VBALD - Variational Bayesian Approximation of Log Determinants

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Abstract

Evaluating the log determinant of a positive definite matrix is ubiquitous in machine learning. Applications thereof range from Gaussian processes, minimum-volume ellipsoids, metric learning, kernel learning, Bayesian neural networks, Determinantal Point Processes, Markov random fields to partition functions of discrete graphical models. In order to avoid the canonical, yet prohibitive, Cholesky $O(n^3)$ computational cost, we propose a novel approach, with complexity $O(n^2)$, based on a constrained variational Bayes algorithm. We compare our method to Taylor, Chebyshev and Lanczos approaches and show state of the art performance on both synthetic and real-world datasets.

1. 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. A common hindrance, appearing in Gaussian graphical models, Gaussian Processes (Rue & Held, 2005; Rasmussen, 2006), sampling, variational inference (MacKay, 2003), metric/kernel learning (Davis et al., 2007; Van Aelst & Rousseeuw, 2009), Markov random fields (Wainwright & 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 $K ∈ R^{n×n}$, the canonical solution involves the Cholesky decomposition, $K = LL^T$. The log determinant is then trivial to calculate as $\log \det(K) = 2 \sum_{i=1}^n \log L_{ii}$. This computation invokes a computational complexity $O(n^3)$ and thus is unfit for purpose for $n > 10^4$, i.e. even a small sample set in the age of big data.

1.1. Related Work

Recent work in machine learning combined stochastic trace estimation with Taylor approximations for Gaussian process parameter learning (Zhang & Leithead, 2007; Boutsidis et al., 2017), reducing the computational cost to matrix vector multiplications (MVMs), $O(n^2)$ for a dense matrix and $O(nnz)$ for a sparse matrix. Variants of the same theme used Chebyshev polynomial approximations, giving a performance improvement over Taylor along with refined error bounds (Han et al., 2015) and the combination of either Chebyshev/Lanczos techniques with structured kernel interpolation (SKI) in order to accelerate MVMs to $O(n + i \log i)$, where $i$ is the number of inducing points (Dong et al., 2017).

This approach relies on an extension of Kronecker and Toeplitz methods, which are limited to low dimensional (typically $D ≤ 5$) 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 $O(\sqrt{\kappa})$ Lanczos steps (Ubaru et al., 2016), where $\kappa$ is the matrix condition number. In many practical cases of interest $\kappa > 10^{10}$ and thus the large number of $\kappa$ matrix vector multiplications becomes prohibitive. We restrict ourselves to the high-dimensional, high-condition number, big data limit.

1.2. Contribution

We recast the problem of calculating log determinants as a constrained variational inference problem, which under the assumption of a uniform prior reduces to maximum entropy spectral density estimation given moment information. We develop a novel 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 ($m > 30$) surpassing the $m \approx 8$ limit of previous MaxEnt algorithms (Granziol & Roberts, 2017; Bandyopadhyay et al., 2005; Mead & Papanicolaou, 1984). We build on the experimental results of (Han et al., 2015) and show state of the art performance on both synthetic and real-world datasets.
2. Motivating example

Determinantal point processes (DPPs) (Macchi, 1975) are probabilistic models capturing global negative correlations. They describe Fermions \(^2\) in Quantum Physics, Eigenvalues of random matrices and non-intersecting random walks.

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 (Bandyopadhyay et al., 2005) to estimate the matrix spectral density in order to calculate the log determinant. Their approach outperforms Chebyshev, Taylor, Lanczos and kernel based approximations, yet begins to show pathologies and increasing error for \(m \geq 8\) moments, due to convergence issues (Granziol & Roberts, 2017), making it unsuitable for machine learning where typical squared exponential kernels have very sharply decaying spectra and thus a larger number of moments is required for high precision.

3. Background

3.1. Log Determinants as a Density Estimation Problem

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

\[
\log \det K = \log \prod_i \lambda_i = \sum_i^n \log \lambda_i = n \mathbb{E}_\mu(\log \lambda). \quad (3)
\]

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:

\[
\mathbb{E}_\mu(\log \lambda) = \int_{\lambda_{\min}}^{\lambda_{\max}} d\mu(\lambda) \log \lambda = \int_{\lambda_{\min}}^{\lambda_{\max}} \sum_i^n \frac{1}{n} \delta(\lambda_i - \lambda) \log \lambda d\lambda. \quad (4)
\]

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,

\[
\log \det \frac{K}{\lambda_u} = n \mathbb{E}_\mu(\log \lambda') = n \mathbb{E}_\mu(\log \lambda) - n \lambda_u. \quad (5)
\]

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

\[
\int_{\lambda_{\min}/\lambda_u}^{\lambda_{\max}/\lambda_u} p(\lambda') \log \lambda' d\lambda' = \int_0^1 p(\lambda') \log \lambda' d\lambda', \quad (6)
\]

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

3.2. Stochastic Trace Estimation

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

\[
\mathbb{E}(zz^t) = mm^t + \Sigma \sum_{m=0}^{\infty} I, \quad (7)
\]

where in the last equality we have assumed that the variable possesses zero mean and unit variance. By the linearity of

\[
\mathbb{E}(\log \det K) = \mathbb{E}(\log |\det K|) = \mathbb{E}(\log \prod_i \lambda_i) = \sum_i^n \mathbb{E}(\log \lambda_i).
\]

which does not cover the class of realistic kernel matrix spectra, notably the popular squared exponential kernel. We develop a method in section 5.2 and an algorithm 5.4 which is capable of handling very high condition numbered matrices.
trace and expectation for any $m \geq 0$ we can write
\[ \sum_{i=1}^{n} \lambda^m = nE(\lambda^m) = \text{Tr}(IK^m) = E(zK^m z^t). \quad (8) \]

In practice we approximate the expectation over all random vectors with a simple Monte Carlo average, i.e. for $d$ random vectors,
\[ E(zK^m z^t) \approx \frac{1}{d} \left( \sum_{j=1}^{d} z_j K^m z_j \right)^{\dagger}, \quad (9) \]

where we take the product of the matrix $K$ with the vector $z_j$, $m$ times, so as to avoid costly $O(n^3)$ matrix multiplication. This allows us to calculate the non-central moments
\[ \text{Var}[\text{Tr}K] = 2\left(\|K\|^2 - \sum_{i=1}^{n} K_{ii}^2 \right). \quad (10) \]

Loose bounds exist on the number of samples $d$ required to get within a fractional error $\epsilon$ with probability $1 - \eta$ (Han et al., 2015),
\[ d \geq 6e^{-2} \log\left(\frac{2}{\eta}\right) \]
\[ \text{Pr}\left[\left|\frac{\text{Tr}_a(K) - \text{Tr}(K)}{\text{Tr}(K)}\right| \leq \epsilon\right] \geq 1 - \eta. \quad (11) \]

as per (Roosta-Khorasani & Ascher, 2015). To get within 1% fractional error with probability 0.9, for example, we require $d = 180,000$ samples. In practice we find that as little as $d = 30$ gives good accuracy however.

4. Polynomial approximations to the Log Determinant

Recent work (Han et al., 2015; Dong et al., 2017; Zhang & Leithhead, 2007) has considered incorporating knowledge of the non-central moments of a normalised eigenspectrum by replacing the logarithm with a finite polynomial expansion,
\[ E(\lambda) = \int_{0}^{1} p(\lambda) \log(\lambda) d\lambda = \int_{0}^{1} p(\lambda) \log(1 - (1 - \lambda)) d\lambda. \quad (12) \]

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.

4.1. Taylor approximations are probabilistically unsound

In the case of a Taylor expansion equation (12) can be written as,
\[ -\int_{0}^{1} p(\lambda) \sum_{i=1}^{n} \frac{(1 - \lambda)^i}{i} \approx -\int_{0}^{1} p(\lambda) \sum_{i=1}^{n} \frac{(1 - \lambda)^i}{i}. \quad (13) \]

The error in this approximation can be written as the difference of the two sums,
\[ -\sum_{i=m+1}^{n} E(\lambda^i), \quad (14) \]

where we have used the Taylor expansion of $\log(1 - x)$ and $E(\lambda)$ 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, 1991), satisfies the conditions of,

1. **Non Negativity**: $p_i \geq 0 \forall i,$
2. **Normalization**: $\sum_i p_i = 1,$
3. **Finite Additivity**: $P(\cup_{n=1}^{N} A_n) = \sum_{n=1}^{N} P(A_n).$ \footnote{for a sequence of disjoint sets $A_n$.}

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,
\[ \int_{0}^{1} [p(\lambda) - q(\lambda)] \log(\lambda) d\lambda \]
\[ = \int_{0}^{1} [p(\lambda) - q(\lambda)] \sum_{i=1}^{\infty} \frac{(1 - \lambda)^i}{i} d\lambda. \quad (15) \]

For this error to be equal to that of our Taylor expansion (14), 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.

For any PD matrix $K$, for which $E_p(1 - \lambda)^i > 0, \forall i \leq m$, for equation (15) to be equal to (14), we must have,

$$\int_0^1 q(\lambda) \sum_{m+1}^{\infty} \frac{(1 - \lambda)^i}{i} d\lambda = 0. \quad (16)$$

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 $\lambda$, which is incompatible with the theory of probability (De Finetti, 1974; Kolmogorov, 1950).

5. Constrained Variational Method

5.1. Variational Bayes

Variational Methods (MacKay, 2003; Fox & Roberts, 2012) in machine learning pose the problem of intractable density estimation from the application of Bayes’ rule as a functional optimization problem,

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)} \approx q(z), \quad (17)$$

and finding finding 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,

$$\log p(x) \geq \mathbb{E}_q[\log p(x, z)] - \mathbb{E}_q[\log q(z)]. \quad (18)$$

It can be shown that the reverse KL divergence between the posterior and the variational distribution, $D_{kl}(q||p)$, can be written as,

$$\log p(x) = \mathbb{E}_q[\log p(x, z)] - \mathbb{E}_q[\log q(z)] + D_{kl}(q||p). \quad (19)$$

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

By assuming the variational distribution to factor over the set of latent variables, the functional form of the variational marginals, subject to the normalisation condition, can be computed using functional differentiation of the dual,

$$\frac{\partial}{\partial Q_i(x_i)} \left\{ -D_{kl}(Q_i(x_i)Q^*(x_i)) - \lambda_i \left( \int Q_i dx_i - 1 \right) \right\}, \quad (20)$$

leading to a Gibbs’ distribution and an iterative update equation.

5.2. Log Determinant as a Variational Inference problem

We consider minimizing the reverse KL divergence between our surrogate posterior $q(\lambda)$ and our prior $p_0(\lambda)$ on the eigenspectrum,

$$D_{kl}(q||p_0) = -H(q) - \int_0^1 q(\lambda) \log p_0(\lambda) d\lambda, \quad (21)$$

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 & Vandenberghe, 2009),

$$-H(q) - \int q(\lambda) \log p_0(\lambda) d\lambda - \sum_{i=0}^m \alpha_i \left( \int_0^1 q(\lambda) \lambda^i d\lambda - \mu_i \right), \quad (22)$$

or alternatively we minimise

$$H(q) + \int q(\lambda) \log p_0(\lambda) d\lambda - \sum_{i=0}^m \alpha_i \left( \int_0^1 q(\lambda) \lambda^i d\lambda - \mu_i \right). \quad (23)$$

5.3. Link to Information Physics

In the field of information physics the minimization of Equation (23) 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 sub-system 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.

These lead to the generalised entropic functional,

$$-\int q(x) \log \frac{q(x)}{m(x)} dx - \sum_i \alpha_i \left( \int_{x \in \mathcal{D}} f_i(x) dx - \mu_i \right). \quad (24)$$

Here the justification for restricting ourselves to a functional is derived from considering the set of all distributions $q_i(\lambda)$ 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; 1957). Conditions for the existence of a solution to this problem have been proved for the case of the Hausdorff moment conditions (Mead & Papanicolaou, 1984), of which our problem is a special case.

5.4. Algorithm

The generalised dual objective function which we minimise is,

\[ S(q, q_0) = \int_0^1 q_0(\lambda) \exp(-[1 + \sum \alpha_i \lambda_i])d\lambda + \sum \alpha_i \mu_i , \]

which can be shown to have gradient

\[ \frac{\partial S(q, q_0)}{\partial \alpha_j} = \mu_j - \int_0^1 q_0(\lambda) \lambda^j \exp(-[1 + \sum \alpha_i \lambda_i])d\lambda , \]

and Hessian

\[ \frac{\partial^2 S(q, q_0)}{\partial \alpha_j \partial \alpha_k} = \int_0^1 q_0(\lambda) \lambda^{j+k} \exp(-[1 + \sum \alpha_i \lambda_i])d\lambda . \]

5.4.1. PRIOR SPECTRAL BELIEF

If we assume complete ignorance over the spectral domain, then the natural maximally entropic prior is the uniform distribution and hence \( q(\lambda) = 1 \). 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,

\[ \frac{\Gamma(\gamma + \beta)}{\Gamma(\gamma) \Gamma(\beta)} \lambda^{\gamma-1}(1 - \lambda)^{\beta-1} . \]

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 (4). We set the parameters of by maximum likelihood, hence,

\[ \gamma = \frac{\mu_1(\mu_1 - \mu_2)}{\mu_2 - \mu_1} , \quad \beta = \left(1 - \frac{1}{\mu_1} \right) \frac{\mu_1(\mu_1 - \mu_2)}{\mu_2 - \mu_1} . \]

5.4.2. ANALYTICAL SURROGATE FORM

Our final equation for \( q(\lambda) \) can be written as,

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

for the beta prior and

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

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

5.4.3. PRACTICAL IMPLEMENTATION

For simplicity we have kept all the formula’s in terms of power moments, however we find vastly improved performance and conditioning when we switch to another polynomial basis. Many alternative and orthogonal Polynomial bases exist (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 significance previously (Yap et al., 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 along the diagonal. The pseudo code is given in Algorithm 1. The Log Determinant is then calculated using Algorithm 2.
Table 1. Absolute relative error for VBALD, Chebyshev & Lanczos methods on varying length-scale $l$, with varying condition number $\kappa$ on squared exponential kernel matrices $K \in \mathbb{R}^{1000 \times 1000}$.

| $\kappa$   | $l$  | VBALD | CHEBYSHEV | LANCZOS |
|------------|------|-------|-----------|---------|
| $3 \times 10^1$ | 0.05 | 0.0014 | 0.0037    | 0.0024  |
| $1.1 \times 10^2$ | 0.15 | 0.0522 | 0.0104    | 0.0024  |
| $1.0 \times 10^3$ | 0.25 | 0.0387 | 0.0795    | 0.0072  |
| $2.4 \times 10^4$ | 0.35 | 0.0263 | 0.2302    | 0.0196  |
| $8.3 \times 10^5$ | 0.45 | 0.0284 | 0.3439    | 0.0502  |
| $4.2 \times 10^6$ | 0.55 | 0.0256 | 0.4089    | 0.0646  |
| $4.3 \times 10^7$ | 0.65 | 0.0048 | 0.5049    | 0.0838  |
| $1.4 \times 10^8$ | 0.75 | 0.0086 | 0.5049    | 0.1050  |
| $4.2 \times 10^9$ | 0.85 | 0.0177 | 0.5358    | 0.1199  |

6. Experiments

In order to test the validity and practical applicability of our proposed Algorithm, we test on both Synthetic and real Kernel matrices. We compare against Chebyshev and Lanczos approaches. For completeness in Figures 2, 3 and 4 we include results from the Taylor expansion. However in light of the consistently superior performance of the Chebyshev approach (Han et al., 2015), the arguments in Section 4.1 and space requirements we do not include Taylor methods in our results tables.

6.1. Synthetic Kernel Data

We simulate the kernel matrices from a Gaussian/Determinental Point Process (Rasmussen & 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 ($0.1$, $0.33$ & $0.66$) with condition numbers $16$, $2 \times 10^7$ & $1.8 \times 10^{11}$ respectively. We use $m = 30$ Moments, $d = 50$ Hutchinson probe vectors and compare VBALD against the Taylor approximation, Chebyshev (Han et al., 2015) and Lanczos (Ubaru et al., 2017). We see that for low condition numbers (Figure 2) The benefit of framing the log determinant as an optimization problem is marginal, whereas for large condition numbers (Figures 3 & 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. Results for a wider range of length scales are shown in Table 6.1.
Table 2. Absolute relative error for VBALD, Chebyshev & Lanczos on SuiteSparse Matrices

| DATASET | m   | VBALD   | CHEBYSHEV | LANCZOS |
|---------|-----|---------|-----------|---------|
| THERMO  | 5   | $1 \times 10^{-2}$ | $5 \times 10^{-2}$ | $3 \times 10^{-3}$ |
| WATER 2 | 5   | $4 \times 10^{-3}$ | $1 \times 10^{-3}$ | $9 \times 10^{-4}$ |
| WATER 1 | 5   | $2 \times 10^{-4}$ | $3 \times 10^{-3}$ | $2 \times 10^{-5}$ |
| JLNRBRNG1| 5 | $3 \times 10^{-2}$ | $3 \times 10^{-2}$ | $2 \times 10^{-3}$ |
| FINAN512| 5   | $9 \times 10^{-3}$ | $8 \times 10^{-2}$ | $1 \times 10^{-5}$ |
| ECOCY 2 | 5   | $1 \times 10^{-2}$ | $1 \times 10^{-2}$ | $3 \times 10^{-2}$ |
| APACHE | 5   | $5 \times 10^{-2}$ | $2 \times 10^{-1}$ | $8 \times 10^{-2}$ |

6.2. Sparse Matrices

Given that the method described above works in general for any positive definite matrices. We look at large sparse spectral problems. Given that good results are reported for Polynomial methods at even a fairly modest number of moments, we consider very very large sparse matrices, such as social networks\(^3\), where we wish to limit the number of non-central moment estimates. We set\( m = d = 5 \) and test on the UFL SuiteSparse dataset. We show our results in table 6.2. VBALD it competitive with Lanczos and we note that similar to the Kernel Matrix case, VBALD does best relative to other methods when the others perform at their poorest, i.e have a relatively large absolute relative error.

6.3. Citations and References

6.4. Software and Data

Acknowledgements

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\(^3\)Facebook, with \(10^9\) users, each with \(~10^3\) friends is equivalent to a dense \(10^6\) matrix

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