matrix Dimension n, Tolerance ϵ
Output: Number of Clusters N_c
Initialize $p(\lambda) \to p(\lambda|\alpha_i) = \exp -[1 + \sum_i \alpha_i x^i]$.
Minimize $\lambda*$ s.t $\frac{dp(\lambda)}{d\lambda}|_{\lambda=\lambda*} \leq \epsilon$
Calculate $N_c = n \int_0^{\lambda*} p(\lambda)d\lambda$

Estimating the Cluster Number using Maximum Entropy: For any smoothed spectral density, which we learn using stochastic trace estimation (Section) and MaxEnt (Algorithm 2), to count the number of near 0 eigenvalues, one simply integrates the spectral density until the first spectral minimum (found using gradient descent) and then multiplies by number of Nodes N, we illustrate this in Algorithm 3.

Experiments

We follow the experimental setup in Section , use $d = 100$ Gaussian random vectors for our stochastic trace estimation, for both MaxEnt and Lanczos (Ubaru, Chen, and Saad, 2017). When comparing MaxEnt with Lanczos we set the number of moments m equal to the number of Lanczos stepsIn order to normalise the moment input we use the normalised Laplacian with eigenvalues bounded by $[0, 2]$ and divide by 2. To make a fair comparison we take the output from Lancsoz (Ubaru, Chen, and Saad, 2017) and apply kernel smoothing (Lin, Saad, and Yang, 2016) before applying our cluster estimator. We explain the details of our kernel smoothing in section .

Algorithm 4 Stochastic Trace Estimation

Input: Number of Random Vectors d, Number of Moments m, Matrix $M^{n\times n}$
Output: Moment Expectations $\mathbb{E}_\mu(\lambda^i)\ \forall i \leq m$
Initialize $\mathbb{E}_\mu(\lambda^i) = 0\ \forall i$
for $i \leq d$ **do**
  Initialize $\vec{z}_d = rand(1, n)$
  for $j \leq m$ **do**
    $\vec{z}_d = M * \vec{z}_d$
    $\mathbb{E}_\mu(\lambda^j) = \mathbb{E}_\mu(\lambda^j) + \frac{1}{d}\vec{z}_d^t * \vec{z}_d$
  end for
end for

Table 2: Fractional error in community detection for synthetic networks using MaxEnt and Lanczos with 80 moments

# OF CLUSTERS (N)	LANCZOS	MAXENT
9 (270)	$\mathbf{3.20 \times 10^{-3}}$	9.70×10^{-3}
30 (900)	1.41×10^{-2}	$\mathbf{6.40 \times 10^{-3}}$
90 (2700)	1.81×10^{-2}	$\mathbf{5.80 \times 10^{-3}}$
240 (7200)	2.89×10^{-2}	$\mathbf{3.50 \times 10^{-3}}$

Synthetic Data

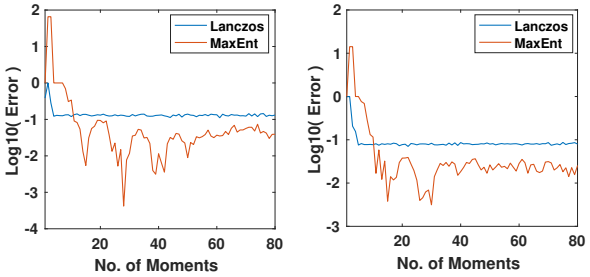
In order to test the robustness of the approach to networks with clusters of different structures, we implement a mixture of Erdös-Rényi , Watts-Strogatz and Barabsi-Albert networks using the Python package *NetworkX* and conduct multiple experiments using networks that have from 9 to 240 clusters, with each cluster containing 30 nodes. We connect the nodes between clusters randomly, with a single inter-cluster connection. We show the results in Table .

To test the performance of our approach for networks that are too big to apply eigen-decomposition, we also generate two large networks by mixing Erdös-Rényi, Watts-Strogatz and Barabsi-Albert networks. The first large network has a size of 201,600 nodes and comprises 350 interconnected clusters whose size varies from 500 to 1000 nodes. The other large network has a size of 404,420 nodes and comprises interconnected 1355 clusters whose size varies from 200 to 800 nodes. The results in Figure **??** show that our MaxEnt approach outperforms Lanczos for both large synthetic networks.

Figure 2: Comparison of Classical and Novel MaxEnt algorithms

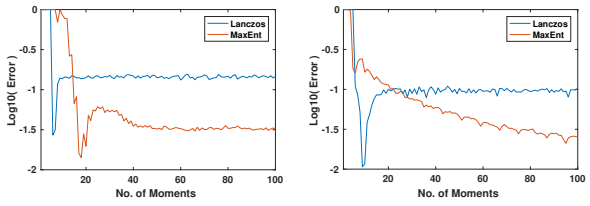
(a) $201,600$ nodes and 305 clusters

(b) $404,420$ nodes and $1,355$ clusters



(c) Email Dataset

(d) Netscience Dataset



Small Real World Data When the number of nodes $n \approx 10^3$, it is possible to compute the eigen-decomposition exactly and hence to benchmark the performance of our algorithm in the real world.

The first real-world dataset we use is the Email network, which is generated using email communication data among $1,005$ members of a large European research institution and is an undirected graph of $n = 1,005$ nodes. We calculate the ground-truth by computing the eigenvalues explicitly and finding the spectral gap near 0. We note that this differs from the value of 42 given by the number of departments at the research institute. A likely reason for this ground truth inflation is that certain departments, Astrophysics, Theoretical Physics and Mathematics for example, may collaborate to such an extent that their division in name may not be reflected in terms of node connection structure.

In order to make a valid comparison, we smooth the implied density using a Gaussian kernel, with $\sigma = 10^{-3}$. We plot the log error against the number of moments for both MaxEnt and Lanczos in Figure **??**, with MaxEnt showing superior performance. We repeat the experiment on the Net Science collaboration network, which represents a co-authorship network of $1,589$ scientists ($n = 1,589$) working on network theory and experiment (Newman, 2006). The results in Figure **??** show that MaxEnt quickly outperforms the Lanczos algorithm after around 20 moments.

Appendix

First order Eigenvalue perturbation

We formalise this intuition by considering a small perturbation of the Laplacian $\tilde{L} = L + \delta L$, where $||\delta L|| \ll ||L||$. Considering the vectors $\vec{u_i}$ to be the normalised eigenvectors of the unperturbed Laplacian L we solve the equation

$$(L + \delta L)(\vec{u_i} + \delta\vec{u_i}) = (\lambda_i + \delta\lambda_i)(\vec{u_i} + \delta\vec{u_i}) \tag{21}$$

Cancelling and dropping second order terms we have

$$\delta L\vec{u_i} + L\delta\vec{u_i} = \lambda_i\delta\vec{u_i} + \delta\lambda_i\vec{u_i} \tag{22}$$

expressing the vector $\delta\vec{u_i}$ in the basis of the eigenvectors $\vec{u_i}$ of L, which can always be done as the L is normal and hence its eigenvectors span the space of $\mathbb{R}^{n\times n}$, hence $\delta\vec{u_i} = \sum_j^n \epsilon_j\vec{u_j}$. Hence we can write equation (22) as

$$\delta L\vec{u_i} + L\sum_j^n \epsilon_j\vec{u_j} = \lambda_i\sum_j^n \epsilon_j\vec{u_j} + \delta\lambda_i\vec{u_i}$$

$$\vec{u_i}^T\delta L\vec{u_i} + \sum_j^n \lambda_j\epsilon_j\vec{u_i}^T\vec{u_j} = \lambda_i\sum_j^n \epsilon_j\vec{u_i}^T\vec{u_j} + \delta\lambda_i\vec{u_i}^T\vec{u_i}$$

$$\vec{u_i}^T\delta L\vec{u_i} = \delta\lambda_i \tag{23}$$

Where we have used the eigenvalue equation $L\vec{u_i} = \lambda_i\vec{u_i}$ and that the eigenvectors are orthonormal $\vec{u_j}^t\vec{u_i} = \delta_{i,j}$. We can now bound this term using the Cauchy-Schwarz inequality

$$\delta\lambda_i = \vec{u_i}^T\delta L\vec{u}_i \leq ||\delta L||\,||\vec{u_i}^T\vec{u}_i|| = ||\delta L|| \tag{24}$$

If we consider the natural variant of the Laplacian, normalised by the number of vertices in the graph, i.e $L_{\text{natural}} = (D - A)/n$, then by adding R vertices between previously disconnected subgraphs, for each vertex, we alter a two diagonal components by $+1$ and two off diagonal components by -1.Thus, using the Frobenius norm, our bound B goes as

$$B = \sqrt{\sum_{i=1}^n\sum_{j=1}^n \left|\delta L_{i,j}\right|^2} = \frac{2R}{n} \tag{25}$$

We note that our derived bound using the Cauchy-Schwarz inequality is exactly the same as Weyl's perturbation theorem for Hermitian matrices, which uses the min-max principle (Bhatia, 2013).

Hence we expect the eigenvalue perturbations to die off as $\mathcal{O}(n^{-1})$ for a constant number of connections between clusters as we increase the number of nodes n in the network. Even if the number of such connections grows with n but is sparse such that the total number is $\mathcal{O}(ns)$ with small sparsity s, the perturbation would only be of order s. For small sparsity s we would expect the spectral gap between the perturbed eigenvalues which were at 0 pre perturbation and the non zero eigenvalues to remain non-negligible. In these cases, we expect our cluster detection algorithm, introduced in the next section to also work.

If we choose to work with the normalised Laplacian defined in (**??**), then for each new connection between previously disconnected components we get a term of the form

$$\sum_{j=1}\left|\left|\frac{1}{\sqrt{d_i d_j}} - \frac{1}{\sqrt{(d_i+1)d_j}}\right|\right|^2 + \frac{2}{(d_i+1)(d_{k+1})}$$
$$+\sum_{l=1}\left|\left|\frac{1}{\sqrt{d_k d_l}} - \frac{1}{\sqrt{(d_k+1)d_l}}\right|\right|^2 \tag{26}$$

where nodes k and i are being connected and nodes j and l are the nodes connected to k and i, respectively. By taking the degrees to be a fraction of the total number of nodes n and taking n to be large we observed a similar n^{-1} scaling. The idea of strong communities being nearly disconnected components, is not novel (McGraw and Menzinger, 2008) and has been used in community detection algorithms (Capocci et al., 2005). However we have not come across a simple exposition of the results from matrix perturbation theory, or the application of the Cauchy-Schwarz inequality to bound the increase in the 0 eigenvalues as a function of node number n or degrees d_i amongst the connected components.

Polynomial approximations to the Log Determinant

Recent work Han, Malioutov, and Shin (2015); Dong et al. (2017); Zhang and Leithead (2007) has considered incorporating knowledge of the non central moments [3] of a normalised eigenspectrum by replacing the logarithm with a fi-

[3] Also using stochastic trace estimation.

nite polynomial expansion,

$$\mathbb{E}_\mu = \int_0^1 p(\lambda)\log(\lambda)d\lambda = \int_0^1 p(\lambda)\log(1-(1-\lambda))d\lambda. \tag{27}$$

Given that $\log(\lambda)$ is not analytic at $\lambda = 0$, it can be seen that, for any density with a large mass near the origin, a very large number of polynomial expansions, and thus moment estimates, will be required to achieve a good approximation, irrespective of the choice of basis.

Taylor approximations are probabilistically unsound

In the case of a Taylor expansion equation (27) can be written as,

$$-\int_0^1 p(\lambda)\sum_{i=1}^{\infty}\frac{(1-\lambda)^i}{i} \approx -\int_0^1 p(\lambda)\sum_{i=1}^{m}\frac{(1-\lambda)^i}{i}. \tag{28}$$

The error in this approximation can be written as the difference of the two sums,

$$-\sum_{i=m+1}^{\infty}\frac{\mathbb{E}_\mu(1-\lambda)^i}{i}, \tag{29}$$

where we have used the Taylor expansion of $\log(1-x)$ and $\mathbb{E}_\mu$ denotes the expectation under the spectral measure.

De-Finetti De Finetti (1974) showed that Kolmogorov's axioms of probability Kolmogorov (1950) could be derived by manipulating probabilities in such a manner so as to not make a sure loss on a gambling system based on them. Such a probabilistic framework, of which the Bayesian is a special case Walley (1991a), satisfies the conditions of,

1. **Non Negativity:** $p_i \geq 0\,\forall i$**,**
2. **Normalization:** $\sum_i p_i = 1$**,**
3. **Finite Additivity:** $P(\cup_{n=1}^N A_n) = \sum_{n=1}^N P(A_n)$**.** [4]

The intuitive appeal of De-Finetti's sure loss arguments, is that they are inherently performance based. A sure loss is a practical cost, which we wish to eliminate.

Keeping within such a very general formulation of probability and thus inference. We begin with complete ignorance about the spectral density $p(\lambda)$ (other than its domain $[0,1]$) and by some scheme after seeing the first m non-central moment estimates we propose a surrogate density $q(\lambda)$. The error in our approximation can be written as,

$$\int_0^1 [p(\lambda)-q(\lambda)]\log(\lambda)d\lambda$$
$$= \int_0^1 -[p(\lambda)-q(\lambda)]\sum_{i=1}^{\infty}\frac{(1-\lambda)^i}{i}d\lambda. \tag{30}$$

For this error to be equal to that of our Taylor expansion (29), our implicit surrogate density must have the first m non-central moments of $(1-\lambda)$ identical to the true spectral density $p(\lambda)$ and all others 0.

[4] for a sequence of disjoint sets A_n.

For any PD matrix K, for which $E_\mu(1-\lambda)^i > 0,\ \forall i \leq m$[5], for equation (30) to be equal to (29), we must have,

$$\int_0^1 q(\lambda)\sum_{m+1}^{\infty}\frac{(1-\lambda)^i}{i}d\lambda = 0. \tag{31}$$

Given that $0 \leq \lambda \leq 1$ and that we have removed the trivial case of the spectral density (and by implication its surrogate) being a delta function at $\lambda = 1$, the sum is manifestly positive and hence $q(\lambda) < 0$ for some λ, which is incompatible with the theory of probability De Finetti (1974); Kolmogorov (1950).

Prior Spectral Belief If we assume complete ignorance over the spectral domain, then the natural maximally entropic prior is the uniform distribution and hence $q(\lambda) = 1$.[6] An alternative prior over the $[0,1]$ domain is the Beta distribution, the maximum entropy distribution of that domain under a mean and log mean constraint,

$$\frac{\Gamma(\gamma+\beta)}{\Gamma(\gamma)\Gamma(\beta)}\lambda^{\gamma-1}(1-\lambda)^{\beta-1}. \tag{32}$$

The log mean constraint is particularly interesting as we know that it must exists for a valid log determinant to exist, as is seen for equation (12). We set the parameters of by maximum likelihood, hence,

$$\gamma = \frac{\mu_1(\mu_1-\mu_2)}{\mu_2-\mu_1^2},\ \beta = \left(\frac{1}{\mu_1}-1\right)\frac{\mu_1(\mu_1-\mu_2)}{\mu_2-\mu_1^2}. \tag{33}$$

Analytical surrogate form Our final equation for $q(\lambda)$ can be written as,

$$q(\lambda) = \frac{\Gamma(\gamma+\beta)}{\Gamma(\gamma)\Gamma(\beta)}\lambda^{\gamma-1}(1-\lambda)^{\beta-1}\times\exp(-[1+\sum_{i=0}^{m}\alpha_i\lambda^i]) \tag{34}$$

for the beta prior and

$$q(\lambda) = \exp(-[1+\sum_{i=0}^{m}\alpha_i\lambda^i]) \tag{35}$$

for the uniform. The exponential factor can be thought of altering the prior beta/uniform distribution so as to fit the observed moment information.

Lagrangian Duality

Consider a generic optimization problem of the form,

$$\begin{aligned} &\text{minimize } f_0(x) \\ &\text{subject to } f_i(x) \leq 0,\ i = 1...m \\ &\text{subject to } h_i(x) = 0,\ i = 1...p \end{aligned} \tag{36}$$

where $x \in \mathbb{R}^n$ and the domain $\mathcal{D} = \bigcap_{i=0}^{m} f_i \cap \bigcap_{i=1}^{p} h_i$. We define the Lagrangian dual function as the infimum of the

[5] we except the trivial case of a Dirac distribution at $\lambda = 1$, which is of no practical interest

[6] Technically as the log determinant exists and is finite, we cannot have any mass at $\lambda = 0$, hence we must set the uniform between some $[\delta\epsilon, 1]$, where $\delta\epsilon > 0$.

Lagrangian over the domain of x,

$$g(\lambda,\nu) = \inf_{x\in\mathcal{D}} L(x,\lambda,\nu) \\ = \inf_{x\in\mathcal{D}}\left(f_0(x) + \sum_{i=1}^{m}\lambda_i f_i(x) + \sum_{i=1}^{p}\nu_i h_i(x)\right). \tag{37}$$

As the dual is the pointwise infimum of a family of affine functions of (λ,ν), it is concave, irrespective of the convexity of f_0, f_i, h_i. Boyd and Vandenberghe (2009). It is easily verifiable due to the net negativity of the two summation terms in $g(\lambda,\nu)$ that the dual provides a lower bound on the optimal value p^* of the primal problem. This is known as weak duality. In the case of equality constraints this bound is tight.

For general inequality constraints the difference between the primal and dual optimal solution (duality gap) is not 0. However, for $f_0...f_m$ convex, affine equality constraints and certain regularity conditions, we have a duality gap of 0, this is known as strong duality. An example of such a constraint qualification is Slater's condition, which states that there is an $x \in$ **relint** $\mathcal{D}$ which satisfies the constraints.

Application to Probability Distributions

We consider a probability distribution $p : \mathcal{R}^n \to \mathcal{R}$ which satisfies the general axioms of non-negativity, associativity and normalizability. This defines a very general space of probability theories, of which the Bayesian formalism is a special case Walley (1991b). Thus $p(x) \geq 0$ for all $x \in C$ and $\int p(x)dx = 1$, where $C \subseteq \mathcal{R}^n$ is convex. The last condition follows from the definition of convexity and the fact that any sum of two real numbers is a real number. Then as any non negative weighting of a convex set preserves convexity,

$$\int_C p(x)x\,dx \in C \tag{38}$$

if the integral exists.

Application to Maximum Entropy

We wish to maximise the entropic functional $\mathcal{S}(p) = -\int p(x)\log p(x)dx$ under certain moment constraints $\int p(x)x^m dx = \mu_m$. This can be written as,

$$\text{minimize } f_0[p(x)] = \int p(x)\log p(x)dx \\ \text{subject to } h_i[p(x)] = \int p(x)x^i dx - \mu_i = 0,\ i = 1...p. \tag{39}$$

Given that the negative entropy is a convex objective and that the moment equality constraints are affine in the variable being optimised over $p(x)$ by strong duality we have an equivalence between the solution of the dual and that of the primal.

It is also clear that the domain defined as the intersection of the constraint sets can never increase upon the addition of an extra constraint. Hence,

$$\inf_{x\in\mathcal{D}=\bigcap_{i=0}^{m} f_i} L(x,\lambda,\nu) \leq \inf_{x\in\mathcal{D}=\bigcap_{i=0}^{m+1} f_i} L(x,\lambda,\nu) \tag{40}$$

and thus the entropy can only decrease when adding an extra constraint. Hence by adding more moment constraints, we always reduce the entropy and given equations (**??**) and (**??**) we necessarily reduce $\mathcal{D}_{kl}(p(x)\|q(x))$, where $p(x), q(x)$ define the true eigenvalue and MaxEnt proposal distributions respectively

KL as a measure of divergence

Using Pinsker's inequality, which is tight up to constant factors, we can relate the KL divergence to both the total variation distance and the total variation norm Cover and Thomas (2012):

$$\delta(P,Q) \leq \sqrt{\frac{1}{2}\mathcal{D}_{kl}(P\|Q)}, \tag{41}$$

where the total variation distance is defined as

$$\delta(P,Q) = sup\{|P(A) - Q(A)|\}\text{where} \in \Sigma. \tag{42}$$

The total variation norm between P and Q can be written as,

$$|P - Q| \leq \sqrt{2\mathcal{D}_{kl}(P\|Q)}. \tag{43}$$

This follows as $2\delta(P,Q) = |P - Q|_1$ where the 1 relates to the $L1$ norm.

Bound on Error of MaxEnt

To calculate the log determinant of the matrix in question, once we have the proposal eigenvalue distribution $q(x)$ we calculate the mean value of $\log(x)$ under the distribution $q(x)$, i.e $\int q(x)\log(x)dx$. We can write the error of our MaxEnt estimate as

$$\epsilon = \left|\int_{x\in\chi}[p(x) - q(x)]\log(x)dx\right| \tag{44}$$

Where $p(x)$ is the true eigenvalue distribution. $\forall p(x), q(x) \geq 0$ it is hence true that,

$$\left|\int_{x\in\chi}(p(x)-q(x))\log(x)dx\right| \leq \int_{x\in\chi}|p(x)-q(x)||\log(x)|dx. \tag{45}$$

From the monotonicity of the function $\log(x)$, we have that $\log(x) \leq \max[|\log(x_{max})|, |\log(x_{min})|$ and rewriting the total variational norm in terms of the KL divergence we have:

$$\epsilon \leq \max[|\log(x_{max})|, |\log(x_{min})|]\sqrt{2\mathcal{D}_{kl}(P\|Q)}. \tag{46}$$

We thus note that by reducing the self entropy of the proposal distribution $q(x)$ we necessarily reduce the maximum possible error of the log determinant estimation. However, given that we do not have an analytic form of $p(x)$, we cannot explicitly calculate $\mathcal{D}_{kl}(P\|Q)$ and hence the bound in its current form is not inherently practical. We leave the estimation of this term and derivation of estimate uncertainty to future work.

Conditions for the existence of a solution to this problem have been proved for the case of the Hausdorff moment conditions Mead and Papanicolaou (1984), of which our problem is a special case.

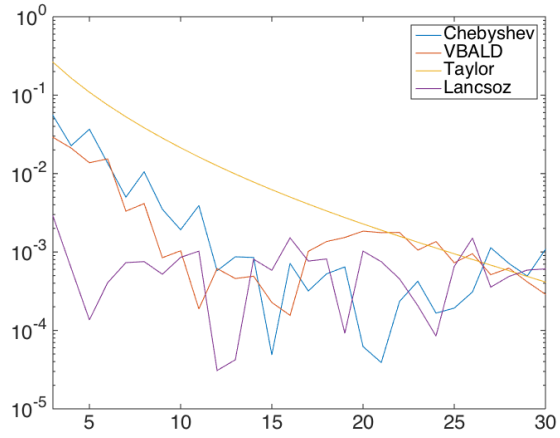


Figure 3: Length Scale = 0.1, Condition number = 16

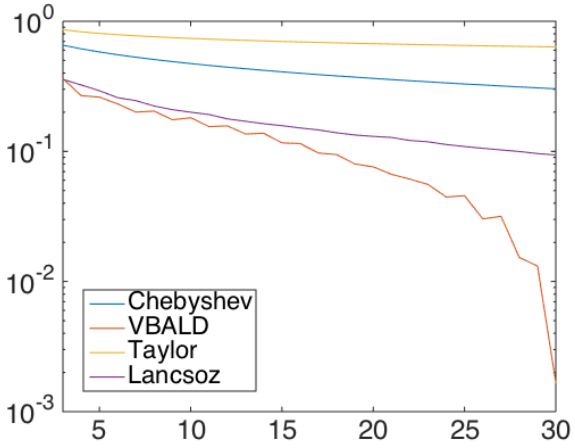


Figure 4: Length Scale = 0.33, Condition number = 2×10^7 Equivalent Chebyshev steps $n = 1200$, Lanczos steps $n \approx 100$.

Figure 5: Comparison of MaxEnt against Taylor, Lanczos and Chebyshev algorithms for calculating the log determinant of synthetic squared exponential kernel matrices of different condition number. The absolute relative error is on the y-axis and number of moments used on the x-axis.

Acknowledgements

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