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Published in:
Computers & Geosciences

Link to article, DOI:
[10.1016/j.cageo.2012.09.004](https://doi.org/10.1016/j.cageo.2012.09.004)

Publication date:
2013

[Link back to DTU Orbit](#)

Citation (APA):
Hansen, T. M., Cordua, K. S., Caroline Looms, M., & Mosegaard, K. (2013). SIPPI: A Matlab toolbox for sampling the solution to inverse problems with complex prior information: Part 1—Methodology. *Computers & Geosciences*, 52, 470-480. <https://doi.org/10.1016/j.cageo.2012.09.004>

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www.elsevier.com/locate/cageo

PII: S0098-3004(12)00313-5
DOI: <http://dx.doi.org/10.1016/j.cageo.2012.09.004>
Reference: CAGEO3018

To appear in: *Computers & Geosciences*

Received date: 22 June 2012
Revised date: 7 September 2012
Accepted date: 10 September 2012

Cite this article as: Thomas Mejer Hansen, Knud Skou Cordua, Majken Caroline Looms and Klaus Mosegaard, SIPPI: A Matlab toolbox for sampling the solution to inverse problems with complex prior information: Part 1 - Methodology, *Computers & Geosciences*, <http://dx.doi.org/10.1016/j.cageo.2012.09.004>

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SIPPI : A Matlab toolbox for sampling the solution to inverse problems with complex prior information: Part 1 - Methodology

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Abstract

From a probabilistic point-of-view, the solution to an inverse problem can be seen as a combination of independent states of information quantified by probability density functions. Typically, these states of information are provided by a set of observed data and some a priori information on the solution. The combined states of information (i.e. the solution to the inverse problem) is a probability density function typically referred to as the a posteriori probability density function. We present a generic toolbox for Matlab and Gnu Octave called SIPPI that implements a number of methods for solving such probabilistically formulated inverse problems by sampling the a posteriori probability density function. In order to describe the a priori probability density function, we consider both simple Gaussian models and more complex (and realistic) a priori models based on higher order statistics. These a priori models can be used with both linear and non-linear inverse problems. For linear inverse Gaussian problems we make use of least-squares and kriging-based methods to describe the a posteriori probability density function directly. For general non-linear (i.e. non-Gaussian) inverse problems we make use of the extended Metropolis algorithm to sample the a posteriori

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probability density function. Together with the extended Metropolis algorithm we use sequential Gibbs sampling that allow computationally efficient sampling of complex a priori models. The toolbox can be applied to any inverse problem as long as a way of solving the forward problem is provided. Here we demonstrate the methods and algorithms available in SIPPI. An application of SIPPI, to a tomographic cross borehole inverse problems, is presented in a second part of this paper.

Keywords: inversion, nonlinear, sampling, a priori, a posteriori

1. Introduction

Inverse problems are abundant in almost any type of scientific research field. An inverse problem occurs when a set of unknown parameters, that describe a physical system, pixel values of an image or some mathematical expression, have to be inferred based on indirect observations of these parameters. Examples of inverse problems are image deblurring, tomographic reconstruction, solutions to certain differential equations, or reconstructing the earth's interior based on surface observations. There are several ways to solve an inverse problem. In a probabilistic formulation the inverse problem can be seen as a way of combining information: Given knowledge about the system (differential equation, physical law, or blurring mechanisms), and a set of observations (signal intensities, pixel values, gravity field), and some prior expectations about the parameters, the goal is to quantify how probable a number of possible scenarios are of explaining the observations and the prior information. A successful probabilistic inversion will, in principle, locate all solutions to the problem and assign a probability to each scenario given the information at hand.

18 In this paper we present a Matlab¹ toolbox (SIPPI), compatible with Gnu
 19 Octave², that can be used to solve inverse problems in a probabilistic formu-
 20 lation. In this formulation the solution to the inverse problem is a probability
 21 density function (pdf) referred to as the *a posteriori* pdf, that describe all
 22 information available about a system. While the toolbox is generally appli-
 23 cable to inverse problems, it has been designed specifically for geophysical
 24 inverse problems, where the model parameters typically describe a 1D-3D
 25 space, such as for example the subsurface of the earth.

26 Initially we lay out the theory of probabilistically formulated inverse prob-
 27 lems. Then we show how so-called *a priori* information about the model
 28 parameters, and uncertainty of data observations can be specified. Finally
 29 we show how realizations of the *a posteriori* pdf can be generated using least
 30 squares based methods, and sampling techniques such as rejection sampling
 31 and Metropolis sampling.

32 In a second part of this manuscript we demonstrate the application of
 33 SIPPI to a cross borehole traveltime tomographic inverse problem, Hansen
 34 et al. (this issue).

35 2. Probabilistic Inverse Problem Theory

36 Consider some data, $\mathbf{d}$, which are indirect measurements of some model
 37 parameters, $\mathbf{m}$, describing a system, such as for example the subsurface of
 38 the Earth. Let $\mathbf{d}$ and $\mathbf{m}$ be related through the function g :

$$\mathbf{d} = g(\mathbf{m}) \quad (1)$$

¹<http://mathworks.com/>

²<http://www.gnu.org/software/octave>

Eq. 1, referred to as the forward problem, can be solved with various degrees of accuracy for a number of physical problems.

Inversion of geophysical data amounts to infer information about the model parameters, $\mathbf{m}$, given some data, $\mathbf{d}$, the forward relation between model parameters and data, g , and a priori existing knowledge about the model parameters. Such an inverse problem can be solved in a variety of ways. In this paper we will deal with the general probabilistic formulation of inverse problems. Note that many types of deterministic inversion methods can be formulated as special cases of the probabilistic inverse theory as we consider here.

Tarantola and Valette (1982b) formulate a probabilistic approach for solving inverse problems where all available states of information is described by pdfs. The solution to the inverse problem is the pdf that combines known states of information. In a typical inverse problem the states of information can be described by the *a priori* pdf and the *likelihood* function. The *a priori* pdf, $\rho_M(\mathbf{m})$, describes prior knowledge about the model parameters. The likelihood function, $L(\mathbf{m})$, is a probabilistic measure of how well a given model $\mathbf{m}$ explains observed data.

The general solution to such a probabilistically formulated inverse problem is the *a posteriori* pdf, which is proportional to the product of the *a priori* pdf and the likelihood function:

$$\sigma_M(\mathbf{m}) = k \rho_M(\mathbf{m}) L(\mathbf{m}) , \quad (2)$$

where the k is a normalization constant and the likelihood is given by

$$L(\mathbf{m}) = \int_{\mathcal{D}} d\mathbf{d} \frac{\rho_D(g(\mathbf{m})) \theta(\mathbf{d}|\mathbf{m})}{\mu_D(\mathbf{d})} \quad (3)$$

61 $\rho_D(\mathbf{d})$ describes *measurement uncertainties*, typically related to uncertainties
 62 in the instrument that records the data. $\theta(\mathbf{d}|\mathbf{m})$ describes the *modelization*
 63 *error*, i.e. the error caused by using an imperfect forward model g or an
 64 imperfect parameterization. $\mu_D(\mathbf{d})$ describes the homogeneous state of infor-
 65 mation that ensures that the parameterization is invariant to changes in the
 66 coordinate system. For the remainder of the text we shall assume that $\mu_D(\mathbf{d})$
 67 can be approximated by a constant. For more details on the homogeneous
 68 pdf see e.g. Mosegaard and Tarantola (2002).

69 The a posteriori pdf describes the distribution of models consistent with
 70 the combined states of information given by the a priori model and the data.

71 The probabilistic formulation of inverse problems allows utilization of the
 72 movie strategy advocated by Tarantola (2005), who suggest to visualize and
 73 compare a sample from the a priori pdf and the a posteriori pdf, respectively,
 74 as movies. The 'prior movie' will make it apparent what prior choices have
 75 been made. The difference between the prior and the posterior movie will
 76 emphasize the effect of using data.

77 2.1. The linear inverse Gaussian problem

78 Consider a linear forward problem, where the data $\mathbf{d}$ is linearly related
 79 to the model parameters $\mathbf{m}$ using the linear operator $\mathbf{G}$, such that $\mathbf{d} = \mathbf{G}\mathbf{m}$.
 80 Let $\mathcal{N}(\mathbf{a}, \mathbf{A})$ refer to a Gaussian distribution with mean $\mathbf{a}$ and covariance $\mathbf{A}$.
 81 If in addition both the a priori model $\mathcal{N}(\mathbf{m}_0, \mathbf{C}_M)$, the noise model $\mathcal{N}(0, \mathbf{C}_d)$
 82 and the modelization error $\mathcal{N}(0, \mathbf{C}_T)$ can be described by a Gaussian pdf,
 83 then the a posteriori pdf (Eq. 2) can be described analytically by a Gaussian
 84 pdf, $\mathcal{N}(\tilde{\mathbf{m}}, \tilde{\mathbf{C}}_M)$ (Tarantola and Valette, 1982a):

$$\tilde{\mathbf{m}} = \mathbf{m}_0 + \mathbf{C}_M \mathbf{G}^t (\mathbf{G} \mathbf{C}_M \mathbf{G}' + \mathbf{C}_D)^{-1} (\mathbf{d}_0 - \mathbf{G} \mathbf{m}_0) \quad (4)$$

$$\tilde{\mathbf{C}}_{\mathbf{M}} = \mathbf{C}_{\mathbf{M}} - \mathbf{C}_{\mathbf{M}} \mathbf{G}^t (\mathbf{G} \mathbf{C}_{\mathbf{M}} \mathbf{G}' + \mathbf{C}_{\mathbf{D}})^{-1} \mathbf{G} \mathbf{C}_{\mathbf{M}} \quad (5)$$

Note that Gaussian measurement errors and modelization errors combine through addition of the covariance operators, such that the combined covariance model is given by $\mathbf{C}_{\mathbf{D}} = \mathbf{C}_d + \mathbf{C}_T$. This allows accounting of Gaussian modelization errors directly as given in Eqs. 4-5, Tarantola (2005).

If $\tilde{\mathbf{m}}$ and $\tilde{\mathbf{C}}_{\mathbf{M}}$ are available from Eqs. 4-5 then samples from the a posteriori pdf can be generated using e.g. Cholesky decomposition of the a posteriori covariance model, Eq. 5 in Le Ravalec et al. (2000).

Sampling the a posteriori pdf of a linear inverse Gaussian problem can also be performed using sequential Gaussian simulation without the need for explicitly computing $\tilde{\mathbf{m}}$ and $\tilde{\mathbf{C}}_{\mathbf{M}}$, Hansen et al. (2006). Hansen and Mosegaard (2008) extend this approach to work with direct sequential simulation. This allows a non-Gaussian a priori distribution of model parameters.

An alternative approach is to use kriging through error simulation, Journel and Huijbregts (1978, p. 495), in a co-kriging formulation as proposed by Gloaguen et al. (2004,2005). This approach may be faster than the methods based on sequential simulation, but is only valid for strictly Gaussian a priori models.

The above mentioned methods rely on the fact that in a linear formulation, data can be seen as weighed averages of the model parameters. While not specifically making the link to inverse problems, such ideas has also been explored by Journel (1999) and Gómez-Hernández et al. (2005).

2.2. The non-linear Inverse problem

The linear and Gaussian assumptions considered above are convenient as they lead to computationally efficient algorithms. However, in reality

the inverse problem is typically non-linear and the Gaussian assumption not valid. This may lead to severe artifacts in the inversion if the least-squares based approaches, as described above, are used. Instead one can use sampling techniques to sample the a posteriori pdf.

Rejection sampling. Perhaps the simplest method to sample the a posteriori pdf is the rejection sampler, that can be implemented as follows

1. Propose a model candidate from the a priori pdf, $\mathbf{m}_{pro}$.
2. Compute $L(\mathbf{m}_{pro})$
3. Accept the proposed model as a realization of the a posteriori pdf with probability

$$P_{acc} = L(\mathbf{m}_{pro})/L_{max} \quad (6)$$

where L_{max} is the maximum value the likelihood function can obtain. Typically the value of L_{max} is not known and must be set to 1. The only requirements for using the method is that one must be able to generate independent realizations of the a priori pdf and compute the corresponding likelihood. The collection of models accepted by the rejection sampling algorithm will be a sample of the a posteriori pdf. The main problem with the rejection sampler is that it is computationally very inefficient for anything but very low dimensional problems.

The extended Metropolis sampler. Mosegaard and Tarantola (1995) propose an extended version of the Metropolis algorithm (Metropolis et al. (1953); Hastings (1970)) that allows sampling the a posteriori pdf of an inverse problem with, in principle, arbitrary complex a priori information as given by Eq. 2. Using the classical Metropolis algorithm one must be able to

132 evaluate the a posteriori probability $\sigma_M(\mathbf{m})$ and, hence, typically also the a
133 priori probability, in order to evaluate Eq. 2.

134 The extended Metropolis algorithm differ from the classical Metropolis
135 algorithm in that one does not need to evaluate the a posteriori probability
136 $\sigma_M(\mathbf{m})$, nor the a priori probability $\rho_M(\mathbf{m})$ of a given model $\mathbf{m}$. If only an
137 algorithm is present that can sample the a priori pdf and a method exist for
138 evaluating the likelihood, $\rho_D(g(\mathbf{m}))$, then the extended Metropolis algorithm
139 will sample the a posteriori pdf.

140 The extended Metropolis algorithm is a Markov Chain Monte Carlo method
141 and can be implemented as a random walk in the space of a priori acceptable
142 models as follows. If initially a realization of the a priori pdf is generated as
143 $\mathbf{m}_{cur}$, and the associated likelihood $L(\mathbf{m}_{cur})$ is evaluated using Eq. 3, then
144 the following algorithm will sample the a posteriori pdf

- 145 1. In the vicinity of $\mathbf{m}_{cur}$, propose a new model candidate, $\mathbf{m}_{pro}$, consistent
146 with the a priori model.
- 147 2. Compute $L(\mathbf{m}_{pro})$
- 148 3. Accept the proposed model with probability $P_{acc} = \min([1, L(\mathbf{m}_{pro})/L(\mathbf{m}_{cur})])$
- 149 4. If the proposed model is accepted, then the transition from $\mathbf{m}_{cur}$ to
150 $\mathbf{m}_{pro}$ is accepted, and the proposed model becomes the current model,
151 $\mathbf{m}_{cur} = \mathbf{m}_{pro}$. Otherwise the random walker stays a location $\mathbf{m}_{cur}$ and
152 $\mathbf{m}_{cur}$ counts again.

153 There are only two requirements for running the extended Metropolis al-
154 gorithm: 1) One must be able to evaluate the likelihood function, Eq. 3.
155 This is most often trivial, even if it may be computationally demanding, as
156 it requires one to solve the forward problem and evaluate the correspond-

157 ing data fit given the noise model. 2) One must be able to sample the a
158 priori pdf such that aperiodicity and irreducibility is ensured, Mosegaard
159 and Sambridge (2002). In addition, it is preferable to be able to control
160 the exploratory nature (often referred to as the step length) of the sampling
161 algorithm, i.e. step 1 in the above algorithm, which is closely linked to the
162 computational efficiency. See Mosegaard and Tarantola (1995) for details on
163 the extended Metropolis algorithm.

164 The sequential Gibbs sampling algorithm provides such a general way to
165 sample complex a priori models, with arbitrary step length ensuring aperiod-
166 icity and irreducibility, Hansen et al. (2012). Sequential Gibbs sampling can
167 be used with any pdf that can be sampled using sequential simulation, which
168 is the case for most of the statistical models developed in the geostatistical
169 community over the last decades. The resampling strategy inherent in the
170 sequential Gibbs sampler was initially proposed by Hansen et al. (2008), and
171 subsequently Irving and Singha (2010) and Mariethoz et al. (2010) proposed
172 similar methods. Hansen et al. (2012) demonstrate how the method is simi-
173 lar to an application of the Gibbs sampler and show that the method leads
174 to a way of sampling the a priori pdf where aperiodicity and irreducibility is
175 ensured.

176 3. SIPPI

177 SIPPI is a Matlab toolbox (SIPPI), compatible with Gnu Octave, that
178 can be used to solve inverse problems in the formulation given by Eqs. 2-3 by
179 allowing **S**ampling the solution to **I**nverse **P**roblems with complex **A** **P**riori
180 **I**nformation.

181 In order to solve a probabilistic framed inverse problem as presented
 182 previously, one needs (at least) three ingredients: 1) a choice of an a priori
 183 model, 2) a choice of how to solve the forward problem, and 3) a choice of a
 184 noise model model that describes the uncertainty of the observed data and
 185 the modelization error. Once these choices have been made one can solve the
 186 inverse problem using any of the applicable inversion methods.

187 SIPPI provides a generic approach to defining the a priori model and the
 188 noise model in form of the two data structures `prior` and `data`.

189 3.1. The a priori model

190 All information about the a priori model is defined in the Matlab struc-
 191 ture called `prior`, which can specify any number of a priori type of models.
 192 For example an a priori choice of a 2D Gaussian velocity field can be spec-
 193 ified in `prior{1}` and a 1D parameter describing a bias correction can be
 194 specified in `prior{2}`. Once the `prior` has been defined, a realization of the
 195 corresponding a priori pdf can be generated by calling

```
m=sippi_prior(prior);
```

196 `m` is a Matlab structure of the same size as `prior`. If 3 types of a priori
 197 models have been defined in `prior{1}`, `prior{2}`, and `prior{3}` then the
 198 corresponding realizations will be stored in `m{1}`, `m{2}`, and `m{3}`. Consid-
 199 ering the example above, `m{1}` will hold a realization of a 2D a priori model,
 200 while `m{2}` will hold a realization of a 1D a priori model. For the remainder
 201 of the text the index `im` will point to a specific number of a priori model,
 202 `prior{im}`.

203 A number of different types of a priori models can be selected using a
 204 `type` field to the `prior` data structure. The following 4 types of a priori
 205 models are available as part of SIPPI:

```
im=1;
prior{im}.type='GAUSSIAN';
prior{im}.type='FFTMA';
prior{im}.type='VISIM';
prior{im}.type='SNESIM';
```

206 **Generalized Gaussian.** `prior{im}.type=GAUSSIAN'` defines a 1D gener-
 207 alized Gaussian distribution;

$$f_{gg}(m_0, \sigma, p) = \frac{p^{1-1/p}}{2\sigma\Gamma(1/p)} \exp\left(-\frac{1}{p} \frac{|m - m_0|^p}{\sigma^p}\right) \quad (7)$$

208 where p is the norm, σ the variance. f_{gg} is symmetric around m_0 , the a priori
 209 mean value. In the limit of $p \rightarrow \infty$ f_{gg} will define a uniform distribution. The
 210 following code defines a 1D Gaussian distribution with mean 10 and standard
 211 deviation 2

```
im=1;
prior{im}.type='GAUSSIAN';
prior{im}.m0=10;
prior{im}.std=2;
```

212 If not set, the `norm` is by default set to 2. The following code defines a 1D
 213 close to uniform distribution in the interval [8,12]

```
im=1;
prior{im}.type='GAUSSIAN';
```

```
prior{im}.m0=10;
prior{im}.std=2;
prior{im}.norm=60;
```

214 A histogram of a sample of size 100000 of these two 1D prior models is shown
215 in Figure 1.

216 [Figure 1 about here.]

217 The FFTMA, VISIM and SNESIM type priors all describe a 1D to 3D a priori
218 model defined on a Cartesian grid, which is defined as (for a 3D case)

```
im=1;
prior{im}.prior.x=[0:1:10]; % X array
prior{im}.prior.y=[0:1:20]; % Y array
prior{im}.prior.z=[0:1:30] ;% Z array
```

219 For a 1D prior only `prior{im}.prior.x` needs to be defined, and for a 2D
220 prior `prior{im}.prior.x` and `prior{im}.prior.y` need to be defined.

221 Both the FFTMA and VISIM type a priori models describe a multivariate
222 Gaussian a priori pdf, which requires the specification of an a priori mean
223 and covariance model. The a priori mean `m0` can be either a scalar, indicating
224 a constant a priori mean model, or a matrix of the size of the a priori model,
225 allowing for a varying a priori mean model. The model of spatial variabil-
226 ity is defined by a, possibly anisotropic, covariance model (equivalent to a
227 semivariogram model) given by the `Cm` (or equivalent the `Va`) field. The spec-
228 ification of the covariance model uses the same notation as used in Pebesma
229 and Wesseling (1998). For example a multivariate Gaussian model defined by

230 a 2D Spherical type covariance model with sill (or variance) 1, a maximum
 231 correlation length of 10 in the direction west to east (i.e. horizontal), and a
 232 perpendicular range (i.e. vertical) of 2.5 (hence an anisotropy factor of 0.25)
 233 and a mean of 10, is given by

```
prior{im}.m0=10;
prior{im}.Cm='1 Sph(10,90,0.25)';
```

234 **FFT Moving Average.** `prior{im}.type='FFTMA'` defines a spatially cor-
 235 related multivariate Gaussian a priori model where a priori realizations are
 236 generated using the FFT Moving Average generator (FFTMA), Le Ravalec
 237 et al. (2000). The FFTMA algorithm is very efficient for generating uncon-
 238 ditional realizations from a multivariate Gaussian model. In addition it also
 239 allows separation of the random component field and the structural parame-
 240 ters that define spatial correlation. We will discuss the use of this feature in
 241 more details later.

242 A 2D FFTMA type a priori model, on a 200x100 grid, can for example be
 243 given by

```
im=1;
prior{im}.type='FFTMA';
prior{im}.prior.x=[0:.1:10]; % X array
prior{im}.prior.y=[0:.1:20]; % Y array
prior{im}.m0=10;
prior{im}.Va='1 Sph(10,90,.25)';
```

244 Figure 2a shows a set of five realizations from this choice of a priori model.

245 [Figure 2 about here.]

246 **VISIM.** `prior{im}.type='VISIM'` defines a spatially correlated multivari-
 247 ate Gaussian a priori model where a priori realizations are generated using
 248 the VISIM algorithm, Hansen and Mosegaard (2008). VISIM can run us-
 249 ing sequential Gaussian simulation, in which case the model parameters are
 250 assumed normally distributed. It can also run using direct sequential simu-
 251 lation, which allows a (non-Gaussian) target distribution to be set that de-
 252 scribes the a priori distribution of the model parameters, while at the same
 253 time ensuring that the a priori chosen mean and covariance will be honored.

254 An a priori model similar to the one described above for the FFTMA type
 255 prior, but with an a priori assumption of a bimodal distribution of model
 256 parameters can be given as

```
im=1;
prior{im}.type='VISIM';
prior{im}.prior.x=[0:1:10]; % X array
prior{im}.prior.y=[0:1:20]; % Y array
prior{im}.m0=10;
prior{im}.Va='1 Sph(10,90,.25)';
% target distribution
N=10000;
prob_chan=0.5;
d1=randn(1,ceil(N*(1-prob_chan)))*.5+8.5;
d2=randn(1,ceil(N*(prob_chan)))*.5+11.5;
d_target=[d1(:);d2(:)];
prior{im}.target=d_target;
```

257 Figure 3 shows a set of five realizations from this VISIM type of a priori
 258 model a) without a specification of a target distribution, and b) using a

target distribution. Once `[m,prior]=sippi_prior(prior)` has been called once, a data structure will be available as `prior{im}.V`, which allows access to all options available for running the VISIM algorithm. See Hansen and Mosegaard (2008) for more details on VISIM.

[Figure 3 about here.]

The FFTMA and VISIM type prior models only allow reproducing the first two moments of the distribution describing the spatial variability, the mean and the covariance (i.e. Gaussian variability between sets of two data points). Maximum entropy is implicitly assumed in higher order moments, Journel and Zhang (2006). This is the reason why geological structures such as for example meandering channels cannot be reproduced by Gaussian statistics. To achieve this one can make use of statistical models based on higher order moments.

SNESIM. `prior{im}.type='SNESIM'` defines an a priori model based on a higher order statistical moments (a multiple point statistical model) describing spatial variability as inferred from a training image.

There are several methods that allow sampling from an a priori model defined by multiple point statistics. Here, we use the SNESIM algorithm, originally developed by Strebelle (2000, 2002), and we make use of the implementation available in the SGeMS software package, Remy et al. (2008). It works by initially extracting a multiple point based statistical model from a training image. Then sequential simulation is used to generate realizations of this statistical model.

282 Optionally the `scaling` and `rotation` field can be speified. `prior{im}.scaling=2`
 283 scales the axis of the training image such that spatial structures appears
 284 twice as large. `prior{im}.rotation=45` rotates the training image 45 de-
 285 grees clockwise.

286 A 2D SNESIM type prior with the training image 'channels.ti' (Figure 4)
 287 rotated 30 degrees and scaled by a factor of 0.75, with two categories ('0'
 288 and '1'), and where the first category '0' reflect a model parameter value of
 289 8, and the second category '1' reflect a value of 12, is given by

```
im=1;
prior{im}.type='SNESIM';
prior{im}.x=[0:.1:10];
prior{im}.y=[0:.1:20];
prior{im}.ti='channels.ti';
prior{im}.index_values=[0 1]; % optional
prior{im}.m_values=[8 12]; % optional
prior{im}.scaling=.75; % optional
prior{im}.rotation=30; % optional
```

290 Figure 5 shows a set of five realizations from this choice of a priori model.
 291 Once `[m,prior]=sippi_prior(prior)` has been called, a data structure will
 292 be available as `prior{im}.S` which allow access to all options available for
 293 running the SNESIM algorithm as implemented in SGeMS. See Remy et al.
 294 (2008) for more details on setting up the SNESIM algorithm.

295 [Figure 4 about here.]

296 [Figure 5 about here.]

297 *Distribution transform.* A normal score transform can be defined for any of
 298 the Gaussian based a priori models, that allow the transformation of the
 299 normally distributed model parameters to any desired distribution, see e.g.
 300 Goovaerts (1997). It requires only that the user defines the 'target' distribu-
 301 tion, in form of a sample of the target distribution in the `d_target` field. For
 302 example a bimodal distribution with increased probability of values around
 303 8.5 and 11.5, can be given by

```
N=10000;
prob_chan=0.5;
d1=randn(1,ceil(N*(1-prob_chan)))*.5+8.5;
d2=randn(1,ceil(N*(prob_chan)))*.5+11.5;
d_target=[d1(:);d2(:)];
prior{im}.d_target=d_target;
```

304 Note that the number N here reflects the size of the sample generated and
 305 used to describe the target distribution in the `d_target` field, and can be
 306 chosen arbitrarily large. The larger the sample, the better accuracy of re-
 307 flecting a specific distribution. An example of combining this distribution
 308 transform with the FFTMA type prior used to generate Figure 2a is shown in
 309 Figure 2b.

310 Note that when using the VISIM type prior one can use a target distri-
 311 bution directly, while ensuring that the chosen a priori covariance model is
 312 still honored. Using the distribution transform with the FFTMA prior will not
 313 preserve the properties of the a priori chosen covariance model.

314 *Randomizing the model of spatial variability.* As mentioned for the 'FFTMA'
 315 prior type model, the structural parameters that describe the a priori model

316 covariance, can be separated from the random number series that defines the
 317 random component. Therefore, all properties of the covariance model can be
 318 treated as model parameters, such as scaling and rotation. The properties of
 319 the model covariance can be perturbed independently of the random number
 320 series defining the random component, Le Ravalec et al. (2000).

321 In order to randomize a specific component of the covariance model, a
 322 GAUSSIAN type prior model needs to be defined for this component. The name
 323 of the specific prior model must be either `range_1`, `range_2`, or `range_3` to
 324 define the range, or one of `ang_1`, `ang_2`, or `ang_3` to define the rotation,
 325 and `m0` to define the a priori mean, and `sill` to define the sill. In addition,
 326 one must set the `prior_master` field to point the prior model that define the
 327 prior for the corresponding FFTMA a priori model.

328 As an example, consider the FFTMA example used to generate Figure 2a.
 329 To randomize the maximum correlation length to be close to uniform between
 330 6 and 14, and randomize the primary rotation angle to be close to uniform
 331 between 40 and 130 degrees (from north) use

```
im=1;
prior{im}.type='gaussian';
prior{im}.name='range_1';
prior{im}.m0=10;
prior{im}.std=4;
prior{im}.norm=80;
prior{im}.prior_master=3;

im=2;
prior{im}.type='gaussian';
```

```
prior{im}.name='ang_1';
prior{im}.m0=90;
prior{im}.std=50;
prior{im}.norm=80;
prior{im}.prior_master=3;

im=3;
prior{im}.type='FFTMA';
prior{im}.prior.x=[0:1:10]; % X array
prior{im}.prior.y=[0:1:20]; % Y array
prior{im}.m0=10;
prior{im}.Va='1 Sph(10,90,.25)';
```

332 Figure 2c shows an example of 5 realizations from such an a priori model.

333 3.1.1. A random walk in the a priori model space

334 To perform a random walk in the prior probability space, as needed by
 335 the extended Metropolis sampler, we make use of sequential Gibbs sampling,
 336 Hansen et al. (2012). An application of the sequential Gibbs sampler es-
 337 sentially amounts to selecting a subset, which can be any subset of model
 338 parameters, and simulate these conditional to the rest of the model param-
 339 eters. The number of chosen model parameters in the subset controls the
 340 exploratory nature (i.e. step-length) of the sequential Gibbs sampler (which
 341 controls the degree of correlation between successive realizations), and hence
 342 the efficiency of the extended Metropolis sampler. All properties of the se-
 343 quential Gibbs sampler is controlled by `seq_gibbs` structure, which is a field
 344 in the `prior` data structure. Two different methods for selecting the subset

of model parameters for conditional re-simulation have been implemented.

Box type subset. If `prior{im}.seq_gibbs.type=1`, then a line/rectangle/cube of model parameters (for the 1D, 2D and 3D case respectively) is selected as the subset used for conditional re-simulation. The width of the box is defined by `prior{im}.seq_gibbs.step`. For example a box with dimension 2x3x4 (in the units of the prior model considered - typically meters) is given by `prior{im}.seq_gibbs.step=[2 3 4]`. The center of the 'box' is chosen randomly

Randomly selected subset. If `prior{im}.seq_gibbs.type=2`, then a randomly selected number of the total number of model parameters is selected as the subset used for conditional resimulation. The number of data used for conditional re-simulation is given by `prior{im}.seq_gibbs.step`. If `prior{im}.seq_gibbs.step` is smaller than 1, it is interpreted as a percentage of the total number of model parameters.

As an example, five iterations of sequential Gibbs sampling can in SIPPI be performed using iterative calls to `sippi_prior` as

```
[m_current,prior]=sippi_prior(prior);
for i=1:5
    [m_proposed,prior]=sippi_prior(prior,m_current);
end
```

Figures 6 and Figure 7 shows examples of using sequential Gibbs sampling with a box type selection and random type selection of model parameters for conditional re-simulation, respectively. The a priori model is in both cases

364 the same as the one used to generate the unconditional realizations of Figure
365 3. The options for the box type re-simulation is

```
prior{im}.seq_gibbs.type=1;  
prior{im}.seq_gibbs.step=[4 4];
```

366 while the options for the random type re-simulation, with only 0.5 % of the
367 total number of model parameter used as conditional data for re-simulation,
368 is

```
prior{im}.seq_gibbs.type=2;  
prior{im}.seq_gibbs.step=0.995;
```

369 The sequential Gibbs sampler can be used with the FFTMA, VISIM, and
370 SNESIM types a priori models. For the 1D GAUSSIAN type a priori model we
371 use an alternate method. Given a current realization of the a priori model, a
372 step length between 0 and 1 will generate a new realization of the prior, in the
373 vicinity of the current realization. A step length of '0' indicates no change,
374 while a step length of '1' will generate a new unconditional realization of the
375 a priori model.

376 Figure 8 shows the first 300 iterations when sampling the same a priori
377 model as sampled in Figure 1 using a step length of 0.25, `prior{im}.seq_gibbs.step=0.25`.
378 After 100000 iterations the histogram of the sampled model parameters re-
379 semble that of Figure 1, and is therefore not shown here.

380 [Figure 6 about here.]

381 [Figure 7 about here.]

382 [Figure 8 about here.]

383 *3.2. Data, data uncertainties, modelization errors and the likelihood function*

384 Observed data must be given in the **data** data structure along with a
 385 description of the noise model. As for the **prior** structure, the **data** structure
 386 may consist of many types of data, where each data type number **id** is
 387 defined in the **data{id}** structure. Observed data are stored in the **d_obs**
 388 field. Uncorrelated uncertainty can be given either in the form of standard
 389 deviation, **d_std**, or variance, **d_var**. A simple data structure with such
 390 uncorrelated uncertainties can be given by

```
id=1;
data{id}.d_obs=[0 3 4]';
data{id}.d_std=[2 2 2]';
```

391 If the data uncertainties are uncorrelated, the noise model can be described
 392 by a generalized Gaussian model as defined in Eq. 7, if the norm of the
 393 generalized Gaussian is set by **data{id}.norm**. If not specified a Gaussian
 394 noise model (using a norm of 2) is chosen by default.

395 The noise model can also be given in form of a correlated Gaussian model,
 396 for both the data noise, $\mathbf{C}_d$ and the modelization error, $\mathbf{C}_T$. The following
 397 will for example specify a correlated Gaussian noise model:

```
id=1;
data{id}.d_obs=[0 3 4]';
data{id}.Cd=[4 0 .1 ; 0 4 0 ; .1 0 4];
```

398 If a Gaussian model for the modelization error, $\mathcal{N}(\mathbf{d}_T, \mathbf{C}_T)$, is available it
 399 can be specified as


```
data{id}.dt=[0 -1 0]';
data{id}.Ct=[4 .1 .1 ; .1 4 .1 ; .1 .1 4];
```

400 where $\mathbf{d}_T$ is a bias correction.

401 One can choose to consider only a subset of the available data using the
402 `i_use` field. To use for example only data number 1 and 3 use

```
id=1;
data{id}.d_obs=[0 3 4]';
data{id}.i_use=[1 3];
```

403 Once the data structure has been setup in `data`, the log-likelihood and
404 the likelihood of a given data response d can be computed using

```
[logL,L,data]=sippi_likelihood(d,data);
```

405 3.3. The forward problem

406 The forward problem is naturally problem dependent, and to use SIPPI,
407 the user needs to supply the solution to the forward problem, wrapped in
408 the m-file `sippi_forward.m`.

409 The input to `sippi_forward.m` is the `forward`, `data` and prior Matlab
410 structures. The `forward` structure can contain information on how to solve
411 the forward problem. The output must be the data obtained by solving the
412 forward problem, in form of the data structure `d` which must be of the same
413 length as the `data` structure, and each entry of `d{id}` must have the same
414 size as `data{id}.d_obs`, or the size of `data{id}.i_use` if a data subset is
415 specified.

416 As an alternative for providing `sippi_forward`, one can provide a generic
417 name for the m-file solving the forward problem by setting `forward.forward_function`.

Part 2 of this paper will provide an example of setting up `sippi_forward.m`,
Hansen et al. (this issue).

When the forward model has been setup, the process of generating an
unconditional realization of the a priori model, `m`, followed by solving the
forward problem and computing the likelihood of `m` can be done using

```
m=sippi_prior(prior);
d=sippi_forward(m,forward,prior,data);
logL=sippi_likelihood(d,data);
```

In the specific case where the forward relation is linear, the linear forward
operator must be specified as the matrix G

```
forward.G
```

such that the forward problem can be solved using $d\{1\} = \text{forward.G} * m\{1\}$.

3.4. Sampling the a posteriori pdf

When the forward problem, `sippi_forward`, and the `prior`, `data`, and
`forward` data structures have been defined, the a posteriori pdf can be sam-
pled using the rejection sampler or the extended Metropolis sampler in the
general non-linear case. In the linear Gaussian case, least-squares based in-
version can be utilized.

3.5. Rejection sampling

Simple rejection sampling, using 30000 iterations, of the a posteriori
pdf can be performed using

```
options.mcmc.nite=30000;
sippi_rejection(data,prior,forward,options);
```

435 By default the $L_{max} = 1$, see Eq. 6. This can be manually changed by
 436 providing the `options.mcmc.Lmax`.

437 3.5.1. Metropolis sampling

438 All available a priori model types and noise models in SIPPI work seam-
 439 lessly as part of the extended Metropolis algorithm. The extended Metropolis
 440 sampling algorithm can be applied using

```
options=sippi_metropolis(data,prior,forward,options);
```

441 The `options` structure define some properties of how the Metropolis algo-
 442 rithm will run.

443 `options.mcmc.nite` determines the number of iterations of the extended
 444 Metropolis algorithm. `options.mcmc.i_sample` sets how often the current
 445 model is saved to disc, measured in number of iterations. `options.mcmc.i_plot`
 446 sets number of iterations between updating figures showing the progress of
 447 the algorithm. If any of these parameters are not set, the following values
 448 will be chosen by default

```
options.mcmc.nite= 30000;  
options.mcmc.i_sample= 500;  
options.mcmc.i_plot: 50
```

449 *Perturbation strategy.* The choice of the number of model parameters to be
 450 perturbed in each iteration of the extended Metropolis algorithm can have
 451 large impact on its computational performance. By default a random type
 452 of model parameter is perturbed in each iteration. Thus if 3 types of a priori
 453 models have been specified in `prior{1}`, `prior{2}`, and `prior{3}`, the prob-
 454 ability of perturbing each individual type of prior model in each iteration is

1/3. This default behaviour can be changed by choosing a perturbation strategy. `options.mcmc.pert_strategy.i_pert` selects the number of a prior model types to perturb, and `options.mcmc.pert_strategy.i_pert_freq` set the relative frequency of each selected type of prior model. Thus, to perturb prior model 1 and 3 (but never model 2), such that prior model 3 is perturbed 9 times as often as prior type 1, one could use

```
options.mcmc.pert_strategy.i_pert=[1 3];
options.mcmc.pert_strategy.i_pert_freq=[1 9];
```

Automatic adjustment of the exploration rate (step length). The exploratory nature of the Metropolis sampling algorithm, controlled by the 'step length', has large impact on its computational demands. A small step-length provides a dense local sampling, but the algorithm will use many iterations to move away from the initial point, i.e. a less exploratory algorithm. A large step length will lead to a very exploratory sampling algorithm that will not get trapped in local minima, but many models that are proposed will be rejected. Gelman et al. (1996) argues that a step-length leading to an acceptance rate in the Metropolis sampler of about 20-40% will lead to a good compromise between exploration and rejection rate. SIPPI allows automatic detection of the step length leading to an acceptance rate specified by `prior{im}.seq_gibbs.P_target`, using the method given by Cordua et al. (2012). Note that the Metropolis sampler will not sample the a posteriori pdf correct until the step-length is fixed, and unchanged. Therefore one can set the number of initial iterations in which adjustment of the step length is allowed using `prior{im}.seq_gibbs.i_update_step_max`. After this, actual sampling of the a posteriori pdf will start, if the algorithm has reached

478 burn-in. `prior{im}.seq_gibbs.i_update_step` sets the number of itera-
 479 tions between updating the step length. `prior{im}.seq_gibbs.step_min`
 480 and `prior{im}.seq_gibbs.step_max` determine the minimum and maximum
 481 allowed step length.

482 The default choice of the step length is to use infinitely long step-length,
 483 resulting in a prior sampler generating statistically independent realization
 484 of the prior in each iteration.

485 As an example, a preferred acceptance ratio of 0.3, adjusted in the first
 486 1000 iterations, allowing step lengths in the interval 1 to 100 (using type 1
 487 data subset), can be specified using:

```
prior{im}.seq_gibbs.type=1;
prior{im}.seq_gibbs.step_min=1;
prior{im}.seq_gibbs.step_max=100;
prior{im}.seq_gibbs.step=100;
prior{im}.seq_gibbs.i_update_step_max=1000;
prior{im}.seq_gibbs.P_target=0.3;
```

488 3.5.2. Linear Gaussian inverse Problems

489 In the specific case where the forward problem is linear, and the a priori
 490 model Gaussian, as defined by the VISIM of FFTMA type a priori model, the
 491 a posteriori pdf can be sampled directly without the need for the Metropolis
 492 algorithm using

```
[m_reals,m_est,Cm_est]=
    sippi_least_squares(data,prior,forward,n_reals,lsq_type);
```

493 `n_reals` sets how many a posteriori realizations, as output in `m_reals`, that
 494 are generated. `lsq_type` determines the method used to solve sample the a

posteriori pdf. `m_est` and `Cm_est` are the a posteriori mean and covariance as given by Eq. 5, and are only available if least squares types of inversion is performed.

Three methods described previously, are available to generate samples of the a posteriori pdf, and can be selected by setting the the `lsq_type` argument when calling `sippi_least_squares`.

`lsq_type='lsq'` use classical least-squares inversion where the complete Gaussian a posteriori pdf can be analytically derived in form of a posteriori mean and covariance of Eqs. 4-5. Then Cholesky decomposition of the a posterior covariance is used to generated realizations of the a posteriori pdf.

`lsq_type='error_sim'` make use of kriging simulation through error simulation to generate a sample of the a posteriori pdf, Journel and Huijbregts (1978); Gloaguen et al. (2005a,b); Hansen and Mosegaard (2008).

`lsq_type='visim'` make use of the VISIM algorithm for sampling the a posteriori pdf, Hansen and Mosegaard (2008). The type of prior model must be chosen as a VISIM type prior model. If the target distribution is set as `prior{im}.target` then VISIM runs as a direct sequential simulation algorithm. If it is not set, VISIM will run as a sequential Gaussian simulation algorithm.

4. Conclusions

A generic Matlab and Gnu Octave toolbox for sampling the a posteriori pdf of linear and non-linear inverse problems has been presented. Prior information about the model parameters can be described by any number of the following types of a priori models: 1) 1D arbitrarily distributed pdf, 2)

519 1D-3D multivariate Gaussian pdf as sampled using the FFTMA method, 3)
 520 1D-3D multivariate Gaussian model as sampled using the VISIM algorithm
 521 (utilizing both sequential Gaussian simulation and direct sequential simula-
 522 tion), or 4) 1D-3D multiple-point based statistical models as sampled using
 523 the SNESIM algorithm.

524 For linear Gaussian inverse problems the a posteriori pdf can be sampled
 525 using 1) traditional least squares inversion combined with Cholesky decom-
 526 position of the a posteriori covariance, 2) sequential Gaussian simulation, 3)
 527 direct sequential simulation and 4) Gaussian simulation through error simu-
 528 lation.

529 For non-linear and non-Gaussian inverse problems the a posteriori pdf can
 530 be sampled using the rejection sampler or the extended Metropolis sampler.
 531 The computational efficiency of the extended Metropolis sampler can be con-
 532 trolled by using a flexible perturbation mechanism, based on sequential Gibbs
 533 sampling, allowing arbitrary long or short step length. The choice of the step
 534 length can optionally be automatized.

535 The combination of the FFTMA method with the extended Metropolis
 536 algorithm allows treating the properties describing the Gaussian a priori
 537 model, to be treated as model parameters, and thus inferred as part of the
 538 inversion.

539 **Acknowledgement**

540 We thank DONG for financial support. Interfacing geostatistical algo-
 541 rithms has been done using the mGstat toolbox, <http://mgstat.sourceforge.net/>.
 542 SIPPI source code can be downloaded from <http://sippi.sourceforge.net/>.

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Figure 1: Histogram of 100000 unconditional realizations from a generalized Gaussian, GAUSSIAN type prior model with norm 60 and 2.

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