GLASS: A General Likelihood Approximate Solution Scheme

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Abstract

We present a technique for constructing suitable posterior probability distributions in situations for which the sampling distribution of the data is not known. This is very useful for modern scientific data analysis in the era of “big data”, for which exact likelihoods are commonly either unknown, computationally prohibitively expensive or inapplicable because of systematic effects in the data. The scheme involves implicitly computing the changes in an approximate sampling distribution as model parameters are changed via explicitly-computed moments of statistics constructed from the data.

1 Introduction

Bayesian inference [1] is now commonly used and understood as being the correct way to learn about models from data. Posteriors for model parameters \( q \) are related via Bayes’ Theorem to the product of priors for the said parameters and the likelihood function, which is the probability for the data \( x \) given the model, considered as a function of the model parameters:

\[
p(q|x) = \frac{p(x|q)p(q)}{p(x)}. \tag{1}
\]

A difficulty presents itself in making accurate inferences if the true likelihood is not known or is unfeasible to repeatedly calculate. Reasons might include systematics in the data rendering an idealized likelihood unusable, or simply computational cost. One might still have an idea for a good choice of statistics to represent the data. This could be inspired say by “robustness” to systematics, by analogy to analysis procedures for idealized cases, or empirically by investigation of simulations. If certain quantities, such as means and variances, are calculable (or estimatable via simulations) as functions of the model parameters in a reasonable amount of time, one might hope to be able to make some plausible inferences. Whilst in the past people have been able to build approximations heuristically (see e.g. [2, 3, 4] in a cosmological context), here we
present a general scheme for constructing suitable likelihoods in such situations. The scheme should be relevant specifically for cosmic microwave background analysis, galaxy redshift surveys and the like, but is of general applicability.

This paper is organised as follows. First, the method is introduced and the main result derived in Sec. 2. Next, examples are presented in Sec. 3. Conclusions and further work are given in Sec. 4. Appendices A, B and C discuss various technical issues regarding the approximation including its derivation, practical use and validity.

2 Basic Procedure

The underlying idea is to use the principle of maximum entropy to construct the broadest (i.e. least presumptive) sampling distribution consistent with a) what one assumes and b) what one has managed to calculate about the statistics of the samples in the context of a model [1]. This, evaluated for the data, is used as the likelihood, which, when multiplied by the prior, gives the approximate posterior for the model given the data as in Eq. (1). (See Appendix A for a complementary motivation for our approach.)

Say, for example, one can calculate the mean \( \langle x \rangle \) and the variance \( \langle \langle x^2 \rangle \rangle \) of some statistic \( x \) for a model parametrized by a parameter \( q \). (We use \( \langle \ldots \rangle \) to denote moments and \( \langle\langle\ldots\rangle\rangle \) to denote cumulants of the indicated quantities.) Before even calculating anything, one might also have a “prior” \( p_0(x) \) on \( x \), such as it being positive for example. One then needs to maximise the entropy,

\[
H(p) = - \int dx \, p(x) \ln \frac{p(x)}{p_0(x)},
\]

using Lagrange multipliers to impose the desired constraints on the distribution along with normalisation of \( p(x) \). This yields

\[
p(x) = \frac{p_0(x) \exp \left(-\lambda_x x - \lambda_{xx} x^2\right)}{\int dx \, p_0(x) \exp \left(-\lambda_x x - \lambda_{xx} x^2\right)}.
\]

Generally, the lagrange multipliers must be solved for numerically, repeatedly evaluating \( \langle x \rangle \) and \( \langle \langle x^2 \rangle \rangle \) as a function of \( \lambda_x \) and \( \lambda_{xx} \) until \( \langle x \rangle(q) \) and \( \langle \langle x^2 \rangle \rangle(q) \) are obtained. The appropriate multipliers may be denoted \( \lambda_x(q) \) and \( \lambda_{xx}(q) \). Substituting these into Eq. (3) gives our approximate sampling distribution for \( x \) for the model with parameter \( q \). If \( x \) is then found to have some value, our approximate likelihood for \( q \) is then given by evaluating Eq. (3) for that \( x \). By analogy with conventional notation in statistical dynamics we denote the denominator of Eq. (3) by \( Z \), and we can introduce the “action” \( S \) (after classical/quantum mechanics) as \( -\log p(x) \):

\[
S(x, q) = -\log p_0(x) + \lambda_x(q) x + \lambda_{xx}(q) x^2 + \log Z(\lambda(q)).
\]

Multiplying by a desired prior on the parameter \( q \), one then has a suitable approximate (unnormalized-) posterior for \( q \) in light of the data \( x \), appropriate for use for inference.

In principle, this procedure is easily extensible to multi-dimensional data \( x^i, i = 1, \ldots, n \), described by multi-dimensional model parameters \( q^a, a = 1, \ldots, m \), and to use higher moments. The Lagrange multipliers become labelled...
by indices, $\lambda_i$, $\lambda_{ij}$, and so on and will be implicit functions of the $q^a$. The entropy becomes a multidimensional integral, and the action is

$$S(x,q) = -\log p_0(x) + \lambda_i x^i + \lambda_{ij} x^i x^j + \lambda_{ijk} x^i x^j x^k + \cdots + \log Z(\lambda(q^a))$$  \hfill (5)

with summation implied over repeated indices. Here parentheses around indices indicate their symmetrization, e.g. $\kappa^{(i} x^{j)} \equiv \frac{1}{2} (\kappa^i x^j + \kappa^j x^i)$, and we take all Lagrange multipliers to be symmetric since any non-symmetric part would not contribute to (5)\(^1\). Now

$$Z(\lambda(q^a)) = \int d^n x p_0(x) e^{-\lambda_i x^i - \lambda_{ij} x^i x^j - \lambda_{ijk} x^i x^j x^k - \cdots}.$$  \hfill (6)

One varies the Lagrange multipliers until all of the desired multi-dimensional moments are matched\(^2\) and the probability for the distribution becomes

$$p(x|q) d^n x = e^{-S(x,q)} d^n x.$$  \hfill (7)

In practice, the procedure rapidly becomes difficult to perform as the dimension increases, because of the increasing difficulty of evaluating the multidimensional numerical integrals required to solve explicitly for the Lagrange multipliers.

However, within a given class of models, we can get away without having to solve explicitly for the Lagrange multipliers as follows. Let us introduce the vector $X$ to denote $(x^i, x^{(i} x^{j)}, x^{(i} x^j x^k), \ldots)^T$. We may indicate a specific component of $X$ with a superscript $I$. (Nb. this component could contain one, two or more powers of the $x^i$.) Similarly, we can introduce $\lambda$ to denote the vector $(\lambda_i, \lambda_{ij}, \ldots)^T$ of associated Lagrange multipliers, with components $\lambda_I$.

Now we derive a set of relations between moments from the distribution given by Eq. (7). From the form of (7), we have:

$$\langle X^I \rangle(\lambda) = \frac{\partial \log Z}{\partial \lambda_I}, \quad \langle \langle X^I X^J \rangle \rangle(\lambda) = \frac{\partial^2 \log Z}{\partial \lambda_J \partial \lambda_I}.$$  \hfill (8, 9)

If we have managed to find $\lambda$ such that the desired $\langle X \rangle(q)$ are obtained in a neighbourhood of $q$, then we can consider differentiating Eq. (8) with respect to $q^a$ (sometimes denoting $\partial/\partial q^a$ by the shorthand $\alpha$):

$$\langle X^I \rangle_\alpha = \frac{\partial^2 \log Z}{\partial \lambda_J \partial \lambda_I} \frac{\partial \lambda_J}{\partial q^a} = \langle \langle X^I X^J \rangle \rangle \lambda_{J,a}. \quad \hfill (10)$$

Meanwhile, differentiating the action (5) with respect to $q^a$ gives

$$S_{\alpha} = \langle X^I - \langle X^I \rangle \rangle_\alpha \lambda_{I,a} \quad \hfill (11)$$

\(^1\)Alternatively one could demand, for example, that only multipliers with non-decreasing indices $i \leq j \leq \cdots \leq k$ are potentially nonzero.

\(^2\)We typically consider matching all moments up to a given order, but in certain circumstances one might wish to match only a subset of the moments. In a two-dimensional problem for example, with variables $x$ and $y$, one might be able to calculate all the first and second moments, but only the “auto” cubic moments $(x^3)$ and $(y^3)$ and not the “cross” ones such as $(x^2 y)$. In that case only the Lagrange multipliers corresponding to considered terms should be varied and the other ones, such as $\lambda_{(x y)}$ in this example, should be ignored/taken to be zero.
with the $\langle X^I \rangle$ term coming from the log $Z$ via Eq. (8). It is worthwhile noting that the "prior" $p_0(x)$ on the data has disappeared explicitly. Now, we should be able to invert Eq. (10) to solve for the $\lambda_{J,a}$ in terms of the derivatives $\langle X^I \rangle_{,a}$ of the first moments and the second cumulants $\langle \langle X^I X^J \rangle \rangle$:

$$\lambda_{,a} = -\langle \langle X X^T \rangle \rangle^{-1} \langle X \rangle_{,a}$$

(12)

(adopting a matrix notation). Substituting into Eq. (11) we obtain our main result:

$$S_{,a} = -(X - \langle X \rangle)^T \langle \langle X X^T \rangle \rangle^{-1} \langle X \rangle_{,a},$$

(13)

in which the Lagrange multipliers do not appear.

The scheme is then to obtain the desired moments of the $X^I$, their derivatives with respect to the $q^a$ and their second cumulants from the theory in question, ideally by calculation or potentially also by simulation. One then uses them in Eq. (13) to obtain the gradient. This gradient is then integrated between two points in parameter space to obtain the difference in $S$ between them.

One option for a likelihood would be to integrate $S_{,a}$ up from a fiducial choice of $q^a$ to the values in question. (Note that as the gradient generally varies along the path and the integration takes this into account, such a likelihood would not generally be a linear expansion in parameter shifts around a fiducial model.) Alternatively one might integrate in steps between two nearby models under consideration in an MCMC chain for example. When models vary smoothly with their parameters, the Romberg integration method (see e.g. [5]) has been found to work well and to converge quickly. In multi-dimensional situations one can choose a path in parameter space and perform a line integral, expressing the one-dimensional gradient along the path in terms of the partial derivatives of $S$ and the rate of change of parameters along the path using the chain rule. (Alternatively, one can use $S_{,a}$ directly in a sampling method that only uses the gradient of the likelihood.)

Equation (13) is framed in terms of the means of the $X^I$, their derivatives with respect to parameters, and their covariance. With the $X^I$ being powers of the $x^i$, such objects are expressible in terms of cumulants of the latter and their derivatives with respect to parameters. This allows one to formulate a version of Eq. (13) “reduced down” from the $X^I$ to the $x^i$, which may be easier to handle if the theory more directly gives cumulants of the $x^i$ rather than of the $X^I$. This is discussed further in Appendix B.

There is an approximation that is not at first sight obvious in this procedure. Equation (13) applies for the distribution defined by Eq. (7). While $\langle X \rangle$ agrees by construction between the underlying sampling distribution and its approximation in (7), not all of the moments required in $\langle \langle X X^T \rangle \rangle$ need necessarily match. So, to use $\langle \langle X X^T \rangle \rangle$ as calculated from the underlying sampling distribution in Eq. (7) constitutes to using an exact result as an approximation to a term in the approximation. In multiple dimensions this can lead to a breakdown in analyticity, causing the change in $S$ to become path-dependent in parameter space. Appendix C further discusses these consistency issues and potential mitigation strategies. In practice, one should include enough terms in $X$ to well-describe the parameter-dependent part of the sampling distribution. Then Eq. (7) should yield a good approximate likelihood. Reassurance in results obtained with the scheme might come through checking for stability under variation of...
the number of moments constrained. The quality of the likelihood might also
be judged empirically by testing its performance on suitable simulations of the
data.

3 Examples

Here we examine the theory for some test cases in which the true sampling
distribution is actually known. The cases are motivated from cosmic microwave
background (CMB) analysis, in which one computes power spectra of spherical
harmonic coefficients of (assumed-Gaussian) fields on the sky (see e.g. [6, 7]).

3.1 Auto Power Spectrum Example

Imagine one has $2l + 1$ independent Gaussianly-distributed variables $y^i$ with
zero mean and the same variance $C$ that we are wishing to learn about. Then
the sampling distribution for the $y^i$ is just a Gaussian,

$$p(y|C)d^{2l+1}y = \frac{d^{2l+1}y}{(2\pi C)^{(2l+1)/2}}e^{-\sum_i \frac{y^i^2}{2C}}$$  \hspace{1cm} (14)

and we can see that a sufficient statistic $\hat{C}$,

$$\hat{C} = \frac{1}{2l+1} \sum_i y^i^2,$$  \hspace{1cm} (15)

exists with sampling distribution

$$p(\hat{C}|C)d\hat{C} \propto \frac{\hat{C}^{l-1/2}d\hat{C}}{C^{l+1/2}}e^{-(l+1/2)\hat{C}/C}.$$  \hspace{1cm} (16)

The associated minus-log-likelihood, normalized to zero at its minimum, is

$$S_{true} = (l + 1/2) \left( \frac{\hat{C}}{C} + \log \frac{C}{\hat{C}} - 1 \right),$$  \hspace{1cm} (17)

where we have dropped a $1/\hat{C}$ which will not affect the change in $S$ with respect
to $C$. Let us apply our method to this problem. We shall use $\hat{C}$ for our $x$, and
choose to work to the lowest order possible, only constraining $\hat{C}$. From Eq. (14)
we can calculate the mean and variance of $\hat{C}$:

$$\langle \hat{C} \rangle = C,$$  \hspace{1cm} (18)

$$\langle \langle \hat{C}^2 \rangle \rangle = \frac{2}{2l+1}C^2.$$  \hspace{1cm} (19)

Substituting in to Eq. (13), we have

$$\frac{\partial S}{\partial C} = - \left( \frac{\hat{C}}{C} - 1 \right) \frac{2l+1}{2C^2}$$  \hspace{1cm} (20)

and integrating this up actually reproduces the exact result (17)!

It is informative to repeat this exercise to the next level in approximation,
considering constraining both $\langle \hat{C} \rangle$ and $\langle \langle \hat{C}^2 \rangle \rangle$, requiring knowledge of up to the
fourth cumulant of $\hat{C}$. One again recovers the exact result, the additional terms cancelling in the formula for $\partial S/\partial C$.

The form (16) of the sampling distribution for $\hat{C}$ is linear in $\hat{C}$ in the exponent. Hence it is expressible exactly with only a finite number of terms in the form (5) that the scheme assumes, explaining why the procedure does so well in this case.

3.2 Correlated Power Spectra Example

The next case to consider is when (14) is generalised for $y$ to become a vector of components, between which cross-correlations may be present. Then the sampling distribution becomes

$$p(y|C)d^{2l+1}y = \frac{d^{2l+1}y}{|2\pi C|^{(2l+1)/2}}e^{-\frac{1}{2} \sum_i y_i^T C^{-1} y_i},$$

with $C$ being the covariance matrix for the components of $y$. The components of the power spectra:

$$\hat{C} \equiv \frac{1}{2l+1} \sum_i y_i y_i^T$$

are again seen to be sufficient statistics for inferences about $C$.

Again, from knowledge of $\langle \hat{C}_{ij} \rangle$ and $\langle \langle \hat{C}_{ij} \hat{C}_{kl} \rangle \rangle$ as a function of the model our procedure recovers the true form of the likelihood:

$$S_{true} = \left( l + 1/2 \right) \left( \text{tr} C^{-1} \hat{C} + \log \frac{|C|}{|\hat{C}|} - 1 \right).$$

Again, we only need the linear constraint; repeating the procedure to quadratic order yields the same result. One can check explicitly that the moments of $\hat{C}$ satisfy Eq. (50) of Appendix C, as needed to get both the first and second moments exactly right with only the linear constraint.

3.3 Cross-Spectrum Example

Our final example is more challenging and might be considered a non-trivial test of the scheme. Taking the case above, for a two-component vector, we may write $C$ as

$$C = \begin{pmatrix} C + N_{11} & C \\ C & C + N_{22} \end{pmatrix}$$

and assume we are interested in making inferences about $C$. (For example, we may imagine the two components to be measurements of the same underlying field contaminated with independent Gaussian noise.) We may not know the noise levels $N_{11}$ and $N_{22}$ well enough to trust using them in a full likelihood using all the components of $C$. Instead, we may try and build a likelihood using the cross-spectrum $\hat{C}_{12}$ alone. Such a likelihood will hopefully be less at risk of bias in inferences about $C$. Actually, an analytic expression for the sampling
distribution for \( \hat{C}_{12} \) is known (see [4] for a recent use in the context of the CMB) which we can use to compare our approximate likelihoods to.

In Fig. 1 we show the distribution of \( \hat{C}_{12} \) for 10,000 realizations and compare this to the aforementioned analytic result.

Given the Gaussianity of the \( y \)'s, we can compute cumulants of the cross spectrum:

\[
\begin{align*}
\langle \hat{C}_{12} \rangle &= C, \\
(2l + 1)\langle \langle \hat{C}_{12}^2 \rangle \rangle &= C^2 + (C + N_{11})(C + N_{22}), \\
(2l + 1)^2\langle \langle \hat{C}_{12}^4 \rangle \rangle &= 2C^4 + 6C(C + N_{11})(C + N_{22}), \\
(2l + 1)^3\langle \langle \hat{C}_{12}^6 \rangle \rangle &= 6(C^6 + (C + N_{11})^2(C + N_{22})^2 \\
&\quad + 6C^2(C + N_{11})(C + N_{22}))
\end{align*}
\]

and so on. Using such cumulants we can numerically integrate up (13) for a selection of degrees of approximation (linear to quartic, requiring from up to quadratic to up to 8th order cumulants) and for a variety of instructive data “realizations”. Indeed, one does well to remember that some data point could be well into the tail of the sampling distribution, particularly for multi-dimensional data. Therefore it is important to check the validity of a likelihood approximation for reasonable models when some of the data is rare. Shown in Figs. 2, 3 and 4 are posteriors for \( C \) (assuming a uniform prior on \( C \)) for \( C = -1.2, 0.8 \) and 4.0 respectively. It is interesting to note how well the approximations work, even for very rare data values. For the low tail value, the basic linear approximation behaves qualitatively correctly for plausible models, and as the degree
Figure 2: Illustration of how the method works when the data value $\hat{C} = -1.2$ comes from the low tail of the sampling distribution, using model parameters as in Fig. 1. Different levels of approximation, coming from fitting up to the first, second, third and fourth moments, are shown, along with the analytic result.

As the approximation increases, the approximation approaches the true posterior. For the high tail value and particularly the middle value, even the linear approximation works relatively well.

Figure 3: As for Fig. 2 but when the data value $\hat{C} = 0.8$ comes from the middle of the sampling distribution, close to the underlying model value of $C = 1$. 
Figure 4: As for Fig. 2 but when the data value $\hat{C} = 4$ comes from the high tail of the sampling distribution.

4 Conclusion and Further Work

The technique presented here has some particular strengths:

**Theoretically-underpinned** The principle of maximum entropy ensures that the procedure uses the information it is given and makes minimal assumptions beyond that.

**Calculation-based** The approximation nowhere requires the use of simulations, rather it requires the calculation of cumulants (though one could indeed numerically estimate some of these, assuming a sufficient number of simulations are available, to use in the scheme if desired).

**Extensible** By looking for any change in the distribution as one adds in further constraints, one can build up a feel of when the approximation is “good enough”. (Tests of the scheme against a limited number of realistic simulations can empirically build confidence in the approximation also.)

For multi-dimensional problems, it would be useful to understand the error in the log-likelihood approximation in more detail coming from the potential path-dependence of the result in the parameters plane. If this error could be estimated to be small it might be possible then, for example, to safely use a linear approximation instead of a quadratic one (even though the argument given in Appendix C suggests that the latter should be more generally applicable). A complementary step would be to develop options for manipulating higher cumulants in order to improve the analyticity of the approximation.

Applications to CMB analysis with multi-dimensional data and tests against simulations will be presented in [8].
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A Complementary Motivation for Matching Moments

Section 2 derives an approximate sampling distribution using maximum entropy, using Lagrange multipliers to enforce the matching of the moments of this approximate distribution with those calculated for the underlying one. Here we present a complementary motivation for matching moments. The starting point is the Kullback-Leiber divergence

$$D_{KL}(p, q) = -\int d^n x \ p(x) \log \frac{q(x)}{p(x)}$$

which quantifies how different the probability distribution $q(x)$ is from $p(x)$. $D_{KL}(p, q)$ can be thought of as the mean of the difference in minus log probability between the approximation $q(x)$ and the true $p(x)$ with the average taken over $p(x)$, and is minimized for $q(x) = p(x)$ (see also the discussion in [9]). Now, imagine we wish to approximate $p(x)$ with a form for $q(x)$ compatible with Eq. (5), i.e.

$$q(x) = p_0(x)e^{-\alpha - \lambda_i x^i - \lambda_{ij} x^i x^j - \cdots}$$

with a finite polynomial in the $x^i$ in the exponent. Here we think of $\alpha$ and the $\lambda_i, \lambda_{ij}, \ldots$ as parameters that we shall vary to minimize $D_{KL}(p, q)$ subject to the constraint that $q(x)$ is normalized. Substituting into (29), we have:

$$D_{KL}(p, q) = \int d^n x \ p(x) \left( \alpha + \lambda_i x^i + \lambda_{ij} x^i x^j + \cdots + \log \frac{p(x)}{p_0(x)} \right).$$

We can impose the normalization constraint with a Lagrange multiplier $\beta$. Varying with respect to $\alpha$

$$\frac{\partial}{\partial \alpha} \left( D_{KL}(p, q) - \beta \int d^n x q(x) \right) = 0$$

$$\Rightarrow \int d^n x \ p(x) - \beta \int d^n x q(x) = 0$$

shows we must take $\beta = 1$. Varying with respect to $\lambda_i \ldots$ and substituting in $\beta = 1$ then tells us that

$$\int d^n x \ p(x)x^i \ldots x^j - \int d^n x q(x)x^i \ldots x^j.$$

Thus after minimization the moments of the $x^i$ that appear in the exponent in (30) computed for the approximate distribution must match those computed for
the underlying distribution. (Note that it is not necessary for the underlying distribution to be explicitly given, only that its appropriate moments be known.)

So, finding the broadest probability distribution consistent with constraints on certain moments yields the same distribution as that coming from minimizing the Kullback-Leibler divergence of the associated functional form from the unknown underlying distribution.

### B Solving for the Lagrange Multiplier Derivatives

Moments/cumulants of the X and their derivatives are derivable from moments/cumulants of the x and their derivatives. Indeed, cumulants of the x are typically the things that are most straightforwardly obtainable from parametric models (or simulations). Hence it is useful to be able to relate X-based quantities to x-based ones. By inspection of Eq. (7), we see that

\[
\frac{\partial Z}{\partial \lambda_{ij}} = -\frac{\partial^2 Z}{\partial \lambda_i \partial \lambda_j},
\]

(35)

\[
\frac{\partial Z}{\partial \lambda_{ijk}} = \frac{\partial^3 Z}{\partial \lambda_i \partial \lambda_j \partial \lambda_k},
\]

(36)

or generally:

\[
-\frac{\partial}{\partial \lambda_{i...j}} \ldots - \frac{\partial}{\partial \lambda_{p...q}} Z = -\frac{\partial}{\partial \lambda_i} \ldots - \frac{\partial}{\partial \lambda_j} \ldots - \frac{\partial}{\partial \lambda_p} \ldots - \frac{\partial}{\partial \lambda_q} Z.
\]

(37)

This allows us to obtain general moments of the X in terms of the moments of the x, giving us a straightforward route to obtaining the cumulants of the X needed for Eq. (13).

The relation (37) above suggests an alternative way of getting at the derivatives of the Lagrange multipliers with respect to the parameters: we may start with the cumulants of the x, and then differentiate them with respect to the parameters q. For example, with x distributed according to Eq. (7), one has

\[
\frac{\partial \langle x^i x^j \rangle}{\partial q^a} = \frac{\partial}{\partial \lambda_r} \left( \frac{\partial^2 \log Z}{\partial \lambda_j \partial \lambda_i} \right) \frac{\partial \lambda_r}{\partial q^a} +
\]

\[
\frac{\partial}{\partial \lambda_{rs}} \left( \frac{\partial^2 \log Z}{\partial \lambda_j \partial \lambda_i} \right) \frac{\partial \lambda_{rs}}{\partial q^a} +
\]

\[
\ldots.
\]

(38)

Using commutativity of partial derivatives, the log Z derivative in the second term for example may then be rewritten as:

\[
\frac{\partial^2}{\partial \lambda_j \partial \lambda_i} \frac{\partial \log Z}{\partial \lambda_{rs}}
\]

(39)
and then we may use
\[
\frac{\partial \log Z}{\partial \lambda_{rs}} = 1 \quad \text{and} \quad \frac{\partial Z}{\partial \lambda_{rs}} = -\frac{1}{Z} \frac{\partial \log Z}{\partial \lambda_{s}} \frac{\partial \log Z}{\partial \lambda_{r}}
\]
(40)
\[
= -\frac{1}{Z} \frac{\partial \log Z}{\partial \lambda_{s}} \left( Z \frac{\partial \log Z}{\partial \lambda_{r}} \right) \quad \text{(41)}
\]
\[
= -\frac{\partial \log Z}{\partial \lambda_{s}} \frac{\partial \log Z}{\partial \lambda_{r}} - \frac{\partial^2 \log Z}{\partial \lambda_{s} \partial \lambda_{r}} \quad \text{(42)}
\]
to express the coefficient of \( \frac{\partial \lambda_{rs}}{\partial q_{a}} \) in terms of cumulants of \( x \). With \( \kappa^{i...j} \) denoting \( \langle\langle x^{i}...x^{j}\rangle\rangle \) derived from a distribution of the form in Eq. (7), we have:
\[
\begin{pmatrix}
\kappa^{i} \\
\kappa^{(ij)} \\
\vdots 
\end{pmatrix}_{,a} = -\begin{pmatrix}
\kappa^{ip} \\
\kappa^{jp} + 2\kappa^{(p}\kappa^{q)} \\
\vdots 
\end{pmatrix} \begin{pmatrix}
\lambda_{p} \\
\vdots 
\end{pmatrix}.
\]
(43)
If we let \( \kappa \) denote the vector \( (\kappa^{i}, \kappa^{(ij)}, ...)^T \) of cumulants of the \( x \) and \( \lambda \) denote the vector \( (\lambda_{p}, \lambda_{(pq)}, ...)^T \) of Lagrange multipliers, then we may write
\[
\kappa_{,a} = -M_{,a}
\]
(44)
defining \( M \) to be the big matrix on the right hand side of Eq. (43). Assuming \( M \) is invertible, we thus have
\[
\lambda_{,a} = -M^{-1}\kappa_{,a},
\]
(45)
to be compared with Eq. (12).

\section*{B.1 Cumulants as Parameters}
It is often natural to choose some of the constrained cumulants as the parameters themselves. For example, one might imagine that some underlying theory determines all of the cumulants of the \( x^{i} \) in terms of a small set of parameters. One might wish to compare different underlying models with different fundamental parameterizations against the same data set. In this case one might first construct a generic likelihood in which the cumulants of the \( x^{i} \) are set directly. For example, if one uses unbiased estimators of parameters as the \( x^{i} \), then by construction their first moments are the parameters. The higher cumulants might then be functions of the same parameters. The higher cumulants might then be functions of the same parameters.

\section*{B.2 Expanding around a Gaussian}
One can take the second derivative of Eq. (45) to find
\[
\lambda_{ab} = M^{-1}M_{,b}M^{-1}\kappa_{,a} - M^{-1}\kappa_{,ab}
\]
(46)
and hence expand the action to second order around a fiducial model. A natural choice for a fiducial model is a gaussian. Then, in conjunction with the suggestions above about using cumulants as the parameters themselves, we can compute the change in the action to second order in the higher cumulants \( \kappa^{ijk} \) and \( \kappa^{ijkl} \). The \( M \) matrix is upper-diagonal for a gaussian and its inverse can be analytically computed. This expansion may be compared to an Edgeworth expansion.
C Consistency of Approximation

Eq. (43) allows one to begin to see for which circumstances a mooted approximation is possible or not. Our procedure consists of setting some of the cumulants $\kappa^I$ as functions of the parameters as desired, and then hoping we can find a set of corresponding $\lambda$ and other cumulants such that Eq. (43) can be consistent. (There is some freedom in the cumulants corresponding to varying the “prior” term $p_0(x).$)

Imagine for example we want a situation in which the dimension of the data matches the number of model parameters, and we think that a likelihood constructed only from constraints on the means of the $x^i$ should suffice. Then only the first (block-)column of the “big” matrix in Eq. (43) is relevant:

$$
\begin{pmatrix}
\kappa^i \\
\kappa^{ij} \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\kappa^{ijp} \\
\kappa^{ijpq} + 2\kappa^{i(pK^q)} \\
\vdots
\end{pmatrix} \cdot \begin{pmatrix}
\lambda_p \\
\lambda_{(pq)} \\
\vdots
\end{pmatrix},
$$

(47)

Given that we can compute covariances, the first (block-)row of Eq. (47) then allows us to solve for some putative $\lambda_{p,a}$. However, the second (block-)row of Eq. (47) also needs to be satisfied, and then the third and so on. One consistent solution, for example, occurs when the covariance is independent of the model and cumulants higher than second order vanish. In one dimension, for arbitrary mean and variance, we can actually successively determine higher and higher cumulants to formally solve all rows of Eq. (47).

A counting argument suggests a general solution however is impossible in dimensions greater than one. First, note that the cumulant with $k$ factors, each one of $n$ variables, has $n(n+1) \cdots (n+k-1)/k!$ independent terms. Then the $k^{th}$ block-row involves $n \cdot n(n+1) \cdots (n+k-1)/k!$ numbers on the left, the $n$ possible derivatives of each of the terms of the $k^{th}$ order cumulant. But the $k^{th}$ block-row of the big matrix has only $n(n+1) \cdots (n+k)/(k+1)!$ numbers to vary, coming from the $k+1^{th}$ order cumulant. This is not enough (for $n > 1$), being a factor of $(n+k)/(k+1)/n$ too small. So, unless appropriate functional relations exist between the cumulants of the model, this form of desired likelihood is unattainable.

By a similar counting argument, allowing the approximate likelihood to involve quadratic constraints does not allow for solutions either. The second (block-)column introduces the $k+2^{th}$ power cumulant, with its $n(n+1) \cdots (n+k+1)/(k+2)!$ numbers, into play,

$$
\begin{pmatrix}
\kappa^i \\
\kappa^{ij} \\
\vdots
\end{pmatrix} = \begin{pmatrix}
\kappa^{ijp} \\
\kappa^{ijpq} + 2\kappa^{i(pK^q)} + 2\kappa^{i(pK^q)}j \\
\vdots
\end{pmatrix} \cdot \begin{pmatrix}
\lambda_p \\
\lambda_{(pq)} \\
\vdots
\end{pmatrix},
$$

(48)

This is a factor $(n+k)(n+k+1)/n/(k+1)/(k+2)$ relative to that needed to match the left hand side, for the $k^{th}$ (block-)row. So, for sufficiently large $k$, $\sim \sqrt{n}$, there is not enough freedom available in the cumulant. Turning this around though, we might only expect difficulties to become acute below some dimensionality up to a given order in the cumulant. As the quadratic approximation needs up to the fourth cumulant, one might suspect the scheme has a chance of working reasonably well for $n \geq 20$. 

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For an alternative perspective, consider Eq. (10) again. If the right hand side is indeed to be the derivatives of analytic functions, we need:

\[
(\lambda_a)_b = (\lambda_b)_a
\]
i.e.

\[
\left(\langle (XX^T)^{-1}X \rangle_a\right)_b = \left(\langle (XX^T)^{-1}X \rangle_b\right)_a
\]

(49)
or

\[
\left(\langle XX^T \rangle_b \langle (XX^T)^{-1}X \rangle \right)_a = \left(\langle XX^T \rangle_a \langle (XX^T)^{-1}X \rangle \right)_b
\]

(50)
to hold. Some of the higher cumulants might then better be chosen in such a way as to satisfy Eq. (50), rather than to be equal to those calculated from the underlying theory.

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