Correlated signal inference by free energy exploration

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The inference of correlated signal fields with unknown correlation structures is of high scientific and technological relevance, but poses significant conceptual and numerical challenges. To address these, we develop the correlated signal inference (CSI) algorithm within information field theory (IFT) and discuss its numerical implementation. To this end, we introduce the free energy exploration (FrEE) strategy for numerical information field theory (NIFTy) applications. The FrEE strategy is to let the mathematical structure of the inference problem determine the dynamics of the numerical solver. FrEE uses the Gibbs free energy formalism for all involved unknown fields and correlation structures without marginalization of nuisance quantities. It thereby avoids the complexity marginalization often impose to IFT equations. FrEE simultaneously solves for the mean and the uncertainties of signal, nuisance, and auxiliary fields, while exploiting any analytically calculable quantity. Here, we develop the FrEE strategies for the CSI of a normal, a log-normal, and a Poisson log-normal IFT signal inference problem and demonstrate their performances via their NIFTy implementations.

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I. INTRODUCTION

A. Correlated signal inference

Correlated signal fields appear in many contexts as descriptions of properties of some spatial or temporal domain, like the atmospheric temperature and velocity, the magnetic field in the Galaxy, a population density, the evolution of a stock price, etc. The detailed knowledge of such fields is of high scientific, technological, sociological, economical, or other interest and rests on data converted into field estimates. As measurements sample the fields usually in a sparse fashion, such estimates require interpolations and extrapolations of field values. Such interpolations are, thanks to the correlation most fields exhibit, usually justified. However, the optimal reconstruction scheme requires precise knowledge about the field correlation structure in order to optimally suppress the measurement noise without over-smoothing the signal. This correlation structure is usually not known a priori and has to be inferred along with the signal field. This complicates the inference substantially, even in case the field statistics is simply Gaussian. Here we will address this correlated signal inference (CSI) problem within the framework of information field theory (IFT) \( \text{IFT} \), the information theory for fields, which is from a mathematical perspective a statistical field theory.

The CSI problem has already been addressed within IFT successfully by renormalization calculations \cite{2}, which led to well functioning signal estimators. In order to improve the accuracy and most importantly the efficiency of such estimators, we re-investigate their derivation in a slightly different manner than done before. In particular, the novel approach provides also uncertainty information on the correlation structure, and takes the impact of this uncertainty for the field estimate into account.

The problem of estimating the mean of a Gaussian random variable from independent samples under an unknown covariance was addressed in a Bayesian setting previously \cite{3,4}. The here discussed method can be regarded as an extension of those works to the multidimensional case with independent variables (here field values). Also this extended problem has been addressed by previous works, most notably by means of the Gibbs sampling technique \cite{5–9}. This latter approach differs from the here used minimal Gibbs free energy approach, but shares with it that the field and its spectrum are inferred simultaneously, and for both uncertainty information is provided.

B. Structure of this work

The structure of this work is as follows. Sect. \( III \) introduces IFT and the Gibbs free energy formalism. Sect. \( III \) discusses the challenges of numerical IFT and the free energy explorer (FrEE) strategy to face them. In Sect. \( IV \) all the available information on the fields we investigate here is mathematically summarized in an information Hamiltonian. In Sect. \( V \) the Gibbs free energy is constructed for the normal field measurement problem. The corresponding log-normal and the Poisson log-normal problems are treated in Appendices \( A \) and \( B \) respectively. The FrEE strategy for the CSI is developed in Sect. \( VI \) and verified with simulations in Sect. \( VII \). Sect. \( VII \) contains our conclusions.

II. INFORMATION FIELD THEORY

A. Basics

The reconstruction of a physical field from observational data faces the problem, that the field degrees of freedom outnumber the constraints given by the data by a huge, if not infinite factor. There are infinitely many field configurations that are fully consistent with any finite set of measurements, even in the absence of measurement noise. Most of those configurations would be discarded as not being plausible. For example in many physical fields strong gradients are rare,
as they either require an improbable concentration of energy, or are rapidly erased by the field evolution.

To diminish the number of possibilities and to exclude unlikely or even nonphysical configurations the plausibility of field configurations should be included in the field reconstruction process. The correct language to combine measurement information and prior knowledge on any quantity is probability theory [10][11].

IFT is just probability theory for fields. It takes advantage of the rich pool of methods developed for quantum field theory for the derivation of optimal field reconstruction methods, which use all available information. This is achieved by a simple identification of the posterior probability $P(\phi|d, I)$ of a field $\phi$, constrained by measurement data $d$ and prior information $I$, with the Gibbs-Boltzmann distribution of a hypothetical energy function $H(d, \phi|I)$ at temperature $T = 1$,

$$P(\phi|d, I) = \frac{P(d, \phi|I)}{Z(d|0, I)} = e^{-\frac{H(d, \phi|I)}{T}}$$

(1)

$$H(d, \phi|I) \equiv -\ln P(d, \phi|I)$$

Here, the field scalar product $j^i \phi = \int dx j^*(x) \phi(x)$ is used, which we, for notational convenience, assume to be symmetric by implicitly using $a^i b^j \equiv \frac{1}{2} (a^i b^j + b^j a^i)$.

The function $H(d, \phi|I)$ therefore summarizes all information on the field, and is thus called the information Hamiltonian in IFT. The partition function $Z(d|j, I)$, which is given by a path integral over all field configurations, is simultaneously a moment generating function, from which any field moment of interest can be calculated via derivation with respect to the information source term $j$. For example the posterior mean is given for $T = 1$ as

$$m = \langle \phi \rangle_{\phi|d} \equiv \int \mathcal{D}\phi \, \phi \, P(\phi|d)$$

$$= \frac{1}{Z(d|j)} \delta \int \mathcal{D}\phi \, e^{-H(d, \phi|I) + j^i \phi}_{j=0}$$

$$= \frac{\delta \ln Z(d|j)}{\delta j}_{j=0}$$

(2)

and its uncertainty covariance as

$$D = \langle (\phi - m)(\phi - m)^\dagger \rangle_{\phi|d, I}$$

$$= \frac{\delta^2 \ln Z(d|j)}{\delta j \delta j^\dagger}_{j=0}.$$  

(3)

Unfortunately, the partition function can only be calculated analytically for a limited class of probability density functionals (PDFs), most notably the Gaussian distribution

$$P(\phi|\Phi) = G(\phi, \Phi) \equiv \frac{1}{\sqrt{|2\pi\Phi|}} \exp \left( -\frac{1}{2} \phi^\dagger \Phi^{-1} \phi \right),$$

(4)

where here $\Phi_{xy} = \langle \phi_x \phi_y^\dagger \rangle_{\phi}$ is the prior field covariance structure. For other PDFs perturbation theoretic, renormalization, or other approximation techniques have to be invoked.

The prior Hamiltonian of a Gaussian field with known covariance

$$H(\phi|\Phi) = \frac{1}{2} \left( \phi^\dagger \Phi^{-1} \phi + \ln |2\pi\Phi| \right)$$

(5)

is quadratic in $\phi$, and therefore contributes only to a free field theory, which can be tackled by linear methods. However, the CSI problem addressed in this work is how to infer a Gaussian field $\phi$ for which the covariance $\Phi$ is not known a priori and has to be estimated from the same data used to estimate $\phi$. This lack of knowledge alone renders an otherwise often easily analytically solvable problem into a complex, non-Gaussian problem, beyond the reach of simple perturbation methods.

The available knowledge on the covariance $\Phi$ is summarized by the hyper-prior $P(\Phi)$. The prior knowledge on the field is then

$$P(\phi) = \int \mathcal{D}\Phi \, P(\phi|\Phi) \, P(\Phi),$$

(6)

which turns the corresponding effective Hamiltonian

$$H(\phi) = -\ln \int \mathcal{D}\Phi \, P(\phi|\Phi) \, P(\Phi)$$

$$= -\ln \int \mathcal{D}\Phi \, e^{-\frac{1}{2} \phi^\dagger \Phi^{-1} \phi} \, P(\Phi) + \frac{1}{2} \ln |2\pi|$$

into a non-quadratic function of $\phi$ unless there is certainty about the correlation structure, $P(\Phi) = \delta(\Phi - \Phi_0)$, in which case Eq. [5] is recovered.

All relevant information is stored in the partition function $Z$. Any moment of the field can be extracted from $Z$. However, the calculation of this can be difficult and therefore approximations are used to calculate field estimates.

**B. Maximum a posteriori**

One popular approximation is the maximum a posteriori (MAP) approximation, which is equivalent to minimizing the joint Hamiltonian $H(d, \phi)$ with respect to the field,

$$\frac{\delta H(d, \phi)}{\delta \phi} \bigg|_{\phi=m_{\text{MAP}}} = 0.$$  

(8)

Ref. [2] showed that this leads to poorly performing signal reconstruction schemes in case the uncertainty on $\Phi$ is on logarithmic scale. Minimizing $H(d, \phi, \Phi)$ simultaneously with respect to $\phi$ and $\Phi$ gives even worse results. On the MAP level, the only well working strategy was to estimate $\Phi$ from maximizing $P(\Phi|d) = \int \mathcal{D}\phi \, P(d, \phi, \Phi)$ and then to use this as given in $P(d, \phi|\Phi)$. This empirical Bayes approach neglects the uncertainties in $\Phi$ and therefore provides overconfident estimates of $\phi$.

When using the MAP approach we just need to minimize the Hamiltonian. This has the advantage that suboptimal steps during the minimization get corrected by later steps and therefore do not affect the outcome. A similar guiding function property is desired for a more accurate estimator of the signal mean. It exists in the form of the Gibbs free energy.
C. Gibbs free energy

The Gibbs free energy can be used to approximate a complex posterior $P(\varphi|d)$ with a simpler probability function $\tilde{P}(\varphi|d)$ \cite{12} for example a Gaussian

$$\tilde{P}(\varphi|d) = \mathcal{G}(\varphi - m, D).$$

For this, the form

$$G(m, D|d) = U(m, D|d) - T \mathcal{S}(D|d)$$

$$= (\mathcal{H}(d, \varphi))_{\tilde{P}(\varphi|d)} + T (\ln \tilde{P}(\varphi|d))_{\tilde{P}(\varphi|d)}$$

is most convenient, as its construction requires only Gaussian averaging to get the internal energy $U$ and the entropy $\mathcal{S}$. The Gibbs free energy has the desired property of being a guiding objective function since its minimum is at the posterior mean and in addition to this its curvature there encodes the uncertainty dispersion:

$$\frac{\delta^2 G}{\delta m \delta m^\dagger} = \mathcal{T} = (\varphi \varphi^\dagger)_{\tilde{P}(\varphi|d)}. \quad (10)$$

The Gibbs free energy was successfully used in Ref. \cite{16} to minimize the effective Hamiltonian in Eq. \cite{7} approximately. To lowest order, the result was identical to that of the empirical Bayes approach discussed above. In order to obtain a more accurate field and covariance estimation, including uncertainty information for both, and hopefully also a numerically more efficient algorithm, we make a different design choice here. We will not use the field covariance marginalized effective theory as given by Eq. \cite{7}, but keep the covariance explicit by investigating

$$P(\varphi, \Phi|d, I) = \frac{P(d|\varphi, I) P(\varphi|\Phi, I) P(\Phi|I)}{P(d|I)}. $$

Thus, the unknown “signal” to be estimated by the Gibbs formalism will be the field $\varphi$ and its prior covariance $\Phi$. The latter is described for homogenous statistics by a strictly power spectrum $P_\varphi(k)$. As this function of the Fourier wavevector $k$ varies often over orders of magnitude, and to enforce its positivity, we actually use the logarithm of the spectrum in comparison to some pivot amplitude $r$ as our unknown parameter $r_k = \ln [P_\varphi(k)/r]$. Together with the unknown field this forms the combined signal vector $s = (\varphi^\dagger, r^\dagger)^\dagger$. For the log-power spectrum a Gaussian approximation of the uncertainty is more appropriate, as it can be positive or negative equally well.

\footnote{The minimal Gibbs free energy approach used here is mathematical identical to the concept of variational inference \cite{13} based on minimal Kullback-Leibler distance of probability distributions \cite{14}. Given that the oldest of these similar, if not identical concepts is the Gibbs free energy \cite{15}, we stick to this term in our naming conventions.}

III. NUMERICAL INFORMATION FIELD THEORY

A. Basics

The equations of IFT have to be solved numerically. These usually involve high dimensional linear or non-linear operators acting on fields, which can not be represented explicitly by handling their matrix elements in computer memory. Instead, these operators have to be represented implicitly by computer routines that perform the action of the operator without representing its matrix elements explicitly. For example the Fourier transformation operator $F$, with $F_{kx} = e^{i k x}$, can be represented by the Fast Fourier Transform (FFT) algorithm. The inverse of such an implicit operators $A$ applied to a vector $b$ has then to be done by a numerical solver for $Ax = b$ that is able to use such implicit operator representations. One such solver is the famous conjugate gradient (CG) method for solving linear systems of equations \cite{17}.

IFT equations usually do not depend explicitly on the size, coordinate system, number of dimensions, or topology of the space the field of interest is living on. They look the same for fields over Cartesian spaces and fields over spheres if the corresponding harmonic spaces are automatically used to express spatial correlation structures. In order to benefit from space invariance and in order to facilitate the implementation of IFT algorithms numerical information field theory (NIFTy) was developed \cite{15,13}. NIFTy permits the user to specify field inference algorithm in a coordinate free manner, so that those can easily be applied to reconstruct fields over varying dimensions and space topologies. It has successfully been used in a number of imaging and signal inference problems \cite{20,28}.

NIFTy already contains an implementation of the empirical Bayes CSI, the so called critical filter method to retrieve a field and its unknown spectrum \cite{2,20,22}. This, however, has three short comings we want to overcome here:

First, the critical filter is relatively slow, as the field and the spectrum estimates are performed separately by iterations. These variables have a large inertia since the mutual dependencies require a combined solution for those. Abstractly speaking, there exists a diagonal and curved valley in the information Hamiltonian of combined field and spectrum Hilbert space. This should be followed downhill, but the critical filter performs only steps in orthogonal directions of which none is parallel to the valley.

Second, the critical filter has no notion of spectral uncertainty. Uncertainty of the spectrum should however be manifest in the inference equations since a field estimator should be more conservative as larger this uncertainty is.

Third, the critical filter is not adapted to non-linear measurement situations. It has been used for such, though, but without a strict IFT derivation.

To address all these issues, but also as a design principle for efficient and consistent signal inference algorithms with NIFTy, we introduce here the free energy exploration (FrEE) strategy.
The FrEE strategy proposes to address signal field inference problems based on the following design principles:

**Form follows function:** The optimal numerical scheme should derive from the properties of a suitable objective function, which is the Gibbs free energy for a given inference problem. We exploit the analytic form of this function as much as possible.

**Free energy exploration:** The Gibbs energy measures the information distance of an assumed, approximate probability distribution from the correct one. Minimizing this distance provides a nearly information optimal approximate (see [20] for a discussion of this), from which a good estimate of the posterior mean and uncertainty can be read off.

**Free fields:** A free field follows Gaussian statistics. Information about field values can then be easily propagated from one location to another. Consequently, inference of Gaussian fields conditional to other fields is easier than inference of self-interacting, non-Gaussian fields. Complex interaction terms in an information Hamiltonian often result from marginalization of nuisance fields. These are better regarded as signal fields to be estimated as well than being marginalized. It can be more efficient numerically to have an explicit representation of a nuisance field than to recalculate its effective forces from the signal field in every computational step. If necessary, we can introduce additional, auxiliary fields to keep track of and/or accumulate knowledge on field properties that are otherwise expensive to re-calculate. If our approximate posterior is free, i.e. Gaussian, marginalization of nuisance parameters can easily be done after the calculation.

**Force-free configurations:** The negative gradient of the Gibbs energy is the force which drives the inference. If, however, a location for which some of the force components vanish can be reached directly, we adapt it.

**No unnecessary accuracy:** The free energy extremal principle guides the inference to the optimal solution from any location in the Hilbert space of the field. Intermediate errors can be corrected later. If the situation is rapidly changing, there is no need to accurately plan for the perfect next step or to accumulate statistics for a stochastically estimated quantity. It is more beneficial to keep moving quickly.

**Stability:** The tight coupling between degrees of freedom of the inference problem, and most notably the concaveness of interesting problems can easily destabilize a finite step size numerical scheme. We propose to increase stabilizing “mass terms” of the dynamics for degrees of freedom that exhibit sign changes of their steps.

In the following, we will construct efficient CSI algorithms based on the FrEE strategy, while trying to be pragmatic.

### C. FrEE recipe

The recipe to tackle inference problems via the FrEE strategy is as follows:

1. Identification of the relevant quantities to be inferred, the signal $s$ in the following. For the CSI problem this is the combined vector $s = (\varphi^T, \tau^T)^T$ describing the field and its log power spectrum.

2. Construction of $\mathcal{H}(d, s) = -\ln p(d|s) - \ln p(s)$, the joint information Hamiltonian, out of likelihood $p(d|s)$ and prior $\ln p(s)$.

3. Choosing an Ansatz for the approximate posterior, here and usually a Gaussian $\tilde{p}(s|d) = \mathcal{G}(s - \bar{s}, S)$. The choice for the representation of the posterior uncertainty dispersion $S$ might require a trade off between accuracy and complexity.

4. Calculation of the internal energy

\[
U(\bar{s}, S|d) = \langle \mathcal{H}(d, s) \rangle |_{\bar{s}, d} \\
= \int \mathcal{D}s \, \mathcal{G}(s - \bar{s}, S) \, \mathcal{H}(d, s),
\]

entropy

\[
S(\bar{s}, S|d) = \int \mathcal{D}s \, \ln \tilde{p}(s|d) = \frac{1}{2} \text{Tr} [1 + \ln(2\pi S)],
\]

and Gibbs free energy

\[
G(\bar{s}, S|d) = U(\bar{s}, S|d) - T S(\bar{s}, S|d),
\]

where $T = 1$.

5. Calculation of the information forces

\[
f_\bar{s} = \frac{\delta G}{\delta \bar{s}} \quad \text{and} \quad f_S = \frac{\delta G}{\delta S}.
\]

For the latter the force-free solution, $f_S = 0$, can often be found analytically and adapted immediately to specify $S$. This might require the evaluation of trace terms, for which we propose the usage of stochastic probing (App. [C]).

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2 For $T = 1$ the Gibbs free energy is – up to an irrelevant constant – identical to the cross information or Kullback-Leibler distance of the posterior approximation $\tilde{p}(s|d)$ to the exact posterior $p(s|d, f)$. For this reason, the temperature $T$ will typically be set to the canonical value of 1. For $T = 0$ the approximate posterior becomes a delta function at the maximum of the correct posterior. For problems with nuisance parameters, as here the field covariance, maximum a posterior estimates can be very sub-optimal 2. We will keep $T$ in the formula, as it permits the exploration of inference schemes in between maximum a posteriori ($T = 0$) and maximum cross information ($T = 1$) or even to increase the uncertainty estimate in a systematic and self consistent fashion in case conservative estimates are required ($T > 1$).
6. Translation of the forces into an optimal step \( \Delta \mathbf{\pi} \) according to a Newton scheme for \( \mathbf{\pi} \):
\[
\Delta \mathbf{\pi} = -\left( \frac{\delta^2 \mathcal{G}}{\delta \mathbf{\pi} \delta \mathbf{\pi}^\dagger} \right)^{-1} \delta \mathcal{G} \mathbf{\pi} = \mathcal{T}^{-1} S f_{\mathbf{\pi}}.
\]

7. Eventually, modification of \( S^{-1} \) in the above step size calculation to ensure spectral positivity needed for a stable numerical Newton scheme. This modification should not prevent the scheme to converge towards the minimum of \( \mathcal{G} \) as characterized by \( f_{\mathbf{\pi}} = 0 \).

8. Implementation and testing of the resulting FrEE solver.

We will follow this FrEE recipe in the following construction of our CSI, and extend it where appropriate.

IV. FIELD KNOWLEDGE

A. Unknown Gaussian field

A continuous field \( \varphi : \Omega \rightarrow \mathbb{K} \) over a metric space \( \Omega \) is assumed to be drawn from a homogeneous Gaussian random process \( \mathcal{P}(\varphi|\Phi) = \mathcal{G}(\varphi, \Phi) \) with harmonic covariance structure \( \Phi = \langle \varphi \varphi^\dagger \rangle_{(\varphi)} \). The corresponding information Hamiltonian is
\[
\mathcal{H}(\varphi|\Phi) = -\ln \mathcal{P}(\varphi|\Phi) = \frac{1}{2} \varphi^\dagger \Phi^{-1} \varphi + \frac{1}{2} \ln |2\pi \Phi|.
\]
(11)

The signal covariance \( \Phi \) is unknown, but we will assume that it to be harmonic, it commutes with the Beltrami-Laplace operator \( \Delta \). This means for \( \Omega = \mathbb{R}^n \) that
\[
\Phi_{xy} = \langle \varphi(x) \varphi(y) \rangle_{(\varphi)} = C_{\varphi}(x - y)
\]
(12)
is translation invariant and only depends on the vector between locations \( x \) and \( y \). Furthermore, we will assume statistical isotropy, such that \( \Phi_{xy} = C_{\varphi}(|x - y|) \) only depends on the distance of \( x \) and \( y \), but not on their orientation. As a consequence, the covariance \( \Phi \) is characterized by a single 1D function, the correlation function \( C_{\varphi}(r) \), and the covariance is diagonal in the harmonic or Fourier space, with the power spectrum \( P_{\varphi}(k) \) on its diagonal. In the following we parametrize this power spectrum in a way that is convenient for the FrEE approach.

B. Unknown harmonic correlation structure

We assume the covariance \( \Phi \) to be diagonal in the harmonic basis of the space \( \Omega \) the field \( \varphi \) lives over, as this is the best generalisation of translation invariant statistics. Harmonic means that the basis functions \( \varphi_{k'} : \Omega \rightarrow \mathbb{K} \) are eigenvectors of the Laplace operator \( \Delta \). For a Cartesian space \( \Omega = \mathbb{R}^n \) this is the Fourier basis, for the sphere \( \Omega = S^2 \), this is the basis given by the spherical harmonic functions.

Let \( \{a_{k'}\}_{k'} \) be a set of orthonormal harmonic eigenvectors \( a_{k'} : \Omega \rightarrow \mathbb{K} \), with corresponding eigenvalues \( \{\lambda_{k'}\}_{k'} \), such that \(-\Delta a_{k'} = \lambda_{k'} a_{k'}\), sorted as \( \lambda_{k'+1} \geq \lambda_{k'} > \lambda_0 = 0 \) for all \( k' > 0 \), and the \( a_{k'} \)'s being orthonormal according to \( a_{k'}^\dagger a_{k'} = \delta_{k'k'} \). The index \( k' \) in principle only labels the different modes, but for the Fourier space, it can be identified with the Fourier wavevectors \( \vec{k} = \vec{k}(k') \), such that \( a_{k'}(\vec{x}) = e^{i \vec{k} \cdot \vec{x}} \) and for the spherical harmonic space with the angular momentum quantum numbers usually (but not here) denoted by \( \ell \) and \( m \). The reason for the prime in the notation \( k' \) will become clear soon.

Then any harmonic covariance can be expressed as
\[
\Phi = \sum_{k'} p_{k'} a_{k'} a_{k'}^\dagger = \sum_{k'} p_{k'} \bar{P}_{k'} \equiv p^\dagger \bar{P},
\]
(13)
where \( p = (p_{k'})_{k'} \) is the unknown spectrum of \( \Phi \) (the set of eigenvalues of \( \Phi \) ordered by \( k' \), the index of the harmonic operator) and \( a_{k'} a_{k'}^\dagger \equiv \bar{P}_{k'} \) are spectral projectors onto the individual basis vectors. We denote with \( \bar{P} = (\bar{P}_{k'})_{k'} \) the vector of all such spectral projectors. The inverse covariance is then
\[
\Phi^{-1} = \sum_{k'} p_{k'}^{-1} a_{k'} a_{k'}^\dagger = \sum_{k'} p_{k'}^{-1} \bar{P}_{k'} = p^{-1} \bar{P},
\]
(14)
where we used the notation convention that a function is applied to a vector component wise in the vector’s natural basis. This also applies to the multiplication or division of vectors, such as \( a b = (a_i b_i)_i \) and \( a/b = (a_i/b_i)_i \).

C. Spectral bands

It can be convenient to group several harmonic modes together, e.g., in case their eigenvalues are so similar that a similar spectral amplitude can be assumed. To this end, we define disjoint and covering sets of spectral modes \( b_k = \{k'_{i_k}, k'_{i_k+1}, \ldots, k'_{i_k+q_k}\} \) with similar harmonic eigenvalues \( \{\lambda_{i_k}, \lambda_{i_k+1}, \ldots, \lambda_{i_k+q_k}\} \) and \( q_k \) entries. A projector into such spectral bands is then
\[
P_k = \sum_{k' \in b_k} a_{k'} a_{k'}^\dagger
\]
(15)
and its trace \( g_k = \text{Tr} P_k \) provides the number of modes per band \( k \). From now on we assume that this grouping has happened and that every \( k \) labels a different \( \lambda_k \). Furthermore, if the number \( n_p \) of spectral bands is small the \( n_p \times n_p \) matrices can be managed explicitly in computer memory. We also use the notation \( \bar{P} = (P_k)_{k} \) for the vector of spectral projector. This implies, e.g., \( \bar{P}^\dagger \bar{P} = \sum_k P_k = \sum_{k' \in b_k} a_{k'} a_{k'}^\dagger = \sum_{k'} a_{k'} a_{k'}^\dagger = \mathbb{I} \). Here and in the following, we use the primed variables \( k', \ell', \) and \( q' \) to denote the original harmonic modes, and the not primed variables \( k, \ell, \) and \( q \) for harmonic bands.

The spectral vector \( p \) parametrizes the covariance \( \Phi = \Phi(p) \). Our a priori knowledge of the covariance
can hence be expressed as $\mathcal{P}(\Phi|p) = \mathcal{P}(p|I)^3$, where $I$ encodes the set of our a priori assumptions. These should encode (i) the unknown magnitude of the spectral amplitudes and (ii) their spatial scale-invariance, such that $i, ii \in I$.

\( i. \) Unknown magnitude of the spectral amplitudes

Without any prior information on the magnitude of the spectral band amplitudes $p = (p_k)_k$, these should be modeled as a falling power law distributions $\mathcal{P}(p_k|i) \propto (p_k / r)^{-\alpha_k}$ with spectral indexes $\alpha = (\alpha_k)_k$ and reference power scale $r$. A magnitude-agnostic prior would be given by $\alpha_k = 1$, a pessimistic by $\alpha_k \geq 1$, and an optimistic by $\alpha_k \leq 1$.

We permit for a lower cut-off of the amplitudes by introducing the dimensionless parameters $q = (q_k)_k$ and the inverse Gamma-distributions

$$\mathcal{P}(p_k|i) \propto \left(\frac{p_k}{r}\right)^{-\alpha_k} \exp\left[-q_k \left(\frac{p_k}{r}\right)^{-1}\right]. \quad (16)$$

Since the spectral magnitudes $\ln(p_k / r) \equiv \tau_k$, play a special role we provide their information Hamiltonian

$$\mathcal{H}(\tau_k|i) = -\ln\left(\mathcal{P}(p_k|i) \left| \frac{\partial p_k}{\partial \tau_k}\right|\right)$$

$$\equiv (\alpha_k - 1) \tau_k + q_k e^{-\tau_k} \quad (17)$$

without any irrelevant $\tau_k$-dependent constants. For later reference, we state

$$p = r e^\tau \quad (18)$$

and note that except for units, $r$ could be absorbed by a redefinition of $\tau \rightarrow \tau + \ln r$. This, however, can easily lead to confusion and therefore we better track $r$ through the formalism.

The Hamiltonian combined for all modes $k$ is

$$\mathcal{H}(\tau|i) \equiv (\alpha - 1)^\dagger \tau + q^\dagger e^{-\tau}, \quad (19)$$

where $\alpha^\dagger = \alpha^\dagger_k \tau_k \equiv \sum_k \alpha_k \tau_k$ denotes the scalar product in the band-harmonic space.

The purely agnostic magnitude prior $i$ with $(\alpha, \tau) = (1, 0)$ does not provide any constraints on the magnitudes, since $\mathcal{H}(\tau|i)$ is agnostic = const.

\( ii. \) Spatial scale-invariance of spectral amplitudes

We further assume that the amplitudes are spatially scale-invariant. The spatial scale $L_k$ of a harmonic mode $k$ is encoded in its eigenvalue with respect to $-\Delta$ according to $\lambda_k = L_k^{-2}$, and the magnitude of its inverse as $\kappa_k = \ln L_k^{-1} = 1/2 \ln \lambda_k$. For Euclidian spaces, $\kappa$ would be the logarithmic length of the Fourier-vector of a mode.

We postulate the existence of a smooth, but unknown function $\tilde{r}(\kappa)$ such that $\tau_k = \tilde{r}(\kappa_k)$. Smoothness is enforced by the prior energy

$$\mathcal{H}(\tilde{r}|ii) \equiv \int_{-\infty}^{\infty} \frac{dk}{2\sigma^2} \left(\frac{\partial^2 \tilde{r}(\kappa)}{\partial \kappa^2}\right)^2$$

$$\equiv \frac{1}{2} \tilde{r}^\dagger \tilde{r} + \frac{1}{2} \tau^\dagger \tau \equiv \mathcal{H}(\tau|ii) \quad (20)$$

where $\sigma$ regulates the strength of the smoothness enforcing. $\sigma = \infty$ encodes no smoothness, since then $\mathcal{H}(\tau|i, \text{ rough}) = \text{const}$, $\sigma = 0$ enforces a single power-law spectrum of $p_k$, and $\sigma = 1$ seems to be a reasonable compromise between these regimes, permitting the spectral index of the power spectrum to change typically by one per $e$-folding in the length scale.

$T$ represents a discretization of the integro-differential operator $\tau$ onto the spectral grid $\{\kappa_k\}_k$.

A straightforward discretization $\tau \rightarrow T$ of the differential operator $T = \Delta^\dagger \Delta$ in Eq. (20) can be found in Refs. [2, 22].

Note that the zero mode $k = 0$ with $a_0(x) = \text{const}$, $\lambda_0 = 0$, and thus $\kappa_0 = 1/2 \ln \lambda_0 = -\infty$ is infinitely distant to all the other modes, which have $k > 0$, $\lambda_k > 0$, and thus $\kappa_k = 1/2 \ln \lambda_k > -\infty$. Therefore the spectral smoothness prior leaves the zero completely unconstrained. Its value has to be determined fully from the data or other prior knowledge.

**Combined spectral Hamiltonian**

The combined spectral Hamiltonian is

$$\mathcal{H}(\tau|I) = \mathcal{H}(\tau|i) + \mathcal{H}(\tau|ii)$$

$$\equiv \frac{1}{2} \tilde{r}^\dagger T \tilde{r} + \tau^\dagger (\alpha - 1)^\dagger \tau + q^\dagger e^{-\tau}, \quad (21)$$

where the direct information sum reflects the independence of the two assumptions $i$ and $ii$.

**D. Measurements**

Measurements source our knowledge on the field and its spectrum. Here, we investigate three measurement situations, the normal field measurement (N), which is the linear measurement of a Gaussian field as given by Eq. (1), the log-normal field measurement (LN), and the Poisson log-normal field measurement (PLN). To focus the discussion, we investigate the normal case in the main text and treat the LN and PLN cases in Appendices A and B respectively.

1. Normal field measurement

A normal field measurement apparatus applies a known linear response $R$ to the Gaussian field $\varphi$. The response transforms the continuous field into a discrete data vector to which noise adds, assumed here to be Gaussian with signal independent and known covariance $N$. Therefore, we have

$$d \equiv R \varphi + n, \quad (22)$$
In case the field covariance $\Phi$ is unknown, the linearity of the data. The mean $m$ of the posterior mean.

The information Hamiltonian of the field and its spectrum

\[ H(d, \varphi | \Phi, N) = H(d | \varphi, N) + H(\varphi | \Phi) \]

\[ = \frac{1}{2} (d - R \varphi)^\dagger N^{-1} (d - R \varphi) \]

\[ + \frac{1}{2} \varphi^\dagger \Phi^{-1} \varphi \]

\[ = \frac{1}{2} (\varphi - m)^\dagger D^{-1} (\varphi - m), \]

with

\[ D^{-1} = \Phi^{-1} + R \sigma^2 N^{-1} R \]

the so called posterior precision matrix and

\[ m = \frac{1}{N} D R \sigma^2 N^{-1} d \]

the posterior mean. $D^{-1}$ is read off from the Hamiltonian and $m$ is found by quadratic completion. The posterior is then Gaussian with mean $m$ and uncertainty covariance $D$,

\[ \mathcal{P}(\varphi | d, \Phi, N) \equiv \mathcal{G}(\varphi - m, D). \]

In this case of known covariance $\Phi$, the mean $m$ is a linear function of the data. The mean $m$ is also called the Wiener filter solution and $D$ the Wiener variance. In case the field covariance $\Phi$ is unknown, the linearity between $m$ and $d$ is not the case any more as we will see later on.

E. Full information Hamiltonian

The information Hamiltonian of the field and its spectrum

\[ H(d, \varphi, \tau | I) = H(d | \varphi, I) + H(\varphi | \Phi, I) + H(\tau | I) \]

\[ = \frac{1}{2} (d - R \varphi)^\dagger N^{-1} (d - R \varphi) \]

\[ + \frac{1}{2} \varphi^\dagger \Phi^{-1} \varphi + \frac{1}{2} \ln 2 | \varphi \Phi^\dagger | \]

\[ + \frac{1}{2} \tau^\dagger (\tau + (\alpha - 1)^\dagger \tau + q^\dagger e^{-\tau}, \]

with $\Phi^{-1} = r^{-1} e^{-\tau}$, consists of Eqs. (1), (24), (A.4), or (B.3) for the normal, log-normal, or Poisson log-normal measurement, respectively. Calculating the corresponding posterior mean and uncertainty poses a complex problem that we address approximately by using the FrEE recipe.

V. FREE ENERGY CONSTRUCTION

A. Gaussian Ansatz

For the construction of the Gibbs free energy we use an approximate Gaussian Ansatz for the posterior of our signal vector $s^\dagger = (\varphi^\dagger, \tau^\dagger)$, consisting of the field its log-spectrum:

\[ \tilde{\mathcal{P}}(s | d) = \mathcal{G}(s - \bar{s}, S) \]

\[ \bar{s} = \left( \begin{array}{c} m \\ t \end{array} \right), \] the posterior mean, and

\[ S = \left( \begin{array}{cc} D & C \\ C^\dagger & \Theta \end{array} \right), \]

the posterior uncertainty covariance.

The posterior mean $\bar{s}$ consists of the mean field $m = (m_x) = \langle \varphi \rangle$ and the mean log-spectrum $t = (t_k)_k = \langle \tau \rangle$.

The signal covariance $S = \langle (s - \bar{s})(s - \bar{s})^\dagger \rangle$ consists of four blocks: 1) the field uncertainty covariance $D = \langle (\varphi - m)(\varphi - m)^\dagger \rangle$, which is a position space operator, $D = (D_{\alpha \gamma} x y) \tau$, 2) the log-spectrum uncertainty covariance $\Theta = \langle (\tau - t)(\tau - t)^\dagger \rangle$, which is a harmonic-band space operator, $\Theta = (\Theta_{\alpha \gamma} x y) \tau$, 3) the cross correlation $C = \langle (\varphi - m)(\tau - t)^\dagger \rangle$, which is an operator that transforms a function over harmonic bands into one in position space, $C = (C_{\alpha \gamma} x k) \tau$, and 4) its adjoint, $C^\dagger = \langle (\tau - t)(\varphi - m)^\dagger \rangle$, which transforms from position space into harmonic bands, $C^\dagger = (C_{\alpha \gamma}^\dagger x k) \tau$.

The unknown parameters $m$, $D$, $t$, $\Theta$, and $C$ depend in a still to be specified fashion on the data $d$. The Gibbs free energy is given in terms of these parameters as

\[ G(\bar{s}, S | d) = U(\bar{s}, S | d) - T S(\bar{s}, S | d). \]

Here

\[ U(\bar{s}, S | d) = \langle H(d, \varphi, \tau | I) \rangle \]

is the internal energy, the full non-Gaussian Hamiltonian of Eq. (1) averaged by the approximate posterior Ansatz Eq. (30). The entropy of the approximate posterior is

\[ S(\bar{s}, S | d) = - \int d s \mathcal{P}(s | d, I) \ln \mathcal{P}(s | d, I) \]

\[ = \langle H(s | d, I) \rangle \]

The unknown parameters $m$, $t$, $D$, $\Theta$, and $C$ derive from a minimization of $G(\bar{s}, S | d)$ with respect to them. Ref. 10 provides implicit formula for this minimum, under certain approximations which seem to be equivalent to setting $C = 0$ and $\Theta = 0$. These implicit formula have to be solved numerically. A frequently used strategy in applications is to iterate the individual implicit formula and to hope for finding a fix point of the coupled system of equations within an acceptable computational time. This strategy is used for example in the D$^3$PO code for photon imaging 25, the RESOLVE code for radio interferometry 23, 24, and the tomography code for Galactic reconstruction.
This iterative strategy is computationally expensive as it converges only slowly.

Here, the minimization of the Gibbs free energy should provide us directly with an implicit numerical scheme in which the different equations are solved simultaneously, not iteratively. This is more efficient and more accurate, if we maintain the spectral uncertainty information as encoded in Θ and C.

### B. The building blocks

The Gibbs free energy consists of an entropy term and an internal energy, which is composed of three terms according to the three Hamiltonian components in Eq. (29) resulting from the likelihood, the field prior, and the spectral hyperprior, respectively.

1. **Entropy**

Thanks to the Gaussian Ansatz in Eq. (30), the entropy is independent of θ,

\[
S(\pi, S|d) = \frac{1}{2} \text{Tr} [1 + \ln (2\pi S)]
\]  
(34)

and therefore the gradients of S with respect to m and t vanish,

\[
\frac{\delta S}{\delta m} = 0, \quad \frac{\delta S}{\delta t} = 0.
\]  
(35)

For later usage, we also provide the gradient of the entropy with respect to the unknown covariance S,

\[
\frac{\delta S}{\delta S} = \frac{1}{2} S^{-1}
\]  
(36)

and its sub-covariances D, Θ, and C. For the latter we need

\[
S^{-1} = \begin{pmatrix}
E^{-1} & -D^{-1}C F^{-1} \\
-D\Theta^{-1}C & F^{-1}
\end{pmatrix}, \quad \text{with}
\]  
(37)

\[
E \equiv D + C \Theta^{-1}C^\dagger \quad \text{and}
\]  
(38)

\[
F \equiv \Theta + C^\dagger D^{-1}C.
\]  

In case C = 0, we would have E = D and F = Θ, but otherwise, the matrix inversion mixes between D and Θ.

The entropy-gradients with respect to the unknown sub-covariances are

\[
\begin{align*}
\frac{\delta S}{\delta D} &= \frac{\delta S}{\delta S} \frac{\delta S}{\delta D} = E^{-1} = (D + C \Theta^{-1}C^\dagger)^{-1}, \\
\frac{\delta S}{\delta \Theta} &= \frac{\delta S}{\delta S} \frac{\delta S}{\delta \Theta} = F^{-1} = (\Theta + C^\dagger D^{-1}C)^{-1}, \\
\frac{\delta S}{\delta C} &= \frac{\delta S}{\delta S} \frac{\delta S}{\delta C} = -E^{-1}C \Theta^{-1}, \quad \text{and}
\]  
(39)

\[
\frac{\delta S}{\delta C^\dagger} = \frac{\delta S}{\delta S} \frac{\delta S}{\delta C^\dagger} = -F^{-1}C^\dagger D^{-1}.
\]  

Here, A : B = Tr (A^\dagger B) is the matrix scalar product. We expect

\[
\left(\frac{\delta S}{\delta C^\dagger}\right)^\dagger = \frac{\delta S}{\delta C^\dagger}
\]  
(40)

and therefore

\[
E^{-1}C \Theta^{-1} = D^{-1}C F^{-1},
\]  
(41)

which is easily verified by inserting the definitions of E and F in Eq. (37).

The entropic forces \(f^S_D = -\delta S/\delta D\) and \(f^S_\Theta = -\delta S/\delta \Theta\) ensure for \(T > 0\) non-vanishing uncertainty covariances, as they push for larger covariances as one can read off from

\[
f^S_D \cdot D = T \text{Tr} \left( \left(1 + D C \Theta^{-1} C^\dagger\right)^{-1} \right) > 0 \quad \text{and}
\]  
(42)

\[
f^S_\Theta \cdot \Theta = T \text{Tr} \left( \left(1 + \Theta C^\dagger D^{-1} C\right)^{-1} \right) > 0.
\]  
(43)

In contrast, the entropic force \(f^S_C = -\delta S/\delta C\) reduces the magnitude of C as

\[
f^S_C \cdot C = -T \text{Tr} \left( \Theta^{-1} C^\dagger D^{-1} C \right) \leq 0.
\]  
(44)

All these forces try to increase the entropy. If not counterbalanced by other forces, they would lead to a state of complete lack of certainty, \(D = \infty\), \(\Theta = \infty\), and \(C = 0\).

2. **Hyperprior**

The spectral prior \(P(\tau)\) is the hyperprior of our problem. Its internal energy is

\[
U_r(\pi, S|d) = \langle H(\tau) \rangle \tilde{\rho} \equiv \frac{1}{2} T^t t + \frac{1}{2} T \Theta + \frac{3}{2} \tau^t \tau + \frac{1}{2} e^{-\tau + \Theta/2}.
\]  
(45)

Here and elsewhere, a dropped \(\tau\) between two vectors indicates component wise multiplication, \((q|t)_k = q_k t_k\), a tilde on a tensor means its diagonal vector in band harmonic basis, \(\Theta_k = \Theta_{kk}\), and a tilde on a vector denotes a tensor with the vector on the diagonal in band harmonic basis, \(\tilde{q}_k = \delta_{kk} q_k\). As a consequence of this notation we find \(\tilde{t} = t\) always, but \(\tilde{\Theta} = \Theta\) only for \(\Theta\) being diagonal in the harmonic basis. Similarly we define \(\tilde{m}_{xy} = \delta_{xy} m_{xx}\) as an operator which is diagonal in position basis and \(\tilde{D}_{xx} = D_{xx}\) the diagonal of D in position basis.

The corresponding non-vanishing gradients of the hyperprior internal energy are

\[
\frac{\delta U_r}{\delta t} = \frac{1}{2} \left( T^t + \tau^t \right),
\]  
(46)

\[
\frac{\delta U_r}{\delta \Theta} = \frac{1}{2} \left( T^t + \tau^t \right), \quad \text{with}
\]  
(47)

\[
t' \equiv \tau - \tilde{\Theta}/2.
\]  

3. **Prior**

The field prior \(P(\varphi; \Phi_r)\) provides the internal energy

\[
U_\varphi(\pi, S|d) = \langle H(\varphi; \Phi_r, I) \rangle \tilde{\rho} \equiv \frac{1}{2} \varphi^t \tau + \frac{1}{2} \sum_k e^{-\varphi_k} w_k, \text{ with}
\]  
(48)

\[
w_k \equiv \text{Tr} \left( P_k \left( (m - C_k) (m - C_k)^\dagger + D \right) \right),
\]  
(49)
and $C_k = (C_{kk})_{x} [3]$. The term $\frac{1}{2} \varphi \tilde{t}$ results from the log-determinant $\ln |2\pi \Phi|$ in $\mathcal{H}(\varphi, \Phi, I)$. The multiplicity $\varphi_k = \text{Tr} \Phi_k$ of a spectral band $k$ sharing the same harmonic eigenvalue $\lambda_k$ enters since the different harmonic modes count separately in the determinant in Eq. (11). This internal energy would simplify in case $C = 0$ to

$$U_\varphi(\varphi, S|d) \equiv \frac{1}{2} \left[ \varphi \tilde{t} + m^\dagger \Phi^{-1}_\varphi m + \text{Tr} (\Phi^{-1}_\varphi \tilde{m}) \right]$$

with $\Phi^{-1}_\varphi \equiv r^{-1} \sum_k \Phi_k e^{-t_k} \equiv r^{-1} \Phi \Gamma e^{-t}$. (46)

In the general case of $C \neq 0$, the associated gradients are

$$\delta U_\varphi \over \delta m^\dagger = \frac{1}{2} \Phi^{-1}_\varphi m - \frac{1}{2r} \sum_k e^{-t_k} \Phi_k C_k,$$

$$\delta U_\varphi \over \delta t = \frac{1}{2} \left( \varphi - r^{-1} \varphi \tilde{t} \right),$$

$$\delta U_\varphi \over \delta D = 1 \Phi^{-1}_\varphi,$$

$$\delta U_\varphi \over \delta \Theta_{kl} = -1 \sum_k e^{-t_k} w_k,$$

$$\delta U_\varphi \over \delta \Theta_k = -1 \sum_k e^{-t_k} \Phi_k (C_k - m).$$

It is interesting that $C$ can diminish the $m$-gradient generated by the prior precision matrix $\Phi^{-1}_\varphi$. Knowing that a more extreme $m$ will imply a higher inferred spectrum and therefore a smaller prior precision matrix, the system reduces the restoring force of the currently assumed spectrum. The last equation states, that in the absence of any other information forces, $C$ would adapt such that $C_k \equiv \Phi_k m$, which is fulfilled by $C_k = \Phi_k m$ as $\hat{F}_k \Phi_k \hat{F}_k = \Phi_k$. $C' \equiv C - C'$ would remove any restoring forces on $m$ from the precision matrix $\Phi^{-1}_\varphi$. There is, however, an entropic force on $C'$ and $C$ given by Eq. (58), which counteracts the pull towards $C'$ and ensures that the prior precision matrix influences the field inference to an appropriate degree.

4. Likelihood

The internal energy of the likelihood term should be denoted by $U_L$ with $L \in \{N, LN, PLN\}$ for the three likelihoods under investigation here. For the linear measurement of a normal field we have

$$U_N(S, S|d) = \mathcal{H}(d|\varphi, N)_{(x|d, I)}$$

$$\frac{1}{2} \text{Tr} \left[ (m m^\dagger + D) R^l N^{-1} R \right]$$

$$-m^\dagger R^l N^{-1} d,$$

$$\frac{\delta U_N}{\delta m} = R^l N^{-1} (R m - d),$$

$$\frac{\delta U_N}{\delta D} = \frac{1}{2} R^l N^{-1} R,$$

and all other gradients vanish. The corresponding results for $U_{LN}$ and $U_{PLN}$ can be found in Appendices [A] and [B] respectively. The likelihood provides a pull on the mean field towards $m' = (R^l N^{-1} R)^{-1} R^l N^{-1} d$, where $(R^l N^{-1} R)^{-1}$ denotes the pseudo inverse of $R^l N^{-1} R$.

C. Gibbs free energy

The Gibbs free energy $G = G(\varphi, S|d)$ is then

$$G \equiv U_L + \frac{1}{2} \varphi \tilde{t} + \frac{1}{2r} \sum_k e^{-t_k} w_k$$

$$+ \frac{1}{2} \varphi \tilde{t} T t + \frac{1}{2} \text{Tr} (T \Theta) + (\alpha - 1)^2 t + q \varphi \tilde{t}$$

$$- \frac{T}{2} \text{Tr} \left[ \ln (S) \right],$$

with $L \in \{N, LN, PLN\}$ and in particular

$$U_L \equiv \frac{1}{2} \text{Tr} \left[ (m m^\dagger + D) R^l N^{-1} R \right]$$

$$-m^\dagger R^l N^{-1} d.$$

VI. FREE ENERGY EXPLORATION

A. FrEE dynamics

The solution of the inference problem should be driven by the Gibbs free force. If $G(\varphi, S|d)$ is the Gibbs free energy of an inference problem, its negative gradient

$$f = \left( f_\varphi \over f_S \right) = -\left( \frac{\delta G}{\delta \varphi} \over \frac{\delta G}{\delta S} \right)$$

in terms of the signal mean $\varphi$ and its uncertainty dispersion $S$ should be the force which drives the dynamics. These forces will now be calculated for the CSI problem of the normal field measurement situation. The corresponding forces are composed according to Eq. (51) from Eqs. (36), (41), (47), and (48).
B. Signal mean

The mean field evolution is driven by the force

\[ f_m = R^t N^{-1} (d - R m) - r^{-1} \sum_k \varpi_k e^{-t^k} (m - C_k) \]

and stops evolving for a static \( \Phi \) as soon as

\[ \frac{m}{N} = (\Phi t^{-1} + R^t N^{-1} R)^{-1} R^t N^{-1} \times \left( d - r^{-1} \sum_k \varpi_k e^{-t^k} C_k \right) \]

(53)

is reached. This is the Wiener filter solution in case \( C = 0 \). However, \( \Phi t^{-1} = r^{-1} \sum_k \varpi_k e^{-t^k} \) evolves as well due to the force

\[ f_t = \theta - \left( \alpha - 1 + \frac{\theta}{2} + T \, t \right), \quad \text{with} \quad \theta = \{ q + \frac{w}{2^r} \} e^{-t^r}. \]

(54)

This stops evolving once

\[ e^{t^k} = \frac{q_k + \frac{1}{2^r} \text{Tr} \left[ \left( (m - C) (m - C)^\dagger + D \right) \varpi_k \right]}{(\alpha - 1 + \frac{\theta}{2} + T \, t)_k} \]

(55)

This formula reduces to the critical filter formula developed in Refs. [2, 10, 20, 22] in case \( C = 0 \) and \( \Theta = 0 \), the latter implying \( t = t' \). For a fixed \( m, D, \Theta, \) and \( C \) this implicit formula can be solved e.g. by iteration. However, these quantities evolve themselves and therefore it is advisable to solve the dynamics of all these quantities simultaneously.

Note, that while \( t' = t - \frac{1}{2^r} \Theta \) appears as the effective log spectrum in \( \Phi t^{-1} \) the dynamics is for \( t \) and also the smoothness enforcing term \( T \, t \) does not involve \( \Theta \).

The required quantity \( w \) needs that \( D = \text{Tr} (P \, D) \) as well as \( C \) are available according to Eq. (45). Also this requests that we investigate the uncertainty covariances \( D, C, \) and \( \Theta \) next.

C. Uncertainty covariances

1. Field uncertainty covariance

The field uncertainty covariance force

\[ f_D = \frac{1}{N} \left[ T \left( D + C \Theta^{-1} C^\dagger \right)^{-1} - \left( \Phi t^{-1} + R^t N^{-1} R \right) \right] \]

vanishes – for fixed \( \Phi t^{-1}, C, \) and \( \Theta \) – for the stationary force-free solution

\[ D = D^* \equiv \frac{T \left( \Phi t^{-1} + R^t N^{-1} R \right)^{-1} - C \Theta^{-1} C^\dagger}{= E \oplus A_D \equiv \Theta}. \]

(57)

It is reasonable to adapt this solution instantaneously at every time step. First, in most applications, there is no hope to store \( D \) in a computer memory. Second, adapting the force-free solution for \( D \) will immediately put us closer to the minimum of the Gibbs free energy \( G \) and therefore speed up the inference.

The term \( E = T \left( \Phi t^{-1} + R^t N^{-1} R \right)^{-1} \) to which \( D \) reduces for \( C = 0 \) was encountered already in Eq. (26) for the natural choice \( T = 1 \). For this term, an implicit representation is possible, as all operator terms in \( E^{-1} \) can be represented as computer routines, and the application of \( E \) to a vector \( j \), \( m = E \, j \), can therefore be obtained from a CG based solving of \( E^{-1} \, \text{m} = j \). If \( C \) and \( \Theta \) are available, \( D \) can therefore be applied to any vector. For later reference, we note, that

\[ D^{-1} = (E - A_D)^{-1} \]

\[ = (1 - E^{-1} A_D)^{-1} E^{-1} \]

(58)

can as well be represented by an implicit routine, based on a CG inversion of \( 1 - E^{-1} A_D \). A numerical necessity is that \( E^{-1} C \Theta^{-1} C^\dagger < 1 \) all the time and therefore that \( \Theta \) stays sufficiently large.

The impact of implicitly solving \( \Delta \) is 0 for \( D \) has to be taken into account by adding the effect any changing quantity affecting \( D \) has on \( G \). Relevant quantities are \( t, C, \Theta, \) and \( D \), since those affect \( D \) according to Eqs. (57), (44), and (43). However, we find the relevant gradients are not changed, as the implicit solution for \( D \) is at a (constrained) minimum of \( G \):

\[ \frac{\delta G}{\delta t_k} \bigg|_{D = D'} \equiv \frac{\delta G}{\delta D} \bigg|_{D = D'} = 0 \text{ as well as} \]

\[ \frac{\delta G}{\delta \Theta} \bigg|_{D = D'} = 0 \text{ for the same reason,} \]

(59)

and so forth.

2. Spectral uncertainty covariance

The uncertainty covariance of the spectral field \( \tau \) has the force

\[ f_\theta = \frac{1}{2} \left[ T \left( \Theta + C^\dagger D^{-1} C \right)^{-1} - (T + \Theta) \right] \]

(60)

acting on it, which drives the \( \Theta \)-evolution until it reaches a stable configuration at

\[ \Theta^* = T \left( T + \Theta \right)^{-1} - C^\dagger D^{-1} C. \]

(61)

We should again adapt the fix point solution \( \Theta = \Theta^* \) immediately at every step of the dynamics. No other

\[ ^5 \text{The extra term} \ A_D = C \Theta^{-1} C^\dagger \text{seems to reduce the field uncertainty covariance} \ D \text{with respect to} \ \theta \text{and the value} \ D \text{has in case of known spectrum (Eq. (26)). However, this conclusion is not correct, as the effective spectrum} \ r \ \text{appearing in} \ D \text{and} \ E \text{is also decreased in the presence of} \ C \sim \Phi, \text{as an inspection of} \ w \text{as given by Eq. (45) reveals. Thus, this extra term just compensates for some otherwise too strong enlargement of the field uncertainty covariance caused by the reduced inferred effective spectrum.} \]


The dynamical equation has to be changed in this case for exactly the same reason as the one we encountered when adapting the temporary fix points for $D$.

For most application, it should be possible to invert $T + \tilde{\theta}$ numerically at every time step, so that an explicit representation of $F = T \left( T + \tilde{\theta} \right)^{-1}$ is available. Its contribution to $\hat{\Theta}$ can be read off, however, the contribution from the term $A_\Theta = C^T D^{-1} C$ is more tricky, as it contains $D^{-1} = (E - C \Theta^{-1} C^T)^{-1}$ that again depends on $\Theta$. We propose to shortcut this infinite recursion by using the following approximations:

$$A_D = C \Theta^{-1} C^T \approx C F^{-1} C^T$$

$$A_\Theta = C^T D^{-1} C \approx C^T E^{-1} C$$

(62)

3. **Uncertainty covariance of field and spectrum**

The $C$-force is

$$f_C = \frac{1}{2r} e^{-t'} \left[ \rho (m - C) \right] - \frac{T}{2} E^{-1} C \Theta^{-1}$$

(63)

Setting the force $f_C$ to zero, we can solve for the operator $C$. To do this, we change into the orthonormal eigenbasis of the $\Theta$ operator, with eigenvalues $\lambda_i$ and corresponding eigenvectors $a_i$, where we can write:

$$\Theta^{-1} = \sum_i \lambda_i^{-1} a_i a_i^\dagger$$

(64)

The operator $C$ can be expressed as:

$$C = \sum_i c_i a_i^\dagger$$

(65)

Multiplying the force $f_C$ by the eigenvector $a_i$ gives us the force on the map $c_i$:

$$f_C a_i = \frac{1}{2r} e^{-t'} \left[ \rho (m a_i - \sum_j c_j a_j^\dagger a_i) \right] - \frac{T}{2} E^{-1} \sum_j c_j a_j^\dagger \sum_l \lambda_l^{-1} a_l a_l^\dagger a_i$$

(66)

Setting this equation to zero and using orthonormality of the eigenvectors, we get:

$$0 = \frac{1}{2r} e^{-t'} \left[ \rho (m a_i - c_i) \right] - \frac{T}{2 \lambda_i} E^{-1} c_i$$

(67)

$$\frac{1}{2r} e^{-t'} \rho m a_i = \left[ \frac{1}{2r} e^{-t'} \rho + \frac{T}{2 \lambda_i} E^{-1} \right] c_i$$

(68)

This can be solved and rewritten as:

$$c_i = \frac{\lambda_i}{r} \left[ (1 + \frac{\lambda_i}{r}) \Phi^{-1} + R^\dagger N^{-1} R \right]^{-1} \Phi^{-1} a_i^\dagger \rho m$$

(69)

The force free operator $C$ can now be constructed out of all maps $c_i$ with corresponding eigenvectors $a_i$. Calculating the whole off-diagonal operator involves the numerical inversion of an operator for each band $i$. For large problems, this computationally expensive task is impracticable and slows down the inference. Therefore, we propose using only the $c_i$ corresponding to the largest eigenvalues $\lambda_i$ of $\Theta$, or to drop $C$ completely.

4. **Precision matrix**

The global signal posterior precision matrix can now be written as

$$S^{-1} = \begin{pmatrix} E^{-1} & -E^{-1} C \Theta^{-1} \\ -\Theta^{-1} C^T E^{-1} & F^{-1} \end{pmatrix},$$

with

$$E^{-1} = T^{-1} \left( \Phi_{x} + R^\dagger N^{-1} R \right)$$

and

$$F^{-1} = T^{-1} (T + \tilde{\theta})$$

being well applicable and therefore also numerically invertible operators. The non-diagonal blocks were written in a form that avoids the operator $D^{-1}$ and particularly ensures that $S^{-1}$ is always self-adjointed.

D. **Fixing the fix point**

The fix point of the system of equations worked out above exhibits a defect. Eqs. 54 and 55 state that at the fix point we should have

$$\theta = \alpha + 1 + \frac{\bar{q}}{2} + T t$$

To simplify matters, let us assume we have an uninformative spectral hyperprior ($\alpha = 1$, $q = 0$), standard temperature ($T = 1$), and the obtained spectrum is power-law like ($T t \approx 0$). Then the spectral uncertainty covariance is $\Theta = \left( T + \frac{\bar{q}}{2} \right)^{-1} - A_\Theta$, which turns out to be very narrow. First, we note that the term $-A_\Theta$ only tightens an already tight variance $F = \left( T + \frac{\bar{q}}{2} \right)^{-1}$. The latter does not depend on the data, as $T$ and $q$ are completely predefined. Thus, the spectral uncertainty seems to be nearly independent of how the measurement was performed, except for a small correction by $-A_\Theta$, which only worsens the problem of a too tight uncertainty covariance. The spectral uncertainty should, however, depend on the data quality and be larger for less informative data. Here it seems, that all signal field degrees of freedom provide confidence to the spectral determination, irrespectively whether they were directly determined by the prior and data (the term $q + \frac{1}{2r} \text{Tr} [(m - C) (m - C)^\dagger \rho]$, or only guessed by a covariance (the term $\frac{1}{2r} \text{Tr} [D F]$ in $w$).

In order to fix this, we propose to modify the formula for $F$ to

$$F = T \left( T + \tilde{\theta} \right)^{-1}$$

with

$$\tilde{\theta} = \left( q + \frac{w'}{2r} \right) e^{-t'}$$

(71)

$$w' = \text{Tr} [(m - C) (m - C)^\dagger \rho] = w - \text{Tr} [D F].$$

This way, the uncertainty information $D$ is not counted when the certainty of $\tau$ is estimated. Effectively, this corresponds to using a reduced number of degrees of freedom $\bar{q}' < q$ while estimating the spectral uncertainty. For our simplified case ($\alpha = 1$, $q = 0$, $T t \approx 0$) we have $\bar{q}' = w'/w$. 

The deeper reason for this defect delivers also a justification for our fixing strategy. The Gibbs free energy approach is equivalent to minimizing the Kullback-Leibler divergence

$$d_{KL}({\hat{P}}||P) = \int \mathcal{D}s \, {\hat{P}}(s|d) \ln \left( \frac{{\hat{P}}(s|d)}{P(s|d)} \right)$$

of our approximated posterior $P(s|d) = \mathcal{G}(s - \pi, D)$ to the correct one, $P(s|d)$. This is, however, only an approximation, and not even the most optimal one. It was shown from first principles in [29] that the information optimal scheme would minimize the inverse Kullback-Leibler divergence, $d_{KL}(P||\hat{P})$. It turns out that this demands that the first and second moments of $P(s|d)$ are calculated and used to specify the Gaussian approximation $P(s|d)$. The Gibbs free energy approach was, however, just introduced to facilitate the calculation of these moments, which are otherwise hard to calculate.

Fortunately, the spectral uncertainty $\sigma_k^2$ of a Gaussian random field in a spectral band $k$ of which $\phi_k$ modes were measured turns out to be $\sigma_k^2 = \frac{2}{T} \phi_k$ in the absence of any prior information ($a = 1, q = 0, T = 0$). The fix proposed above just introduces a correction so that only the number of effectively measured spectral degrees of freedom, $\phi'$, and not the total number, $\phi$, are used in the calculation of spectral uncertainty such that in the prior free case the well known result $\sigma_k^2 = \frac{2}{T} \phi_k$ is recovered.

### E. Numerical steps

#### 1. Notation

Let $z = (m, t, c, D, \Theta)$ be the argument vector of the Gibbs free energy $G(z)$ we intend to minimize, or, alternatively, the vector of the fields we track dynamically, $z = (m, t, A_x, A_\Theta, D, \Theta, \ldots)$: We split $z = (x, y)$ into the part for which we follow explicitly the gradient dynamics, $x = (m, t) = \pi$, and the part evolving implicitly or estimated stochastically $y = (c, A_x, A_\Theta, D, \Theta, \ldots)$.

The FrEE dynamics for $x$ is driven by its Gibbs free energy force

$$f = -\frac{\partial G(x, y)}{\partial x},$$

which imposes on $x$ the velocity

$$\frac{dx}{dt} = \Gamma f.$$
The operator $\Gamma$ steers the algorithm. We get a Newton scheme if $\Gamma = S = (\delta^2 G / \delta x \delta x^\dagger)^{-1}$ and the time steps are $\delta t = 1$, such that

$$x \leftarrow x + \Gamma f.$$  \hspace{1cm} (75)

In case of non-convex problems, $S$ can develop temporarily negative eigenvalues, which would spoil the numerical scheme.

To avoid this problem, we propose to steer the degrees of freedom of $x$ individually by adding a mass matrix-like term,

$$\Gamma = (S^{-1} + \hat{\eta})^{-1},$$  \hspace{1cm} (76)

with a suitably chosen damping vector $\eta$ with $\eta > 0$ in all components. $\eta = \lambda$ with a global tuning parameter $\lambda$ would correspond to Levenberg’s algorithm \[31] and $\hat{\eta} = \lambda f f^\dagger$ would to the Levenberg–Marquardt algorithm \[32]. Here, we pragmatically propose to tune the components of $\eta$ on the fly.

To this end, we set $\eta = S^{-1} \eta'$ to introduce with $S^{-1} = (E^{-1}, F^{-1})^\dagger$ typical scales, so that $\eta'$ is dimensionless. The latter is component wise steered via

$$\eta' \leftarrow \eta' \begin{cases} f_{\eta'}^\text{acc} \quad \delta x_n \delta x_{n-1} > 0 \\ f_{\eta'}^\text{break} \quad \delta x_n \delta x_{n-1} \leq 0 \end{cases}$$  \hspace{1cm} (77)

where $\delta x_n$ is the update vector of step $n$ and $f_{\eta'}^\text{acc} = 0.5$ and $f_{\eta'}^\text{break} = 3$ are our empirical choices for the numerical tuning parameters. $\eta' \geq 0.3$ is ensured in every step, to keep the scheme ready to damp any degree of freedom that starts to get unstable.

This way, any oscillating parameter gets damping. When the scheme reached the minimum, all parameters will oscillate around the equilibrium position and $\delta x_n \delta x_{n-1}$ will have random signs.

3. Implementation simplifications

Not all the discussed terms are essential in every situation. The related critical filter scheme for CSI lacks many of the here discussed terms, but provides acceptable results. Therefore, a number of simplifications are adapted here to reduce the computational complexity:

- The terms $A_D$ and $A_D$ are approximated as in Eq. \[62]. This truncates the mutual dependence of the $D$ and $T$ operators.

- The field-to-spectral uncertainty cross-correlation term $C$ is set to zero in most numerical runs, as no significant effect of it on the numerical speed, or the results could be
detected. An inspection of \( C \) in Sect. VII A 2 reveals that it is of a low relative amplitude in the test cases we investigate.

- Steering was only applied to the \( t \)-dimension, the spectral components of \( x \). In case of very stiff problems, an extension to \( m \) might be necessary. This will be used for the LN problem presented below, which is stiff due to a response function mimicking a radio interferometer.

- The CG used to calculate steps of the Newton scheme was run with moderate accuracy, as all steps are only intermediate. Experiments with low accuracy CG had a worse performance.

The implementation of the CSI algorithm was done in NIFTy 1.0 [19].

VII. EXAMPLES

To illustrate the performance for normal (N), log-normal (LN), and Poisson-log-normal (PLN) fields, the CSI algorithm was applied to mock data generated with such statistics. We report about the results.

A. Normal field

1. Spatial and spectral reconstruction

A normal field, the power spectrum of its generating statistical process, noisy data tracing a Gaussian-convolved version of the field, and the reconstruction of the field and its spectrum are displayed in Fig. 1. The field is well reconstructed within the uncertainties, which are much smaller than the scatter of the data. The power spectrum, however, is reconstructed with an overconfidence in the higher spectral bins (darkly shaded in the bottom right panel of Fig. 1) unless the fix to the effectively measured degrees of freedom as described in Sect. VII D is applied (lightly shaded). It is very apparent that this correction is necessary as the Gaussian point spread function has erased a large part of the information of the signal field spectrum on small spatial scales. We will adapt this correction for the remaining discussion of the N example and also for the LN and PLN examples.

2. Spectral uncertainty structure

The CSI algorithm provides the full spectral uncertainty covariance matrix, which in its corrected form (see discussion in Sect. VII D) is displayed for our example in the top left panel of Fig. 2. The large uncertainty of the highest Fourier band powers is obviously correlated, as the spectral smoothness prior prevents these from varying independently. The eigenvalues of this uncertainty covariance matrix span two orders of magnitude (top right panel). The eigenvector \( a_0 \) corresponding to the largest eigenvalue (see bottom left panel) expresses the substantial and correlated uncertainty of the small-scale power spectrum (see bottom right corner of top left panel). The next important eigenvector \( a_1 \) allows for structure in this part of the spectrum via a sign change and captures the main spectral uncertainty for large spatial scales (see top left corner of top left panel).

Finally, Fig. 2 displays the corresponding \( c \)-fields, that were calculated according to Eq. (69), and which form, together with their eigenvectors, the spectral uncertainty covariance operator \( C \) according to \( C = \sum_i c_i a_i^t \) (Eq. (65)). The \( c_i \)-field expresses how the reconstruction \( m \) changes with a change of the spectrum according to the corresponding spectral uncertainty eigenvector \( a_i \) and vice versa. As the \( c \)-fields are filtered versions of the reconstruction \( m \), a scaled version of this is displayed in Fig. 2 for comparison.
B. Log-normal field

A LN field is a good representation of diffuse emission on the celestial sphere, as it is strictly positive, spatially correlated, and varies over orders of magnitude in intensity. To present the performance of the CSI algorithm for LN fields with non-trivial measurement response, we adapt an idealized radio interferometric measurement situation. The brightness field (top left panel of Fig. 3) is measured in its Fourier representation at the Fourier locations indicated (top right panel). This is a very incomplete coverage, with about 80% of the necessary image information missing. Consequently, the back projected data (bottom right panel), the so called dirty image in radio astronomical language, is a relative poor representation of the true sky. In particular it contains areas with nonphysically negative flux densities. The CSI reconstruction (bottom left) managed to recover all brighter structures well, and a good fraction of the dim emission regions.

The simultaneously recovered power spectrum is shown in Fig. 4. Although the power spectrum uncertainty correction of Sect. (VI D) is applied, the true and reconstructed spectra deviate by a few sigma for some of the intermediate spectral bands. The origin of this discrepancy is not completely clear, as it could be due to the neglected $C$ terms, just a statistical fluctuation, an expression of the strong non-Gaussianity of the underlying probabilities, or – most likely – a combination of such factors.

C. Poisson Log-Normal Field

Finally, the performance of CSI on PLN reconstruction problems should be shown. Such problems occur for example in astronomical imaging with photon counts. Fig. 5 shows a PLN field, data drawn from it, and the reconstruction of the field and its spectrum. The real signal and spectrum lie well within the corresponding uncertainties.

VIII. CONCLUSION

Correlated signal inference (CSI) poses numerical challenges. We address these by the Free Energy Exploration (FrEE) strategy. This proposes to simplify the inference problem via the construction of a Gaussian approximation of the posterior, to reconstruct nuisance and hyper-prior quantities explicitly, and to use stochastic probing of expensive operator properties, as well as to automatically steer the step size of the individual signal and power spectrum components. The resulting NIFTY implementation of CSI accurately reconstructed normal, log-normal, and Poisson log-normal fields as well as the power spectra of their
generative processes. Uncertainty information on all these quantities is provided alongside. CSI is therefore mature for the usage on real data applications, since prototypes of a radio interferometric and a photon count imaging algorithm performed well. Furthermore, the FrEE strategy seems also to be sufficiently robust to be applied to other signal inference problems in information field theory.

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Appendix A: Log-normal model

1. Field measurement

Many measured signal fields are strictly positive and vary rather in magnitude than on a linear scale. An example for such is the sky brightness \( s \). Here a log-normal model is more appropriate where a Gaussian field \( \varphi = \ln s \) is exponentiated before linearly measured. Thus, we have

\[
d = \text{Re}\varphi + n
\]

and consequently

\[
P(d|\varphi, \text{LN}) = \mathcal{G}(d - \text{Re}\varphi, N)
\]

as well as

\[
\mathcal{H}(d|\varphi, \text{LN}) \equiv \frac{1}{2} (d - \text{Re}\varphi)^\dagger N^{-1} (d - \text{Re}\varphi).
\]

In case of known field covariance \( \Phi \), the joint Hamiltonian

\[
\mathcal{H}(d, \varphi|\Phi, \text{LN}) = \mathcal{H}(d|\varphi, \text{LN}) + \mathcal{H}(|\varphi, \Phi)
\]

\[
\equiv \frac{1}{2} \varphi^\dagger \Phi^{-1} \varphi + \frac{1}{2} (d - \text{Re}\varphi)^\dagger N^{-1} (d - \text{Re}\varphi).
\]

does not permit a linear estimate of the posterior mean field \( m = \langle \varphi|d, \varphi, \text{LN} \rangle \) or mean signal \( \tilde{s} = \langle \text{e}^\varphi |d, \varphi, \text{LN} \rangle \). An unknown covariance further complicates this problem considerably.

2. Likelihood contribution

The LN-likelihood internal energy and its gradients,

\[
U_{\text{LN}}(m, D|d) = \langle \mathcal{H}(d|\varphi, \text{LN}) |(\varphi, d, t) \rangle
\]

\[
\equiv \frac{1}{2} \int dx \int dy \left( R^t N^{-1} R \right)_{xy}
\]

\[
\times e^{m_x^\dagger + m_y^\dagger + D_{xy}}
\]

\[
- e^{m_x^\dagger} R^t N^{-1} d,
\]

with

\[
m' = m + \frac{1}{2} \tilde{D}, \text{ and }
\]

\[
\delta U_{\text{LN}} \bigg/ \delta m_x = e^{m_x^\dagger} \int dx \left( R^t N^{-1} R \right)_{xy} e^{m_x^\dagger + D_{xy}}
\]

\[
- (R^t N^{-1} d)_x,
\]

\[
\delta U_{\text{LN}} \big/ \delta D_{xy} = \frac{1}{2} \left( R^t N^{-1} R \right)_{xy} e^{m_x^\dagger + m_y^\dagger + D_{xy}}
\]

are a bit intricate due to the \( e^{D_{xy}} \) terms. These would require, in principle, an explicit calculation of all these matrix elements, which is currently completely out of reach for megapixel sized field inference problems requiring to track 10^{12} entries of \( D \). We will therefore replace \( D_{xy} \rightarrow \frac{1}{2} \left( \tilde{D}_x + \tilde{D}_y \right) \), with \( \epsilon \in [0, 1], \epsilon = 1 \) is a reasonable approximation if the field correlation volume exceeds largely the footprint of the point spread function (and the noise covariance is diagonal). This might be the case for highly resolving imaging instruments. \( \epsilon = 0 \) should be a suitable approximation in case it is exactly the other way around, as it is the case in interferometry and tomography, where the instrument data are influenced by extended integration regions.

With this approximation, we define \( m' = m' + \frac{1}{2} \tilde{D} + m + \frac{1}{2} \tilde{D} \) and \( R_m = \text{Re}\tilde{m} \) so that

\[
\delta U_{\text{LN}} \big/ \delta m = R_{m'} N^{-1} R e^{m'} - R_{m''} N^{-1} \equiv -j,
\]

\[
\delta U_{\text{LN}} \big/ \delta D_{xy} = \frac{1}{2} \left( R_{m'} N^{-1} R_{m''} - j \right).
\]

During the Gibbs free energy decent of the algorithm, the term \(-j\) is omitted in the last equation, to ensure positive definiteness of \( S \).

Appendix B: Poisson Log-normal model

1. Field measurement

Here, the signal \( s = e^\varphi \) is again log-normal, but the measurement is Poissonian and therefore subject to signal dependent shot noise. The signal response \( R \) only determines the expected number \( \mu = \langle d|d, s, \text{PLN} \rangle \) of counts according to

\[
\mu = R e^\varphi + b, \quad \text{(B1)}
\]
where \( b \) is the background count rate, here assumed to be known. An individual datum \( d_i \in \mathbb{N} \) follows the Poisson distribution

\[
P(d_i|m) = \frac{P^d_i}{d_i!} e^{-m_i}
\]  

(B2)

independently of the other data. Therefore,

\[
\mathcal{H}(d|\varphi, \text{PLN}) \approx 1^T R e^{\varphi} - d^T \ln (R e^{\varphi} + b),
\]

(B3)

where the logarithm has to be applied component wise. The joint Hamiltonian in case of known covariance

\[
\mathcal{H}(d, \varphi|\Phi, \text{PLN}) = \mathcal{H}(d|\varphi, \text{PLN}) + \mathcal{H}(\varphi|\Phi)
\]

(B4)

\[
= \frac{1}{2} \varphi^T \Phi^{-1} \varphi + 1^T R e^{\varphi} - d^T \ln (R e^{\varphi} + b)
\]

also does not permit simple linear estimate of the posterior mean field \( m = \langle \varphi \rangle|d, \Phi, \text{PLN} \rangle \) or mean signal

\[
\pi = \langle e^{\varphi} \rangle|d, \Phi, \text{PLN} \rangle.
\]

It is interesting to note that in case of no background \( b = 0 \), a local response \( R_{i\alpha} = r, \delta(x - x_i) \) and a restriction of the field to the measured locations, \( \phi = \langle \phi(x_i) \rangle \), its Hamiltonian

\[
\mathcal{H}(d, \phi|\Phi, \text{PLN}, b = 0, r) \approx \frac{1}{2} \partial^T \Phi^{-1} \phi + \ln |\Phi| - d^T \phi + e^{\varphi}
\]

(B5)

becomes structurally similar to that of the log-spectrum given by Eq. (21).

2. Likelihood contribution

The PLN-likelihood internal energy is

\[
U_{\text{PLN}}(m, D|d) = \langle \mathcal{H}(d|\varphi, \text{LN}) \rangle|\varphi(d, t) \rangle
\]

\[
\approx 1^T R e^{m' - d^T \ln (R e^{m' + b})} \tilde{\varphi}_{\varphi(D)}
\]

(B6)

where

\[
\langle \ln (R e^{m' + b}) \rangle_i = \ln \left( \frac{R^i e^{m' + b_i}}{R^i e^{m'' + b_i}} \right)
\]

(B7)

with

\[
\langle \ln (1 + \varepsilon_i) \rangle = 0 + \langle \varepsilon_i \rangle - \frac{1}{2} \langle \varepsilon_i^2 \rangle + \ldots
\]

\[
= \int dx \int dy e^{m'_i + m'_y} (1 - e^{D_{xy}}) R_{i\alpha} R_{i\beta}
\]

\[
\times 2 \left( R^i e^{m' + b_i} \right)^2
\]

(B8)

as correction term.

The gradients are then

\[
\frac{\delta U_{\text{PLN}}}{\delta m_i} \approx e^{m'_i} \left( 1 - \frac{d}{\mu} \right)^T R
\]

\[
- \sum_i \frac{d_i}{\mu_i} e^{m'_i} R_{i\alpha} \int dy e^{m'_y} (1 - e^{D_{xy}}) R_{i\beta}
\]

\[
+ \sum_i \frac{d_i}{\mu_i} R_{i\alpha} e^{m'_y} \int dz \left( \int dy e^{m'_i + m'_y} (1 - e^{D_{xy}}) R_{i\gamma} R_{i\beta} \right),
\]

(B9)

with \( \mu = R e^{m'} + b \), and

\[
\frac{\delta U_{\text{PLN}}}{\delta D_{xy}} \approx \frac{1}{2} \delta_{xy} e^{m'_y} \left( 1 - \frac{d}{\mu} \right)^T R
\]

\[
- \sum_i \frac{d_i}{\mu_i} \delta_{xy} e^{m'_y} R_{i\alpha} \int dy e^{m'_y} (1 - e^{D_{xy}}) R_{i\beta}
\]

\[
+ \sum_i \frac{d_i}{\mu_i} \delta_{xy} e^{m'_y} R_{i\alpha} \int dz \int dy e^{m'_i + m'_y} (1 - e^{D_{xy}}) R_{i\gamma} R_{i\beta}
\]

\[
+ e^{m'_i + m'_y} e^{D_{xy}} \sum_i \frac{d_i}{\mu_i} R_{i\alpha} R_{i\beta}
\]

Using as for the LN case the approximation \( D_{xy} \approx \frac{1}{2} (D_{xx} + D_{yy}) \) in exponents, the notation \( m'' = m' + \frac{1}{2} \tilde{D} \) and \( R_m = R e^{m''} \), we get

\[
\frac{\delta U_{\text{PLN}}}{\delta m} \approx \left( 1 - \frac{d}{\mu} \right)^T R_{m'}
\]

\[
- d^T \mu^{-2} \left( R_{m'} R_{m''} - R_{m''} R e^{m''} \right)
\]

\[
+ d^T \mu^{-3} R_{m'} \left[ \left( R e^{m''} \right)^2 - \left( R e^{m''} \right)^2 \right]
\]

\[
\approx \frac{1}{2} \left( R^i_{m'} d \mu^{-2} R_{m''} - \frac{j}{2} \right)
\]

(B10)

(B11)

In the implementation of the PLN reconstruction only the first term in Eq. (B10) is actually used, as the others are small corrections. During the Gibbs free energy decent of the algorithm, the term \( j \) is omitted in the last equation, to ensure positive definiteness of \( S \). It is, however used when the minimum is reached, to calculate the correct covariances. Note that

\[
j \approx \left( 1 - \frac{d}{\mu} \right)^T R_{m'}
\]

\[
+ 2 \varepsilon d^T \mu^{-2} R_{m'} \tilde{D} R_{m'}
\]

\[
- 2 \varepsilon d^T \mu^{-3} R e^{m''} R_{m'} \tilde{D} R_{m'} + \mathcal{O}(\varepsilon^2)
\]

(B12)

has only a significant contribution of order \( \mathcal{O}(\varepsilon) \) if the background \( b \) is large.
Appendix C: Operator probing

We propose to treat terms like $\hat{D}$ as independent, dynamically evolving quantities. Since we rarely have an explicit representations of $D$, which explicitly carries matrix elements required for these quantities of interest, an expensive and noisy stochastic estimation invoking the implicit representation of $D$ has to be performed. While doing this, we should take care to retain any already obtained information on these quantities for the sake of reducing noise and computational costs.

As detailed below, each such quantity $A \in \{ \hat{D}, A_x, A_A \}$ can be estimated stochastically by calculating the trace of a specific operator $\mathcal{O}_A$ by probing

$$A \equiv \text{Tr}[\mathcal{O}_A] = \langle \xi | \mathcal{O}_A \xi \rangle_{(\xi)} , \quad \text{(C1)}$$

where we will use only a finite number of white noise samples $\xi \leftarrow \mathcal{P}(\xi) = \mathcal{G}(\xi, 1)$ to estimate the average.

The diagonal $\hat{D}$ of the field uncertainty dispersions provides diagnostically valuable uncertainty quantification, as $\varphi = m_x \pm \hat{D}_x^{1/2}$ in colloquial language. Furthermore, knowing $\hat{D}$ is also required by the FrEE dynamics in case of the LN- and PLN-lielihoods (see Appendices A and B). We write

$$\hat{D}_x \equiv D_{xx} = \text{Tr}[\mathcal{O}_x D] = \langle \xi | \mathcal{O}_x D \xi \rangle_{(\xi)} \equiv \langle \xi | (D_{xx}) \xi \rangle_{(\xi)} . \quad \text{(C2)}$$

where the $*$ operator vector projects out the position space diagonal of a matrix $D$ if applied to this with the matrix scalar product $\text{Tr}(\mathcal{O} D) = \hat{D}$. Thus we have $\mathcal{O}_D = \mathcal{O} D$. Since $\hat{D} \in [0, \Phi]$ we clip these values. The harmonic space field uncertainty

$$\hat{D}_h \equiv \text{Tr}[\mathcal{P}_k D] = \langle \xi | \mathcal{P}_k D \xi \rangle_{(\xi)}$$

can be obtained by stochastic probing the operator $\mathcal{P}_D = \mathcal{P} D$. While doing so, we should use a minimum of prior information on the values of $D$. First $\hat{D} \geq 0$ since $D$ is a covariance. From $D \leq \Phi = r \mathcal{P} \mathcal{E}$ we conclude

$$\hat{D} \leq \text{Tr}[\mathcal{P} \Phi] = r \mathcal{P} \mathcal{E} \hat{D} \equiv \Phi \mathcal{P}$$

and therefore enforce $\hat{D}_h \in [0, \Phi \mathcal{P}]$ by clipping any value outside of this interval.

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