Partition function approach to non-Gaussian likelihoods: Formalism and expansions for weakly non-Gaussian cosmological inference

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ABSTRACT
Non-Gaussian likelihoods, ubiquitous throughout cosmology, are a direct consequence of nonlinearities in the physical model. Their treatment requires Monte-Carlo Markov-chain or more advanced sampling methods for the determination of confidence contours. As an alternative, we construct canonical partition functions as Laplace-transforms of the Bayesian evidence, from which MCMC-methods would sample microstates. Cumulants of order $n$ of the posterior distribution follow by direct $n$-fold differentiation of the logarithmic partition function, recovering the classic Fisher-matrix formalism at second order. We connect this approach for weakly non-Gaussianities to the DALI- and Gram-Charlier expansions and demonstrate the validity with a supernova-likelihood on the cosmological parameters $\Omega_m$ and $w$. We comment on extensions of the canonical partition function to include kinetic energies in order to bridge to Hamilton Monte-Carlo sampling, and on ensemble Markov-chain methods, as they would result from transitioning to macrocanonical partition functions depending on a chemical potential. Lastly we demonstrate the relationship of the partition function approach to the Cramér-Rao boundary and to information entropies.

Key words: redshift-luminosity data – dark energy – statistics

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In physical systems, Monte-Carlo Markov-chain methods and in particular the the Metropolis-Hastings algorithm (Metropolis 1953) provide an efficient and physically transparent way of sampling microstates from an ensemble, and became indispensable in simulations in statistical physics. They are an efficient numerical tool to compute thermodynamical quantities from a model of the microscopic dynamics of a system. As such, they provide an alternative to the computation of partition functions: Even though they contain the complete physical information of a system in thermodynamic equilibrium and allow the derivation of all state variables and their relationships, their analytical computation is only technically possible for reasonably simple systems, for instance for ideal gases, but fails for systems with interactions, the Ising-model in three dimensions being a famous example. Sampling with the Metropolis-Hastings algorithm generates microstates with a relative occurrence given by the Boltzmann-factor $p \propto \exp(-\beta e)$ with $\beta$ being the inverse temperature and $e$ the energy difference of the states, effectively sampling from the canonical ensemble.

In parallel, sampling from a posterior distribution with a MCMC-method has become a central tool in cosmology (starting from Lewis & Bridle 2002). There, MCMC-sampling is used to explore the shape of likelihoods as it offers tremendous computational advantages over simple grid-based evaluations, in particular in highly dimensional parameter spaces. Technically, the Metropolis-Hastings algorithm generates parameter tuples $\theta^*$ as samples which occur at a probability which is proportional to the posterior distribution $p(\theta|y)$ given the experimental data $y$. For this purpose, one requires the logarithmic likelihood, or in the case of a Gaussian error model, the $\chi^2$-functional, which itself combines the information about the data prediction for a given set of model parameters $\theta^*$, as well as the magnitude of the experimental error and the statistical independence of the data in the form of a data covariance.

A prior distribution $\pi(\theta) \propto \exp(-\phi(\theta))$, reflecting the state of knowledge on the parameters $\theta$ before the measurement, can be incorporated by replacing $\chi^2(y|\theta)/2$ with $\chi^2(y|\theta)/2 + \phi(\theta)$. The exponential relationship $\mathcal{L} \propto \exp(-\chi^2(y|\theta)/2)$ between $\chi^2(y|\theta)$ and the likelihood $\mathcal{L}$ is completely analogous to the probability $p$ for a microstate with energy $\Delta V$ to occur in statistical physics, where a thermal bath is able to provide this energy at the Boltzmann probability $p = \exp(-\beta \Delta V)$. The fact that in statistical inference the Metropolis-Hastings algorithm samples microstates from the partition function can therefore be illustrated with physical analog: Effectively, $V(y) = \chi^2(y|\theta)/2 + \phi(\theta)$ plays the role of a potential, on which a particle with coordinates $\theta^*$ performs a thermal random walk. Then, the probability of finding the particle at a certain location corresponds to the posterior distribution $p(\theta|y) \propto \exp(-\chi^2(y|\theta)/2 - \phi(\theta))$ and is numerically evaluated as the sample density in $\theta^*$.

As cosmological likelihoods have in general non-Gaussian shapes and are joint distributions in a large number of parameters with possibly strong degeneracies between them, analytical methods are difficult to employ beyond the second order. As soon as a Gaussian approximation to the likelihood is permissible, though, the Fisher-formalism can play its strength (Tegmark et al. 1997), and has found applications throughout cosmology (for instance, Bassett et al. 2009, 2011; Coe 2009; Elsner & Wandelt 2012; Refregier et al. 2011; Amara & Kitching 2011; Raveri et al. 2016). Extensions to the Fisher-matrix formalism including higher-order derivatives for dealing with non-Gaussian likelihoods have been constructed that are able to capture non-Gaussian shapes of distributions (Wolz et al. 2012; Giesel et al. 2021; Schäfer & Reischke 2016; Sellentin et al. 2014) and that can treat systematic errors in addition to statistical errors (Amara & Refregier 2007; Taburet et al. 2009; Kitching & Taylor 2011; Schäfer & Heisenberg 2012; Kitching et al. 2009; Loverde et al. 2007).

Motivated by the paper by Jaynes (1957), who clarified that thermodynamics is in reality a theory of information, we aim to continue to use ideas from thermodynamics in statistical inference and to establish analytical methods akin to the partition functions of statistical physics in order to understand the relation between the physical model and the shape of the likelihood. For this purpose, we summarise the construction of canonical partition functions from which a MCMC-algorithm would sample microstates in Sect. 2. The recovery of the conventional Fisher-formalism in this formalism is demonstrated in Sect. 3, where we show es well the unbiasedness of Gaussian likelihoods and the Cramer-Rao limit. The central analytical result of our paper is summarised in Sect. 4, where we expand the partition function approach beyond the realm of linear models to non-Gaussian posterior distributions and bridge between the DALI-expansion (Sellentin et al. 2014) and the more conventional Gram-Charlier parameterisation. In Sect. 5 we show how information entropies, in particular the Shannon-entropy, are directly from Monte-Carlo Markov-chain samples and from differentiation of the partition function are equivalent, and construct an analytic approximation of the posterior distribution with a Gram-Charlier-series. Finally, a discussion in Sect. 7 concludes the article.

Throughout the paper, we adopt the summation convention and make the choice to denote parameter tuples $\theta^*$ and data tuples $y^*$ as vectors with contravariant indices; Greek indices are reserved for quantities in parameter space and Latin indices for objects in data space. With these conventions, the data covariance $C^{ij} = \langle y^i y^j \rangle - \langle y^i \rangle \langle y^j \rangle$ is a contravariant tensor with $C_{ji}$ as its covariant inverse, $C^{ij}C_{jk} = \delta^i_k$. Similarly, the Fisher-matrix $F_{ij}$ is a covariant tensor, allowing to write quadratic forms like $\chi^2 = F_{ij} \theta^i \theta^j$, and to define an inverse $F^{-\theta^i}_j$, $F_{ij} F^{ji} = \delta^i_j$. For an example application in cosmology, we consider supernova-constraints in the frame of a flat wCDM-family of FLRW-cosmologies with the matter density $\Omega_m$ and the dark energy equation of state parameter $w$ as parameters. Flatness implies that the density parameter of dark energy is given by $1 - \Omega_m$, and it suffices for demonstration purposes to assume a $w$ that is constant in time.
2 PARTITION FUNCTIONS AND METROPOLIS-HASTINGS SAMPLING

The Bayes-theorem

\[ p(\theta|y) = \frac{L(y|\theta)p(\theta)}{p(y)} \]

is the foundation of inference as it relates the posterior distribution \( p(\theta|y) \) of the model parameter(s) \( \theta \) given the data \( y \) to the likelihood \( L(y|\theta) \) and the prior distribution \( p(\theta) \). The posterior distribution is properly normalised by the Bayesian evidence \( p(y) \),

\[ p(y) = \int d\theta L(y|\theta)p(\theta). \]

For distributions from the exponential family, \( L(y|\theta) \propto \exp(-\chi^2(y|\theta)/2) \) with the \( \chi^2 \)-functional and \( p(\theta) \propto \exp(-\phi(\theta)) \) with the logarithmic prior \( \phi \) one can reformulate the evidence,

\[ p(y) = \int d\theta \exp \left( -\frac{1}{2} \chi^2(y|\theta) + \phi(\theta) \right). \]

Enabling Laplace-transforms by introducing sources \( J_\alpha \) and scaling the exponent with an inverse temperature \( \beta \) leads to an expression reminiscent of a canonical partition function

\[ Z[\beta, J_\alpha] = \int d\theta \exp \left( -\beta \frac{1}{2} \chi^2(y|\theta) + \phi(\theta) \right) \exp(\beta J_\alpha \theta^\alpha) \]

where the (inverse) temperature \( \beta \) and the sources \( J_\alpha \) play the role of state variables.

Then, the cumulants of the posterior distribution of order \( n \) follow from \( n \)-fold derivation of with respect to the sources \( J_\alpha \), i.e. the expectation value is given by

\[ \kappa^n = \langle \theta^n \rangle = \frac{\partial}{\partial J_\alpha} \left( \frac{1}{\beta} \ln Z[\beta, J_\alpha] \right) \bigg|_{J_\alpha=0}. \]

evaluated at \( J_\alpha = 0 \), as well as the covariance by

\[ \kappa^{n \alpha \beta} = \langle \theta^n \theta^\alpha \theta^\beta \rangle - \langle \theta^n \rangle \langle \theta^\alpha \rangle \langle \theta^\beta \rangle = \frac{\partial^2}{\partial J_\alpha \partial J_\beta} \left( \frac{1}{\beta} \ln Z[\beta, J_\alpha] \right) \bigg|_{J_\alpha=0}. \]

and at higher order corresponding to skewness

\[ \kappa^{n \alpha \beta \gamma} = \langle \theta^n \theta^\alpha \theta^\beta \theta^\gamma \rangle - \langle \theta^n \rangle \langle \theta^\alpha \rangle \langle \theta^\beta \rangle \langle \theta^\gamma \rangle - \langle \theta^n \theta^\alpha \rangle \langle \theta^\beta \rangle \langle \theta^\gamma \rangle + 2 \langle \theta^n \rangle \langle \theta^\alpha \rangle \langle \theta^\beta \rangle = \frac{\partial^3}{\partial J_\alpha \partial J_\beta \partial J_\gamma} \left( \frac{1}{\beta} \ln Z[\beta, J_\alpha] \right) \bigg|_{J_\alpha=0}, \]

and a non-Gaussian kurtosis

\[ \kappa^{n \alpha \beta \gamma \delta} = \langle \theta^n \theta^\alpha \theta^\beta \theta^\gamma \theta^\delta \rangle - \langle \theta^n \theta^\alpha \theta^\beta \rangle \langle \theta^\gamma \theta^\delta \rangle - \langle \theta^n \theta^\alpha \theta^\gamma \rangle \langle \theta^\beta \theta^\delta \rangle - \langle \theta^n \theta^\beta \theta^\gamma \rangle \langle \theta^\alpha \theta^\delta \rangle = \frac{\partial^4}{\partial J_\alpha \partial J_\beta \partial J_\gamma \partial J_\delta} \left( \frac{1}{\beta} \ln Z[\beta, J_\alpha] \right) \bigg|_{J_\alpha=0}, \]

all taken at \( J_\alpha = 0 \) after differentiation; the dependence on temperature \( \beta \) is lost due to the differentiation operating on \( \ln Z[\beta, J_\alpha] \). It is remarkable that differentiation of the partition function yields the expectation values of the parameters \( \langle \theta^n \rangle \) and not the best-fit values.

Commonly, one uses Monte-Carlo Markov-chain methods such as the Metropolis-Hastings algorithm to sample microstates which correspond to parameter tuples \( \theta^\alpha \) from the partition function \( Z \). From these samples one can compute estimates for the cumulants, or equivalently, of the moments, as the two are related by Faa di Bruno’s formula (Johnson 2002). Here, we advocate instead that the cumulants up to the order of non-Gaussianity that one decides to truncate the expansion, are given by possibly numerical differentiation of the logarithmic partition function, and that this approach yields an analytic approximation to the posterior distribution \( p(\theta|y) \).

3 (NON)LINEAR MODELS AND (NON)GAUSSIAN LIKELIHOODS

3.1 Linear models

Linear models together with a Gaussian error process on the data have particularly convenient properties in data analysis. The \( \chi^2 \)-functional for data \( y \) with an inverse data covariance \( C_{ij} \), resulting from \( C_{ij} = (y'y') \langle y'y \rangle \), for a model that is linear in the parameters, \( y'_{\text{model}} = A'y^\theta \), is given by a quadratic form

\[ \chi^2 = (y' - A'y^\theta)^T C_{ij} (y' - A'y^\theta) = y'C_{ij} y - 2 y'C_{ij} A'_i \theta^\alpha + A'_i A'_j \theta^\alpha \theta^\beta = c - 2 Q_{ij} \theta^\alpha + F_{ij} \theta^\alpha \theta^\beta. \]

The quadratic term \( A'_i A'_j \theta^\alpha \theta^\beta \) is identified as the Fisher-matrix \( F_{ij} \), with the Jacobian \( A'_i = \partial y'/\partial \theta^\alpha \) taking care of the change of basis between parameter space and data space. Consequently, likelihoods of linear models are Gaussian in the data as well as in the parameters,

\[ L(y|\theta) \propto \exp \left( -\frac{1}{2} \chi^2(y|\theta) \right). \]
and unless the prior \( \pi(\theta) \) deviates from being constant or Gaussian itself, the posterior distribution \( p(\theta|y) \) will be Gaussian, too.

The best-fit parameter tuple \( \tilde{\theta} \) is readily computed by minimisation of \( \chi^2 \) as a function of the parameters \( \theta^r \).

\[
\frac{\partial}{\partial \theta^r} \chi^2 = -2Q_{\beta,\alpha} \frac{\partial \theta^r}{\partial \theta^r} + F_{\alpha,\beta} \frac{\partial \theta^r}{\partial \beta} \theta^r \theta^r \theta^r = -2Q_{\beta,\alpha} + F_{\alpha,\beta} \theta^r \theta^r = 0 \quad \rightarrow \quad \tilde{\theta} = F^{\alpha,\beta} Q_{\alpha,\beta} = \Lambda_{\alpha,\beta} \theta^r
\]

(11)

recovering estimation with the inverse Jacobian \( \Lambda_{\alpha,\beta} = \partial \theta^r / \partial \theta^r \): In fact, the estimate is unbiased because the true model \( \theta^r \) would generate the data \( y = A^r \theta^r \), such that \( \theta^r = A^r A^r \theta^r = \theta^r \).

Constructing the partition function for such a linear model amounts to

\[
Z(\beta, J_0) = \int dy \exp \left( \frac{\beta}{2} F_{\alpha,\beta} \theta^r \theta^r + \beta Q_{\alpha,\beta} \theta^r \right) \exp (\beta J_0 \theta^r),
\]

(12)

where the Gaussian integrals can be carried out to yield

\[
Z(\beta, J_0) = \sqrt{\frac{2\pi}{\beta}} \frac{1}{\det(F)} \exp \left( \frac{1}{2} F_{\alpha,\beta} (J_0 + Q_{\alpha,\beta}) \right) \exp \left( \frac{1}{2} F_{\alpha,\beta} J_0 \right)
\]

(13)

with the inverse Fisher-matrix \( F^{\alpha,\beta} \). Here, we have dropped the irrelevant normalisation \( \exp(-c/2) \) of the likelihood and disregarded any prior \( \pi(\theta) \) for simplicity.

The expectation value of the posterior distribution, or equivalently, the first cumulant \( \kappa^\mu \) follows directly from differentiation of \( \ln Z(\beta, J_0) / \beta \), evaluated at \( \beta_j = 0 \), keeping in mind that the Fisher-matrix and its inverse are symmetric,

\[
\kappa^\mu = \left. \frac{\partial}{\partial \mu} \left( \frac{1}{\beta} \ln Z(\beta, J_0) \right) \right|_{\beta_j} = \left. \frac{F^{\alpha,\beta} J_0}{2} \left( \delta_{\alpha,\beta} \delta^\mu_{\gamma} + \delta_{\alpha,\gamma} \delta^\mu_{\beta} \right) \right|_{\beta_j} = F^{\mu,\gamma}
\]

(14)

and because one recovers the result from the direct calculation in eqn. (11): For a symmetric distribution, most likely value and expectation value coincide with the true parameter value: \( \kappa^\alpha = \langle \theta^\alpha \rangle = \tilde{\theta}_\alpha \), and incidentally \( \theta^\alpha = \theta^r \), too, as a reflection of the Gaussian-Markov theorem in this formalism.

The second cumulant \( \kappa^{\mu,\nu} \), corresponding to the parameter covariance, is computed as

\[
\kappa^{\mu,\nu} = \left. \frac{\partial^2}{\partial \mu \partial \nu} \left( \frac{1}{\beta} \ln Z(\beta, J_0) \right) \right|_{\beta_j} = \left. \frac{F^{\alpha,\beta} J_0}{2} \left( 2 \delta_{\alpha,\mu} \delta_{\nu,\beta} + \delta_{\alpha,\nu} \delta_{\mu,\beta} \right) \right|_{\beta_j} = F^{\mu,\nu}
\]

(15)

Consequently, as any higher-order cumulants are zero, the posterior distribution \( p(\theta|y) \) is necessarily Gaussian, with the Fisher-matrix as the inverse covariance and is centered on the expectation value:

\[
p(\theta|y) = \sqrt{\frac{\det(F)}{2\pi}} \exp \left( -\frac{1}{2} F_{\mu,\nu} (\theta^\mu - \kappa^\mu)^2 \right),
\]

(16)

because \( F_{\mu,\nu} F^{\nu,\rho} = F_{\mu,\rho} \kappa^{\rho,\nu} = \delta_{\mu,\rho} \).

### 3.2 Cramér-Rao inequality

Generally, the (co)variance of posterior distributions \( p(\theta|y) \) is bounded from below by the inverse \( 1/F \) of the Fisher-information \( F \), as stated by the Cramér-Rao inequality,

\[
\kappa^{(2)} \geq \frac{1}{F}, \quad \text{with} \quad F = \left( \frac{\partial^2 \chi^2(\theta|y)}{\partial \theta^r \partial \theta^r} \right) / 2,
\]

(17)

averaged over the parameters \( \theta \), where the logarithmic likelihood \( \ln L \) corresponds for a Gaussian error process to \( -\chi^2/2 \). The partition-function formalism provides a way to derive this relationship because any cumulant of the posterior distribution is given by differentiation of \( \ln Z(\beta, J_0) / \beta \) with respect to the source terms \( J \) and because the partition function \( Z \) reflects the specific functional dependence of \( \chi^2(\theta|y) \) on the parameters \( \theta \) themselves. Therefore, it is sensible to ask whether there is a particular \( \chi^2(\theta|y) \) that minimises the variance for a fixed value of the Fisher information. Essentially, this amounts to carrying out a functional minimisation of \( \kappa^{(2)} \) with respect to \( \chi^2(\theta|y)/2 \):

\[
\delta \kappa^{(2)} = \delta \left( \theta^r - \langle \theta^r \rangle \right) \cdot \delta \chi^2(\theta|y)/2 = \delta \frac{\partial \chi^2(\theta|y)/2}{\partial \theta^r} \ln Z(\beta, J_0) \bigg|_{\beta_j} = \frac{\partial^2 \chi^2(\theta|y)/2}{\partial \theta^r \partial \theta^r} \ln Z(\beta, J_0) \bigg|_{\beta_j} = 0
\]

(18)

where we focus for now on unit temperature \( \beta = 1 \) and on the univariate case, for simplicity, as well as a constant prior distribution \( \pi(\theta) \).

Fixing the value of the Fisher information to \( F \), the expectation value of the distribution to \( \langle \theta \rangle \) and the normalisation to one can be done by incorporating three Lagrange-multipliers \( \alpha, \beta \) and \( \gamma \),

\[
\delta \kappa^{(2)} \rightarrow \delta \kappa^{(2)} + \alpha \delta \left( \frac{\partial}{\partial \theta^r} \chi^2(\theta|y)/2 \right) = F + \beta \delta \left[ \langle \theta^r \rangle - \mu \right] + \gamma \delta \left( \int d\theta^r \exp \left( \frac{\chi^2(\theta|y)/2}{2} \right) - 1 \right).
\]

(19)

Collecting all terms leads to the variation

\[
\int d\theta^r \exp \left( \frac{\chi^2(\theta|y)/2}{2} \right) \theta^r + 2\langle \theta^r \rangle \theta^r + \alpha \left( 2 \frac{\partial^2 \chi^2(\theta|y)/2}{\partial \theta^r \partial \theta^r} - \frac{\partial}{\partial \theta^r} \frac{\partial \chi^2(\theta|y)/2}{\partial \theta^r} \right) \theta^r + \beta \theta^r + \gamma \left( \frac{\chi^2}{2} \right) = 0
\]

(20)
using the relation $\delta((\theta^2)^2) = 2(\theta) \delta(\theta)$ and the fact that every term is proportional to $1/Z$, such that the term in the square brackets needs to vanish. Abbreviating the negative logarithmic likelihood as $q = \chi^2(\theta;\gamma)$ and using primes to denote the derivative with respect to $\theta$ yields the differential equation

$$\theta^2 - 2(\theta) \theta + \alpha(2q'' - q') + \beta \theta + \gamma = 0. \tag{21}$$

As a polynomial, the solution $q$ can only be consistent if its second derivative and the square of its first derivative do no generate powers of $\theta$ higher than 2. Therefore, a sensible ansatz would be

$$q = \chi^2(\theta;\gamma) = \frac{1}{2}F(\theta - \mu)^2 \tag{22}$$

which is readily shown to solve the variational problem with $\alpha = 1/F^2$, $\beta = 0$ and the (irrelevant) normalisation $\gamma = \mu - 2/F$. Substituting back into the expression for $\chi^2$ leads directly to the value $1/F$, in fulfilment of the Cramér-Rao inequality.

The multivariate case is slightly more complicated and requires $n$ individual Lagrange-multipliers $\beta^\nu$ for enforcing the means $\langle \theta^\nu \rangle$ of the distribution, replacing eqn. (21) by

$$\theta^\nu - ((\theta^\nu)^2 + \theta^\nu(\theta^\nu')) + \alpha n \sum \frac{\partial^2 q}{\partial q^\nu \partial q^\mu} + \beta \theta^\nu + \gamma = 0, \quad \text{with the definition} \quad F_{\nu\mu} = n \left( \frac{\partial^2}{\partial \theta^\nu \partial \theta^\mu} \chi^2(\theta;\gamma) \right). \tag{23}$$

Then, the same arguments as in the univariate case lead to a quadratic form

$$q = \chi^2(\theta;\gamma) = \frac{1}{2}F_{\nu\mu}(\theta^\nu - (\theta^\nu))(\theta^\nu - (\theta^\nu')). \tag{24}$$

In summary, the minimum variance for a fixed Fisher-information is realised by a quadratic $\chi^2(\theta;\gamma)$-functional, or equivalently, a Gaussian posterior distribution $p(\theta|y)$. Commonly, $\chi^2$ is a convex function of the parameters $\theta^\nu$, otherwise there can not be a global minimum for uniquely defining the best fitting parameters $\theta^\nu$. Consequently, the functional to be minimised is convex, too: $\exp(-\chi^2/2)$ is convex if $\chi^2$ is convex. Multiplying $\exp(-\chi^2)$ with strictly positive functions $q_{\nu'}$ or $\theta^\nu$ does not change convexity, which implies that the functional variation has yielded a minimum for the variance for a given Fisher information $F$.

### 3.3 Nonlinear models

Nonlinear models are notably more complicated: Neither is the $\chi^2$-functional quadratic in the parameters nor is the likelihood $L$ of Gaussian shape, simply because the function $y^\nu = A^\nu \theta^\nu$ with a constant $A^\nu$, or equivalently, because $\partial y^\nu / \partial \theta^\mu$ becomes a function of $\theta^\nu$ itself. But in the language of partition functions, this means that they are neither of Gaussian form, nor would the differentiations truncate after second order: The posterior distribution becomes genuinely non-Gaussian. But the cumulants of order $n$ with $n \geq 3$ remain computable, at least numerically, from the partition function. In this sense, the partition function formalism provides an approximation for non-Gaussian posterior distributions at a given order. At least for weak non-Gaussianities, which would be the case if a linearisation of the physical model over the allowed parameter space is applicable, the partition function can be decomposed into a Gaussian part and a non-Gaussian correction, written in terms of Hermite-polynomials, linking to the Gram-Charlier-expansion for weakly non-Gaussian distributions. From this moment on, we always assume a rescaling of the model such that the fiducial parameter values are zero, $\langle \theta^\nu \rangle = \kappa^\nu = 0$, simplifying the notation tremendously.

### 4 WEAKLY NON-GAUSSIAN LIKELIHOODS

#### 4.1 Higher cumulants

When introducing a weak non-Gaussianity, e.g. through introducing a model where the parameters are not quite linearly linked to the data the partition function factorizes into a Gaussian and a non-Gaussian part. The non-Gaussianity is introduced in the $\chi^2$-functional as

$$\chi^2 = \frac{1}{2}F_{\nu\mu} \theta^\nu - \sum_{k=3}^{N} \frac{1}{k!} C_{\mu_1 \ldots \mu_k} \theta^{\mu_1} \ldots \theta^{\mu_k}, \tag{25}$$

i.e. with a Taylor-expansion of $\chi^2$ beyond quadratic order, as it would naturally arise in nonlinear models. The coefficients in the Taylor expansion are assumed to be small compared to the entries of the covariance matrix $F_{\nu\mu}$, and the minus-sign of the nonlinear term $C_{\mu_1 \ldots \mu_k}$ is chosen out of convenience. This allows to separate the Gaussian from the non-Gaussian part in the partition function.

$$Z[\beta, J_\nu] = \int \exp \left( - \frac{\beta}{2} F_{\nu\mu} \theta^\nu \theta^\mu + \sum_{k=3}^{N} \frac{1}{k!} C_{\mu_1 \ldots \mu_k} \theta^{\mu_1} \ldots \theta^{\mu_k} + \beta J_\nu \theta^\nu \right) \approx \int \exp \left( - \frac{\beta}{2} F_{\nu\mu} \theta^\nu \theta^\mu + \beta J_\nu \theta^\nu \right) \left( 1 + \beta \sum_{k=3}^{N} \frac{1}{k!} C_{\mu_1 \ldots \mu_k} \theta^{\mu_1} \ldots \theta^{\mu_k} \right) \tag{26}$$

In a next step the computation of the moments is replaced with a differentiation with respect to the sources $J_\nu$. The partition function
can then be expressed as

\[ Z[\beta, J_\alpha] = \left( 1 + \beta \sum_{k=1}^{\infty} \frac{1}{k!} C_{\mu_1 \cdots \mu_k} \frac{\partial}{\partial J_{\mu_1}} \cdots \frac{\partial}{\partial J_{\mu_k}} \right) \int \text{d}^\theta \exp \left( -\frac{\beta}{2} F_{\mu \nu} \theta^\mu \theta^\nu + \beta J_{\mu} \theta^\mu \right) \]

\[ = \sqrt{\frac{2\pi}{\beta}} \left( \frac{1}{\det(F)} \right)^{\frac{1}{2}} \left( 1 + \beta \sum_{k=1}^{\infty} \frac{1}{k!} C_{\mu_1 \cdots \mu_k} \frac{\partial}{\partial J_{\mu_1}} \cdots \frac{\partial}{\partial J_{\mu_k}} \right) \]

\[ = \sqrt{\frac{2\pi}{\beta}} \left( \frac{1}{\det(F)} \right)^{\frac{1}{2}} \exp \left( \frac{\beta}{2} F^{\mu \nu} J_\mu J_\nu \right) \left( 1 + \beta \sum_{k=3}^{\infty} \frac{1}{k!} C_{\mu_1 \cdots \mu_k} \frac{\partial}{\partial J_{\mu_1}} \cdots \frac{\partial}{\partial J_{\mu_k}} \exp \left( \frac{\beta}{2} F^{\mu \nu} J_\mu J_\nu \right) \right) \]  

The first factor in this equation is equivalent to the partition function for a linear model as given in eqn. (13). Here the mean values are set to zero. The second factor in the equation is the contribution of non-Gaussianities to the partition function. With the definitions

\[ Z_G[\beta, J_\alpha] = \sqrt{\frac{2\pi}{\beta}} \left( \frac{1}{\det(F)} \right)^{\frac{1}{2}} \exp \left( \frac{\beta}{2} F^{\mu \nu} J_\mu J_\nu \right) \]  

as well as

\[ Z_{NG}[\beta, J_\alpha] = \left( 1 + \beta \sum_{k=3}^{\infty} \frac{1}{k!} C_{\mu_1 \cdots \mu_k} \frac{\partial}{\partial J_{\mu_1}} \cdots \frac{\partial}{\partial J_{\mu_k}} \exp \left( \frac{\beta}{2} F^{\mu \nu} J_\mu J_\nu \right) \right) \]

a factorization of the partition function into a contribution due to its Gaussian part and the influence of the non-Gaussianities can be observed,

\[ Z[\beta, J_\alpha] = Z_G[\beta, J_\alpha] Z_{NG}[\beta, J_\alpha]. \]

Using the fact that the inverse Fisher matrix can be Cholesky decomposed as \( F^{\mu \nu} = L^{\mu \nu} L^{\nu \mu} \) the non-Gaussian part can be expressed in terms of multivariate Hermite polynomials of the form

\[ H^{(\nu_1 \cdots \nu_k)}(J) = \exp \left( \frac{1}{2} J_\alpha \delta^{\alpha \beta} J_\beta \right) \frac{(-1)^k}{\beta} \frac{\partial^k}{\partial J_{\nu_1} \cdots \partial J_{\nu_k}} \exp \left( \frac{1}{2} J_\alpha \delta^{\alpha \beta} J_\beta \right) \]

as

\[ Z_{NG}[\beta, J_\alpha] = \left( 1 + \beta \sum_{k=3}^{\infty} \frac{(-1)^k}{k!} C_{\mu_1 \cdots \mu_k} L^{\mu_1}_{\nu_1} \cdots L^{\mu_k}_{\nu_k} H^{(\nu_1 \cdots \nu_k)}(\mathbf{I} \mathbf{L}) \right). \]

When computing cumulants the logarithm of these quantities is considered and the contributions of the Gaussian and non-Gaussian part can be expressed as a sum. Up to first order in the non-Gaussianities the expression is

\[ \ln Z[\beta, J_\alpha] = \ln Z_G[\beta, J_\alpha] + \ln Z_{NG}[\beta, J_\alpha] \approx \frac{\beta}{2} F^{\mu \nu} J_\mu J_\nu + \sum_{k=3}^{\infty} \frac{(-1)^k}{k!} C_{\mu_1 \cdots \mu_k} L^{\mu_1}_{\nu_1} \cdots L^{\mu_k}_{\nu_k} H^{(\nu_1 \cdots \nu_k)}(\mathbf{I} \mathbf{L}) + \text{const.} \]

Note that in eqn. (26) the approximation can be performed to higher order in the non-Gaussianities for the cost of including higher order Hermite polynomials in the result. The factorization itself can still be performed.

For non-vanishing expectation values such that

\[ \frac{\chi^2}{2} = \frac{\beta}{2} F^{\mu \nu} J_\mu J_\nu + \mu_\sigma \sigma^\sigma - \sum_{k=3}^{\infty} \frac{(-1)^k}{k!} C_{\mu_1 \cdots \mu_k} \theta^{\mu_1} \cdots \theta^{\mu_k} \]

the Gaussian term is modified by a term linear in the sources

\[ Z_G[\beta, J_\alpha] = \frac{\beta}{2} F^{\mu \nu} J_\mu J_\nu - \beta \mu^\mu J_\alpha, \]

and consequently, the non-Gaussian term in the partition function remains unchanged. The higher order cumulants of the posterior can be computed as

\[ \kappa^{\nu_1 \cdots \nu_k} = \left. \frac{\partial^k}{\partial J_{\nu_1} \cdots \partial J_{\nu_k}} \left( \frac{1}{\beta} \ln Z[\beta, J_\alpha] \right) \right|_{\beta=0} \approx \left. \frac{\partial^k}{\partial J_{\nu_1} \cdots \partial J_{\nu_k}} \left( \frac{1}{2} F^{\mu \nu} J_\mu J_\nu - \sum_{k=3}^{\infty} \frac{(-1)^k}{k!} C_{\mu_1 \cdots \mu_k} L^{\mu_1}_{\nu_1} \cdots L^{\mu_k}_{\nu_k} H^{(\nu_1 \cdots \nu_k)}(\mathbf{I} \mathbf{L}) \right) \right|_{\beta=0} \]

The first and second cumulants already contain contributions from the odd and even Hermite polynomials in the non-Gaussian term respectively. The higher cumulants are completely determined by the non-Gaussian term. The question whether non-Gaussianities are genuine or just an artefact of an unfortunate choice of random variables and could therefore in principle removed by a suitable coordinate transform can be traced to the existence of curvature on the manifold whose metric is given by the Fisher-matrix \( F_{\mu \nu} \) (see the foundational work by Amari 2016). Applications in cosmology are discussed in Giesel et al. (2021), and variations of the Fisher-matrix over the parameter manifold and the resulting non-Gaussianities in Schäfer & Reischke (2016) and Reischke et al. (2017).
4.2 Gram-Charlier series

The cumulants of a weakly non-Gaussian posterior allow to reconstruct it using the multivariate Gram-Charlier series. It can be written as

$$ p(\theta | y) = \frac{1}{(2\pi)^{\frac{1}{2}} \sqrt{\det(\Sigma)}} \exp \left( -\frac{1}{2} \Sigma_{\alpha \beta} \theta^\alpha \theta^\beta \right) \left( 1 + \frac{1}{3!} \sum_{n=0}^{\infty} \frac{C_{\alpha_1 \alpha_2 \ldots \alpha_n}}{n!} \left( L_{\alpha_1} \ldots L_{\alpha_n} H_{\beta_1, \ldots, \beta_k} (L(\theta - \mu)) \right) \right). $$

where the mean value of the distribution is chosen as the first cumulant of the posterior while the covariance matrix is the inverse of the second cumulant. The Hermite polynomials in this expression again follow the definition in eqn. (33). Due to the covariance matrix chosen as unity in this definition the multidimensional Hermite polynomials factorize into one dimensional ones. The variable transformation necessary to achieve this form can be seen in the argument of the Hermite polynomials. This accounts for the Cholesky decomposed second cumulants in their prefactors.

In the following the Gram-Charlier series is used to reconstruct a probability distribution of the form

$$ p(\theta | y) = \frac{1}{(2\pi)^{\frac{1}{2}} \sqrt{\det(\Sigma)}} \exp \left( -\frac{1}{2} \Sigma_{\alpha \beta} \theta^\alpha \theta^\beta \right) \left( 1 + \frac{1}{3!} \sum_{n=0}^{\infty} \frac{C_{\alpha_1 \alpha_2 \ldots \alpha_n}}{n!} \left( S_{\alpha_1 \theta^\alpha \theta^\beta} \right) ^n \right). $$

Note that this is a first order approximation in the coefficients $C_{\alpha_1 \alpha_2 \ldots \alpha_n}$ to a posterior with a third order non-Gaussianity. For small coefficients it is possible to compute the cumulants of this posterior according to eqn. (38) they can then be inserted into expression eqn. (39). The results of that reconstruction are depicted in Fig. 1 for a toy model of non-Gaussianity.

As demonstrated in the above example it is possible to approximately construct cumulants for a given expansion coefficient in the DALI expansion. However, it is worth noting that even the first order in the DALI expansion does not correspond to any specific order in the Gram-Charlier expansion. This can be seen by considering

$$ \exp \left( -\frac{1}{2} F_{\alpha_1 \alpha_2 \ldots \alpha_n} \theta^\alpha \theta^\beta + \frac{1}{3!} S_{\alpha_1 \theta^\alpha \theta^\beta} \theta^\gamma \theta^\delta \right) = \exp \left( -\frac{1}{2} F_{\alpha_1 \alpha_2 \ldots \alpha_n} \theta^\alpha \theta^\beta \right) \sum_{n=0}^{\infty} \frac{1}{n!} \left( S_{\alpha_1 \theta^\alpha \theta^\beta} \theta^\gamma \theta^\delta \right) ^n. $$

Terms in this expansion that are of order $3^r$ in the parameters $\theta$ can only be obtained by including an ever increasing order expansion in the Gram-Charlier series. This is why the Gram-Charlier series seems to be incompatible with a straightforward expansion of the logarithmic likelihood in terms of a polynomial as done in DALI (Sellentin et al. 2014; Sellentin 2015). One clearly needs a large number of terms to be able to describe even moderately non-Gaussian distributions, set aside issues with non-positive definite probability densities, as pointed out in Cramér (1999).

5 PARTITIONS, BAYESIAN EVIDENCES AND ENTROPY MEASURES

5.1 Entropy measures

The partition function $Z(\beta, J_n)$ evaluated at unit temperature $\beta = 1$ and for vanishing sources $J_n = 0$ falls back onto the Bayes evidence as the normalising factor for the posterior distribution,

$$ Z[\beta, J_n = 0] = \int d^\alpha \theta \exp \left( -\beta \frac{1}{2} \chi^2(\theta) + \phi(\theta) \right) \text{ such that } Z[\beta = 1, J_n = 0] = p(y), $$

which is exactly the normalisation of the posterior distribution $p(\theta | y)$, according to eq. (1). It is an interesting thought to derive the Shannon-entropy $S$ of the posterior distribution,

$$ S = -\int d^\alpha \theta p(\theta | y) \ln p(\theta | y) $$

Figure 1. Reconstruction of non-Gaussianity of second order using the Gram-Charlier series. The left plot shows the posterior constructed according to eqn. (40) and a Gaussian (dashed) with the same width in comparison. The middle (dashed) is the Gram-Charlier series to first order in the non-Gaussianities. The dashed lines in the right depict the Gram-Charlier series to second order in the non-Gaussianities.
5.2 Hamilton Monte-Carlo partitions

Extensions to the partition function \( Z[\beta, J_n] \) could consist of including a kinetic term

\[
Z[\beta, J_n] = \int \frac{d^np}{(2\pi)^p} \int d^q \theta^{(q)} \exp \left( -\beta \frac{p^2}{2m} + \frac{1}{2} \chi^2(\theta | \beta) + \phi(\theta) \right) \exp(\beta J_n \theta^q) = \int \frac{d^np}{(2\pi)^p} \int d^q \theta^{(q)} \exp \left( -\beta \mathcal{H}(p, \theta) \right) \exp(\beta J_n \theta^q)
\]

which would correspond to Hamilton-Monte Carlo Markov-chains, with a Hamilton function

\[
\mathcal{H}(p, \theta) = \frac{p^2}{2m} + \frac{1}{2} \chi^2(\theta | \beta) + \phi(\theta)
\]
not only reflecting potential, but also kinetic energy (for an application in cosmology, see Jasche & Kitaura 2010; Kitaura & Ensslin 2008). The integrals in the partition sum separate always, such that there is no influence of the \(d^r p\)-integration on the cumulants of \(p(\theta|y)\), explicitly for instance for a linear model with a flat prior as discussed in eqn. (13)

\[
Z[\beta, J_\alpha] = \int \frac{d^r p}{(2\pi)^r} \int d\theta \exp\left(-\beta \left[ \frac{p^2}{2m} + \frac{1}{2} \chi^2(\theta|y) + \phi(\theta) \right] \right) \exp(\beta J_\alpha \theta^\alpha) = \sqrt{\frac{m^r}{\beta^r \det(F)}} \exp \left( \frac{\beta}{2} F^{\alpha\beta} J_\alpha J_\beta \right),
\]

however, the inclusion of momentum degrees of freedom can make the sampling more efficient, in particular in the case of strong degeneracies.

5.3 Ensemble Monte-Carlo partitions

Having \(N\) instead of a single Monte-Carlo Markov-chain bridges towards ensemble Markov-methods (Foreman-Mackey et al. 2013): If the chains are non-interacting, this would amount to a factorising \(N\)-particle partition \(Z[\beta, J_\alpha, N]\)

\[
Z[\beta, J_\alpha, N] = Z[\beta, J_\alpha]^N
\]

suggesting the question whether one could introduce a fugacity \(z\) that controls the number \(N\) of Markov-chains, effectively defining a macrocanonical partition

\[
Z[\beta, J_\alpha, z] = \sum_N Z[\beta, J_\alpha, N] z^N = \sum_N \left( z Z[\beta, J_\alpha] \right)^N.
\]

Adding a Gibbs-factor \(1/N!\) seems superfluous as the chains are perfectly distinguishable.

6 APPLICATION TO SUPERNOVA DATA

As a topical example for a non-Gaussian likelihood from cosmology we consider constraints on \(\Omega_m\) and \(w\) from the distance redshift relation of supernovae (Riess et al. 1998; Goobar & Leibundgut 2011), where we focus on spatially flat FLRW-cosmologies with a constant dark energy equation of state, and derive constraints on \(\Omega_m\) and \(w\) for the Union2.1-data set (Suzuki et al. 2012; Amanullah et al. 2010; Kowalski et al. 2008). For these cases, the distance modulus \(y(z)\) as a function of redshift \(z\) is given by

\[
y(z, \Omega_m, w) = 10 + 5 \log \left( \left( 1 + z \right) H_0 \int_0^z dz' \frac{1}{\sqrt{\Omega_m (1+z')^2 + (1-\Omega_m)(1+z')^{2(1+w)}}} \right),
\]

with the relevant integral, for this type of cosmology, being expressible in terms of a hypergeometric function \( _2F_1 \) (Arutjunjan et al. 2022)

\[
\int du \frac{1}{\sqrt{A u^2 + B u}} = -\frac{2u}{\sqrt{A u^2 + B u}} + \frac{1}{\sqrt{A}} _2F_1 \left( \frac{1}{2}, \frac{1}{2}; 1; -\frac{A u}{\sqrt{A u^2 + B u}} \right) + \text{const.}
\]

Expressing the likelihood for the two parameters \(\Omega_m\) and \(w\) for Gaussian errors \(\sigma_i\) in the distance moduli \(y_i\) yields a simplified expression, where we neglect correlations between the data points,

\[
L(y|\Omega_m, w) \propto \exp \left(-\frac{1}{2} \chi^2(y|\Omega_m, w) \right) \quad \text{with} \quad \chi^2(y|\Omega_m, w) = \sum_i \left( \frac{y_i - y(z_i, \Omega_m, w)}{\sigma_i} \right)^2,
\]

which we use for the construction of partition functions \(Z[\beta, J_\alpha]\) and for implementation in a Monte-Carlo Markov-chain. For simplicity, we employ a flat prior \(p(\Omega_m, w)\) on the two cosmological parameters and drive the MCMC-sampling with a straightforward Metropolis-Hastings algorithm. The model for the distance modulus as a function of the model parameters \(\Omega_m\) and \(w\) is clearly nonlinear, giving rise to a non-Gaussian likelihood, on which we demonstrate the a Gram-Charlier-type expansion, with cumulants derived from differentiation of the partition function \(\ln Z[\beta, J_\alpha]\). These differentiation are done by finite differencing of a numerically integrated partition function, where we have verified the numerical precision in toy examples.

In the case that the partition function cannot be computed exactly or be approximated analytically it can be constructed from a Monte-Carlo Markov-chain sampling from a posterior distribution by computing an expectation value of \(\exp(J_\alpha \theta^\alpha)\)

\[
Z[\beta = 1, J_\alpha] = \langle \exp(J_\alpha \theta^\alpha) \rangle \approx \frac{1}{N} \sum_{i=1}^N \exp(J_i \theta^\alpha_i),
\]

Here, \(i\) denotes the \(i\)-th sample generated by the Metropolis-Hastings algorithm. This allows to find the cumulants following the first part of eqn. (38) and to construct the partition function for a given \(J_\alpha\). The cumulants can then be computed through finite differencing with respect to all \(J_\alpha\).

The numerical precision can be verified by computing moments of order \(a + b\) of the posterior using the samples drawn by the Monte-Carlo Markov-chain, which are distributed according to the posterior distribution. They are computed as

\[
\langle \Omega_m^a w^b \rangle = \int d\Omega_m dw \rho(\Omega_m, w|y) \Omega_m^a w^b \approx \frac{1}{N} \sum_{i=1}^N (\Omega_m^a w^b)_i.
\]
The subject of this paper was an analytical approach to inference in cosmology with Gaussian and weakly non-Gaussian distributions, with supernova constraints on $\Omega_m$ and $w$ as a topical example from cosmology with a weakly non-Gaussian likelihood. Our motivation was the statistical model behind Monte-Carlo Markov-chain methods routinely used in likelihood evaluation with the hope to develop analytical methods that can be implemented in reality. The subject of this paper was an analytical approach to inference in cosmology with Gaussian and weakly non-Gaussian distributions, with supernova constraints on $\Omega_m$ and $w$ as a topical example from cosmology with a weakly non-Gaussian likelihood. Our motivation was the statistical model behind Monte-Carlo Markov-chain methods routinely used in likelihood evaluation with the hope to develop analytical methods that can be implemented in reality.
methods that extend the Fisher-matrix formalism beyond second order and that allow an approximative description of non-Gaussian posterior distributions.

(i) It is a known result how the Bayes-evidence $p(y)$ can be extended to a partition function $Z(\beta, J_\mu)$, by introducing an inverse temperature $\beta$ and by carrying out a Laplace-transform of the actual model parameter $\theta^\mu$ to source variables $J_\mu$. Cumulants of the posterior distribution $p(\theta|y)$ of order $n$ would follow from $n$-fold differentiation of the logarithmic partition function. An MCMC-algorithm would sample microstates from this partition function, so that the determination of cumulants of order $n$ would be possible from estimating all moments up to order $n$ and assembling them according to Faa di Bruno’s formula: Instead, we aim to compute the integral defining the partition function directly, numerically if necessary, and determine the cumulants by finite differencing.

(ii) We recover analytically the well-known Fisher-matrix formalism for linear models from our approach. The partition-function is of Gaussian shape and has an analytical solution, again of Gaussian form. The sequence of cumulants truncates at second order such that one obtains a Gaussian posterior distribution $p(\theta|y)$. While the first cumulant becomes equal to the true model parameters as expected due to the Gauß-Markov theorem, the second cumulant (or the covariance) is given by the inverse Fisher-matrix. We were able to show within the partition function-formalism by functional extremisation the Cramér-Rao inequality, i.e. that the inverse Fisher-matrix is in fact a lower bound to the variance and that this bound is reached for a $\chi^2$ that is quadratic in the parameters, or equivalently, a linear model.

(iii) The partition function gives a direct access to higher-order cumulants and Gram-Charlier expansions of the posterior distribution. Cumulants of arbitrary order $n$ follow by $n$-fold differentiation, and we have validated the numerics in comparison to MCMC-sampling in toy-examples. More importantly, though, is the factorisation of the partition function of a nonlinear model into a Gaussian and non-Gaussian part, where in the case of weak non-Gaussianities the corresponding term can be Taylor-expanded, leading straight to the Gram-Charlier expansion of weakly non-Gaussian distributions.

(iv) It is straightforward to show that derivatives of order $n$ of the logarithmic partition function with respect to inverse temperature $\beta$ correspond to cumulants of the $\chi^2(y|\theta)$-function. Motivated by the result from statistical mechanics, where one defines the Helmholtz free energy $F(\beta)$ as $-\ln Z(\beta)$ and where the entropy $S$ is given by $\beta^2 \partial F(\beta)/\partial \beta^2$ we showed that the Shannon-entropy of the posterior distribution $p(\theta|y)$ follows analogously. Extension of the partition function to include kinetic terms would lead to Hamilton Monte-Carlo partitions. We showed that quadratic kinetic terms would not change the value of cumulants of the posterior distribution.

(v) Application of our formalism to supernova data showed that the posterior distribution $p(\Omega_m, w|y)$ for the two cosmological parameters $\Omega_m$ and $w$ can be evaluated easily to fourth order in the cumulants by finite differentiation of $\ln Z$, and that the cumulants correspond well numerically to estimates from samples obtained in MCMC-sampling.

We intend to pursue the idea of ensemble MCMC-methods controlled by a fugacity $\beta$ further, and hope to find methods to evaluate Bayes-evidences in the partition function formalism, as well as bridge to measures of statistical consistency (Raveri et al. 2020; Raveri & Hu 2019). Changes in fugacity $\beta$ as a state variable would yield a pathway of controlling the sampling analogous to changing $\beta$ in simulated annealing.

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DATA AVAILABILITY STATEMENT

Our python-toolkit for the automatic computation of multivariate cumulants and the corresponding Gram-Charlier-expansion is available on request.

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