Bayesian reconstruction of the cosmological large-scale structure: methodology, inverse algorithms and numerical optimization

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ABSTRACT

We address the inverse problem of cosmic large-scale structure reconstruction from a Bayesian perspective. For a linear data model, a number of known and novel reconstruction schemes, which differ in terms of the underlying signal prior, data likelihood, and numerical inverse extra-regularization schemes are derived and classified. The Bayesian methodology presented in this paper tries to unify and extend the following methods: Wiener-filtering, Tikhonov regularization, Ridge regression, Maximum Entropy, and inverse regularization techniques. The inverse techniques considered here are the asymptotic regularization, the Jacobi, Steepest Descent, Newton-Raphson, Landweber-Fridman, and both linear and non-linear Krylov methods based on Fletcher-Reeves, Polak-Ribiére, and Hestenes-Stiefel Conjugate Gradients. The structures of the up-to-date highest-performing algorithms are presented, based on an operator scheme, which permits one to exploit the power of fast Fourier transforms. Using such an implementation of the generalized Wiener-filter in the novel ARG0-software package, the different numerical schemes are benchmarked with 1-, 2-, and 3-dimensional problems including structured white and Poissonian noise, data windowing and blurring effects. A novel numerical Krylov scheme is shown to be superior in terms of performance and fidelity. These fast inverse methods ultimately will enable the application of sampling techniques to explore complex joint posterior distributions. We outline how the space of the dark-matter density field, the peculiar velocity field, and the power spectrum can jointly be investigated by a Gibbs-sampling process. Such a method can be applied for the redshift distortions correction of the observed galaxies and for time-reversal reconstructions of the initial density field.

Key words: large-scale structure of Universe – galaxies: distances and redshifts – methods: data analysis – methods: statistical – methods: numerical – techniques: image processing

1 INTRODUCTION

According to our current picture of cosmogenesis, the galaxies, galaxy clusters, galaxy filaments, and giant voids forming the cosmic large-scale structure (LSS) are products of gravitational instability, which pulls increasingly more matter onto the tiny primordial seed density fluctuations generated at the very first epoch of inflation. The shape and size of the cosmic matter distribution reflects the initial conditions set during or shortly after Big Bang, as well as the interplay of the gravitational self-attraction of matter and the diluting action of the Hubble expansion of cosmic space. Valuable information about the properties and the origin of the cosmic inventory are encoded in the LSS, however, on small-scales, that information is being erased through dynamical non-linear processes.

Our goal is to extract as much of this information as possible from astronomical measurements, which introduce uncertainties and, consequently, degeneracies. Therefore, we have to adapt an information-theoretical approach to solve the reconstruction problem of cosmography. The Bayesian framework turns out to be the most general approach as we will discuss later. In this paper we present the novel ARG0-software package, which reconstructs the three-dimensional density field from the information provided by galaxy surveys with different Bayesian and inverse methods. Here we focus our study on understanding the Bayesian theoretical background and the required algorithmic aspects. Further extensions of the code in which the power-spectrum and the peculiar velocities can be jointly sampled are presented and tested on mock galaxy catalogues. Some of the preliminary results are presented and future development is outlined.

The large number of telescopes performing galaxy surveys with increasing depth, sky coverage, and accuracy in position and distance (or redshift) determination provide us with superb data on

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1 Algorithm for the Reconstruction of Galaxy-traced Over-densities
the cosmic matter distribution at an exponentially increasing rate. One problem is that the discrete objects these instruments reveal to us, the galaxies, are the result of a complex non-linear evolution of cosmic matter combined with complicated astrophysical processes such as star formation. A translation of the galaxy data into the much better understood large-scale dark matter (DM) distribution, which would be much easier to analyze for imprints of cosmologically interesting effects, is far from trivial. The discrete nature of galaxies introduces certain noise, usually modeled by shot noise. Moreover, the partially understood galaxy-formation process inserts systematic uncertainties. In addition, the limited volume of surveys adds complications beyond the problems of galaxy-distance determination being contaminated by observational and velocity redshift-distortions. All these complications have to be dealt with simultaneously and in a controlled fashion. Since it cannot be assumed that the correct or optimal values for the various degrees of freedom of the problem (bias factors, redshift-corrections, etc.) will be guessed a priori, repeated and iterative data analysis is mandatory in order to achieve a high-fidelity and well-understood cosmic map. For example, a correction of redshift-distortions of the galaxies requires the gravitational potential generated by the matter distribution, which would be much easier to analyze for imprints of cosmological interest.

Repeated generation of cosmic matter maps increases the urge to face another challenge, the scaling of the performance of the underlying map-generation algorithms with the data size. Since the matter-density information displayed at a location on a map may depend on all input data (galaxy positions), any algorithm optimized to information theory scales super-linearly. With increasing survey sizes, increasing requirements for spatial resolution and volume coverage, and the need to frequently re-iterate the map-generation step, the algorithm has to scale closely to linear with data size, otherwise its application is strongly limited. Former applications in cosmography suffered from such inconvenient performance-scaling, and an effort has to be made to develop simultaneously high-performance and accurate methods.

The work presented in this paper develops the general methodology of Bayesian reconstruction of the cosmic matter distribution, based on the invaluable pioneering work of many other scientists, which will be discussed below, and extends this work to a series of new applications. Existing and novel map making algorithms are summarized in terms of a classification of their Bayesian likelihood and prior functions. The implementation, optimization, and comparison of various numerical schemes are addressed in detail. This provides a starting point for a correct information-theory approach to cosmography. Many additional problems, not addressed in this paper, such as the galaxy bias, will also have to be solved before accurate maps of the dark matter distribution in our still mysterious Universe can be generated.

Such an undertaking would be highly rewarded in the short and long run. An accurate map of the cosmic matter distribution would be valuable for a manifold of direct scientific applications. These range from structure-formation analysis, to cosmological parameter estimation via power-spectrum measurements, dark energy studies, galaxy-cluster identification and galaxy-bias studies. Accurate cosmic maps would help to determine weak signals associated with the large-scale structure such as the integrated Sachs-Wolf (ISW) effect, or the extended Sunyaev-Zel’dovich (SZ) effect, the detection of which relies on the construction of optimal statistical filters for these signals.

Finally, one could argue that mapping the distribution of matter in the Universe represents a response to mankind’s curiosity in its aim to discover terra incognita and find an orientation in space and time on cosmological scales and, therefore, should be a goal in itself.

In the remainder of this introduction we give the sources of uncertainties, we present an overview of existent and new Bayesian reconstruction methods, subsequently we briefly describe the algorithmic development presented in this paper, and in the final part we give a more detailed overview of the structure of this paper.

1.1 Classes of uncertainty

Several classes of uncertainties related to the density-field reconstruction from galaxy surveys demand a statistical approach. Some of the uncertainties are intrinsic to the nature of the underlying signal (the dark matter). Other uncertainties are intrinsic to the nature of the observable (the galaxies). And finally there are uncertainties due to degeneracies which appear through the observation and data mining process.

(i) Intrinsic stochastic character: cosmic variance

In cosmology it is generally assumed that the structure of the Universe comes from some infinitesimal quantum fluctuations which were frozen out and stretched by an inflationary phase (see Guth [1981]; Guth & P<sup>2</sup> [1982]; Starobinsky [1982]; Hawking [1982].

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2 A map of galaxy counts can be generated by an algorithm with linear scaling to data size however, it is not an optimal representation of the underlying matter field.
distortions operator (for a detailed derivation see Hamilton 1998).
In the non-linear regime, these efforts include a velocity dispersion factor (the dispersion-model) corresponding to an exponential pairwise velocity distribution function with no mean streaming (see Ballinger et al. 1996). Scoccimarro (2004) presents an exact relationship between real-space and redshift-space two-point statistics through the pairwise velocity distribution function including all non-linearities. More complex methods of correcting for redshift-distortions were classified by Schmoldt et al. (1999) into iterative methods, which uses the redshift-space density to calculate a peculiar velocity field, and then iteratively corrects the density field distortions (Yahil et al. 1994; Kaiser & Stebbings 1991).

The other class decomposes the redshift-space density in radial and angular basis functions from which the radial redshift-distortion is corrected (see e.g. Lahav 1994; Nusser & Davis 1994; Fisher et al. 1995; Schmoldt et al. 1999 and more recently Percival 2005). Below, we propose a Bayesian method to correct for the linear and non-linear redshift-distortions in a statistical way (see section 2.5).

(iv) Observational uncertainties: measurements
The action of measurement introduces uncertainties, either due to the instruments, e.g. blurring by the telescope, or due to the observational strategy, which is included in the noise term, the selection function, and the mask effects (see Zaroubi et al. 1995, for a pioneering work in the LSS field). Ignoring selection functions, windowing, or blurring will lead to strongly biased reconstructions, which are far from the real signal, and thus allow only very limited interpretation of the true physical picture. A numerical implementation of these effects is presented in section (sec:operators). The influence of these effects will then be analyzed separately and tested with our code. The results are presented in section (4). Though ARGO demonstrates its capability to handle these uncertainties, further work is required in order to apply it to real data. Particular expressions for the selection function according to the redshift survey under study, as well, as masks, etc., have to be implemented.

(v) Mathematical/numerical representation uncertainties: aliasing effects
Some uncertainties are not intrinsic to the observable, but originate from the mathematical representation one chooses. Treating galaxies as counts in cells or with other mass-assignment schemes will smear out the information about their measured position for which one has to correct (see section 3.3.2) in order to derive other quantities, like the power-spectrum (see section 2.6.2).

From all the points mentioned above we conclude, that extracting the underlying dark matter density field from the luminous matter distribution given by galaxy redshift surveys poses a classical signal reconstruction problem. A Bayesian network depicting the relation of these uncertainties is shown in fig. (1).

1.2 Bayesian reconstruction methods
Any Bayesian statistical approach requires the definition of a likelihood and a prior. The former is the probability distribution function describing the process generating the observational data. It can be interpreted as a distance measure of the observed data to the underlying signal, as we will discuss below. The prior stands for the distribution function modeling our prior knowledge on the signal to be recovered. Mathematically it can be shown that it regularizes the estimator in the presence of noise (see section 2.5.1).

Two kinds of priors have to be distinguished, informative priors, in which the previous physical knowledge about the signal is encoded, and non-informative priors, which try to give objective estimators.
for the underlying signal based on purely information-theoretical arguments. Here, three non-informative priors are considered: flat priors (see section 2.5.5) with a constant probability distribution function (PDF), entropic priors based on Shannon’s notion of information (see section 2.5.9), and Jeffrey’s prior based on invariant statistical structures under transformation of variables (see section 2.5.8). Finally, a maximization or sampling of the posterior distribution, which is proportional to the product of the likelihood and the prior, has to be done to complete the Bayesian estimation. The maximization of the posterior is called the maximum a posteriori method (MAP). The maximum likelihood (ML) and maximum entropy method (MEM) are particular cases of the MAP with flat priors and entropic priors, respectively. Complex posterior distribution functions may be sampled iteratively from conditional PDFs in a Markov Chain Monte Carlo fashion (MCMC), see section 2.6. We show how different choices for these distribution functions together with the estimation procedure lead to different reconstruction algorithms, which consequently have distinct application fields (see table 1). A review of existing methods is presented and new applications for the large-scale structure reconstruction, which naturally emerge within the Bayesian formalism, are developed.

In this work we consider Poissonian and Gaussian likelihoods for the galaxy distribution. The former has been previously considered in image restoration especially for deconvolution purposes (see Richardson 1972; Lucy 1974). For example, the Richardson-Lucy algorithm can be derived as the ML of a Poissonian likelihood (see Shepp & Vardi 1982, and appendix D). Here an image can be regarded as photon counts in cells represented by a Poissonian distribution. However, one should notice that this likelihood does not represent the galaxy-formation process. From a pure image reconstruction perspective, it can still be interesting for LSS estimations, because it naturally represents the discrete nature of a galaxy distribution. The Gaussian likelihood allows the incorporation of arbitrary noise structures through the variance. The CMB map-making algorithms, which aim to convert time-ordered data received from satellites into a map of the CMB signal on the sky as a projection on the sphere, usually use this likelihood. In this case, the ML leads to the simple COBE-filter first derived by Janssen & Gulkis (1992). Nevertheless, the complex scanning strategies and foreground removal can add unlimited complexity to these algorithms (e.g. Natoli et al. 2001; Doré et al. 2001; Stompor et al. 2002; Keihanen et al. 2005; Yvon & Mäkelä 2005).

For the LSS the Gaussian prior arises as the natural informative prior due to the arguments discussed above. We propose a novel algorithm: GAPMAP, which maximizes the posterior with a Gaussian prior and a Poissonian likelihood (see section 2.5.5) and appendix E. In contrast, the Gaussian likelihood with the Gaussian prior leads to the well-known Wiener-filter, which has been used for the LSS reconstruction (see Fisher et al. 1994; Hoffman 1994; Lahav et al. 1994; Lahav 1994; Zaroubi et al. 1995; Fisher et al. 1995; Webster et al. 1997; Zaroubi et al. 1999; Schmoldt et al. 1999; Erdogdu et al. 2004; 2006) and for CMB-mapping (see e.g. Bunn et al. 1994; Tegmark 1997). It is also known to give optimal results in terms of yielding the least square error, see the pioneering work of Rybicki & Press (1992) and Zaroubi et al. 1995. We present in this paper a fast Wiener-filer extra-regularized with Krylov methods as we will see below (see table 2 for a summary of different Krylov methods).

Intrinsic primordial non-Gaussianities can be imprinted in the seed fluctuations depending on the particular theory responsible for the amplification of the fluctuations coming from the early Universe. To find such deviations, non-informative priors, which give non-linear estimates for the underlying signal are required. Entropic priors are well suited here, and have been previously applied for CMB studies. We extend this work for LSS reconstructions and develop the corresponding maximum entropy method for Gaussian and Poissonian likelihoods (see section 2.5.9 and appendix D).

Sampling methods have the advantage of determining the shape of distributions and, thus, leading to a natural estimate of the uncertainty of the estimator. Moreover, the mean can be calculated easily from the sample and is known to give more accurate results than the maximum in the case of asymmetric PDFs (see e.g. Tunnell 1996).

As an example, Hobson & McLachlan (2003) proposed a SZ-cluster detection algorithm using the Metropolis-Hasting algorithm method based on a Poissonian prior distribution, which is designed to find discrete objects. Recently Sutton & Wandelt (2006) developed a reconstruction method for radio-astronomy that samples from the multiplicity function (see eq. 11). Alternative approaches to the maximum likelihood for CMB-mapping algorithms try to jointly reconstruct the CMB-map with its power-spectrum using Gibbs-sampling techniques (Wandelt et al. 2004; O’Dwyer et al. 2004; Eriksen et al. 2007). This approach is especially efficient with respect to other MCMC methods because the transition probability matrix moves the system in each step of the chain. For this special case the importance ratio is always one (see e.g. Negi 1993). This MCMC method requires, however, the complete knowledge of the full conditional PDFs in order to sample from them. Note, that the Gaussian prior for the signal simultaneously represents the likelihood for the power-spectrum given the signal, which in this case is an inverse Gamma function for the power-spectrum (see section 2.6.2). This distribution naturally samples the power-spectrum, which strongly deviates from Gaussianity.

With the aim of estimating the power-spectrum in an objective way, non-informative priors are used. Usually a flat prior is taken for the power-spectrum. Alternatively, Jeffrey’s prior, for which we give a derivation based on Fisher information (see appendix E), can be used. Alternatively, an entropic prior could also be taken.

Other attempts have been made to estimate the power-spectrum from the LSS based on the distribution of galaxies. A modified Gaussian PDF with a log-normal mean has been used in this approach (see Percival 2003). The same kind of concept, using a modified Gaussian distribution to sample deviations from Gaussianity, has been applied to SZ-cluster detection by Pierpaoli & Anthoine (2003).

In this paper we propose to apply a Gibbs-sampling algorithm to jointly sample the underlying three-dimensional density field with the power-spectrum and the peculiar velocities, which can be used to correct for the redshift-distortions. Note, that the peculiar velocities can also be used to trace the initial density fluctuations back in time as we will discuss below.

1.3 Algorithmic development

In this paper we focus our work on the numerical optimization of inverse techniques to show that a joint estimation of the LSS matter density field and its parameters is feasible (see sections 3 & 4).

The calculation of the reconstructions, either through maximization or through sampling, requires the inversion of certain matrices. For the Wiener-filter, for instance, the reconstruction problem consists in one of its steps on the inversion of the correlation matrix of the data. The methods used in this field so far calculated this matrix and inverted it mainly using the Singular Value Decomposition algorithm that scales as $O(n^3)$ for a $n \times n$ matrix (see e.g.
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Zaroubi et al. [1995]. However, this approach seems to be hopeless in light of the overwhelming amounts of data coming from different surveys and the possibility of combining them. We made special effort to implement an algorithm in which the involved matrices would not need to be stored taking advantage of an operator formalism, which we worked out here for different reconstruction methods (see table 3 and section 3.3). Such a formalism also allows fast iterative numerical methods that speed the inverse step up to a formalism, which we worked out here for different reconstruction cases would not need to be stored taking advantage of an operator for iterative schemes (see appendix I and section 3.3). Particular detailed derivations are presented in the appendix.

1.4 Structure of the paper

This paper is structured as follows: in section 2 we state the problem of signal reconstruction, then we define the data model. Subsequently, we introduce a general statistical perspective within a Bayesian framework from which different solutions to the reconstruction problem are presented, including Wiener-filtering, the COBE-filter, a novel GAPMAP algorithm with a Poissonian likelihood and a Gaussian prior, Jeffrey’s prior and the Maximum Entropy method (MEM). Markov Chain Monte Carlo methods (MCMC) that sample the global probability distribution function of the signal and all underlying parameters are presented as the ideal approach to achieve a full Bayesian solution of the reconstruction problem. In the numerical method section 3, different iterative inverse schemes which have been implemented in ARGO are presented, including a very efficient novel scheme. The operator formalism is worked out for four novel algorithms in large-scale structure reconstruction. The efficiency of the different inverse schemes is tested with the Wiener-filter under different reconstruction cases with synthetic data, including structured noise, blurring, selection function effects, and windowing in section 4. Particular detailed derivations are presented in the appendix.

2 BAYESIAN APPROACH TO SIGNAL RECONSTRUCTION

The reconstruction of a signal (here: DM distribution) given a set of measurements (here: galaxy catalogues) is usually a highly degenerate problem, as we have discussed above, where the signal is under-sampled and modified by systematic and intrinsic errors due to the nature of the observable. This is indeed the situation that we are facing, since most of the galaxy redshift surveys have partial sky coverage and the discrete nature of galaxies introduces shot noise.

An expression for the data as a function of the real signal has to be modeled in a first step. The reconstruction problem is classically seen as the inverse of this functional dependence. The solution to this problem is far from being trivial and essential issues, like solution existence, solution uniqueness, and instability of the solving process, have to be considered. Regarding the solution existence, there will be no model that exactly fits the data, since the mathematical model of the physics of the system is approximate and the data contain noise. That forces us to look for optimal solutions, rather than exact solutions. We will have to deal especially with the last two points mentioned above, uniqueness and stability, because an infinite set of possible solutions can fit the data and because of the ill-conditioned character of the system we are treating. A regularization method that stabilizes the inverse process by imposing additional constraints will be required. We show below how the Bayesian framework permits us to do a regularization in a natural way and furthermore to jointly estimate the signal and its parameters. The calculation of the Bayesian estimators will require extra-regularization techniques, which will be presented in section 3. We will start posing the inverse problem by defining the model of the data.

2.1 Data model

The galaxy formation process is known to be a complicated, non-linear and probably non-local process, as mentioned in the introduction. Thus, attempts to invert the galaxy distribution into the original DM distribution suppose a great challenge. It is known that, given some bias factor between the amplitude of the galaxy and the DM fluctuations, the galaxy power-spectrum on large scales fits well to the expected DM spectrum predicted from CMB observations. Detailed studies reveal that the bias factor is not universal, but depends on galaxy type, galaxy formation time, redshift, etc. The data model connecting the signal (DM distribution) to our observable (galaxy counts) is in consequence complex, non-linear and non-local. The main goal of this paper is to develop a Bayesian framework that permits one to split the dependencies into separated problems, which can then be jointly tackled with physical and statistical techniques. In principle, also the bias of the galaxies can be sampled (see discussion in the introduction). However, this is out of the scope of this paper.

Here we present a linear data model which can easily be extended to a simple non-linear data model by a non-linear weighting scheme (e.g. by weighting the galaxies according to their apparent luminosity). Nevertheless, many of the uncertainties we are facing, such as the convolution effects due to the blurring of a telescope, the pixelization scheme, the mask effects due to the observation strategy, or the selection effects due to the limited sensitivity of the detectors, can be described with a linear model. This linear model will contain non-linear information in the noise term.

2.1.1 Linear data model

The general linear reconstruction problem formally can be written as the inverse problem of recovering the signal $s$ from the observations $d$ related in the following way

$$d(x) = \int dy R(x, y)s(y),$$

(1)

where $R$ represents the kernel of the Fredholm integral equation of the first kind defined by (1), with noise on the signal $s$ being expressed by the superscript $\epsilon$. Discretizing eq. (1) and assuming
where the \( m \times 1 \) vector \( d \) represents the data points resulting from the measurements (here: galaxy counts), the statistical noise and the underlying signal are a \( m \times 1 \) vector \( \epsilon \), and a \( n \times 1 \) vector \( s \) respectively. The object that operates on the signal is the response function matrix \( R \) which commonly describes blurring effects caused by the atmosphere, the point-spread function (PSF) of the telescope or the detector response function of the detectors of the instrument.

Let us denote the physical observation process encoded in the \( R \)-matrix as \( R \cdot s \). We are interested in the selection function of the survey \( f_{s} \) with the corresponding masks \( f_{s} \), which can also be included in \( R \). One has to be careful with the data model defined in eq.\(^2\) As several authors point out, there is a correlation between the underlying signal \( s \) and the level of shot noise produced by the discrete distribution of galaxies (see e.g. Seljak 1998). Since, by definition, additive noise assumes no correlation with the signal – otherwise we would have signal content in the noise – we define the effective noise \( \epsilon \) as the product of a structure function \( f_{S\epsilon} \), which could be correlated with the signal, with a random noise component \( \epsilon_{N} \) that is uncorrelated with the signal. Given the above definitions, the effective noise \( \epsilon \) is uncorrelated with the signal. We may then rewrite eq.\(^2\) in continuous representation as

\[
d(x) = \int d\mathbf{y} R_{D}(\mathbf{x}, \mathbf{y}) f_{s}(\mathbf{y}) f_{M}(\mathbf{y}) s(\mathbf{y}) + f_{S\epsilon}(s(x)) \epsilon_{N}(x) \tag{3}
\]

where \( R(x, y) = R_{D}(x, y) f_{s}(y) f_{M}(y) \) and \( \epsilon(x) = f_{S\epsilon}(s(x)) \epsilon_{N}(x) \). In practice, we will assume white noise (i.e. constant noise in Fourier space), \( \epsilon_{N} = \epsilon W_{N} \). However, none of the presented techniques in this paper depend on this simplification. Some of the previous studies of large-scale structure reconstruction also included the inverse of the linear redshift-distortion operators as a matrix multiplying \( R \) (see e.g. Lahav et al. 1994). Such an operator cannot easily be found for the non-linear regime. Earlier works try to correct the non-linear redshift-distortions with an additional factor in the power-spectrum analogous to Kaiser’s factor (see Kaiser 1987; Ballinger et al. 1996; Erdo˘gdu et al. 2004). Here, we propose a Bayesian solution to the signal reconstruction problem as it will be discussed later.

In most cases, the signal will be strongly under-constrained due to under-sampling, i.e. \( n \gg m \), which is nearly unavoidable due to partial sky coverage of surveys. The linear equation (eq.\(^2\)) to be inverted is a rank-deficient system. Such systems are characterized by non-uniqueness, since the matrix \( R \) has a nontrivial null space. By superposition, any linear combination of the null space models (models \( s_{0} \) that satisfy \( R s_{0} = 0 \)) can be added to a particular solution leading to infinite solutions. Consequently, we cannot discriminate between situations where the solution is truly zero (see for example Aster et al. 2005). As is well known, a direct inversion of eq.\(^2\) (\( R^{-1} d \)) will amplify the statistical noise and lead to an unstable solution (see e.g. Zaroubi et al. 1993). Instead, a regularization method, which often follows several steps, has to be applied. The first step consists of finding an expression for an estimator of the signal \( s \) that approximately satisfies the data model (eq.\(^2\)) and copes with the noise. Further regularization methods are usually required in a second step to actually calculate the estimator. This happens whenever some ill-posed linear or non-linear operators have to be inverted. We shall distinguish between noise regularization and inverse regularization according to the first and the second step, respectively. As Zaroubi et al. (1995) pointed out, using a mean variance estimator alone does not completely solve the inverse problem. Therefore, they proposed the singular value decomposition algorithm (SVD) to extra-regularize these problems. However, this method requires one to calculate the correlation matrix of the data implying a slow algorithm, scaling as \( O(n^3) \), and needs large storage facilities. We will show that a Bayesian approach is a natural regularizer for the noise, which then can be regularized further for the inverse purpose with efficient methods that scale as \( O(n \log_{2} n) \) (see section\(^3\)). Let us address the problem of signal reconstruction from a statistical inference perspective.

### 2.2 Inversion via statistical estimator

In parametric modeling it is assumed that observational data have been generated by random processes with probability density distributions, depending on the model parameters (see for example Robert 2001). Statistical analysis in this context is essentially an inverse method, which aims at retrieving the causes (here reduced to the parameters of the probabilistic generating mechanism) from the effects (here summarized by the observations).

Traditionally, one tries to find a way where the available information is optimally used and a unique estimator is selected from an infinite set of solutions. One of the classical approaches consists of minimizing the variance of the residuals, which is the variance of the discrepancy between the estimator and the set of possible realizations consistent with the data (see Rybicki & Press 1992). This conjecture is reasonable because the least deviation from the set of true signals is searched. The estimator obtained in this way is called the least squares quadratic (LSQ) estimator. However, a transparent statement of the statistical assumptions is missing in this method, contrary to the Bayesian approach used in this work as will be shown below. Moreover, Bayesian statistics allows sampling the PDF of the system under consideration in a natural way. Strictly speaking, one does not look for a unique estimator in this framework. Nevertheless, a summary of the PDF can be given by the mean of the sample (see section\(^2\)).

The most general approach to determine an estimator, however, should be based on the global (joint) PDF over all relevant quantities, like the signal \( s \) and all model parameters \( p \), without neglecting any possible dependences. Let us assume that \( P(s, p \mid d) \), the joint PDF of the system under consideration, depends on the signal \( s \) and a series of additional parameters \( p \), given the observations \( d \). One solution would then be to calculate the expectation of the signal over the joint PDF space

\[
E_{\text{joint}}(s) \equiv \int ds dp \left[ P(s, p \mid d) \right] s \equiv \langle s \rangle_{(s, p \mid d)} \tag{4}
\]

where we have introduced the ensemble average \( \langle s \rangle_{(s, p \mid d)} \) with the subscript representing the PDF over which the integral is done \( P(s, p \mid d) \rightarrow (s, p \mid d) \). Expression (4) can consequently be read as the ensemble average over all possible signals and parameters. The joint PDF is unfortunately quite hard to calculate directly, and the integral in eq.\(^4\) is computationally too expensive for realistic cases as it involves many parameters and a large amount of data. To disentangle the uncertainties in parameter and signal

\(^3\) Sometimes, however, the ensemble angles will denote the estimator of some signal or parameter in a more general sense, like the maximum likelihood or the maximum a posteriori (see sections\(^2\) and\(^3\) respectively). Note that a bracket formalism could be introduced at this point, in which eq.\(^4\) would be represented in the following way: \( [s]_{s[p,d]} \).
2.3 Bayesian approach

Given a data model, one can usually find an expression for the sampling distribution, i.e. the probability of obtaining the data given the signal and some additional parameters \( p, P(d | s, p) \). This is much less difficult than a direct calculation of the posterior \( P(s | d, p) \).

We need an expression which relates both the sampling and the posterior distribution given by Bayes theorem. The derivation of Bayes theorem is straightforward from the joint PDF of the signal and the data, using the product rule and the fact that the joint PDF is invariant under permutations of its arguments.\(^4\) Bayes theorem can be expressed by the following equation

\[
P(s | d, p, I) = \frac{P(d | s, p, I)P(s | p, I)}{P(d | p, I)},
\]

where \( P(s | p, I) \) represents the prior knowledge about the signal, as it models the signal before any observations occur. The PDF given by \( P(d | p, I) \) stands for the so-called evidence that is treated as the normalization of the posterior

\[
P(d | p, I) = \int ds \, P(d | s, p, I)P(s | p, I).
\]

It is worth mentioning that all the probabilities are conditional to the underlying physical picture, or prior information \( I \). This has to be explicitly considered in case of model comparisons. In the following sections, we will present the steps for completing a Bayesian analysis, starting with the likelihood, then discussing the importance of the prior, and finishing with sampling through the joint signal and parameter space. Note that different choices for these three components (likelihood, prior, and sampling) lead to different classes of reconstruction algorithms. An overview of the different reconstruction scheme implementations based on this classification can be found in table 1.

2.4 The likelihood

The likelihood function is formally any function of the parameters \( \theta \) proportional to the sample density (see \[\text{eq. (4)}\])

\[
\mathcal{L}(\theta | d) \propto P(d | \theta).
\]

Many inference approaches are based on the likelihood function, justified by the likelihood principle, which states that the information obtained by an observation \( d \) about \( \theta \) is entirely contained in the likelihood function \( \mathcal{L}(\theta | d) \). To be specific, if \( d_1 \) and \( d_2 \) are two observations depending on the same parameter \( \theta \) such that there exists a constant \( c \) satisfying \( \mathcal{L}(\theta | d_1) = c \mathcal{L}(\theta | d_2) \) for every \( \theta, d_1 \) and \( d_2 \) then bring the same information about \( \theta \) and must hence lead to identical inferences (see \[\text{Robert (2001)}\]).

Maximum likelihood (ML) methods, for example, rely on the likelihood principle with an estimator of the parameters given by

\[
(\theta)_{\text{ML}} = \arg\sup_{\theta} \mathcal{L}(\theta | d),
\]

i.e., the value of \( \theta \) that maximizes the probability density at \( d \).

Bayesian methods take also advantage of the likelihood principle incorporating the decision-related requirement of the inferential problem through the definition of a prior distribution (see section 2.5). The definition of the likelihood is the first step in a Bayesian framework to determine the posterior distribution (see \[\text{eq. (7)}\]). In using galaxy redshift surveys to trace the matter distribution, we have to deal with the discrete nature of the data sample. Thus the likelihood may be derived here for Poissonian statistics.

2.4.1 Poissonian likelihood

The likelihood of our galaxy distribution may be approximately represented by a Poissonian distribution (the real statistics should describe the much more complex galaxy formation process). Under the assumption of independent and identically distributed (iid) observations, this yields

\[
\mathcal{L}(s | d, p) \propto \exp\left(-\left[ (R s')_i + c_i \right] \right) \frac{[R s']_i + c_i]^{d'_i}}{d'_i!},
\]

where \( d'_i \) are the galaxy counts per cell \( i \) and the real, positive signal of the expectation value of the number of galaxies is given by \( s'_i = \frac{m}{b s_i} (1 + b s_i) \), with \( s_i = \delta s_i = \frac{N_{\rho}}{\rho} \) the DM over-density, our target signal. The quantity \( N_{\rho} \) stands for the mean number of galaxies, \( \rho \) represents the mean density and \( b \) the bias factor. All these quantities are redshift-dependent. The additional parameters \( p \) in this case would be represented by some background \( c_i \) and would enter into the operator \( R \) that modifies the signal \( s \).

For a similar application in astronomy see \[\text{Lahav & Gull (1989) and Robinson (1991)}\]. If \( d'_i \) is not an integer, e.g. due to some interpolation process, a Gamma function may be used instead of the factorial, \( d'_i! \rightarrow \Gamma(d'_i + 1) \).

2.4.2 Gaussian likelihood

When the number of counts is large the Poisson distribution can be approximated by the normal distribution. In that case, the likeli-
hood can be given by a Gaussian distributed noise

\[ \mathcal{L}(s \mid d, p) \propto \frac{1}{(2\pi)^{m} \text{det}(N)^{1/2}} \exp \left( -\frac{1}{2} \epsilon^{\text{T}} N^{-1} \epsilon \right) \]

\[ P(d \mid s, p) \propto \exp \left[ -\frac{1}{2} \chi^2(s) \right], \quad (12) \]

where \( N \equiv \langle \epsilon \epsilon^{\text{T}} \rangle \) is the covariance matrix of the noise \( \epsilon \equiv d - R s \), and

\[ \chi^2(s) = (d - R s)^{\text{T}} N^{-1} (d - R s). \quad (13) \]

The parameters \( p \) determine the structure of the noise \( \epsilon \) (and therefore the structure of the covariance matrix \( N \)), and also enter into the operator \( R \). We give different expressions for the noise covariance matrix \( N \) in section (3.3).

Note that \( \chi^2 \) coincides with the square of the Mahalanobis distance,\(^6\) between \( d \) and \( R s \), and also coincides with the squared \( N^{-1} \)-norm of the error

\[ \chi^2(s) = D_{\text{Mah}}^2(d, R s)_{\text{N}^{-1}} = ||\epsilon||_{N^{-1}}^2. \quad (14) \]

In this case, the ML will correspond to the least squares of the error. It will minimize the \( \chi^2(s) \) and hence minimize the Mahalanobis distance between the data and the noise-free data model. Therefore, the ML is equivalent to searching the estimator that fits the data better without constraining the model for the signal. Let us study the prior that precisely sets constraints on the signal \( s \).

### 2.5 The prior

A second step in Bayesian analysis is to specify the prior distribution for the signal, which contains the prior knowledge about the signal before the measurements were carried out. For little informative data it can strongly affect the posterior distribution and thus modify any inference based on it. For this reason, frequentists criticize Bayesian methods as being subjective. Other definitions of probability, like the frequentist, however, can be shown in most of the situations to be particular cases of the Bayesian approach (see e.g. [Tanner 1996]), implying the use of an implicit prior. The advantage of defining the prior knowledge about the system under consideration is that the interpretation of the results is straightforward, especially because assumptions flowing into the inference procedure are clearly stated. Once the prior is defined, we can obtain the maximum a posteriori (MAP) estimator, by maximizing the posterior distribution, which is proportional to the likelihood multiplied by the prior,

\[ \hat{\theta}_{\text{MAP}} = \arg \sup_{\theta} P(\theta \mid d). \quad (15) \]

Note that there is a crucial difference to the maximum likelihood estimator (eq. 10) due to the incorporation of the prior information.

#### 2.5.1 Bayes and regularization methods: the prior as a regularizer

Looking at the log-probabilities, we see that the MAP estimator maximizes the following quantity using Bayes theorem

\[ (\log P(\theta \mid d) \propto \log P(d \mid \theta) P(\theta)) \]

\[ Q = \log P(d \mid \theta) + \log P(\theta). \quad (16) \]

If we assume that the error is Gaussian distributed, (which is a fair assumption if there is no prior information about the noise), and we parameterize the prior of the parameter, say the signal \( s \), we can rewrite eq. (16) as (2Q \rightarrow Q)

\[ Q = -\chi^2(s) + \alpha f_p(s), \quad (17) \]

where we absorbed the factor 2 in the Lagrangian multiplier \( \alpha \), and \( f_p \) represents the penalty function that obliges the estimator to fulfill some constraint on the parameter \( s \), to the detriment of the \( \chi^2(s) \) that strongly relies on the data. If we further assume that \( N^{-1} = I \) (say we have white noise), the Mahalanobis distance reduces to the Euclidean distance

\[ (D_{\text{Mah}}^2(d, R s)|_{\text{N}^{-1} = I} = D_{\text{Euc}}^2(d, R s)), \]

and the quantity one wants to minimize reads

\[ ||\epsilon||^2 + \alpha ||s||^2, \quad (18) \]

which then becomes the Tikhonov regularization method [Tikhonov 1963]. The parameter \( \alpha \) is called the regularization parameter. These methods lead to linear filters and are essentially identical to Wiener-filtering [Foster 1961], which will be presented in the next section. Note that Tikhonov regularization is equivalent to MAP of a Gaussian likelihood with noise covariance matrix \( N = I \) and Gaussian prior, with signal covariance matrix \( S = \alpha^{-1} I \). Nevertheless, the penalty function \( f_p \) in general can be a non-linear function of the parameter to be estimated (say the signal \( s \)) leading to non-linear estimators. We will introduce MEM as such an example. Tikhonov regularization can also be generalized to non-linear problems by introducing a non-linear kernel operator \( R(s) \).

Summarizing the exposed theory of signal reconstruction, we might interpret the likelihood as some distance measure between the data and the noise-free model of the data, and the prior as some constraint that tightens the estimator to the model of the signal. We have shown here that the classical methods of signal reconstruction, like the Tikhonov regularization, are particular cases of the Bayesian approach. The inclusion of a prior can be regarded as a natural regularization, in the sense that the regularization term is provided by a (physical) model of the true signal. In appendix C we discuss the relation between other regularization methods and the Bayesian approach. In the following sections we introduce different priors that are relevant for large-scale structure reconstruction and are implemented in ARGO.

#### 2.5.2 Gaussian prior

The distribution of the primordial density field should be very close to Gaussianity according to most of the inflationary scenarios [Guth 1981, Linde 1982, Albrecht & Steinhardt 1982]. In fact, the measurements of the CMB show very small deviations from Gaussianity (see e.g. Komatsu et al. 2003). Non-Gaussianities in the matter distribution arose mainly from non-linear gravitational collapse. The non-linear regime of structure formation is responsible for the strong radial redshift-distortions, the finger-of-god effect, limiting...
Table 1. Classification of reconstruction methods in astrophysics based on the prior (columns) and likelihood (rows). Note that most of the reconstruction algorithms in other research areas, such as tomography, where Tikhonov-regularization is widely used, or the algebraic reconstruction technique (ART), which is based on the asymptotic regularization, fall into the class of Wiener-filtering schemes as we show in section (2.5.1) and appendix L. The differences in the ML CMB-map-making algorithms reside mainly in the modeling of the complex noise structure that arises due to the scanning strategies of the satellites and in the various foreground removal methods. The LSS Wiener-filtering methods, on the other hand, are based on the different input data, either galaxy-positions or peculiar velocities. The discrete object detection (Hobson & McLachlan 2003) algorithm was developed to find Sunyaev-Zel’dovich clusters. This is also the case for the modified Gaussian by Pierpaoli & Anthoine (2005). The reconstruction of the power-spectrum is also listed here. In CMB the joint map and power-spectrum estimation is done by MAGIC (section 2.5.9 and appendix J), and in LSS by GAPMAP (section 2.6.2). This paper covers three new areas in LSS (GAPMAP, MEMG, MEMP) and presents four novel algorithms with which reconstructions can be done very fast.

| Likelihood   | Prior                  | Non-informative priors | Entropic (MEM) | Informative priors (MAP) |
|--------------|------------------------|------------------------|----------------|--------------------------|
| Gaussian     |                        |                        |                |                          |
| -Radio       |                        |                        |                |                          |
| -CMB         |                        |                        |                |                          |
| COBE:        | Janssen & Gulkis (1992)| Sutton & Wandelt (2006)#|                |                          |
|              | Tegmark (1997)         | Masinger et al. (1997) |                |                          |
| ROMA:        | Natoli et al. (2001)   |                        |                |                          |
| MAPCUMBA:    | Doré et al. (2001)     |                        |                |                          |
| MAXIMA:      | Stompor et al. (2002)  |                        |                |                          |
| MAGIC*:      | Wandelt et al. (2004)  | MAGIC*:                |                |                          |
| MIRAGE:      | Yvon & Mayet (2005)    |                        |                |                          |
| MADAM:       | Keihanen et al. (2005) |                        |                |                          |
| -LSS         |                        |                        |                |                          |
|              |                        |                        |                |                          |
| Poissonian   |                        |                        |                |                          |
|              |                        |                        |                |                          |
| Inverse Gamma|                        |                        |                |                          |
| -CMB         |                        | MAGIC*:                |                |                          |
|              |                        | O’Dwyer et al. (2004)# |                |                          |
|              |                        | Larson et al. (2007)#  |                |                          |
|              |                        | Eriksen et al. (2007)# |                |                          |
| -LSS         |                        | ARGO*:                 |                |                          |
|              |                        | (section 2.6.2)        |                |                          |
| Modified Gaussian|                  |                        |                |                          |
| -CMB         |                        | Pierpaoli & Anthoine (2005)# |         |                          |
| -LSS         |                        | Percival (2005)#       |                |                          |

*developed and presented in this paper; ** developed, tested and presented in this paper; # able to sample PDFs

We have left out the reconstruction methods that are focused on the cosmological initial conditions, since they address a different problem and, in general, cannot be classified in terms of the PDFs listed in this table. Neither can other reconstruction algorithms based on geometrical arguments, like Voronoi, Delaunay tessellations, friends-of-friends schemes or cloud-in-cell interpolation schemes, be classified here.
the accuracy of reconstructions. Previous attempts to correct for these distortions have modified the power-spectrum by introducing a Lorentzian factor (see e.g. [Ballinger et al 1996; Erdogdu et al 2004]. In section (2.6) we propose an alternative way to do this in a Bayesian framework, where peculiar velocities are sampled together with the three dimensional map of the matter distribution. For the underlying DM density fluctuation we will assume a Gaussian prior. This is a crude approximation for the density field at the present epoch of the Universe, especially on small-scales. It is, however, a valid description on large-scales and allows to incorporate non-linear corrections in a MCMC fashion, as will be discussed in section (2.6). Following Bardeen et al. (1986) we may thus write the PDF of the signal as a multivariate Gaussian distribution

\[ P(s \mid p) = \frac{1}{(2\pi)^n|\text{det}(S)|^{1/2}} \exp \left( -\frac{1}{2} s^T S^{-1} s \right), \]

(20)

with \( S \) being the covariance matrix of the signal (\( S = S(p) = \langle s s^\dagger \rangle_{(s \mid p)} \)). This formula emphasizes the high dimensional character of the problem (n dimensions of the signal reconstruction, with n being typically between 10^3 and 10^9).

2.5.3 Gaussian prior and Gaussian likelihood: the Wiener-filter

The Gaussian prior together with the Gaussian likelihood lead to the Wiener-filter, completing the square for the signal in the exponent of the posterior distribution (see Zaroubi et al. (1998) and appendix A).

\[ P(s \mid d, p) \propto \exp \left( -\frac{1}{2} \left[ s^T S^{-1} s + (d - R s)^T N^{-1} (d - R s) \right] \right) \]

\[ = \exp \left( -\frac{1}{2} \left[ (s - \langle s \rangle_{WF})^T (\sigma_{WF}^2)^{-1} (s - \langle s \rangle_{WF}) \right] \right), \]

(21)

where the Wiener-filter used to calculate the estimator from the data \( \langle s \rangle_{WF} = F_{WF} \) is given by

\[ F_{WF} = (S^{-1} + R^T N^{-1} R)^{-1} R^T N^{-1}, \]

(22)

and the corresponding covariance is

\[ \sigma_{WF}^2 = (r^T r)^{-1}_{WF} = (S^{-1} + R^T N^{-1} R)^{-1}, \]

(23)

with \( r = s - \langle s \rangle_{WF} \) being the residual. A similar filter to the Wiener-filter can be obtained by the LSQ estimation (\( \text{for an explicit derivation see Zaroubi et al. (1998)} \) and appendix [B]) leading to the following expression

\[ \langle s \rangle_{LSQ} = \langle s d^\dagger \rangle (d d^\dagger)^{-1} d, \]

(24)

where the correlation matrix of the signal and the data \( \langle s d^\dagger \rangle \) is multiplied by the inverse of the autocorrelation matrix of the data \( (d d^\dagger)^{-1} \). Given that the signal and the noise are uncorrelated \( \langle s \sigma^2 \rangle = 0 \), the correlation matrix of the signal and the data reduces to: \( \langle s d^\dagger \rangle = SR^\dagger \). Thus, the filter in eq. (24) can be reformulated as

\[ F_{LSQ} = SR^\dagger (R S R^\dagger + \langle N \rangle_{(s \mid p)})^{-1}. \]

(25)

\[ \text{Note that in this case, the least squares are referred to the residuals} \ r, \text{instead of the difference between the real signal} \ s \text{and the estimated signal} \ \langle s \rangle_{LSQ} \text{, \( \|r\|^2 = \|s - \langle s \rangle_{LSQ}\|^2 \), where the prior on} \ s \text{is given in a more implicit way by assuming a linear relation between the estimator and the data and statistical homogeneity.} \]

The noise covariance matrix for the LSQ estimator will differ from the one in the likelihood, if there is a signal dependence in the structure function of the noise term as it is the case for a Poissonian-like distribution.

From the structure of the LSQ filter \( F_{LSQ} \) (eq. 25), one could postulate another expression for the Wiener-filter given by:

\[ F_{WF} = SR^\dagger (R S R^\dagger + N)^{-1}. \]

(26)

We show in appendix C that both expressions for the Wiener-filter (eqs. 22 and 26) are equivalent. From now on, we will call eq. 26 the data-space representation of the Wiener-filter, and eq. 22 the signal-space representation of the Wiener-filter. Note, that the LSQ estimator will coincide with the Wiener-filter after performing an ensemble average over all possible signal realizations: \( \langle s \rangle_{LSQ} = \langle \langle s \rangle_{WF} \rangle_{(s \mid p)} \).

The following notation can be introduced for the posterior PDF

\[ P(s \mid d, p) \propto G(s - \langle s \rangle_{WF}, \sigma_{WF}^2), \]

(27)

i.e. given a dataset \( d \) derived from a Gaussian process, the possible signals are Gaussian distributed around the Wiener-filter reconstruction \( \langle s \rangle_{WF} \) with a covariance \( \sigma_{WF}^2 \). The parameters \( p \) enter the operator \( R \), including also the cosmological parameters that determine the signal covariance matrix \( S \). We will discuss in section 2.6.2 how to sample \( S \) and to determine cosmological parameters.

A remarkable characteristic of the Wiener-filter is that it suppresses the signal in the presence of a high noise level resulting in the null estimator and gives just the deblurred data when noise is negligible. In this sense it is a biased estimator, since its covariance matrix has less power than the original one. Some attempts have been made to derive an equivalent unbiased estimator (see Zaroubi 2002). However, one might be especially interested in obtaining a conservative estimator. Sampling the joint PDF will fill the missing modes (see e.g. Wandelt et al. 2004) and in this way complete the signal in regions where it is under-sampled or the signal to noise ratio is low. It is interesting to note that the Wiener Filter coincides with the MAP estimator in the case of a Gaussian prior on \( s \) and a Gaussian likelihood (\( \langle s \rangle_{WF} = \langle s \rangle_{MAP} \)). Performing the integral of the conditional PDF (see eq. 5) one obtains the same estimator again, thus \( \langle s \rangle_{WF} = \langle s \rangle_{(s \mid d, p)} \). This is a very important result, since it permits one to sample the conditional PDF. We propose to exploit this property for the joint estimation of the signal and its power-spectrum as is done in the CMB (see Wandelt et al. 2004) and section 2.6.2.

2.5.4 Gaussian prior and Poissonian likelihood: the GAPMAP estimator

The Gaussian likelihood constitutes a valid approximation when the Poissonian character of the distribution is appropriately modeled in the noise correlation matrix \( N \). However, one would rather describe a discrete sampling process like a galaxy survey with a Poissonian likelihood. Unfortunately, there is no filter available for such a case. Thus, we present a novel iterative equation for the MAP estimator with a Gaussian prior and a Poissonian likelihood, which we call GAPMAP (see appendix C for a derivation)

\[ s^{j+1} = SR^\dagger \exp \left( -\frac{1}{2} \left[ (R S R^\dagger + b s^j)^{-1} \right] d' \right). \]

(28)
2.5.5 Flat prior

With the aim of deriving objective posterior distributions, non-informative prior distributions are introduced. A non-informative prior would suggest that any value is reasonable. Flat priors where the probability distribution is assumed to be constant are thus very often applied. Note, however, that these are improper priors, since the integral of these distributions diverges to infinity. In this case, the posterior is proportional to the likelihood. The maximum likelihood solution coincides in this way with the MAP estimator assuming a flat prior \((\hat{\theta})_{\text{ML}} = (\hat{\theta})_{\text{MAP}}|n_{\alpha})\).

2.5.6 Flat prior and Gaussian likelihood: the COBE-filter

In CMB map-making algorithms it is common to use the so-called COBE-filter (see Jansen & Gulkis 1992; Tegmark 1997), which can easily be derived by maximizing the likelihood given in eq. (22)

\[
F_{\text{COBE}} = (R^T N^{-1} R)^{-1} R^T N^{-1}.
\]

This filter has the property that among all unbiased linear estimators (with a noise of zero mean), it leads to the minimum variance (Natoli et al. 2001). Here unbiased means that the statistical mean of the estimator is equal to the true signal. This is, however, only fulfilled when the inverse of \(R^T N^{-1} R\) exists (see appendix C). The covariance for the COBE-filter can be found to be

\[
\sigma^2_{\text{COBE}} = \langle r r^T \rangle_{\text{COBE}} = \langle R^T N^{-1} R \rangle^{-1}.
\]

Note that, in general, the following relation holds: \(\sigma^2_{\text{VF}} \leq \sigma^2_{\text{COBE}}\), as a comparison to eq. (23) shows. Tegmark (1997) claims that several linear filters like the COBE or the Wiener-filter conserve information by comparing the Fisher information matrix corresponding to the filtered signal to the one of the un-filtered time ordered data. This property apparently permits one to perform cosmological parameter estimation from the reconstructed signal after filtering the data. However, linear filters conserve information only if they are invertible, which is not provided for realistic cases as we show in appendix H. A consistent estimation of cosmological parameters has to be done in a full Bayesian framework by estimating the joint PDF of the signal and the parameters, as we will see in section 2.6.2 (Wandelt et al. 2004).

2.5.7 Flat prior and Poissonian likelihood: the Richardson-Lucy algorithm

A widely used deblurring algorithm in astronomy and medical tomography is the Richardson-Lucy algorithm (Richardson 1972; Lucy 1974), which was shown to be the maximum likelihood solution with a Poissonian likelihood by Shepp & Vardi (1982). We show the derivation in appendix H as a simplified case with respect to eq. (23). The Richardson-Lucy algorithm cannot prevent serious noise amplifications in the restoration process (see e.g. Carasso 1999). This is a natural consequence when a prior that regularizes the solution is missing. A toy application is presented in section 2.5.3.

2.5.8 Jeffrey’s prior

Other non-informative priors have been suggested based on invariant statistical structures under transformation of variables in a Bayesian formalism. Considering a one-to-one transformation in the one-dimensional case of the parameter: \(\phi = f(\theta)\), the equivalence between the respective prior densities is expressed by

\[
P(\phi) = P(\theta) \left| \frac{\partial f}{\partial \phi} \right|^{-1}.
\]

This relation is satisfied by Jeffrey’s prior \(P(\theta) \propto |J(\theta)|^{1/2}\), where \(J(\theta)\) is the Fisher information

\[
J(\theta) = \left( \frac{\partial \log P(d|\theta)}{\partial \theta} \right) (d \theta) = -\left( \frac{\partial^2 \log P(d|\theta)}{\partial \theta^2} \right) (d \theta),
\]

and where we have assumed the following regularity condition \(\int d \theta P(d|\theta) = 0\). Relation (31) can be proved easily by doing the evaluation \(J(\phi) = -\left( \frac{\partial^2 \log P(d|\phi)}{\partial \phi^2} \right) (d \phi)^2 = J(\theta) \left| \frac{\partial f}{\partial \phi} \right|^2\) (see e.g. Gelman et al. 2004). Note, however, that in the multidimensional case, Jeffrey’s prior may lead to incoherences or even paradoxes (see e.g. Berger & Bernard 1992; Robert 2001). Jeffrey’s prior is applied adequately, when not even the order of magnitude of the parameter to be estimated is known a priori. We derive Jeffrey’s ignorance prior for the 3-D power-spectrum \((S = \text{diag}(P_\delta(k)))^6\) in appendix I (see section 2.6.2 for an application of this prior).

2.5.9 Entropic prior and Maximum Entropy method

Another approach searches the least informative model compatible with the data using a prior based on Boltzmann’s definition of entropy \(S^B\) (or equivalently, Shannon’s notion of information, see Shannon 1948).

\[
P(s|p) = \exp(\alpha S^B),
\]

and maximizing the resulting posterior distribution, being \(\alpha\) some constant, and \(s\) the so-called hidden image (or signal). This inference procedure is called the Maximum Entropy method (MEM). Jaynes 1963, 1968; Frieden 1972; Gull & Daniell 1978; Gull 1989; Skilling 1989; Maisinger et al. 1997; Hobson et al. 1998). For a review see Narayan & Nityananda (1984). From now on we will represent the underlying signal by \(s\) in the framework of MEM. The MEM can be considered as MAP estimation with an entropic prior.

The particular expression for the entropy depends on the statistical formulation of the non-informative prior. Let us think of a positive signal as a grid with \(q\) cells, with each cell \(i\) having a certain intensity value \(s_i, i = 1, \ldots, q\), with an uncertainty on each value given by \(\pm\alpha^{-1}\). Then we define some discrete quantas \(n_i\) on each cell related to the intensity through the uncertainty: \(n_i = \alpha s_i\). The signal can be guessed by distributing the \(n_i\) quantas in the grid. In this way, the image is modeled in this way analogously to the energy configuration space of a thermo-dynamical system. If we further demand each cell to be \(\text{iid}\), the number of ways this object can occur is given by the multiplicity

\[
W = \frac{N_i!}{n_1! n_2! \ldots n_q!},
\]

6 The generalization to the multidimensional case leads to the following matrix form: \(J_{ij}(\theta) \equiv \left( \frac{\partial \log P(d|\theta)}{\partial \theta} \frac{\partial \log P(d|\theta)}{\partial \theta} \right) (d \theta) (d \theta)\) (see appendix H).

7 Here the autocorrelation matrix \(S\) is represented in k-space. We will discuss this in further detail in section 2.5.10.

10 Not to be confused by the signal autocorrelation \(S\).
with $N_q$ being the total amount of *quantas* to be distributed in all cells $(N_q = \sum n_i)$. The probability of any particular result is then given by the multinomial distribution

$$P(s' \mid p) = W q^{-N_q}.$$  

(35)

[Sutton & Wandelt 2006] propose to sample from the multiplicity function directly to perform reconstructions in radioastronomy. By using Stirling’s formula for the factorials $(n! \sim n^e \cdot e^{-n})$ we can write

$$\log P(s' \mid p) = -\alpha \sum s'_i \log s'_i + \text{const.}$$  

(36)

Comparing this expression with eq. (33), we recover Shannon’s definition of entropy ($S_E^\pm = \sum s'_i \log s'_i$). The expression that is commonly used for the entropy is a generalization of Shannon’s formula by Skilling that can be derived based on consistency arguments within probabilistic information theory for positive and additive distributions (PADs) [Skilling 1989].

This generalization implies the definition of a Lebesgue measure $(m)$ for the integral of some function of the hidden image to represent the entropy

$$S_E^\pm(s' \mid p) = \sum \left[ s'_i - m_i - s'_i \log \left( s'_i / m_i \right) \right].$$  

(37)

here in its discretized form. Skilling’s expression for the entropy can also be derived by considering a *team of monkeys* throwing balls at $q$ cells at random with Poissonian expectation $\mu_i$: $P(n(\mu) = \prod \mu_i^{n_i} e^{-\mu_i} / n_i)!$, where $n_i = \alpha s_i$ and $\mu = \alpha m_i$ [Skilling 1989]. For a review on further expressions for the entropy see [Molino et al. 2001].

The global maximum of $S_E^\pm$ over $s$ in the absence of further constraints is found to be $s' = m$. Consequently, $m$ can also be thought of as a prior model for the image. However, this expression for the entropy will allow reconstructing positive signals only. [Zaroubi et al. 1995] propose to define $s' = p$ and $m = p_0$, to avoid the possibility of having a negative distribution for $s$.

According to [Gull & Skilling 1997], the MEM can be extended to reconstruct distributions, which can be either positive or negative, as in the case of density fluctuations. Such distributions can be described as the difference between two subsidiary positive distributions (PADs)

$$s = u - v,$$

(38)

relative to a common model $m$:

$$S_E^\pm(u, v \mid p) = \sum \left[ u_i - 2 m_i - u_i \log (u_i/m_i) \right] + \sum \left[ v_i - 2 m_i - v_i \log (v_i/m_i) \right].$$  

(39)

One can see from eq. (38) that $\partial S_E^\pm / \partial u = -\partial S_E^\pm / \partial v$, hence yielding

$$uv = m^2.$$  

(40)

From the relations given by eqs. (38) and (40), it is easy to derive

$$u = \frac{1}{2} (w + s).$$  

(41)

11 The “+” symbol in $S_E^+$ denotes that the definition is only valid for positive signals $s$.

12 The “−” symbol in $S_E^-$ denotes that the definition is valid for positive and negative signals $s$. 

TheMaximum Entropy method gives a non-linear estimator of the underlying signal that one wants to reconstruct. This method is especially interesting to study deviations from Gaussianity [Maisinger et al. 1997; Hobson et al. 1998]. It is equivalent to maximize $\chi^2$ with a Lagrangian multiplier, which includes a penalty function given by the entropy. Maximum Entropy in this context searches the hidden image that adds the least additional information to the data.

The quantity we need to maximize is given by

$$Q_E(s \mid p) = \alpha S_E(s \mid p) + \log L(s \mid d, p),$$  

(44)

where the log $L$ is given by eq. (13) or eq. (14). The equation we want to solve is

$$\nabla Q_E(s \mid p) = 0.$$  

(45)

In section 2.4, different iterative algorithms to solve this non-linear problem will be discussed. The required expressions for the gradient of $Q_E^\pm$ and its curvature for positive and positive/negative expressions of the entropy (eqs. 37 and 43) and for both Gaussian and Poissonian likelihoods are presented in appendix B.

Note that in the limit of low density fluctuations, i.e. in the linear regime, the expression of the entropy reduces to the quadratic entropy (eventually with an offset of the origin of $s$), $S_E^\pm(s \mid p) \approx -\sum s_i^2 / 2m_i$. This expression is very similar to a Gaussian prior for the signal with a variance given by $m$. In that case Maximum Entropy leads to the Wiener-filter.

### 2.6 Markov Chain Monte Carlo: sampling the joint PDF

The drawback of the maximization methods hitherto mentioned, is that they find a unique estimator that is most probably subject to the chosen values for the required parameters. As already mentioned, the complete characterization of a system is contained in the joint PDF in the product space of possible signals and parameters. Thus, it would be desirable to sample from this PDF to find the region of highest confidence for our estimator. This is possible using Markov Chain Monte Carlo (MCMC). The importance of sampling from the joint PDF and the viability of doing that with MCMCs has already been discussed in other contexts in astronomy [Hobson & McLachlan 2003; Jewell et al. 2004; Wandelt et al. 2004]. With the MCMC method, the whole system can be moved in its configuration space by updating all variables successively in a Monte Carlo fashion, until the system relaxes (burns-in) and reaches the highest density region.

The expectation of the $i$-th parameter ($\theta_i$) can be calculated by the so-called ergodic average, which is given by the mean of the sample

$$\langle \theta_i \rangle \mid (\theta, d) \approx \frac{1}{N_b} \sum_{t=0}^{N_b-1} \theta_i^t,$$

(46)

with $N_b$ being the size of the sample drawn once the Markov Chain has *burned-in*. In general, the mean estimator is more reliable than the maximum of the distribution, especially in cases with deviations from Gaussianity (see e.g. Gelman et al. 2004). The MCMC
method permits one to approximately solve the integral in eq. 4 through expression 46.

2.6.1 Gibbs sampling

The most straightforward MCMC method is the Gibbs sampler (Geman & Geman 1984), also known as the heatbath algorithm. The Gibbs algorithm samples from the joint PDF by repeatedly replacing each component with a value drawn from its distribution conditional on the current values of all other components. This process can be seen as a Markov Chain with transition probabilities \( \pi_k \) for \( k = 1, \ldots, n \),

\[
\pi_k(\theta, \theta') = P(\theta_k' | \{ \theta_i : i \neq k \}) \cdot \prod_{i \neq k} \delta_k(\theta_i, \theta_i'),
\]

(47)

where \( \delta_k(\theta_i, \theta_i') = \{(\theta_1, \ldots, \theta_{k-1}, \theta_{k+1}, \ldots, \theta_n) \) (see e.g. Neal 1993) and \( \delta_k \) is the Kroenecker delta-function. The Gibbs sampler starts with some initial values \( \theta^{(0)} = (\theta_1^{(0)}, \ldots, \theta_n^{(0)}) \) and obtains new updates \( \theta^{(i)} = (\theta_1^{(i)}, \ldots, \theta_n^{(i)}) \) from the previous step \( \theta^{(i-1)} \) through successive generation of values

\[
\theta_1^{(i)} \sim P(\theta_1 | \{ \theta^{(i-1)}_j : i \neq 1 \})
\]
\[
\theta_2^{(i)} \sim P(\theta_2 | \{ \theta_1^{(i)}, \theta^{(i-1)}_j : i > 2 \})
\]
\[
\vdots
\]
\[
\theta_n^{(i)} \sim P(\theta_n | \{ \theta^{(i)}_i : i \neq n \})
\]

(48)

In this way a random walk on the vector \( \theta \) is performed by making subsequent steps in low-dimensional subspaces, which span the full product space. This is similar to individual collisions of particles in a mechanical system that drives a many-body system to an equilibrium distribution for all degrees of freedom. We are especially interested in this sampling method because of its efficiency that permits us to tackle large dimensional problems in contrast to other algorithms, which include acceptance and rejection rules. See Wandelt et al. (2004) for applications in CMB-mapping and power-spectrum estimation. However, in the case where the particular distribution function is unknown or cannot be explicitly expressed rejection sampling methods will be necessary (see section 2.3.3). Like the Metropolis-Hastings algorithm (Metropolis et al. 1953; Hastings 1970).

The MCMC method can be applied to perform simultaneously the reconstruction of the density field and the estimation of other parameters, such as the power-spectrum, the peculiar velocities, the bias, or the cosmological parameters (see fig. 1). We propose in the next sections two novel applications of this method to power-spectrum estimation from a galaxy redshift survey and redshift-distortion corrections, which can also be used in a joint algorithm. Note, that a higher degree of complexity can be achieved in the schemes we present here by going beyond linear perturbation theory or considering higher moments of the density field.

2.6.2 Joint signal and power-spectrum estimation: sampling the cosmic variance with data augmentation

The joint PDF considered here is given by the joint PDF of the signal and the power-spectrum \( P(s, S(d)) \). For the initial guess either an expression for the power-spectrum can be applied (see e.g. Efstathiou et al. 1992; Peacock & Dodds 1994; Smith et al. 1998; Eisenstein & Hu 1999), or the power-spectrum of the CMB can be taken and calculated for the required redshifts with some transfer functions (see e.g. Eisenstein & Hu 1999). Then the following sampling processes are iterated until the chain "burns-in"

\[
s^{(j+1)} \sim P(s | S^{(j)}, d),
\]

(49)

\[
S^{(j+1)} \sim P(S | s^{(j+1)}),
\]

(50)

The DM signal is sampled with the following PDF (see section 2.5.2)

\[
P(s | S^{(j)}, d) \propto G\left(s - F_{WF}(S^{(j)})d, \sigma^2_{WF}(S^{(j)})\right).
\]

(51)

The Wiener reconstruction is known to give a biased estimator, which attenuates the power especially for the modes where the noise becomes important, as discussed in section 2.5.3. This filtering effect has to be compensated by adding a fluctuating term with statistics according to the correct covariance (see Wandelt et al. 2004)

\[
s^{(j)} = (s^{(j)})_{WF} + y^{(j)}_{WF}.
\]

(52)

To generate the data augmentation \( y^{(j)}_{WF} \), one has to solve the following set of equations (see Eriksen et al. 2007)

\[
y^{(j)}_{WF} = \left((S^{(j)})^{-1} + \sigma^2_{WF}\sigma^2_{WF}^{-1}\right)^{-1}\left((S^{(j)})^{-1/2}x_{G_1} + \sigma^2_{WF}^{-1/2}x_{G_2}\right),
\]

where \( x_{G_1} \) and \( x_{G_2} \) are two independent Gaussian variables. One can show by direct calculation that \( y^{(j)}_{WF} \) has a covariance given by \( \sigma^2_{WF} \). To stabilize the inversion Eriksen et al. (2007) suggest using the following expression derived from the previous one by factorizing the square-root of the power-spectrum

\[
y^{(j)}_{WF} = \left((S^{(j)})^{1/2} + \sigma^2_{WF}^{-1/2}\sigma^2_{WF}^{-1}\sigma^2_{WF}^{-1}\right)^{-1}\left(x_{G_1} + (S^{(j)})^{1/2}x_{G_2}\right).
\]

(54)

Accordingly, the reconstruction step can be done by solving the following set of equations based on the signal-space representation of the Wiener-filter (eq. 22)

\[
s^{(j)}_{WF} = \left((S^{(j)})^{1/2} + \sigma^2_{WF}^{-1/2}\sigma^2_{WF}^{-1}\sigma^2_{WF}^{-1}\right)^{-1}\left((S^{(j)})^{1/2}x\right) + \sigma^2_{WF}^{-1/2}d.
\]

(55)

This allows to perform the inversion for the fluctuating term and for the reconstruction in one step. An alternative way, permits us to use the data-space representation of the Wiener-filter by generating the fluctuations with a constrained realization (see Bertschinger 1987; Hoffman & Ribak 1991; Ganon & Hoffman 1993)

\[
y^{(j)}_{WF} = \tilde{s}^{(j)} - F_{WF}\tilde{d}^{(j)},
\]

(56)

using two auxiliary Gaussian random fields \( \tilde{s} \) and \( \tilde{c} \) with zero mean and correlation \( \langle \tilde{s}\tilde{s}^\dagger \rangle = S \) and \( \langle \tilde{c}\tilde{c}^\dagger \rangle = N \) respectively. Further we set \( \tilde{d} = R\tilde{s} + \tilde{c} \). This method has the advantage that non-linear reconstructions can be obtained with N-body simulation. \[\text{Note: this is not appropriate, due to the inverse of the response operator (see appendix C).}\]

\[\text{Note: however, that a Gaussian constrained realization is good enough for power-spectrum estimation especially when one is interested in the tracers of the linear regime, like the baryon acoustic oscillations, or the gravitational potential for the ISW-effect. Sampling with constrained N-body reconstructions requires a much deeper development, since the whole cosmological parameter space has to be scanned.}\]

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(see Bistolas & Hoffman [1998]). It can be shown that the term in eq. (56) has the appropriate Wiener covariance (see appendix [2]). Each reconstruction step can then be done in one step with the direct Wiener representation by solving the following equations

\[ s^{(j)} = \tilde{g}^{(j)} + F_{\text{WF}} (d - \tilde{d}^{(j)}). \]  

(57)

The power-spectrum can be sampled by an inverse gamma function, which we derive here for the case of the 3D power-spectrum (see Wandelt et al. (2004), for the analogous CMB case)

\[ P(S \mid s) \propto P(S)P(s \mid S). \]  

(58)

Assuming a Gaussian signal \( s \) (see eq. (20)) this yields

\[ P(P_{\delta}(k) \mid s^{(j)}) \propto P(P_{\delta}(k)) \prod_{k} \frac{1}{\sqrt{P_{\delta}(k)}} \exp \left( -\frac{|s^{(j)}(k)|^2}{2P_{\delta}(k)} \right), \]  

(59)

with \( S = \text{diag}(P_{\delta}(k)) \). The prior \( P(P_{\delta}(k)) \) can be chosen to be flat \( (P(P_{\delta}(k)) = \text{const}) \) or instead Jeffrey’s prior can be used \( (P(P_{\delta}(k)) \propto P_{\delta}(k)^{-1}) \), see section (2.5.8) and appendix I. Note, that the likelihood for the power-spectrum given by eq. (59) is clearly non-Gaussian.

2.6.3 Joint signal and peculiar velocities estimation: redshift-distortions correction

We propose to sample the peculiar velocities in a MCMC fashion (see section 2.6), analogous to the case of the power-spectrum (see Wandelt et al. (2004) and section 2.6.2). We draw realizations of the matter field given the data, a power-spectrum and assumed galaxy peculiar velocities

\[ s^{(j+1)} \sim P(s \mid v^{(j)}, S, d). \]  

(60)

The velocities are subsequently sampled too:

\[ v^{(j+1)} \sim P(v \mid s^{(j+1)}). \]  

(61)

In each step where we sample the peculiar velocity, the redshift-distortion can be corrected using

\[ r^{(j+1)} = z - v^{(j+1)} \]  

(62)

We propose to sample the peculiar velocities from a PDF with a mean \( \langle \psi \rangle_M \) given by the linear theory \( v_{LT} \) and a velocity dispersion \( \sigma_v \) depending on the local value of the over-density,

\[ P(v \mid s^{(j)}) \propto G \left( v - \langle \psi \rangle_M (s^{(j)}), \sigma_v^2 (s^{(j)}) \right), \]  

(63)

where we have taken a Gaussian distribution, but this could be extended to other PDFs.

3 NUMERICAL METHOD

In order to efficiently sample the joint PDF, as it is required in MCMC methods (see section 2.6), fast inverse algorithms need to be considered to regularize the solution. General iterative inverse methods scale as \( \mathcal{O}(n^3) \) since they imply matrix multiplications of a \( n \times n \) matrix in an iterative fashion (at most \( n \)-steps until convergence). This makes the study of the joint PDFs as presented in section 2.6, at a first glance, un-feasible. However, a proper formulation of the problem in an operator formalism allows treating the matrices as operators that have to be neither calculated nor stored. Within this operator formalism, the inversion methods we present here speed up to a scaling of \( \mathcal{O}(n \log_2 n) \). We start with a general formulation of iterative methods and subsequently present the different schemes that we have implemented in ARGO. Since a preconditioning treatment can dramatically enhance the performance of iterative schemes (see our numerical experiments in section 4), we pay special attention to this point in the derivation of the different schemes.

3.1 Iterative inverse and regularization methods: a unified formulation of different linear methods

Let us consider a region \( D \) in the \( n \)-dimensional Euclidean space \( E^n \) and denote \( L_2(D) \) the Hilbert space of all complex measurable square integrable functions \( \int_D d^nz |g(z)|^2 < \infty \) with inner product \( ^{\text{c}} \)

\[ \langle g | s \rangle = \int_D d^nz \overline{g(z)} s(z), \]  

(64)

and norm of \( g \in L_2(D) \)

\[ ||g|| = ( \langle g | g \rangle )^{1/2}. \]  

(65)

Let \( \Psi \) be a subspace of the Hilbert space \( L_2(D) \) with the conditions that every element \( \psi \in \Psi \) must satisfy being smoothness, limit behavior at the boundary \( D \), etc. Let us now consider the linear operator \( A \), defined on the linear manifold \( \Psi \), and suppose that \( A \) is a positive definite, i.e. \( \langle A \psi | \psi \rangle \geq 0 \) for all \( \psi \in \Psi \). The kind of inverse problem we are interested in belongs to the stationary problems of the form

\[ A \psi = f, \]  

(66)

since, for example, for the COBE-filter we have to invert \( A(s)_{\text{COBE}} = \mathbf{R}^\top \mathbf{N}^{-1} \mathbf{d} \), with \( \psi = \langle s \rangle_{\text{COBE}}, A = \mathbf{R}^\top \mathbf{N}^{-1} \mathbf{R} \) and \( f = \mathbf{R}^\top \mathbf{N}^{-1} \mathbf{d} \), and for the Wiener-filtering we have \( \psi = \langle \mathbf{S}^\top \rangle_{\text{WF}}^{-1} \langle s \rangle_{\text{WF}}, A = \mathbf{R}^\top \mathbf{S} \mathbf{R} + \mathbf{N} \) and \( f = \mathbf{d} \). Eq. (66) has the same structure as eq. (2), but without a noise term. Hence, a regularization method is again required.

3.1.1 Minimization of the quadratic form

Another way of approaching the linear inverse problem is the minimization of a quadratic form given by

\[ Q_A(\psi) = \frac{1}{2} \langle A \psi | \psi \rangle - \langle f | \psi \rangle + c. \]  

(67)

The gradient of \( Q_A \) leads to

\[ \frac{dQ_A}{d\psi}(\psi) \equiv Q_A'(\psi) = A \psi - f, \]  

(68)

assuming that the operator \( A \) is self-adjoint. Setting the gradient to zero, one obtains eq. (65). The surface defined by a quadratic form with a positive definite matrix \( A \) is shaped like a paraboloid bowl (see e.g. Shewchuk [1994]). This ensures the existence of a unique minimum or, equivalently, the convergence of appropriate algorithms.

15 Here a Dirac type notation is introduced. It should not be confused with the ensemble average notation, which does not have a bulk in-between.

16 This expression can be written in matrix notation as \( \psi^\dagger A \psi \geq 0 \), where \( \psi^\dagger \) is the conjugate and transpose of the vector \( \psi \).
3.1.2 Solution of the non-stationary problem: asymptotic regularization

Here, a unified framework for the regularization methods that we have implemented in ARGO is given based on the asymptotic regularization. Nevertheless, an original Bayesian motivation to the asymptotic solution is presented in appendix L.

The stationary problem (eq. 66) can be replaced by a non-stationary equation, which relaxes to the equilibrium solution as the time step \( \tau \) becomes small:

\[
\frac{\partial \psi}{\partial \tau} + A \psi = f.
\]  

We seek solutions of the form

\[
\psi = \sum_i \psi_i u_i,
\]

with a spectrum for the operator \( A \)

\[
A u_i = \lambda_i u_i.
\]

Expanding \( f \) in this basis, yields

\[
f = \sum_i f_i u_i.
\]

Then we get the following relations for the Fourier coefficients in the stationary case

\[
\lambda_i \psi_i = f_i,
\]

and for the non-stationary case

\[
\frac{\partial \psi_i(t)}{\partial \tau} + \lambda_i \psi_i(t) = f_i,
\]

which lead to the following solutions

\[
\psi = \sum_i \frac{f_i}{\lambda_i} u_i,
\]

and

\[
\psi(t) = \sum_i \frac{f_i}{\lambda_i} (1 - e^{-\lambda_i t}) u_i,
\]

for the stationary and non-stationary cases, respectively. Since the spectrum of a positive definite operator \( A \) is real, \( \lambda_i > 0 \), it follows that \( \lim_{\tau \to \infty} \psi_{\text{non-stationary}} = \psi_{\text{stationary}} \).

The non-stationary problem can be solved using difference methods with respect to \( \tau \)

\[
\psi^{\tau+1} = \psi^\tau + \tau^\prime M^\prime (f - A \psi^\tau),
\]

with \( \{M^\prime\} \) being a set of non-singular matrices and \( \{\tau^\prime\} \) being a sequence of real parameters. Here we concentrate on a constant, self-adjoint matrix \( M \). Let us rewrite eq. (77) as

\[
\psi^{\tau+1} = \psi^\tau + \tau^\prime M \xi^\prime,
\]

with the residuals given by

\[
\xi^\prime = f - A \psi^\prime.
\]

The error vectors are defined as

\[
\eta^\prime = \psi^\prime - \psi^\tau,
\]

where \( \psi^\prime = A^{-1} f \) is the exact solution. The matrix \( M \) and the real number \( \{\tau^\prime\} \) are chosen to speed up convergence. M usually represents the preconditioning of eq. (77) and \( \tau^\prime \) can be interpreted as the time step (see appendix M), and is also called relaxation parameter. Here truncation regularization occurs by quitting the iteration loop. Some stopping rules are therefore required. In the case where no noise regularization was conducted in the first step, they crucially define the noise regularization. In the other cases, they mostly determine algorithmic performance and accuracy. At this point we are interested in the regularization for the inverse purpose, since we have already found expressions which regularize the noise (e.g. Wiener-filter, or MEM). However, the results presented in section 4 show that in some cases truncation leads to better results (see discussion in section 4.3). In the following sections, we will show how different iterative schemes are based on the general formula given by eq. (77). It is worth mentioning that other methods that we do not discuss in this paper, like the algebraic reconstruction technique (ART, see Gordon 1974), can also be expressed through this formula.

3.1.3 Jacobi method

The Jacobi iteration method splits the operator \( A \) in two matrices

\[
A = D + B,
\]

where \( D \) contains the diagonal elements of \( A \) and \( B \) contains the off-diagonal elements. From eq. (69) one follows

\[
\psi = D^{-1} (f - B \psi).
\]

Substituting \( B \) by \( A - D \) one gets the following iteration scheme

\[
\psi^{\tau+1} = \psi^\tau + D^{-1} (f - A \psi^\tau),
\]

The Jacobi method turns out to be a particular case of the iteration scheme given by eq. (77) with a preconditioning matrix given by \( M = D^{-1} \) and \( \tau^\prime = 1 \). This method can, must be optimized by increasing the timestep \( \tau^\prime \) by a certain percentage if the solution converges and decreasing the timestep if the solution diverges. An optimal timestep is hard to find, because the spectrum of the operator \( A \) has to be known (see appendix M).

3.1.4 Steepest Descent method

The steepest descent method searches the minimum of the quadratic form by choosing the direction in which \( Q_A \) decreases most rapidly. This direction is given by the residual

\[
- Q_A^\prime (\psi^\prime) = f - A \psi^\prime = \xi^\prime.
\]

The form of the iteration scheme is thus given by eq. (78), with the length of the step in the direction of the residual given by \( \tau^\prime \). Steepest descent looks for the optimal length which minimizes the quadratic form with respect to \( \tau^\prime \)

\[
0 = \frac{dQ_A}{d\tau^\prime} (\psi^{\tau+1}) = \langle Q_A (\psi^{\tau+1}) \psi^{\tau+1} \rangle = \langle \xi^{\tau+1} | M \xi^{\tau+1} \rangle.
\]

This implies that subsequent searching directions must be orthogonal (say \( M = I \)). Starting from this condition it is straightforward to derive the expression for \( \tau^\prime \). It is only necessary to use the definition of residual for \( \xi^{\tau+1} \) and substitute \( \psi^{\tau+1} \) from eq. (78).

\[
\tau^\prime = \frac{\langle \xi^\prime | M \xi^\prime \rangle}{\langle \xi^\prime | M \xi^\prime \rangle}.
\]

Both the calculation of the factors \( \tau^\prime \) and the residuals \( \xi^\prime \) imply applying the operator \( A \) each time on different vectors. It is possible, however, to reduce the operation of \( A \) to the same vector for

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every iteration, but the residuals, must be calculated in a different way. Multiplying both sides of eq. (78) by \(-A\) and adding \(f\), one obtains the following relation for the residuals
\[
\xi^{j+1} = \xi^j - \tau^j AM\xi^j. \tag{87}
\]
Notice that the vector \(AM\xi^j\) already appears in the expression for \(\tau^j\), and consequently saves one operation. However, expression (79) has to be periodically used with the feedback of \(\psi^j\), to avoid the accumulation of floating-point roundoff error. The disadvantage of this method is that it ends up searching repeatedly in the same direction. This is especially severe when the quadratic form is highly deformed, which occurs when the matrix \(A\) deviates from the unity matrix. We will see, however, that the newest descent competes with any other method when the preconditioning is effective, and thus the stretched shape of the quadratic form is brought close to a spherical symmetric shape. Preconditioning should not imply too many operations; that is the reason why the inverse of the matrix, which contains only the diagonal elements of \(A\), is usually taken for preconditioning. This will work especially fine when the operator \(A\) is diagonally dominant, which in our case occurs when nearly full-sky data are available.

3.1.5 Krylov methods: Conjugate Gradients

To make the iteration scheme more efficient, Conjugate Gradients proposes to search each time in a different direction. This is achieved by imposing \(A\)-orthogonality to two different \((i \neq j)\) searching vectors \(\mu^i\) and \(\mu^j\):
\[
\langle \mu^i | \mu^j \rangle_A \equiv \langle A\mu^i | \mu^j \rangle = 0, \tag{88}
\]
which are then said to be conjugated. In the preconditioned case, the searching vectors are multiplied by \(M\) so that the conjugacy has to be formulated in the following way:
\[
\langle M\mu^j | M\mu^i \rangle_A = 0 \quad \text{(for} \quad i \neq j). \tag{89}
\]

The iteration scheme is given by substituting the residuals in eq. (78) by the new searching vectors \{\mu^j\}
\[
\psi^{j+1} = \psi^j + \tau^j M\mu^j. \tag{90}
\]

By subtracting \(\psi^*\) we obtain an equation for the errors, \(\eta^{j+1} = \eta^j + \tau^j M\mu^j\).
\[
\xi^{j+1} = -A\eta^{j+1}, \tag{91}
\]
we can derive the recurrent formula for the residuals
\[
\xi^{j+1} = -A(\eta^j + \tau^j M\mu^j) = \xi^j - \tau^j AM\xi^j. \tag{92}
\]

Here again, expression (79) has to be used periodically with the feedback of \(\psi^j\) to avoid the accumulation of floating-point roundoff error. The optimal length of the step is found by minimizing the quadratic form
\[
0 = \frac{dQ_A}{d\tau}(\psi^{j+1}) = -\langle \xi^{j+1} | M\mu^j \rangle = \langle \eta^{j+1} | M\mu^j \rangle_A. \tag{93}
\]
Substituting expression (90) in (92) we then obtain
\[
\tau^j = -\frac{\langle \eta^j | M\mu^j \rangle_A}{\langle M\mu^j | M\mu^j \rangle_A} = \frac{\langle \xi^j | M\xi^j \rangle}{\langle M\xi^j | M\mu^j \rangle_A}. \tag{94}
\]
It can be shown that this formula is equivalent to the following expression
\[
\tau^j = \frac{\langle \xi^j | M\xi^j \rangle}{\langle M\mu^j | M\mu^j \rangle_A}. \tag{95}
\]

Using \(\langle \xi^j | M\mu^j \rangle = \langle \xi^j | M\xi^j \rangle \) (see appendix \textbf{K}).

To generate \(A\)-orthogonal searching vectors one could think of Gram-Schmidt-conjugation
\[
\mu^j = \xi^j + \sum_{k=0}^{j-1} \beta^{jk} \mu^k. \tag{96}
\]

Here it was assumed that the residuals \(\{\xi^j\}\) form a set of linearly independent vectors (see appendix \textbf{K}). The expression for the factors \(\beta^{jk}\) can be derived by calling \(A\)-orthogonality in eq. (96)
\[
\langle M\mu^j | M\mu^j \rangle_A = \langle M\xi^j | M\mu^j \rangle_A + \sum_{k=0}^{j-1} \beta^{jk} \langle M\mu^k | M\mu^j \rangle_A = 0 = \langle M\xi^j | M\mu^j \rangle_A + \beta^{j+1} \langle M\mu^j | M\mu^j \rangle_A. \tag{97}
\]
One obtains the following formula for the factors
\[
\beta^{j+1} = \frac{\langle M\xi^j | M\mu^{j+1} \rangle_A}{\langle M\mu^{j+1} | M\mu^j \rangle_A}. \tag{98}
\]
where \(i < j\) according to eq. (96).

This method seems to require too much memory, as apparently all previous searching vectors must be stored to calculate the new one. However, only one \(\beta\)-factor remains in the sum in eq. (96), as we show in appendix \textbf{K}.

Hence, Gram-Schmidt orthogonalization can be simplified to the following expression
\[
\mu^{j+1} = \xi^{j+1} + \beta^{j+1} \mu^j, \tag{99}
\]

where
\[
\beta^{j+1} = \frac{\langle M\xi^j | M\mu^{j+1} \rangle_A}{\langle M\mu^{j+1} | M\mu^j \rangle_A}. \tag{100}
\]

with \(\text{EXP}\) meaning expensive, since the numerator of \(\beta\) apparently requires an extra \(A\) operation. This additional operation can be saved by taking the vector \(AM\mu^j\) from \(\tau^j\) or with alternative methods (see table 2 and appendix \textbf{K}), like the Fletcher-Reeves method (Fletcher & Reeves 1964)
\[
\beta^{j+1}_\text{FR} = \frac{\langle \xi^{j+1} | M\xi^{j+1} \rangle}{\langle \xi^{j+1} | M\xi^j \rangle}, \tag{101}
\]
the Polak-Ribiére formula (Polak & Ribiére 1969)
\[
\beta^{j+1}_\text{PR} = \frac{\langle \xi^{j+1} | M(\xi^{j+1} - \xi^j) \rangle}{\langle \xi^{j+1} | \xi^j \rangle}, \tag{102}
\]
or the Hestenes-Stiefel expression (Hestenes & Stiefel 1952)
\[
\beta^{j+1}_\text{HS} = -\frac{\langle \xi^{j+1} | M(\xi^{j+1} - \xi^j) \rangle}{\langle \mu^j | M(\xi^{j+1} - \xi^j) \rangle}. \tag{103}
\]

However, \(\beta\text{EXP}\) turns out to be a very efficient scheme, which behaves far more stably than the rest (see section 4). Since the \(\beta\)-formulae (eq. 100) are mathematically equivalent, one could think of combining them in a single scheme finding numerically different solutions. However, this kind of hybrid scheme remains to be thoroughly studied.

Formula (99) shows that new searching vectors are built from

\[\beta^{j+1} \neq 0\text{ for } j = 0, \ldots, n-1, \quad \text{for } i < j. \]
a linear combination of the current residual and the previous searching vector. Since the subsequent residuals are given by the linear combination of the previous residual and the A-operator applied to the searching vector, the manifold where the solution is being searched is spanned by the residuals and the so-called Krylov space. The latter is built by applying the A operator to the basis vector successively. In this manifold, curved quadratic forms appear to be spherical and thus the searching process becomes more effective. It is possible to derive the Conjugate Gradients method by minimizing the A-norm of the error: \( \min ||\eta||_A \) (see e.g. Marchuk 1982). In this sense an optimal solution to the inverse problem can be found even if no unique solution exists. Conjugate Gradients works, even if the operator A is not a positive definite (for a discussion see e.g. Shewchuk 1994). It can easily be shown that Conjugate Gradients converges at most in \( n \)-steps, with \( n \) being the number of pixels/vector columns (see e.g. Shewchuk 1994).

### 3.2 Non-linear inverse methods

Non-linear inverse methods are especially required in reconstruction algorithms that do not assume a Gaussian distribution. The iterative method given in eq. (28), which makes use of a Poissonian likelihood, can alternatively be solved with the methods presented in this section. The same applies to the MEM, where zeros of the likelihood, can alternatively be solved with the methods presented in appendix K. The FR and the PR methods are tested against the EXP algorithm in section 4.

| \( D_m \) | \( N_l \) | \( \langle \xi^j | M \xi^{j+1} \rangle \) | \( \langle \xi^j | M (\xi^{j+1} - \xi^j) \rangle \) | \( \langle \xi^j | -M (\xi^{j+1} - \xi^j) \rangle \) | \( -\langle M \xi^{j+1} | M \xi^j \rangle \) | \\hline
| FR | PR | N3/D1 | — | — | EXP |
| N1/D2 | N2/D2 | — | — | — | — |
| N1/D3 | N2/D3 | — | — | — | — |
| N1/D4 | HS | N3/D4 | — | — | EXP |
| N1/D5 | N2/D5 | — | — | — | — |

Table 2. Formulae for the \( \beta \)-factor: \( \beta^{j+1}_m = \frac{N_l}{N_l} \). Three of the methods are discussed in the literature: FR (Fletcher-Reeves), PR (Polak-Ribière), and HS (Hestenes-Stiefels). The rest of the formulae are derived in this paper using equivalence relations derived in appendixes 5 and 6. The FR and the PR methods are tested against the EXP algorithm in section 4.

### 3.2.1 Newton-Raphson method

One of the most extended non-linear inverse methods is the so-called Newton-Raphson method (for an application in MEMs see Mässinger et al. 1997; Hobson et al. 1998), which can easily be derived by doing a Taylor expansion of the function under study and truncating it at the first order

\[
\psi^{j+1} = \psi^j + (\nabla A(\psi^j))^{-1}(f - A(\psi^j)).
\]

This method requires the inverse of the gradient of A, which for the cases we are interested in is the inverse of a Hessian matrix. Recalling the problem of finding extrema of a function as presented in section 3.1.1 and taking into account eq. (84), the previous equation can be rewritten as

\[
\psi^{j+1} = \psi^j + (\nabla \nabla Q_A(\psi^j))^{-1} \nabla Q_A(\psi^j),
\]

where \( \nabla \nabla Q_A \equiv \partial Q_A / \partial \psi^j \partial \psi^m \) is the Hessian matrix of \( Q_A \). For a direct derivation of this equation, we require a Taylor expansion until the second order of \( Q_A \), which is where the non-linearity arises. The MEM can be solved with expression (105) by doing the substitutions: \( Q_A \rightarrow Q^h \) and \( \psi^j \rightarrow s^j \). Here the quantity \( Q^h \) is implicitly approximated by its quadratic expansion \( Q_A \). Calculating the inverse of the Hessian \( (\nabla \nabla Q_A(\psi^j))^{-1} \) implies solving a linear ill-posed problem in each iteration of the scheme (108). Some solutions have been found to regularize this scheme, like the Levenberg-Marquardt method (see Hankel 1997) or the regularized Gauss-Newton method (see e.g. Blaschke et al. 1997).

### 3.2.2 Landweber-Fridman method

Alternative algorithms to the above mentioned Newton-Raphson class of methods do not need to invert the Hessian matrix and can thus simultaneously speed up and stabilize the inversion process. The Landweber-Fridman algorithm belongs to the class of methods based on steepest descent

\[
\psi^{j+1} = \psi^j + (\nabla A(\psi^j))\frac{1}{2}(f - A(\psi^j)).
\]
Making the same substitutions as for eq. (108), we obtain
\[ \psi^{j+1} = \psi^j - (\nabla \nabla Q_A(\psi^j))^\dagger \nabla Q_A(\psi^j). \] (110)

Here just the adjoint of the Hessian must be taken \((\nabla \nabla Q_A(\psi^j))^\dagger\). For a convergence analysis of this method see Hanke et al. (1995).

### 3.2.3 Non-linear Krylov methods

Another class of methods that do not require one to invert the Hessian matrix are the Krylov-based methods, which we have exposed in the previous section. The difference with respect to the linear case mainly resides in the calculation of the residuals. There are alternative expressions for the time step \(\tau^j\), which we have exposed in the previous section. The residuals are updated now by the negation of the gradient of the quadratic form that approximates the function under consideration \(\xi^j = -\nabla Q_A(\psi^j)\) (see eq. 84). The step size is given by
\[ \tau^j = \frac{\langle \nabla Q_A(\psi^j) | M \mu^j \rangle}{\langle M \mu^j | \nabla Q_A(\psi^j) \rangle}. \] (111)

The derivation of this expression (see appendix [C]) is based on the second order Taylor expansion of \(Q_A\). That is why Krylov algorithms which use this formula are called Newton-Krylov methods. There are alternative expressions for the time step \(\tau^j\) where the Hessian is approximated and does not need to be explicitly calculated, like those using a secant approximation. For various implementations of non-linear Krylov methods see, for example, Shewchuk (1994).

### 3.3 Operator formalism

The iterative methods presented so far require an operator formalism to become efficient. In this formalism, matrices should be represented in such a way that their action can be expressed as simple operations, like sums and multiplications. In order to achieve this, one has to carefully choose the adequate representation, in which the individual matrix components are diagonal, though the whole matrix may not be. In this section, we present the different operators under consideration (see table 3) in k-space and real-space and discuss their optimal representation. In this way, we can take advantage of the fast Fourier-transform methods (FFTs) that scale as \(n \log_2 n\), with \(n\) being the length of the arrays, and which ultimately determine the speed of the algorithm.

#### 3.3.1 Fourier-transform definitions and dimensionality of the problem

Let us introduce the following definitions of the \(N_D\)-dimensional forward and inverse Fourier-transforms just to make clear our notation
\[ \hat{x}(k) \equiv \text{FT} \{x(r)\} \equiv \int d^{N_D} r \exp(\imath k \cdot r) x(r), \] (112)
and
\[ x(r) \equiv \text{IFT} \{\hat{x}(k)\} \equiv \int d^{N_D} k \left( \frac{2\pi}{N_D} \right)^{N_D} \exp(-\imath k \cdot r) \hat{x}(k), \] (113)
respectively.

In general, the reconstruction problem has three spatial dimensions \((N_D = 3)\), with the corresponding discrete array lengths for the real-space and k-space vectors given by \(r = (r_x, r_y, r_z)\) and \(k = (k_x, k_y, k_z)\). Each component has the following range:
\[ r_x = \frac{L_x}{n_x} [0, n_x - 1], r_y = \frac{L_y}{n_y} [0, n_y - 1], r_z = \frac{L_z}{n_z} [0, n_z - 1] \] and
\[ k_x = \frac{\pi}{L_x} [0, n_x - 1], k_y = \frac{\pi}{L_y} [0, n_y - 1], k_z = \frac{\pi}{L_z} [0, n_z - 1]. \]
where the volume of the Universe under consideration is given by \(V = L_x \times L_y \times L_z\) in \([\text{Mpc}/h]^3\), and the box containing that volume is divided into \(n = n_x \times n_y \times n_z\) cells, with \(n\) being the length of the array \(x\). In the following, we will treat the operators as being continuous. However, the discrete implementation can be derived in a straightforward way (for a discussion on the relation between discrete and continuous representations see Martel (2005)). Note that the methods presented here can be applied in arbitrary dimensions.

The number of dimensions \(N_D\) is thus kept as a free parameter.

In our convention, vectors defined in real-space have plain notation \((x)\) and in k-space they are denoted with hats \((\hat{x})\). Matrices, however, have two hats in k-space. We represent convolutions with circles "\(\circ\)" and multiplications with dots "\(\cdot\)". Due to the convolution theorem, where convolutions are shown to be equal to convolutions in the counter space, we can either omit hats if they are present or include them if they are not, and replace circles with dots and vice versa "\(\hat{\cdot} \leftrightarrow \circ \)" to change from one representation to the other.

All the numerical iterative inversion schemes (see section [B]) of the different reconstruction algorithms (section [C]) require only a small number of basic operators, listed in table (3). To show how the operators listed in table [3] can efficiently be applied we derive their action on an arbitrary vector.

#### 3.3.2 Data model: the response operator and its transpose

Let us first remember the data model given in eq. (3), and suppose that the operator \(R_D\) is given by a convolution in real-space with some blurring function \(f_D\)
\[ d(r) \equiv \int d^{N_D} r' f_D(r - r') f_S(r') f_M(r') s(r') + f_{SP}(r) \epsilon(r). \] (117)

The operator \(R\) acting on an arbitrary vector \(x\) is thus given by
\[ R \{x\} (r) \equiv \int d^{N_D} r' f_D(r - r') f_S(r') f_M(r') \{x(r')\}. \] (118)

The selection function and the masks should conveniently be multiplied in real-space to save convolutions
\[ f_{SM}(r) \equiv f_S(r) f_M(r). \] (119)

Accordingly, the same operation as in eq. (118) leads to
\[ \hat{R} \{\hat{x}\} (k) = \hat{f}_D(k) \int \frac{d^{N_D} r}{(2\pi)^{N_D}} \hat{f}_{SM} (k - q) \{\hat{x}(q)\}, \] (120)
\[ \hat{f}_B \cdot \hat{f}_{SM} \circ \{\hat{x}\}, \]
in k-space. Here we have introduced the operator notation in which the equations have to be read from right to left. The braces show the sequence in which the subsequent operations have to be performed in the algorithm. The analogous operation for the adjoint \(R^\dagger\) can be derived from the definition of the response operator in real space (see eq. 118) leading to
\[ R^\dagger \{x\} (r) = f_S(r) f_M(r) \int d^{N_D} r' f_D(r' - r') \{x(r')\}. \] (121)

In k-space it yields
\[ R^\dagger \{\hat{x}\} (k) = \hat{f}_{SM} \circ [\hat{f}_B \cdot \{\hat{x}\}](k). \] (122)
\[
\mathbb{R}S^1 R(\hat{x})(k) = f_B(k) \int d^{N_D}q f_{SM}(k - q) \int d^{N_D}q' P_N(q')(2\pi)^N \delta_D(q - q') \int d^{N_D}k' f_{SM}(k' - q') f_B(k')(\hat{x}(k'))
\]

\[
\mathbb{R}^N R^N R(\hat{x})(k) = f_B(k) \int d^{N_D}q f_{SM}(k - q) \int d^{N_D}q' P_N(q')(2\pi)^N \delta_D(q - q') \int d^{N_D}k' f_{SM}(k' - q') f_B(k')(\hat{x}(k'))
\]

\[
\mathbb{R}^N N_W^\dagger R(\hat{x})(k) = f_B(k) \int d^{N_D}q f_{SM}(k - q) \int d^{N_D}q' N_W^{-1}(q - q') f_B(q') \int d^{N_D}k' f_{SM}(q' - k') f_B(k')(\hat{x}(k'))
\]

**Figure 2.** Here the action on an arbitrary vector \(\hat{x}\) of the most complex operators that appear in table 3 is shown. The upper one is required for Wiener-filtering and represents the signal term in the covariance matrix of the data. The middle and lower ones stand for the inverse of the ML variance (eq 30) and are required for the COBE-filter, the MEMG and for sampling purposes with the Wiener-filter. The equations have to be read from right to left. The braces show the order in which the operations have to be done from top to bottom. One has to be very careful with the correct conjugation of the different functions. Note that, contrary to naive expectations, the conjugation of the first selection function \(f_{SM}\) to be applied in the upper operation disappears.
The data model consists of two terms 
\[
\begin{align*}
\text{sources (such as galaxies) on a grid. The most popular assign-
\text{ment sum}
\end{align*}
\] 
Consequently, the covariance matrix of the data is given by the following sum 
\[
\langle \hat{d}(k)\hat{d}'(k') \rangle(s,p) = \langle \hat{\alpha}(k)\hat{\alpha}(k') \rangle(s,p) + \langle \hat{\epsilon}(k)\hat{\epsilon}(k') \rangle(s,p),
\]
where we have assumed that the noise is uncorrelated to the signal, which is consistent with our data model. Even though the structure function may be correlated with the signal 
\[
\langle \hat{\epsilon}(k)\hat{f_{SM}}(k') \rangle(s,p) \neq 0,
\]
the random noise part is not 
\[
\langle \hat{\epsilon}(k)\hat{f_{N}}(k') \rangle(s,p) = 0.
\]
We will calculate the different terms of the data covariance matrix and other related operators in the next sections.

### 3.3.4 Covariance matrix of the data: the signal term
Here it becomes necessary to choose the Fourier representation, since it is there that the signal-autocorrelation matrix appears to be diagonal in the form of a power spectrum (eq. 128). Taking into account statistical homogeneity for the signal 
\[
\langle \hat{s}(k)\hat{s}(k') \rangle(s,p) = (2\pi)^N\delta_D(k - k')P_{S}(k'),
\]
with \(\delta_D\) being the Dirac-delta function, we can derive the expression for the signal covariance matrix term 
\[
\langle \hat{f}_{R}\rangle(k,k') = \langle \hat{\alpha}(k)\hat{\alpha}(k') \rangle(s,p) \langle \hat{f}_{SM}(k - q)\hat{f}_{SM}(k' - q) \rangle(s,p).
\]
For its action on a vector (see fig. 2), we get
\[
\langle \hat{f}_{R} \rangle \hat{x}(k) = \hat{f}_{B}(k)\int (2\pi)^N\delta_D\hat{x}(q)\hat{f}_{SM}(k - q)\hat{f}_{SM}(k' - q)\hat{f}_{SM}(k - q')\hat{f}_{SM}(k' - q').
\]
and consequently
\[
\langle \hat{R}\rangle \hat{x}(k) = \int (2\pi)^N\delta_D\hat{x}(q)\hat{f}_{SM}(k - q)\hat{f}_{SM}(k' - q)\hat{f}_{SM}(k - q')\hat{f}_{SM}(k' - q').
\]
The inverse of the signal-autocorrelation matrix can be solved trivially in Fourier-space:
\[
\hat{S}^{-1} = \text{diag}(P_{S}(k)^{-1}).
\]
Hence, the inverse square root yields
\[
\hat{S}^{-1/2} = \text{diag}(P_{S}(k)^{-1/2}).
\]

### 3.3.5 Covariance matrix of the data: the noise term
Here, we will consider the noise covariance matrix corresponding to the definition of the likelihood. Note, that this expression is equivalent to the noise term in eq. 127 if the noise structure function has no signal dependence (see discussion in section 2.5.3). We
assume, analogous to the case of the signal, statistical homogeneity for \( C_{N} \)
\[
\langle \hat{e}_N(k) \overline{C_{N}(k')} \rangle_{(\epsilon_p)} = (2\pi)^{N_D} \delta_D(k - k') P_N(k'),
\]
and then derive the expression for the noise covariance matrix
\[
\hat{N}(k, k') = \langle \hat{e}(k) \overline{\hat{e}(k')} \rangle_{(\epsilon_p)} = \int \frac{d^{N_D} q}{(2\pi)^{N_D}} \hat{f}_{SF}(k - q) P_N(q) \hat{f}_{SF}(q - k').
\]

Its action on a vector yields
\[
\hat{N}\{\hat{x}\}(k) = \int \frac{d^{N_D} k'}{(2\pi)^{N_D}} \langle \hat{e}(k) \overline{\hat{e}(k')} \rangle_{(\epsilon_p)} \{\hat{x}(k')\} = \int \frac{d^{N_D} q}{(2\pi)^{N_D}} \hat{f}_{SF}(k - q) P_N(q) \int \frac{d^{N_D} k'}{(2\pi)^{N_D}} \langle \hat{e}(k) \overline{\hat{e}(k')} \rangle_{(\epsilon_p)} \{\hat{x}(k')\} \hat{f}_{SF}(q - k').
\]

In the case where there is no structure function, the noise-autocorrelation reduces to
\[
\hat{\hat{N}}(k, k') = (2\pi)^{N_D} \delta_D(k - k') P_N(k').
\]

Then, its action is given by
\[
\hat{\hat{N}}\{\hat{x}\}(k) = P_N\{\hat{x}\}(k).
\]

The corresponding inverse operation is
\[
\hat{N}^{-1}\{\hat{x}\}(k) = P_N^{-1} \cdot \{\hat{x}\}(k).
\]

Consequently, we obtain (see fig. 4)
\[
R^{\prime} \hat{N}^{-1}_{N} R\{\hat{x}\}(k) = \hat{f}_{SF} \circ \{f_B \circ \{P^{-1}_N \cdot \{f_B \circ \{ \hat{f}_{SF} \circ \{\hat{x}\} \}\}\}\}(k),
\]
and
\[
R^{\prime} \hat{N}^{-1}_{N} \{\hat{x}\}(k) = \hat{f}_{SF} \circ \{f_B \circ \{P^{-1}_N \cdot \{\hat{x}\} \}\}(k).
\]

The inverse square root of \( \hat{N} \) can now be calculated and leads to
\[
\hat{\hat{N}}^{-1/2}(k) = \text{diag}(P^{-1/2}_N(k)).
\]

The operation \( R^{\prime} \hat{N}^{-1/2}_{N} \{\hat{x}\} \) can then be obtained by doing the following substitution \( \hat{N}^{-1}_{N} \rightarrow \hat{\hat{N}}^{-1/2}_{N} \) in eq. (139)
\[
R^{\prime} \hat{N}^{-1/2}_{N} \{\hat{x}\}(k) = \hat{f}_{SF} \circ \{f_B \circ \{P^{-1/2}_N \cdot \{\hat{x}\} \}\}(k).
\]

We are especially interested in the case of white noise (\( P_N = P_{WN} = \text{const} \)) with a structure function (given by the Poissonian shot noise)
\[
\hat{N}_{WN}(k, k') = P_{WN} \int \frac{d^{N_D} q}{(2\pi)^{N_D}} \hat{f}_{SF}(k - q) \hat{f}_{SF}(q - k').
\]

The corresponding action yields
\[
\hat{N}_{WN}\{\hat{x}\}(k) = P_{WN} \int \frac{d^{N_D} q}{(2\pi)^{N_D}} \hat{f}_{SF}(k - q) f_{SF}(q - k') \cdot f_{SF}(\hat{x}(k')).
\]

It can be seen from this equation, that the preferential representation now is in real-space, where \( N \) is diagonal
\[
N_{WN}(r, r') = \delta_D(r - r') C_{WN} f_{SF}^2(r'),
\]
with \( C_{WN} = \text{IFT}[P_{WN}] \) being a constant. The inverse operation yields
\[
\hat{N}_{WN}^{-1}\{\hat{x}\}(r) = (C_{WN} f_{SF}^2)^{-1} \cdot \{\hat{x}\}(r).
\]

Hence, the inverse square root yields
\[
N_{WN}^{-1/2}(r, r') = \delta_D(r - r') C_{WN} f_{SF}^{-1/2} \langle\{\hat{x}\}(r)\rangle.
\]

Then we get (see fig. 2)
\[
R^{\prime} \hat{N}^{-1/2}_{WN} R\{\hat{x}\}(k) = \hat{f}_{SF} \circ \{f_B \circ \{\hat{N}^{-1}_{WN} \circ \{f_B \circ \{ \hat{f}_{SF} \circ \{\hat{x}\} \}\}\}\}(k),
\]
and consequently
\[
R^{\prime} \hat{N}^{-1}_{WN} \{\hat{x}\}(k) = \hat{f}_{SF} \circ \{f_B \circ \{\hat{N}^{-1}_{WN} \circ \{\hat{x}\} \}\}(k).
\]

To calculate \( R^{\prime} \hat{N}^{-1/2}_{WN} \{\hat{x}\} \) one has to do the following substitution \( \hat{N}^{-1}_{WN} \rightarrow \hat{\hat{N}}^{-1/2}_{WN} \) in eq. (149)
\[
R^{\prime} \hat{N}^{-1/2}_{WN} \{\hat{x}\}(k) = \hat{f}_{SF} \circ \{f_B \circ \{\hat{\hat{N}}^{-1/2}_{WN} \circ \{\hat{x}\} \}\}(k).
\]

In summary, we showed that the action of the different operators on a vector required for the different reconstruction estimators (see table 3) can be calculated in a straightforward way, as an ordered series of products and convolutions. Note that whenever we need to perform a convolution, we change to the counter space representation with FFTs and do multiplications there.

4 EFFICIENCY AND QUALITY VALIDATION OF THE INVERSE METHODS WITH THE WIENER-FILTER

In this section the Wiener-filter implemented in ARG0 is tested with the different linear inverse algorithms presented in the section of numerical methods (3) under several conditions determined by structured noise, blurring, selection function effects and windowing.

The inverse methods that we test here are the Jacobi (J), the Steepest Descent (SD), and several Krylov methods, like the Fletcher-Reeves (FR), the Polak-Ribiere (PR), and the EXP Conjugate Gradients method (see section 3.1.5 and appendix B3). This

\[ \text{In order to avoid aliasing effects one has to adequately perform zero-p} \]
scheme has not been previously discussed in the literature and turns out to be very efficient as will be discussed below. Many other Krylov methods (see table 2) can be built from simple equivalence relations, as we show in appendix B. However, only the methods mentioned above are taken into account here, as we consider them to be sufficiently representative. The extra-regularization we propose with these Krylov methods converts the Wiener-filtering in a hybrid Tikhonov-Krylov space regularization method. In addition, we also test the Wiener-filter that uses hermitian redundancy as derived in appendix B. We call the Wiener-filter defined by the mapping equation (B5) the conjugated Wiener-filter (CJ), whereas the Wiener-filter defined by eq. (B5) has no extra suffix.

With the aim of having full control over the synthetic data, we generate Gaussian random field with the Peacock & Dodds (1994) formula for the power spectrum. The resulting real density field is denoted by \( \delta_{\text{real}} \equiv \delta_\rho \), and the reconstruction by \( \delta_{\text{rec}} \equiv \psi \). The signals are discretized and arranged as vectors given by \([k + n_x \times (j + n_y \times i)]\), where \( i \in [0, n_x - 1], j \in [0, n_y - 1], \) and \( k \in [0, n_z - 1] \). The algorithmic part of the reconstruction methods shown in section 3 does not change with the dimensionality, but solely the length of the vectors given by \( n = n_x \times n_y \times n_z \) change and thus also the dimension of the involved matrices. The formulation of the matrices is explained in detail in section 3.3. The Fourier transforms must be accordingly called with the dimensions under consideration, which occurs in ARGO by switching between the different FFTs given by FFTW. In addition, the power spectrum that is used for the reconstruction has to be set up with the corresponding length and the data have to be correctly rearranged to their original dimensions \([i][j][k] \leftarrow [k + n_x \times (j + n_y \times i)]\) after their manipulation.

### 4.2 Multi-dimensional test cases

ARGO has been implemented such that the global dimension \( N_{\text{D}} \) (see section 3.3) and even the length in each dimension \((n_x, n_y, n_z)\), can be chosen arbitrarily. Our tests in one-, two- and three dimensions show that the results do not differ qualitatively. The convergence behavior changes with the length of the arrays \((n = n_x \times n_y \times n_z)\) as \( n \log_2 n \) fully determined by the FFTs, as we showed in section 3. For the demonstration cases in this paper, we have selected the two-dimensional tests with \( 128 \times 128 = 16384 \) pixels. However, three dimensional tests were also carried out leading to the same conclusions.

#### 4.2.1 Qualitative and quantitative measurement of the quality of the reconstruction

To give a quantitative measurement of the quality of the reconstructions, we define the correlation coefficient \( r \) between the reconstructed and the real density field by

\[
r \equiv \frac{\sum_i \delta_{\text{rec}} \psi_i}{\sqrt{\sum_i \delta_{\text{rec}}^2 \psi_i^2}}.
\]

This statistical quantity is not very sensitive to the overall distribution and yields good values (close to unity) in some cases even with poor reconstructions (see section 3.2.5). The pixel to pixel plot of the real density field against the reconstruction is highly informative because the scatter in the alignment of the pixels around the line of perfect correlation (45° slope) gives a qualitative goodness of the reconstruction. In general, the quality of the recovered density map is better represented by the Euclidean distance between the real and the reconstructed signals. The ensemble average of this quantity can also be regarded as an action or loss function that leads to the Wiener-filter through minimization (see appendix B). Here we introduce the volume-averaged squared Euclidean distance:

\[
D^2_{\text{Eucl}}(\psi, \delta_\rho) \equiv \frac{1}{V} \int d^N \Delta r \, \left( \psi(r) - \delta_\rho(r) \right)^2,
\]

with \( V = L_x \times L_y \times L_z \). We further normalize the Euclidean distance through the following definition

\[
D^2_{\text{Eucl}}(\psi, \delta_\rho) \equiv \frac{D^2_{\text{Eucl}}(\psi, \delta_\rho)}{D^2_{\text{Eucl}}(\psi_0, \delta_\rho)},
\]

where \( \psi_0 \) is the zero vector. We define the convergence tolerance criterion based on the squared Euclidean distance between subsequent reconstructions

\[
t_{\text{tol}}^{1+1} \equiv D^2_{\text{Eucl}}(\psi^{1+1}, \psi^1).
\]

We prefer this criterion with respect to the squared residuals \( ||\epsilon||^2 \) (see eq. 29) because all the tests show that no further statistical quality improvement in the reconstructions is reached after \( t_{\text{tol}}^{1+1} \), as can be inferred from the correlation coefficients \( r \) and the normalized squared Euclidean distances \( D^2_{\text{Eucl}}(\psi, \delta_\rho) \).

#### 4.2.2 Numerical performance with and without preconditioning

Here we analyze the convergence behavior of the different inverse schemes with and without preconditioning. We start by considering a Gaussian random field with some structured noise that increases.

---

20 We use GARFIELDS: G AUSSIAN Random FIELDS, a program we developed to generate Gaussian random fields from a given power spectrum. The method can be found in detail in Martel (2005).

21 FFTW is a C subroutine library for computing fast discrete Fourier transforms in one or more dimensions of arbitrary input size and of both real and complex data: http://www.fftw.org/

22 \( G(0, 1) \): zero mean and variance 1.
radially and is modulated by a random noise component. As a preconditioning expression, the diagonal part of the data covariance matrix is chosen, which is given by the sum of

\[
(RSFR)_{kk} = \frac{1}{f_B(k)} \int \frac{d^Nq}{(2\pi)^N} f_{SM}(k-q) P_S(q) f_{SM}(q-k) f_B(k) = P_B(k) \left( \int \frac{d^Nq}{(2\pi)^N} P_{SM}(k-q) P_S(q) \right) \quad (155)
\]

and

\[
\hat{N}(k) = \frac{1}{P_{SF} \circ P_N} \int \frac{d^Nq}{(2\pi)^N} f_{SM}(k-q) P_N(q) f_{SM}(q-k) \int \frac{d^Nq}{(2\pi)^N} P_{SM}(k-q) P_N(q) \quad (156)
\]

where we have used the following definitions: \(P_B \equiv ||f_B||^2\), \(P_{SM} \equiv ||f_{SM}||^2\) and \(P_{SF} \equiv ||f_{SF}||^2\). We can thus calculate the preconditioning matrix \(M\) required for the different schemes (section 3) by just inverting each diagonal component. The results summarized in figs. 4 and 5 show important differences between the reconstructions done with (on the left side of fig. 5) and without (on the right side of fig. 5) preconditioning. Some of the methods just speed up, like the various EXP methods or the SD scheme. Others, however, are stabilized and manage to converge to the solution only after preconditioning, like the J, the FR and the CPR methods.

Without preconditioning, the latter converges extremely quickly to a wrong solution. This is due to the fact that we did not impose the following stabilization: \(\beta_{PR} = \max(\beta_{PR}, 0)\) in this calculation (see Shewchuk 1994, for a discussion). However, our tests show that upon imposing this stabilization the PR-method becomes significantly slower than the rest. On the other hand, the EXP-Krylov methods behave most stably and converge very quickly. In the preconditioned case, we see that all methods converge to the same statistical result, as we can infer from the correlation coefficient \(r\) and \(D^2_{\text{rescl}}(\psi, \delta_p)\), except for the PR scheme that yields slightly less optimal results (see the green line in comparison to the rest in panel e). We have tested preconditioning in the rest of the examples and could confirm the results presented in this section. Preconditioning turns out to be necessary to achieve fast algorithms. In the next subsections we present results with a Poissonian distribution (fig. 6) and with blurring (fig. 7). Their corresponding numerical efficiency tests are shown in fig. (8). The same kind of studies are done with a simulated selection function (fig. 9) and with a mask (fig. 10). Their respective numerical behaviour can be seen in fig. (11).

4.2.3 Poissonian distribution

In this study case, we investigate the reconstruction of a Gaussian field based on a Poissonian distribution. This model is far from reality, where much more complex processes are known to occur (see discussion in section 4.1.1). However, we can model a non-Gaussian process in this way and test how good the Wiener-filter reconstruction works under such circumstances. Here the assumed data model does not coincide with the one that has generated the

\[
\theta = \frac{1}{\sqrt{2\pi}} \int \frac{d^Nq}{(2\pi)^N} f_B(k) P_S(q) f_B(k) \quad (157)
\]
Figure 4. Structured noise treatment: The upper left picture shows the real signal. The upper right picture is the input signal, where some random noise that increases radially was added. Note that the scale of the colourbar changes from a maximum overdensity of 20 to 70. The lower left picture shows the reconstruction. The reconstructions using different numerical methods implemented in ARGO are indistinguishable. In the lower right image, the real density field is plotted against the reconstructed density field pixel by pixel without any smoothing. The numerical performance of this reconstruction case is shown in the next figure.

data. However, the Poissonian noise can be modeled in the noise matrix of the Wiener-filtering through the structure function $f_S$.

The results presented in fig. (6) show very good agreement between the reconstruction and the real underlying density field (compare panels a and e). The convergence behaviour and statistical goodness is plotted in the left side of fig. (8), panels a, c and e. There we can see that the FR and PR methods do not converge rapidly (see yellow and green curves in panel a). On the contrary, the J, SD, and EXP schemes are very efficient (panel e) and lead to very similar results (panels c and e).

4.2.4 Blurring effects: deconvolution

In this numerical experiment we tested the blurring effects by convolving the density field with a Gaussian. The result is shown in fig. (7), panel b. We see how the small structures are smoothed out and only the larger ones prevail. Some noise with a structure function was added to the signal. However, the noise was kept low with the aim of investigating primarily the blurring effect. The results of the reconstruction that considers only the noise does not change much with respect to the input signal, as can be expected. However, the extra-regularized Wiener-filtering deblurs the image applying eqs. (130) and (131), and yields the figure shown in panel c. We see how much of the small scale structure is restored and the peaks become enhanced. The correlation between this reconstruction and the original signal (panel e) is significantly better than for the case where the blurring is ignored (panel f). We can see in fig. (8) that the deconvolution algorithm is very fast for all the methods except for the FR-scheme. The PR-method is the fastest, but it leads to slightly worse results (see the green curve in panels c and e). The EXP turns out to be more efficient than the J and SD methods in this case.

4.2.5 Selection function effects

For this case we use a modified data model in which the selection function also affects the noise

$$d = f_S \cdot (s + f_{SP} \cdot \epsilon_{WN}),$$

with $f_S \in [0, 1]$, simulating the fading strength of the signal with increasing distance. The results are plotted in fig. (9), where the structure of the signal can be seen to become indistinguishable in radial direction (see panel b). Taking only the noise into account leads to very poor reconstructions (see panel d). On the contrary,
Figure 5. Numerical performance with and without preconditioning: Here the convergence behaviour and the goodness of the reconstructions using different inversion algorithms can be seen. The pictures on the left show the methods using preconditioning, whereas the pictures on the right do not use preconditioning. The upper plots show the squared Euclidean distance between successive reconstructions. The plots in the middle show the normalized Euclidean distance between the different reconstructions and the true signal. The lower plots show the evolution of the statistical correlation coefficient between reconstruction and signal. We see from panel c and panel e that after less than 10 iterations the reconstructions do not significantly improve with most of the inversion algorithms. The different inversion algorithms used are: Jacobi (J), Steepest Descent (SD), Conjugate Gradients (CG), Fletcher Reeves (FR), and Polak Ribière (PR). We also tested a more expensive variant that uses one additional operation of the involved matrix (EXP) and one other variant (CJ), where a degree of freedom in the mapping equation for the Wiener-filter is used.
Figure 6. Poissonian noise: Here two stochastic processes are underlying the input signal. First the Gaussian random field that generates the signal in panel a, which is then Poisson sampled leading to the signal in panel b. The reconstruction in panel c is shown to be in good agreement with the underlying signal. The pixel values are correctly distributed as can be seen in panel d.

by also considering the selection function effects, the structures are resolved even at contours where only 10% of the signal plus noise is left (see panel e). As can be appreciated in panels e and f there is an improvement in the correlation between the real density field and the reconstructed signal. Panel e shows a higher correlation coefficient, but the quality enhancement of the reconstruction can be seen better in the distribution of the density values for each pixel. How the points are correctly spread along the diagonal line can be verified there. The longer Euclidean distance to the real density field shows the quantitative difference very clearly, by just comparing the pink curve with the rest (fig. 11 and panel c). It is worth mentioning that although the PR test seems to give a comparable result to the calculation that ignores the selection function. The final correlation coefficient in panel e shows that the reconstructions actually strongly differ and panel c shows that the quality of the recovered signal is notably better for the former experiment.

In addition, we tested the same selection function affecting only the underlying signal with a model given by

\[ d = f_S \cdot a + f_{SP} \cdot \epsilon_{WN}, \]  

and obtained the same qualitative results.

4.3 Windowing effects

In this section we investigate the mask effects that introduce coupling between different modes in Fourier-space so that the data covariance matrix is no longer diagonal. The input signal is given in panel b of fig. (10). The noisy signal from panel b in fig. (4) was cut in stripes to simulate observed regions. We compare two reconstructions here, the first one ignores windowing effects given in panel d and a second reconstruction employs the proper treatment of the boundary through \( f_M \) in the algorithm (see eqs. 130 and 131). The statistical correlation is given in panels e and f, respectively. Our experiments show better results not only for the latter reconstruction in the un-sampled region (Ω), represented by the red dots in panels e and f in fig. (10), but also in the sampled regions (Ω). The global correlation \( r \) is significantly improved. Whereas the distribution of the black dots, the values of the densities in the observed regions, does not apparently change, the distribution of the un-sampled red dots clearly does. These are distributed around the zero value for the case where windowing is ignored because a zero signal is assumed by \( \text{ARGO} \) in the \( \Omega \) region. In contrast we see that the red dots are distributed along the diagonal line when edge effects are considered. This is equivalent to a propagation of the information to the un-sampled regions or the appropriate interpolation and extrapolation of signals. Looking at the numerical
Figure 7. Blurring treatment: Here the signal (panel a) was convolved with a gaussian modeling blurring effects, as shown in panel b. Some low noise with a structure function was added. Panel c shows the deblurred result. Panel d takes only the noise into account. We see in panel f the correlation between the input signal and the true signal, because the noise is negligible. The correlation coefficient is thus very high, however, the alignment of the pixels in the plot is not correct. Overdensities and underdensities tend to be underestimated, which is consistent with the blurring effect. The reconstruction given in panel e corrects this effect and consequently a higher correlation coefficient is achieved.
Figure 8. Poissonian noise and numerical performance (panels a, c, e): Here the convergence behaviour and quality of the reconstruction is comparable for the J, SD, EXP methods. The FR and PR schemes do not present a fast convergence (panel a). Nevertheless, the FR scheme (yellow curve) seems to lead to the correct solution (panels c and e). The PR formula, on the contrary, stagnates at reconstructions that have much lower quality compared to the rest of the schemes. Blurring treatment and numerical performance (panels b, d, f): In this study case, the EXP algorithm seems to work better than the rest of the schemes. Although the PR formula converges very rapidly (green curve in panel b), it leads to a lower quality reconstruction (panels d and f). The FR scheme converges to the same solution as the J, SD, and EXP algorithms, however, with a slower convergence (yellow curve in panel b). The J and SD methods have an overall good behaviour in this case, but still converge significantly slower than the EXP scheme (their convergence is identical black and red curves are overplotted). The reconstruction considering just the noise is very poor, because the noise is negligible in this case (pink curves).
Figure 9. Selection function treatment: Here selection function effects were simulated with a function that takes values between zero and one, decreasing exponentially in radial direction. The contours show different values of this function. Panel a shows the real density field. Panel b shows the input data, where the true signal was multiplied in real space with the selection function and a radially increasing noise was added. The reconstruction and its correlation with the true signal are represented in panel c and e, respectively. The reconstruction ignoring selection effects by taking only the noise into account leads to panels d and f. The reconstruction given in panel d is very conservative and smooths the overdensities out due to noise suppression. This leads to a high correlation coefficient, though the individual pixels are clearly not correctly aligned (panel f). Panel c, on the contrary, shows more structures that are enhanced due to consideration of the selection function effects. This correctly distributes the pixels, as can be seen in panel e. The correlation coefficient seems to be significantly better than in panel f, however, a better measure of the overall quality of the reconstruction can be seen in next figure.
Figure 10. Windowing treatment: Here the edge effects are shown in two dimensions. The true signal was multiplied by a windowing function that is one in the observed region ($\Omega$) and zero in the unknown region ($\bar{\Omega}$). The sampled regions are given by the vertical stripes. In addition, a radially increasing noise was added (see panel b). Panel c shows the reconstruction handling the edge effects. Panel d represents the result taking only the noise into account. We see in panel e how the information is propagated into the unsampled regions leading to a closer resemblance of the real signal, whereas the noise is just suppressed in panel d. Panels e and f show the correlation coefficients for the whole reconstructed region, split into the sampled (black dots) and the unsampled regions (red dots). Note that the red dots are strongly aligned around the zero value in panel f, whereas they are correctly spread in panel e, statistically representing the information propagation process mentioned above.
Figure 11. Selection function treatment and numerical performance (panels a, c, e): The same color coding is used as in fig. (5) panel a, except for additional curve (represented in pink) that indicates the reconstruction in which the selection effects are ignored. Panel a shows the squared Euclidean distance between subsequent reconstructions. The squared Euclidean distance between the reconstruction and the true density field is plotted in panel c, showing a huge difference between the reconstruction which takes only the noise into account and ignores the selection function and the rest of the methods. Note that the statistical correlation $r$ is also much better for the case where the selection effects are properly treated (panel e). One concludes from the three plots, that the SD and EXP methods (red, blue and violet curves) clearly converge faster to a more or equally optimal solution in comparison with the rest of the methods. The J scheme shows a significantly slower convergence (black curve in panel a). The PR algorithm stagnates at poorer reconstructions as can be seen in panel e. Windowing treatment and numerical performance (panels b, d, f): In this case, the PR shows extremely good results: fast convergence (panel b) and a high correlation coefficient (panel d). However, the Euclidean distance is slightly bigger than for the rest of the methods, except for the pink curve (ignoring windowing effects). The FR method is disastrous in this study case and diverges from the solution as can be seen in panel f. The J, SD, and EXP methods show good and stable results. The J and SD algorithms give extremely similar results. Although their convergence behaviour is similar to the EXP schemes, the latter give slightly better results: smaller values for the Euclidean distance and higher values for the correlation coefficient (violet curves in panels d and f, respectively).
performance in fig. reveals that most of the methods behave very similarly, except for the PR and FR schemes that deviate from the rest. The former converges rapidly to a good solution that has a higher correlation (see green curve in panel f), but a slightly worse Euclidean distance to the true signal. The FR on the other hand converges extremely slowly. The correlation coefficient is at a stage where it becomes dramatically worse (see yellow curve in panel f). The smaller Euclidean distance is no measure for the quality in this case because these low values can be achieved when the reconstruction is very conservative (closer to zero) and has no structure. Notice how many schemes start with better values for that distance measure (see panel d). The EXP methods converge faster and the CJ version leads to even slightly better results (see violet curve in panels d and f).

It is also worth mentioning that the best reconstructions in terms of high correlation coefficients and low Euclidean distances to the underlying signal are achieved only after three iterations for the J, SD, and EXP methods, prior to numerical convergence. We furthermore tested ARG0 under extreme noise conditions in which the inversion diverges and produces density values that approach infinity. At early iterations, extremely good reconstructions were produced. These examples underline the regularization character of the inversion schemes under consideration in this paper. However, for the cases we are interested in, where the noise is mainly determined by the discrete sampling of galaxies, no additional stopping rules are required and the inversion algorithms can be run until full convergence.

5 SUMMARY AND CONCLUSIONS

The goal of this work is to exploit the Bayesian formalism to develop methods that reconstruct the underlying dark-matter distribution from the discrete sample of galaxies and their three-dimensional positions provided by galaxy redshift surveys. Such a general Bayesian analysis permits one to innovate methods and push this field forward to develop more accurate reconstruction algorithms.

We show how a series of uncertainties demand a statistical approach (see figure and section). Some of the uncertainties are intrinsic to the nature of the underlying signal (the dark matter) and have a stochastic character, the cosmic variance. Other uncertainties are intrinsic to the nature of the observable (the galaxies) and lead to a kind of shot noise, galaxy-bias and redshift-distortions. Additional uncertainties, such as windowing, selection function effects and blurring effects, arise due to the observation process. The degeneracies that are produced by such uncertainties require regularization techniques, which should converge to optimal solutions. We discuss the different Bayesian approaches specified through different options for the likelihood and the prior, and see how natural regularizations can be performed by the prior-choice (see section). Moreover, we see how the definition of particular likelihoods and priors define classes of algorithms, each specific to a different problem approach (see table).

We develop new algorithms in this Bayesian framework which account for the discrete nature of a galaxy distribution by taking a Poissonian likelihood. This is done for the case of a Gaussian prior leading to the GAPMAP estimator (see section and appendix) and for the case of an entropic prior (see section and appendix). The Maximum Entropy method is studied in detail as a non-informative prior, which does not assume a particular pattern for the underlying signal. This can be interesting when searching for intrinsic deviations from Gaussianity (see section and references therein).

We extend the Wiener-filter (see section and appendix) and propose novel algorithms to do a joint estimation of the density field, its power-spectrum, and the peculiar velocities of the galaxies (see section). We also address the possibility of extending such work to determine cosmological parameters and the bias between galaxies and dark matter.

Such an aim requires a large number of repeated reconstructions, which can be only achieved with highly efficient inverse algorithms. We develop here the necessary numerical schemes in a preconditioned way for linear and non-linear inverse problems (see section and appendix). Such iterative schemes acquire their real power only in an operator formalism, which we derive in detail for different Bayesian methods (see section). A novel Krylov formula (see section and appendix) turns out to be superior in terms of performance and fidelity, as we show in section.

The novel ARG0-software package is presented in this paper. Different inverse schemes are tested with the Wiener-filter implemented in ARG0 under several conditions determined by structured noise, blurring, selection function effects and windowing (see section).

We conclude that fast three-dimensional reconstructions of the large-scale structure scaling as with (with being the total number of grid cells) can be done with hybrid Wiener-Krylov iterative schemes under an operator formalism, which takes advantage of the speed of FFTs. This opens new horizons of possibilities, such as joint parameter and signal estimation, in the field of large-scale structure reconstruction.

It is our goal to apply such techniques to reconstruct the underlying density field, the power-spectrum and the peculiar velocities from galaxy surveys. Still, different problems, such as galaxy-bias studies, have to be further analysed. However, we are confident that such issues can be tackled from an information-theory approach.

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APPENDIX A: THE WIENER-FILTER AS A BAYESIAN ESTIMATOR

Let us recall eq. (21) which comes from Bayes theorem assuming a Gaussian prior and a Gaussian likelihood

\[ P(s | d, p) \propto \exp \left( -\frac{1}{2} \left[ s^T S^{-1} s + (d - Rs)^T N^{-1} (d - Rs) \right] \right). \]  

(A1)

If we just look at the log-posterior distribution we have

\[ \log P(s | d, p) \propto s^T S^{-1} s + (d - Rs)^T N^{-1} (d - Rs) \]

(A2)

We can combine the first two terms to one term: \( s^T (\sigma_{WF}^2)^{-1} s \), with \( (\sigma_{WF}^2)^{-1} \equiv (S^{-1} + R^T N^{-1} R) \). Since we want to obtain a log-posterior of the form

\[ \log P(s | d, p) \propto (s - \langle s \rangle_{WF})^T (\sigma_{WF}^2)^{-1} (s - \langle s \rangle_{WF}) \]

(A3)

with \( \langle s \rangle_{WF} = F_{WF} d \), we can identify the third and the fourth term of eq. (A3) with the corresponding terms in eq. (A3)

\[ -s^T R^T N^{-1} d = -s^T (\sigma_{WF}^{-1}) F_{WF} d, \]  

(A4)

and

\[ -d^T N^{-1} R s = -d^T F_{WF}^T (\sigma_{WF}^2)^{-1} s, \]  

(A5)

respectively. The remaining term depends only on the data and is thus factorized in the posterior distribution function as part of the evidence. From both eq. (A3) and eq. (A5) we conclude that the Wiener-filter has the form

\[ F_{WF} = \sigma_{WF}^{-1} R^T N^{-1} = (S^{-1} + R^T N^{-1} R)^{-1} R^T N^{-1}. \]  

(A6)

This is the natural Bayesian representation in contrast to expression (26), which is the outcome of a generalized LSQ approach (see appendix B and discussion in section 2.5.3). It can be shown that both expressions for the Wiener-filter are mathematically equivalent (see appendix C).

\[ \text{APPENDIX B: THE MAPPING EQUATION FOR THE WIENER-FILTER IN K-SPACE} \]

Following the concept of minimum variance (e.g. Rybicki & Press 1992; Zaroubi et al. 1995), we define an action given by the normalized volume integral of the square of the difference between the reconstruction (\( \psi \)) and the ensemble of different possible realizations of the density field (\( s = \delta_s \))

\[ A = \langle \frac{1}{V} \int d^3 r \left[ \psi(r) - s(r) \right]^2 \rangle_{(s,e,p)}. \]  

(B1)

From the statistical point of view, the action \( A \) is the loss function that has to be minimized. Note that this action can be expressed as the ensemble average of the squared Euclidean distance between the real density field \( s \) and the reconstruction \( \psi \)

\[ A = \frac{1}{V} \langle D_{\text{Eul}}(\psi, s) \rangle_{(s,e,p)}. \]  

(B2)

Transferring expression (B1) into Fourier space yields

\[ A = \frac{1}{V} \int \frac{d^3 k}{(2\pi)^3} \left[ \langle \hat{\psi}(k)\hat{\psi}(k) \rangle_{(s,e,p)} + \langle \hat{s}(k)\hat{s}(k) \rangle_{(s,e,p)} \right. \]

\[ - \langle \hat{\psi}(k)\hat{s}(k) \rangle_{(s,e,p)} - \langle \hat{s}(k)\hat{\psi}(k) \rangle_{(s,e,p)} \right]. \]  

(B3)

Assuming a linear relation between the reconstruction \( \psi \) and the data \( d \)

\[ \hat{\psi}(k) = \int \frac{d^3 k'}{(2\pi)^3} \hat{F}(k, k') \hat{d}(k'), \]  

(B4)

and statistical homogeneity \( \langle \hat{s}(k)\hat{s}(k') \rangle_{(s,e,p)} = (2\pi)^3 \delta_D (k - k') P_s(k') \), yields

\[ A = \frac{1}{V} \int \frac{d^3 k}{(2\pi)^3} \left[ \hat{F}(k, k') \int \frac{d^3 q}{(2\pi)^3} \hat{F}(q, k') \hat{d}(q) \hat{d}(q) \right. \]

\[ + (2\pi)^3 \delta_D (k - k') \langle \hat{s}(k')\hat{s}(k') \rangle_{(s,e,p)} \]

\[ - \hat{F}(k, k') \langle \hat{d}(k')\hat{s}(k') \rangle_{(s,e,p)} \]

\[ - \hat{F}(k, k') \langle \hat{s}(k')\hat{d}(k') \rangle_{(s,e,p)} \]. \]  

(B5)

Now the action is minimized with respect to the linear operator,

\[ \frac{\partial A}{\partial \hat{F}} = 0, \]

to obtain the following mapping equation

\[ \int \frac{d^3 q}{(2\pi)^3} \hat{F}(k, q) \hat{d}(q) \hat{d}(q) \rangle_{(s,e,p)} = \langle \hat{s}(k) \hat{d}(k') \rangle_{(s,e,p)}. \]  

(B6)

The desired filter can be thus expressed as the correlation matrix between the signal and the data multiplied by the inverse of the autocorrelation matrix of the data (see Zaroubi et al. 1995).

\[ F = \langle sd^T \rangle \langle dd^T \rangle^{-1}. \]  

(B7)

This filter is the LSQ estimator (see eq. 23). It is identical to the Wiener-filter in case the noise term has no signal-dependent structure function or after applying an ensemble average over all possible signals on the noise covariance matrix. Note, that eq. (B6) allows us to substitute \( k' \) by \(-k'\), which is equivalent to the conjugation of \( \hat{d}(k') \) due to the hermitian redundancy of real numbers

\[ \int \frac{d^3 q}{(2\pi)^3} \hat{F}(k, q) \hat{d}(q) \hat{d}(q) \rangle_{(s,e,p)} = \langle \hat{s}(k) \hat{d}(k') \rangle_{(s,e,p)}. \]  

(B8)

The linear operator one obtains in this way is different, but fulfills the same requirements. We compare both cases in section 4. Let us see how one would apply such a filter. The covariance matrix of the data is given by

\[ \langle \hat{d}(k)\hat{d}(k') \rangle_{(s,e,p)} = \langle \hat{s}(k)\hat{d}(k') \rangle_{(s,e,p)} + \langle \hat{d}(k)\hat{d}(k') \rangle_{(s,e,p)}, \]  

(B9)

and its action on some vector by

\[ \int \frac{d^3 k'}{(2\pi)^3} \langle \hat{d}(k)\hat{d}(k') \rangle_{(s,e,p)} \hat{\tilde{e}}(k') \rangle_{(s,e,p)} = \hat{f}_B \circ \left[ \hat{f}_{\text{SM}} \circ \left[ P_s \circ \left[ \hat{f}_{\text{SM}} \circ \left[ \hat{f}_B \circ \{ \hat{e} \} \right] \right] \right] \right](k), \]  

(B10)

\[ \int \frac{d^3 k'}{(2\pi)^3} \langle \hat{s}(k)\hat{d}(k') \rangle_{(s,e,p)} \hat{\tilde{e}}(k') \rangle_{(s,e,p)} = \hat{f}_{\text{SP}} \circ \left[ P_N \circ \left[ \hat{f}_{\text{SP}} \circ \{ \hat{e} \} \right] \right](k). \]  

(B11)

The correlation matrix between the data and the signal applied to that vector yields

\[ \int \frac{d^3 k'}{(2\pi)^3} \langle \hat{s}(k)\hat{d}(k') \rangle_{(s,e,p)} \hat{\tilde{e}}(k') \rangle_{(s,e,p)} = P_s \circ \left[ \hat{f}_{\text{SM}} \circ \left[ \hat{f}_B \circ \{ \hat{e} \} \right] \right](k). \]  

(B12)

We see that the difference with respect to the operations derived in section 2.3 resides in the conjugation of certain functions.
APPENDIX C: DATA-SPACE AND SIGNAL-SPACE REPRESENTATIONS FOR THE WIENER-FILTER

Here we show the equivalence between the data-space and the signal-space representations for the Wiener-filter (see section 2.5.3). In a first approach, we start assuming that the inverse of the response operator exists \((R^{-1})\). Then after some operations the equivalence can be shown for both the Wiener-filter

\[
F_{WF} = (S^{-1} + R'N^{-1}R)^{-1}R'N^{-1},
\]

\[
= (S^{-1}(R'R^{-1}N + R^{-1}N)^{-1},
\]

\[
= \sigma^2_{WF}(R'R^{-1}N + N)^{-1}, \tag{C1}
\]

and the covariance

\[
\sigma^2_{WF} = (S^{-1} + R'N^{-1}R)^{-1},
\]

\[
= \sigma^2_{WF}(R + RSR^{-1}N^{-1}R)^{-1},
\]

\[
= \sigma^2_{WF}(R + RSR^{-1}N^{-1}R)^{-1}. \tag{C2}
\]

Note that the covariance given by eq. (C2) has limited practical use, since it requires the inverse of the response operator \(R\), which is in general a singular matrix. To find a data-space representation for the covariance one has to introduce the concept of constrained realizations (see section 2.6.2 and appendix D). In order to find a general proof for the equivalence between the data-space and the signal-space representation of the Wiener-filter, we have to look at the residuals

\[
\sigma^2_{WF} = (r'r') = \langle(s - F_{WF}d)(s - F_{WF}d)\rangle \tag{C3}
\]

\[
= S - \sigma^2_{WF}F_{WF}^{-1} - F_{WF}RS + F_{WF}(RSR^{-1} + N)F_{WF}^{-1},
\]

where we have done the substitution: \(d = Rs + \epsilon\) and \(\langle s\epsilon \rangle = 0\). The first two terms lead to the Wiener covariance, as we show here

\[
S - \sigma^2_{WF}F_{WF}^{-1} = (S\sigma^2_{WF}^{-1} - \sigma^2_{WF}F_{WF}^{-1}\sigma^2_{WF}^{-1})\sigma^2_{WF}
\]

\[
= (S(S^{-1} + R'N^{-1}R) - S\sigma^2_{WF}^{-1}R)\sigma^2_{WF}
\]

\[
= \sigma^2_{WF}, \tag{C4}
\]

where we have used the signal-space relation obtained in section A. \(F_{WF} = \sigma^2_{WF}R'N^{-1}\). Consequently, the last two terms of eq. (C4) have to cancel out

\[
0 = -F_{WF}RS + F_{WF}(RSR^{-1} + N)F_{WF}^{-1}
\]

\[
0 = F_{WF}(-RS + (RSR^{-1} + N)F_{WF}^{-1}). \tag{C5}
\]

Now we take the transpose and conjugate of the last equation and factorize the data correlation matrix out (which is always invertible, since the noise covariance matrix is invertible)

\[
0 = (F_{WF} - \sigma^2_{WF}(RSR^{-1} + N)^{-1})(RSR^{-1} + N)F_{WF}^{-1}. \tag{C6}
\]

The last equation motivates the data-space representation of the Wiener-filter without performing squares, i.e. without demanding the Filter to be optimal \((\partial\sigma^2_{WF}/\partial F_{WF} = 0)\), which is already imposing some regularity condition on \(F_{WF}\). Note that we also obtain the trivial zero solution \((F_{WF} = 0)\), which is equivalent to \(R = 0\) or \(N = \infty\) with covariance \(\sigma^2 = S\). Since the data-space and the signal-space representation have the same null-spaces eq. (C6) already proves the equivalence between the data-space and the signal-space representations for the Wiener-filter. Nevertheless, let us directly test this equivalence

\[
SR^1(RSR^2 + N)^{-1} \equiv \sigma^2_{WF}R'N^{-1}
\]

\[
SR^1 \equiv \sigma^2_{WF}R'N^{-1}(RSR^2 + N)
\]

\[
RS \equiv (RSR^2 + N)N^{-1}R\sigma^2_{WF}
\]

\[
RS \equiv RSR^2N^{-1}R + R
\]

\[
RS(RSR^2 + N)^{-1} \equiv RSR^2N^{-1}R + R
\]

\[
R + RSR^2N^{-1}R \equiv RSR^2N^{-1}R + R. \tag{C7}
\]

Since the left-hand-side is equal to the right-hand-side both representations are equivalent. Note that we did not assume the response operator to be invertible. We solely demanded that the inverse of the signal and of the noise covariance matrices can be built (\(\exists S^{-1}\) and \(\exists N^{-1}\)). This implies that the covariance matrix and the inverse of the data autocorrelation matrix exist (\(\exists(S^{-1} + R'N^{-1}R)^{-1}\) and \(\exists(RSR^2 + N)^{-1}\)), as we required in our proof.

APPENDIX D: COVARIANCE OF A CONSTRAINED REALIZATION

Following [Hoffman & Ribak (1991); Ganon & Hoffman (1993); Bistolas & Hoffman (1998)] we can generate a synthetic realization with

\[
y = \tilde{s} - F_{WF}d, \tag{D1}
\]

If the following relations hold \(\langle \tilde{s}\tilde{s} \rangle = S\), \(\langle \tilde{\epsilon}\tilde{\epsilon} \rangle = N\) and \(\langle \tilde{\epsilon}\tilde{\epsilon} \rangle = 0\) then we obtain

\[
\langle yy \rangle = \langle (s - F_{WF}d)(s - F_{WF}d) \rangle \tag{D2}
\]

\[
= S - \sigma^2_{WF}F_{WF}^{-1} - F_{WF}RS + F_{WF}(RSR^{-1} + N)F_{WF}^{-1}
\]

We can identify these terms with eq. (C4). Thus, following relation is fulfilled

\[
\langle y'y' \rangle = \langle rr' \rangle = \sigma^2_{WF}. \tag{D3}
\]

APPENDIX E: GAPMAP: MAP WITH A GAUSSIAN PRIOR AND A POISSONSSIAN LIKELIHOOD

Remember \(P(s \mid d, p) \propto \mathcal{L}(d \mid s, p)P(s \mid p)\) to be extremized. First we write the log-likelihood taking the logarithm of eq. (12)

\[
\log \mathcal{L}(s \mid d, p) = \sum_i \left[ -\langle Rs' \rangle_i - c_i + d'_i \log \left( \langle Rs' \rangle_i + c_i \right) - \log (d'_i) \right]. \tag{E1}
\]

Then we differentiate with respect to the signal to yield

\[
\frac{\partial \log \mathcal{L}(s \mid d, p)}{\partial s_k} = \sum_i \left[ R_{ik}b_{mp} \left( -1 + \sum_j (R_{ij}s_j + c_j)^{-1}d'_j \right) \right].
\]

The same exercise for the Gaussian prior leads to

\[
\frac{\partial \log P(s \mid p)}{\partial s_k} = - \sum_j s_{kj}^{-1} s_j. \tag{E2}
\]

\[\text{Note that the realization does not need to be Gaussian distributed, but just fulfill these requirements.}\]
Now we demand \(0 = \partial \log P(s \mid d, p) / \partial s_k\) to get an equation for the MAP estimator. After applying \(S\) to the equation we obtain
\[
s_k^j = - \sum_i \sum_j \left[ S_k R_{ik} b \tau_{R} \left( -1 + \left( \sum_m R_{im} \tau_{R} (1 + b s_m^i) + c_i \right)^{-1} d_i^j \right) \right].
\]  
(E3)

Adding the index \(j\) and \(j\) to \(s\) on lhs and rhs respectively, an iteration scheme is formed
\[
s_k^{j+1} = - \sum_i \sum_j \left[ S_k R_{ik} b \tau_{R} \left( -1 + \left( \sum_m R_{im} \tau_{R} (1 + b s_m^i) + c_i \right)^{-1} d_i^j \right) \right].
\]  
(E4)

Let us simplify this algorithm for positive signals \(s^i\) in matrix notation
\[
s'^{j+1} = \tau^2 \sigma^2 \tau^{-1} \bar{\sigma}^2 \tau^{-1} \left[ -1 + \text{diag}(R \sigma^2 + c)^{-1} d' \right] + \tau^2 ,
\]  
(E5)

where we made the following substitutions \(b \rightarrow 1\) and \(\tau_{R}\) → \(\bar{\tau}\), with \(\bar{\tau}\) being the average of the positive signal.

### APPENDIX F: POISSON MAXIMUM LIKELIHOOD

The context in which the Richardson-Lucy algorithm is applied has positive intensity signals and the kernel \(R\) in eq. [1] is understood as a blurring function that can be expressed mathematically as a convolution with the true signal \(s\). We will further assume no background (\(c = 0\)) so that the log-likelihood of eq. (12) can be written as
\[
\log \mathcal{L}(s' \mid d', p) = \sum_i \left[ - (R s')_i + d'_i \log((R s')_i) - \log(d'_i) \right],
\]  
(F1)

differentiating with respect to the signal yields
\[
0 = \frac{\partial \log \mathcal{L}(s' \mid d', p)}{\partial s_k} = \sum_i \left[ R_{ik} \left( -1 + (R s')_i \right)^{-1} d'_i \right].
\]  
(F2)

We can multiply this equation with the signal \(s'\) and make an iterative method which coincides with Richardson-Lucy algorithm
\[
s'^{j+1} = \text{diag}(R \text{diag}(R s')^{-1} d') s',
\]  
(F3)

with \(R \bar{1} = \bar{1}\) due to the convolution operation.

### APPENDIX G: COBE-FILTER

We briefly show here that the COBE-filter is an unbiased estimator only and only if the response matrix is invertible.

\[
\langle \langle s \rangle \rangle_{\text{COBE}} \langle d(s, p) \rangle = \langle (R \bar{1} \bar{1} R^{-1}) (R \bar{1} \bar{1} R^{-1}) (R \bar{1} \bar{1} R^{-1}) \rangle_{(d(s, p))},
\]  
\[
= (R \bar{1} \bar{1} R^{-1}) (R \bar{1} \bar{1} R^{-1}) (R \bar{1} \bar{1} R^{-1}) \langle \delta(s + \epsilon) (d(s, p)) \rangle,
\]  
\[
= (R \bar{1} \bar{1} R^{-1}) (R \bar{1} \bar{1} R^{-1}) \langle \delta(s + \epsilon) \rangle,
\]  
\[
= s, \text{ if } R \text{ is invertible.}
\]  
(G1)

### APPENDIX H: LINEAR FILTERS NEED TO BE INVERTIBLE TO CONSERVE INFORMATION

The Fisher information matrix \(J\) for a Gaussian distribution\(^{25}\) with zero mean and covariance matrix \(C\) calculated by Vogeley & Szalay (1996) has the form
\[
J_{ij} = \frac{1}{2} \text{tr} \left( G_i G_j \right),
\]  
(H1)

with
\[
G_i = C^{-1} C_i,
\]  
(H2)

where the comma notation \(C_i\) stands for the derivative with respect to the parameter \(\theta_i\). Following Tegmark (1997), we calculate the Fisher information matrix \(J\) for the filtered and unfiltered signal. Let us assume a linear filter \(L\), which provides us with an estimator of the signal
\[
\langle \langle s \rangle \rangle_L \equiv LD.
\]  
(H3)

The correlation matrix of the estimator yields
\[
C^{\text{est}} = \langle (\langle s \rangle_L, \langle s \rangle_L) \rangle_{(s, \epsilon | p)} = L L^\dagger \left( \left( R S R^\dagger + N \right) \right) L.
\]  
(H4)

We get then
\[
C^{L} = \left( R S R^\dagger + N \right) L^\dagger \left( R S R^\dagger + N \right)^{-1} L L^\dagger \left( R S R^\dagger + N \right),
\]  
(H5)
\[
C^{\text{data}} = \left( R S R^\dagger + N \right) L^\dagger \left( R S R^\dagger + N \right)^{-1} L (R S R^\dagger + N),
\]  
(H6)

If we now insert expression \((H6)\) in the Fisher matrix \((H1)\), we get
\[
J^{\text{est}}_{ij} = \frac{1}{2} \text{tr} \left( G_{ij}^{\text{est}} \right),
\]  
(H7)
\[
= \frac{1}{2} \text{tr} \left( L C^{\text{data}} L^\dagger \left( R S R^\dagger + N \right) L C^{\text{data}} \right).
\]  
(H8)

In general, this will differ from the Fisher matrix of the data. If we assume, however, that the linear operator is invertible \((R L^{-1})\), then eq. \((H11)\) reduces to
\[
J^{\text{est}}_{ij} = \frac{1}{2} \text{tr} \left( L^{-1} G_{ij}^{\text{data}} G_{ij}^{\text{data}} L \right).
\]  
(H9)

Invoking that the trace of a product of matrices is invariant under cyclic permutations, we see that
\[
J^{\text{est}}_{ij} = \frac{1}{2} \text{tr} \left( G_{ij}^{\text{data}} G_{ij}^{\text{data}} \right) = J^{\text{data}}_{ij}.
\]  
(H10)

This shows the result that any linear invertible filter conserves information, regardless of the parameters that one wants to estimate. However, one should be careful with this statement because linear filters are, in general, not invertible unless the data and signal space have the same dimension, the noise is non-zero for any frequency, and the \(R\)- and \(S\)-matrices are invertible. Usually the data and signal space will differ and the \(R\)-matrix will not be exactly invertible.

---

\(^{25}\) Here a Gaussian likelihood is assumed, but the result does not rely on the Gaussianity of the data (see e.g. Schmal 1998).
APPENDIX I: JEFFREY’S PRIOR FOR THE 3-DIMENSIONAL POWER SPECTRUM

Let us start by assuming a Gaussian likelihood:

\[ P(s \mid P_3(k)) \propto \prod_k \frac{1}{\sqrt{2\pi P_3(k)}} \exp\left(-\frac{|s(k)|^2}{2P_3(k)}\right). \]  

The log-likelihood is then given by

\[ \log \left( P(s \mid P_3(k)) \right) \propto \sum_k \left[ \log \left( P_3(k) \right) + |s(k)|^2 / P_3(k) \right]. \]  

We now need the second derivatives of the log-likelihood with respect to the parameter \( P_3(k) \)

\[ \frac{\partial^2}{\partial P_3(k)^2} \log \left( P(s \mid P_3(k)) \right) \propto \left[ -\frac{1}{P_3^2(k)} + \frac{2|s(k)|^2}{P_3^2(k)} \right]. \]

The next step consists of calculating the Fisher information by performing the integral

\[ J(P_3(k)) = \left( \frac{\partial^2}{\partial P_3(k)^2} \log \left( P(s \mid P_3(k)) \right) \right)_{(s \mid p)} \propto \frac{1}{P_3(k)}, \]

where we have taken into account that \( P_3(k) = \langle |s(k)|^2 \rangle_{(s \mid p)} \). Finally the square-root of the Fisher information leads to Jeffrey’s prior

\[ P(P_3(k)) = \sqrt{J(P_3(k))} \propto P_3(k)^{-1}. \]

Following Wandelt et al. (2004) we can argue in a more intuitive way that \( P(P_3(k)) \propto P_3(k)^{-1} \) is a solution to a measure invariant under scale transformations of the form

\[ P(P_3(k)) \propto P(\alpha P_3(k)) \alpha P_3(k) \]

(here we have generalized this result to the 3-dimensional power spectrum).

APPENDIX J: MEM WITH GAUSSIAN AND POISSONIAN LIKELIHOODS

The quantity to maximize is given by

\[ Q^E(s \mid p) = \alpha \mathcal{S}^E(s \mid p) + \log \mathcal{L}(s \mid d, p). \]  

After some calculations we see that the gradient of the entropy for PADs is

\[ \nabla S^E_\pm(s' \mid p)_i = -\log \left( \frac{s'_j}{m_i} \right), \]

and for positive and negative distributions

\[ \nabla S^E_\pm(s \mid p)_i = -\log \left( \frac{w_i + s_i}{m_i} \right). \]

We took into account that \( \partial w_i / \partial s_j = s_i / w_i \delta_{ij} \). It is then more straightforward to calculate the \( S^E \) curvature for PADs

\[ \nabla \nabla S^E_\pm(s' \mid p) = -\text{diag}(s')^{-1}, \]

and for positive and negative distributions,

\[ \nabla \nabla S^E_\pm(s \mid p) = -\text{diag}(w)^{-1}. \]

Analogously, we calculate the gradient of the log \( \mathcal{L}(s \mid d) \) for the Gaussian case valid for positive \( (s') \) and positive and negative signals \( (s_\pm) \)

\[ \nabla \log \mathcal{L}_C(s \mid d, p)_i = -\frac{1}{2} \nabla \nabla \mathcal{X}'(s)_i = -\left( \mathbf{R} \mathbf{N}^{-1} (\mathbf{R} s - d) \right)_i, \]

and the corresponding curvature

\[ \nabla \nabla \log \mathcal{L}_C(s \mid d, p) = -\frac{1}{2} \nabla \nabla \mathcal{X}'(s) = -\mathbf{R} \mathbf{N}^{-1} \mathbf{R}. \]

The Poissonian case leads to

\[ \nabla \log \mathcal{L}_P(s \mid d, p)_i = b_w \sum_k \left[ R_{kl} \left( -1 + \langle \sum_j R_{kj} s'_j + c_k \rangle^{-1} d_k \right) \right] \]

\[ = b_w \left[ \mathbf{R} \left( \mathbf{I} + \text{diag}((\mathbf{R} s') + c)^{-1} \mathbf{d} \right) \right]_i, \]

and

\[ \nabla \nabla \log \mathcal{L}_P(s \mid d, p)_{ij} = -b_w \sum_k \left[ R_{kl} \left( \sum_i R_{ki} s'_i + c_k \right)^{-2} R_{kj} d'_k \right] \]

\[ = -b_w \left[ \mathbf{R} \left( \text{diag}((\mathbf{R} s') + c)^{-2} \mathbf{R} \mathbf{d} \right) \right]_{ij}. \]

Note that when dealing with over-density fields one should do the following substitution: \( s'_i = \tau_{ij} (1 + b s_i) \) in the last two expressions.

Summing up, we have the following gradient of \( Q^E \) for PADs

\[ \nabla Q^E_{\pm}(s' \mid p)_i = -\alpha \log \left( \frac{s'_i}{m_i} \right) + \nabla \log \mathcal{L}(s' \mid d, p)_i, \]

and for positive and negative distributions

\[ \nabla Q^E_{\pm}(s \mid p)_i = -\alpha \log \left( \frac{w_i + s_i}{m_i} \right) + \nabla \log \mathcal{L}(s \mid d, p)_i, \]

and the corresponding curvatures

\[ \nabla \nabla Q^E_{\pm}(s' \mid d, p) = -\alpha \text{diag}(s')^{-1} + \nabla \nabla \log \mathcal{L}(s' \mid d, p), \]

\[ \nabla \nabla Q^E_{\pm}(s \mid d, p) = -\alpha \text{diag}(w)^{-1} + \nabla \nabla \log \mathcal{L}(s \mid d, p). \]

The corresponding likelihood (Gaussian or Poissonian) has to be inserted in each of the expressions for the gradient or curvature of \( Q^E \). For the choice of an optimal regularization constant \( \alpha \) see e.g. Maisinger et al. (1997) and Hobson et al. (1998).

APPENDIX K: KRYLOV METHODS: CONJUGATE GRADIENTS

K1 Orthogonality between the residuals and the searching vectors

Eq. (23) tells us that each error vector \( \eta^{j+1} \) is \( A \)-orthogonal to the previous searching vector \( \mathbf{M} \mu^j \). Since all different searching vectors \( \mathbf{M} \mu^j \) are \( A \)-orthogonal to each other by construction, and the error vectors are given by the linear combination of the previous error vector and the previous searching vector (eq. (20)), it follows that each error vector \( \eta^{j+1} \) is \( A \)-orthogonal to all previous searching vectors \( \mu^i \), i.e. for \( i \leq j \),

\[ \langle \eta^{j+1} | \mu^i \rangle_A = 0. \]  

(K1)

Using eq. (21) we can write eq. (K1) as

\[ \langle \xi^{j+1} | \mu^i \rangle = 0, \]  

(K2)

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being \( i \leq j \).

Applying the inner product between the searching vectors \( \mathbf{M} \mu^i \) and the recurrent formula for the residuals (eq. 92), we get
\[
\langle \xi^{j+1} | \mathbf{M} \mu^i \rangle = \langle \xi^j | \mathbf{M} \mu^i \rangle - \tau^j \langle \mathbf{M} \mu^i | \mathbf{M} \mu^i \rangle_A.
\] (K3)

For \( i \neq j \) this equation reduces to
\[
\langle \xi^{j+1} | \mathbf{M} \mu^i \rangle = \langle \xi^j | \mathbf{M} \mu^i \rangle.
\] (K4)

From eq. (K2) and eq. (K4) we conclude that for \( i < j \),
\[
\langle \xi^j | \mathbf{M} \mu^i \rangle = 0.
\] (K5)

**K2** The set of residuals as a basis of linearly independent vectors

Taking the Gram-Schmidt orthogonalization scheme (eq. 50) and multiplying it with the residuals, we obtain
\[
\langle \xi^i | \mathbf{M} \xi^j \rangle = \langle \xi^i | \mathbf{M} \xi^j \rangle + \sum_{k=0}^{j-1} \beta^{ij} \langle \xi^i | \mathbf{M} \xi^k \rangle.
\] (K6)

Using the result obtained in the appendix [K1] (eq. 55), one shows the orthogonality (strictly orthogonal, if \( \mathbf{M} = \mathbf{I} \)) between any different residuals (for \( i \neq j \))
\[
\langle \xi^i | \mathbf{M} \xi^j \rangle = 0.
\] (K7)

For \( i = j \) by combining (K3) and (K5) we get the relation we used in equation 95
\[
\langle \xi^i | \mathbf{M} \mu^i \rangle = \langle \xi^i | \mathbf{M} \xi^i \rangle.
\] (K8)

**K3** Formulae for the \( \beta \)-factor

From the scalar product between eq. 92 and the residual \( \xi^i \)
\[
\langle \xi^{j+1} | \mathbf{M} \xi^i \rangle = \langle \xi^j | \mathbf{M} \xi^i \rangle - \tau^j \langle \mathbf{M} \mu^i | \mathbf{M} \xi^i \rangle_A,
\] (K9)

it is clear that the \( \beta \)-factors are all zero except for one. Notice that the denominator in \( \beta \), given by \( \langle \mathbf{M} \mu^i | \mathbf{M} \xi^i \rangle_A \) cancels out if neither \( i = j + 1 \) nor \( i = j \). The latter is excluded according to the definition of \( \beta \) (see eqs. 96 and 98). Gram-Schmidt orthogonalization thus simplifies to eq. 99, with
\[
\beta_{\text{EXP}}^{j+1} = \frac{\langle \mathbf{M} \xi^{j+1} | \mathbf{M} \mu^i \rangle_A}{\langle \mathbf{M} \mu^i | \mathbf{M} \mu^i \rangle_A}.
\] (K10)

Other expressions for this factor can be derived by replacing \( i = j + 1 \) in eq. (K9)
\[
\langle \mathbf{M} \mu^i | \mathbf{M} \xi^{j+1} \rangle_A = -\frac{1}{\tau^j} \langle \xi^{j+1} | \mathbf{M} \xi^i \rangle_A.
\] (K11)

Substituting this expression in eq. 98 and using the formula for \( \tau^j \) (eq. 95) one obtains the Fletcher-Reeves equation
\[
\beta_{\text{PR}}^{j+1} = \frac{\langle \xi^{j+1} | \mathbf{M} \xi^{j+1} \rangle}{\langle \xi^j | \mathbf{M} \xi^j \rangle}.
\] (K12)

Polak-Ribière formula can now be obtained trivially by taking expression (K2) into account. Let us do an invariant operation by adding \( -\langle \xi^i | \mathbf{M} \xi^i \rangle \) to the nominator in Fletcher-Reeves formula
\[
\langle \xi^{j+1} | \mathbf{M} \xi^{j+1} \rangle - \langle \xi^i | \mathbf{M} \xi^j \rangle = (\langle \xi^{j+1} | \mathbf{M} \xi^{j+1} \rangle - \langle \xi^i | \mathbf{M} \xi^i \rangle),
\] (K13)

which immediately leads to Polak-Ribière expression
\[
\beta_{\text{PR}}^{j+1} = \frac{\langle \xi^{j+1} | \mathbf{M} (\xi^{j+1} - \xi^j) \rangle}{\langle \xi^j | \mathbf{M} \xi^j \rangle}.
\] (K14)

In order to get Hestenes-Stiefels formula one has to consider eqs. 58 and 55 in the denominator of \( \beta_{\text{PR}} \)
\[
\langle \xi^j | \mathbf{M} \xi^i \rangle = \langle \mu^i | \mathbf{M} \xi^j \rangle = \langle \mu^i | \mathbf{M} \xi^i \rangle,
\] (K15)

resulting in the following expression
\[
\beta_{\text{HS}}^{j+1} = -\frac{\langle \xi^{j+1} | \mathbf{M} (\xi^{j+1} - \xi^j) \rangle}{\langle \mu^i | \mathbf{M} (\xi^{j+1} - \xi^j) \rangle}.
\] (K16)

Due to the relations derived in this appendix other equivalent formulæ for \( \beta \) (summarized in table 2) can be found, which differ in their numerical behavior. Note that from the 16 possible schemes presented here, only 3 are discussed in the literature.

**K4** Preconditioned non-linear time step

The function under consideration is expanded until the second order around \( \tau \mathbf{M} \mu^i \) according to eq. 69
\[
Q_A(\psi^j + \tau \mathbf{M} \mu^i)
\] (K17)

\[\simeq Q_A(\psi^j) + \tau^j (\nabla Q_A(\psi^j) | \mathbf{M} \mu^i) + \frac{\tau^{j^2}}{2} (\mathbf{M} \mu^i | \mathbf{M} \mu^i)_{\nabla \nabla Q_A(\psi^j)}.\] (K18)

Then the derivative with respect to the searching vector is done to find the extremum
\[
\frac{d}{d\tau} Q_A(\psi^j + \tau \mathbf{M} \mu^i)
\]
\[\simeq (\nabla Q_A(\psi^j) | \mathbf{M} \mu^i) + \tau^j (\mathbf{M} \mu^i | \mathbf{M} \mu^i)_{\nabla \nabla Q_A(\psi^j)}.\] (K19)

By setting this equation to zero, one finds an expression for the time step
\[
\tau^j = -\frac{(\nabla Q_A(\psi^j) | \mathbf{M} \mu^i)}{(\mathbf{M} \mu^i | \mathbf{M} \mu^i)_{\nabla \nabla Q_A(\psi^j)}}.
\] (K20)

**APPENDIX I: BAYES, TIKHONOV, ASYMPTOTIC REGULARIZATION AND LEARNING ALGORITHMS**

We want to solve eq. 66 from a Bayesian perspective. Let us assume a Gaussian likelihood with covariance \( \mathbf{I} \)
\[
\mathcal{L}(\psi | \mathbf{f}, \mathbf{p}) = G(f - A\psi, \mathbf{I}),
\] (L1)

which is a fair assumption in the absence of noise (eq. 66) is equivalent to eq. 2 without noise, \( \epsilon = 0 \). Let us further assume a Gaussian prior around a prior solution \( \psi^* \) with covariance \( \tau \mathbf{M}^{-1} \)
\[
P(\psi | p) = G(\psi - \psi^*, \tau \mathbf{M}^{-1}).
\] (L2)

We can now calculate the MAP which coincides in this case with the mean of the posterior. Let us look at the quantity given by the log-posterior PDF
\[
||\mathbf{f} - A\psi||^2 + \tau ||\psi - \psi^*||^2 \mathbf{M}.
\] (L3)
which is a generalization of Tikhonov regularization. Minimizing the negative log-posterior yields the following equation for the Bayesian estimator \( \langle \psi \rangle_B \)

\[
A^\dagger (A\langle \psi \rangle_B - f) + \tau^{-1} M (\langle \psi \rangle_B - \psi^*) = 0. \tag{L4}
\]

If we now choose \( M = A^\dagger M^{-1} \) (\( M \) is an invertible matrix) we get

\[
A^\dagger (M^{-1} (\psi^* - \langle \psi \rangle_B) + \tau (f - A\langle \psi \rangle_B)) = 0, \tag{L5}
\]

This equation will be fulfilled if the following equality holds

\[
\langle \psi \rangle_B = \psi^* + \tau M (f - A\langle \psi \rangle_B). \tag{L6}
\]

The estimator \( \langle \psi \rangle_B \) for the solution to the inverse problem (eq. (65)) is expressed in eq. (L6) as the prior solution \( \psi^* \) plus a correction term given by the residual \( f - A\langle \psi \rangle_B \). Since only the residual based on the prior solution is known, the following substitution must be done on the right-hand-side (rhs) \( \langle \psi \rangle_B \rightarrow \psi^* \) leading to

\[
\langle \psi \rangle_B \approx \psi^* + \tau M (f - A\psi^*). \tag{L7}
\]

This can be interpreted as an iterative scheme, in which the estimator is the update \( j + 1 \) (\( \langle \psi \rangle_B \rightarrow \psi^{j+1} \) on the left-hand-side (lhs)) of the estimator at the previous step \( j \) (\( \psi^* \rightarrow \psi^j \) on the rhs)

\[
\psi^{j+1} = \psi^j + \tau M (f - A\psi^j). \tag{L8}
\]

In this way, we have found the general iterative method (eq. 77) derived with the asymptotic regularization in section 3.1.2. From the Bayesian point of view, this scheme could be interpreted as a learning algorithm, in which the estimator of the solution to the inverse problem is calculated from the prior solution and becomes itself the prior solution for the subsequent iteration.

APPENDIX M: PRECONDITIONING

We can enhance the convergence of the iteration methods by multiplying the matrix we want to invert by another matrix that is close to its inverse

\[
MA\psi = Mf, \tag{M1}
\]

with \( M \sim A^{-1} \). Let us show this by deriving eq. (77) in a different way. We can invert \( MA \) using the Neumann expansion for the inverse of an operator

\[
\psi = (MA)^{-1} Mf = \sum_{i=0}^{\infty} (I - MA)^{i} Mf. \tag{M2}
\]

This iteration scheme will converge if \( \|I - MA\| < 1 \). Let us introduce the following notation

\[
\psi \equiv \sum_{i=0}^{\infty} \psi[i], \tag{M3}
\]

\[
\psi^j \equiv \sum_{i=0}^{j} \psi[i], \tag{M4}
\]

with

\[
\psi[i] \equiv (I - MA)^{i} Mf. \tag{M5}
\]

It follows that

\[
\psi[i + 1] = (I - MA)\psi[i], \tag{M6}
\]

and summing over \( i \) we get

\[
\sum_{i=0}^{j} \psi[i + 1] = \sum_{i=0}^{j} \psi[i] - \sum_{i=0}^{j} MA\psi[i]. \tag{M7}
\]

Manipulating the indices, we see that

\[
\sum_{i=0}^{j} \psi[i + 1] = \sum_{i=0}^{j+1} \psi[i] - \psi[0]. \tag{M8}
\]

Combining the last two equations we obtain eq. (77)

\[
\psi^{j+1} = \psi^j + M (f - A\psi^j), \tag{M9}
\]

with

\[
\psi[0] = \psi^0 = Mf. \tag{M10}
\]

The meaning of the preconditioning matrix \( M \) is clear when we look at eq. (M2). There it can be seen that a much more rapid convergence is obtained if \( (I - MA) \) is close to zero, that is if \( M \) is close to the inverse of \( A \).

\footnote{The iteration time step \( \tau \) has been absorbed here in the matrix \( M \).}