User's Manual
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Quantification of Uncertainty for Estimation, Simulation, and Optimization (QUESO)

Editors:
Kemelli C. Estacio-Hiroms
Ernesto E. Prudencio
Nicholas P. Malaya
Manav Vohra
Damon McDougall

Center for Predictive Engineering and Computational Sciences (PECOS)
Institute for Computational and Engineering Sciences (ICES)
The University of Texas at Austin
Austin, TX 78712, USA

Abstract

QUESO stands for Quantification of Uncertainty for Estimation, Simulation and Optimization and consists of a collection of algorithms and C++ classes intended for research in uncertainty quantification, including the solution of statistical inverse and statistical forward problems, the validation of mathematical models under uncertainty, and the prediction of quantities of interest from such models along with the quantification of their uncertainties.

QUESO is designed for flexibility, portability, easy of use and easy of extension. Its software design follows an object-oriented approach and its code is written on C++ and over MPI. It can run over uniprocessor or multiprocessor environments.

QUESO contains two forms of documentation: a user's manual available in PDF format and a lower-level code documentation available in web based/HTML format.

This is the user's manual: it gives an overview of the QUESO capabilities, provides procedures for software execution, and includes example studies.

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Preface

The QUESO project started in 2008 as part of the efforts of the recently established Center for Predictive Engineering and Computational Sciences (PECOS) at the Institute for Computational and Engineering Sciences (ICES) at The University of Texas at Austin.

The PECOS Center was selected by the National Nuclear Security Administration (NNSA) as one of its new five centers of excellence under the Predictive Science Academic Alliance Program (PSAAP). The goal of the PECOS Center is to advance predictive science and to develop the next generation of advanced computational methods and tools for the calculation of reliable predictions on the behavior of complex phenomena and systems (multiscale, multidisciplinary). This objective demands a systematic, comprehensive treatment of the calibration and validation of the mathematical models involved, as well as the quantification of the uncertainties inherent in such models. The advancement of predictive science is essential for the application of Computational Science to the solution of realistic problems of national interest.

The QUESO library is released as open source under Version 2.1 of the GNU Lesser General Public License and is available for free download world-wide. See https://www.gnu.org/licenses/lgpl-2.1.html for more information on the LGPLv2.1 software use agreement.

Contact Information:
Paul T. Bauman, Kemelli C. Estacio-Hiroms or Damon McDougall,
Institute for Computational and Engineering Sciences
1 University Station C0200
Austin, Texas 78712
email: pecos-dev@ices.utexas.edu
web: http://pecos.ices.utexas.edu

Referencing the QUESO Library

When referencing the QUESO library in a publication, please cite the following:

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  author    = "Ernesto Prudencio and Karl W. Schulz",
  title     = {The Parallel C++ Statistical Library 'QUESO':
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  series    = {Lecture Notes in Computer Science},
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   Author      = {Kemelli C. Estacio-Hiroms and Ernesto E. Prudencio},
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  Year   = {2008-2013}
}
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QUESO Development Team

The QUESO development team currently consists of Paul T. Bauman, Sai Hung Cheung, Kemelli C. Estacio-Hiroms, Nicholas Malaya, Damon McDougall, Kenji Miki, Todd A. Oliver, Ernesto E. Prudencio, Karl W. Schulz, Chris Simmons, and Rhys Ulerich.

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We would also like to thank James Martin, Roy Stogner and Lucas Wilcox for interesting discussions and constructive feedback.

Target Audience

QUESO is a collection of statistical algorithms and programming constructs supporting research into the uncertainty quantification (UQ) of models and their predictions. UQ may be a very complex and time consuming task, involving many steps: decide which physical model(s) to use; decide which reference or experimental data to use; decide which discrepancy models to use; decide which quantity(ies) of interest (QoI) to compute; decide which parameters to calibrate; perform computational runs and collect results; analyze computational results, and eventually reiterate; predict QoI(s) with uncertainty.

The purpose of this manual is not to teach UQ and its methods, but rather to introduce QUESO library so it can be used as a tool to assist and facilitate the uncertainty quantification of the user's application. Thus, the target audience of this manual is researchers who have solid background in Bayesian methods, are comfortable with UNIX concepts and the command line, and have knowledge of a programming language, preferably C/C++. Bellow we suggest some useful literature:

1. Probability, statistics, random variables [12, 13, 29];
2. Bayes' formula [5, 15, 31, 42];
3. Markov chain Monte Carlo (MCMC) methods [4, 17, 21, 22, 23, 33, 36, 39, 40];
4. Monte Carlo methods [43];
5. Kernel density estimation [46];
6. C++ [32, 37];
7. Message Passing Interface (MPI) [56, 54];
8. UNIX/Linux (installation of packages, compilation, linking);
9. MATLAB/GNU Octave (for dealing with output files generated by QUESO); and
10. UQ issues in general [10].

CHAPTER 1

Introduction

QUESO is a parallel object-oriented statistical library dedicated to the research of statistically robust, scalable, load balanced, and fault-tolerant mathematical algorithms for the quantification of uncertainty (UQ) of mathematical models and their predictions.

The purpose of this chapter is to introduce relevant terminology, mathematical and statistical concepts, statistical algorithms, together with an overall description of how the user's application may be linked with the QUESO library.

1.1 Preliminaries

Statistical inverse theory reformulates inverse problems as problems of statistical inference by means of Bayesian statistics: all quantities are modeled as random variables, and probability distribution of the quantities encapsulates the uncertainty observed in their values. The solution to the inverse problem is then the probability distribution of the quantity of interest when all information available has been incorporated in the model. This (posterior) distribution describes the degree of confidence about the quantity after the measurement has been performed [33].

Thus, the solution to the statistical inverse problem may be given by Bayes' formula, which express the posterior distribution as a function of the prior distribution and the data represented through the likelihood function.

The likelihood function has an open form and its evaluation is highly computationally expensive. Moreover, simulation-based posterior inference requires a large number of forward calculations to be performed, therefore fast and efficient sampling techniques are required for posterior inference.

It is often not straightforward to obtain explicit posterior point estimates of the solution, since it usually involves the evaluation of a high-dimensional integral with respect to a possibly non-smooth posterior distribution. In such cases, an alternative integration technique is the Markov chain Monte Carlo method: posterior means may be estimated using the sample mean from a series of random draws from the posterior distribution.

QUESO is designed in an abstract way so that it can be used by any computational model, as long as a likelihood function (in the case of statistical inverse problems) and a quantity of interest (QoI) function (in the case of statistical forward problems) is provided by the user application.

QUESO provides tools for both sampling algorithms for statistical inverse problems, following Bayes' formula, and statistical forward problems. It contains Monte Carlo solvers (for autocorrelation, kernel density estimation and accuracy assessment), MCMC (e.g. Metropolis Hastings [39, 23]) as well as the DRAM [21] (for sampling from probability distributions); it also has the capacity to handle many chains or sequences in parallel, each chain or sequence itself demanding many computing nodes because of the computational model being statistically explored [41].

1.2 Key Statistical Concepts

A computational model is a combination of a mathematical model and a discretization that enables the approximate solution of the mathematical model using computer algorithms and might be used in two different types of problems: forward or inverse.

Any computational model is composed of a vector $\boldsymbol{\theta}$ of n *parameters*, *state variables* $\mathbf{u}$, and *state equations* $\mathbf{r}(\boldsymbol{\theta}, \mathbf{u}) = \mathbf{0}$. Once the solution $\mathbf{u}$ is available, the computational model also includes extra functions for e.g. the calculation of *model output data* $\mathbf{y} = \mathbf{y}(\boldsymbol{\theta}, \mathbf{u})$, and the *prediction* of a vector $\mathbf{q} = \mathbf{q}(\boldsymbol{\theta}, \mathbf{u})$ of m quantities of interest (QoI),

Parameters designate all model variables that are neither state variables nor further quantities computed by the model, such as: material properties, coefficients, constitutive parameters, boundary conditions, initial conditions, external forces, parameters for modeling the model error, characteristics of an experimental apparatus (collection of devices and procedures), discretization choices and numerical algorithm options.

In the case of a forward problem, the parameters $\boldsymbol{\theta}$ are given and one then needs to compute $\mathbf{u}$, $\mathbf{y}$ and/or $\mathbf{q}$. In the case of an inverse problem, however, experimental data $\mathbf{d}$ is given and one then needs to *estimate* the values of the parameters $\boldsymbol{\theta}$ that cause $\mathbf{y}$ to best fit $\mathbf{d}$.

Figure 1.2.1 represents general inverse and forward problems respectively.

There are many possible sources of uncertainty on a computational model. First, $\mathbf{d}$ need not be equal to the actual values of observables because of errors in the measurement process. Second, the values of the input parameters to the phenomenon might not be precisely known. Third, the appropriate set of equations governing the phenomenon might not be well understood.

Computational models can be classified as either deterministic or stochastic – which are the ones of interest here. In deterministic models, all parameters are assigned numbers, and

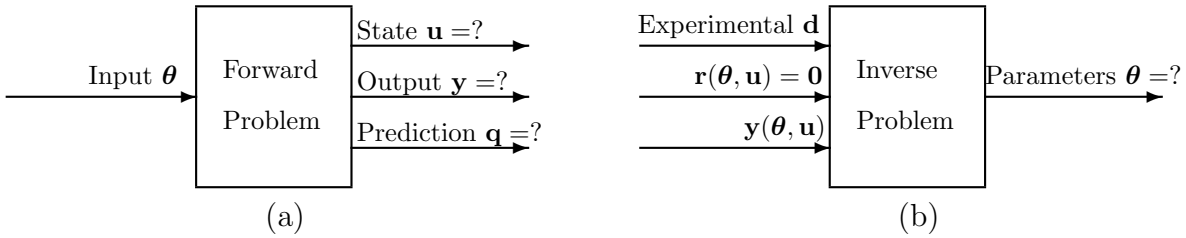


Figure 1.2.1: The representation of (a) a generic forward problem and (b) a generic inverse problem.

no parameter is related to the parametrization of a random variable (RV) or field. As a consequence, a deterministic model assigns a number to each of the components of quantities $\mathbf{u}$, $\mathbf{y}$ and $\mathbf{q}$. In stochastic models, however, at least one parameter is assigned a probability density function (PDF) or is related to the parametrization of a RV or field, causing $\mathbf{u}$, $\mathbf{y}$ and $\mathbf{q}$ to become random variables. Note that not all components of $\boldsymbol{\theta}$ need to be treated as random. As long as at least one component is random, $\boldsymbol{\theta}$ is a random vector, and the problem is stochastic.

In the case of forward problems, statistical forward problems can be represented very similarly to deterministic forward problems, as seen in Figure 1.2.2. In the case of inverse problems, as depicted in Figure 1.2.3, however, the conceptual connection between deterministic and statistical problems is not as straightforward.

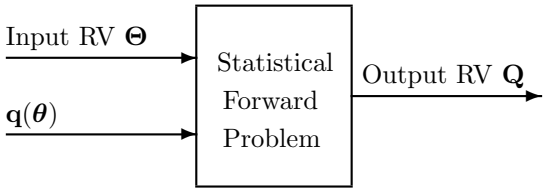


Figure 1.2.2: The representation of a statistical forward problem. $\boldsymbol{\Theta}$ denotes a random variable related to parameters, $\boldsymbol{\theta}$ denotes a realization of $\boldsymbol{\Theta}$ and $\mathbf{Q}$ denotes a random variable related to quantities of interest.

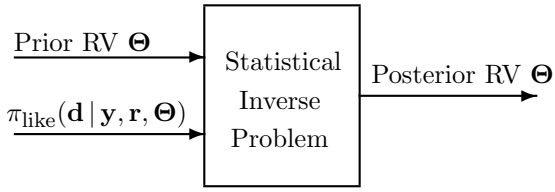


Figure 1.2.3: The representation of a statistical inverse problem. $\boldsymbol{\Theta}$ denotes a random variable related to parameters, $\boldsymbol{\theta}$ denotes a realization of $\boldsymbol{\Theta}$ and $\mathbf{r}$ denotes model equations, $\mathbf{y}$ denotes some model output data and $\mathbf{d}$ denotes experimental data.

QUESO adopts a Bayesian analysis [33, 42] for statistical inverse problems, interpreting

the posterior PDF

$$\pi_{\text{posterior}}(\boldsymbol{\theta}|\mathbf{d}) = \frac{\pi_{\text{prior}}(\boldsymbol{\theta})\pi_{\text{likelihood}}(\mathbf{d}|\boldsymbol{\theta})}{\pi(\mathbf{d})} \tag{1.2.1}$$

as the solution. Such solutions combine the prior information $\pi_{\text{prior}}(\boldsymbol{\theta})$ of the parameters, the information $\pi(\mathbf{d})$ on the data, and the likelihood $\pi_{\text{likelihood}}(\mathbf{d}|\boldsymbol{\theta})$ that the model computes certain data values with a given set of input parameters.

This semantic interpretation of achieving a posterior knowledge on the parameters (on the model) after combining some prior model knowledge with experimental information provides an important mechanism for dealing with uncertainty. Although mathematically simple, is not computationally trivial.

1.3 The Software Stack of an Application Using QUESO

An application using QUESO falls into three categories: a statistical inverse problem (IP), a statistical forward problem (FP), or combinations of both. In each problem the user might deal with up to five vectors of potentially very different sizes: parameters $\boldsymbol{\theta}$, state $\mathbf{u}$, output $\mathbf{y}$, data $\mathbf{d}$ and QoIs $\mathbf{q}$.

Algorithms in the QUESO library require the supply of a likelihood routine $\pi_{\text{like}} : \mathbb{R}^n \to \mathbb{R}_+$ for statistical inverse problems and of a QoI routine $\mathbf{q} : \mathbb{R}^n \to \mathbb{R}^m$ for statistical forward problems. These routines exist at the application level and provide the necessary bridge between the statistical algorithms in QUESO, model knowledge in the model library and scenario and experimental data in the disk space. Figure 1.3.1 shows the software stack of a typical application that uses QUESO. In the figure, the symbol $\boldsymbol{\theta}$ represents a vector of $n \geqslant 1$ parameters.

Even though QUESO deals directly with $\boldsymbol{\theta}$ and $\mathbf{q}$ only, it is usually the case the one of the other three vectors ($\mathbf{u}$, $\mathbf{y}$ and $\mathbf{d}$) will have the biggest number of components and will therefore dictate the size of the minimum parallel environment to be used in a problem. So, for example, even though one processor might be sufficient for handling $\boldsymbol{\theta}$, $\mathbf{y}$, $\mathbf{d}$ and $\mathbf{q}$, eight processors at least might be necessary to solve for $\mathbf{u}$. QUESO currently only requires that the amounts n and m can be handled by the memory available to one processor, which allows the analysis of problems with thousands of parameters and QoIs, a large amount even for state of the art UQ algorithms.

QUESO currently supports three modes of parallel execution: an application user may simultaneously run:

(a) multiple instances of a problem where the physical model requires a single processor, or

(b) multiple instances of a problem where the physical model requires multiple processors, or

(c) independent sets of types (a) and (b).

For example, suppose an user wants to use the Metropolis-Hastings (MH) algorithm to solve a statistical IP, and that 1,024 processors are available. If the physical model is simple

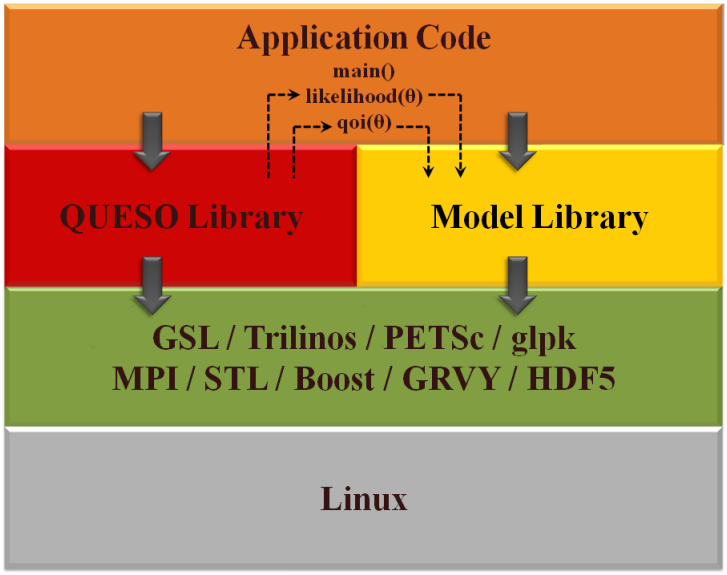


Figure 1.3.1: An application software stack. QUESO requires the input of a likelihood routine $\pi_{\text{like}} : \mathbb{R}^n \to \mathbb{R}_+$ for IPs and of a QoI routine $\mathbf{q} : \mathbb{R}^n \to \mathbb{R}^m$ for FPs. These application level routines provide the bridge between the statistical algorithms in QUESO, physics knowledge in the model library, and relevant experimental (calibration and validation) data.

enough to be handled efficiently by a single processor, then the user can run 1,024 chains simultaneously, as in case (a). If the model is more complex and requires, say, 16 processors, then the user can run 64 chains simultaneously, as in case (b), with 16 processors per chain. QUESO treats this situation by using only 1 of the 16 processors to handle the chain. When a likelihood evaluation is required, all 16 processors call the likelihood routine simultaneously. Once the likelihood returns its value, QUESO puts 15 processors into idle state until the routine is called again or the chain completes. Case (c) is useful, for instance, in the case of a computational procedure involving two models, where a group of processors can be split into two groups, each handling one model. Once the two-model analysis end, the combined model can use the full set of processors.[1]

1.4 Algorithms for solving Statistical Inverse Problems

The goal of inference is to characterize the posterior PDF, or to evaluate point or interval estimates based on the posterior [27]. Samples from posterior can be obtained using Markov chain Monte Carlo (MCMC) which require only pointwise evaluations of the unnormalized posterior. The resulting samples can then be used to either visually present the posterior or its marginals, or to construct sample estimates of posterior expectations. Examples of

[1]The parallel capabilities of QUESO have been exercised on the Ranger system of the TACC [2] with up to 16k processors.

MCMC are: the Metropolis-Hastings (MH) algorithm [39, 23], the Delayed Rejection (DR) algorithm [17, 40], and Adaptive Metropolis (AM) [22] which are combined together in the Delayed Rejection Adaptive Metropolis, DRAM, algorithm [21]. The DRAM is implemented in QUESO and available for the solution of SIP. MCMC methods are well-established and documented [4, 17, 21, 22, 23, 33, 36, 39, 40]; thus only brief description of the DRAM algorithm is presented in Section 1.4.1.

During model construction, errors arising from imperfect modeling and uncertainties due to incomplete information about the system and its environment always exist; thus, there has been a crescent interest in Bayesian model class updating and selection [9, 7, 8].

Model updating refers to the methodology that determines the most plausible model for a system, given a prior PDF. One stochastic method that handles model updating successfully is the multilevel method. Throughout the years, sereveral versions of the same method have been implemented as improvements of its predecessors [3, 9, 8]. QUESO hosts the novel Adaptive Multilevel Stochastic Simulation Algorithm (AMSSA) [8], which is described in Section 1.4.2. For details about the method, please refer to [8].

1.4.1 DRAM Algorithm

DRAM is a combination of two ideas for improving the efficiency of Metropolis-Hastings type Markov chain Monte Carlo (MCMC) algorithms, Delayed Rejection and Adaptive Metropolis [34].

Random walk Metropolis-Hasting algorithm with Gaussian proposal distribution is useful in simulating from the posterior distribution in many Bayesian data analysis situations. In order for the chain to be efficient, the proposal covariance must somehow be tuned to the shape and size of the target distribution. This is important in highly nonlinear situations, when there are correlation between the components of the posterior, or when the dimension of the parameter is high. The problem of adapting the proposal distribution using the chain simulated so far is that when the accepted values depend on the history of the chain, it is no longer Markovian and standard convergence results do not apply. One solution is to use adaptation only for the burn-in period and discard the part of the chain where adaptation has been used. In that respect, the adaptation can be thought as automatic burn-in. The idea of diminishing adaptation is that when adaptation works well, its effect gets smaller and we might be able to prove the ergodicity properties of the chain even when adaptation is used throughout the whole simulation. This is the ideology behind AM adaptation. On the other hand, the DR method allows the use of the the current rejected values without losing the Markovian property and thus allows to adapt locally to the current location of the target distribution.

In Adaptive Metropolis [22] the covariance matrix of the Gaussian proposal distribution is adapted on the fly using the past chain. This adaptation destroys the Markovian property of the chain, however, it can be shown that the ergodicity properties of the generated sample remain. How well this works on finite samples and on high dimension is not obvious and must be verified by simulations.

Starting from initial covariance $C^{(0)}$, the target covariance is updated at given intervals from the chain generated so far.

$$C^{(i)} = s_d \, cov(\text{chain}_1 : \text{chain}_i) + s_d \varepsilon I_d,$$

the small number ε prevents the sample covariance matrix from becoming singular. For the scaling factor, the value $s_d = 2.4^2/d$ is standard optimal choice for Gaussian targets, d being the dimension of the target [15]. A standard updating formula for the sample covariance matrix can be used, so that the whole chain does not need to reside in the computer memory.

With the Delayed rejection method [40], it becomes possible to make use of several tries after rejecting a value by using different proposals while keep the reversibility of the chain. Delayed rejection method (DR) works in the following way. Upon rejection a proposed candidate point, instead of advancing time and retaining the same position, a second stage move is proposed. The acceptance probability of the second stage candidate is computed so that reversibility of the Markov chain relative to the distribution of interest is preserved. The process of delaying rejection can be iterated for a fixed or random number of stages, let's say n_{stages}. The higher stage proposals are allowed to depend on the candidates so far proposed and rejected. Thus DR allows partial local adaptation of the proposal within each time step of the Markov chain still retaining the Markovian property and reversibility.

The first stage acceptance probability in DR is the standard MH acceptance and it can be written as

$$\alpha_1(\mathbf{a}, \mathbf{x}^{(1)}) = \min \left\{ 1, \frac{\pi(\mathbf{x}^{(1)})}{\pi(\mathbf{a})} \cdot \frac{q_1(\mathbf{x}^{(1)}, \mathbf{a})}{q_1(\mathbf{a}, \mathbf{x}^{(1)})} \right\},$$

Here $\mathbf{a}$ is the current point, $\mathbf{x}^{(1)}$ is the proposed new value drawn from the distribution $q_1(\mathbf{a}, \cdot)$, and π is the target distribution. If $\mathbf{x}^{(1)}$ is rejected, a second candidate $\mathbf{x}^{(2)}$ is drawn from $q_2(\mathbf{a}, \mathbf{x}^{(1)}, \cdot)$ using the acceptance probability

$$\alpha_2(\mathbf{a}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) = \min \left\{ 1, \frac{\pi(\mathbf{x}^{(2)}) q_1(\mathbf{x}^{(2)}, \mathbf{x}^{(1)}) q_2(\mathbf{x}^{(2)}, \mathbf{x}^{(1)}, \mathbf{a}) [1 - \alpha_1(\mathbf{x}^{(2)}, \mathbf{x}^{(1)})]}{\pi(\mathbf{a}) q_1(\mathbf{a}, \mathbf{x}^{(1)}) q_2(\mathbf{a}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}) [1 - \alpha_1(\mathbf{a}, \mathbf{x}^{(1)})]} \right\}$$

i.e., it depends not only on the current position of the chain but also on what we have just proposed and rejected.

As the reversibility property is preserved, this method also leads to the same stationary distribution π as the standard MH algorithm. The procedure can be iterated further for higher-stage proposals. The Gaussian proposal at each stage i is defined as:

$$q_i(\underbrace{\mathbf{a}, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(i-1)}}_{i \text{ terms}}, \mathbf{z}) = e^{-\frac{1}{2}\{[\mathbf{z}-\mathbf{a}]^T \cdot [\mathbf{C}]^{-1} \cdot [\mathbf{z}-\mathbf{a}]\}} \tag{1.4.1}$$

where the covariance matrix $\mathbf{C}$ and the scalings for the higher-stage proposal covariances $1 = \gamma_1 \leqslant \gamma_2 \leqslant \ldots \leqslant \gamma_{n_{\text{stages}}}$ are given.

If q_i denotes the proposal at the i-th stage, the acceptance probability at that stage is:

$$\alpha_i(\mathbf{a}, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(i)}) = \min \left\{ 1, \frac{\pi(\mathbf{x}^{(i)})}{\pi(\mathbf{a})} \cdot q_{\text{fraction}} \cdot \alpha_{\text{fraction}} \right\}. \tag{1.4.2}$$

where the expressions q_{fraction} and α_{fraction} are given by

$$q_{\text{fraction}} = \frac{q_1(\mathbf{x}^{(i)}, \mathbf{x}^{(i-1)})}{q_1(\mathbf{a}, \mathbf{x}^{(1)})} \frac{q_2(\mathbf{x}^{(i)}, \mathbf{x}^{(i-1)}, \mathbf{x}^{(i-2)})}{q_2(\mathbf{a}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)})} \cdots \frac{q_i(\mathbf{x}^{(i)}, \mathbf{x}^{(i-1)}, \ldots, \mathbf{x}^{(1)}, \mathbf{a})}{q_i(\mathbf{a}, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(i-1)}, \mathbf{x}^{(i)})}$$

and

$$\alpha_{\text{fraction}} = \frac{[1 - \alpha_1(\mathbf{x}^{(i)}, \mathbf{x}^{(i-1)})]}{[1 - \alpha_1(\mathbf{a}, \mathbf{x}^{(1)})]} \frac{[1 - \alpha_2(\mathbf{x}^{(i)}, \mathbf{x}^{(i-1)}, \mathbf{x}^{(i-2)})]}{[1 - \alpha_2(\mathbf{a}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)})]} \cdots \frac{[1 - \alpha_{i-1}(\mathbf{x}^{(i)}, \mathbf{x}^{(i-1)}, \ldots, \mathbf{x}^{(1)})]}{[1 - \alpha_{i-1}(\mathbf{a}, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(i-1)})]}.$$

Since all acceptance probabilities are computed so that reversibility with respect to π is preserved separately at each stage, the process of delaying rejection can be interrupted at any stage that is, we can, in advance, decide to try at most, say, 3 times to move away from the current position, otherwise we let the chain stay where it is. Alternatively, upon each rejection, we can toss a p-coin (i.e., a coin with head probability equal to p), and if the outcome is head we move to a higher stage proposal, otherwise we stay put [21].

The smaller overall rejection rate of DR guarantees smaller asymptotic variance of the estimates based on the chain. The DR chain can be shown to be asymptotically more efficient that MH chain in the sense of Peskun ordering (Mira, 2001a).

Haario, et al. 2006 [21] combine AM and DR into a method called DRAM, in what they claim to be a straightforward possibility amongst the possible different implementations of the idea, and which is described in this section.

In order to be able to adapt the proposal, all you need some accepted points to start with.

One "master" proposal is tried first – i.e., the proposal at the first stage of DR is adapted just as in AM: the covariance $C^{(1)}$ is computed from the points of the sampled chain, no matter at which stage these points have been accepted in the sample path. After rejection, a try with modified version of the first proposal is done according to DR. A second proposal can be one with a smaller covariance, or with different orientation of the principal axes. The most common choice is to always compute the covariance $C^{(i)}$ of the proposal for the i-th stage ($i = 2, \ldots, n_{\text{stages}}$) simply as a scaled version of the proposal of the first stage,

$$C^{(i)} = \gamma_i C^{(1)}$$

where the scale factors γ_i can be somewhat freely chosen. Then, the master proposal is adapted using the chain generated so far, and the second stage proposal follows the adaptation in obvious manner.

The requirements for the DRAM algorithm are:

- Number $n_{\text{pos}} \geqslant 2$ of positions in the chain;
- Initial guess $\mathbf{m}^{(0)}$;
- Number of stages for the DR method: $n_{\text{stages}} \geqslant 1$;

- For $1 \leqslant i \leqslant n_{\text{stages}}$, functions $q_i : \underbrace{\mathbb{R}^N \times \ldots \times \mathbb{R}^N}_{(i+1) \text{ times}} \to \mathbb{R}_+$, such that $q_i(\mathbf{a}, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(i-1)}, \cdot)$ is a PDF for any $(\mathbf{a}, \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(i-1)}) \in \underbrace{\mathbb{R}^N \times \ldots \times \mathbb{R}^N}_{i \text{ times}}$; i.e., choose q_i as in Equation (1.4.1);
- Recursively define $\alpha_i : \underbrace{\mathbb{R}^n \times \ldots \times \mathbb{R}^n}_{(i+1) \text{ times}} \to [0,1], \quad 1 \leqslant i \leqslant n_{\text{stages}}$ according to Equation (1.4.2).

Recalling that a sample is defined as:

$$\text{a sample } = \mathbf{a} + \mathbf{C}^{1/2}\mathcal{N}(0, I).$$

a simple, but useful, implementation of DRAM is described in Algorithm 1.

There are six variables in the QUESO input file used to set available options for the DRAM algorithm, which are described in 3.3.4. Here, they are presented presented bellow together with their respective definition in Algorithm 1.

`ip_mh_dr_maxNumExtraStages:` defines how many extra stages should be considered in the DR loop (n_{stages});

`ip_mh_dr_listOfScalesForExtraStages:` defines the list s of scaling factors that will multiply the covariance matrix (values of γ_i);

`ip_mh_am_adaptInterval:` defines whether or not there will be a period of adaptation;

`ip_mh_am_initialNonAdaptInterval:` defines the initial interval where the proposal covariance matrix will not be changed (n_0);

`ip_mh_am_eta:` is a factor used to scale the proposal covariance matrix, usually set to be $2.4^2/d$, where d is the dimension of the problem [36, 21] (s_d);

`ip_mh_am_epsilon:` is the covariance regularization factor (ε).

1.4.2 Adaptive Multilevel Stochastic Simulation Algorithm

In this section we rewrite the Bayesian formula (1.2.1) by making explicit all the implicit model assumptions. Such explication demands the use of probability logic and the concept of a stochastic system model class (model class for short); as these concepts enable the comparison of competing model classes.

Let M_j be one model class; the choice of $\boldsymbol{\theta}$ specifies a particular predictive model in M_j, and, for brevity, we do not explicitly write $\boldsymbol{\theta}_j$ to indicate that the parameters of different model classes may be different, but this should be understood. Based on M_j, one can use data D to compute the updated relative plausibility of each predictive model in the set defined by M_j. This relative plausibility is quantified by the *posterior* PDF $\pi(\boldsymbol{\theta}|\mathbf{D}, M_j)$.

Algorithm 1 DRAM algorithm [36].

Input: Number of positions in the chain $n_{\text{pos}} \geqslant 2$; initial guess $\mathbf{m}^{(0)}$; initial first stage proposal covariance $C^{(0)}$; $n_{\text{stages}} \geqslant 1$; and functions $q_i : \underbrace{\mathbb{R}^N \times \ldots \times \mathbb{R}^N}_{(i+1) \text{ times}} \to \mathbb{R}_+$

Select s_d ; // scaling factor
Select ε ; // covariance regularization factor
Select n_0 ; // initial non-adaptation period
for $i \leftarrow 1$ **to** n_{stages} **do** // n_{stages} is the number of tries allowed
  Select γ_i ; // scalings for the higher-stage proposal covariances
end
repeat
  Set $ACCEPT \leftarrow false$ Set $i \leftarrow 1$
  // After an initial period of simulation, adapt the master proposal (target) covariance using the chain generated so far:
  if $k \geqslant n_0$ **then**
    $C^{(1)} = s_d Cov(\mathbf{m}^{(0)}, \ldots, \mathbf{m}^{(k-1)}) + s_d \varepsilon I_d$
  end
  // n_{stages}-DR loop:
  repeat
    Generate candidate $\mathbf{c}^{(i)} \in \mathbb{R}^N$ by sampling $q_i(\mathbf{m}^{(k)}, \mathbf{c}^{(1)}, \ldots, \mathbf{c}^{(i-1)}, \cdot)$; // q_i is the proposal probability density
    if $\mathbf{c}^{(i)} \notin supp(\pi)$ **then**
      $i \leftarrow i + 1$
    end
    if $\mathbf{c}^{(i)} \in supp(\pi)$ **then**
      Compute $\alpha_i(\mathbf{m}^{(k)}, \mathbf{c}^{(1)}, \ldots, \mathbf{c}^{(i-1)}, \mathbf{c}^{(i)})$; // acceptance probability
      Generate a sample $\tau \sim \mathcal{U}((0, 1])$
      if $(\alpha_i < \tau)$ **then** $i \leftarrow i + 1$;
      if $(\alpha_i \geqslant \tau)$ **then** ACCEPT$\leftarrow$true;
    end
    $C^{(i)} = \gamma_i C^{(1)}$; // Calculate the higher-stage proposal as scaled versions of $C^{(1)}$, according to the chosen rule
  until *(ACCEPT=false) and* $(i \leqslant n_{stages})$;
  if *(ACCEPT=true)* **then**
    Set $\mathbf{m}^{(k+1)} \leftarrow \mathbf{c}^{(i)}$
  end
  if *(ACCEPT=false)* **then**
    Set $\mathbf{m}^{(k+1)} \leftarrow \mathbf{m}^{(k)}$
  end
  Set $k \leftarrow k + 1$
until $(k + 1 < n_{pos})$;

Bayes theorem allows the update of the probability of each predictive model M_j by combining measured data D with the prior PDF into the posterior PDF:

$$\begin{aligned}\pi_{\text{posterior}}(\boldsymbol{\theta}|\mathbf{D}, M_j) &= \frac{f(\mathbf{D}|\boldsymbol{\theta}, M_j) \cdot \pi_{\text{prior}}(\boldsymbol{\theta}|M_j)}{\pi(\mathbf{D}, M_j)} \\ &= \frac{f(\mathbf{D}|\boldsymbol{\theta}, M_j) \cdot \pi_{\text{prior}}(\boldsymbol{\theta}|M_j)}{\int f(\mathbf{D}|\boldsymbol{\theta}, M_j) \cdot \pi_{\text{prior}}(\boldsymbol{\theta}|M_j)\, d\boldsymbol{\theta}}\end{aligned} \tag{1.4.3}$$

where the denominator expresses the probability of getting the data $\mathbf{D}$ based on M_j and is called the evidence for M_j provided by $\mathbf{D}$; $\pi_{\text{prior}}(\boldsymbol{\theta}|M_j)$ is the prior PDF of the predictive model $\boldsymbol{\theta}$ within M_j; and the likelihood function $f(\mathbf{D}|\boldsymbol{\theta}, M_j)$ expresses the probability of getting $\mathbf{D}$ given the predictive model $\boldsymbol{\theta}$ within M_j – and this allows stochastic models inside a model class M_j to be compared.

When generating samples of posterior PDF $\pi_{\text{posterior}}(\boldsymbol{\theta}|D, M_j)$ in order to forward propagate uncertainty and compute QoI RV's, it is important to take into account potential multiple modes in the posterior. One simple idea is to sample increasingly difficult intermediate distributions, accumulating "knowledge" from one intermediate distribution to the next, until the target posterior distribution is sampled. In [8], an advanced stochastic simulation method, referred to as Adaptive Multi Level Algorithms, is proposed which can generate posterior samples from $\pi_{\text{posterior}}(\boldsymbol{\theta}|\mathbf{D}, M_j)$ and compute the log of the evidence $p(\mathbf{D}|\boldsymbol{\theta}, M_j)$ at the same time by adaptively moving samples from the prior to the posterior through an adaptively selected sequence of intermediate distributions [7].

Specifically, the intermediate distributions are given by:

$$\pi_{\text{int}}^{(\ell)}(\boldsymbol{\theta}|\mathbf{D}) = f(\boldsymbol{\theta}|\mathbf{D}, M_j)^{\tau_\ell} \cdot \pi_{\text{prior}}(\boldsymbol{\theta}|M_j), \quad \ell = 0, 1, \ldots, L, \tag{1.4.4}$$

for a given $L > 0$ and a given sequence $0 = \tau_0 < \tau_1 < \ldots < \tau_L = 1$ of exponents.

In order to compute the model evidence $\pi(\mathbf{D}|M_j)$ where:

$$\pi(\mathbf{D}|M_j) = \int f(\boldsymbol{\theta}|\mathbf{D}, M_j) \cdot \pi_{\text{prior}}(\boldsymbol{\theta}|M_j)\, d\boldsymbol{\theta}, \tag{1.4.5}$$

the use of intermediate distribution is also beneficial. For that, recall that

$$\begin{aligned}\pi(\mathbf{D}|M_j) &= \int f(\boldsymbol{\theta})\pi(\boldsymbol{\theta})\, d\boldsymbol{\theta} \\ &= \int f\ \pi\, d\boldsymbol{\theta} \\ &= \int f^{1-\tau_{L-1}} f^{\tau_{L-1}-\tau_{L-2}} \ldots f^{\tau_2-\tau_1} f^{\tau_1}\ \pi\, d\boldsymbol{\theta} \\ &= c_1 \int f^{1-\tau_{L-1}} f^{\tau_{L-1}-\tau_{L-2}} \ldots f^{\tau_2-\tau_1} \frac{f^{\tau_1}\ \pi}{c_1}\, d\boldsymbol{\theta} \\ &= c_2 c_1 \int f^{1-\tau_{L-1}} f^{\tau_{L-1}-\tau_{L-2}} \ldots \frac{f^{\tau_2-\tau_1} f^{\tau_1}\ \pi}{c_2 c_1}\, d\boldsymbol{\theta} \\ &= c_L c_{L-1} \cdots c_2 c_1.\end{aligned} \tag{1.4.6}$$

Assuming that the prior PDF is normalized (it integrates to one) and if τ_ℓ is small enough, then Monte Carlo method can be efficiently applied to calculate c_ℓ in Equation (1.4.6). Due to numerical (in)stability, it is more appropriate to calculate the estimators:

$$\tilde{c}_i = \ln c_i, \quad i = 1, \ldots, L. \tag{1.4.7}$$

Combining Equations (1.4.6) and (1.4.7), we have:

$$\ln[\pi(\mathbf{D}|M_j)] = \tilde{c}_L + \tilde{c}_{L-1} + \ldots + \tilde{c}_2 + \tilde{c}_1.$$

Computing the log of the evidence instead of calculating the evidence directly is attractive because the evidence is often too large or too small relative to the computer precision. The posterior probability can be calculated readily in terms of the log evidence, allowing overflow and underflow errors to be avoided automatically [7].

Now let's define some auxiliary variables for $k = 1, \ldots, n_{\text{total}}^{(\ell)}$:

- k-th sample at the ℓ-th level:

$$\boldsymbol{\theta}^{(\ell)[k]}, \quad \ell = 0, 1, \ldots, L \tag{1.4.8}$$

- Plausibility weight:

$$\begin{aligned} w^{(\ell)[k]} &= \frac{f(\boldsymbol{\theta}^{(\ell)[k]}|\mathbf{D}, M_j)^{\tau_\ell} \cdot \pi_{\text{prior}}(\boldsymbol{\theta}^{(\ell)[k]}, M_j)}{f(\boldsymbol{\theta}^{(\ell)[k]}|\mathbf{D}, M_j)^{\tau_{\ell-1}} \cdot \pi_{\text{prior}}(\boldsymbol{\theta}^{(\ell)[k]}, M_j)} = \frac{f^{(\tau_\ell)}(\mathbf{D}|\boldsymbol{\theta}^{(\ell)[k]}, M_j)}{f^{(\tau_{\ell-1})}(\mathbf{D}|\boldsymbol{\theta}^{(\ell)[k]}, M_j)}, \\ &= f^{(\tau_\ell - \tau_{\ell-1})}(\mathbf{D}|\boldsymbol{\theta}^{(\ell)[k]}, M_j), \quad \ell = 0, 1, \ldots, L \end{aligned} \tag{1.4.9}$$

- Normalized plausibility weight:

$$\tilde{w}^{(\ell)[k]} = \frac{w^{(\ell)[k]}}{\sum_{s=1}^{n_{\text{total}}^{(\ell)}} w^{(\ell)[s]}}, \quad \ell = 0, 1, \ldots, L \tag{1.4.10}$$

- Effective sample size:

$$n_{\text{eff}}^{(\ell)} = \frac{1}{\sum_{s=1}^{n_{\text{total}}^{(\ell)}} \left(\tilde{w}^{(\ell)[s]}\right)^2} \tag{1.4.11}$$

- Estimate for the sample covariance matrix for $\pi_{\text{int}}^{(\ell)}$:

$$\Sigma = \sum_{m=1}^{n_{\text{total}}^{(\ell-1)}} \tilde{w}_m (\boldsymbol{\theta}^{(\ell-1)[m]} - \overline{\boldsymbol{\theta}})(\boldsymbol{\theta}^{(\ell-1)[m]} - \overline{\boldsymbol{\theta}})^t, \quad \text{where} \quad \overline{\boldsymbol{\theta}} = \sum_{m=1}^{n_{\text{total}}^{(\ell-1)}} \tilde{w}_m \boldsymbol{\theta}^{(\ell-1)[m]} \tag{1.4.12}$$

so we can define the discrete distribution:

$$P^{(\ell)}(k) = \tilde{w}^{(\ell)[k]}, \quad k = 1, 2, \ldots, n_{\text{total}}^{(\ell)}. \tag{1.4.13}$$

The ML algorithm consists of a series of resampling stages, with each stage doing the following: given $n_{\text{total}}^{(\ell)}$ samples from $\pi_{\text{int}}^{(\ell)}(\boldsymbol{\theta}|\mathbf{D})$, denoted by $\boldsymbol{\theta}^{(\ell)[k]}, k = 1...n_{\text{total}}^{(\ell)}$ obtain samples from $\pi_{\text{int}}^{(\ell+1)}(\boldsymbol{\theta}|\mathbf{D})$, denoted by $\boldsymbol{\theta}^{(\ell+1)[k]}, k = 1...n_{\text{total}}^{(\ell+1)}$.

This is accomplished by: given the samples $\boldsymbol{\theta}^{(\ell)[k]}, k = 1...n_{\text{total}}^{(\ell)}$, in Equation (1.4.8), from $\pi_{\text{int}}^{(\ell)}(\boldsymbol{\theta}|\mathbf{D})$, we compute the plausibility weights $w^{(\ell)[k]}$ given in Equation (1.4.9) with respect to $\pi_{\text{int}}^{(\ell+1)}(\boldsymbol{\theta}|\mathbf{D})$. Then we re-sample the uncertain parameters according to the normalized weights $\tilde{w}^{(\ell)[k]}$, given in Equation (1.4.10), through the distribution in Equation (1.4.13). This is possible due to the fact that for large $n_{\text{total}}^{(\ell)}$ and $n_{\text{total}}^{(\ell+1)}$, then $\boldsymbol{\theta}^{(\ell+1)[k]}, k = 1...n_{\text{total}}^{(\ell+1)}$ will be distributed as $\pi_{\text{int}}^{(\ell+1)}(\boldsymbol{\theta}|\mathbf{D})$ [9].

The choice of $\tau_\ell, \ell = 1, \ldots, L-1$ is essential. It is desirable to increase the τ values slowly so that the transition between adjacent PDFs is smooth, but if the increase of the τ values is too slow, the required number of intermediate stages (L value) will be too large [9]. More intermediate stages mean more computational cost. In the ML method proposed by [8] and implemented in QUESO, τ_ℓ is computed through a bissection method so that:

$$\beta_{\text{min}}^{(\ell)} < \frac{n_{\text{eff}}^{(\ell)}}{n_{\text{total}}^{(\ell)}} < \beta_{\text{max}}^{(\ell)} \tag{1.4.14}$$

1.4.2.1 AMSSA Algorithm

Based on the above results, and recalling that the series of intermediate PDFs, $\pi_{\text{int}}^{(\ell)}(\boldsymbol{\theta}|\mathbf{D})$, start from the prior PDF and ends with the posterior PDF, Algorithm 2 can be applied both to draw samples from the posterior PDF, $\pi_{\text{posterior}}(\boldsymbol{\theta}|\mathbf{D}, M_j)$, and to estimate the evidence $\pi(\mathbf{D}, M_j)$.

Steps 43 and 44 in Algorithm 2 are accomplished by sampling the distribution in Equation (1.4.13) a total of $n_{\text{total}}^{(\ell)}$ times. The selected indices k determine the samples $\boldsymbol{\theta}^{(\ell)[k]}$ to be used as initial positions, and the number of times an index k is selected determines the size of the chain beginning at $\boldsymbol{\theta}^{(\ell)[k]}$.

At each level ℓ, many computing nodes can be used to sample the parameter space collectively. Beginning with $\ell = 0$, the computing nodes: (a) sample $\pi_{\text{int}}^{(\ell)}(\boldsymbol{\theta}|\boldsymbol{D}, M_j)$; (b) select some of the generated samples ("knowledge") to serve as initial positions of Markov chains for the next distribution $\pi_{\text{int}}^{(\ell+1)}(\boldsymbol{\theta}|\boldsymbol{D}, M_j)$; and (c) generate the Markov chains for $\pi_{\text{int}}^{(\ell+1)}(\boldsymbol{\theta}|\boldsymbol{D}, M_j)$.

The process (a)–(b)–(c) continues until the final posterior distribution is sampled. As ℓ increases, the selection process tends to value samples that are located in the regions of high probability content, which gradually "appear"as τ_ℓ increases. So, as ℓ increases, if the "good" samples selected from the ℓ-th level to the (ℓ+1)-th level are not redistributed among computing nodes before the Markov chains for the (ℓ+1)-th level are generated, the "lucky" computing nodes (that is, the ones that had, already at the initial levels, samples in the

Algorithm 2 Detailed description of the Adaptive Multilevel Stochastic Simulation Algorithm proposed by [8].

Input: for each $\ell = 0, \ldots, L$: the total amount of samples to be generated at ℓ-th level ($n^{(\ell)}_{\text{total}} > 0$) and the thresholds ($0 < \beta^{(\ell)}_{\text{min}} < \beta^{(\ell)}_{\text{max}} < 1$) on the effective sample size of the ℓ-th level

Output: $\boldsymbol{\theta}^{(m)[k]}, k = 1, \ldots, n^{(m)}_{\text{total}}$; which are asymptotically distributed as $\pi_{\text{posterior}}(\boldsymbol{\theta}|\mathbf{D}, M_j)$

Output: $\prod_\ell c_\ell$; which is asymptotically unbiased for $\pi(\mathbf{D}, M_j)$

33 Set $\ell = 0$

34 Set $\tau_\ell = 0$

35 Sample prior distribution, $\pi_{\text{prior}}(\boldsymbol{\theta}|M_j)$, $n^{(0)}_{\text{total}}$ times ; `// i.e, obtain` $\boldsymbol{\theta}^{(0)[k]}, k = 1, \ldots, n^{(0)}_{\texttt{total}}$

36 **while** $\tau_\ell < 1$ **do**

`/* At the beginning of the` ℓ`-th level, we have the samples` $\boldsymbol{\theta}^{(\ell-1)[k]}, k = 1 \ldots n^{(\ell-1)}_{\texttt{total}}$ `from` $\pi^{(\ell-1)}_{\texttt{int}}(\boldsymbol{\theta}|\mathbf{D})$`, Equation (1.4.4). */`

37 Set $\ell \leftarrow \ell + 1$; `// begin next level`

38 Compute plausibility weights $w^{(\ell)[k]}$ via Equation (1.4.9) Compute normalized weights $\tilde{w}^{(\ell)[k]}$ via Equation (1.4.10) Compute $n^{(\ell)}_{\text{eff}}$ via Equation (1.4.11)

39 Compute τ_ℓ so that Equation (1.4.14) is satisfied **if** $\tau_\ell > 1$ **then**

40 $\tau_\ell \leftarrow 1$ Recompute $w^{(\ell)[k]}$ and $\tilde{w}^{(\ell)[k]}$

41 **end**

42 Compute an estimate for the sample covariance matrix for $\pi^{(\ell)}_{\text{int}}$ via Equation (1.4.12)

43 Select, from previous level, the initial positions for the Markov chains

44 Compute sizes of the chains ; `// the sum of the sizes` $= n^{(\ell)}_{\texttt{total}}$

45 Redistribute chain initial positions among processors

`/* Then the` $n^{(\ell)}_{\texttt{total}}$ `samples` $\boldsymbol{\theta}^{(\ell)[k]}$`, from` $\pi^{(\ell)}_{\texttt{int}}(\boldsymbol{\theta})$ `are generated by doing the following for` $k = 1, \ldots, n^{(\ell)}_{\texttt{total}}$`: */`

46 Generate chains: draw a number k' from a discrete distribution $P^{(\ell)}(k)$ in Equation (1.4.13) via Metropolis-Hastings ; `// i.e., obtain` $\boldsymbol{\theta}^{(\ell)[k]} = P^{(l)[k]}$

47 Compute $c_\ell = \frac{1}{n^{(\ell-1)}_{\text{total}}} \left(\sum_{s=1}^{n^{(\ell-1)}_{\text{total}}} w_s \right)$; `// recall that` $\pi(\mathbf{D}|M_j) = \prod_\ell c_\ell$`, Equation (1.4.5)`

48 **end**

final posterior regions of high probability content) will tend to accumulate increasingly more samples in the next levels. This possible issue is avoided maintaining a balanced computational load among all computing nodes, which is handled in the ML by the step in Line 45.

Running the step in Line 45 of Algorithm 2 is then equivalent of solving the following problem: given the number of processors N_p, the total number of runs n_{total} and the number of runs n_j (to be) handled by the j-th processor; distribute N_t tasks among the N_p processors so that each processor gets its total number n_j of program runs, $j = 1, \ldots, N_p$, the closest

possible to the mean $\bar{n} = n_{\text{total}}/N_p$. This parallel implementation of the algorithm is proposed in [8], and it has been implemented in QUESO by the same authors/researchers.

1.5 Algorithms for solving the Statistical Forward Problem

The Monte Carlo method is commonly used for analyzing uncertainty propagation, where the goal is to determine how random variation, lack of knowledge, or error affects the sensitivity, performance, or reliability of the system that is being modeled [43].

Monte Carlo works by using random numbers to sample, according to a PDF, the 'solution space' of the problem to be solved. Then, it iteratively evaluates a deterministic model using such sets of random numbers as inputs.

Suppose we wish to generate random numbers distributed according to a positive definite function in one dimension $P(x)$. The function need not be normalized for the algorithm to work, and the same algorithm works just as easily in a many dimensional space. The random number sequence x_i, $i = 0, 1, 2, \ldots$ is generated by a random walk as follows:

1. Choose a starting point x_0
2. Choose a fixed maximum step size δ.
3. Given a x_i, generate the next random number as follows:
   (a) Choose x_{trial} uniformly and randomly in the interval $[x_i - \delta, x_i + \delta]$.
   (b) Compute the ratio $w = \dfrac{P(x_{\text{trial}})}{P(x_i)}$.
   Note that P need not be normalized to compute this ratio.
   (c) If $w > 1$ the trial step is in the right direction, i.e., towards a region of higher probability.
   Accept the step $x_{i+1} = x_{\text{trial}}$.
   (d) If $w < 1$ the trial step is in the wrong direction, i.e., towards a region of lower probability. We should not unconditionally reject this step! So accept the step conditionally if the decrease in probability is smaller than a random amount:
      i. Generate a random number r in the interval $[0, 1]$.
      ii. If $r < w$ accept the trial step $x_{i+1} = x_{\text{trial}}$.
      iii. If $w \leq r$ reject the step $x_{i+1} = x_i$. Note that we don't discard this step! The two steps have the same value.

There are essentially two important choices to be made. First, the initial point x_0 must be chosen carefully. A good choice is close to the maximum of the desired probability distribution. If this maximum is not known (as is usually the case in multi-dimensional problems), then the random walker must be allowed to thermalize i.e., to find a good starting configuration: the

algorithm is run for some large number of steps which are then discarded. Second, the step size must be carefully chosen. If it is too small, then most of the trial steps will be accepted, which will tend to give a uniform distribution that converges very slowly to $P(x)$. If it is too large the random walker will step right over and may not ' 'see" important peaks in the probability distribution. If the walker is at a peak, too many steps will be rejected. A rough criterion for choosing the step size is for the

$$\text{Acceptance ratio} = \frac{\text{Number of steps accepted}}{\text{Total number of trial steps}}$$

to be around 0.5.

An implementation of Monte Carlo algorithm is described in Algorithm 3.

Algorithm 3 Detailed description of the Monte Carlo Algorithm proposed by [39].

Input: Starting point x_0, step size δ, number of trials M, number of steps per trial N, unnormalized density or probability function $P(x)$ for the target distribution.

Output: Random number sequence x_i, $i = 0, 1, 2, \ldots$

```
for i = 0...M do
    for j = 0...N do
        Set x_trial ← x_i + (2 RAND([0,1]) − 1)δ  Set w = P(x_trial)/P(x)  Set accepts ← 0
        if w ≥ 1 then // uphill
            x_{i+1} ← x_trial ;                                   // accept the step
            accepts ← accepts+1
        else // downhill
            Set r ← RAND([0,1])  if r < w then // but not too far
                x_{i+1} ← x_trial ;                               // accept the step
                accepts ← accepts+1
            end
        end
    end
end
```

Monte Carlo is implemented in QUESO and it is the chosen algorithm to compute a sample of the output RV (the QoI) of the SFP for each given sample of the input RV.

CHAPTER 2

Installation

This chapter covers the basic steps that a user will need follow when beginning to use QUESO: how to obtain, configure, compile, build, install, and test the library. It also presents both QUESO source and installed directory structure, some simple examples and finally, introduces the user on how to use QUESO together with the user's application.

This manual is current at the time of printing; however, QUESO library is under active development. For the most up-to-date, accurate and complete information, please visit the online QUESO Home Page[1].

2.1 Getting started

In operating systems which have the concept of a superuser, it is generally recommended that most application work be done using an ordinary account which does not have the ability to make system-wide changes (and eventually break the system via (ab)use of superuser privileges).

Thus, suppose you want to install QUESO and its dependencies on the following directory:

```
$HOME/LIBRARIES/
```

so that you will not need superuser access rights. The directory above is referred to as the QUESO installation directory (tree).

There are two main steps to prepare your LINUX computing system for QUESO library: obtain and install QUESO dependencies, and define a number of environmental variables.

[1] https://github.com/libqueso

These steps are discussed bellow.

2.1.1 Obtain and Install QUESO Dependencies

QUESO interfaces to a number of high-quality software packages to provide certain functionalities. While some of them are required for the successful installation of QUESO, other may be used for enhancing its performance. QUESO dependencies are:

1. C and C++ compilers. Either `gcc` or `icc` are recommended [50, 53].
2. **Autotools**: The GNU build system, also known as the Autotools, is a suite of programming tools (Automake, Autoconf, Libtool) designed to assist in making source-code packages portable to many Unix-like systems [51].
3. **STL**: The Standard Template Library is a C++ library of container classes, algorithms, and iterators; it provides many of the basic algorithms and data structures of computer science [28]. The STL usually comes packaged with your compiler.
4. **GSL**: The GNU Scientific Library is a numerical library for C and C++ programmers. It provides a wide range of mathematical routines such as random number generators, special functions and least-squares fitting [14]. The lowest version of GSL required by QUESO is GSL 1.10.
5. **Boost**: Boost provides free peer-reviewed portable C++ source libraries, which can be used with the C++ Standard Library [49]. QUESO requires Boost 1.35.0 or newer.
6. **MPI**: The Message Passing Interface is a standard for parallel programming using the message passing model. E.g. Open MPI [56] or MPICH [54]. QUESO requires MPI during the compilation step; however, you may run it in serial mode (e.g. in one single processor) if you wish.

QUESO also works with the following optional libraries:

1. **GRVY**: The Groovy Toolkit (GRVY) is a library used to house various support functions often required for application development of high-performance, scientific applications. The library is written in C++, but provides an API for development in C and Fortran [52]. QUESO requires GRVY 0.29 or newer.
2. **HDF5**: The Hierarchical Data Format 5 is a technology suite that makes possible the management of extremely large and complex data collections [18]. The lowest version required by QUESO is HDF5 1.8.0.
3. **GLPK**: The GNU Linear Programming Kit package is is a set of routines written in ANSI C and organized in the form of a callable library for solving large-scale linear programming, mixed integer programming, and other related problems [38]. QUESO works with GLPK versions newer than or equal to GLPK 4.35.

4. **Trilinos**: The Trilinos Project is an effort to develop and implement robust algorithms and enabling technologies using modern object-oriented software design, while still leveraging the value of established libraries. It emphasizes abstract interfaces for maximum flexibility of component interchanging, and provides a full-featured set of concrete classes that implement all abstract interfaces [25, 24]. QUESO requires Trilinos release to be newer than or equal to 11.0.0. **Remark:** An additional requirement for QUESO work with Trilinos is that the latter must have enabled both Epetra and Teuchos libraries.

The majority of QUESO output files is MATLAB®/GNU Octave compatible [19, 55]. Thus, for results visualization purposes, it is recommended that the user have available either one of these tools.

2.1.2 Prepare your LINUX Environment

This section presents the steps to prepared the environment considering the user LINUX environment runs a BASH-shell. For other types of shell, such as C-shell, some adaptations may be required.

Before using QUESO, the user must first set a number of environmental variables, and indicate the full path of the QUESO's dependencies (GSL and Boost) and optional libraries.

For example, supposing the user wants to install QUESO with two additional libraries: HDF5 and Trilinos. Add the following lines to append the location of QUESO's dependencies and optional libraries to the `LD_LIBRARY_PATH` environment variable:

```
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
  $HOME/LIBRARIES/gsl-1.15/lib/:\
  $HOME/LIBRARIES/boost-1.53.0/lib/:\
  $HOME/LIBRARIES/hdf5-1.8.10/lib/:\
  $HOME/LIBRARIES/trilinos-11.2.4/lib:
```

which can be placed in the user's `.bashrc` or other startup file.

In addition, the user must set the following environmental variables:

```
$ export CC=gcc
$ export CXX=g++
$ export MPICC=mpicc
$ export MPICXX=mpic++
$ export F77=fort77
$ export FC=gfortran
```

2.2 Obtaining a Copy of QUESO

The latest supported public release of QUESO is available in the form of a tarball (tar format compressed with gzip) from QUESO Home Page: https://github.com/libqueso.

Suppose you have copied the file '`queso-0.56.0.tar.gz`' into `$HOME/queso_download/`. Then just follow these commands to expand the tarball:

```
$ cd $HOME/queso_download/
$ tar xvf queso-0.56.0.tar.gz
$ cd queso-0.56.0     #enter the directory
```

Naturally, for versions of QUESO other than 0.56.0, the file names in the above commands must be adjusted.

2.2.1 Recommended Build Directory Structure

Via Autoconf and Automake, QUESO configuration facilities provide a great deal of flexibility for configuring and building the existing QUESO packages. However, unless a user has prior experience with Autotools, we strongly recommend the following process to build and maintain local builds of QUESO (as an example, see note on Section 2.6). To start, we defined three useful terms:

Source tree - The directory structure where the QUESO source files are located. A source tree is is typically the result of expanding an QUESO distribution source code bundle, such as a tarball.

Build tree - The tree where QUESO is built. It is always related to a specific source tree, and it is the directory structure where object and library files are located. Specifically, this is the tree where you invoke `configure, make`, etc. to build and install QUESO.

Installation tree - The tree where QUESO is installed. It is typically the `prefix` argument given to QUESO's configure script; it is the directory from which you run installed QUESO executables.

Although it is possible to run `./configure` from the source tree (in the directory where the configure file is located), we recommend separate build trees. The greatest advantage to having a separate build tree is that multiple builds of the library can be maintained from the same source tree [25].

2.3 Configure QUESO Building Environment

QUESO uses the GNU Autoconf system for configuration, which detects various features of the host system and creates Makefiles. The configuration process can be controlled through environment variables, command-line switches, and host configuration files. For a complete list of switches type:

```
$ ./configure  --help
```

from the top level of the source tree (exemplified as `$HOME/queso_download/queso-0.56.0` in this report).

This command will also display the help page for QUESO options. Many of the QUESO configure options are used to describe the details of the build. For instance, to include HDF5, a package that is not currently built by default, append `--with-hdf5=DIR`, where `DIR` is the root directory of HDF5 installation, to the configure invocation line.

QUESO default installation location is '`/usr/local`', which requires superuser privileges. To use a path other than '`/usr/local`', specify the path with the '`--prefix=PATH`' switch. For instance, to follow the suggestion given in Section 2.1, the user should append '`--prefix=$HOME/LIBRARIES`'.

Therefore, the basic steps to configure QUESO using Boost, GSL (required), HDF5 and Trilinos (optional) for installation at '`$HOME/LIBRARIES/QUESO-0.56.0`' are:

```
$  ./configure --prefix=$HOME/LIBRARIES/QUESO-0.56.0 \
  --with-boost=$HOME/LIBRARIES/boost-1.53.0 \
  --with-gsl=$HOME/LIBRARIES/gsl-1.15 \
  --with-hdf5=$HOME/LIBRARIES/hdf5-1.8.10 \
  --with-trilinos=$HOME/LIBRARIES/trilinos-11.2.4
```

Note: the directory '`$HOME/LIBRARIES/QUESO-0.56.0`' does not need to exist in advance, since it will be created by the command `make install` described in Section 2.4.

2.4 Compile, Check and Install QUESO

In order to build, check and install the library, the user must enter the following three commands sequentially:

```
$ make
$ make check       # optional
$ make install
```

Here, `make` builds the library, confidence tests, and programs; `make check` conducts various test suites in order to check the compiled source; and `make install` installs QUESO library, include files, and support programs.

The files are installed under the installation tree (refer to Section 2.2.1), e.g. the directory specified with '`--prefix=DIR`' in Section 2.3. The directory, if not existing, will be created automatically.

By running `make check`, several printouts appear in the screen and you should see messages such as:

```
----------------------------------------------------------------------
(rtest): PASSED: Test 1 (TGA Validation Cycle)
----------------------------------------------------------------------
```

The tests printed in the screen are tests under your QUESO build tree, i.e., they are located at the directory `$HOME/queso_download/queso-0.56.0/test` (see Section 2.7 for the complete list of the directories under QUESO build tree). These tests are used as part of the periodic QUESO regression tests, conducted to ensure that more recent program/code changes have not adversely affected existing features of the library.

2.5 QUESO Developer's Documentation

QUESO code documentation is written using Doxygen [57], and can be generated by typing in the build tree:

```
$ make docs
```

A directory named `docs` will be created in `$HOME/queso_download/queso-0.56.0` (the build tree; your current path) and you may access the code documentation in two different ways:

1. HyperText Markup Language (HTML) format: `docs/html/index.html`, and the browser of your choice can be used to walk through the HTML documentation.
2. Portable Document Format (PDF) format: `docs/queso.pdf`, which can be accessed thought any PDF viewer.

2.6 Summary of Installation Steps

Supposing you have downloaded the file 'queso-0.56.0.tar.gz' into `$HOME/queso_download/`. In a BASH shell, the basic steps to configure QUESO using GRVY, Boost and GSL for installation at '`$HOME/LIBRARIES/QUESO-0.56.0`' are:

```
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
  $HOME/LIBRARIES/gsl-1.15/lib/:\
  $HOME/LIBRARIES/boost-1.53.0/lib/:\
  $HOME/LIBRARIES/hdf5-1.8.10/lib/:\
  $HOME/LIBRARIES/trilinos-11.2.4/lib:
$ export CC=gcc
$ export CXX=g++
$ export MPICC=mpicc
$ export MPICXX=mpic++
$ export F77=fort77
$ export FC=gfortran
$ cd $HOME/queso_download/                #enter source dir
$ gunzip < queso-0.56.0.tar.gz  | tar xf -
$ cd $HOME/queso_download/queso-0.56.0   #enter the build dir
$ ./configure --prefix=$HOME/LIBRARIES/QUESO-0.56.0 \
  --with-boost=$HOME/LIBRARIES/boost-1.53.0 \
```

```
  --with-gsl=$HOME/LIBRARIES/gsl-1.15 \
  --with-hdf5=$HOME/LIBRARIES/hdf5-1.8.10 \
  --with-trilinos=$HOME/LIBRARIES/trilinos-11.2.4
$ make
$ make check
$ make install
$ make docs
$ ls $HOME/LIBRARIES/QUESO-0.56.0 #listing QUESO installation dir
>>  bin  include  lib  examples
```

2.7 The Build Directory Structure

The QUESO build directory contains three main directories, `src`, `examples` and `test`. They are listed below and more specific information about them can be obtained with the Developer's documentation from Section 2.5 above.

1. `src`: this directory contains the QUESO library itself, and its main subdirectories are:

   (a) `basic/`: contain classes for dealing with vector sets, subsets and spaces, scalar and vector functions and scalar and vector sequences

   (b) `core/`: contain classes that handle QUESO environment, and vector/matrix operations

   (c) `stats/`: contain classes that implement vector realizers, vector random variables, statistical inverse and forward problems; and the Monte Carlo and the Metropolis-Hasting solvers

   Details of QUESO classes are presented in Chapter 3.

2. `examples`: examples of different applications, with distinct levels of difficulty, using QUESO. The following examples have been thoroughly documented and are included in Chapter 6:

   (a) `gravity/`: inference of the acceleration of gravity via experiments and a solution of a SIP; and forward propagation of uncertainty in the calculation of the distance traveled by a projectile. It is presented in detail in Section 6.3.

   (b) `simpleStatisticalForwardProblem/`: simplest example of how to use QUESO to solve a SFP, described in detail in Section 6.2.

   (c) `simpleStatisticalInverseProblem/`: simplest example of how to use QUESO to solve a SIP, thoroughly described in Section 6.1.

   (d) `validationCycle/`: presents a combination of SIP and SFP to solve a thermogravimetric analysis problem; this problem has the majority of its code in `*.h` files, with templated routines. This example is described in Section 6.4.

(e) `validationCycle2/`: also presents a combination of SIP and SFP to solve a thermogravimetric analysis problem; but the majority of its code is in `*.C` files.

All the examples presented in Chapter 6 come with the mathematical formulation, their translation into code, the options input file required by QUESO and auxiliary Matlab (GNU Octave compatible) files for data visualization.

The build directory contains only the source files. The executables are available under the QUESO installation directory, together with example of Makefiles that may be used to re-build the examples without the need of re-building the library.

3. `test`: a set of tests used as part of the periodic QUESO regression tests, conduct to ensure that more recent program/code changes have not adversely affected existing features of the library, as described in Section 2.4.

   (a) `gsl_tests`

   (b) `t01_valid_cycle/`

   (c) `t02_sip_sfp/`

   (d) `t03_sequence/`

   (e) `t04_bimodal/`

   (f) `test_Environment/`

   (g) `test_GaussianVectorRVClass/`

   (h) `test_GslMatrix/`

   (i) `test_GslVector/`

   (j) `test_uqEnvironmentOptions/`

   These tests can optionally be called during QUESO installation steps by entering the instruction: `make check`.

2.8 The Installed Directory Structure

After having successfully executed steps described in Sections 2.1–2.4, the QUESO installed directory will contain four subdirectories:

1. `bin`: contains the executable `queso_version`, which provides information about the installed library. The code bellow presents a sample output:

```
kemelli@margarida:~/LIBRARIES/QUESO-0.56.0/bin$ ./queso_version
---------------------------------------------------------------
QUESO Library: Version = 0.56.0 (56.0)

Development Build
```

```
Build Date    = 2013-07-12 12:36
Build Host    = margarida
Build User    = kemelli
Build Arch    = i686-pc-linux-gnu
Build Rev     = 40392

C++ Config    = mpic++ -g -O2 -Wall

Trilinos DIR = /home/kemelli/LIBRARIES/trilinos-11.2.4
GSL Libs      = -L/home/kemelli/LIBRARIES/gsl-1.15/lib -lgsl -lgslcblas
    -lm
GRVY DIR      =
GLPK DIR      =
HDF5 DIR      =
-----------------------------------------------------------------
kemelli@margarida:~/LIBRARIES/QUESO-0.56.0/bin$
```

2. `lib`: contains the static and dynamic versions of the library. The full to path to this directory, e.g., `$HOME/LIBRARIES/QUESO-0.56.0/lib` should be added to the user's `LD_LIBRARY_PATH` environmental variable in order to use QUESO library with his/her application code:

```
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
 $HOME/LIBRARIES/QUESO-0.56.0/lib
```

   Note that due to QUESO being compiled/built with other libraries (GSL, Boost, Trilinos and HDF5), `LD_LIBRARY_PATH` had already some values set in Section 2.1.2.

3. `include`: contains the library `.h` files.

4. `examples`: contains the same examples of QUESO build directory, and listed in Section 2.7, together with their executables and Matlab files that may be used for visualization purposes. A selection of examples are described in details in Chapter 6; the user is invited understand their formulation, to run them and understand their purpose.

2.9 Create your Application with the Installed QUESO

Prepare your environment by either running or saving the following command in your `.bashrc` (supposing you have a BASH-shell):

```
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
 $HOME/LIBRARIES/QUESO-0.56.0/lib
```

Suppose your application code consists of the files: `example_main.C`, `example_qoi.C`, `example_likelihood.C, example_compute.C` and respective `.h` files. Your application code may be linked with QUESO library through a Makefile such as the one displayed as follows:

```
QUESO_DIR = $HOME/LIBRARIES/QUESO-0.56.0/
BOOST_DIR = $HOME/LIBRARIES/boost-1.53.0/
GSL_DIR = $HOME/LIBRARIES/gsl-1.15/
GRVY_DIR = $HOME/LIBRARIES/grvy-0.32.0
TRILINOS_DIR = $HOME/LIBRARIES/trilinos-11.2.4/

INC_PATHS = \
  -I. \
  -I$(QUESO_DIR)/include \
  -I$(BOOST_DIR)/include/boost-1.53.0 \
  -I$(GSL_DIR)/include \
  -I$(GRVY_DIR)/include \
  -I$(TRILINOS_DIR)/include \

LIBS = \
  -L$(QUESO_DIR)/lib -lqueso \
  -L$(BOOST_DIR)/lib -lboost_program_options \
  -L$(GSL_DIR)/lib -lgsl \
  -L$(GRVY_DIR)/lib -lgrvy \
  -L$(TRILINOS_DIR)/lib -lteuchoscore -lteuchoscomm -lteuchosnumerics \
  -lteuchosparameterlist -lteuchosremainder -lepetra

CXX = mpic++
CXXFLAGS += -O3 -Wall -c

default: all

.SUFFIXES: .o .C

all:  ex_gsl

clean:
  rm -f *~
  rm -f *.o
%   rm -f example_gsl

ex_gsl: example_main.o example_likelihood.o example_qoi.o example_compute.o
  $(CXX) example_main.o example_likelihood.o example_qoi.o \
         example_compute.o -o example_gsl $(LIBS)

%.o: %.C
  $(CXX) $(INC_PATHS) $(CXXFLAGS) $<
```

CHAPTER 3

C++ Classes in the Library

QUESO is is a parallel object-oriented statistical library dedicated to the research of statistically robust, scalable, load balanced, and fault-tolerant mathematical algorithms for the quantification of uncertainty in realistic computational models and predictions related to natural and engineering systems.

Classes in QUESO can be divided in four main groups: core, templated basic, templated statistical and miscellaneous. The classed that handle environment (and options), vector and matrix classes are considered *core* classes. Classes implementing vector sets and subsets, vector spaces, scalar functions, vector functions, scalar sequences and vector sequences are *templated basic* classes; they are necessary for the definition and description of other entities, such as RVs, Bayesian solutions of IPs, sampling algorithms and chains. Vector realizer, vector RV, statistical IP (and options), MH solver (and options), statistical FP (and options), MC solver (and options) and sequence statistical options are part of *templated statistical* classes. And finally, the *miscellaneous* classes consist of C and FORTRAN interfaces.

3.1 Core Classes

QUESO core classes are the classes responsible for handling the environment (and options), vector and matrix operations. They are described in the following sections.

3.1.1 Environment Class (and Options)

The `Environment` class sets up the environment underlying the use of the QUESO library by an executable. This class is virtual. It is inherited by `EmptyEnvironment` and `FullEnvironment`.

The QUESO environment class is instantiated at the application level, right after `MPI_Init(&argc,&argv)`. The QUESO environment is required by reference by many constructors in the QUESO library, and is available by reference from many classes as well.

The constructor of the environment class requires a communicator, the name of an options input file, and the eventual prefix of the environment in order for the proper options to be read (multiple environments can coexist, as explained further below).

The environment class has four primary tasks:

1. Assigns rank numbers, other than the world rank, to nodes participating in a parallel job,
2. Provides MPI communicators for generating a sequence of vectors in a distributed way,
3. Provides functionality to read options from the options input file (whose name is passed in the constructor of this environment class), and
4. Opens output files for messages that would otherwise be written to the screen (one output file per allowed rank is opened and allowed ranks can be specified through the options input file).

Let $S \geqslant 1$ be the number of problems a QUESO environment will be handling at the same time, in parallel. S has default value of 1 and is an option read by QUESO from the input file provided by the user. The QUESO environment class manages five types of communicators, referred to as:

1. *world*: MPI_WORLD_COMM;
2. *full*: communicator passed to the environment constructor, of size F and usually equal to the world communicator;
3. *sub*: communicator of size F/S that contains the number of MPI nodes necessary to solve a statistical IP or a statistical FP;
4. *self*: MPI_SELF_COMM, of size 1; and
5. *inter0*: communicator of size S formed by all MPI nodes that have subrank 0 in their respective subcommunicators.

A *subenvironment* in QUESO is the smallest collection of processors necessary for the proper run of the model code. An *environment* in QUESO is the collection of all subenvironments, if there is more than one subenvironment.

Each subenvironment is able to generate a statistical inverse problem and/or a statistical forward problem; that is, each subenvironment is able to handle a "sub" Markov chain (a sequence) of vectors and/or a "sub" Monte Carlo sequence of output vectors. The "sub" sequences can be seen as forming a "unified" sequence in a distributed way. Indeed, the virtual class `VectorSequence` provides "sub" and "unified" statistical operations.

Thus, if the model code requires 16 processors to run and the user decides to run 64 Markov chains in parallel, then the environment will consist of a total of $F = 1024$ processors and $S = 64$ subenvironments, each subenvironment with $F/S = 16$ processors. Any given computing node in a QUESO run has potentially five different ranks. Each subenvironment is assigned a subid varying from 0 (zero) to $S - 1$, and is able to handle a statistical IP and/or a statistical FP. That is, each subenvironment is able to handle a *sub* Markov chain (a sequence) of vectors and/or a *sub* MC sequence of output vectors. The *sub* sequences form an unified sequence in a distributed way. QUESO takes care of the unification of results for the application programming and for output files. Of course, if the user is solving just one statistical problem with just one MPI node, then all ranks are equal to zero.

A QUESO subenvironment eventually prints messages to its own output file. In order for that to happen, the requirements are:

1. option `m_subDisplayFileName`, a string, must be different than the default value `"."`;
2. option `m_subDisplayAllowedSet`, a set of sub ids, must contain the id of the sub environment wanting to write a message to the output file;
3. the previous requirement is automatically satisfied if the option `m_subDisplayAllowAll`, a boolean, is set to 1 (the default value is 0);
4. the processor wanting to write a message to the output file must have sub rank 0 (zero).

If all requirements are satisfied, then QUESO will generate a file with name `<m_subDisplayFileName>_sub<sub id>.txt`. For instance, if `m_subDisplayFileName` is '`pROblem_775_`' then a node of sub rank 0 in sub environment 17 will write a message to the file '`pROblem_775_sub17.txt`'. The class responsible for reading options one can pass to a QUESO environment through an input file is the `EnvironmentOptions` class.

Figure 3.1.1 depicts class diagram for the environment class and Figure 3.1.2 display its collaboration graph; and Figure 3.1.3 displays environment options class. Finally, the input file options for a QUESO environment, i.e., the options the user may set in his/her input file when using QUESO together with the application of interest, is presented in Table 3.1.1.

3.1.2 Vector

The Vector class handles all the vector operations carried out in QUESO, and currently has two derived classes: `GslVector` and `TeuchosVector`. `GslVector` is based on the GSL vector structure; whereas `TeuchosVector` is based on Trilinos Teuchos vector structure [25], and therefore, it is only available if QUESO was compiled with Trilinos.

A class diagram for `Vector` class is presented in Figure 3.1.4.

3.1.3 Matrix

The Matrix class handles all the matrix operations carried out in QUESO. Analogously to the vector class case described in the previous section, matrix class currently has two derived

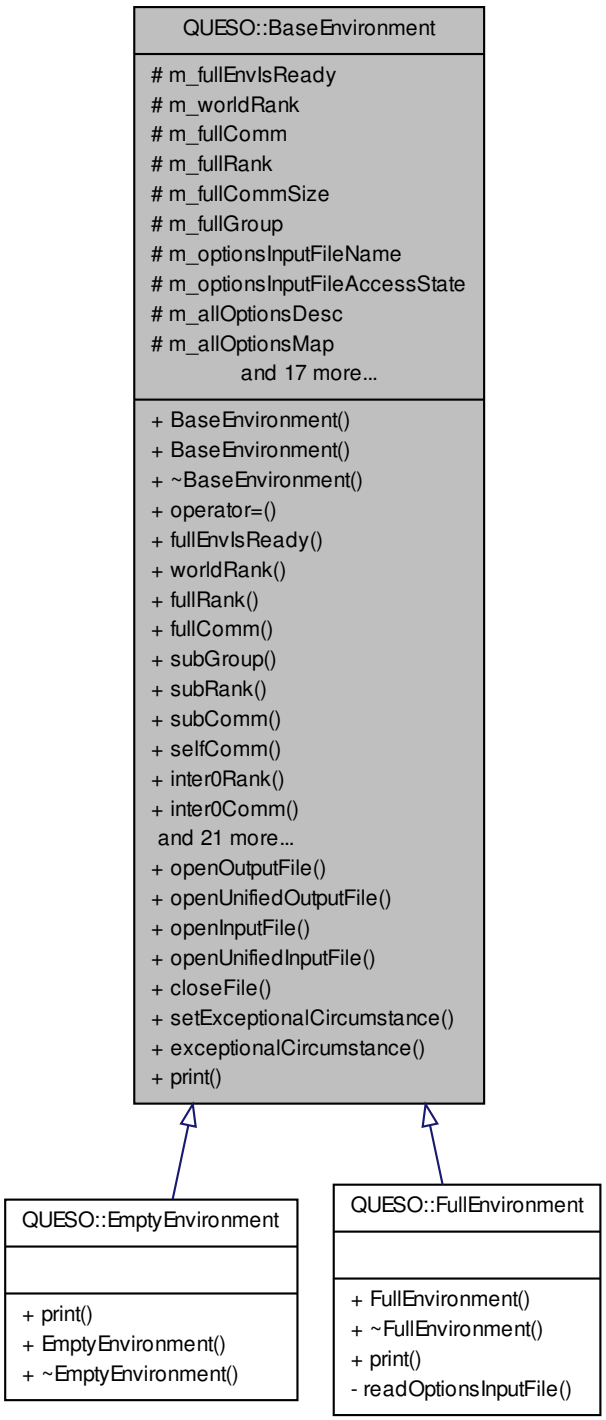


Figure 3.1.1: The class diagram for the Environment class described in Section 3.1.1.

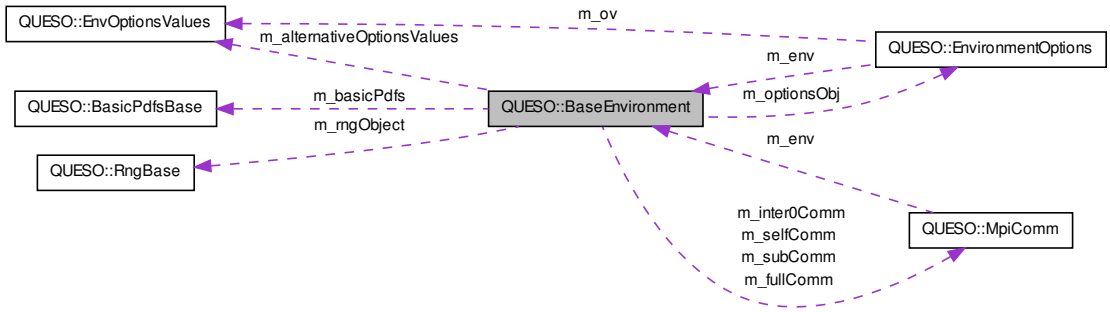


Figure 3.1.2: Collaboration graph for the environment class described in Section 3.1.1.

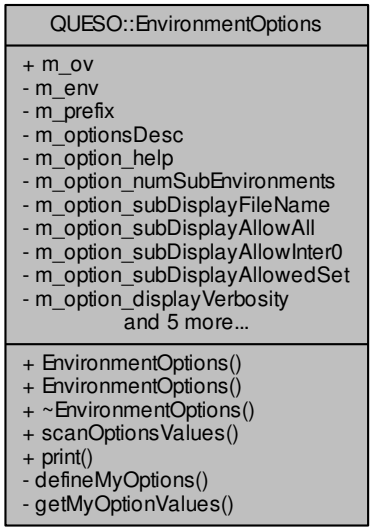


Figure 3.1.3: The environment options class with its attributes and methods.

Table 3.1.1: Input file options for a QUESO environment.

Option name	Default value	Description
⟨PREFIX⟩env_help		Produces help message for environment class
⟨PREFIX⟩env_numSubEnvironments	1	Number of subenvironments
⟨PREFIX⟩env_subDisplayFileName	"."	Output filename for sub-screen writing
⟨PREFIX⟩env_subDisplayAllowAll	0	Allows all subenvironments to write to output file
⟨PREFIX⟩env_subDisplayAllowedSet	""	Subenvironments that will write to output file
⟨PREFIX⟩env_displayVerbosity	0	Sets verbosity
⟨PREFIX⟩env_syncVerbosity	0	Sets syncronized verbosity
⟨PREFIX⟩env_seed	0	Set seed

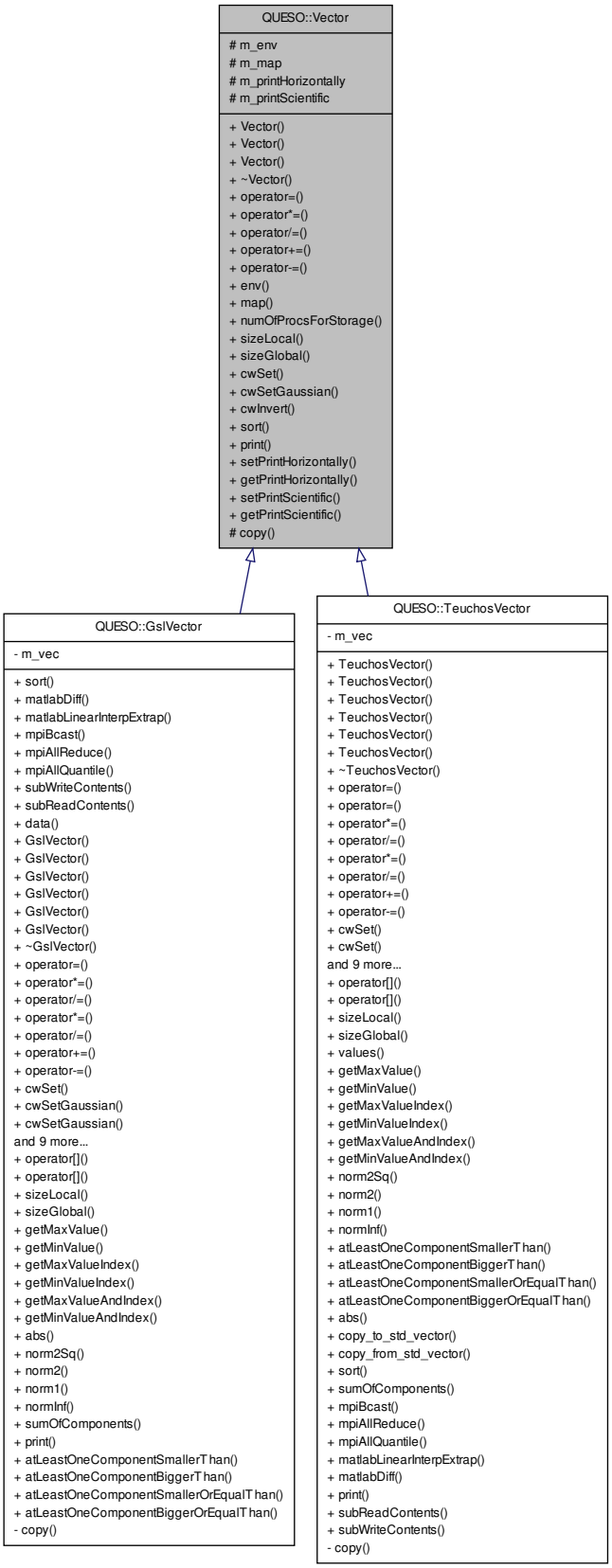


Figure 3.1.4: The class diagram for the vector class described in Section 3.1.2.

classes: `GslMatrix` and `TeuchosMatrix`. `GslMatrix` is based on the GSL matrix structure; whereas `TeuchosMatrix` is based on Trilinos Epetra matrix structure.

A class diagram for `Matrix` is presented in Figure 3.1.5; it displays its protected attributes together with its member functions. Again, the diagram displays in some detail the inherited classes `GslMatrix` and `TeuchosMatrix`.

3.2 Templated Basic Classes

The classes in this group are: vector sets, subsets and spaces (Section 3.2.1), scalar and vector function classes (Section 3.2.2), and scalar and vector sequences (Section 3.2.3).

These classes constitute the core entities necessary for the formal mathematical definition and description of other entities, such as random variables, Bayesian solutions of inverse problems, sampling algorithms and chains.

3.2.1 Vector Set, Subset and Vector Space Classes

The vector set class is fundamental for the proper handling of many mathematical entities. Indeed, the definition of a scalar function such as $\pi : \mathbf{B} \subset \mathbb{R}^n \to \mathbb{R}$ requires the specification of the domain $\mathbf{B}$, which is a *subset* of the *vector space* $\mathbb{R}^n$, which is itself a *set*. Additionally, SIPs need a likelihood routine $\pi_{\text{like}} : \mathbb{R}^n \to \mathbb{R}_+$, and SFPs need a QoI routine $\mathbf{q} : \mathbb{R}^n \to \mathbb{R}^m$; the *sets* $\mathbb{R}^n$, $\mathbb{R}^m$, etc., are *vector spaces*.

The relationship amongst QUESO classes for handling sets, namely `VectorSet`; subsets, namely `VectorSubset`; and vector spaces, namely `VectorSpace` is sketched in Figure 3.2.1. An attribute of the *subset* class is the *vector space* which it belongs to, and in fact a reference to a vector space is required by the constructor of the subset class. An example of this case is the definition of a scalar function such as $\pi : \mathbf{B} \subset \mathbb{R}^n \to \mathbb{R}$ above.

The power of an object-oriented design is clearly featured here. The intersection subset derived class `IntersectionSubset` is useful for handling a posterior PDF on Equation (1.2.1), since its domain is the intersection of the domain of the prior PDF with the domain of the likelihood function.

3.2.2 Scalar Function and Vector Function Classes

Joint PDF, marginal PDF, and CDF are all examples of scalar functions present in statistical problems. QUESO currently supports basic PDFs such as uniform and Gaussian and also more complex PDFs, such as the ones coming from a Bayesian analysis. They are implemented in the classes `UniformJointPdf`, `GaussianJointPdf`, and `BayesianJointPdf`, respectively. The posterior PDF may be represented within QUESO by `GenericJointPdf`. See Diagram 3.2.2 for the scalar function class.

The handling of vector functions within QUESO is also quite straightforward. Indeed, the definition of a vector function $\mathbf{q} : \mathbf{B} \subset \mathbb{R}^n \to \mathbb{R}^m$ requires only the extra specifi-

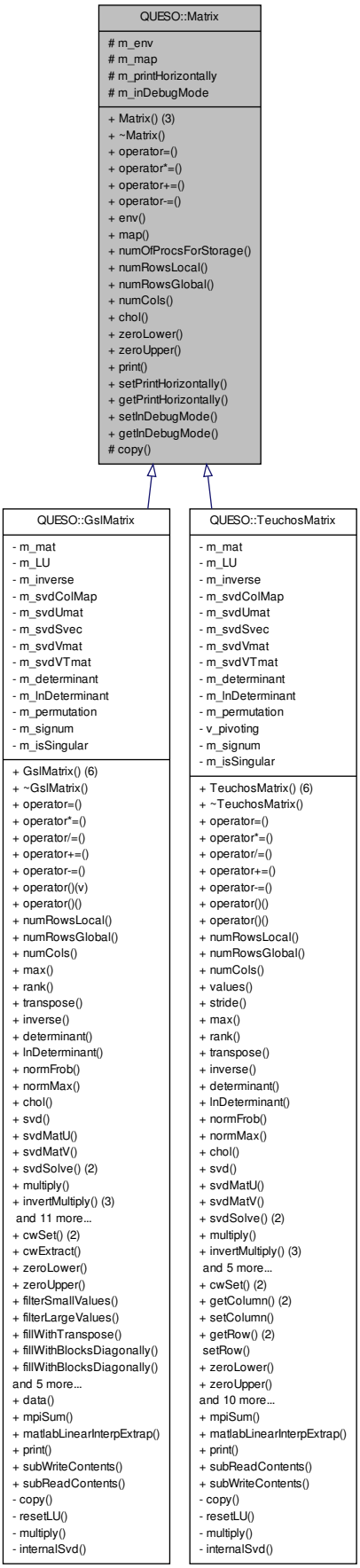


Figure 3.1.5: The class diagram for the matrix class.

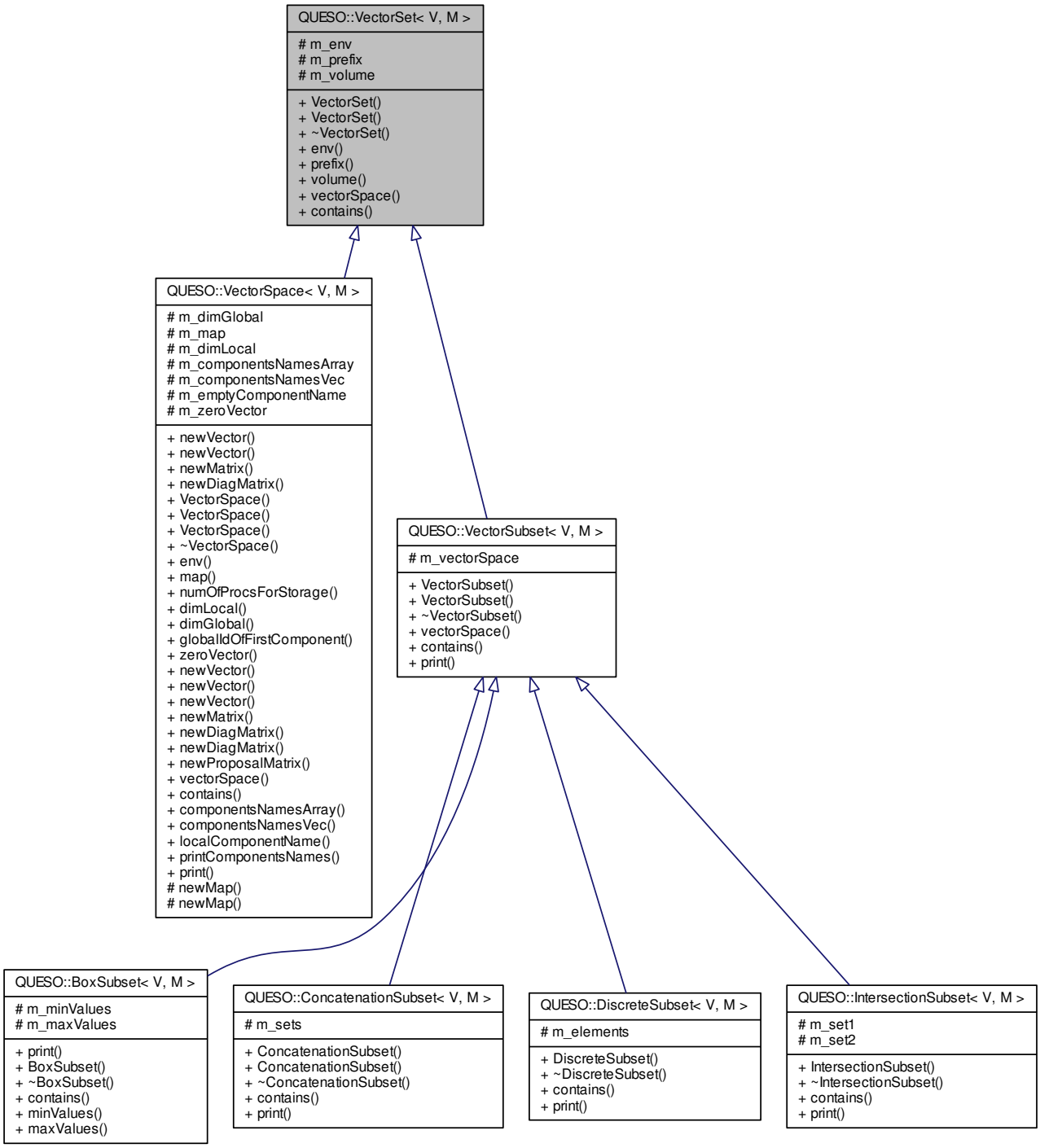


Figure 3.2.1: The class diagram for vector set, vector subset and vector space classes, described in Section 3.2.1.

cation of the image vector space $\mathbb{R}^m$. The classes representing the vector function class `GenericVectorFunction` and `ConstantVectorFunction` are derived from `BaseVectorFunction` and are presented in Diagram 3.2.3

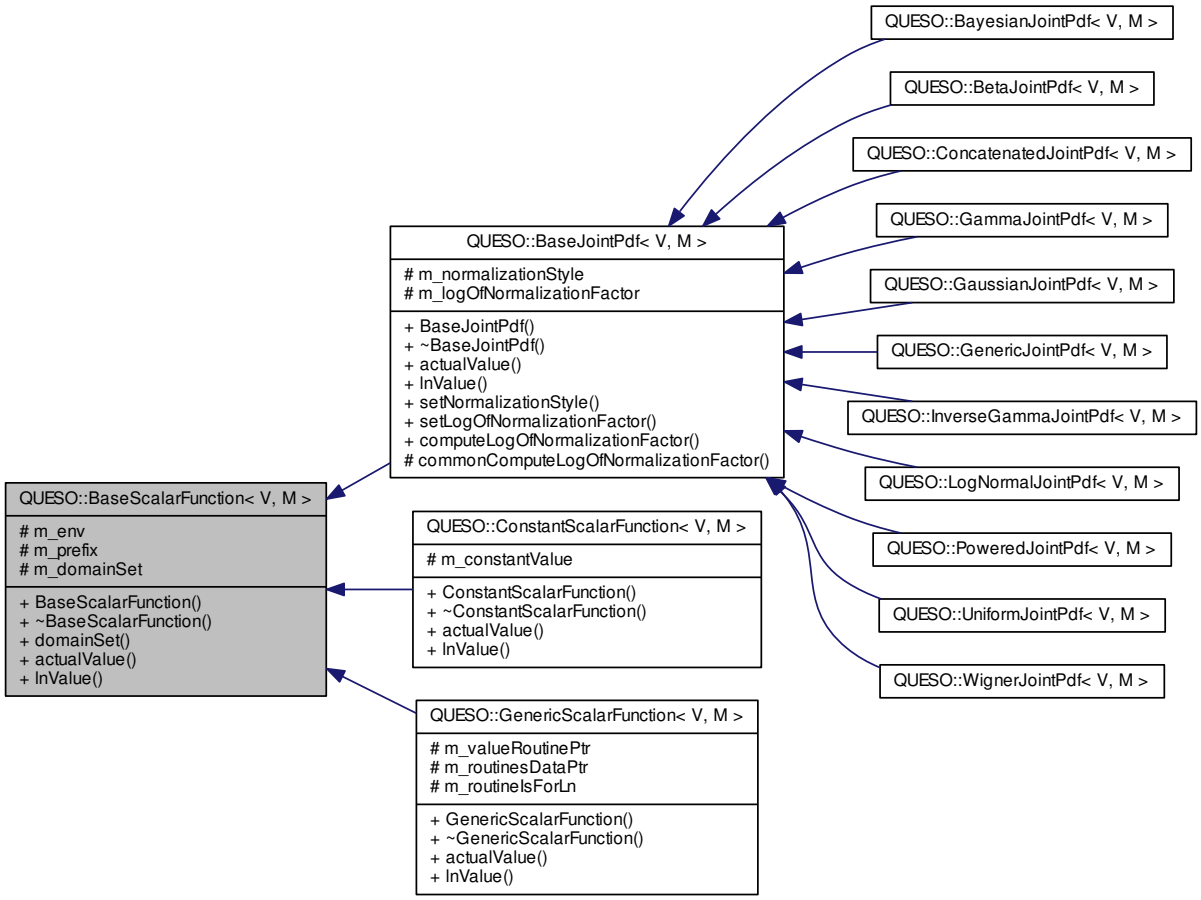


Figure 3.2.2: The class diagram for the scalar function class.

3.2.3 Scalar Sequence and Vector Sequence Classes

The scalar sequence class contemplates *scalar* samples generated by an algorithm, as well as operations that can be done over them, e.g., calculation of means, variances, and convergence indices. Similarly, the vector sequence class contemplates *vector* samples and operations such as means, correlation matrices and covariance matrices.

Figures 3.2.4 and 3.2.5 display the class diagram for the scalar sequence and vector sequence classes, respectively.

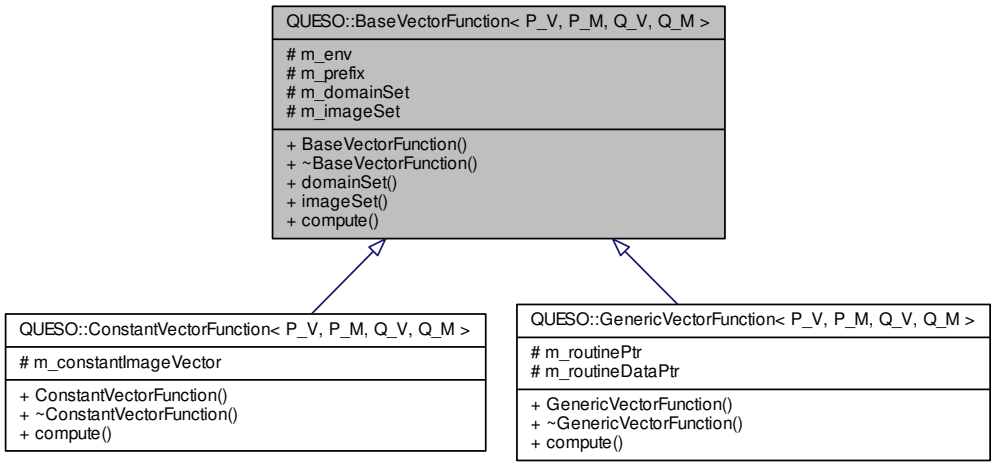


Figure 3.2.3: The class diagram for the vector function class described in Section 3.2.2.

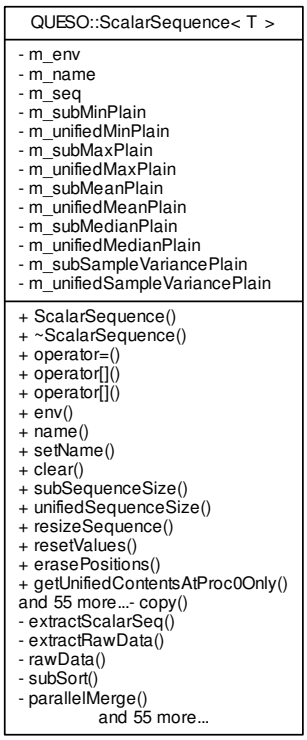


Figure 3.2.4: The class diagram for the scalar sequence class.

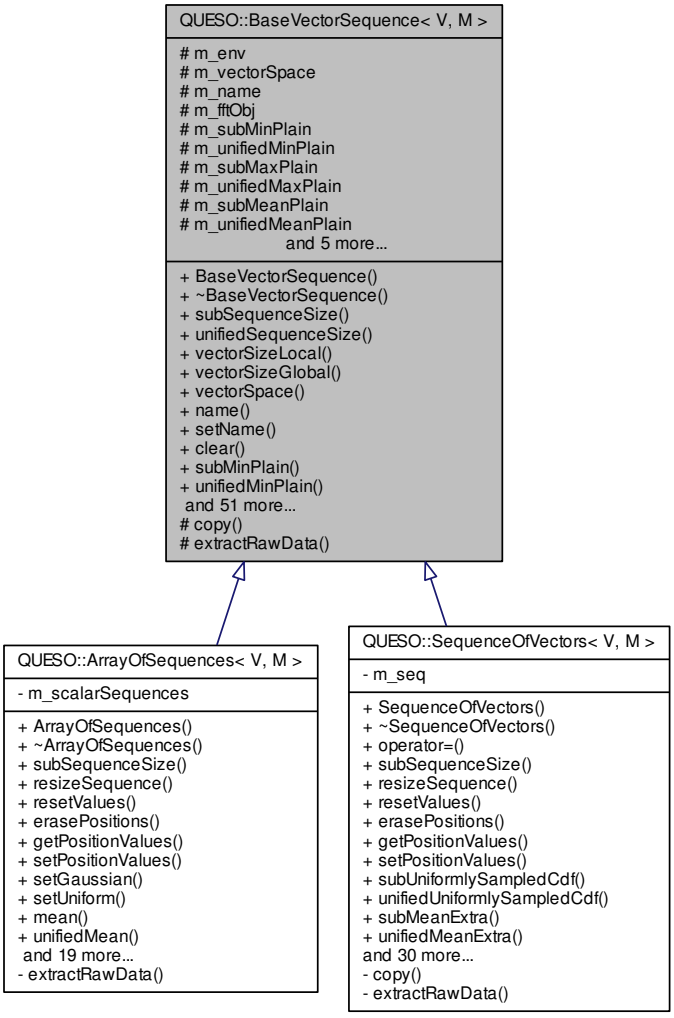


Figure 3.2.5: The class diagram for the vector sequence class.

3.3 Templated Statistical Classes

The classes in this group are: vector realizer, vector random variable, statistical inverse problem (and options), Metropolis-Hastings solver (and options), statistical forward problem (and options), Monte Carlo solver (and options), and Sequence statistical options.

For QUESO, a SIP has two input entities, a prior RV and a likelihood routine, and one output entity, the posterior RV, as shown in Chapter 1, Figure 1.2.3. Similarly, a SFP has two input entities, a input RV and a QoI routine, and one output entity, the output RV, as shown in Figure 1.2.2.

3.3.1 Vector Realizer Class

A *realizer* is an object that, simply put, contains a `realization()` operation that returns a sample of a vector RV. QUESO currently supports several realizers:

- uniform, implemented in `UniformVectorRealizer`,
- Gaussian, implemented in `GaussianVectorRealizer`,
- Log Normal, implemented in `LogNormalVectorRealizer`,
- Gamma, implemented in `GammaVectorRealizer`,
- Inverse Gamma, implemented in `InverseGammaVectorRealizer`, and
- Beta, , implemented in `BetaVectorRealizer`,

which are all derived from the base class `BaseVectorRealizer`.

QUESO conveniently provides the class `ConcatenatedVectorRealizer`, which allows two distinct realizers to be concatenated. It also contains a *sequence realizer* class for storing samples of a MH algorithm.

3.3.2 Vector Random Variable Class

Vector RVs are expected to have two basic functionalities: compute the value of its PDF at a point, and generate realizations following such PDF. The joint PDF (`BaseJointPdf` and derived classes, see Section 3.2.2) and vector realizer (`BaseVectorRealizer` and derived classes, see Section 3.3.1) classes allow a straightforward definition and manipulation of vector RVs. Similarly to the vector realizer class above, QUESO also allows users to form new RVs through the concatenation of existing RVs (class `ConcatenatedVectorRV`).

QUESO currently supports a few vector RVs such as uniform, Gaussian, Gamma and Beta, as depicted in Diagram 3.3.1. A derived class called *generic vector RV* allows QUESO to store the solution of an statistical IP: a *Bayesian joint PDF* becomes the PDF of the posterior RV, while a *sequence vector realizer* becomes the realizer of the same posterior RV.

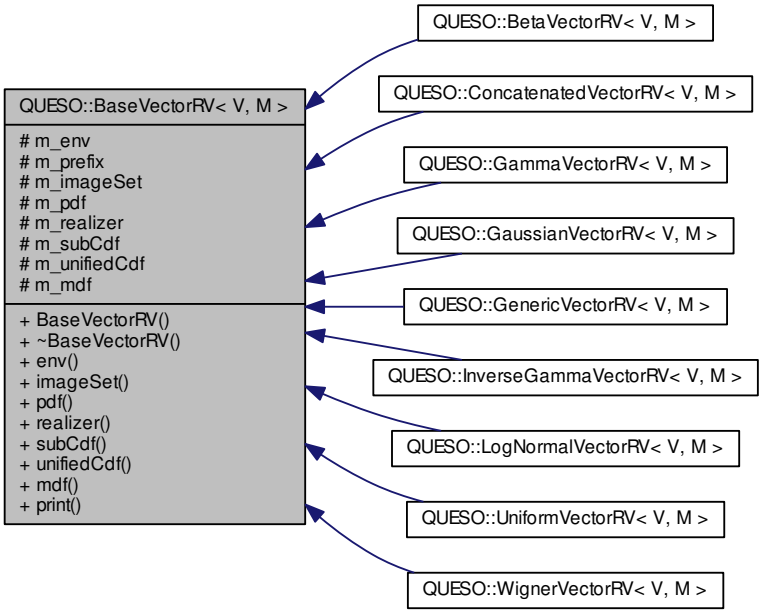


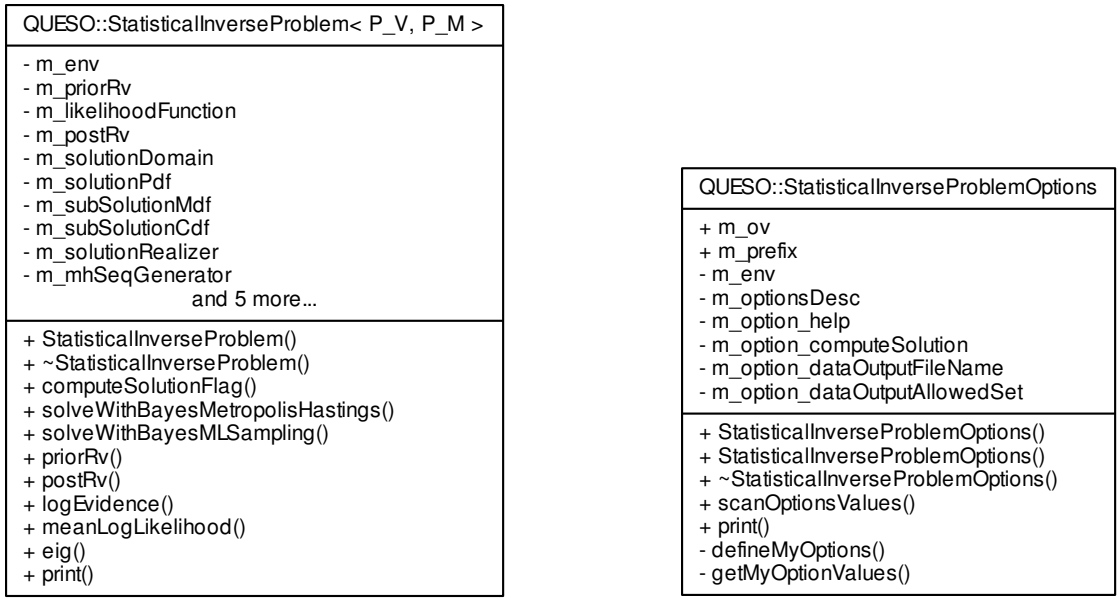
Figure 3.3.1: The class diagram for the vector random variable class.

3.3.3 Statistical Inverse Problem (and Options)

Similarly to its mathematical concepts, a SIP in QUESO also expects two input entities, a prior RV and a likelihood routine, and one output entity, the posterior RV. The SIP is represented in QUESO through the templated class `StatisticalInverseProblem<P_V,P_M>`, which is illustrated in Figure 3.3.2a. One important characteristic of the QUESO design is that it separates 'what the problem is' from 'how the problem is solved'. The prior and the posterior RV are instances of the `BaseVectorRv<V,M>` class, while the likelihood function is an instance of the `BaseScalarFunction<V,M>` class.

The solution of a SIP is computed by calling either `solveWithBayesMetropolisHastings()` or `solveWithBayesMLSampling()`, which are member functions of the class `StatisticalInverseProblem<P_V,P_M>` class. Upon return from a solution operation, the posterior RV is available through the `postRv()` member function. More details are provided about `solveWithBayesMetropolisHastings()` and `solveWithBayesMLSampling()` in Sections 3.3.4 and 3.3.5, respectively.

Figure 3.3.2b displays the `StatisticalInverseProblemOptions` class, i.e. that class that handles a variety of options for solving the SIP. Such options may be provided to QUESO by the user's input file; and they are listed in Table 3.3.1.



(a) StatisticalInverseProblem (b) StatisticalInverseProblemOptions

Figure 3.3.2: The statistical inverse problem class, which implements the representation in Figure 1.2.3, and statistical inverse problem options class.

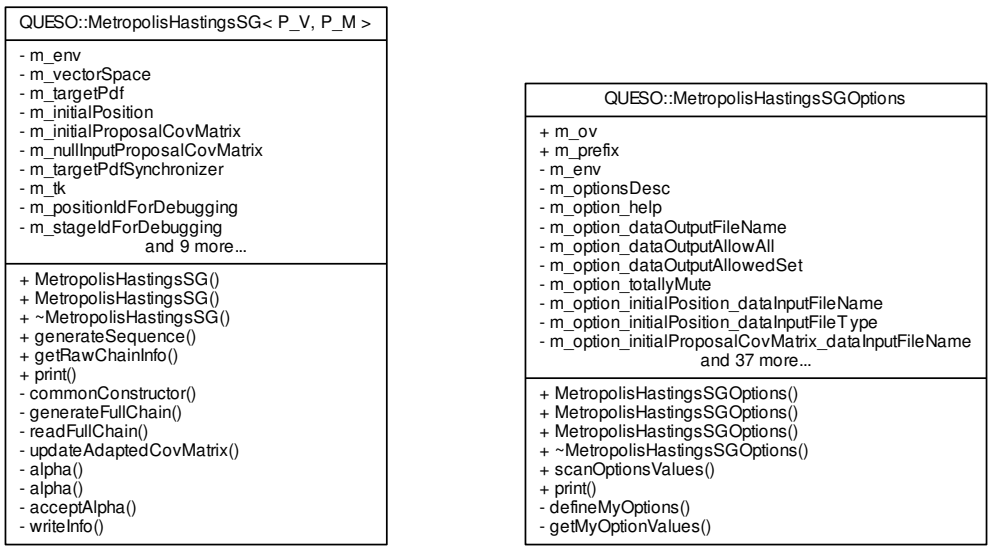
Table 3.3.1: Input file options for a QUESO statistical inverse problem.

Option name	Default Value	Description
`⟨PREFIX⟩ip_help`		Produces help message for statistical inverse problem
`⟨PREFIX⟩ip_computeSolution`	`1`	Computes solution process
`⟨PREFIX⟩ip_dataOutputFileName`	`"."`	Name of data output file
`⟨PREFIX⟩ip_dataOutputAllowedSet`	`""`	Subenvironments that will write to data output file

3.3.4 Metropolis-Hastings Solver (and Options)

The templated class that represents a Metropolis-Hastings generator of samples in QUESO is `MetropolisHastingsSG<P_V,P_M>`, where SG stands for 'Sequence Generator'. This class implements the DRAM algorithm of Haario, Laine, Mira and Saksman [21] together with an operation named `generateSequence()` based on the core routine at the MCMC toolbox for MATLAB [35].

The Metropolis-Hastings sequence generator class is depicted in Figure 3.3.3a; the Metropolis-Hastings sequence generator options class is depicted in Figure 3.3.3b. A collaboration graph for the Metropolis-Hastings class is presented in Figure 3.3.4; and the options are presented in Table 3.3.2.



(a) MetropolisHastingsSG (b) MetropolisHastingsSGOptions

Figure 3.3.3: The Metropolis-Hastings sequence generator class and the Metropolis-Hastings sequence generator options class.

3.3.5 Multilevel Solver (and Options)

The templated class that represents a Multilevel generator of samples in QUESO is `MLSampling<P_V,P_M>`. This class implements the Adaptive Multilevel Stochastic Simulation Algorithm of Cheung and Prudencio [8]. The Multilevel sequence generator class is assisted by two extra classes, `MLSamplingOptions` and `MLSamplingLevelOptions`, for handling the options to be used.

The Multilevel class, the Multilevel options and level options classes are depicted in Figure 3.3.5. A collaboration graph for the Multilevel class is presented in Figure 3.3.6; whereas its associated options are presented in Table 3.3.3.

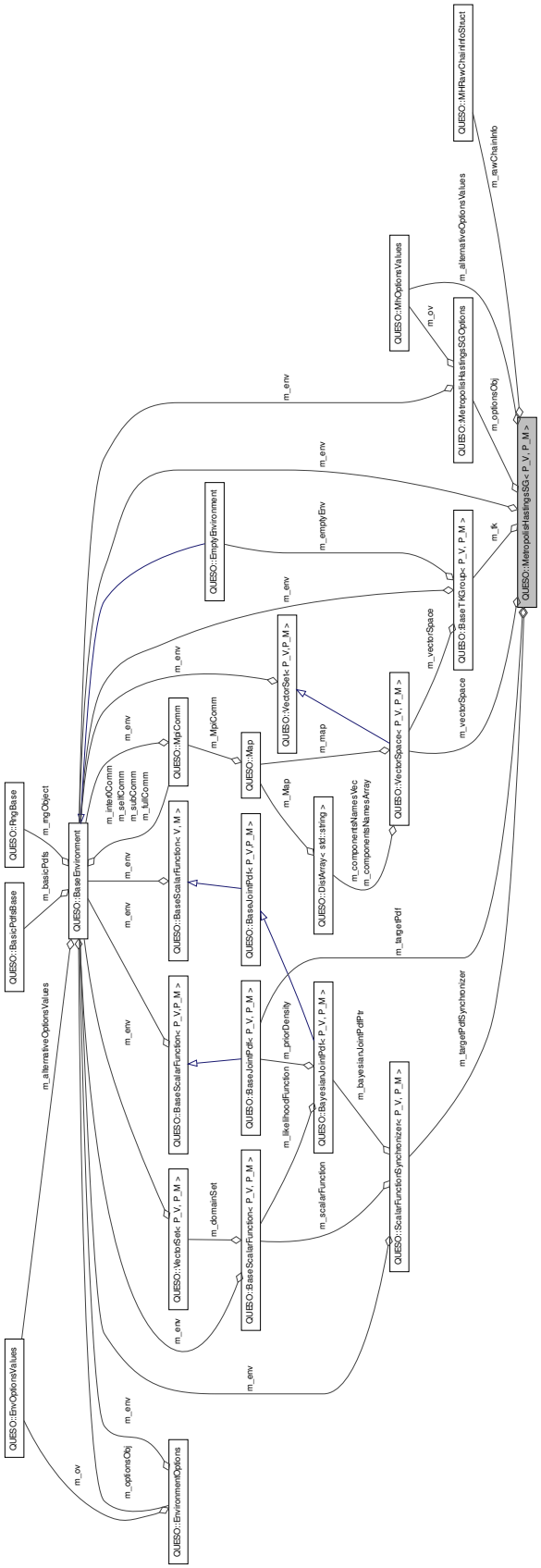
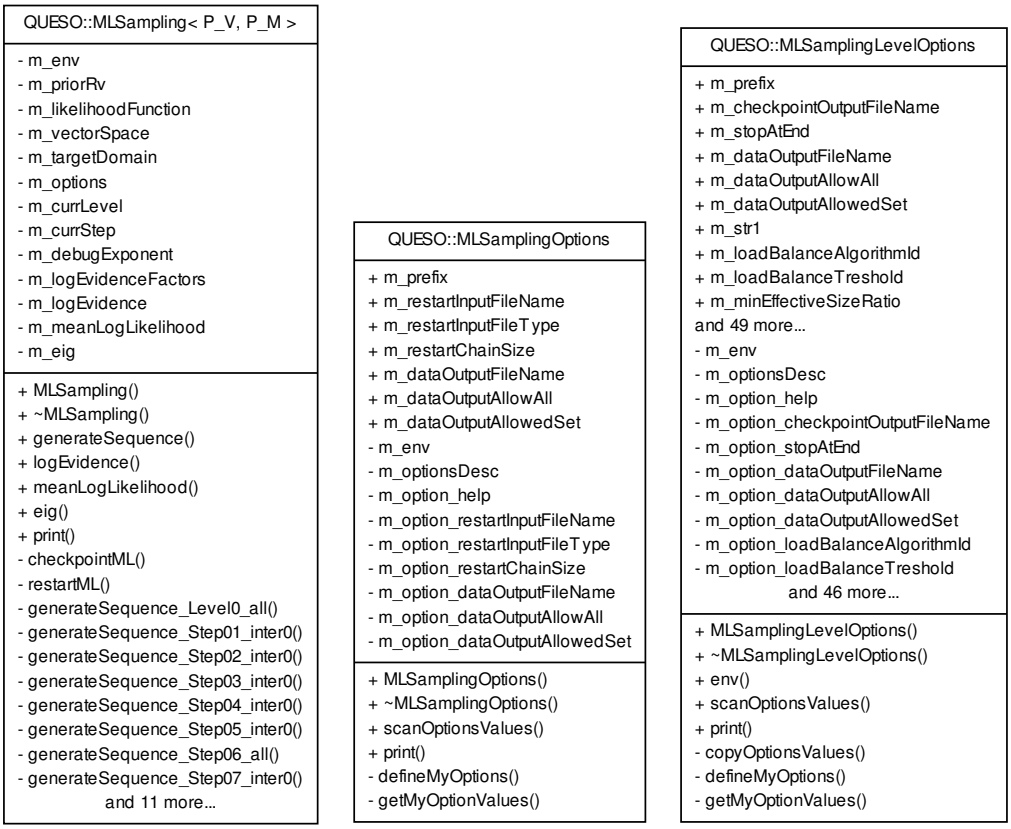


Figure 3.3.4: Collaboration graph of the Metropolis-Hastings sequence generator class.

Table 3.3.2: Input file options for a QUESO Metropolis-Hastings solver.

Option Name	Default Value
⟨PREFIX⟩mh_dataOutputFileName	"."
⟨PREFIX⟩mh_dataOutputAllowAll	0
⟨PREFIX⟩mh_initialPositionDataInputFileName	"."
⟨PREFIX⟩mh_initialPositionDataInputFileType	"m"
⟨PREFIX⟩mh_initialProposalCovMatrixDataInputFileName	"."
⟨PREFIX⟩mh_initialProposalCovMatrixDataInputFileType	"m"
⟨PREFIX⟩mh_rawChainDataInputFileName	"."
⟨PREFIX⟩mh_rawChainDataInputFileType	"m"
⟨PREFIX⟩mh_rawChainSize	100
⟨PREFIX⟩mh_rawChainGenerateExtra	0
⟨PREFIX⟩mh_rawChainDisplayPeriod	500
⟨PREFIX⟩mh_rawChainMeasureRunTimes	1
⟨PREFIX⟩mh_rawChainDataOutputPeriod	0
⟨PREFIX⟩mh_rawChainDataOutputFileName	"."
⟨PREFIX⟩mh_rawChainDataOutputFileType	"m"
⟨PREFIX⟩mh_rawChainDataOutputAllowAll	0
⟨PREFIX⟩mh_filteredChainGenerate	0
⟨PREFIX⟩mh_filteredChainDiscardedPortion	0.
⟨PREFIX⟩mh_filteredChainLag	1
⟨PREFIX⟩mh_filteredChainDataOutputFileName	"."
⟨PREFIX⟩mh_filteredChainDataOutputFileType	"m"
⟨PREFIX⟩mh_filteredChainDataOutputAllowAll	0
⟨PREFIX⟩mh_displayCandidates	0
⟨PREFIX⟩mh_putOutOfBoundsInChain	1
⟨PREFIX⟩mh_tkUseLocalHessian	0
⟨PREFIX⟩mh_tkUseNewtonComponent	1
⟨PREFIX⟩mh_drMaxNumExtraStages	0
⟨PREFIX⟩mh_drDuringAmNonAdaptiveInt	1
⟨PREFIX⟩mh_amKeepInitialMatrix	0
⟨PREFIX⟩mh_amInitialNonAdaptInterval	0
⟨PREFIX⟩mh_amAdaptInterval	0
⟨PREFIX⟩mh_amAdaptedMatricesDataOutputPeriod	0
⟨PREFIX⟩mh_amAdaptedMatricesDataOutputFileName	"."
⟨PREFIX⟩mh_amAdaptedMatricesDataOutputFileType	"m"
⟨PREFIX⟩mh_amAdaptedMatricesDataOutputAllowAll	0
⟨PREFIX⟩mh_amEta	1.
⟨PREFIX⟩mh_amEpsilon	1×10^{-5}
⟨PREFIX⟩mh_enableBrooksGelmanConvMonitor	0
⟨PREFIX⟩mh_BrooksGelmanLag	100



(a) MLSampling (b) MLSamplingOptions (c) MLSamplingLevelOptions

Figure 3.3.5: The Multilevel sequence generator options class (3.3.5a) and its associated classes for handling options.

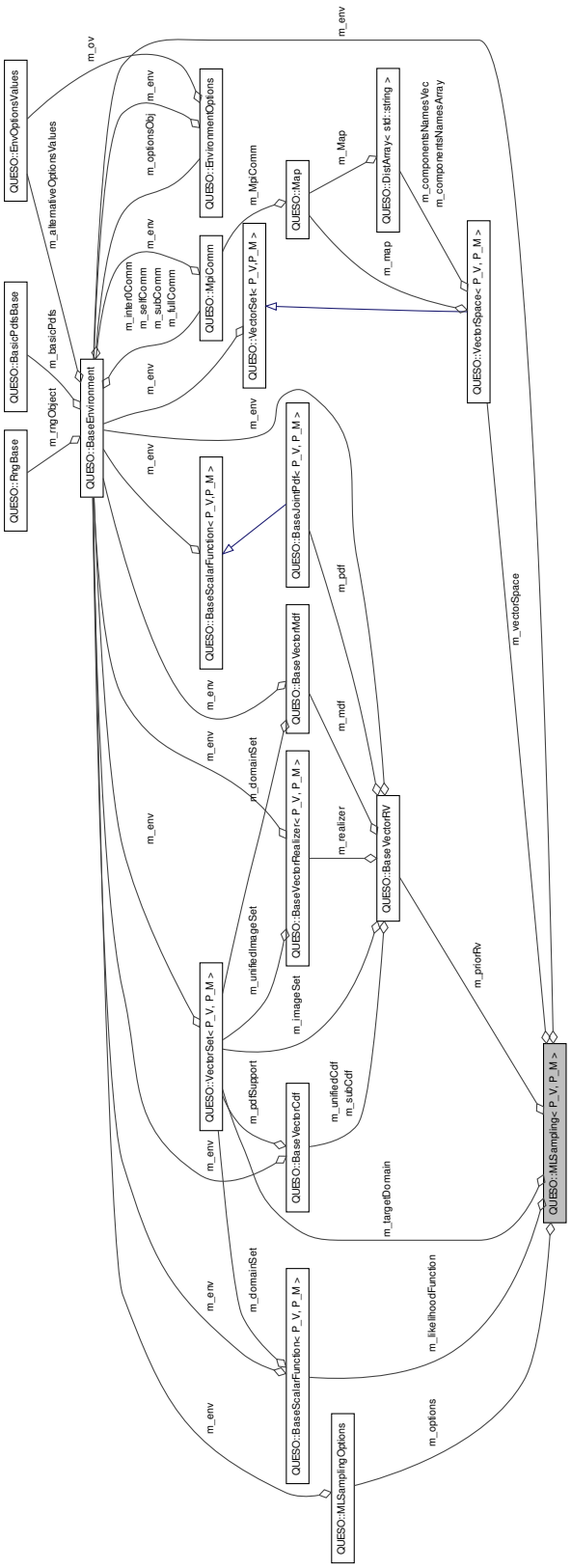


Figure 3.3.6: Collaboration graph of the Multilevel sampling class.

Table 3.3.3: Input file options for a QUESO Multilevel solver (to be continued).

Option Name	Default Value
⟨PREFIX⟩ml_restartOutput_levelPeriod	0
⟨PREFIX⟩ml_restartOutput_baseNameForFiles	"."
⟨PREFIX⟩ml_restartOutput_fileType	"m"
⟨PREFIX⟩ml_restartInput_baseNameForFiles	"."
⟨PREFIX⟩ml_restartInput_fileType	"m"
⟨PREFIX⟩ml_stopAtEnd	0
⟨PREFIX⟩ml_dataOutputFileName	"."
⟨PREFIX⟩ml_dataOutputAllowAll	0
⟨PREFIX⟩ml_loadBalanceAlgorithmId	2
⟨PREFIX⟩ml_loadBalanceTreshold	1.0
⟨PREFIX⟩ml_minEffectiveSizeRatio	0.85
⟨PREFIX⟩ml_maxEffectiveSizeRatio	0.91
⟨PREFIX⟩ml_scaleCovMatrix	1
⟨PREFIX⟩ml_minRejectionRate	0.50
⟨PREFIX⟩ml_maxRejectionRate	0.75
⟨PREFIX⟩ml_covRejectionRate	0.25
⟨PREFIX⟩ml_minAcceptableEta	0.
⟨PREFIX⟩ml_totallyMute	1
⟨PREFIX⟩ml_initialPositionDataInputFileName	"."
⟨PREFIX⟩ml_initialPositionDataInputFileType	"m"
⟨PREFIX⟩ml_initialProposalCovMatrixDataInputFileName	"."
⟨PREFIX⟩ml_initialProposalCovMatrixDataInputFileType	"m"
⟨PREFIX⟩ml_rawChainDataInputFileName	"."
⟨PREFIX⟩ml_rawChainDataInputFileType	"m"
⟨PREFIX⟩ml_rawChainSize	100
⟨PREFIX⟩ml_rawChainGenerateExtra	0
⟨PREFIX⟩ml_rawChainDisplayPeriod	500
⟨PREFIX⟩ml_rawChainMeasureRunTimes	1
⟨PREFIX⟩ml_rawChainDataOutputPeriod	0
⟨PREFIX⟩ml_rawChainDataOutputFileName	"."
⟨PREFIX⟩ml_rawChainDataOutputFileType	"m"
⟨PREFIX⟩ml_rawChainDataOutputAllowAll	0
⟨PREFIX⟩ml_filteredChainGenerate	0
⟨PREFIX⟩ml_filteredChainDiscardedPortion	0.
⟨PREFIX⟩ml_filteredChainLag	1
⟨PREFIX⟩ml_filteredChainDataOutputFileName	"."
⟨PREFIX⟩ml_filteredChainDataOutputFileType	"m"
⟨PREFIX⟩ml_filteredChainDataOutputAllowAll	0
⟨PREFIX⟩ml_displayCandidates	0
⟨PREFIX⟩ml_putOutOfBoundsInChain	1
⟨PREFIX⟩ml_tkUseLocalHessian	0
⟨PREFIX⟩ml_tkUseNewtonComponent	1
⟨PREFIX⟩ml_drMaxNumExtraStages	0
⟨PREFIX⟩ml_drScalesForExtraStages	0
⟨PREFIX⟩ml_drDuringAmNonAdaptiveInt	1
⟨PREFIX⟩ml_amKeepInitialMatrix	0
⟨PREFIX⟩ml_amInitialNonAdaptInterval	0
⟨PREFIX⟩ml_amAdaptInterval	0
⟨PREFIX⟩ml_amAdaptedMatricesDataOutputPeriod	0
⟨PREFIX⟩ml_amAdaptedMatricesDataOutputFileName	"."
⟨PREFIX⟩ml_amAdaptedMatricesDataOutputFileType	"m"
⟨PREFIX⟩ml_amAdaptedMatricesDataOutputAllowAll	0
⟨PREFIX⟩ml_amEta	1.
⟨PREFIX⟩ml_amEpsilon	1.e-5

3.3.6 Statistical Forward Problem (and Options)

A SFP in QUESO also has two input entities, the input (parameter) RV and a QoI function, and one output entity, the QoI RV. The SIP is represented through the templated class `StatisticalForwardProblem<P_V,P_M,Q_V,Q_M >`, which diagram is presented in Figure 3.3.7a. Again, the types `P_V` and `Q_V` of vectors and types `P_M` and `Q_M` of matrices, where `P_` stands for 'parameter' and `Q_` stands for 'quantities of interest'.

The input RV and the output QoI RV are instances of the `BaseVectorRv<P_V,P_M>` class, while the QoI function is an instance of `BaseVectorFunction<P_V,P_M,Q_V,Q_M>`. In the template parameters, the prefix `P_` refers to the parameters, whereas the prefix `Q_` refers to the QoIs.

In order to find the solution of a SFP, one must call the `solveWithMonteCarlo()` member function of the `StatisticalForwardProblem<P_V,P_M>` class. Upon return from a solution operation, the QoI RV is available through the `qoiRv()` member function. Such QoI RV is able to provide: a vector realizer through the operation `'qoiRv().realizer()'`, which returns an instance of the class `'uqBaseVectorRealizer<Q_V,Q_M>'`.

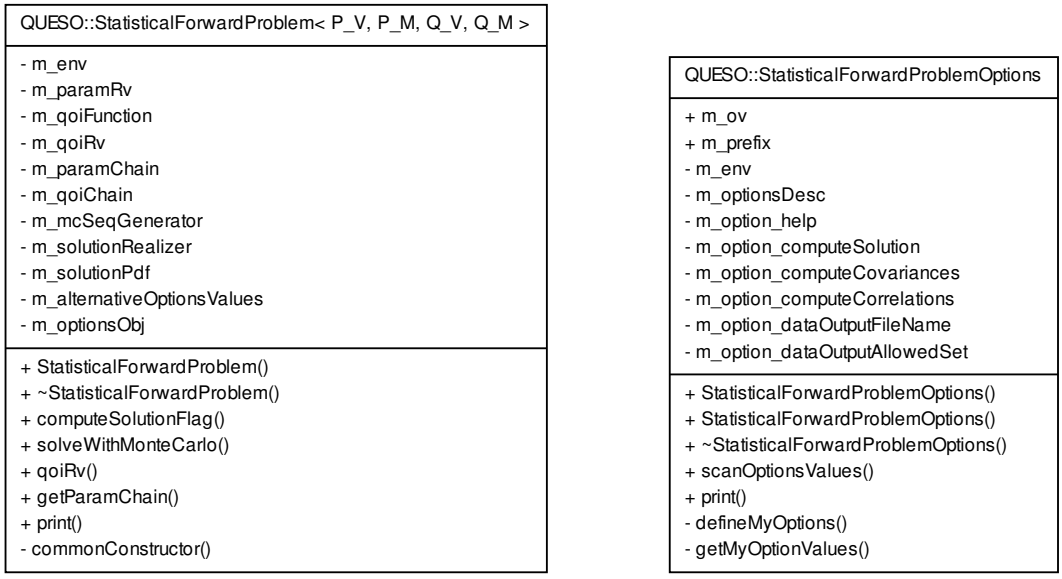
Figure 3.3.7b displays the statistical forward problem options class, i.e. that class that handles a variety of options for solving the SFP. Such options may be provided to QUESO at the user's input file; and they are listed in Table 3.3.4. In the table, `p-q` stands for parameter–quantity of interest.

Table 3.3.4: Input file options for a QUESO statistical forward problem.

Option Name	Default Value	Description
⟨PREFIX⟩fp_computeSolution	1	Computes the solution process
⟨PREFIX⟩fp_computeCovariances	1	Compute p-q covariances
⟨PREFIX⟩fp_computeCorrelations	1	Compute p-q correlations
⟨PREFIX⟩fp_dataOutputFileName	"."	Name of data output file
⟨PREFIX⟩fp_dataOutputAllowedSet	""	Subenvironments that will write to data output file

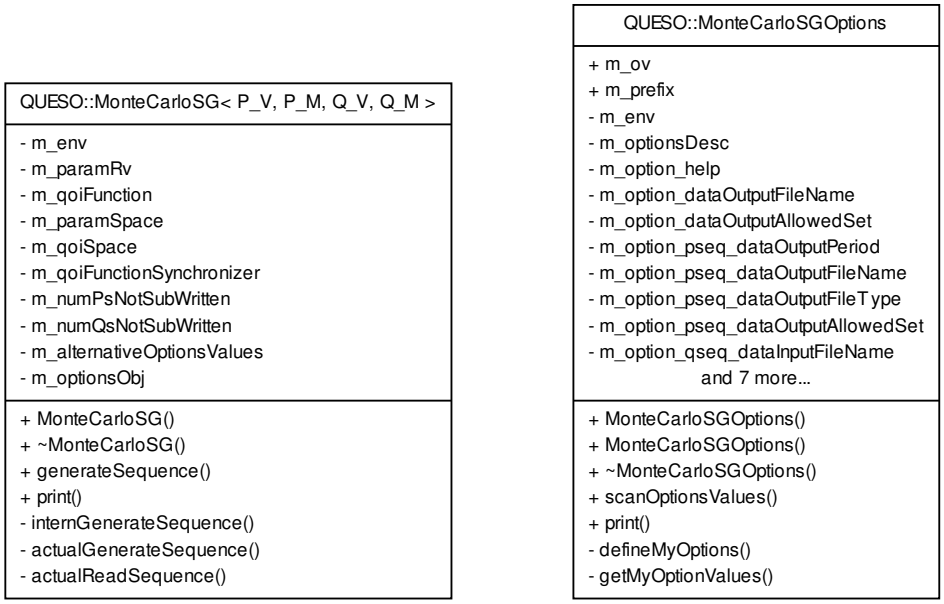
3.3.7 Monte Carlo Solver (and Options)

The templated class that implements a Monte Carlo generator of samples within QUESO is `MonteCarloSG<P_V,P_M,Q_V,Q_M>`, as illustrated in Figure 3.3.8a. This class has the requirement that the image set of the vector random variable and the domain set of the QoI function belong to vector spaces of equal dimensions. If the requirements are satisfied, the class constructor reads input options that begin with the string '`<PREFIX>_mc_`' (See Table 3.3.5). Options reading is handled by class `MonteCarloOptions`, which is illustrated in Figure 3.3.8b.



(a) StatisticalForwardProblem (b) StatisticalForwardProblemOptions

Figure 3.3.7: The statistical forward problem class, which implements the representation in Figure 1.2.2, and the statistical forward problem options class.



(a) MonteCarloSG (b) MonteCarloSGOptions

Figure 3.3.8: The Monte Carlo sequence generator class and the Monte Carlo sequence generator options class.

Table 3.3.5: Input file options for a QUESO statistical forward problem solved via Monte Carlo algorithm.

Option Name	Default Value
⟨PREFIX⟩mc_dataOutputFileName	"."
⟨PREFIX⟩mc_dataOutputAllowedSet	
⟨PREFIX⟩mc_pseq_dataOutputFileName	"."
⟨PREFIX⟩mc_pseq_dataOutputAllowedSet	
⟨PREFIX⟩mc_qseq_dataInputFileName	"."
⟨PREFIX⟩mc_qseq_size	100
⟨PREFIX⟩mc_qseq_displayPeriod	500
⟨PREFIX⟩mc_qseq_measureRunTimes	0
⟨PREFIX⟩mc_qseq_dataOutputFileName	"."
⟨PREFIX⟩mc_qseq_dataOutputAllowedSet	

3.4 Miscellaneous Classes and Routines

As the name suggests, QUESO miscellaneous classes and routines have a variety of routines. For instance, the function `MiscReadDoublesFromString` is used for reading the options input files and assigning the values to the respective variables, in `uqMonteCarloSGOptions::getMyOptionValues` and in `MetropolisHastingsSGOptions::getMyOptionValues`.

QUESO class `BaseOneDGrid` generates grids necessary for calculating the CDF of a RV; it is required by class `ArrayOfOneDGrids`, which, in turn, is used in both classes: `StatisticalForwardProblem` and `StatisticalInverseProblem`.

CHAPTER 4

Important Remarks

At this point, the user may feel comfortable and ready to start his/her validation and calibration exercises using QUESO. There are, however, a few quite important remarks that will make the linkage of the QUESO Library with the user application code possible. They are addressed in the following sections.

4.1 Revisiting Input Options

Input options are read from the QUESO input file, whose name is required by the constructor of the QUESO environment class. Herein, suppose that no prefix is defined, i.e., nothing will precede the input variables names (`PREFIX = ""` in Tables 3.1.1 – 3.3.5). An example of the use of prefixes may be found in the input file `tgaCycle.inp` under the subdirectory `/examples/validationCycle/` of QUESO installation tree.

The first part of a input file commonly handles the environment options. he variable assignment `env_numSubEnvironments = 1` indicates to QUESO that only one subenvironment should be used. The variable assignment `env_subDisplayFileName = outputData/ display` create both the subdirectory `outputData/` and a file named `display_sub0.txt` that contains all the options listed in the input file together with more specific information, such as the chain run time and the number of delayed rejections. The existence of file `display_sub0.txt` allows, for instance, the user in verifying the actual parameters read by QUESO.

For an SIP, the user may set up variables related to the DRAM algorithm. Six important variables are: `ip_mh_dr_maxNumExtraStages` defines how many extra candidates will be generated; `ip_mh_dr_listOfScalesForExtraStages` defines the list s of scaling factors that will multiply the covariance matrix. The variable `ip_mh_am_initialNonAdaptInterval` de-

fines the initial interval in which the proposal covariance matrix will not be changed; whereas `ip_mh_am_adaptInterval` defines the size of the interval in which each adapted proposal covariance matrix will be used. `ip_mh_am_eta` is a factor used to scale the proposal covariance matrix, usually set to be $2.4^2/d$, where d is the dimension of the problem [36, 21]. Finally, `ip_mh_am_epsilon` is the covariance regularization factor used in the DRAM algorithm.

For a SFP, the variable assignment `fp_computeSolution = 1` tells QUESO to compute the solution process; the assignment `fp_computeCovariances = 1`, instructs QUESO to compute parameter–QoI covariances, and analogously, `fp_computeCorrelations = 1` inform QUESO to compute parameter–QoI correlations. The name of the data output file can be set with variable `fp_dataOutputFileName arg`; and `fp_dataOutputAllowedSet` defines which subenvironments will write to data output file.

An example a complete input file used by QUESO to solve a SIP–SFP is presented in Section 6.3.5; however every application example included in QUESO build and installation directories `examples` has an options input file and the user is invited to familiarize him/herself with them.

4.2 Revisiting Priors

QUESO offers a variety of prior distributions: uniform, Gaussian, Beta, Gamma, Inverse Gamma, and Log Normal. Also, QUESO presents the option of concatenating any of those priors, through the Concatenated prior.

Concatenated priors are employed in problems with multiple random parameters. They allow one random parameter to have a different prior distribution then other; i.e., one variable may have a uniform prior distribution whereas other may have a Gaussian prior distribution.

It is important to notice that, in order to set a Gaussian prior, besides providing the mean, the user must also supply the variance, not the standard deviation.

4.3 Running with Multiple Chains or Monte Carlo Sequences

As presented in the previous section, the variable `env_numSubEnvironments` determines how many subenvironments QUESO will work with. Thus, if `env_numSubEnvironments=1`, then only one subenvironment will be used, and QUESO will use only one set on Monte Carlo chains of size defined by ones of the variables `ip_mh_rawChain_size` or `fp_mc_qseq_size`, depending either the user is solving a SIP or a SFP.

If the user wants to run QUESO with multiple chains or Monte Carlo sequences, then two variables have to be set in QUESO input file: `env_numSubEnvironments =` N_s, with $N_s > 1$ is the number of chains and/or Monte Carlo sequences of samples; and `env_seed =` $-z$, with $z \geqslant 1$, so that each processor sets the seed to value MPI_RANK+z. It is crucial that `env_seed` takes a negative value, otherwise all chain samples are going to be the same.

Also, the total number N_p of processors in the full communicator, usually named MPI_COMM_WORLD, needs to be a multiple of N_s.

4.4 Running with Models that Require Parallel Computing

It is possible to run QUESO with models that require parallel computing as long as total number of processors N_p is multiple of the number of subenvironments N_s. QUESO will internally create N_s subcommunicators, each of size N_p/N_s, and make sure that the likelihood and QoI routines are called for all processors in these subcommunicators – the likelihood/QoI routine will have available a communicator of size N_p/N_s. For instance, if $N_p = 2048$ and $N_s = 16$, then each likelihood/QoI will have available a communicator of size 128. s Each subcommunicator is accessible through `env.subComm()`. At the end of the simulation, there will be a total of N_s chains.

The user, however, must keep in mind the possible occurrence of race condition, especially in the case where the application is a black box and files are being accessed constantly (e.g. data is being written and read).

4.5 A Requirement for the DRAM Algorithm

Besides setting up the variables related to the DRAM algorithm in the input file, as described in Section 4.1 above, the user must also provide an initialized covariance matrix before calling the DRAM solver, `solveWithBayesMetropolisHastings(...)`, in his/her application code.

It is worth to note that this is rather a DRAM requirement [36], not a QUESO limitation. An example of the instantiation and initialization of a proposal covariance matrix and its subsequent use is presented in lines 145-147 of Listings 6.27, Section 6.3.4.

CHAPTER 5

Global Sensitivity Analysis

Global sensitivity analysis (GSA) involves a quantitative assessment of variability in the model output or quantity of interest (QoI) due to uncertain model parameters. Variance based approaches relying on pseudo-random sampling of prior distributions of the parameters have been used effectively [11, 47, 45]. However, it can be understood that estimating the sensitivity indices ('first order effect' and 'total effect') can be computationally intensive especially in situations where a complex multiphysics model is simulated for a considered set of parameter samples. In order to mitigate such computational costs, alternative strategies involving construction and application of cheap surrogates for the models have been developed. Examples include polynomial chaos expansions [61, 16] which have been used extensively for physics-based models and admit simple analytical expressions for computing the sensitivity indices [59, 58]. Other examples include response surfaces based on Kriging, and radial basis functions [20].

Surrogate models, however, are not the central theme of this chapter. Instead, we focus our attention on exploiting QUESO to perform a prior based, parametric GSA. As mentioned earlier, the analysis helps determine relative contribution to the variance of the QoI and thus the relative importance of the stochastic model parameters. Potentially, such an analysis could help reduce the dimensionality of an inverse problem. In the following section, we provide a mathematical framework for the first order effect and total effect sensitivity indices as well as a brief survey of existing estimators for these indices. In section 5.2, we provide an algorithm based on [44] for using QUESO to perform a prior-based parametric GSA and further demonstrate its implementation using a simple exercise involving sensitivity analysis of the slope and intercept of a straight line.

5.1 Sensitivity Indices

Consider a model, $\mathcal{G}(\boldsymbol{\theta})$, where $\boldsymbol{\theta}$ denotes a vector of model parameters. Variance based measures for the first order effect and total effect sensitivity indices can be computed as discussed below.

5.1.1 First Order Effect

The first order effect sensitivity index $\mathcal{S}(\theta_i)$ for a specific model parameter (θ_i) quantifies relative contribution to the variance of the QoI strictly due to (θ_i) and does not consider its interactions with other parameters. Mathematically, this is expressed as follows:

$$\mathcal{S}(\theta_i) = \frac{\mathbb{V}_{\theta_i}(\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{G}|\theta_i])}{\mathbb{V}(\mathcal{G})} \tag{5.1.1}$$

where θ_i is the i^{th} parameter for which the first order effect index is to be computed and $\boldsymbol{\theta}_{\sim i}$ denotes a vector of all parameters except θ_i. The quantity, $\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{G}|\theta_i]$ denotes the mean estimate of the model output taken over all possible values of $\boldsymbol{\theta}_{\sim i}$ while using a fixed value of θ_i. The outer variance of this expectation is hence computed over all possible values of θ_i. The quantity, $\mathbb{V}_{\theta_i}(\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{G}|\theta_i])$ can also be understood as the expected reduction in variance due to fixed θ_i. It is normalized by, $\mathbb{V}(\mathcal{G})$, i.e. the total variance of of the model output.

5.1.2 Total Effect

The total effect sensitivity index $\mathcal{T}(\theta_i)$ for a specific model parameter (θ_i) quantifies relative contribution to the variance of the QoI due to (θ_i) and accounts for its interactions with other parameters. Mathematically, this is expressed as follows:

$$\mathcal{T}(\theta_i) = \frac{\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathbb{V}_{\theta_i}(\mathcal{G}|\boldsymbol{\theta}_{\sim i})]}{\mathbb{V}(\mathcal{G})} \tag{5.1.2}$$

$$= 1 - \frac{\mathbb{V}_{\boldsymbol{\theta}_{\sim i}}(\mathbb{E}_{\theta_i}[\mathcal{G}|\boldsymbol{\theta}_{\sim i}])}{\mathbb{V}(\mathcal{G})} \tag{5.1.3}$$

where $\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathbb{V}_{\theta_i}(\mathcal{G}|\boldsymbol{\theta}_{\sim i}))$ is the expected variance when all parameters except θ_i could be fixed. We can also interpret $\mathcal{T}(\theta_i)$ using the quantity, $\mathbb{V}_{\boldsymbol{\theta}_{\sim i}}(\mathbb{E}_{\theta_i}[\mathcal{G}|\boldsymbol{\theta}_{\sim i}])$ which denotes the expected reduction in variance when all parameters except θ_i could be fixed.

5.1.3 Estimation of $\mathcal{S}(\theta_i)$ and $\mathcal{T}(\theta_i)$

In order to estimate the first order effect and the total effect sensitivity indices, we need to numerically estimate the quantities, $\mathbb{V}_{\theta_i}(\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{G}|\theta_i])$ and $\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathbb{V}_{\theta_i}(\mathcal{G}|\boldsymbol{\theta}_{\sim i})]$ respectively. Tabulated below are commonly used estimators. As discussed in [44], we consider two independent

set of samples denoted by the matrices, $\boldsymbol{A}$ and $\boldsymbol{B}$. Additionally, we consider derived sets of samples denoted by the matrices, $\boldsymbol{A}_{\boldsymbol{B}}^{(i)}$ where all columns are from $\boldsymbol{A}$ except the i^{th} column which is from $\boldsymbol{B}$. Similarly, we can construct the matrix, $\boldsymbol{B}_{\boldsymbol{A}}^{(i)}$ as well.

	Estimator	Reference
$\mathbb{V}_{\theta_i}(\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{G}\|\theta_i])$	$\frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{A})_k f(\boldsymbol{B}_{\boldsymbol{A}}^{(i)})_k - f_0^2$	Sobol 1990 [47]
	$\frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{B})_k (f(\boldsymbol{A}_{\boldsymbol{B}}^{(i)})_k - f(\boldsymbol{A})_k)$	Saltelli 2010 [44]
	$\mathbb{V}(\mathcal{G}) - \frac{1}{2N}\sum_{k=1}^{N} (f(\boldsymbol{B})_k - f(\boldsymbol{A}_{\boldsymbol{B}}^{(i)})_k)^2$	Jansen 1999 [30]
$\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathbb{V}_{\theta_i}(\mathcal{G}\|\boldsymbol{\theta}_{\sim i})]$	$\mathbb{V}(\mathcal{G}) - \frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{A})_k f(\boldsymbol{A}_{\boldsymbol{B}}^{(i)})_k + f_0^2$	Homma 1996 [26]
	$\frac{1}{N}\sum_{k=1}^{N} f(\boldsymbol{A})_k (f(\boldsymbol{A})_k - f(\boldsymbol{A}_{\boldsymbol{B}}^{(i)})_k)$	Sobol 2007 [48]
	$\frac{1}{2N}\sum_{k=1}^{N} (f(\boldsymbol{A})_k - f(\boldsymbol{A}_{\boldsymbol{B}}^{(i)})_k)^2$	Jansen 1999 [30]

Table 5.1.1: Commonly used estimators and corresponding references for $\mathbb{V}_{\theta_i}(\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{G}|\theta_i])$ and $\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathbb{V}_{\theta_i}(\mathcal{G}|\boldsymbol{\theta}_{\sim i})]$.

Statistical forward problem (SFP) can be solved with QUESO by computing the QoI for pseudo-random samples drawn from the posterior distribution as discussed in 3.3.6. However, for GSA, we need to generate two independent data sets comprising pseudo-random samples for the model parameters, drawn from their individual prior distributions. QoIs are estimated for both sets of samples as well derived matrices for the model parameters, as discussed earlier.

In the following section, we present a simple application involving sensitivity analysis of the slope and y-intercept of a straight line. SFP on samples from prior distributions of the model parameters is solved to generate the data which can further be used to compute the first order effect and total effect sensitivity indices.

5.2 Application

We consider the following equation for a straight line:

$$y = mx + c \tag{5.2.1}$$

The slope, m and the y-intercept, c are considered to be uniformly distributed in the intervals, [2, 5] and [3, 7] respectively. For reference purposes, we provide an algorithm followed by the C++ code which interfaces with QUESO to generate the required data for GSA as follows. In order to estimate the first order effect and the total effect sensitivity indices, we solve the forward problem in QUESO to generate the required set of data. Specifically, we need to generate $(2n+2)$ data files for n model parameters. Hence, in the present case, we need 6 data files as listed and described below. Note that the pseudorandom samples pertaining to the individual model parameters are given by their respective columns. In this

case, column 1 corresponds to the slope, m and column 2 corresponds to the y-intercept, c. Moreover, y in the above equation is regarded as the QoI.

1. `qoi_samplesA.txt`: Pseudo-random samples and corresponding QoI estimates, regarded as set $\boldsymbol{A}$.

2. `qoi_samplesB.txt`: Pseudo-random samples and corresponding QoI estimates, regarded as set $\boldsymbol{B}$.

3. `m_qoi_samplesAi.txt`: All columns from set $\boldsymbol{A}$ except the i^{th} (i=1) column which is from set $\boldsymbol{B}$ and corresponding QoI estimates.

4. `m_qoi_samplesBi.txt`: All columns from set $\boldsymbol{B}$ except the i^{th} (i=1) column which is from set $\boldsymbol{A}$ and corresponding QoI estimates.

5. `c_qoi_samplesAi.txt`: All columns from set $\boldsymbol{A}$ except the i^{th} (i=2) column which is from set $\boldsymbol{B}$ and corresponding QoI estimates.

6. `c_qoi_samplesBi.txt`: All columns from set $\boldsymbol{B}$ except the i^{th} (i=2) column which is from set $\boldsymbol{A}$ and corresponding QoI estimates.

In the above list, let us denote files in 3–6 as the set of derived files. The following algorithm provides a sequence of steps as well as snippets of code which could be used to generate the set of data files to compute the sensitivity indices. Relevant source files have also been included later in this section.

Algorithm: Generating data for GSA

1: **procedure** SOLVING SFP WITH QUESO
2: Instantiate a QoI object (`qoi_mc`):
`Qoi_mc<> qoi_mc("qoi_", paramDomain, qoiSpace);`
3: Instantiate the forward problem (`fp_mc`):
`QUESO::StatisticalForwardProblem<> fp_mc("", NULL, priorRv, qoi_mc, qoiRv);`
4: Solve the forward problem to generate the data file, `qoi_samplesA.txt` i.e. set $\boldsymbol{A}$.
`fp_mc.solveWithMonteCarlo(NULL);`
5: Repeat steps 2–4 to generate the data file, `qoi_samplesB.txt` i.e. set $\boldsymbol{B}$.
6: Use the two sets of data, $\boldsymbol{A}$ and $\boldsymbol{B}$, to generate intermediate data files comprising samples, $\boldsymbol{A}_{\boldsymbol{B}}^{(i)}$ and $\boldsymbol{B}_{\boldsymbol{A}}^{(i)}$ for both m and c.
7: Repeat steps 2–4 four times to generate the derived files: `m_qoi_samplesAi.txt`, `m_qoi_samplesBi.txt`, `c_qoi_samplesAi.txt` and `c_qoi_samplesAi.txt`. (Instead of estimating the QoI for pseudorandom samples from the prior, the QoI is now computed for the set of samples in corresponding intermediate data files generated in the previous step.)
8: Compute $\mathcal{S}(\theta_i)$ and $\mathcal{T}(\theta_i)$ using the set of 6 data files generated in previous steps.
9: **end procedure**

The source code for generating the required set of data files is provided by the header file, `sensitivity_mc.h` and the corresponding source file, `sensitivity_mc.C` as follows.

```
#ifndef QUESO_EXAMPLE_SENSITIVITY_MC_H
#define QUESO_EXAMPLE_SENSITIVITY_MC_H

#include <queso/VectorFunction.h>
#include <queso/DistArray.h>
#include <fstream>

template<class P_V = QUESO::GslVector, class P_M = QUESO::GslMatrix,
   class Q_V = QUESO::GslVector, class Q_M = QUESO::GslMatrix>
class Qoi_mc : public QUESO::BaseVectorFunction<P_V, P_M, Q_V, Q_M>
{
public:
  Qoi_mc(const char * prefix, const QUESO::VectorSet<P_V, P_M> & domainSet,
      const QUESO::VectorSet<Q_V, Q_M> & imageSet);
  virtual ~Qoi_mc();
  virtual void compute(const P_V & domainVector, const P_V * domainDirection,
    Q_V & imageVector, QUESO::DistArray<P_V *> * gradVectors,
    QUESO::DistArray<P_M *> * hessianMatrices,
    QUESO::DistArray<P_V *> * hessianEffects) const;

private:
  double x_loc;
  mutable double m,c,mf,cf,count;
  mutable std::fstream qoi_samples;
  mutable std::fstream samples;

};

#endif
```

Listing 5.1: File `sensitivity_mc.h`.

```
1  #include <cmath>
2  #include <fstream>
3  #include <iomanip> // for setprecision
4
5  #include <queso/GslVector.h>
6  #include <queso/GslMatrix.h>
7  #include <sensitivity_mc.h>
8
9  template<class P_V, class P_M, class Q_V, class Q_M>
10 Qoi_mc<P_V, P_M, Q_V, Q_M>::Qoi_mc(const char * prefix,
11     const QUESO::VectorSet<P_V, P_M> & domainSet,
12     const QUESO::VectorSet<Q_V, Q_M> & imageSet)
13   : QUESO::BaseVectorFunction<P_V, P_M, Q_V, Q_M>(prefix, domainSet, imageSet),
14     x_loc(3)
15 {
16 }
17
18 template<class P_V, class P_M, class Q_V, class Q_M>
19 Qoi_mc<P_V, P_M, Q_V, Q_M>::~Qoi_mc()
20 {
21   // Deconstruct here
22 }
23
24 template<class P_V, class P_M, class Q_V, class Q_M>
25 void
26 Qoi_mc<P_V, P_M, Q_V, Q_M>::compute(const P_V & domainVector,
```

```
27      const P_V * domainDirection,
28      Q_V & imageVector, QUESO::DistArray<P_V *> * gradVectors,
29      QUESO::DistArray<P_M *> * hessianMatrices,
30      QUESO::DistArray<P_V *> * hessianEffects) const
31  {
32    if (domainVector.sizeLocal() != 2) {
33      queso_error_msg("domainVector does not have size 2");
34    }
35    if (imageVector.sizeLocal() != 1) {
36      queso_error_msg("imageVector does not have size 1");
37    }
38
39    qoi_samples.open ("c_qoi_samplesAi.txt", std::fstream::in | std::fstream::out | std::
        fstream::app);
40
41   // ----Generate Qoi using samples from a text files -------------
42   count++;
43   samples.open ("./files_sense/c_samples_Ai.txt", std::fstream::in | std::fstream::out | std::
        fstream::app);
44
45   int cou = 1;
46
47   while (samples >> mf >> cf){
48         if (cou == count){
49            m = mf;
50      c = cf;
51          break;
52         }
53         cou++;
54   }
55
56  // ------- Generate Qoi using pseudo-random MC samples ------------
57  //  std::cout << "m = " << domainVector[0] << std::endl;
58  //  m = domainVector[0];  // Sample of the RV 'line slope'
59  //  c = domainVector[1];  // Sample of the RV 'y-intercept'
60    double y_obs = 0.0;
61    y_obs = m*x_loc + c;
62
63    qoi_samples << std::setprecision(4) << y_obs << "\t\t" << m << "\t\t" << c << std::endl;
64
65    imageVector[0] = y_obs;
66    qoi_samples.close();
67    samples.close();
68  }
69
70  template class Qoi_mc<QUESO::GslVector, QUESO::GslMatrix, QUESO::GslVector,
```

Listing 5.2: File `sensitivity_mc.C`.

As shown in lines, 42–54 in the above listing for `sensitivity_mc.C`, in order to generate the set of derived files, we compute the QoI by reading samples from corresponding intermediate files (such as `c_samples_Ai.txt` in this case). Whereas, for generating the pair of files, `qoi_samplesA.txt` and `qoi_samplesB.txt`, we compute the QoI for pseudo-random samples drawn from the prior distributions for m and c as shown in lines, 57–59 which are commented in the present case.

5.3 Results

In this section, we provide results for the first order effect sensitivity index as computed using approximations from Sobol [47] and Saltelli *et al.* [44] for the quantity, $\mathbb{V}_{\theta_i}(\mathbb{E}_{\boldsymbol{\theta}_{\sim i}}[\mathcal{G}|\theta_i])$ as provided in Table 5.1.1.

In Figure 5.3.1(a), we perform a convergence study for the first order effect sensitivity index, $\mathcal{S}(\theta_i)$. It is observed that for a small number of samples (< 5000), estimates from both, Sobol and Saltelli estimators exhibit large oscillations with increase in sample size indicating that the estimates have not yet converged to a stable value. Moreover, we observe large discrepancies are observed between estimates obtained from the two estimators in this regime. However, as we increase the sample size above 10000, it the two estimators seem to converge to stable values that are in close agreement. This phenomenon underscores the need for a large enough sample size for computing the sensitivity indices using pseudo-random sampling techniques. Optimizing the required number of samples in a way that the sensitivity indices are estimated within reasonable accuracy with the least possible sample size is a challenging task and depends on the map from the uncertain model parameters to the quantity of interest.

Figure 5.3.1(b), illustrates estimates for $\mathcal{S}(\theta_i)$ for the slope, m and the y-intercept, c based on 25000 samples. For both parameters, estimates from Sobol [47] and Saltelli *et al.* [44] are in close agreement. Moreover, the QoI (y) is observed to be much more sensitive to the uncertainty in the slope as compared to the y-intercept.

5.4 Concluding Remarks

Global Sensitivity Analysis can be a computationally challenging task especially if it involves model estimates for a complex multiphysics problem. However, in case the forward solve of the model is inexpensive, one can exploit the SFP machinery in QUESO to compute the sensitivity indices as demonstrated with the help of a simple example in this chapter. Moreover, when stochastic formulations are proposed to capture the inadequacy in a model, parametric sensitivity analysis based on prior distributions of the stochastic parameters can potentially reduce the dimensionality of an inverse problem. Depending upon the nature of the problem, one can benefit from valuable insight into relative importance of the parameters with much fewer samples than required for convergence of the estimates as observed in the case of the straight line problem discussed in this chapter.

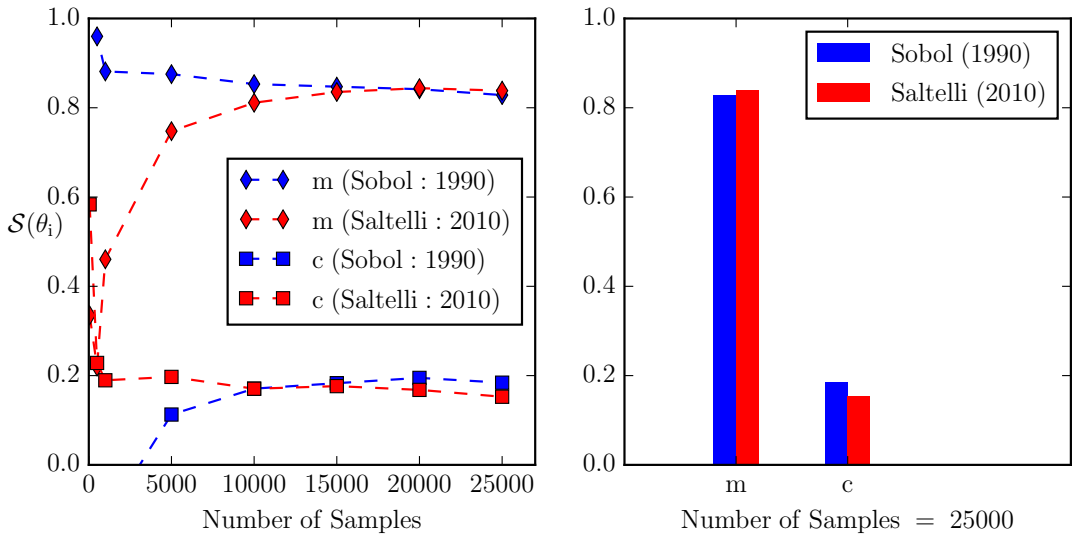


Figure 5.3.1: (a) Analysis of convergence for the first order sensitivity indices for slope, m and y-intercept, c with increasing sample size. (b) Bar-graph representation of estimates for $\mathcal{S}(\theta_i)$ based on estimators suggested by Sobol [47] and Saltelli *et al.* [44] using 25000 pseudo-random samples.

CHAPTER 6

QUESO Examples

This chapter assumes that the user has successfully installed QUESO and its dependencies. It presents a variety of examples of how to use QUESO in order to develop applications.

There are examples that solve a statistical inverse problem (Sections 6.1, 6.5, 6.6 and 6.7), a statistical forward problem (Section 6.2) or a combination of both, where the solution of the former serves as input to the later (Sections 6.3 and 6.4). Three of the first four examples (Sections 6.1, 6.3 –6.4) use the DRAM algorithm for solving the SIP, and the last three examples use the Multilevel algorithm. Each section presents:

- the mathematical models for the SIP and/or the SFP;
- the application codes that translate the mathematical language into C++ using the QUESO classes and algorithms;
- the input file that contains a list of options for either the Markov chain Monte Carlo algorithm or the Multilevel algorithm (in case of SIPs) and the Monte Carlo algorithm (in case of SFPs) which will be used by QUESO classes and algorithms;
- examples of Makefiles which may be used to link the code with QUESO library;
- how to plot figures using Matlab/GNU Octave and the output data generated by each application.

All the examples presented in this chapter may be found under the directory `examples` in both QUESO installation and build directories and are compatible with QUESO 0.56.0.

Note: Even though the Multilevel method is a methodology very useful for stochastic system model class comparison (model updating, model selection, model validation) [6], such tasks are not discussed in this manual. Thus the explicit dependency of the statistical variables on the predictive model in the set M_j as presented in Section 1.4.2 are omitted herein.

6.1 simpleStatisticalInverseProblem

According to the Bayesian paradigm, the unobservable parameters in a statistical model are treated as random. When no data is available, a prior distribution is used to quantify our knowledge about the parameter. When data are available, we can update our prior knowledge using the conditional distribution of parameters, given the data. The transition from the prior to the posterior is possible via the Bayes theorem:

$$\pi_{\text{posterior}}(\boldsymbol{\theta}|\mathbf{d}) = \frac{\pi_{\text{prior}}(\boldsymbol{\theta})\pi_{\text{likelihood}}(\mathbf{d}|\boldsymbol{\theta})}{\pi(\mathbf{d})}$$

In this example, suppose a random variable of interest with two parameters $\boldsymbol{\theta} \in \mathbb{R}^2$ has a uniform prior distribution, and suppose that a suitable likelihood has normal distribution with mean $\boldsymbol{\mu}$ and covariance matrix $\mathbf{C}$, given by:

$$\boldsymbol{\mu} = \begin{pmatrix} -1 \\ 2 \end{pmatrix} \quad \text{and} \quad \mathbf{C} = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}. \tag{6.1.1}$$

Therefore, we have:

$$\pi_{\text{prior}}(\boldsymbol{\theta}) \propto 1$$

and

$$\pi_{\text{like}}(\boldsymbol{\theta}) \propto \exp\left(-\frac{1}{2}\left[(\boldsymbol{\theta}-\boldsymbol{\mu})^T[\mathbf{C}^{-1}](\boldsymbol{\theta}-\boldsymbol{\mu})\right]\right),$$

where

$$\boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \in \mathbb{R}^2.$$

Therefore, posterior PDF is given by:

$$\pi_{\text{post}}(\boldsymbol{\theta}) \propto e^{-\frac{1}{2}\left\{(\boldsymbol{\theta}-\boldsymbol{\mu})^T[\mathbf{C}^{-1}](\boldsymbol{\theta}-\boldsymbol{\mu})\right\}}. \tag{6.1.2}$$

In this example, we can replace the values for the mean and covariance matrix given in Equation (6.1.1) into Equation (6.1.2), in order to analytically compute both the posterior PDF:

$$\begin{aligned} \pi_{\text{post}}(\boldsymbol{\theta}) &= \frac{1}{4\pi}\exp\left(-\frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\mu})^T[\mathbf{C}^{-1}](\boldsymbol{\theta}-\boldsymbol{\mu})\right) \\ &= \frac{1}{4\pi}\exp\left(-\frac{1}{8}(\theta_1+1)^2 - \frac{1}{2}(\theta_2-2)^2\right), \end{aligned}$$

and the marginal results for θ_1 and θ_2:

$$\begin{aligned} \pi_{\text{post}}(\theta_1) &= \frac{1}{2\sqrt{2\pi}}\exp\left(-\frac{1}{8}(\theta_1+1)^2\right), \\ \pi_{\text{post}}(\theta_1) &= \frac{1}{\sqrt{2\pi}}\exp\left(-\frac{1}{2}(\theta_2-2)^2\right). \end{aligned} \tag{6.1.3}$$

Recall that the posterior PDF given in Equation (6.1.2) can be sampled through the expression:

$$\boldsymbol{\mu} + \mathbf{C}^{1/2}\mathcal{N}(0, I), \tag{6.1.4}$$

where $\mathcal{N}(0, I)$ designates a Gaussian joint PDF of zero mean and unit covariance matrix, and $\mathbf{C}^{1/2}$ is given by:

$$\mathbf{C}^{1/2} = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}.$$

Thus, in this simple statistical inverse problem, we use QUESO implementation of the Markov chain algorithm to sample the posterior (6.1.2) via Expression (6.1.4) and compare the calculated marginal results for θ_1 and θ_2 against the analytical formulas given in Equation (6.1.3).

Note: Due to the possibility to compare QUESO sampling algorithms to analytical expressions, this example is also used in the verification procedures and regression tests within QUESO, and it is reproduced in the directory `tests/t02_sip_sfp`.

6.1.1 Running the Example

To run the executable provided (available after QUESO installation), enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/
$ cd examples/simpleStatisticalInverseProblem
$ rm outputData/*
$ ./exSimpleStatisticalInverseProblem_gsl example.inp
$ matlab
   $ simple_ip_plots      # inside matlab
   $ exit                 # inside matlab
$ ls -l outputData/*.png
 simple_ip_autocorrelation_raw_filt.png  simple_ip_hist_filt.png
 simple_ip_cdf_filt.png                  simple_ip_hist_raw.png
 simple_ip_cdf_raw.png                   simple_ip_kde_filt.png
 simple_ip_chain_pos_filt.png            simple_ip_kde_raw.png
```

As a result, the user should have created several of PNG figures containing marginal posterior PDF, chain positions, histograms, cumulative density distributions and autocorrelation of both parameters. The name of the figure files have been chosen to be informative, as shown in the Listing above.

It is worth noting presence of an argument passed to the executable in the example, namely '`example.inp`'. The argument is a input file to be provided to QUESO with options for the solution of the SIP and/or SFP; and it is always required. Each option in the input file is related to one (or more) of the QUESO classes, and is presented throughout Chapter 3.

6.1.2 Example Code

The source code for the example is composed of 5 files: `example_main.C` (Listing 6.1), `example_likelihood.h` and `example_likelihood.C` (Listings 6.2 and 6.3), `example_compute.h` and `example_compute.C` (Listings 6.4 and 6.5).

```
#include <example_compute.h>

int main(int argc, char* argv[])
{
  // Initialize environment
#ifdef QUESO_HAS_MPI
  MPI_Init(&argc,&argv);

  UQ_FATAL_TEST_MACRO(argc != 2,
                      QUESO::UQ_UNAVAILABLE_RANK,
                      "main()",
                      "input file must be specified in command line as argv[1], just after
                          executable argv[0]");

  QUESO::FullEnvironment* env =  new QUESO::FullEnvironment(MPI_COMM_WORLD,argv[1],"",NULL);
#else
  QUESO::FullEnvironment* env =  new QUESO::FullEnvironment(argv[1],"",NULL);
#endif

  // Compute
  compute(*env);

  // Finalize environment
  delete env;
#ifdef QUESO_HAS_MPI
  MPI_Finalize();
#endif

  return 0;
}
```

Listing 6.1: File `example_main.C`.

```
#ifndef EX_LIKELIHOOD_H
#define EX_LIKELIHOOD_H

#include <queso/GslMatrix.h>

struct
likelihoodRoutine_DataType
{
  const QUESO::GslVector* meanVector;
  const QUESO::GslMatrix* covMatrix;
};

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect);

#endif
```

Listing 6.2: File `example_likelihood.h`.

```
#include <example_likelihood.h>

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect)
{
  // Logic just to avoid warnings from INTEL compiler
  const QUESO::GslVector* aux1 = paramDirection;
  if (aux1) {};
  aux1 = gradVector;
  aux1 = hessianEffect;
  QUESO::GslMatrix* aux2 = hessianMatrix;
  if (aux2) {};

  // Just checking: the user, at the application level, expects
  // vector 'paramValues' to have size 2.
  UQ_FATAL_TEST_MACRO(paramValues.sizeGlobal() != 2,
                      QUESO::UQ_UNAVAILABLE_RANK,
                      "likelihoodRoutine()",
                      "paramValues vector does not have size 2");

  // Actual code
  //
  // This code exemplifies multiple Metropolis-Hastings solvers, each calling this likelihood
  // routine. In this simple example, only node 0 in each subenvironment does the job even
  // though there might be more than one node per sub-environment. In a more realistic
  // situation, if the user is asking for multiple nodes per subenvironment, then the model
  // code in the likelihood routines might really demand more than one node. Here we use
  // 'env.subRank()' only. A realistic application might want to use either 'env.subComm()'
  // or 'env.subComm().Comm()'.

  double result = 0.;
  const QUESO::BaseEnvironment& env = paramValues.env();
  if (env.subRank() == 0) {
    const QUESO::GslVector& meanVector =
      *((likelihoodRoutine_DataType *) functionDataPtr)->meanVector;
    const QUESO::GslMatrix& covMatrix  =
      *((likelihoodRoutine_DataType *) functionDataPtr)->covMatrix;

    QUESO::GslVector diffVec(paramValues - meanVector);

    result= scalarProduct(diffVec,covMatrix.invertMultiply(diffVec));
  }
  else {
    // Do nothing;
  }

  return -.5*result;
}
```

Listing 6.3: File `example_likelihood.C`.

```
#ifndef EX_COMPUTE_H
#define EX_COMPUTE_H

#include <queso/Environment.h>

void compute(const QUESO::FullEnvironment& env);

#endif
```

Listing 6.4: File `example_compute.h`.

```
#include <example_compute.h>
#include <example_likelihood.h>
#include <queso/GenericScalarFunction.h>
#include <queso/GslMatrix.h>
#include <queso/UniformVectorRV.h>
#include <queso/StatisticalInverseProblem.h>

void compute(const QUESO::FullEnvironment& env) {
  // Step 1 of 5: Instantiate the parameter space
  QUESO::VectorSpace<QUESO::GslVector,QUESO::GslMatrix>
    paramSpace(env, "param_", 2, NULL);

  // Step 2 of 5: Instantiate the parameter domain
  QUESO::GslVector paramMins(paramSpace.zeroVector());
  paramMins.cwSet(-INFINITY);
  QUESO::GslVector paramMaxs(paramSpace.zeroVector());
  paramMaxs.cwSet( INFINITY);
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomain("param_",paramSpace,paramMins,paramMaxs);

  // Step 3 of 5: Instantiate the likelihood function object
  QUESO::GslVector meanVector(paramSpace.zeroVector());
  meanVector[0] = -1;
  meanVector[1] =  2;

  QUESO::GslMatrix covMatrix(paramSpace.zeroVector());
  covMatrix(0,0) = 4.; covMatrix(0,1) = 0.;
  covMatrix(1,0) = 0.; covMatrix(1,1) = 1.;

  likelihoodRoutine_DataType likelihoodRoutine_Data;
  likelihoodRoutine_Data.meanVector = &meanVector;
  likelihoodRoutine_Data.covMatrix  = &covMatrix;

  QUESO::GenericScalarFunction<QUESO::GslVector,QUESO::GslMatrix>
    likelihoodFunctionObj("like_",
                          paramDomain,
                          likelihoodRoutine,
                          (void *) &likelihoodRoutine_Data,
                          true); // routine computes [ln(function)]

  // Step 4 of 5: Instantiate the inverse problem
  QUESO::UniformVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    priorRv("prior_", paramDomain);
  QUESO::GenericVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    postRv("post_", paramSpace);
  QUESO::StatisticalInverseProblem<QUESO::GslVector,QUESO::GslMatrix>
    ip("", NULL, priorRv, likelihoodFunctionObj, postRv);

  // Step 5 of 5: Solve the inverse problem
  QUESO::GslVector paramInitials(paramSpace.zeroVector());
  paramInitials[0] = 0.1;
```

```
  paramInitials[1] = -1.4;

  QUESO::GslMatrix proposalCovMatrix(paramSpace.zeroVector());
  proposalCovMatrix(0,0) = 8.; proposalCovMatrix(0,1) = 4.;
  proposalCovMatrix(1,0) = 4.; proposalCovMatrix(1,1) = 16.;

  ip.solveWithBayesMetropolisHastings(NULL,paramInitials, &proposalCovMatrix);

  return;
}
```

Listing 6.5: File `example_compute.C`.

6.1.3 Input File

QUESO reads an input file for solving statistical problems. In the case of a SIP, it expects a list of options for MCMC (or Multilevel), together with options for QUESO environment; such as the amount of processors to be used and the seed for its random algorithms. Note that the names of the variables have been designed to be informative:

`env:` refers to QUESO environment;

`ip:` refers to inverse problem;

`mh:` refers to Metropolis-Hastings;

`dr:` refers to delayed rejection;

`am:` refers to adaptive Metropolis;

`rawChain:` refers to the raw, entire chain;

`filteredChain:` refers to a filtered chain (related to a specified `lag`);

The options used for solving this simple SIP are displayed in Listing 6.6.

```
###############################################
# UQ Environment
###############################################
#env_help                 = anything
env_numSubEnvironments   = 1
env_subDisplayFileName   = outputData/display
env_subDisplayAllowAll   = 0
env_subDisplayAllowedSet = 0
env_displayVerbosity     = 2
env_syncVerbosity        = 0
env_seed                 = 0

###############################################
# Statistical inverse problem (ip)
###############################################
#ip_help                  = anything
ip_computeSolution      = 1
ip_dataOutputFileName   = outputData/sipOutput
ip_dataOutputAllowedSet = 0

###############################################
# 'ip_': information for Metropolis-Hastings algorithm
###############################################
#ip_mh_help                = anything
ip_mh_dataOutputFileName   = outputData/sipOutput
```

```
ip_mh_dataOutputAllowedSet = 0 1

ip_mh_rawChain_dataInputFileName    = .
ip_mh_rawChain_size                 = 32768
ip_mh_rawChain_generateExtra        = 0
ip_mh_rawChain_displayPeriod        = 50000
ip_mh_rawChain_measureRunTimes      = 1
ip_mh_rawChain_dataOutputFileName   = outputData/ip_raw_chain
ip_mh_rawChain_dataOutputAllowedSet = 0 1
ip_mh_rawChain_computeStats         = 1

ip_mh_displayCandidates             = 0
ip_mh_putOutOfBoundsInChain         = 1
ip_mh_tk_useLocalHessian            = 0
ip_mh_tk_useNewtonComponent         = 1
ip_mh_dr_maxNumExtraStages          = 1
ip_mh_dr_listOfScalesForExtraStages = 5.
ip_mh_am_initialNonAdaptInterval    = 0
ip_mh_am_adaptInterval              = 100
ip_mh_am_eta                        = 1.92
ip_mh_am_epsilon                    = 1.e-5

ip_mh_filteredChain_generate             = 1
ip_mh_filteredChain_discardedPortion     = 0.
ip_mh_filteredChain_lag                  = 16
ip_mh_filteredChain_dataOutputFileName   = outputData/ip_filt_chain
ip_mh_filteredChain_dataOutputAllowedSet = 0 1
```

Listing 6.6: Options for QUESO library used in application code (Listings 6.1-6.5).

6.1.4 Create your own Makefile

Makefiles are special format files that together with the make utility will help one to compile and automatically build and manage projects (programs). Listing 6.7 presents a Makefile, named '`Makefile_sip_example_margarida`', that may be used to compile the code and create the executable `simple_sip_example`. Naturally, it must be adapted to the user's settings, i.e., it has to have the correct paths for the user's libraries that have actually been used to compile and install QUESO (see Sections 2.1–2.4).

```
QUESO_DIR = /path/to/queso
BOOST_DIR = /path/to/boost
GSL_DIR   = /path/to/gsl

INC_PATHS = \
   -I. \
   -I$(QUESO_DIR)/include \
   -I$(BOOST_DIR)/include \
   -I$(GSL_DIR)/include

LIBS = \
   -L$(QUESO_DIR)/lib -lqueso \
   -L$(BOOST_DIR)/lib -lboost_program_options \
   -L$(GSL_DIR)/lib -lgsl

CXX = mpic++
CXXFLAGS += -g -Wall -c
```

```
default: all

.SUFFIXES: .o .C

all:       example_sip

clean:
   rm -f *~
   rm -f *.o
   rm -f simple_sip_example

example_sip: example_main.o example_likelihood.o example_compute.o
   $(CXX) example_main.o \
          example_likelihood.o \
          example_compute.o \
          -o simple_sip_example $(LIBS)

%.o: %.C
   $(CXX) $(INC_PATHS) $(CXXFLAGS) $<
```

Listing 6.7: Makefile for the application code in Listings 6.1-6.5

Thus, to compile, build and execute the code, the user just needs to run the following commands in the same directory where the files are:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/examples/simpleStatisticalInverseProblem/
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
  $HOME/LIBRARIES/gsl-1.15/lib/:\
  $HOME/LIBRARIES/boost-1.53.0/lib/:\
  $HOME/LIBRARIES/hdf5-1.8.10/lib:\
  $HOME/LIBRARIES/QUESO-0.56.0/lib
$ make -f Makefile_example_margarida
$ ./simple_sip_example example.inp
```

The '`export`' instruction above is only necessary if the user has not saved it in his/her `.bashrc` file.

6.1.5 Data Post-Processing and Visualization

There are a few Matlab-ready commands that are very helpful tools for post-processing the data generated by QUESO when solving statistical inverse problems. This section discusses the results computed by QUESO with the code of Section 6.1.2, and shows how to use Matlab for the post-processing of such results. Only the essential Matlab commands are presented; for the complete/detailed codes, please refer to file '`simple_ip_plots.m`'.

According to the specifications of the input file in Listing 6.6, a folder named '`outputData`' containing the following files should be created: `display_sub0.txt, ip_filt_chain_sub0.m, ip_raw_chain_sub0.m, sipOutput_sub0.m, ip_filt_chain.m, ip_raw_chain.m`

The code bellow shows how to load the data provided by QUESO during the solution process of the SIP described, in the form of chains of positions.

```
% inside Matlab
>> clear all
>> simple_ip_plots
```

Listing 6.8: Matlab code for loading the data in both raw and filtered chains of the SIP, by calling the file `simple_ip_plots.m`.

6.1.5.1 Autocorrelation Plots

The code presented in Listing 6.9 uses Matlab function `autocorr` to generate Figure 6.1.1 which presents the autocorrelation of the parameters θ_1 and θ_2 in both cases: raw and filtered chain.

```
% inside Matlab
% theta_1
>> nlags=10;
>> [ACF_raw, lags] = autocorr(ip_mh_rawChain_unified(:,1), nlags, 0);
>> [ACF_filt, lags] = autocorr(ip_mh_filtChain_unified(:,1), nlags, 0);
>> [ACF_raw2, lags2] = autocorr(ip_mh_rawChain_unified(:,2), nlags, 0);
>> [ACF_filt2, lags3] = autocorr(ip_mh_filtChain_unified(:,2), nlags, 0);
>> plot(lags,ACF_raw,'b--*',lags,ACF_filt,'b*-',lags2,ACF_raw2,'g--*',lags2,ACF_filt2,'g*-','
    linewidth',3);
>> h=legend('\theta_1, raw chain','\theta_1, filtered chain','\theta_2, raw chain','\theta_2,
     filtered chain','location','northeast');
```

Listing 6.9: Matlab code for the autocorrelation plots depicted in Figure 6.1.1.

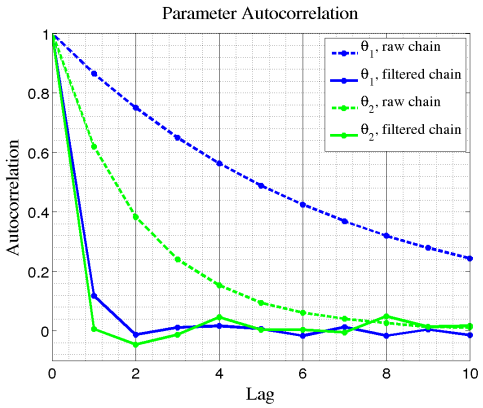


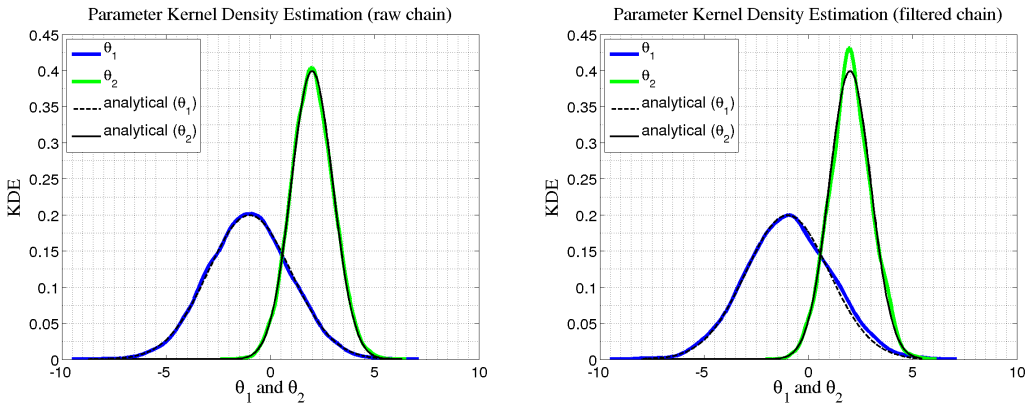
Figure 6.1.1: Autocorrelation plots obtained with QUESO for the SIP.

6.1.5.2 KDE Plots

Matlab function `[f,xi] = ksdensity(x)` (kernel smoothing density estimate) computes a probability density estimate of the sample in the vector `x`. `f` is the vector of density values evaluated at the points in `xi`. The estimate is based on a normal kernel function, using a window parameter ('width') that is a function of the number of points in `x`. The density is evaluated at 100 equally spaced points that cover the range of the data in x. In order to estimate the KDE of the parameters, it is used together with the option '`pdf`'.

```
% Inside Matlab
% Raw chain
>> [f,x] = ksdensity(ip_mh_rawChain_unified(:,1),'function','pdf');
>> [f2,x2] = ksdensity(ip_mh_rawChain_unified(:,2),'function','pdf');
>> x_p1=sort(ip_mh_rawChain_unified(:,1)); %analytical
>> f_p1=(exp(-(x_p1+1).*(x_p1+1)/8))/2/sqrt(2*pi);
>> x_p2=sort(ip_mh_rawChain_unified(:,1));
>> f_p2=(exp(-(x_p2-2).*(x_p2-2)/2))/sqrt(2*pi);
>> plot(x,f,'b',x2,f2,'g','linewidth',4);
>> hold;
>> plot(x_p1,f_p1,'--k',x_p2,f_p2,'-k','linewidth',2);
>> h=legend('\theta_1', '\theta_2', 'analytical (\theta_1)', 'analytical (\theta_2)', '
    location', 'northwest');
```

Listing 6.10: Matlab code for the KDE plots displayed in the left of Figure 6.1.2.



(a) Raw chain (b) Filtered chain

Figure 6.1.2: Kernel Density Estimation. QUESO results for estimation of the KDE of θ_1 and θ_2 are plotted against the analytical expressions $\pi_{\text{post}}(\theta_1) = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{1}{8}(\theta_1+1)^2\right)$ and $\pi_{\text{post}}(\theta_2) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(\theta_2-2)^2\right)$, respectively.

6.1.5.3 Covariance and Correlation Matrices

Matlab function `cov` calculates the covariance matrix for a data matrix (where each column represents a separate quantity), and `corr` calculates the correlation matrix.

Listing 6.39 presents the Matlab steps for calculating the covariance and correlation matrices for the parameters θ_1 and θ_2.

```
% inside Matlab
>> cov_matrix_theta1_theta2 = cov(ip_mh_rawChain_unified)

cov_matrix_theta1_theta2 =

    3.8729    0.0259
    0.0259    1.0050

>> corr_matrix_theta1_theta2 = corr(ip_mh_rawChain_unified)
```

```
corr_matrix_theta1_theta2 =

    1.0000    0.0132
    0.0132    1.0000
```

Listing 6.11: Matlab code for finding covariance and correlation matrices.

6.2 simpleStatisticalForwardProblem

In this simple statistical forward problem (SFP), suppose that the quantity of interest $\mathbf{q}$ is a function of a random variable $\boldsymbol{\theta}$ of two parameters, namely $\mathbf{q} : \mathbb{R}^{\mathbf{2}} \to \mathbb{R}$ such as:

$$\mathbf{q}(\boldsymbol{\theta}) = \theta_1 + \theta_2, \quad \forall \boldsymbol{\theta} = (\theta_1, \theta_2) \in \mathbb{R}^2. \tag{6.2.1}$$

Suppose also that the parameters in θ have Gaussian distribution with mean $\boldsymbol{\mu}$ and covariance matrix $\mathbf{C}$ given by:

$$\boldsymbol{\mu} = \begin{pmatrix} -1 \\ 2 \end{pmatrix} \quad \text{and} \quad \mathbf{C} = \begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}. \tag{6.2.2}$$

Notice that since the solution $\mathbf{Q}$ of this SFP is the sum of two random variables $\boldsymbol{\Theta}_1$ and $\boldsymbol{\Theta}_2$, and since these two random variables independent Gaussian by assumption, should have:

$$E[\mathbf{Q}] = E[\boldsymbol{\Theta}_1] + E[\boldsymbol{\Theta}_2] = -1 + 2 = 1 \quad \text{and} \quad V[\mathbf{Q}] = V[\boldsymbol{\Theta}_1] + V[\boldsymbol{\Theta}_2] = 4 + 1 = 5 \tag{6.2.3}$$

where E and V indicate expectation and variance, respectively. Thus the analytical expression for the solution $\mathbf{Q}$ is this SFP is the one-dimensional Gaussian distribution of mean 1 and variance 5:

$$\mathbf{Q}(x) = \frac{1}{\sqrt{10\pi}} \exp\left(-\frac{1}{10}(x-1)^2\right) \tag{6.2.4}$$

In this example, we use QUESO Monte Carlo algorithm to sample from the QoI given in Equation (6.2.1) and analyze it. Since the parameters have known independent Gaussian distributions, the results obtained by QUESO via sampling the QoI, in Equation (6.2.1), should match the Gaussian distribution given in Equation (6.2.4).

Note: Due to the possibility to compare QUESO sampling algorithms to an analytical expression, this example is also used in the verification procedures and regression tests within QUESO. In fact it is the second part of the test `tests/t02_sip_sfp`.

6.2.1 Running the Example

To run the executable provided (available after QUESO installation), enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/
$ cd examples/simpleStatisticalForwardProblem
$ rm outputData/*
$ ./exSimpleStatisticalForwardProblem_gsl example.inp
$ matlab
   $ simple_fp_plots      # inside matlab
   $ exit                 # inside matlab
$ ls -l outputData/*.png
 simple_fp_autocorrelation_qoi.png  simple_fp_chain_pos_param.png
 simple_fp_hist_qoi.png             simple_fp_cdf_qoi.png
 simple_fp_chain_pos_qoi.png        simple_fp_kde_qoi.png
```

As a result, the user should have created several of PNG figures containing marginal posterior PDF, chain positions of the parameters and the QoI, histogram, cumulative density distribution and autocorrelation. The name of the figure files have been chosen to be informative, as shown in the Listing above.

6.2.2 Example Code

The source code for the SFP example is composed of 5 files: `simple_sfp_example_main.C` (Listing 6.12), `simple_sfp_example_qoi.h` and `simple_sfp_example_qoi.C` (Listings 6.13 and 6.14), `simple_sfp_example_compute.h` and `simple_sfp_example_compute.C` (Listings 6.15 and 6.16).

```
#include <simple_sfp_example_compute.h>

int main(int argc, char* argv[])
{
  // Initialize environment
#ifdef QUESO_HAS_MPI
  MPI_Init(&argc,&argv);

  UQ_FATAL_TEST_MACRO(argc != 2, QUESO::UQ_UNAVAILABLE_RANK, "main()",
                      "input file must be specified in command line as argv[1], just after
                          executable argv[0]");
  QUESO::FullEnvironment* env =
    new QUESO::FullEnvironment(MPI_COMM_WORLD,argv[1],"",NULL);
#else
  QUESO::FullEnvironment* env =
    new QUESO::FullEnvironment(argv[1],"",NULL);
#endif

  // Compute
  compute(*env);

  // Finalize environment
  delete env;
#ifdef QUESO_HAS_MPI
  MPI_Finalize();
#endif

  return 0;
}
```

Listing 6.12: File `simple_sfp_example_main.C`.

```
#ifndef __EX_QOI_H__
#define __EX_QOI_H__

#include <queso/GslMatrix.h>
#include <queso/DistArray.h>

struct
qoiRoutine_DataType
{
  double coef1;
  double coef2;
};

void
qoiRoutine(
  const QUESO::GslVector&                    paramValues,
  const QUESO::GslVector*                    paramDirection,
  const void*                                functionDataPtr,
        QUESO::GslVector&                    qoiValues,
        QUESO::DistArray<QUESO::GslVector*>* gradVectors,
        QUESO::DistArray<QUESO::GslMatrix*>* hessianMatrices,
        QUESO::DistArray<QUESO::GslVector*>* hessianEffects);

#endif
```

Listing 6.13: File `simple_sfp_example_qoi.h`.

```
#include <simple_sfp_example_qoi.h>

void
qoiRoutine(
  const QUESO::GslVector&                    paramValues,
  const QUESO::GslVector*                    paramDirection,
  const void*                                functionDataPtr,
        QUESO::GslVector&                    qoiValues,
        QUESO::DistArray<QUESO::GslVector*>* gradVectors,
        QUESO::DistArray<QUESO::GslMatrix*>* hessianMatrices,
        QUESO::DistArray<QUESO::GslVector*>* hessianEffects)
{
  // Logic just to avoid warnings from INTEL compiler
  const QUESO::GslVector* aux1 = paramDirection;
  if (aux1) {};
  QUESO::DistArray<QUESO::GslVector*>* aux2 = gradVectors;
  if (aux2) {};
  aux2 = hessianEffects;
  QUESO::DistArray<QUESO::GslMatrix*>* aux3 = hessianMatrices;
  if (aux3) {};

  // Just checking: the user, at the application level, expects
  // vector 'paramValues' to have size 2 and
  // vector 'qoiValues' to have size 1.
  UQ_FATAL_TEST_MACRO(paramValues.sizeGlobal() != 2,
                      QUESO::UQ_UNAVAILABLE_RANK,
                      "qoiRoutine()",
                      "paramValues vector does not have size 2");

  UQ_FATAL_TEST_MACRO(qoiValues.sizeGlobal() != 1,
                      QUESO::UQ_UNAVAILABLE_RANK,
                      "qoiRoutine()",
                      "qoiValues vector does not have size 1");

  // Actual code
```

```
  //
  // This code exemplifies multiple Monte Carlo solvers, each calling this qoi routine.
  // In this simple example, only node 0 in each sub-environment does the job even though
  // there might be more than one node per sub-environment.
  // In a more realistic situation, if the user is asking for multiple nodes per sub-
  // environment, then the model code in the qoi routine might really demand more than one
  // node. Here we use 'env.subRank()' only. A realistic application might want to use
  // either 'env.subComm()' or 'env.subComm().Comm()'.

  const QUESO::BaseEnvironment& env = paramValues.env();
  if (env.subRank() == 0) {
    double coef1 = ((qoiRoutine_DataType *) functionDataPtr)->coef1;
    double coef2 = ((qoiRoutine_DataType *) functionDataPtr)->coef2;
    qoiValues[0] = (coef1*paramValues[0] + coef2*paramValues[1]);
  }
  else {
    qoiValues[0] = 0.;
  }

  return;
}
```

Listing 6.14: File `simple_sfp_example_qoi.C`.

```
#ifndef __EX_COMPUTE_H__
#define __EX_COMPUTE_H__

#include <queso/Environment.h>

void compute(const QUESO::FullEnvironment& env);

#endif
```

Listing 6.15: File `simple_sfp_example_compute.h`.

```
#include <simple_sfp_example_compute.h>
#include <simple_sfp_example_qoi.h>
#include <queso/GslMatrix.h>
#include <queso/StatisticalForwardProblem.h>
#include <queso/GenericVectorFunction.h>
#include <queso/GaussianVectorRV.h>

void compute(const QUESO::FullEnvironment& env) {

  // Step 1 of 6: Instantiate the parameter space
  QUESO::VectorSpace<QUESO::GslVector,QUESO::GslMatrix>
    paramSpace(env, "param_", 2, NULL);

  // Step 2 of 6: Instantiate the parameter domain
  QUESO::GslVector paramMins(paramSpace.zeroVector());
  paramMins.cwSet(-INFINITY);
  QUESO::GslVector paramMaxs(paramSpace.zeroVector());
  paramMaxs.cwSet( INFINITY);
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomain("param_",paramSpace,paramMins,paramMaxs);

  // Step 3 of 6: Instantiate the qoi space
  QUESO::VectorSpace<QUESO::GslVector,QUESO::GslMatrix>
    qoiSpace(env, "qoi_", 1, NULL);
```

```
  // Step 4 of 6: Instantiate the qoi function object
  qoiRoutine_DataType qoiRoutine_Data;
  qoiRoutine_Data.coef1 = 1.;
  qoiRoutine_Data.coef2 = 1.;
  QUESO::GenericVectorFunction<QUESO::GslVector,QUESO::GslMatrix,
                               QUESO::GslVector,QUESO::GslMatrix>
    qoiFunctionObj("qoi_",
                   paramDomain,
                   qoiSpace,
                   qoiRoutine,
                   (void *) &qoiRoutine_Data);

  // Step 5 of 6: Instantiate the forward problem
  // Parameters are Gaussian RV
  QUESO::GslVector meanVector( paramSpace.zeroVector() );
  meanVector[0] = -1;
  meanVector[1] = 2;

  QUESO::GslMatrix covMatrix = QUESO::GslMatrix(paramSpace.zeroVector());
  covMatrix(0,0) = 4.;
  covMatrix(0,1) = 0.;
  covMatrix(1,0) = 0.;
  covMatrix(1,1) = 1.;

  QUESO::GaussianVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    paramRv("param_",paramDomain,meanVector,covMatrix);

  QUESO::GenericVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    qoiRv("qoi_", qoiSpace);

  QUESO::StatisticalForwardProblem<QUESO::GslVector,QUESO::GslMatrix,
                                   QUESO::GslVector,QUESO::GslMatrix>
    fp("", NULL, paramRv, qoiFunctionObj, qoiRv);

  // Step 6 of 6: Solve the forward problem
  fp.solveWithMonteCarlo(NULL);

  return;
}
```

Listing 6.16: File `simple_sfp_example_compute.C`.

6.2.3 Input File

In the case of a SFP, QUESO expects a list of options for Monte Carlo algorithm, together with options for QUESO environment; such as the name of the output files and which sub-environments will write to to them. Note that the names of the variables have been designed to be informative:

`env:` refers to QUESO environment;

`fp:` refers to forward problem;

`mc:` refers to Monte Carlo;

`pseq:` refers to the parameter sequence; and

`qseq:` refers to the quantity of interest sequence.

The options used for solving this simple SFP are displayed in Listing 6.17.

```
#######################################################
# UQ Environment
#######################################################
env_numSubEnvironments   = 1
env_subDisplayFileName   = outputData/display
env_subDisplayAllowAll   = 0
env_subDisplayAllowedSet = 0
env_displayVerbosity     = 2
env_syncVerbosity        = 0
env_seed                 = 0

#######################################################
# Statistical forward problem (fp)
#######################################################
fp_computeSolution      = 1
fp_computeCovariances   = 1
fp_computeCorrelations  = 1
fp_dataOutputFileName   = outputData/sfpOutput
fp_dataOutputAllowedSet = 0 1

#######################################################
# 'fp_': information for Monte Carlo algorithm
#######################################################
fp_mc_dataOutputFileName   = outputData/sfpOutput
fp_mc_dataOutputAllowedSet = 0 1

fp_mc_pseq_dataOutputFileName   = outputData/fp_p_seq
fp_mc_pseq_dataOutputAllowedSet = 0 1

fp_mc_qseq_size                 = 20000
fp_mc_qseq_displayPeriod        = 2000
fp_mc_qseq_measureRunTimes      = 1
fp_mc_qseq_dataOutputFileName   = outputData/fp_q_seq
fp_mc_qseq_dataOutputAllowedSet = 0 1
```

Listing 6.17: File name `simple_sfp_example.inp` with options for QUESO library used in application code (Listings 6.12–6.16).

6.2.4 Create your own Makefile

Listing 6.33 presents a Makefile, named '`Makefile_sfp_example_margarida`', that may be used to compile the code and create the executable `simple_sfp_example`. Naturally, it must be adapted to the user's settings, i.e., it has to have the correct paths for the user's libraries that have actually been used to compile and install QUESO.

```
QUESO_DIR = /path/to/queso
BOOST_DIR = /path/to/boost
GSL_DIR   = /path/to/gsl

INC_PATHS = \
   -I. \
   -I$(QUESO_DIR)/include \
   -I$(BOOST_DIR)/include \
   -I$(GSL_DIR)/include

LIBS = \
   -L$(QUESO_DIR)/lib -lqueso \
```

```
    -L$(BOOST_DIR)/lib -lboost_program_options \
    -L$(GSL_DIR)/lib -lgsl

CXX = mpic++
CXXFLAGS += -g -Wall -c

default: all

.SUFFIXES: .o .C

all:       example_sfp

clean:
   rm -f *~
   rm -f *.o
   rm -f simple_sfp_example

example_sfp: simple_sfp_example_main.o simple_sfp_example_qoi.o simple_sfp_example_compute.
    o
   $(CXX) simple_sfp_example_main.o \
          simple_sfp_example_qoi.o \
          simple_sfp_example_compute.o \
          -o simple_sfp_example $(LIBS)

%.o: %.C
   $(CXX) $(INC_PATHS) $(CXXFLAGS) $<
```

Listing 6.18: Makefile for the application code in Listings 6.12–6.16

Thus, to compile, build and execute the code, the user just needs to run the following commands in the same directory where the files are:

```
$ cd HOME/LIBRARIES/QUESO-0.56.0/examples/simpleStatisticalForwardProblem
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
  $HOME/LIBRARIES/gsl-1.15/lib/:\
  $HOME/LIBRARIES/boost-1.53.0/lib/:\
  $HOME/LIBRARIES/hdf5-1.8.10/lib:\
  $HOME/LIBRARIES/QUESO-0.56.0/lib
$ make -f Makefile_sfp_example_margarida
$ ./simple_sfp_example simple_sfp_example.inp
```

The '`export`' instruction above is only necessary if the user has not saved it in his/her `.bashrc` file.

6.2.5 Data Post-Processing and Visualization

This section discusses the results computed by QUESO with the code of Section 6.2.2, and shows how to use Matlab for the post-processing of the data generated by QUESO when solving SFPs. Only the essential Matlab commands are presented; for the complete/detailed codes, please refer to file '`simple_fp_plots.m`'.

According to the specifications of the input file in Listing 6.17, a folder named '`outputData`' containing the following files should be created: `display_sub0.txt`, `fp_p_seq.m`, `fp_p_seq_sub0.m`, `fp_q_seq.m`, `fp_q_seq_sub0.m`, and `sfpOutput_sub0.m`.

The code below shows how to load the data provided by QUESO during the solution

process of the SFP described, in the form of chains of positions.

```
% inside Matlab
>> clear all
>> fp_p_seq.m
>> fp_q_seq.m
```

Listing 6.19: Matlab code for loading the data in both parameter and QoI chains of the SFP.

Alternatively, the user may call the file `simple_fp_plots.m`, which contains the above commands, together with a variety of others, for data visualization:

```
% inside Matlab
>> clear all
>> simple_fp_plots
```

Listing 6.20: Matlab code for loading the data in both parameter and QoI chains of the SFP, by calling the file `simple_fp_plots.m`.

6.2.5.1 Histogram Plots

In order to plot a histogram of the QoI, you may use the pre-defined Matlab function `hist`. The Matlab code presented in Listing 6.21 below shows how to create the Figure 6.2.1.

```
% inside Matlab
>> fp_q_seq  %if commands of Listings 3.19/3.20 have not been called
>> nbins=20;
>> hist(fp_mc_QoiSeq_unified,nbins);
>> title('QoI Histogram','fontsize',20);
>> xlabel('QoI=\theta_1+\theta_2','fontname', 'Times', 'fontsize',20)
>> ylabel('Frequency','fontsize',20);
```

Listing 6.21: Matlab code for the QoI histogram plot.

6.2.5.2 KDE Plot

Matlab function `ksdensity` (Kernel smoothing density estimate) together with the option '`pdf`' may be used to estimate the KDE of the QoI.

```
% inside Matlab
>> fp_q_seq  %if commands of Listing 5.19 have not been called
>> [fi,xi] = ksdensity(fp_mc_QoiSeq_unified,'function','pdf');
>> x=sort(fp_mc_QoiSeq_unified);
>> mu=1;
>> sigma2=5;
>> f=(exp(-(x-mu).*(x-mu)/sigma2/2))/sqrt(2*pi*sigma2);
>> plot(xi,fi,'-m','linewidth',4);
>> hold;
>> plot(x,f,'--k','linewidth',2);
>> h=legend('QoI = \theta_1+\theta_2','analytical','location','northwest');
```

Listing 6.22: Matlab code for the KDE displayed in Figure 6.2.2

6.2.5.3 CDF Plot

Matlab function `ksdensity` with `'cdf'` option may also be used for plotting the Cumulative Distribution Function of the QoI.

```
% inside Matlab
>> fp_q_seq  %if commands of Listing 5.19 have not been called
>> [f,xi] = ksdensity(fp_mc_QoiSeq_unified,'function','cdf');
>> plot(xi,f,'-m','linewidth',3)
```

Listing 6.23: Matlab code for the QoI CDF plot displayed in Figure 6.2.3.

6.3 gravity

This section presents an example of how to use QUESO in order to develop an application that solves a statistical inverse problem (SIP) and a statistical forward problem (SFP), where the solution of the former serves as input to the later. During the SIP, the acceleration due to gravity for an object in free fall near the surface of the Earth is inferred. During the SFP, the distance traveled by a projectile launched at a given angle and altitude is calculated using the calibrated magnitude of the acceleration of gravity.

In this section we describe a statistical forward problem of predicting the described in Section 6.3.1.

6.3.1 Statistical Inverse Problem

A possible deterministic mathematical model for the vertical motion of an object in free fall near the surface of the Earth is given by

$$h(t) = -\frac{1}{2}gt^2 + v_0 t + h_0. \tag{6.3.1}$$

where v_0 $[m/s]$ is the initial velocity, h_0 $[m]$ is the initial altitude, $h(t)$ $[m]$ is the altitude with respect to time, t $[s]$ is the elapsed time, and g $[m/s^2]$ is the magnitude of the acceleration due to gravity (the parameter which cannot be directly measured and will be statistically inferred).

6.3.1.1 Experimental Data

We assume that the experiment of allowing an object to fall from different altitudes with zero initial velocity has been repeatedly conducted (See Figure 6.3.1). The data collected, e.g. $\mathbf{d}$, is displayed in Table 6.3.1; the standard deviations, σ's, refer to the uncertainties in the measured times during the experiment execution [1].

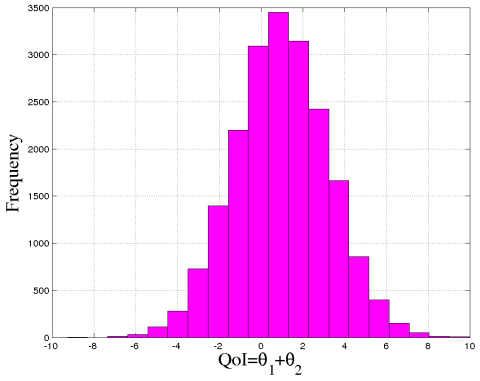


Figure 6.2.1: QoI histogram.

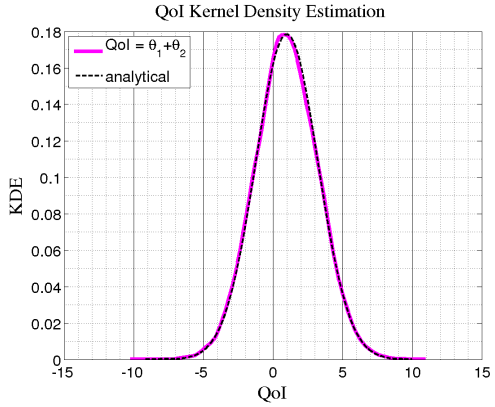


Figure 6.2.2: Kernel Density Estimation. QUESO results are plotted against the PDF of a Gaussian distribution $Q(x) = \frac{1}{\sqrt{10\pi}} \exp\left(-\frac{1}{10}(x-1)^2\right)$, where $\mu = 1$ and $\sigma^2 = 5$.

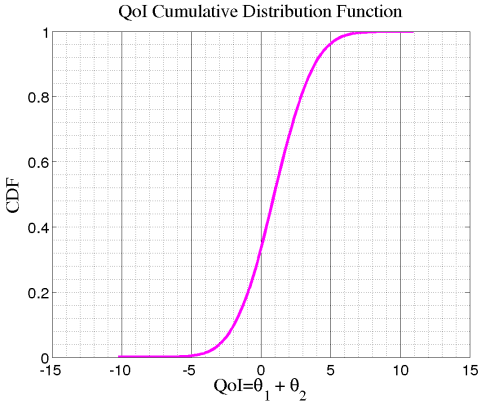


Figure 6.2.3: Cumulative Distribution Function.

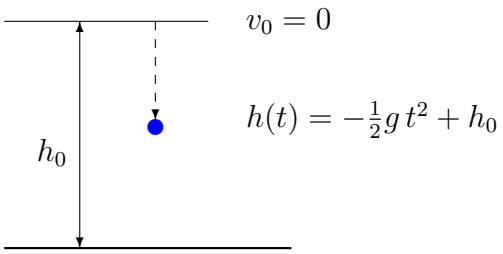


Figure 6.3.1: An object falls from altitude h_0 with zero initial velocity ($v_0 = 0$).

Table 6.3.1: Measurement data $\mathbf{d}$ of size $n_d = 14$. The object falls from altitude h_0 in t seconds, with standard deviation of σ seconds in the time measurement [1].

altitude $[m]$	time $[s]$	Std. Dev. σ $[s]$
10	1.41	0.02
20	2.14	0.12
30	2.49	0.02
40	2.87	0.01
50	3.22	0.03
60	3.49	0.01
70	3.81	0.03
80	4.07	0.03
90	4.32	0.03
100	4.47	0.05
110	4.75	0.01
120	4.99	0.04
130	5.16	0.01
140	5.26	0.09

6.3.1.2 The Prior RV, Likelihood and Posterior RV

In a straightforward classical interpretation of Bayesian inference, the prior signifies the modeler's honest opinion about the unknown. For the gravity inference problem, let's assume that gravity varies uniformly in the interval [8,11], or, in other words, we chose uniform prior distribution in that interval:

$$\pi_{\text{prior}} = \mathcal{U}(8, 11). \tag{6.3.2}$$

We choose the usual likelihood function:

$$\pi_{\text{like}}(\mathbf{d}|\boldsymbol{\theta}) \propto \exp\left\{-\frac{1}{2}[\mathbf{y}(\boldsymbol{\theta}) - \mathbf{d}]^T \left[\mathbf{C}(\boldsymbol{\theta})\right]^{-1} [\mathbf{y}(\boldsymbol{\theta}) - \mathbf{d}]\right\}, \tag{6.3.3}$$

where $\mathbf{C}(\boldsymbol{\theta})$ is a given covariance matrix, $\mathbf{d}$ denotes experimental data, $\mathbf{y}(\boldsymbol{\theta})$ is the model

output data.

Recalling the deterministic model for the acceleration of gravity (6.3.1) with zero initial velocity, the information provided in Table 6.3.1, and Equation (6.3.3); and, additionally, invoking the nomenclature used in Section 1.2, we have:

$$\boldsymbol{\theta} \stackrel{\text{def.}}{=} g, \quad \mathbf{y}(\boldsymbol{\theta}) = \begin{bmatrix} \sqrt{\frac{2h_1}{g}} \\ \sqrt{\frac{2h_2}{g}} \\ \vdots \\ \sqrt{\frac{2h_{n_d}}{g}} \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_{n_d} \end{bmatrix}, \quad \mathbf{C}(\boldsymbol{\theta}) = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \sigma_{n_d}^2 \end{bmatrix}, \tag{6.3.4}$$

where $n_d = 14$ is the number of data points in Table 6.3.1.

Now we are ready to evoke Bayes' formula in order to obtain the posterior PDF $\pi_{\text{post}}(\boldsymbol{\theta})$:

$$\pi_{\text{post}}(\boldsymbol{\theta}|\mathbf{d}) \propto \pi_{\text{like}}(\mathbf{d}|\boldsymbol{\theta})\, \pi_{\text{prior}}(\boldsymbol{\theta}). \tag{6.3.5}$$

6.3.2 Statistical Forward Problem

Projectile motion refers to the motion of an object projected into the air at an angle, e.g. a soccer ball being kicked, a baseball being thrown, or an athlete long jumping. Supposing the object does not have a propulsion system and neglecting air resistance, then the only force acting on the object is a constant gravitational acceleration g.

A possible deterministic two-dimensional mathematical model for the vertical motion of an object projected from near the surface of the Earth is given by

$$v_x = v_{0x} \tag{6.3.6}$$

$$v_y = v_{0y} - gt \tag{6.3.7}$$

$$x = v_{0x} t \tag{6.3.8}$$

$$h = h_0 + v_{0y} t - \frac{1}{2} g t^2 \tag{6.3.9}$$

where h_0 is the initial height, $x = x(t)$ is the distance traveled by the object, $\boldsymbol{v_0} = (v_{0x}, v_{0y})$ is the initial velocity, $v_{0x} = v_0 \cos(\alpha)$, $v_{0y} = v_0 \sin(\alpha)$, and $v_0 = \|\boldsymbol{v_0}\|^2$. Figure 6.3.2 displays the projectile motion of an object in these conditions.

For this example, we assume that $h_0 = 0$ m, $\alpha = \pi/4$ radians, $v_0 = 5$ m/s, all deterministic variables; and g is the solution of the SIP described in Section 6.3.1.

Since a PDF is assigned to parameter g; thus, the output of the mathematical model (6.3.6) becomes a random variable, thus we have a statistical forward problem.

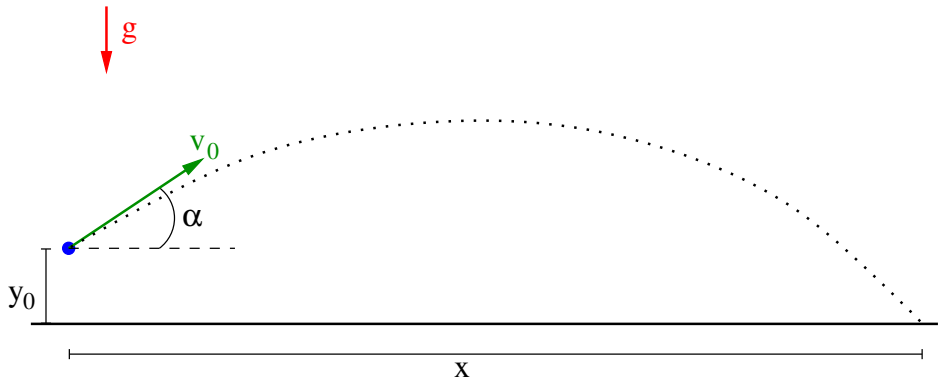


Figure 6.3.2: Object traveling with projectile motion.

6.3.2.1 The Input RV, QoI Function and Output RV

The input random variable for the statistical forward problem is the acceleration of gravity g, which is also the solution (posterior PDF) of the inverse problem described in Section 6.3.1. The output random variable for this example is the distance x traveled by an object in projectile motion. Note that, since there is uncertainty in the parameter g (g is given as a PDF), one can expect that this uncertainty will be propagated to x, which will also be given as a PDF.

Combining the expressions in Equation 6.3.6 and rearranging them, we have that QoI function for x is:

$$x = \frac{v_0 \cos\alpha}{g}\left(v_0 \sin\alpha + \sqrt{(v_0 \sin\alpha)^2 + 2g\,y_0}\right). \tag{6.3.10}$$

where y is the distance traveled and our quantity of interest (QoI).

6.3.3 Running the Example

To run the executable provided (available after QUESO installation), enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/examples/gravity
$ rm outputData/*
$ ./gravity_gsl gravity_inv_fwd.inp
```

The console output of the program is:

```
kemelli@violeta:~/LIBRARIES/QUESO-0.56.0/examples/gravity$ ./gravity_gsl gravity_inv_fwd.inp
-----------------------------------------------------------------------
QUESO Library: Version = 0.56.0 (56.0)

Development Build

Build Date    = 2013-04-29 17:05
Build Host    = violeta
Build User    = kemelli
Build Arch    = x86_64-unknown-linux-gnu
Build Rev     = 38998M
```

```
C++ Config   = mpic++ -g -O2 -Wall

Trilinos DIR =
GSL Libs     = -L/home/kemelli/LIBRARIES/gsl-1.15/lib -lgsl -lgslcblas -lm
GRVY DIR     =
GLPK DIR     =
HDF5 DIR     = /home/kemelli/LIBRARIES/hdf5-1.8.10
-----------------------------------------------------------------------------------------------------

Beginning run at Mon Apr 29 17:27:32 2013

MPI node of worldRank 0 has fullRank 0, belongs to subEnvironment of id 0, and has subRank 0
MPI node of worldRank 0 belongs to sub communicator with full ranks 0
MPI node of worldRank 0 also belongs to inter0 communicator with full ranks 0, and has
    inter0Rank 0


Beginning run of 'Gravity + Projectile motion' example at Mon Apr 29 17:27:32 2013

 my fullRank = 0
 my subEnvironmentId = 0
 my subRank = 0
 my interRank = 0

Beginning 'SIP -> Gravity estimation' at Mon Apr 29 17:27:32 2013

Solving the SIP with Metropolis Hastings

Beginning 'SFP -> Projectile motion' at Mon Apr 29 17:27:33 2013

Solving the SFP with Monte Carlo

Ending run of 'Gravity + Projectile motion' example at Mon Apr 29 17:27:33 2013

Ending run at Mon Apr 29 17:27:33 2013
Total run time = 1 seconds
kemelli@violeta:~/LIBRARIES/QUESO-0.56.0/examples/gravity$
```

Listing 6.24: Console output of program `gravity_gsl`

In order to generate chain plots, histograms, KDEs, etc., the user may use Matlab/GNU Octave and call the following command lines:

```
$ matlab
   $ gravity_plots_ip      # inside matlab
   $ gravity_plots_fp      # inside matlab
   $ exit                  # inside matlab
$ ls -l outputData/*.png
  sfp_gravity_autocorrelation.png  sfp_gravity_cdf.png
  sfp_gravity_chain_pos.png        sfp_gravity_hist.png
  sfp_gravity_kde.png              sip_gravity_autocorrelation_raw_filt.png
  sip_gravity_cdf_filt.png         sip_gravity_cdf_raw.png
  sip_gravity_chain_pos_filt.png   sip_gravity_chain_pos_raw.png
  sip_gravity_hist_filt.png        sip_gravity_hist_raw.png
  sip_gravity_kde_filt.png         sip_gravity_kde_raw.png
```

As a result, the user should have created several of PNG figures containing marginal posterior PDF, chain positions of the parameters and the QoI, histogram, cumulative density distribution and autocorrelation. The name of the figure files have been chosen to be infor-

mative, as shown in the listing above.

6.3.4 Example Code

The source code for the SIP and the SFP is composed of 7 files. Three of them are common for both problems: `gravity_main.C, gravity_compute.h` and `gravity_compute.C`; they combine both problems and use the solution of the SIP (the posterior PDF for the gravity) as an input for the SFP and are presented, respectively, in Listings 6.25, 6.26 and 6.27. Two of files specifically handle the SIP: `gravity_likelihood.h`, and `gravity_likelihood.C`, and are displayed in Listings 6.28 and 6.29. Finally, the files specific for the SFP are `gravity_qoi.h` and `gravity_qoi.C`, and they are presented in Listings 6.30 and 6.31.

```
 /*--------------------------------------------------------------------
 * Brief description of this file:
 *
 * This is an example of how to use QUESO classes and algorithms in order to define and solve
 * a statistical inverse problem (SIP) and/or a statistical forward problem (SFP).
 * The SIP consists on calibrating the magnitude 'g' of acceleration gravity using
 * measurements of the time that it takes for an object in free fall to reach the ground from
 * a given height and zero initial velocity. The solution of the SIP is the posterior
 * probability density function (PDF) of 'g'.
 * The SFP consists of calculating the maximum distance traveled by an object in projectile
 * motion. The posterior PDF of 'g' from the SIP might be used as input to the SFP.
 *
 * The code consists of 7 files:
 * - 'gravity_main.C' (this file)
 * - 'gravity_compute.C' (the driving application code)
 * - 'gravity_compute.h'
 * - 'gravity_likelihood.C' (necessary for the SIP)
 * - 'gravity_likelihood.h'
 * - 'gravity_qoi.C' (necessary for the SFP)
 * - 'gravity_qoi.h'
 *--------------------------------------------------------------------*/

#include <gravity_compute.h>

int main(int argc, char* argv[])
{
  // Initialize QUESO environment
#ifdef QUESO_HAS_MPI
  MPI_Init(&argc,&argv);
  QUESO::FullEnvironment* env =
    new QUESO::FullEnvironment(MPI_COMM_WORLD,argv[1],"",NULL);
#else
  QUESO::FullEnvironment* env =
    new QUESO::FullEnvironment(argv[1],"",NULL);
#endif

  // Call application
  computeGravityAndTraveledDistance(*env);

  // Finalize QUESO environment
  delete env;
#ifdef QUESO_HAS_MPI
  MPI_Finalize();
#endif

  return 0;
}
```

Listing 6.25: File `gravity_main.C`.

```
#define EX_COMPUTE_H

#include <queso/Environment.h>

void computeGravityAndTraveledDistance(const QUESO::FullEnvironment& env);

#endif
```

Listing 6.26: File `gravity_compute.h`.

```
 * This file is divided in two parts:
 * - the first one handles the statistical inverse problem (SIP) for estimating
 *   the magnitude 'g' of gravity acceleration; and
 * - the second part handles the statistical forward problem (SFP) for
 *   predicting the maximum distance traveled by a projectile.
 *
 * The SIP definition requires a user defined likelihood function; refer to
 * files 'gravity_likelihood.h' and 'gravity_likelihood.C'. The SFP definition
 * requires a user defined qoi function; refer to files 'gravity_qoi.h' and
 * 'gravity_qoi.C'.
 */

#include <cmath>
#include <sys/time.h>

#include <queso/GslMatrix.h>
#include <queso/GenericScalarFunction.h>
#include <queso/GenericVectorFunction.h>
#include <queso/GaussianVectorRV.h>
#include <queso/UniformVectorRV.h>
#include <queso/GenericVectorRV.h>
#include <queso/StatisticalInverseProblem.h>
#include <queso/StatisticalForwardProblem.h>

#include <gravity_compute.h>
#include <gravity_likelihood.h>
#include <gravity_qoi.h>

void computeGravityAndTraveledDistance(const QUESO::FullEnvironment& env) {
  struct timeval timevalNow;

  gettimeofday(&timevalNow, NULL);
  if (env.fullRank() == 0) {
    std::cout << "\nBeginning run of 'Gravity + Projectile motion' example at "
              << ctime(&timevalNow.tv_sec)
              << "\n my fullRank = "          << env.fullRank()
              << "\n my subEnvironmentId = " << env.subId()
              << "\n my subRank = "           << env.subRank()
              << "\n my interRank = "         << env.inter0Rank()
               << std::endl << std::endl;
  }

  // Just examples of possible calls
  if ((env.subDisplayFile()       ) &&
      (env.displayVerbosity() >= 2)) {
    *env.subDisplayFile() << "Beginning run of 'Gravity + Projectile motion' example at "
                          << ctime(&timevalNow.tv_sec)
```

```
                          << std::endl;
  }
  env.fullComm().Barrier();
  env.subComm().Barrier();  // Just an example of a possible call

  //=====================================================================
  // Statistical inverse problem (SIP): find posterior PDF for 'g'
  //=====================================================================
  gettimeofday(&timevalNow, NULL);
  if (env.fullRank() == 0) {
    std::cout << "Beginning 'SIP -> Gravity estimation' at "
              << ctime(&timevalNow.tv_sec)
              << std::endl;
  }

  //-----------------------------------------------------
  // SIP Step 1 of 6: Instantiate the parameter space
  //-----------------------------------------------------
  QUESO::VectorSpace<> paramSpace(env, "param_", 1, NULL);

  //-----------------------------------------------------
  // SIP Step 2 of 6: Instantiate the parameter domain
  //-----------------------------------------------------
  QUESO::GslVector paramMinValues(paramSpace.zeroVector());
  QUESO::GslVector paramMaxValues(paramSpace.zeroVector());

  paramMinValues[0] = 8.;
  paramMaxValues[0] = 11.;

  QUESO::BoxSubset<> paramDomain("param_", paramSpace, paramMinValues,
      paramMaxValues);

  //-----------------------------------------------------
  // SIP Step 3 of 6: Instantiate the likelihood function
  // object to be used by QUESO.
  //-----------------------------------------------------
  Likelihood<> lhood("like_", paramDomain);

  //-----------------------------------------------------
  // SIP Step 4 of 6: Define the prior RV
  //-----------------------------------------------------
  QUESO::UniformVectorRV<> priorRv("prior_", paramDomain);

  //-----------------------------------------------------
  // SIP Step 5 of 6: Instantiate the inverse problem
  //-----------------------------------------------------
  // Extra prefix before the default "rv_" prefix
  QUESO::GenericVectorRV<> postRv("post_", paramSpace);

  // No extra prefix before the default "ip_" prefix
  QUESO::StatisticalInverseProblem<> ip("", NULL, priorRv, lhood, postRv);

  //-----------------------------------------------------
  // SIP Step 6 of 6: Solve the inverse problem, that is,
  // set the 'pdf' and the 'realizer' of the posterior RV
  //-----------------------------------------------------

  QUESO::GslVector paramInitials(paramSpace.zeroVector());
  priorRv.realizer().realization(paramInitials);

  QUESO::GslMatrix proposalCovMatrix(paramSpace.zeroVector());
  proposalCovMatrix(0,0) = std::pow(std::abs(paramInitials[0]) / 20.0, 2.0);

  ip.solveWithBayesMetropolisHastings(NULL, paramInitials, &proposalCovMatrix);

```

```
  //=============================================================
  // Statistical forward problem (SFP): find the max distance
  // traveled by an object in projectile motion; input pdf for 'g'
  // is the solution of the SIP above.
117 //=============================================================
  gettimeofday(&timevalNow, NULL);
  std::cout << "Beginning 'SFP -> Projectile motion' at "
            << ctime(&timevalNow.tv_sec)
            << std::endl;
122
  //-----------------------------------------------------
  // SFP Step 1 of 6: Instantiate the parameter *and* qoi spaces.
  // SFP input RV = FIP posterior RV, so SFP parameter space
  // has been already defined.
127 //-----------------------------------------------------
  QUESO::VectorSpace<> qoiSpace(env, "qoi_", 1, NULL);

  //-----------------------------------------------------
  // SFP Step 2 of 6: Instantiate the parameter domain
132 //-----------------------------------------------------

  // Not necessary because input RV of the SFP = output RV of SIP.
  // Thus, the parameter domain has been already defined.

137 //-----------------------------------------------------
  // SFP Step 3 of 6: Instantiate the qoi object
  // to be used by QUESO.
  //-----------------------------------------------------
  Qoi<> qoi("qoi_", paramDomain, qoiSpace);
142
  //-----------------------------------------------------
  // SFP Step 4 of 6: Define the input RV
  //-----------------------------------------------------

147 // Not necessary because input RV of SFP = output RV of SIP
  // (postRv).

  //-----------------------------------------------------
  // SFP Step 5 of 6: Instantiate the forward problem
152 //-----------------------------------------------------
  QUESO::GenericVectorRV<> qoiRv("qoi_", qoiSpace);

  QUESO::StatisticalForwardProblem<> fp("", NULL, postRv, qoi, qoiRv);

157 //-----------------------------------------------------
  // SFP Step 6 of 6: Solve the forward problem
  //-----------------------------------------------------
  std::cout << "Solving the SFP with Monte Carlo"
            << std::endl << std::endl;
162 fp.solveWithMonteCarlo(NULL);

  gettimeofday(&timevalNow, NULL);
  if ((env.subDisplayFile()       ) &&
      (env.displayVerbosity() >= 2)) {
167   *env.subDisplayFile() << "Ending run of 'Gravity + Projectile motion' example at "
                            << ctime(&timevalNow.tv_sec)
                            << std::endl;
  }
  if (env.fullRank() == 0) {
172   std::cout << "Ending run of 'Gravity + Projectile motion' example at "
            << ctime(&timevalNow.tv_sec)
            << std::endl;
  }
}
```

Listing 6.27: File `gravity_compute.C`. The first part of the code (lines 60–150) handles the statistical forward problem, whereas the second part of the code (lines 151–216) handles the statistical forward problem.

```
class Likelihood : public QUESO::BaseScalarFunction<V, M>
{
public:
  Likelihood(const char * prefix, const QUESO::VectorSet<V, M> & domain);
  virtual ~Likelihood();
  virtual double lnValue(const V & domainVector, const V * domainDirection,
      V * gradVector, M * hessianMatrix, V * hessianEffect) const;
  virtual double actualValue(const V & domainVector, const V * domainDirection,
      V * gradVector, M * hessianMatrix, V * hessianEffect) const;

private:
  std::vector<double> m_heights; // heights
  std::vector<double> m_times;   // times
  std::vector<double> m_stdDevs; // uncertainties in time measurements
};

#endif
```

Listing 6.28: File `gravity_likelihood.h`.

```
#include <queso/StatisticalInverseProblem.h>
#include <queso/ScalarFunction.h>
#include <queso/VectorSet.h>

#include <gravity_likelihood.h>

template<class V, class M>
Likelihood<V, M>::Likelihood(const char * prefix,
    const QUESO::VectorSet<V, M> & domain)
  : QUESO::BaseScalarFunction<V, M>(prefix, domain),
    m_heights(0),
    m_times(0),
    m_stdDevs(0)
{
  // Data available in /inputData/data02.dat
  double const heights[] = {10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110,
                            120, 130, 140};

  double const times  [] = {1.41, 2.14, 2.49, 2.87, 3.22, 3.49, 3.81, 4.07,
                            4.32, 4.47, 4.75, 4.99, 5.16, 5.26};

  double const stdDevs[] = {0.020, 0.120, 0.020, 0.010, 0.030, 0.010, 0.030,
                            0.030, 0.030, 0.050, 0.010, 0.040, 0.010, 0.09};

  std::size_t const n = sizeof(heights) / sizeof(*heights);
  m_heights.assign(heights, heights + n);
  m_times.assign(times, times + n);
  m_stdDevs.assign(stdDevs, stdDevs + n);
}

template<class V, class M>
Likelihood<V, M>::~Likelihood()
```

```
{
  // Deconstruct here
}

template<class V, class M>
double
Likelihood<V, M>::lnValue(const V & domainVector, const V * domainDirection,
    V * gradVector, M * hessianMatrix, V * hessianEffect) const
{
  double g = domainVector[0];

  double misfitValue = 0.0;
  for (unsigned int i = 0; i < m_heights.size(); ++i) {
    double modelTime = std::sqrt(2.0 * m_heights[i] / g);
    double ratio = (modelTime - m_times[i]) / m_stdDevs[i];
    misfitValue += ratio * ratio;
  }

  return -0.5 * misfitValue;
}

template<class V, class M>
double
Likelihood<V, M>::actualValue(const V & domainVector,
    const V * domainDirection, V * gradVector, M * hessianMatrix,
    V * hessianEffect) const
{
  return std::exp(this->lnValue(domainVector, domainDirection, gradVector,
        hessianMatrix, hessianEffect));
}

template class Likelihood<QUESO::GslVector, QUESO::GslMatrix>;
```

Listing 6.29: File `gravity_likelihood.C`.

```
#define QUESO_EXAMPLE_GRAVITY_QOI_H

#include <queso/VectorFunction.h>
#include <queso/DistArray.h>

template<class P_V = QUESO::GslVector, class P_M = QUESO::GslMatrix,
         class Q_V = QUESO::GslVector, class Q_M = QUESO::GslMatrix>
class Qoi : public QUESO::BaseVectorFunction<P_V, P_M, Q_V, Q_M>
{
public:
  Qoi(const char * prefix, const QUESO::VectorSet<P_V, P_M> & domainSet,
      const QUESO::VectorSet<Q_V, Q_M> & imageSet);
  virtual ~Qoi();
  virtual void compute(const P_V & domainVector, const P_V * domainDirection,
      Q_V & imageVector, QUESO::DistArray<P_V *> * gradVectors,
      QUESO::DistArray<P_M *> * hessianMatrices,
      QUESO::DistArray<P_V *> * hessianEffects) const;

  void setAngle(double angle);
  void setInitialVelocity(double velocity);
  void setInitialHeight(double height);

private:
  double m_angle;
  double m_initialVelocity;
  double m_initialHeight;
};
```

```
#endif
```

Listing 6.30: File gravity_qoi.h.

```
#include <queso/GslVector.h>
#include <queso/GslMatrix.h>
#include <gravity_qoi.h>

template<class P_V, class P_M, class Q_V, class Q_M>
Qoi<P_V, P_M, Q_V, Q_M>::Qoi(const char * prefix,
    const QUESO::VectorSet<P_V, P_M> & domainSet,
    const QUESO::VectorSet<Q_V, Q_M> & imageSet)
  : QUESO::BaseVectorFunction<P_V, P_M, Q_V, Q_M>(prefix, domainSet, imageSet),
    m_angle(M_PI / 4.0),
    m_initialVelocity(5.0),
    m_initialHeight(0.0)
{
}

template<class P_V, class P_M, class Q_V, class Q_M>
Qoi<P_V, P_M, Q_V, Q_M>::~Qoi()
{
  // Deconstruct here
}

template<class P_V, class P_M, class Q_V, class Q_M>
void
Qoi<P_V, P_M, Q_V, Q_M>::compute(const P_V & domainVector,
    const P_V * domainDirection,
    Q_V & imageVector, QUESO::DistArray<P_V *> * gradVectors,
    QUESO::DistArray<P_M *> * hessianMatrices,
    QUESO::DistArray<P_V *> * hessianEffects) const
{
  if (domainVector.sizeLocal() != 1) {
    queso_error_msg("domainVector does not have size 1");
  }
  if (imageVector.sizeLocal() != 1) {
    queso_error_msg("imageVector does not have size 1");
  }

  double g = domainVector[0];  // Sample of the RV 'gravity acceleration'
  double distanceTraveled = 0.0;
  double aux = m_initialVelocity * std::sin(m_angle);
  distanceTraveled = (m_initialVelocity * std::cos(m_angle) / g) *
    (aux + std::sqrt(std::pow(aux, 2) + 2.0 * g * m_initialHeight));

  imageVector[0] = distanceTraveled;
}

template class Qoi<QUESO::GslVector, QUESO::GslMatrix, QUESO::GslVector,
                   QUESO::GslMatrix>;
```

Listing 6.31: File gravity_qoi.C.

6.3.5 Input File

QUESO reads an input file for solving statistical problems. In the case of a SIP, it expects a list of options for MCMC, while in case of SFP it expects a list of options for Monte Carlo. The input file '`gravity_inv_fwd.inp` used in this example is presented in Listing 6.32.

```
###############################################
# UQ Environment
###############################################
env_numSubEnvironments   = 1
env_subDisplayFileName   = outputData/display_env
env_subDisplayAllowAll   = 0
env_subDisplayAllowedSet = 0 1 2 3 4 5 6 7
env_displayVerbosity     = 2
env_seed                 = -1

###############################################
# Statistical inverse problem (ip)
###############################################
ip_computeSolution      = 1
ip_dataOutputFileName   = outputData/sip_gravity
ip_dataOutputAllowedSet = 0 1

###############################################
# Information for Metropolis-Hastings algorithm
###############################################
ip_mh_dataOutputFileName   = outputData/sip_gravity
ip_mh_dataOutputAllowedSet = 0 1

ip_mh_rawChain_dataInputFileName    = .
ip_mh_rawChain_size                 = 20000
ip_mh_rawChain_generateExtra        = 0
ip_mh_rawChain_displayPeriod        = 2000
ip_mh_rawChain_measureRunTimes      = 1
ip_mh_rawChain_dataOutputFileName   = outputData/sip_gravity_raw_chain
ip_mh_rawChain_dataOutputAllowedSet = 0 1 2 3 4 5 6 7

ip_mh_displayCandidates             = 0
ip_mh_putOutOfBoundsInChain         = 0
ip_mh_dr_maxNumExtraStages          = 3
ip_mh_dr_listOfScalesForExtraStages = 5. 10. 20.
ip_mh_am_initialNonAdaptInterval    = 0
ip_mh_am_adaptInterval              = 100
ip_mh_am_eta                        = 1.98    #(2.4^2)/d, d is the dimension of the problem
ip_mh_am_epsilon                    = 1.e-5

ip_mh_filteredChain_generate             = 1
ip_mh_filteredChain_discardedPortion     = 0.
ip_mh_filteredChain_lag                  = 20
ip_mh_filteredChain_dataOutputFileName   = outputData/sip_gravity_filtered_chain
ip_mh_filteredChain_dataOutputAllowedSet = 0 1

###############################################
# Statistical forward problem (fp)
###############################################
fp_help                 = anything
fp_computeSolution      = 1
fp_computeCovariances   = 1
fp_computeCorrelations  = 1
fp_dataOutputFileName   = outputData/sfp_gravity
fp_dataOutputAllowedSet = 0 1
```

```
#############################################
# 'fp_': information for Monte Carlo algorithm
#############################################
fp_mc_help                  = anything
fp_mc_dataOutputFileName    = outputData/sfp_gravity
fp_mc_dataOutputAllowedSet = 0 1

fp_mc_pseq_dataOutputFileName    = outputData/sfp_gravity_p_seq
fp_mc_pseq_dataOutputAllowedSet = 0 1

fp_mc_qseq_dataInputFileName     = .
fp_mc_qseq_size                  = 16384
fp_mc_qseq_displayPeriod         = 20000
fp_mc_qseq_measureRunTimes       = 1
fp_mc_qseq_dataOutputFileName    = outputData/sfp_gravity_qoi_seq
fp_mc_qseq_dataOutputAllowedSet = 0 1
```

Listing 6.32: Some options for QUESO library used in application code (Listings 6.25-6.29).

Moreover, for the gravity inverse problem, one may notice that QUESO will use the Metropolis-Hastings algorithm to sample the posterior PDF (indicated by the prefix `mh_` in the variable names) without adaptive steps (indicated by the zero value assigned to the variable `ip_mh_am_initialNonAdaptInterval`, which can also be achieved by setting zero to `ip_mh_am_adaptInterval`) and with delayed rejection (indicated by the one-value assigned to the variable `ip_mh_dr_maxNumExtraStages`).

6.3.6 Create your own Makefile

Listing 6.33 presents a Makefile, named `Makefile_example_violeta`, that may be used to compile the code and create the executable `gravity_gsl`. Naturally, it must be adapted to the user's settings, i.e., it has to have the correct paths for the user's libraries that were actually used to compile and install QUESO (see Sections 2.1–2.4).

```
QUESO_DIR = /path/to/queso
BOOST_DIR = /path/to/boost
GSL_DIR   = /path/to/gsl

INC_PATHS = \
   -I. \
   -I$(QUESO_DIR)/include \
   -I$(BOOST_DIR)/include \
   -I$(GSL_DIR)/include

LIBS = \
   -L$(QUESO_DIR)/lib -lqueso \
   -L$(BOOST_DIR)/lib -lboost_program_options \
   -L$(GSL_DIR)/lib -lgsl

CXX = mpic++
CXXFLAGS += -g -Wall -c

default: all

.SUFFIXES: .o .C

all:       example_gravity_gsl
```

```
clean:
   rm -f *~
   rm -f *.o
   rm -f gravity_gsl

example_gravity_gsl: gravity_main.o gravity_likelihood.o gravity_compute.o gravity_qoi.o
   $(CXX) gravity_main.o \
          gravity_likelihood.o \
          gravity_compute.o \
          gravity_qoi.o \
          -o gravity_gsl $(LIBS)

%.o: %.C
   $(CXX) $(INC_PATHS) $(CXXFLAGS) $<
```

Listing 6.33: Makefile for the application code in Listings 6.25-6.29

6.3.7 Running the Gravity Example with Several Processors

Even though the application described in Section 6.3.4 is a serial code, it is possible to run it using more than one processor, i.e., in parallel mode. Supposing the user's workstation has $N_p = 8$ processors, then, the user my choose to have $N_s = 8$, 4 or 2 subenvironments. This complies with the requirement that the total number of processors in the environment must be a multiple of the specified number of subenvironments.

Thus, to build and run the application code with $N_p = 8$, and $N_s = 8$ subenvironments, the must set the variable `env_numSubEnvironments = 8` in the input file (Listing 6.32) and enter the following command lines:

```
cd $HOME/LIBRARIES/QUESO-0.56.0/examples/gravity/
mpirun -np 8 ./gravity_gsl gravity_inv_fwd.inp
```

The steps above will create a total number of 8 raw chains, of size defined by the variable `ip_mh_rawChain_size`. QUESO internally combines these 8 chains into a single chain of size 8 $\times$ `ip_mh_rawChain_size` and saves it in a file named according to the variable `ip_mh_rawChain_dataOutputFileName`. QUESO also provides the user with the option of writing each chain – handled by its corresponding processor – in a separate file, which is accomplished by setting the variable `ip_mh_rawChain_dataOutputAllowedSet = 0 1 ... Ns-1`.

Note: Although the discussion in the previous paragraph refers to the raw chain of a SIP, the analogous is true for the filtered chains (SIP), and for the samples employed in the SFP (`ip_mh_filteredChain_size`, `fp_mc_qseq_size` and `fp_mc_qseq_size`, respectively).

6.3.8 Data Post-Processing and Visualization

According to the specifications of the input file in Listing 6.32, both a folder named `outputData` and a the following files should be generated:

```
sfp_gravity_sub0.m,          sip_gravity_sub0.m,
sfp_gravity_p_seq.m,         sip_gravity_filtered_chain.m,,
sfp_gravity_p_seq_sub0.m     sip_gravity_filtered_chain_sub0.m,
sfp_gravity_qoi_seq.m,       sip_gravity_raw_chain.m,
sfp_gravity_qoi_seq_sub0.m   sip_gravity_raw_chain_sub0.m,
display_env_sub0.txt
```

In this section, a convenient capability of QUESO of internally handling possible conflicts in chain size is presented. Recalling the input file `gravity_inv_fwd.inp` presented in Listing 6.32, one may notice that the raw chain size for the SIP is chosen to have 20000 positions (`ip_mh_rawChain_size = 20000`); the lag of the filtered chain is chosen to be 20 (`ip_mh_filteredChain_lag = 20`) and the chain size for the SFP has 16384 positions (`fp_mc_qseq_size = 16384`). Because the solution of the SIP, ie, the posterior PDF, is used as input PDF for the SFP, QUESO internally sets `fp_mc_qseq_size = 20000`, as can be seen in the file `display_env_sub0.txt`. The file `display_env_sub0.txt` contains information from the subenvironment '0' that was generated during the run of the application code.

6.3.8.1 Statistical Inverse Problem

There are a few Matlab-ready commands that are very helpful tools for post-processing the data generated by QUESO when solving statistical inverse problems. This section discusses the results computed by QUESO with the code of Section 6.3.4, and shows how to use Matlab for the post-processing of such results.

6.3.8.1.1 Chain Plots

It is quite simple to plot, using Matlab, the chain of positions used in the DRAM algorithm implemented within QUESO. The sequence of Matlab commands presented in Listing 6.34 generates the graphic depicted in Figure 6.3.3a. Figure 6.3.3b is obtained analogously.

```
% inside Matlab
>> sip_gravity_raw_chain
>> plot(ip_mh_rawChain_unified)
>> ylabel('\theta=g','fontsize',20);
>> xlabel('Number of positions','fontsize',20);
>> title('DRAM Chain Positions (raw)','fontsize',20);
```

Listing 6.34: Matlab code for the chain plot.

6.3.8.1.2 Histogram Plots

In order to plot histograms of the parameter using either the raw chain or the filtered chain, you simply have to use the pre-defined Matlab function `hist`.

```
% inside Matlab
>> sip_gravity_raw_chain
>> nbins=100;
>> hist(ip_mh_rawChain_unified,nbins)
```

```
>> title('Parameter Histogram (raw chain)','fontsize',20);
>> xlabel('Gravity (m/s^2)','fontsize',20);
>> ylabel('Frequency','fontsize',20);
>> grid on;
```

Listing 6.35: Matlab code for the histogram plot.

6.3.8.1.3 KDE Plots

Matlab function `ksdensity` (Kernel smoothing density estimate) together with the option `'pdf'` may be used for plotting the KDE of the parameter.

```
% inside Matlab
>> sip_gravity_raw_chain
>> [f,xi] = ksdensity(ip_mh_rawChain_unified,'function','pdf');
>> plot(xi,f,'-b','linewidth',3)
>> title('Parameter Kernel Density Estimation','fontsize',20);
>> xlabel('Gravity (m/s^2)','fontsize',20);
>> ylabel('KDE','fontsize',20);
>> grid on;
```

Listing 6.36: Matlab code for the KDE plot.

6.3.8.1.4 CDF Plots

Matlab function `ksdensity` (Kernel smoothing density estimate) with `'cdf'` option may also be used for plotting the Cumulative Distribution Function of the parameter.

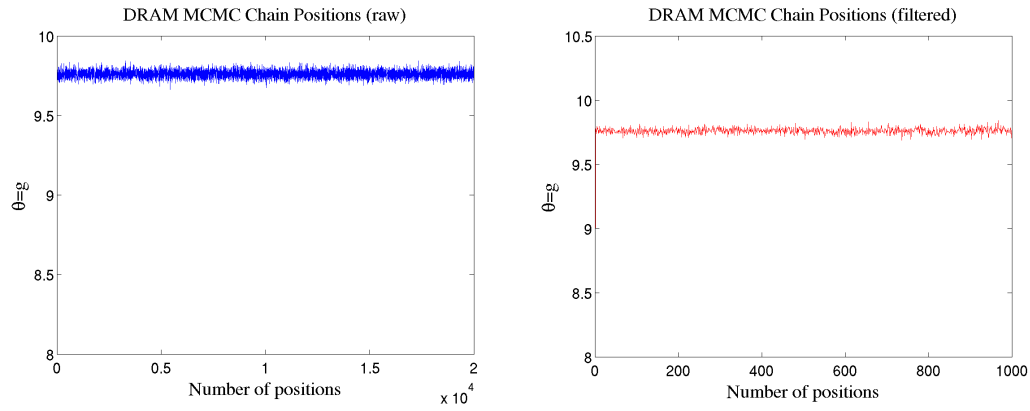
```
% inside Matlab
>> sip_gravity_raw_chain
>> [f,xi] = ksdensity(ip_mh_rawChain_unified,'function','cdf');
>> plot(xi,f,'-b','linewidth',3)
>> title('Parameter Cumulative Distribution Function','fontsize',20);
>> xlabel('Gravity (m/s^2)','fontsize',20);
>> ylabel('CDF','fontsize',20);
>> grid on;
```

Listing 6.37: Matlab code for the CDF plot.

6.3.8.1.5 Autocorrelation Plots

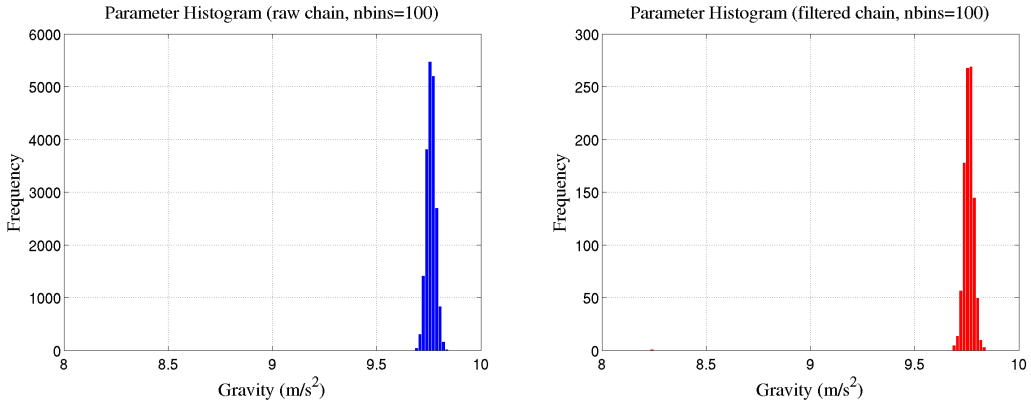
The code presented in Listing 6.38 uses matlab function `autocorr` to generate Figure 6.3.7 which presents the autocorrelation of the parameter g in both cases: raw and filtered chain.

```
% inside Matlab
>> sip_gravity_raw_chain
>> sip_gravity_filtered_chain
>> nlags=10;
>> [ACF_raw,lags,bounds]= autocorr(ip_mh_rawChain_unified, nlags, 0);
>> [ACF_filt,lags,bounds]=autocorr(ip_mh_filtChain_unified,nlags, 0);
>> plot(lags,ACF_raw,'bo-',lags,ACF_filt,'r*-','linewidth',3);
>> ylabel('Autocorrelation for \theta=g','fontsize',20);
>> xlabel('Lag','fontsize',20);
>> title('Parameter Autocorrelation','fontsize',20);
```



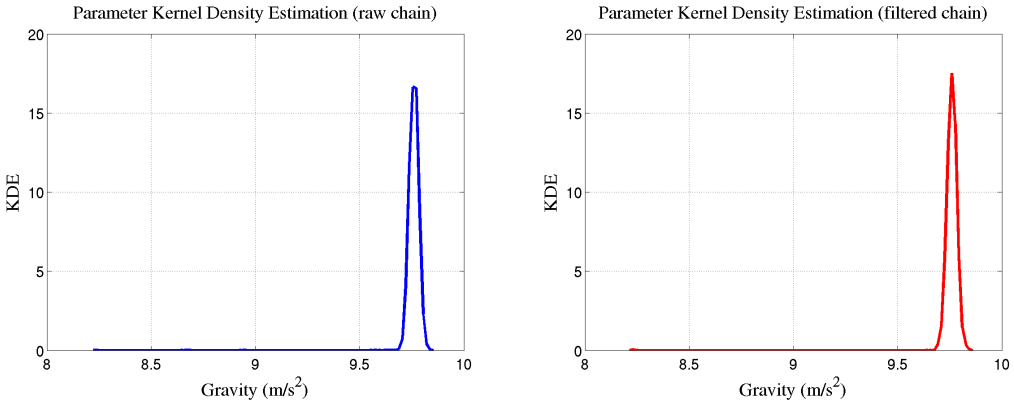
(a) Raw chain (b) Filtered chain

Figure 6.3.3: MCMC raw chain with 20000 positions and a filtered chain with lag of 20 positions.



(a) Raw chain (b) Filtered chain

Figure 6.3.4: Histograms of parameter $\theta = g$.



(a) Raw chain (b) Filtered chain

Figure 6.3.5: Kernel Density Estimation.

```
>> grid on;
>> h=legend('raw chain','filtered chain','location','northeast');
>> set(h,'fontsize',16);
```

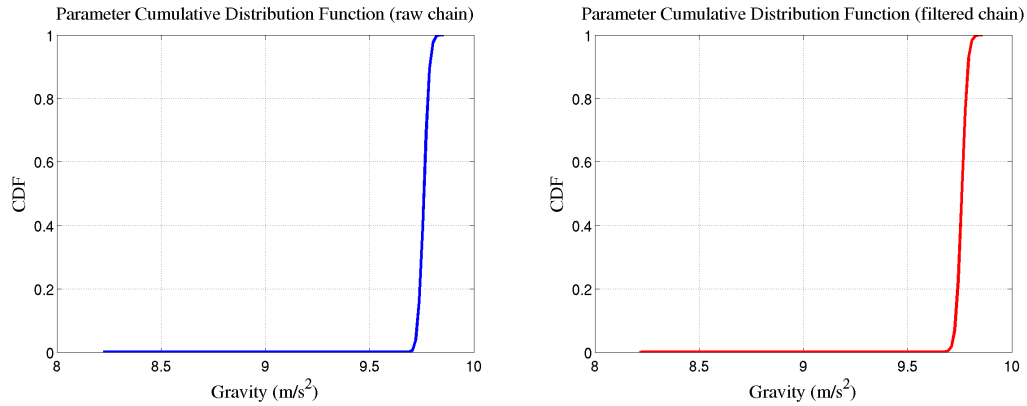
Listing 6.38: Matlab code for the autocorrelation plots.

6.3.8.1.6 Covariance and Correlation Matrices

Matlab function `cov` calculates the covariance matrix for a data matrix (where each column represents a separate quantity), and `corr` calculates the correlation matrix. Since our statistical inverse problem has only one parameter (the acceleration g due to gravity), both covariance and correlation matrices have dimension 1×1, i.e., they are scalars.

```
% inside Matlab
>> sip_gravity_raw_chain;
>> cov_matrix_g = cov(ip_mh_rawChain_unified)

cov_matrix_g =

   6.8709e-04
>> corr_matrix_g = corr(ip_mh_rawChain_unified)

corr_matrix_g =

     1
>>
```

Listing 6.39: Matlab code for finding the covariance matrix.



(a) Raw chain (b) Filtered chain

Figure 6.3.6: Cumulative Distribution Function.

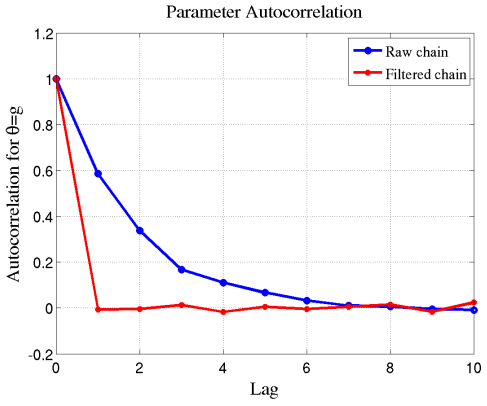


Figure 6.3.7: Autocorrelation plots.

6.3.8.2 Statistical Forward Problem

6.3.8.2.1 Chain Plots

It is quite simple to plot, using Matlab, the chain of positions generated by the Monte Carlo algorithm implemented within QUESO and called during the solution of the statistical forward problem. The sequence of Matlab commands presented bellow generates the graphic depicted in Figure 6.3.8a.

```
% inside Matlab
>> sfp_gravity_qoi_seq.m
>> plot(fp_mc_QoiSeq_unified);
>> ylabel('QoI','fontsize',20);
>> xlabel('Number of positions','fontsize',20);
>> title('MC Chain Positions','fontsize',20);
```

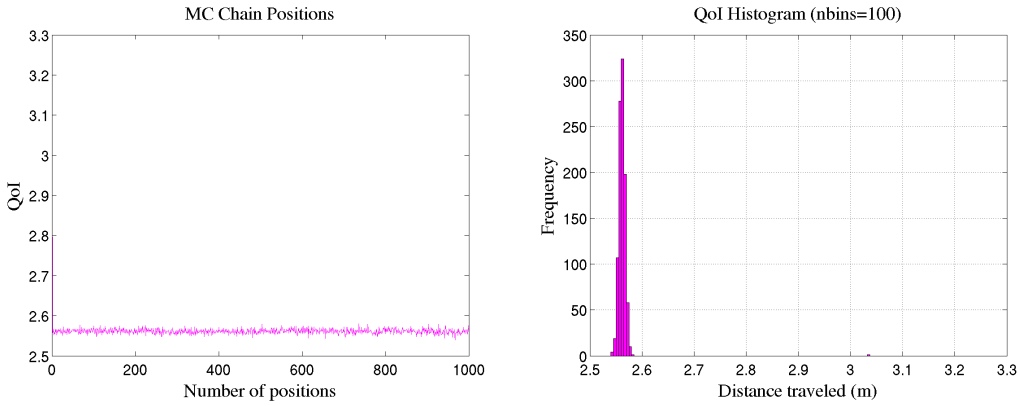
Listing 6.40: Matlab code for the chain plot.

6.3.8.2.2 Histogram Plots

In order to plot a histogram of the QoI, you may use the pre-defined Matlab function `hist`. The Matlab code presented in below shows how to create the Figure 6.3.8b.

```
>> sfp_gravity_qoi_seq.m
>> nbins=100;
>> hist(fp_mc_QoiSeq_unified);
>> title('QoI Histogram','fontsize',20);
>> xlabel('Distance traveled (m)','fontsize',20);
>> ylabel('Frequency','fontsize',20);
>> grid on;
```

Listing 6.41: Matlab code for the QoI histogram plot.



(a) Chain positions (b) Hystogram

Figure 6.3.8: MC chain positions and histogram of QoI = d.

6.3.8.2.3 KDE Plots

Matlab function `ksdensity` (Kernel smoothing density estimate) together with the option `'pdf'` may be used for plotting the KDE of the he QoI, displayed in Figure 6.3.9a.

```
% inside Matlab
>> sfp_gravity_qoi_seq.m
>> [f,xi] = ksdensity(fp_mc_QoiSeq_unified,'function','pdf');
>> plot(xi,f,'-b','linewidth',3)
>> title('QoI Kernel Density Estimation ','fontsize',20);
>> xlabel('Distance traveled (m)','fontsize',20);
>> ylabel('KDE','fontsize',20);
>> grid on;
```

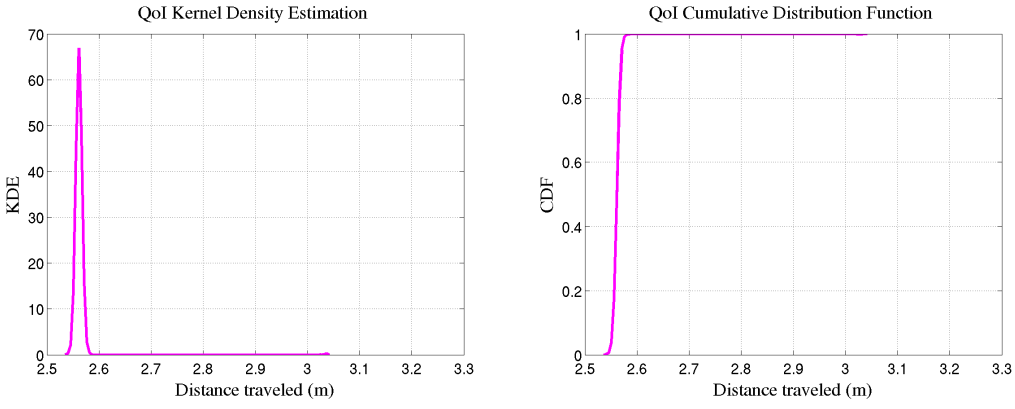
Listing 6.42: Matlab code for the QoI KDE plot.

6.3.8.2.4 CDF Plots

Matlab function `ksdensity` (Kernel smoothing density estimate) with `'cdf'` option may also be used for plotting the Cumulative Distribution Function of the QoI, displayed in Figure 6.3.9b.

```
% inside Matlab
>> sfp_gravity_qoi_seq.m
>> [f,xi] = ksdensity(fp_mc_QoiSeq_unified,'function','cdf');
>> plot(xi,f,'-b','linewidth',3)
>> title('QoI Cumulative Distribution Function ','fontsize',20);
>> xlabel('Distance traveled (m)','fontsize',20);
>> ylabel('CDF','fontsize',20);
>> grid on;
```

Listing 6.43: Matlab code for the QoI CDF plot.



(a) KDE (b) CDF

Figure 6.3.9: Kernel Density Estimation and Cumulative Distribution Function of QoI.

6.3.8.2.5 Autocorrelation Plots

The code presented in Listing 6.44 uses Matlab function `autocorr` to generate Figure 6.3.10, which presents the autocorrelation of the QoI d.

```
% inside Matlab
>> sfp_gravity_qoi_seq.m
>> nlags=10;
>> [ACF, lags, bounds] = autocorr(fp_mc_QoiSeq_unified, nlags, 0);
>> plot(lags,ACF,'bo-','linewidth',3);
>> ylabel('Autocorrelation for QoI = d','fontsize',20);
>> xlabel('Lag','fontsize',20);
>> title('QoI Autocorrelation','fontsize',20);
>> grid on;
```

Listing 6.44: Matlab code for the QoI autocorrelation plot.

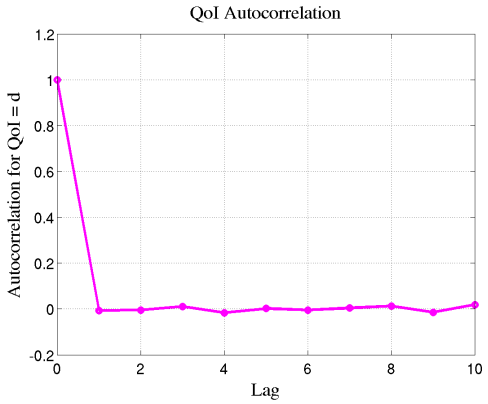


Figure 6.3.10: Autocorrelation plot.

6.3.8.2.6 Covariance and Correlation Matrices

For a matrix input `X`, where each row is an observation, and each column is a variable, the Matlab function `cov(X)` may be used to calculate the covariance matrix.

Thus, in order to calculated the covariance matrix between the parameter and the quantity of interest sequences generated by Monte Carlo sampler with QUESO, one may simply define `X=[fp_mc_ParamSeq_unified fp_mc_QoiSeq_unified]`. The code presented in Listing 6.45 shows the usage of Matlab commands for finding such the matrix.

```
% inside Matlab
>> sfp_gravity_qoi_seq;
>> sfp_gravity_p_seq;
>> X=[fp_mc_ParamSeq_unified fp_mc_QoiSeq_unified];
>> cov_p_QoI = cov(X)

cov_p_QoI =
    [ 2.826e-03   -8.555e-04 ]
    [-8.555e-04    2.599e-04 ]
```

Listing 6.45: Matlab code for the matrix of covariance between parameter g and QoI d.

Analogously, the Matlab function `corrcoef(X)` returns a matrix of correlation coefficients calculated from an input matrix `X` whose rows are observations and whose columns are variables. In order to calculated the correlation matrix between the parameter and the QoI sequences, one may simply define `X=[fp_mc_ParamSeq_unified fp_mc_QoiSeq_unified]`.

```
% inside Matlab
>> sfp_gravity_qoi_seq;
>> sfp_gravity_p_seq;
>> X=[fp_mc_ParamSeq_unified fp_mc_QoiSeq_unified];
>> corr_p_QoI = corrcoef(X)

corr_p_QoI =
    [ 1.000e+00   -9.981e-01 ]
    [-9.981e-01    1.000e+00 ]
>>
```

Listing 6.46: Matlab code for the matrix of correlation between parameter g and quantity of interest d.

6.4 validationCycle

This is the last and more complex of all QUESO examples. In this example, we numerically solve a statistical inverse problem related to a thermogravimetric experiment, where a material sample has its mass measured while loosing it through a controlled heating process.

Given a simple mass evolution model that has a temperature profile and material properties as input parameters, and given thermogravimetric measurements with prescribed variances, the statistical inverse problems ask for the specification of the random variables that represent the unknown material properties. We compute probability density functions with the Bayesian approach and compute sets of realizations through the Metropolis-Hastings algorithm with delayed rejection.

We qualitatively analyze the sensitivity of the solutions with respect to problem characteristics, namely "amount" of data and "quality" of data, and also with respect to algorithm options, namely chain initial position, number of delayed rejections and chain size.

6.4.1 Thermogravimetric Experiments and a Simple Model

Suppose a given material sample of initial mass m_0 and at initial temperature T_0 is heated with constant heating rate β (K/min). Heating is maintained until the sample fully ablates (decomposes). The sample mass $m(T)$ is measured at temperatures $T > T_0$. Let $w(T) = m(T)/m_0$ denote the mass fraction.

It is convenient to transform the kinetic equation to a *per unit temperature* form by dividing through by β. Thus, a simple approach to the simulation of a thermogravimetric phenomenon consists on modeling the sample as a homogeneous material of scalar properties $A > 0$ and $E > 0$ whose relative mass w obeys the following initial value ordinal differential equation

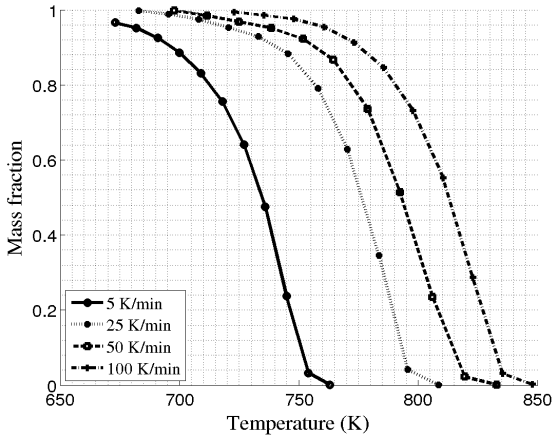


Figure 6.4.1: Mass fraction decay over temperature given different heating rates. Data from J. A. Conesa, R. F. Marcilla and J. A. Caballero, "Thermogravimetric studies on the thermal decomposition of polyethylene", *J. Anal. Appl. Pyrolysis*, 36(1):1-15, 1996

problem:

$$\begin{cases} \dfrac{dw}{dt} &= -\dfrac{Aw}{\beta}\exp\left(-\frac{E}{RT}\right), \quad t \geqslant 0, \\ \\ w(0) &= 1, \end{cases} \tag{6.4.1}$$

where the kinetic parameters A and E are referred to, respectively, as pre-exponential factor (min^{-1}) and activation energy (J/mol).

In this combined SIP–SFP, we calibrate both model parameters A and E given the mathematical model in Equation (6.4.1) and experimental data (Section 6.4.2.3). Then the inferred values for A and E are then used for uncertainty propagation on the remaining mass fraction at time $t = 3.9$ s when $\beta = 250$ K/min, i.e., our quantity of interest is $w(t = 3.9)$.

6.4.2 Statistical Inverse Problem

Let $\mathbf{m} = (A, E)$ be the vector of model parameters and $M = \mathbb{R}^2_+$ be the space of model parameters. Let V_T denote the space of functions $f : \mathbb{R}_+ \to \mathbb{R}_+$ that are weakly differentiable. V_T will be the space of temperature profiles. Finally, let V_w denote the space of functions $f : \mathbb{R}_+ \to [0, 1]$ that are weakly differentiable. V_w will be the space of relative mass evolutions. We will denote by

$$w(\mathbf{m}, T) \in V_w$$

the solution of Equation (6.4.1) for given $\mathbf{m} \in M$ and $T \in V_T$.

6.4.2.1 Misfit Functions $\mathcal{F}(\mathbf{m})$

Let V_S denote the space of all functions $f : \mathbb{R}_+ \to \mathbb{R}_+$ that are square-Lebesgue-integrable over any finite interval. V_S will be the space of misfit weight functions. Let V_σ denote the

space of all functions $f : \mathbb{R}_+ \to \mathbb{R}_+^*$ such that $1/f$ is square-Lebesgue-integrable over any finite interval. V_σ will be the space of variance functions.

Given a reference relative mass evolution function $d \in V_w$, a temperature profile $T \in V_T$, and some $t_{\text{F}} > 0$, let $\mathcal{F} : M \to \mathbb{R}$ be the functional defined by

$$\mathcal{F}(\mathbf{m}) = \int_0^{t_{\text{F}}} \{[w(\mathbf{m}, T)](t) - d(t)\}^2 \cdot S(t)\ dt,$$

or simply

$$\mathcal{F}(\mathbf{m}) = \int_0^{t_{\text{F}}} (w - d)^2 \cdot S\ dt. \tag{6.4.2}$$

The functional (6.4.2) is general enough for our studies, since it can properly describe not only the case where one has continuous measurements d, but also the case of a finite set of N_{meas} discrete measurements $0 \leqslant d_j \leqslant 1$, $1 \leqslant i \leqslant N_{\text{meas}}$ at instants $0 \leqslant t_1 < t_2 < \ldots < t_{N_{\text{meas}}}$.

In the case of continuous measurements, for instance, one can set

$$\mathcal{F}_1(\mathbf{m}) = \int_0^{t_{\text{F}}} \{[w(\mathbf{m}, T)](t) - d(t)\}^2 \cdot \frac{1}{\sigma^2(t)}\ dt,$$

for some given variance function $\sigma^2 \in V_S$ satisfying $\sigma(t) > 0$ for all $t \geqslant 0$.

On the other hand, when measurements are discrete and a corresponding finite set of variances $\sigma_j^2 > 0,\ j = 1, 2, \ldots, N_{\text{meas}}$ is given, one can set

$$\mathcal{F}_2(\mathbf{m}) = \int_0^{t_F} \{[w(\mathbf{m}, T)](t) - \hat{d}(t)\}^2 \cdot \left[\sum_{j=1}^{N_{\text{meas}}} \frac{\delta(t - t_j)}{\hat{\sigma}^2(t)}\right] dt,$$

where $\hat{d} \in V_w$ and $\hat{\sigma} \in V_\sigma$ are any functions satisfying $\hat{d}(t_j) = d_j$ and $\hat{\sigma}(t_j) = \sigma_j$, $j = 1, 2, \ldots, N_{\text{meas}}$, in which case the functional simply becomes

$$\mathcal{F}_2(\mathbf{m}) = \sum_{j=1}^{N_{\text{meas}}} \frac{\{[w(\mathbf{m}, T)](t_j) - d_j\}^2}{\sigma_j^2},$$

assuming, without loss of generality, that $t_F \geqslant t_{N_{\text{meas}}}$.

6.4.2.2 Bayesian Approach: Prior RV, Likelihood and Posterior RV

In deterministic inverse problems treat the unknown parameters as scalars or vectors and the goal is the calculation of their best values according to a given criteria, usually least squares, e.g. solving the unconstrained optimization problem

$$\min_{\mathbf{m} \in M} \mathcal{F}(\mathbf{m}). \tag{6.4.3}$$

In statistical inverse problems, the unknown parameters are treated as random variables (RVs) and the goal is the specification of their probability density functions (PDFs) [33].

Applying the Bayesian approach

$$\pi_{\text{posterior}}(\mathbf{m}) \propto \pi_{\text{prior}}(\mathbf{m}) \cdot \pi_{\text{likelihood}}(\mathbf{m})$$

we have that for the TGA SIP, the prior distribution and the likelihood are, respectively:

$$\pi_{\text{prior}}(\mathbf{m}) \propto e^{-\frac{1}{2}V(\mathbf{m})} \quad \text{and} \quad \pi_{\text{likelihood}}(\mathbf{m}) \propto e^{-\frac{1}{2}\mathcal{F}(\mathbf{m})}.$$

Thus, we chose parameters (A, E) to have joint uniform prior PDF over the open square domain, i.e.:

$$\pi_{\text{prior}} = \mathcal{U}((1.0 \times 10^{10}, 5.0 \times 10^{11}) \times (4.0 \times 10^{5}, 6.0 \times 10^{5})).$$

6.4.2.3 Data from experiments

Table 6.4.1 presents the data collected in the TGA experiment.

Observation index "i"	Temperature T_i (K)	Relative mass $m^*_{\text{obs},i}$ (%)	Variance V_i
1	673.034	96.5855	0.1
2	682.003	95.1549	0.1
3	690.985	92.5048	0.1
4	699.979	88.6353	0.1
5	708.989	83.0585	0.1
6	718.02	75.5306	0.1
7	727.089	64.1003	0.1
8	735.96	47.5474	0.1
9	744.904	23.6777	0.1
10	754.062	03.2234	0.1
11	763.049	00.0855448	0.1

Table 6.4.1: Experimental data.

6.4.3 Statistical Forward Problem

In spacecraft design, ablation is used to both cool and protect mechanical parts and/or payloads that would otherwise be damaged by extremely high temperatures. Two principal applications are heat shields for spacecraft entering a planetary atmosphere from space and cooling of rocket engine nozzles [60].

Suppose that an object about to re-enter the Earth atmosphere has a thermal protection layer (shield) of composition of the same sample material described in Section 6.4.2. Also, as the object re-enters the atmosphere, its shield loses mass according to Equation (6.4.1). The initial sample temperature is $T_0 = 0.1$ K and it is then heated with constant rate $\beta = 5$ K/m.

We are interested in answering the following question: at scenario $\beta = 250$ K/min, what is the remaining mass fraction at time $t = 3.9$ s? In other words, the quantity of interest is $w(t = 3.9s)$.

6.4.3.1 The Input RV, QoI Function and Output RV

The input random variables for this SFP are the inferred parameters A and E which are the solution (posterior PDF) of the inverse problem described in Section 6.4.2. The output random variable for this example is the remaining mass fraction at 3.9 s, i.e. $w(t = 3.9)$. Note that, since there is uncertainty in the parameters A and E (both given as PDFs), one can expect that this uncertainty will be propagated to $w(t = 3.9)$, which will also be given as a PDF. Finally, the QoI function for w is the solution of the Equation (6.4.1) evaluated when $t = 3.9$ s, which is calculated using numerical integration with adjustable and acceptable time-stepping using GSL function `gsl_odeiv_evolve_apply`[1].

6.4.4 Running the Example

To run the executable provided (available after QUESO installation), and generate figures for the chains, PDFs, CDFs, etc., enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.50.0/examples/validationCycle
$ rm outputData/*
$ ./exTgaValidationCycle_gsl tagCycle.inp
$ matlab
   $ tga_cycle_plot.m     # inside matlab
   $ exit                 # inside matlab
$ ls -l outputData/*.png
  cal_parameter1_prior.png                cal_parameter2_prior.png
  cal_val_parameter1_PDF.png              cal_val_parameter2_PDF.png
  cal_val_parameter1_CDF.png              cal_val_parameter2_CDF.png
  cal_val_parameter1_autocorr.png         cal_val_parameter2_autocorr.png
  cal_val_QoI_CDF.png                     cal_val_QoI_PDF.png
  cal_val_QoI_autocorrelation.png
```

As a result, the user should have created several of PNG figures containing marginal posterior PDF, chain positions of the parameters and the QoI, histogram, cumulative density distribution and autocorrelation. The name of the figure files have been chosen to be informative, as shown in the Listing above.

6.4.5 TGA Example Code

The program example given in this paper is compatible with version 0.56.0 of QUESO. The source code for the example is composed of 5 files: `exTgaValidationCycle_gsl.C` (Listing 6.47), `exTgaValidationCycle_appl.h` (Listing 6.48), `exTgaValidationCycle_likelihood.h` (Listing 6.49) and `exTgaValidationCycle_qoi.C` (Listing 6.50).

[1] http://www.gnu.org/software/gsl/manual/html_node/Evolution.html#index-gsl_005fodeiv2_005fevolve_005fapply

```
/* This is an example of how to define and run a PECOS validation cycle for a
 * thermogravimetric analysis (TGA) model
 * using QUESO classes and algorithms. The code itself is in the templated
 * routine 'uqAppl(*env)'. This routine is called right after the initialization
 * of the MPI environment and of the QUESO environment and is available in
 * file 'exTgaValidationCycle_gsl.C'.
 *
 * It is easier to understand this example after undertanding three other simpler
 * examples:
 * (1) examples/simpleStatisticalInverseProblem/src/example_main.C
 * (2) examples/simpleStatisticalForwardProblem/src/simple_sfp_example_main.C
 * (3) examples/gravity/src/gravity_main.C
 *
 * Example (1) focuses on the templated class StatisticalInverseProblem<P_V,P_M>.
 * Example (2) focuses on the templated class StatisticalForwardProblem<P_V,P_M,Q_V,Q_M>.
 * Example (3) focuses on both classes, since it uses the solution of the inverse problem
 * as input to the forward problem.
 *
 * This example with TGA uses both statistical problem templated classes, twice each in
 * fact, but it also:
 * - uses the templated class ValidationCycle<P_V,P_M,Q_V,Q_M>,
 * - reads experimental data from files in order to compute the likelihood function
 *   at candidate parameter vectors generated by the Metropolis-Hastings algorithm, and
 * - compares the qoi cdfs computed from the two statistical forward problems at
 *   the prediction scenario.
 *--------------------------------------------------------------------------
 *-------------------------------------------------------------------------- */

#include <exTgaValidationCycle_appl.h>
#include <queso/GslMatrix.h>
#include <queso/EnvironmentOptions.h>

int main(int argc, char* argv[])
{
  //*****************************************************
  // Initialize environment
  //*****************************************************
#ifdef QUESO_HAS_MPI
  MPI_Init(&argc,&argv);
#endif

  QUESO::EnvOptionsValues* envOptionsValues = NULL;
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
  UQ_FATAL_TEST_MACRO(argc != 2,
                      QUESO::UQ_UNAVAILABLE_RANK,
                      "main()",
                      "input file must be specified in command line as argv[1], just after
                          executable argv[0]");
#ifdef QUESO_HAS_MPI
  QUESO::FullEnvironment* env = new QUESO::FullEnvironment(MPI_COMM_WORLD,argv[1],"",
      envOptionsValues);
#else
  QUESO::FullEnvironment* env = new QUESO::FullEnvironment(argv[1],"",envOptionsValues);
#endif

#else
  envOptionsValues = new QUESO::EnvOptionsValues();
  envOptionsValues->m_subDisplayFileName    = "outputData/display";
  envOptionsValues->m_subDisplayAllowedSet.insert(0);
  envOptionsValues->m_subDisplayAllowedSet.insert(1);
  envOptionsValues->m_displayVerbosity      = 2;
  envOptionsValues->m_seed                  = 0;

#ifdef QUESO_HAS_MPI
```

```
  QUESO::FullEnvironment* env = new QUESO::FullEnvironment(MPI_COMM_WORLD,"","",
      envOptionsValues);
#else
  QUESO::FullEnvironment* env = new QUESO::FullEnvironment("","",envOptionsValues);
#endif
#endif

  //*****************************************
  // Run application
  //*****************************************
  uqAppl<QUESO::GslVector, // type for parameter vectors
         QUESO::GslMatrix, // type for parameter matrices
         QUESO::GslVector, // type for qoi vectors
         QUESO::GslMatrix  // type for qoi matrices
        >(*env);

  //*****************************************
  // Finalize environment
  //*****************************************
  delete env;
  delete envOptionsValues;
#ifdef QUESO_HAS_MPI
  MPI_Finalize();
#endif
  return 0;
}
```

Listing 6.47: File `exTgaValidationCycle_gsl.C`.

```
#ifndef EX_TGA_VALIDATION_CYCLE_APPL_H
#define EX_TGA_VALIDATION_CYCLE_APPL_H

#define UQ_EXAMPLES_USES_QUESO_INPUT_FILE

#include <exTgaValidationCycle_likelihood.h>
#include <exTgaValidationCycle_qoi.h>
#include <queso/ValidationCycle.h>
#include <queso/VectorSubset.h>
#include <queso/UniformVectorRV.h>
#include <queso/GenericScalarFunction.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_odeiv.h>

//Just declaration: actual code is below
template<class P_V,class P_M,class Q_V,class Q_M>
void
uqAppl_LocalComparisonStage(QUESO::ValidationCycle<P_V,P_M,Q_V,Q_M>& cycle);

template<class P_V,class P_M,class Q_V,class Q_M>
void
uqAppl_UnifiedComparisonStage(QUESO::ValidationCycle<P_V,P_M,Q_V,Q_M>& cycle);

//*****************************************************
// The driving routine "uqAppl()": called by main()
// There are 5 main tasks:
// 1) initilization
// 2) the 'calibration stage'
// 3) the 'validation stage'
// 4) the 'comparison stage'
// 5) memory release
// Tasks 2, 3 and 4 constitute the actual validation cycle.
//*****************************************************
```

```
template<class P_V,class P_M,class Q_V,class Q_M>
void
uqAppl(const QUESO::BaseEnvironment& env)
{
  if (env.fullRank() == 0) {
    std::cout << "Beginning run of 'uqTgaExample' example\n"
              << std::endl;
  }

  int iRC;
  struct timeval timevalRef;
  struct timeval timevalNow;

  //*****************************************************
  // Task 1 of 5: instantiation of basic classes
  //*****************************************************

  // Instantiate the parameter space
  std::vector<std::string> paramNames(2,"");
  paramNames[0] = "A_param";
  paramNames[1] = "E_param";
  QUESO::VectorSpace<P_V,P_M> paramSpace(env,"param_",paramNames.size(),&paramNames);

  // Instantiate the parameter domain
  P_V paramMinValues(paramSpace.zeroVector());
  paramMinValues[0] = 2.40e+11;
  paramMinValues[1] = 1.80e+05;
  P_V paramMaxValues(paramSpace.zeroVector());
  paramMaxValues[0] = 2.80e+11;
  paramMaxValues[1] = 2.20e+05;
  QUESO::BoxSubset<P_V,P_M> paramDomain("param_",
                                        paramSpace,
                                        paramMinValues,
                                        paramMaxValues);

  // Instantiate the qoi space
  std::vector<std::string> qoiNames(1,"");
  qoiNames[0] = "TimeFor25PercentOfMass";
  QUESO::VectorSpace<Q_V,Q_M> qoiSpace(env,"qoi_",qoiNames.size(),&qoiNames);

  // Instantiate the validation cycle
  QUESO::ValidationCycle<P_V,P_M,Q_V,Q_M> cycle(env,
                                                "", // No extra prefix
                                                paramSpace,
                                                qoiSpace);

  //*****************************************************
  // Task 2 of 5: calibration stage
  //*****************************************************

  iRC = gettimeofday(&timevalRef, NULL);
  if (iRC) {}; // just to remove compiler warning
  if (env.fullRank() == 0) {
    std::cout << "Beginning 'calibration stage' at " << ctime(&timevalRef.tv_sec)
              << std::endl;
  }

  // Inverse problem: instantiate the prior rv
  QUESO::UniformVectorRV<P_V,P_M> calPriorRv(
    "cal_prior_", // Extra prefix before the default "rv_" prefix
    paramDomain);

  // Inverse problem: instantiate the likelihood function object (data + routine)
  likelihoodRoutine_Data<P_V,P_M> calLikelihoodRoutine_Data(env,
                                                            "scenario_5_K_min.dat",
```

```
                                                                "scenario_25_K_min.dat",
                                                                "scenario_50_K_min.dat");

  QUESO::GenericScalarFunction<P_V,P_M> calLikelihoodFunctionObj("cal_like_",
                                                                paramDomain,
                                                                likelihoodRoutine<P_V,P_M>,
                                                                (void *) &
                                                                    calLikelihoodRoutine_Data
                                                                    ,
                                                                true); // the routine
                                                                    computes [ln(function)]

  // Inverse problem: instantiate it (posterior rv is instantiated internally)
  QUESO::SipOptionsValues* calIpOptionsValues = NULL;
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  calIpOptionsValues = new QUESO::SipOptionsValues();
  calIpOptionsValues->m_computeSolution      = true;
  calIpOptionsValues->m_dataOutputFileName   = "outputData/tgaCalOutput";
  calIpOptionsValues->m_dataOutputAllowedSet.insert(0);
  calIpOptionsValues->m_dataOutputAllowedSet.insert(1);
#endif
  cycle.instantiateCalIP(calIpOptionsValues,
                         calPriorRv,
                         calLikelihoodFunctionObj);

  // Inverse problem: solve it, that is, set 'pdf' and 'realizer' of the posterior rv
  P_V paramInitialValues(paramSpace.zeroVector());
  if (env.numSubEnvironments() == 1) {
    // For regression test purposes
    paramInitialValues[0] = 2.41e+11;
    paramInitialValues[1] = 2.19e+05;
  }
  else {
    calPriorRv.realizer().realization(paramInitialValues);
  }

  QUESO::MhOptionsValues* calIpMhOptionsValues = NULL;
  P_M* calProposalCovMatrix = cycle.calIP().postRv().imageSet().vectorSpace().
      newProposalMatrix(NULL,&paramInitialValues);
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  QUESO::SsOptionsValues ssOptionsValues1;
  QUESO::SsOptionsValues ssOptionsValues2;

  ssOptionsValues1.m_initialDiscardedPortions.resize(9);
  ssOptionsValues1.m_initialDiscardedPortions[0] = 0.;
  ssOptionsValues1.m_initialDiscardedPortions[1] = 0.05;
  ssOptionsValues1.m_initialDiscardedPortions[2] = 0.10;
  ssOptionsValues1.m_initialDiscardedPortions[3] = 0.15;
  ssOptionsValues1.m_initialDiscardedPortions[4] = 0.20;
  ssOptionsValues1.m_initialDiscardedPortions[5] = 0.25;
  ssOptionsValues1.m_initialDiscardedPortions[6] = 0.30;
  ssOptionsValues1.m_initialDiscardedPortions[7] = 0.35;
  ssOptionsValues1.m_initialDiscardedPortions[8] = 0.40;
  ssOptionsValues1.m_autoCorrComputeViaDef       = false;
  ssOptionsValues1.m_autoCorrComputeViaFft       = true;
  ssOptionsValues1.m_autoCorrSecondLag           = 2;
  ssOptionsValues1.m_autoCorrLagSpacing          = 2;
  ssOptionsValues1.m_autoCorrNumLags             = 15;
  ssOptionsValues1.m_autoCorrDisplay             = true;
  ssOptionsValues1.m_autoCorrWrite               = true;
  ssOptionsValues1.m_kdeCompute                  = false;
  ssOptionsValues1.m_covMatrixCompute            = true;
  ssOptionsValues1.m_corrMatrixCompute           = true;
```

```
  ssOptionsValues2.m_initialDiscardedPortions.resize(1);
  ssOptionsValues2.m_initialDiscardedPortions[0] = 0.;
  ssOptionsValues2.m_autoCorrComputeViaDef       = false;
  ssOptionsValues2.m_autoCorrComputeViaFft       = true;
  ssOptionsValues2.m_autoCorrSecondLag           = 2;
  ssOptionsValues2.m_autoCorrLagSpacing          = 2;
  ssOptionsValues2.m_autoCorrNumLags             = 15;
  ssOptionsValues2.m_autoCorrDisplay             = true;
  ssOptionsValues2.m_autoCorrWrite               = true;
  ssOptionsValues2.m_kdeCompute                  = true;
  ssOptionsValues2.m_kdeNumEvalPositions         = 250;
  ssOptionsValues2.m_covMatrixCompute            = true;
  ssOptionsValues2.m_corrMatrixCompute           = true;

  calIpMhOptionsValues = new QUESO::MhOptionsValues(&ssOptionsValues1,&ssOptionsValues2);
  calIpMhOptionsValues->m_dataOutputFileName   = "outputData/tgaCalOutput";
  calIpMhOptionsValues->m_dataOutputAllowedSet.insert(0);
  calIpMhOptionsValues->m_dataOutputAllowedSet.insert(1);

  calIpMhOptionsValues->m_rawChainDataInputFileName     = ".";
  calIpMhOptionsValues->m_rawChainSize                  = 1048576;
  calIpMhOptionsValues->m_rawChainGenerateExtra         = false;
  calIpMhOptionsValues->m_rawChainDisplayPeriod         = 20000;
  calIpMhOptionsValues->m_rawChainMeasureRunTimes       = true;
  calIpMhOptionsValues->m_rawChainDataOutputFileName    = "outputData/file_cal_ip_raw";
  calIpMhOptionsValues->m_rawChainDataOutputAllowedSet.insert(0);
  calIpMhOptionsValues->m_rawChainDataOutputAllowedSet.insert(1);
  calIpMhOptionsValues->m_rawChainComputeStats          = true;

  calIpMhOptionsValues->m_displayCandidates         = false;
  calIpMhOptionsValues->m_putOutOfBoundsInChain     = true;
  calIpMhOptionsValues->m_tkUseLocalHessian         = false;
  calIpMhOptionsValues->m_tkUseNewtonComponent      = true;
  calIpMhOptionsValues->m_drMaxNumExtraStages       = 1;
  calIpMhOptionsValues->m_drScalesForExtraStages.resize(1);
  calIpMhOptionsValues->m_drScalesForExtraStages[0] = 5.;
  calIpMhOptionsValues->m_amInitialNonAdaptInterval = 0;
  calIpMhOptionsValues->m_amAdaptInterval           = 100;
  calIpMhOptionsValues->m_amEta                     = 1.92;
  calIpMhOptionsValues->m_amEpsilon                 = 1.e-5;

  calIpMhOptionsValues->m_filteredChainGenerate             = true;
  calIpMhOptionsValues->m_filteredChainDiscardedPortion     = 0.;
  calIpMhOptionsValues->m_filteredChainLag                  = 20;
  calIpMhOptionsValues->m_filteredChainDataOutputFileName   = ".";
  calIpMhOptionsValues->m_filteredChainDataOutputAllowedSet.insert(0);
  calIpMhOptionsValues->m_filteredChainDataOutputAllowedSet.insert(1);
  calIpMhOptionsValues->m_filteredChainComputeStats         = true;
#endif
  cycle.calIP().solveWithBayesMetropolisHastings(calIpMhOptionsValues,
                                                 paramInitialValues,
                                                 calProposalCovMatrix);
  delete calProposalCovMatrix;
  delete calIpMhOptionsValues;

  // Forward problem: instantiate it (parameter rv = posterior rv of inverse problem; qoi rv
      is instantiated internally)
  double beta_prediction         = 250.;
  double criticalMass_prediction = 0.;
  double criticalTime_prediction = 3.9;

  qoiRoutine_Data<P_V,P_M,Q_V,Q_M> calQoiRoutine_Data;
  calQoiRoutine_Data.m_beta         = beta_prediction;
  calQoiRoutine_Data.m_criticalMass = criticalMass_prediction;
```

```
  calQoiRoutine_Data.m_criticalTime = criticalTime_prediction;

  QUESO::SfpOptionsValues* calFpOptionsValues = NULL;
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  calFpOptionsValues = new QUESO::SfpOptionsValues();
  calFpOptionsValues->m_computeSolution      = true;
  calFpOptionsValues->m_computeCovariances   = true;
  calFpOptionsValues->m_computeCorrelations  = true;
  calFpOptionsValues->m_dataOutputFileName   = "outputData/tgaCalOutput";
  calFpOptionsValues->m_dataOutputAllowedSet.insert(0);
  calFpOptionsValues->m_dataOutputAllowedSet.insert(1);
#endif
  cycle.instantiateCalFP(calFpOptionsValues,
                         qoiRoutine<P_V,P_M,Q_V,Q_M>,
                         (void *) &calQoiRoutine_Data);

  // Forward problem: solve it, that is, set 'realizer' and 'cdf' of the qoi rv
  QUESO::McOptionsValues* calFpMcOptionsValues = NULL;
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  QUESO::SsOptionsValues ssOptionsValues3;
  QUESO::SsOptionsValues ssOptionsValues4;

  ssOptionsValues3.m_initialDiscardedPortions.resize(1);
  ssOptionsValues3.m_initialDiscardedPortions[0] = 0.;

  ssOptionsValues3.m_kdeCompute                  = true;
  ssOptionsValues3.m_kdeNumEvalPositions         = 250;
  ssOptionsValues3.m_covMatrixCompute            = true;
  ssOptionsValues3.m_corrMatrixCompute           = true;

  ssOptionsValues4.m_initialDiscardedPortions.resize(1);
  ssOptionsValues4.m_initialDiscardedPortions[0] = 0.;


  ssOptionsValues4.m_autoCorrComputeViaDef       = false;
  ssOptionsValues4.m_autoCorrComputeViaFft       = true;
  ssOptionsValues4.m_autoCorrSecondLag           = 2;
  ssOptionsValues4.m_autoCorrLagSpacing          = 1;
  ssOptionsValues4.m_autoCorrNumLags             = 15;
  ssOptionsValues4.m_autoCorrDisplay             = true;
  ssOptionsValues4.m_autoCorrWrite               = true;
  ssOptionsValues4.m_kdeCompute                  = true;
  ssOptionsValues4.m_kdeNumEvalPositions         = 250;
  ssOptionsValues4.m_covMatrixCompute            = true;
  ssOptionsValues4.m_corrMatrixCompute           = true;

  calFpMcOptionsValues = new QUESO::McOptionsValues(&ssOptionsValues3,&ssOptionsValues4);
  calFpMcOptionsValues->m_dataOutputFileName   = "outputData/tgaCalOutput";
  calFpMcOptionsValues->m_dataOutputAllowedSet.insert(0);
  calFpMcOptionsValues->m_dataOutputAllowedSet.insert(1);

  calFpMcOptionsValues->m_pseqDataOutputFileName   = ".";
  calFpMcOptionsValues->m_pseqDataOutputAllowedSet.insert(0);
  calFpMcOptionsValues->m_pseqDataOutputAllowedSet.insert(1);
  calFpMcOptionsValues->m_pseqComputeStats         = true;

  calFpMcOptionsValues->m_qseqDataInputFileName    = ".";
  calFpMcOptionsValues->m_qseqSize                 = 1048576;
  calFpMcOptionsValues->m_qseqDisplayPeriod        = 20000;
  calFpMcOptionsValues->m_qseqMeasureRunTimes      = true;
  calFpMcOptionsValues->m_qseqDataOutputFileName   = "outputData/file_cal_fp_qoi2";
  calFpMcOptionsValues->m_qseqDataOutputAllowedSet.insert(0);
  calFpMcOptionsValues->m_qseqDataOutputAllowedSet.insert(1);
```

```
  calFpMcOptionsValues->m_qseqComputeStats         = true;
#endif
  cycle.calFP().solveWithMonteCarlo(calFpMcOptionsValues); // no extra user entities needed
      for Monte Carlo algorithm
  delete calFpMcOptionsValues;

  iRC = gettimeofday(&timevalNow, NULL);
  if (env.fullRank() == 0) {
    std::cout << "Ending 'calibration stage' at "        << ctime(&timevalNow.tv_sec)
              << "Total 'calibration stage' run time = " << timevalNow.tv_sec - timevalRef.
                  tv_sec
              << " seconds\n"
              << std::endl;
  }

  //*****************************************************
  // Task 3 of 5: validation stage
  //*****************************************************

  iRC = gettimeofday(&timevalRef, NULL);
  if (env.fullRank() == 0) {
    std::cout << "Beginning 'validation stage' at " << ctime(&timevalRef.tv_sec)
              << std::endl;
  }

  // Inverse problem: no need to instantiate the prior rv (= posterior rv of calibration
      inverse problem)

  // Inverse problem: instantiate the likelihood function object (data + routine)
  likelihoodRoutine_Data<P_V,P_M> valLikelihoodRoutine_Data(env,
                                                            "scenario_100_K_min.dat",
                                                            NULL,
                                                            NULL);

  QUESO::GenericScalarFunction<P_V,P_M> valLikelihoodFunctionObj("val_like_",
                                                            paramDomain,
                                                            likelihoodRoutine<P_V,P_M>,
                                                            (void *) &
                                                                valLikelihoodRoutine_Data
                                                                ,
                                                            true); // the routine
                                                                computes [ln(function)]

  // Inverse problem: instantiate it (posterior rv is instantiated internally)
  QUESO::SipOptionsValues* valIpOptionsValues = NULL;
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  valIpOptionsValues = new QUESO::SipOptionsValues();
  valIpOptionsValues->m_computeSolution      = true;
  valIpOptionsValues->m_dataOutputFileName   = "outputData/tgaValOutput";
  valIpOptionsValues->m_dataOutputAllowedSet.insert(0);
  valIpOptionsValues->m_dataOutputAllowedSet.insert(1);
#endif
  cycle.instantiateValIP(valIpOptionsValues,
                         valLikelihoodFunctionObj);

  // Inverse problem: solve it, that is, set 'pdf' and 'realizer' of the posterior rv
  QUESO::MhOptionsValues* valIpMhOptionsValues = NULL;

  const QUESO::SequentialVectorRealizer<P_V,P_M>*
    tmpRealizer = dynamic_cast< const QUESO::SequentialVectorRealizer<P_V,P_M>* >(&(cycle.
        calIP().postRv().realizer()));

  // Use 'realizer()' because the post. rv was computed with Metr. Hast.
  P_M* valProposalCovMatrix = cycle.calIP().postRv().imageSet().vectorSpace().
```

```
      newProposalMatrix(
          &tmpRealizer->unifiedSampleVarVector(),
          &tmpRealizer->unifiedSampleExpVector()); // Use these values as the initial values

#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  QUESO::SsOptionsValues ssOptionsValues5;
  QUESO::SsOptionsValues ssOptionsValues6;

  ssOptionsValues5.m_initialDiscardedPortions.resize(9);
  ssOptionsValues5.m_initialDiscardedPortions[0] = 0.;
  ssOptionsValues5.m_initialDiscardedPortions[1] = 0.05;
  ssOptionsValues5.m_initialDiscardedPortions[2] = 0.10;
  ssOptionsValues5.m_initialDiscardedPortions[3] = 0.15;
  ssOptionsValues5.m_initialDiscardedPortions[4] = 0.20;
  ssOptionsValues5.m_initialDiscardedPortions[5] = 0.25;
  ssOptionsValues5.m_initialDiscardedPortions[6] = 0.30;
  ssOptionsValues5.m_initialDiscardedPortions[7] = 0.35;
  ssOptionsValues5.m_initialDiscardedPortions[8] = 0.40;
  ssOptionsValues5.m_autoCorrComputeViaDef       = false;
  ssOptionsValues5.m_autoCorrComputeViaFft       = true;
  ssOptionsValues5.m_autoCorrSecondLag           = 2;
  ssOptionsValues5.m_autoCorrLagSpacing          = 2;
  ssOptionsValues5.m_autoCorrNumLags             = 15;
  ssOptionsValues5.m_autoCorrDisplay             = true;
  ssOptionsValues5.m_autoCorrWrite               = true;
  ssOptionsValues5.m_kdeCompute                  = false;
  ssOptionsValues5.m_covMatrixCompute            = true;
  ssOptionsValues5.m_corrMatrixCompute           = true;

  ssOptionsValues6.m_initialDiscardedPortions.resize(1);
  ssOptionsValues6.m_initialDiscardedPortions[0] = 0.;
  ssOptionsValues6.m_autoCorrComputeViaDef       = false;
  ssOptionsValues6.m_autoCorrComputeViaFft       = true;
  ssOptionsValues6.m_autoCorrSecondLag           = 2;
  ssOptionsValues6.m_autoCorrLagSpacing          = 2;
  ssOptionsValues6.m_autoCorrNumLags             = 15;
  ssOptionsValues6.m_autoCorrDisplay             = true;
  ssOptionsValues6.m_autoCorrWrite               = true;
  ssOptionsValues6.m_kdeCompute                  = true;
  ssOptionsValues6.m_kdeNumEvalPositions         = 250;
  ssOptionsValues6.m_covMatrixCompute            = true;
  ssOptionsValues6.m_corrMatrixCompute           = true;

  valIpMhOptionsValues = new QUESO::MhOptionsValues(&ssOptionsValues5,&ssOptionsValues6);
  valIpMhOptionsValues->m_dataOutputFileName   = "outputData/tgaValOutput";
  valIpMhOptionsValues->m_dataOutputAllowedSet.insert(0);
  valIpMhOptionsValues->m_dataOutputAllowedSet.insert(1);

  valIpMhOptionsValues->m_rawChainDataInputFileName    = ".";
  valIpMhOptionsValues->m_rawChainSize                 = 1048576;
  valIpMhOptionsValues->m_rawChainGenerateExtra        = false;
  valIpMhOptionsValues->m_rawChainDisplayPeriod        = 20000;
  valIpMhOptionsValues->m_rawChainMeasureRunTimes      = true;
  valIpMhOptionsValues->m_rawChainDataOutputFileName   = "outputData/file_val_ip_raw";
  valIpMhOptionsValues->m_rawChainDataOutputAllowedSet.insert(0);
  valIpMhOptionsValues->m_rawChainDataOutputAllowedSet.insert(1);
  valIpMhOptionsValues->m_rawChainComputeStats         = true;

  valIpMhOptionsValues->m_displayCandidates         = false;
  valIpMhOptionsValues->m_putOutOfBoundsInChain     = true;
  valIpMhOptionsValues->m_tkUseLocalHessian         = false;
  valIpMhOptionsValues->m_tkUseNewtonComponent      = true;
  valIpMhOptionsValues->m_drMaxNumExtraStages       = 1;
  valIpMhOptionsValues->m_drScalesForExtraStages.resize(1);
```

```
  valIpMhOptionsValues->m_drScalesForExtraStages[0] = 5.;
  valIpMhOptionsValues->m_amInitialNonAdaptInterval = 0;
  valIpMhOptionsValues->m_amAdaptInterval           = 100;
  valIpMhOptionsValues->m_amEta                     = 1.92;
  valIpMhOptionsValues->m_amEpsilon                 = 1.e-5;

  valIpMhOptionsValues->m_filteredChainGenerate             = true;
  valIpMhOptionsValues->m_filteredChainDiscardedPortion     = 0.;
  valIpMhOptionsValues->m_filteredChainLag                  = 20;
  valIpMhOptionsValues->m_filteredChainDataOutputFileName   = ".";
  valIpMhOptionsValues->m_filteredChainDataOutputAllowedSet.insert(0);
  valIpMhOptionsValues->m_filteredChainDataOutputAllowedSet.insert(1);
  valIpMhOptionsValues->m_filteredChainComputeStats         = true;
#endif
  cycle.valIP().solveWithBayesMetropolisHastings(valIpMhOptionsValues,
                                                 tmpRealizer->unifiedSampleExpVector(),
                                                 valProposalCovMatrix);
  delete valProposalCovMatrix;
  delete valIpMhOptionsValues;

  // Forward problem: instantiate it (parameter rv = posterior rv of inverse problem;
  // qoi rv is instantiated internally)
  qoiRoutine_Data<P_V,P_M,Q_V,Q_M> valQoiRoutine_Data;
  valQoiRoutine_Data.m_beta         = beta_prediction;
  valQoiRoutine_Data.m_criticalMass = criticalMass_prediction;
  valQoiRoutine_Data.m_criticalTime = criticalTime_prediction;

  QUESO::SfpOptionsValues* valFpOptionsValues = NULL;
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  valFpOptionsValues = new QUESO::SfpOptionsValues();
  valFpOptionsValues->m_computeSolution      = true;
  valFpOptionsValues->m_computeCovariances   = true;
  valFpOptionsValues->m_computeCorrelations  = true;
  valFpOptionsValues->m_dataOutputFileName   = "outputData/tgaValOutput";
  valFpOptionsValues->m_dataOutputAllowedSet.insert(0);
  valFpOptionsValues->m_dataOutputAllowedSet.insert(1);
#endif
  cycle.instantiateValFP(valFpOptionsValues,
                         qoiRoutine<P_V,P_M,Q_V,Q_M>,
                         (void *) &valQoiRoutine_Data);

  // Forward problem: solve it, that is, set 'realizer' and 'cdf' of the qoi rv
  QUESO::McOptionsValues* valFpMcOptionsValues = NULL;
#ifdef UQ_EXAMPLES_USES_QUESO_INPUT_FILE
#else
  QUESO::SsOptionsValues ssOptionsValues7;
  QUESO::SsOptionsValues ssOptionsValues8;

  ssOptionsValues7.m_initialDiscardedPortions.resize(1);
  ssOptionsValues7.m_initialDiscardedPortions[0] = 0.;
  ssOptionsValues7.m_kdeCompute                  = true;
  ssOptionsValues7.m_kdeNumEvalPositions         = 250;
  ssOptionsValues7.m_covMatrixCompute            = true;
  ssOptionsValues7.m_corrMatrixCompute           = true;

  ssOptionsValues8.m_initialDiscardedPortions.resize(1);
  ssOptionsValues8.m_initialDiscardedPortions[0] = 0.;
  ssOptionsValues8.m_autoCorrComputeViaDef       = false;
  ssOptionsValues8.m_autoCorrComputeViaFft       = true;
  ssOptionsValues8.m_autoCorrSecondLag           = 2;
  ssOptionsValues8.m_autoCorrLagSpacing          = 1;
  ssOptionsValues8.m_autoCorrNumLags             = 15;
  ssOptionsValues8.m_autoCorrDisplay             = true;
  ssOptionsValues8.m_autoCorrWrite               = true;
```

```
  ssOptionsValues8.m_kdeCompute                  = true;
  ssOptionsValues8.m_kdeNumEvalPositions         = 250;
  ssOptionsValues8.m_covMatrixCompute            = true;
  ssOptionsValues8.m_corrMatrixCompute           = true;

  valFpMcOptionsValues = new QUESO::McOptionsValues(&ssOptionsValues7,&ssOptionsValues8);
  valFpMcOptionsValues->m_dataOutputFileName   = "outputData/tgaValOutput";
  valFpMcOptionsValues->m_dataOutputAllowedSet.insert(0);
  valFpMcOptionsValues->m_dataOutputAllowedSet.insert(1);

  valFpMcOptionsValues->m_pseqDataOutputFileName   = ".";
  valFpMcOptionsValues->m_pseqDataOutputAllowedSet.insert(0);
  valFpMcOptionsValues->m_pseqDataOutputAllowedSet.insert(1);
  valFpMcOptionsValues->m_pseqComputeStats         = true;

  valFpMcOptionsValues->m_qseqDataInputFileName    = ".";
  valFpMcOptionsValues->m_qseqSize                 = 1048576;
  valFpMcOptionsValues->m_qseqDisplayPeriod        = 20000;
  valFpMcOptionsValues->m_qseqMeasureRunTimes      = true;
  valFpMcOptionsValues->m_qseqDataOutputFileName   = "outputData/file_val_fp_qoi2";
  valFpMcOptionsValues->m_qseqDataOutputAllowedSet.insert(0);
  valFpMcOptionsValues->m_qseqDataOutputAllowedSet.insert(1);
  valFpMcOptionsValues->m_qseqComputeStats         = true;
#endif
  cycle.valFP().solveWithMonteCarlo(valFpMcOptionsValues); // no extra user entities needed
      for Monte Carlo algorithm
  delete valFpMcOptionsValues;

  delete valFpOptionsValues;
  delete valIpOptionsValues;
  delete calFpOptionsValues;
  delete calIpOptionsValues;

  iRC = gettimeofday(&timevalNow, NULL);
  if (env.fullRank() == 0) {
    std::cout << "Ending 'validation stage' at "        << ctime(&timevalNow.tv_sec)
              << "Total 'validation stage' run time = " << timevalNow.tv_sec - timevalRef.
                  tv_sec
              << " seconds\n"
              << std::endl;
  }

  //*******************************************************
  // Task 4 of 5: comparison stage
  //*******************************************************

  iRC = gettimeofday(&timevalRef, NULL);
  if (env.fullRank() == 0) {
    std::cout << "Beginning 'comparison stage' at " << ctime(&timevalRef.tv_sec)
              << std::endl;
  }

  uqAppl_LocalComparisonStage(cycle);
  if (env.numSubEnvironments() > 1) {
    uqAppl_UnifiedComparisonStage(cycle);
  }

  iRC = gettimeofday(&timevalNow, NULL);
  if (env.fullRank() == 0) {
    std::cout << "Ending 'comparison stage' at "        << ctime(&timevalNow.tv_sec)
              << "Total 'comparison stage' run time = " << timevalNow.tv_sec - timevalRef.
                  tv_sec
              << " seconds\n"
              << std::endl;
  }
```

```
  //*****************************************************
  // Task 5 of 5: release memory before leaving routine.
  //*****************************************************

  if (env.fullRank() == 0) {
    std::cout << "Finishing run of 'uqTgaExample' example"
              << std::endl;
  }

  return;
}

//*****************************************************
// The 'local comparison stage' of the driving routine "uqAppl()"
//*****************************************************
template<class P_V,class P_M,class Q_V,class Q_M>
void
uqAppl_LocalComparisonStage(QUESO::ValidationCycle<P_V,P_M,Q_V,Q_M>& cycle)
{
  if (cycle.calFP().computeSolutionFlag() &&
      cycle.valFP().computeSolutionFlag()) {
  }

  return;
}

//*****************************************************
// The 'unified comparison stage' of the driving routine "uqAppl()"
//*****************************************************
template<class P_V,class P_M,class Q_V,class Q_M>
void
uqAppl_UnifiedComparisonStage(QUESO::ValidationCycle<P_V,P_M,Q_V,Q_M>& cycle)
{
  if (cycle.calFP().computeSolutionFlag() &&
      cycle.valFP().computeSolutionFlag()) {
  }

  return;
}
#endif // EX_TGA_VALIDATION_CYCLE_APPL_H
```

Listing 6.48: File `exTgaValidationCycle_appl.h`.

```
#ifndef EX_TGA_VALIDATION_CYCLE_LIKELIHOOD_H
#define EX_TGA_VALIDATION_CYCLE_LIKELIHOOD_H

#include <queso/Environment.h>
#include <queso/Defines.h>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_odeiv.h>
#include <cmath>

#define R_CONSTANT 8.314472

//*****************************************************
// The ODE (state dot) function
//*****************************************************
int func(double t, const double Mass[], double f[], void *info)
{
  double* params = (double *)info;
  double A     = params[0];
```

```
  double E    = params[1];
  double beta = params[2];

  f[0] = -A*Mass[0]*std::exp(-E/(R_CONSTANT*t))/beta;

  return GSL_SUCCESS;
}

//*****************************************************
// The (user defined) data class that carries the data
// needed by the (user defined) likelihood routine
//*****************************************************
template<class P_V, class P_M>
struct
likelihoodRoutine_Data
{
  likelihoodRoutine_Data(const QUESO::BaseEnvironment& env,
                         const char* inpName1,
                         const char* inpName2,
                         const char* inpName3);
 ~likelihoodRoutine_Data();

  double              m_beta1;
  double              m_variance1;
  std::vector<double> m_Te1; // temperatures
  std::vector<double> m_Me1; // relative masses

  double              m_beta2;
  double              m_variance2;
  std::vector<double> m_Te2; // temperatures
  std::vector<double> m_Me2; // relative masses

  double              m_beta3;
  double              m_variance3;
  std::vector<double> m_Te3; // temperatures
  std::vector<double> m_Me3; // relative masses

  const QUESO::BaseEnvironment* m_env;
};

template<class P_V, class P_M>
likelihoodRoutine_Data<P_V,P_M>::likelihoodRoutine_Data(
  const QUESO::BaseEnvironment& env,
  const char* inpName1,
  const char* inpName2,
  const char* inpName3)
  :
  m_beta1    (0.),
  m_variance1(0.),
  m_Te1      (0),
  m_Me1      (0),
  m_beta2    (0.),
  m_variance2(0.),
  m_Te2      (0),
  m_Me2      (0),
  m_beta3    (0.),
  m_variance3(0.),
  m_Te3      (0),
  m_Me3      (0),
  m_env      (&env)
{
  // Read experimental data
  if (inpName1) {
    m_Te1.resize(11,0.);
    m_Me1.resize(11,0.);
```

```
  // Open input file on experimental data
  FILE *inp;
  inp = fopen(inpName1,"r");

  // Read kinetic parameters and convert heating rate to K/s
  int aux1 = fscanf(inp,"%lf %lf",&m_beta1,&m_variance1);
  m_beta1 /= 60.;

  if(aux1) {}; // just to eliminate warnings

  unsigned int numObservations = 0;
  double tmpTe;
  double tmpMe;
  while (fscanf(inp,"%lf %lf",&tmpTe,&tmpMe) != EOF) {
    UQ_FATAL_TEST_MACRO((numObservations >= m_Te1.size()),
                        env.fullRank(),
                        "uqAppl(), in uqTgaEx4.h",
                        "input file 1 has too many observations");
    m_Te1[numObservations] = tmpTe;
    m_Me1[numObservations] = tmpMe;
    numObservations++;
  }
  UQ_FATAL_TEST_MACRO((numObservations != m_Te1.size()),
                      env.fullRank(),
                      "uqAppl(), in uqTgaEx4.h",
                      "input file 1 has a smaller number of observations than expected");

  // Close input file on experimental data
  fclose(inp);
}

// Read experimental data
if (inpName2) {
  m_Te2.resize(11,0.);
  m_Me2.resize(11,0.);

  // Open input file on experimental data
  FILE *inp;
  inp = fopen(inpName2,"r");

  // Read kinetic parameters and convert heating rate to K/s
  int aux2 = fscanf(inp,"%lf %lf",&m_beta2,&m_variance2);
  m_beta2 /= 60.;

  if(aux2) {}; // just to eliminate warnings

  unsigned int numObservations = 0;
  double tmpTe;
  double tmpMe;
  while (fscanf(inp,"%lf %lf",&tmpTe,&tmpMe) != EOF) {
    UQ_FATAL_TEST_MACRO((numObservations >= m_Te2.size()),
                        env.fullRank(),
                        "uqAppl(), in uqTgaEx4.h",
                        "input file 2 has too many observations");
    m_Te2[numObservations] = tmpTe;
    m_Me2[numObservations] = tmpMe;
    numObservations++;
  }
  UQ_FATAL_TEST_MACRO((numObservations != m_Te2.size()),
                      env.fullRank(),
                      "uqAppl(), in uqTgaEx4.h",
                      "input file 2 has a smaller number of observations than expected");

  // Close input file on experimental data
```

```
    fclose(inp);
  }

  // Read experimental data
  if (inpName3) {
    m_Te3.resize(11,0.);
    m_Me3.resize(11,0.);

    // Open input file on experimental data
    FILE *inp;
    inp = fopen(inpName3,"r");

    // Read kinetic parameters and convert heating rate to K/s
    int aux3 = fscanf(inp,"%lf %lf",&m_beta3,&m_variance3);
    m_beta3 /= 60.;

    if(aux3) {}; // just to eliminate warnings

    unsigned int numObservations = 0;
    double tmpTe;
    double tmpMe;
    while (fscanf(inp,"%lf %lf",&tmpTe,&tmpMe) != EOF) {
      UQ_FATAL_TEST_MACRO((numObservations >= m_Te3.size()),
                          env.fullRank(),
                          "uqAppl(), in uqTgaEx4.h",
                          "input file 3 has too many observations");
      m_Te3[numObservations] = tmpTe;
      m_Me3[numObservations] = tmpMe;
      numObservations++;
    }
    UQ_FATAL_TEST_MACRO((numObservations != m_Te3.size()),
                        env.fullRank(),
                        "uqAppl(), in uqTgaEx4.h",
                        "input file 3 has a smaller number of observations than expected");

    // Close input file on experimental data
    fclose(inp);


  }
}

template<class P_V, class P_M>
likelihoodRoutine_Data<P_V,P_M>::~likelihoodRoutine_Data()
{
}

//*****************************************************
// The actual (user defined) likelihood routine
//*****************************************************
template<class P_V,class P_M>
double
likelihoodRoutine(
  const P_V&  paramValues,
  const P_V*  paramDirection,
  const void* functionDataPtr,
  P_V*        gradVector,
  P_M*        hessianMatrix,
  P_V*        hessianEffect)
{
  double resultValue = 0.;

  const QUESO::BaseEnvironment& env = *(((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)
      ->m_env);
```

```
  env.subComm().Barrier();
  //env.syncPrintDebugMsg("Entering likelihoodRoutine()",1,env.fullComm());

  // Compute likelihood for scenario 1
  double betaTest = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->m_beta1;
  if (betaTest) {
    double A                        = paramValues[0];
    double E                        = paramValues[1];
    double beta                     = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_beta1;
    double variance                 = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_variance1;
    const std::vector<double>& Te   = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_Te1;
    const std::vector<double>& Me   = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_Me1;
    std::vector<double> Mt(Me.size(),0.);

    double params[]={A,E,beta};

    // integration
    const gsl_odeiv_step_type *T   = gsl_odeiv_step_rkf45; //rkf45; //gear1;
          gsl_odeiv_step      *s   = gsl_odeiv_step_alloc(T,1);
          gsl_odeiv_control   *c   = gsl_odeiv_control_y_new(1e-6,0.0);
          gsl_odeiv_evolve    *e   = gsl_odeiv_evolve_alloc(1);
          gsl_odeiv_system     sys = {func, NULL, 1, (void *)params};

    double t = 0.1, t_final = 1900.;
    double h = 1e-3;
    double Mass[1];
    Mass[0]=1.;

    unsigned int i = 0;
    double t_old = 0.;
    double M_old[1];
    M_old[0]=1.;

    double misfit=0.;
    //unsigned int loopSize = 0;
    while ((t < t_final) && (i < Me.size())) {
      int status = gsl_odeiv_evolve_apply(e, c, s, &sys, &t, t_final, &h, Mass);
      UQ_FATAL_TEST_MACRO((status != GSL_SUCCESS),
                          paramValues.env().fullRank(),
                          "likelihoodRoutine()",
                          "gsl_odeiv_evolve_apply() failed");
      //printf("t = %6.1lf, mass = %10.4lf\n",t,Mass[0]);
      //loopSize++;

      while ( (i < Me.size()) && (t_old <= Te[i]) && (Te[i] <= t) ) {
        Mt[i] = (Te[i]-t_old)*(Mass[0]-M_old[0])/(t-t_old) + M_old[0];
        misfit += (Me[i]-Mt[i])*(Me[i]-Mt[i]);
        //printf("%i %lf %lf %lf %lf\n",i,Te[i],Me[i],Mt[i],misfit);
        i++;
      }

      t_old=t;
      M_old[0]=Mass[0];
    }
    resultValue += misfit/variance;

    //printf("loopSize = %d\n",loopSize);
    if ((paramValues.env().displayVerbosity() >= 10) && (paramValues.env().fullRank() == 0))
        {
      printf("In likelihoodRoutine(), A = %g, E = %g, beta = %.3lf: misfit = %lf, likelihood
          = %lf.\n",A,E,beta,misfit,resultValue);
```

```
  }

  gsl_odeiv_evolve_free (e);
  gsl_odeiv_control_free(c);
  gsl_odeiv_step_free   (s);
}

// Compute likelihood for scenario 2
betaTest = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->m_beta2;
if (betaTest > 0.) {
  double A                        = paramValues[0];
  double E                        = paramValues[1];
  double beta                     = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
      m_beta2;
  double variance                 = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
      m_variance2;
  const std::vector<double>& Te   = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
      m_Te2;
  const std::vector<double>& Me   = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
      m_Me2;
  std::vector<double> Mt(Me.size(),0.);

  double params[]={A,E,beta};

  // integration
  const gsl_odeiv_step_type *T   = gsl_odeiv_step_rkf45; //rkf45; //gear1;
        gsl_odeiv_step      *s   = gsl_odeiv_step_alloc(T,1);
        gsl_odeiv_control   *c   = gsl_odeiv_control_y_new(1e-6,0.0);
        gsl_odeiv_evolve    *e   = gsl_odeiv_evolve_alloc(1);
        gsl_odeiv_system     sys = {func, NULL, 1, (void *)params};

  double t = 0.1, t_final = 1900.;
  double h = 1e-3;
  double Mass[1];
  Mass[0]=1.;

  unsigned int i = 0;
  double t_old = 0.;
  double M_old[1];
  M_old[0]=1.;

  double misfit=0.;
  //unsigned int loopSize = 0;
  while ((t < t_final) && (i < Me.size())) {
    int status = gsl_odeiv_evolve_apply(e, c, s, &sys, &t, t_final, &h, Mass);
    UQ_FATAL_TEST_MACRO((status != GSL_SUCCESS),
                        paramValues.env().fullRank(),
                        "likelihoodRoutine()",
                        "gsl_odeiv_evolve_apply() failed");
    //printf("t = %6.1lf, mass = %10.4lf\n",t,Mass[0]);
    //loopSize++;

    while ( (i < Me.size()) && (t_old <= Te[i]) && (Te[i] <= t) ) {
      Mt[i] = (Te[i]-t_old)*(Mass[0]-M_old[0])/(t-t_old) + M_old[0];
      misfit += (Me[i]-Mt[i])*(Me[i]-Mt[i]);
      //printf("%i %lf %lf %lf %lf\n",i,Te[i],Me[i],Mt[i],misfit);
      i++;
    }

    t_old=t;
    M_old[0]=Mass[0];
  }
  resultValue += misfit/variance;

  //printf("loopSize = %d\n",loopSize);
```

```
    if ((paramValues.env().displayVerbosity() >= 10) && (paramValues.env().fullRank() == 0))
        {
      printf("In likelihoodRoutine(), A = %g, E = %g, beta = %.3lf: misfit = %lf, likelihood
          = %lf.\n",A,E,beta,misfit,resultValue);
    }

    gsl_odeiv_evolve_free (e);
    gsl_odeiv_control_free(c);
    gsl_odeiv_step_free   (s);
  }

  // Compute likelihood for scenario 3
  betaTest = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->m_beta3;
  if (betaTest > 0.) {
    double A                        = paramValues[0];
    double E                        = paramValues[1];
    double beta                     = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_beta3;
    double variance                 = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_variance3;
    const std::vector<double>& Te   = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_Te3;
    const std::vector<double>& Me   = ((likelihoodRoutine_Data<P_V,P_M> *) functionDataPtr)->
        m_Me3;
    std::vector<double> Mt(Me.size(),0.);

    double params[]={A,E,beta};

    // integration
    const gsl_odeiv_step_type *T   = gsl_odeiv_step_rkf45; //rkf45; //gear1;
          gsl_odeiv_step      *s   = gsl_odeiv_step_alloc(T,1);
          gsl_odeiv_control   *c   = gsl_odeiv_control_y_new(1e-6,0.0);
          gsl_odeiv_evolve    *e   = gsl_odeiv_evolve_alloc(1);
          gsl_odeiv_system     sys = {func, NULL, 1, (void *)params};

    double t = 0.1, t_final = 1900.;
    double h = 1e-3;
    double Mass[1];
    Mass[0]=1.;

    unsigned int i = 0;
    double t_old = 0.;
    double M_old[1];
    M_old[0]=1.;

    double misfit=0.;
    //unsigned int loopSize = 0;
    while ((t < t_final) && (i < Me.size())) {
      int status = gsl_odeiv_evolve_apply(e, c, s, &sys, &t, t_final, &h, Mass);
      UQ_FATAL_TEST_MACRO((status != GSL_SUCCESS),
                          paramValues.env().fullRank(),
                          "likelihoodRoutine()",
                          "gsl_odeiv_evolve_apply() failed");
      //printf("t = %6.1lf, mass = %10.4lf\n",t,Mass[0]);
      //loopSize++;

      while ( (i < Me.size()) && (t_old <= Te[i]) && (Te[i] <= t) ) {
        Mt[i] = (Te[i]-t_old)*(Mass[0]-M_old[0])/(t-t_old) + M_old[0];
        misfit += (Me[i]-Mt[i])*(Me[i]-Mt[i]);
        //printf("%i %lf %lf %lf %lf\n",i,Te[i],Me[i],Mt[i],misfit);
        i++;
      }

      t_old=t;
      M_old[0]=Mass[0];
```

```
    }
    resultValue += misfit/variance;

    //printf("loopSize = %d\n",loopSize);
    if ((paramValues.env().displayVerbosity() >= 10) && (paramValues.env().fullRank() == 0))
        {
      printf("In likelihoodRoutine(), A = %g, E = %g, beta = %.3lf: misfit = %lf, likelihood
          = %lf.\n",A,E,beta,misfit,resultValue);
    }

    gsl_odeiv_evolve_free (e);
    gsl_odeiv_control_free(c);
    gsl_odeiv_step_free   (s);
  }

  env.subComm().Barrier();
  //env.syncPrintDebugMsg("Leaving likelihoodRoutine()",1,env.fullComm());

  return -.5*resultValue;
}

#endif // EX_TGA_VALIDATION_CYCLE_LIKELIHOOD_H
```

Listing 6.49: File `exTgaValidationCycle_likelihood.h`.

```
#ifndef EX_TGA_VALIDATION_CYCLE_QOI_H
#define EX_TGA_VALIDATION_CYCLE_QOI_H

#include <queso/Defines.h>
#include <queso/DistArray.h>
#include <gsl/gsl_odeiv.h>

//*****************************************************
// The (user defined) data class that carries the data
// needed by the (user defined) qoi routine
//*****************************************************
template<class P_V,class P_M,class Q_V, class Q_M>
struct
qoiRoutine_Data
{
  double m_beta;
  double m_criticalMass;
  double m_criticalTime;
};

// The actual (user defined) qoi routine
template<class P_V,class P_M,class Q_V,class Q_M>
void qoiRoutine(const P_V&                    paramValues,
                const P_V*                    paramDirection,
                const void*                   functionDataPtr,
                      Q_V&                    qoiValues,
                      QUESO::DistArray<P_V*>* gradVectors,
                      QUESO::DistArray<P_M*>* hessianMatrices,
                      QUESO::DistArray<P_V*>* hessianEffects)
{
  double A             = paramValues[0];
  double E             = paramValues[1];
  double beta          = ((qoiRoutine_Data<P_V,P_M,Q_V,Q_M> *) functionDataPtr)->m_beta;
  double criticalMass  = ((qoiRoutine_Data<P_V,P_M,Q_V,Q_M> *) functionDataPtr)->
      m_criticalMass;
  double criticalTime  = ((qoiRoutine_Data<P_V,P_M,Q_V,Q_M> *) functionDataPtr)->
      m_criticalTime;
```

```
  double params[]={A,E,beta};

  // integration
  const gsl_odeiv_step_type *T   = gsl_odeiv_step_rkf45; //rkf45; //gear1;
        gsl_odeiv_step      *s   = gsl_odeiv_step_alloc(T,1);
        gsl_odeiv_control   *c   = gsl_odeiv_control_y_new(1e-6,0.0);
        gsl_odeiv_evolve    *e   = gsl_odeiv_evolve_alloc(1);
        gsl_odeiv_system     sys = {func, NULL, 1, (void *)params};

  double temperature = 0.1;
  double h = 1e-3;
  double Mass[1];
  Mass[0]=1.;

  double temperature_old = 0.;
  double M_old[1];
  M_old[0]=1.;

  double crossingTemperature = 0.;
  //unsigned int loopSize = 0;
  while ((temperature < criticalTime*beta) &&
         (Mass[0]     > criticalMass     )) {
    int status = gsl_odeiv_evolve_apply(e, c, s, &sys, &temperature, criticalTime*beta, &h,
        Mass);
    UQ_FATAL_TEST_MACRO((status != GSL_SUCCESS),
                        paramValues.env().fullRank(),
                        "qoiRoutine()",
                        "gsl_odeiv_evolve_apply() failed");
    //printf("t = %6.1lf, mass = %10.4lf\n",t,Mass[0]);
    //loopSize++;

    if (Mass[0] <= criticalMass) {
      crossingTemperature = temperature_old + (temperature - temperature_old) * (M_old[0]-
          criticalMass)/(M_old[0]-Mass[0]);
    }

    temperature_old=temperature;
    M_old[0]=Mass[0];
  }

  if (criticalMass > 0.) qoiValues[0] = crossingTemperature/beta; // QoI = time to achieve
      critical mass
  if (criticalTime > 0.) qoiValues[0] = Mass[0];                  // QoI = mass fraction
      remaining at critical time

  //printf("loopSize = %d\n",loopSize);
  if ((paramValues.env().displayVerbosity() >= 3) && (paramValues.env().fullRank() == 0)) {
    printf("In qoiRoutine(), A = %g, E = %g, beta = %.3lf, criticalTime = %.3lf, criticalMass
        = %.3lf: qoi = %lf.\n",A,E,beta,criticalTime,criticalMass,qoiValues[0]);
  }

  gsl_odeiv_evolve_free (e);
  gsl_odeiv_control_free(c);
  gsl_odeiv_step_free   (s);

  return;
}

#endif // EX_TGA_VALIDATION_CYCLE_QOI_H
```

Listing 6.50: File `exTgaValidationCycle_qoi.h`.

6.4.6 Input File

The input file used with this TGA SIP–SFP QUESO provides QUESO with options for its environments, and for both MCMC and Monte-Carlo algorithms. It is displayed in Listing 6.51.

```
###############################################
# UQ Environment
###############################################
#env_help                 = anything
env_numSubEnvironments   = 1
env_subDisplayFileName   = outputData/display
env_subDisplayAllowAll   = 0
env_subDisplayAllowedSet = 0 1
env_displayVerbosity     = 2
env_syncVerbosity        = 0
env_seed                 = 0

###############################################
# Calibration (cal) stage: statistical inverse problem (ip)
###############################################
cycle_cal_ip_help                  = anything
cycle_cal_ip_computeSolution       = 1
cycle_cal_ip_dataOutputFileName    = outputData/tgaCalOutput
cycle_cal_ip_dataOutputAllowedSet = 0 1

###############################################
# 'cal_ip_': information for Metropolis-Hastings algorithm
#
# '_size' examples 16K   128K   1M      2M      16M
#                  16384 131072 1048576 2097152 16777216
###############################################
cycle_cal_ip_mh_help                  = anything
cycle_cal_ip_mh_dataOutputFileName    = outputData/tgaCalOutput
cycle_cal_ip_mh_dataOutputAllowedSet = 0 1

cycle_cal_ip_mh_initialPosition_dataInputFileName          = . # inputData/initPos
cycle_cal_ip_mh_initialPosition_dataInputFileType          = m
cycle_cal_ip_mh_initialProposalCovMatrix_dataInputFileName = . # inputData/
    adaptedMatrix_am910000
cycle_cal_ip_mh_initialProposalCovMatrix_dataInputFileType = m
cycle_cal_ip_mh_rawChain_dataInputFileName     = . # outputData/file_cal_ip_raw_input
cycle_cal_ip_mh_rawChain_size                  = 1048576
cycle_cal_ip_mh_rawChain_generateExtra         = 0
cycle_cal_ip_mh_rawChain_displayPeriod         = 20000
cycle_cal_ip_mh_rawChain_measureRunTimes       = 1
cycle_cal_ip_mh_rawChain_dataOutputFileName    = outputData/file_cal_ip_raw
cycle_cal_ip_mh_rawChain_dataOutputAllowedSet = 0 1

cycle_cal_ip_mh_displayCandidates              = 0
cycle_cal_ip_mh_putOutOfBoundsInChain          = 1
cycle_cal_ip_mh_tk_useLocalHessian             = 0
cycle_cal_ip_mh_tk_useNewtonComponent          = 1
cycle_cal_ip_mh_dr_maxNumExtraStages           = 1
cycle_cal_ip_mh_dr_listOfScalesForExtraStages = 5. 4. 3.
cycle_cal_ip_mh_am_initialNonAdaptInterval     = 0 # 10000
cycle_cal_ip_mh_am_adaptInterval               = 100 # 10000
cycle_cal_ip_mh_am_adaptedMatrices_dataOutputPeriod    = 60000
cycle_cal_ip_mh_am_adaptedMatrices_dataOutputFileName = . # outputData/adaptedMatrix
cycle_cal_ip_mh_am_adaptedMatrices_dataOutputFileType = m
cycle_cal_ip_mh_am_eta                         = 1.92
cycle_cal_ip_mh_am_epsilon                     = 1.e-5

cycle_cal_ip_mh_filteredChain_generate             = 1
```

```
cycle_cal_ip_mh_filteredChain_discardedPortion     = 0.
cycle_cal_ip_mh_filteredChain_lag                  = 20
cycle_cal_ip_mh_filteredChain_dataOutputFileName   = .
cycle_cal_ip_mh_filteredChain_dataOutputAllowedSet = 0 1

##################################################
# Calibration (cal) stage: statistical forward problem (fp)
##################################################
cycle_cal_fp_help                 = anything
cycle_cal_fp_computeSolution      = 1
cycle_cal_fp_computeCovariances   = 1
cycle_cal_fp_computeCorrelations  = 1
cycle_cal_fp_dataOutputFileName   = outputData/tgaCalOutput
cycle_cal_fp_dataOutputAllowedSet = 0 1

##################################################
# 'cal_fp_': information for Monte Carlo algorithm
#
# '_size' examples 16K   128K   1M      2M      16M
#                  16384 131072 1048576 2097152 16777216
##################################################
cycle_cal_fp_mc_help                 = anything
cycle_cal_fp_mc_dataOutputFileName   = outputData/tgaCalOutput
cycle_cal_fp_mc_dataOutputAllowedSet = 0 1

cycle_cal_fp_mc_pseq_dataOutputFileName   = .
cycle_cal_fp_mc_pseq_dataOutputAllowedSet = 0 1

cycle_cal_fp_mc_qseq_dataInputFileName    = . # outputData/file_cal_fp_qoi1
cycle_cal_fp_mc_qseq_size                 = 1048576
cycle_cal_fp_mc_qseq_displayPeriod        = 20000
cycle_cal_fp_mc_qseq_measureRunTimes      = 1
cycle_cal_fp_mc_qseq_dataOutputFileName   = outputData/file_cal_fp_qoi2
cycle_cal_fp_mc_qseq_dataOutputAllowedSet = 0 1

##################################################
# Validation (val) stage: statistical inverse problem (ip)
##################################################
cycle_val_ip_help                 = anything
cycle_val_ip_computeSolution      = 1
cycle_val_ip_dataOutputFileName   = outputData/tgaValOutput
cycle_val_ip_dataOutputAllowedSet = 0 1

##################################################
# 'val_ip_': information for Metropolis-Hastings algorithm
#
# '_size' examples 16K   128K   1M      2M      16M
#                  16384 131072 1048576 2097152 16777216
##################################################
cycle_val_ip_mh_help                 = anything
cycle_val_ip_mh_dataOutputFileName   = outputData/tgaValOutput
cycle_val_ip_mh_dataOutputAllowedSet = 0 1

cycle_val_ip_mh_rawChain_dataInputFileName    = . # outputData/file_val_ip_raw_input
cycle_val_ip_mh_rawChain_size                 = 1048576
cycle_val_ip_mh_rawChain_generateExtra        = 0
cycle_val_ip_mh_rawChain_displayPeriod        = 20000
cycle_val_ip_mh_rawChain_measureRunTimes      = 1
cycle_val_ip_mh_rawChain_dataOutputFileName   = outputData/file_val_ip_raw
cycle_val_ip_mh_rawChain_dataOutputAllowedSet = 0 1

cycle_val_ip_mh_displayCandidates             = 0
cycle_val_ip_mh_putOutOfBoundsInChain         = 1
cycle_val_ip_mh_tk_useLocalHessian            = 0
cycle_val_ip_mh_tk_useNewtonComponent         = 1
```

```
cycle_val_ip_mh_dr_maxNumExtraStages          = 1
cycle_val_ip_mh_dr_listOfScalesForExtraStages = 5. 4. 3.
cycle_val_ip_mh_am_initialNonAdaptInterval    = 0
cycle_val_ip_mh_am_adaptInterval              = 100
cycle_val_ip_mh_am_eta                        = 1.92
cycle_val_ip_mh_am_epsilon                    = 1.e-5

cycle_val_ip_mh_filteredChain_generate             = 1
cycle_val_ip_mh_filteredChain_discardedPortion     = 0.
cycle_val_ip_mh_filteredChain_lag                  = 20
cycle_val_ip_mh_filteredChain_dataOutputFileName   = .
cycle_val_ip_mh_filteredChain_dataOutputAllowedSet = 0 1

#################################################
# Validation (val) stage: statistical forward problem (fp)
#################################################
cycle_val_fp_help                  = anything
cycle_val_fp_computeSolution       = 1
cycle_val_fp_computeCovariances    = 1
cycle_val_fp_computeCorrelations   = 1
cycle_val_fp_dataOutputFileName    = outputData/tgaValOutput
cycle_val_fp_dataOutputAllowedSet = 0 1

#################################################
# 'val_fp_': information for Monte Carlo algorithm
#
# '_size' examples 16K    128K    1M      2M      16M
#                  16384 131072 1048576 2097152 16777216
#################################################
cycle_val_fp_mc_help                  = anything
cycle_val_fp_mc_dataOutputFileName    = outputData/tgaValOutput
cycle_val_fp_mc_dataOutputAllowedSet = 0 1

cycle_val_fp_mc_pseq_dataOutputFileName    = .
cycle_val_fp_mc_pseq_dataOutputAllowedSet = 0 1


cycle_val_fp_mc_qseq_dataInputFileName     = . # outputData/file_val_fp_qoi1
cycle_val_fp_mc_qseq_size                  = 1048576
cycle_val_fp_mc_qseq_displayPeriod         = 20000
cycle_val_fp_mc_qseq_measureRunTimes       = 1
cycle_val_fp_mc_qseq_dataOutputFileName    = outputData/file_val_fp_qoi2
cycle_val_fp_mc_qseq_dataOutputAllowedSet = 0 1
```

Listing 6.51: File name `tgaCycle.inp` with options for QUESO library used in application code (Listings 6.47-6.49).

6.4.7 Data Post-Processing and Visualization

According to the specifications of the input file in Listing 6.51, both a folder named `outputData` and a the following files should be generated:

```
file_cal_ip_raw.m         file_val_ip_raw.m
file_cal_ip_raw_sub0.m    file_val_ip_raw_sub0.m
file_cal_fp_qoi2.m        file_val_fp_qoi2.m
file_cal_fp_qoi2_sub0.m   file_val_fp_qoi2_sub0.m
tgaCalOutput_sub0.m       tgaValOutput_sub0.m
```

`display_sub0.txt`

The sequence of Matlab commands is identical to the ones presented in Sections 6.1.5, 6.2.5 and 6.3.8; therefore, are omitted here. The reader is invited to explore the Matlab file `tga_cycle_plot.m` for details of how the figures have been generated.

6.4.7.1 KDE Plots of Parameters

Matlab function `ksdensity` (Kernel smoothing density estimate) together with the option '`pdf`' may be used to estimate the KDE of the parameters, as illustrated in Figure 6.4.2.

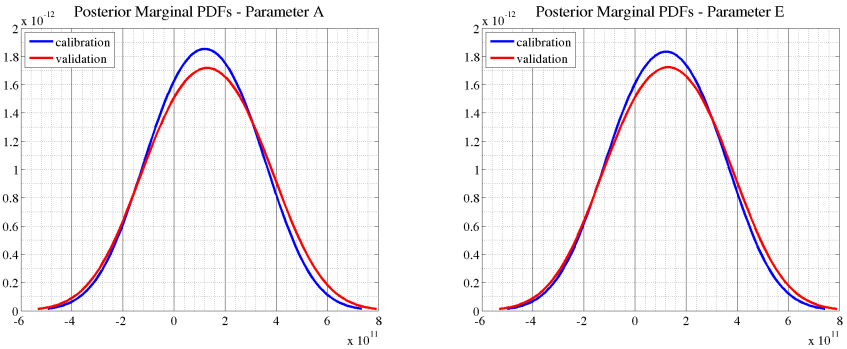


Figure 6.4.2: Posterior distributions of parameters A and E.

6.4.7.2 CDF Plots of Parameters

Matlab function `ksdensity` with `'cdf'` option may also be used for plotting the Cumulative Distribution Function of each one of the parameters, as illustrated in Figure 6.4.3.

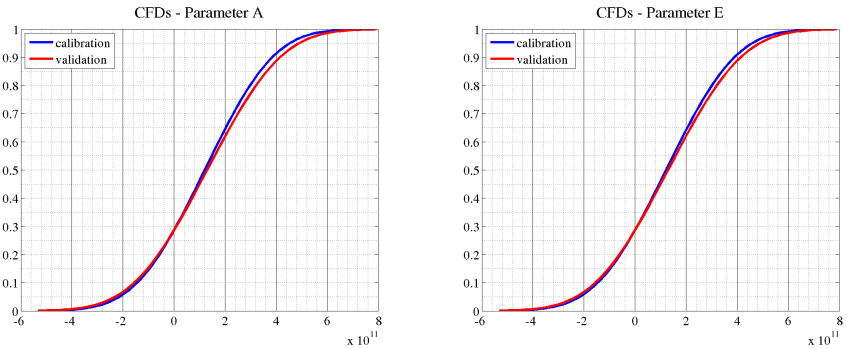


Figure 6.4.3: Cumulative density functions of parameters A and E.

6.4.7.3 Autocorrelation Plots of Parameters

Figure 6.4.4 presents the autocorrelation of the parameters A and E in both cases: calibration and validation stages.

6.4.7.4 KDE, CDF and Autocorrelation Plots of QoI

Figures 6.4.5a and 6.4.5b present PDF and CDF of QoI, respectively and Figure 6.4.6 presents its autocorrelation.

6.5 modal

This example presents a combination of two statistical inverse problems in one. It presents the capability of the Multilevel method in sampling from a target distribution that has either one or two modes (distinct peaks). The random variable of interest has three parameters, i.e., $\boldsymbol{\theta} = (\theta_1, \theta_2, \sigma^2) \in \mathbb{R}^3$, where the third parameter may be seen as variation.

The example also it gives the user the opportunity to chose either one single type of prior distribution, uniform, for the three components of the random variable, or two different priors: a uniform and a beta distribution.

Choosing between a one-mode or a two-mode target distribution is done at execution level, as presented in the following code line:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/
$ cd examples/modal
$ rm outputData/*
$ ./modal_gsl example.inp <num_of_nodes>
```

where `<num_of_nodes>` is either 1 or 2.

6.5.1 One-mode distribution

In this case, the target distribution is assumed to have only one mode. Suppose also that the random variable $\boldsymbol{\theta}$ can either have a uniform prior distribution for all its components, i.e.:

$$\pi_{\text{prior}} = \mathcal{U}([0,3]) \times \mathcal{U}([0,3]) \times \mathcal{U}([0,0.3]).$$

or, the prior distribution is defined as a combination of uniform prior for θ_1 and θ_2, with a beta prior for σ^2:

$$\pi_{\text{prior}} = \mathcal{U}([0,3]) \times \mathcal{U}([0,3]) \times \mathcal{B}(\alpha,\beta), \quad \text{with} \quad \alpha = 3 \quad \text{and} \quad \beta = 0.09709133373799.$$

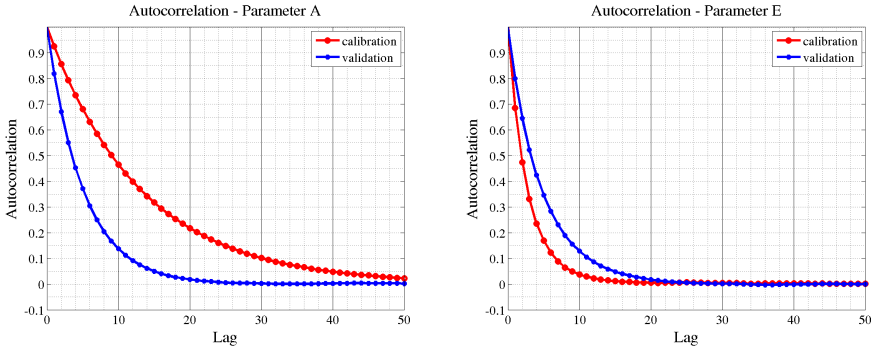
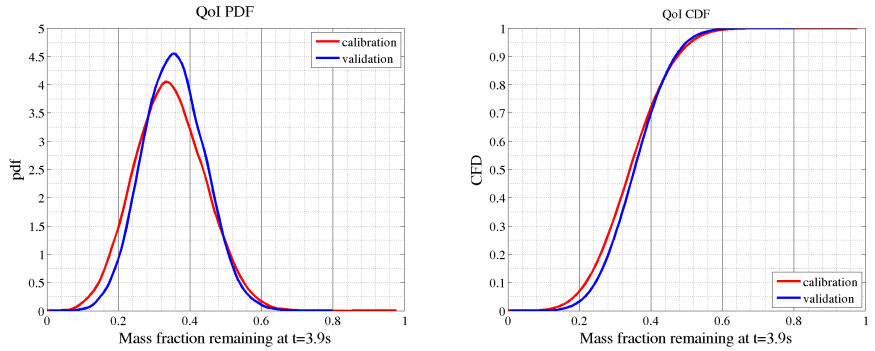


Figure 6.4.4: Autocorrelation of parameters A and E (filtered chain).



(a) QoI PDF (b) QoI CDF

Figure 6.4.5: QoI PDF and CDF, during calibration and validation stages.

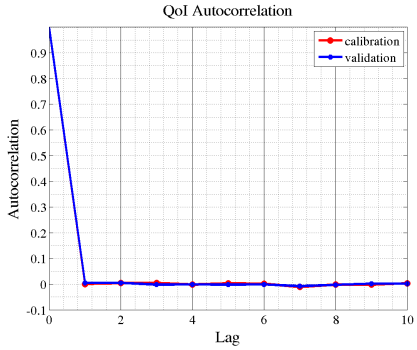


Figure 6.4.6: QoI autocorrelation.

The likelihood function is defined as follows:

$$f(\mathbf{D}|\boldsymbol{\theta}) = -\frac{5}{2}\log\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}\left[\left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}}-72.0470\right)^2 + \right.$$
$$+\left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}}-71.8995\right)^2 +$$
$$+\left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}}-72.2801\right)^2 + \quad (6.5.1)$$
$$+\left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}}-71.9421\right)^2 +$$
$$\left.+\left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}}-72.3578\right)^2\right].$$

6.5.1.1 Running the One-Mode Example

To run the executable provided considering a one-mode distribution, enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/
$ cd examples/modal
$ rm outputData/*
$ ./modal_gsl example.inp 1      #one mode!
$ matlab
   $  plot_modal_all_levels_1mode  # inside matlab
   $ exit                          # inside matlab
$ ls -l outputData/*.png
modal_1_mode_kde_target.png  modal_1_mode_level_1.png  modal_1_mode_level_5.png
modal_1_mode_kde_theta1.png  modal_1_mode_level_2.png  modal_1_mode_level_6.png
modal_1_mode_kde_theta2.png  modal_1_mode_level_3.png  modal_1_mode_level_7.png
modal_1_mode_kde_theta3.png  modal_1_mode_level_4.png
```

Listing 6.52: Running the example with a one-mode distribution.

As a result, the user should have created several of PNG figures scatter plots of each one of the levels and the kernel density estimation of the parameters, for each level in the Multilevel method. The name of the figure files have been chosen to be informative, as shown in the Listing above.

6.5.2 Two-mode distribution

In this case, the target distribution is assumed to have two modes. Suppose that $\boldsymbol{\theta}$ has a either uniform distribution for all its components, i.e.:

$$\pi_{\text{prior}} = \mathcal{U}([0,3]) \times \mathcal{U}([0,3]) \times \mathcal{U}([0,0.3]).$$

or, the prior distribution is defined as a combination of uniform prior for the θ_1, with a beta prior for θ_2:

$$\pi_{\text{prior}} = \mathcal{U}([0,3]) \times \mathcal{U}([0,3]) \times \mathcal{B}(\alpha,\beta), \quad \text{with} \quad \alpha = 3 \quad \text{and} \quad \beta = 0.08335837191688.$$

The likelihood function is defined as follows:

$$\begin{aligned} f(\mathbf{D}|\boldsymbol{\theta}) = -5\log\left(2\pi\sigma^2\right) - \frac{1}{2\sigma^2}\Bigg[& \left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}} - 72.0470\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}} - 71.8995\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}} - 72.2801\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}} - 71.9421\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2+10\sqrt{\theta_1^2+4\theta_2^2}} - 72.3578\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2-10\sqrt{\theta_1^2+4\theta_2^2}} - 28.0292\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2-10\sqrt{\theta_1^2+4\theta_2^2}} - 27.3726\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2-10\sqrt{\theta_1^2+4\theta_2^2}} - 27.5388\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2-10\sqrt{\theta_1^2+4\theta_2^2}} - 27.0357\right)^2 + \\ & + \left(10\sqrt{10\theta_1+20\theta_2-10\sqrt{\theta_1^2+4\theta_2^2}} - 27.1588\right)^2 \Bigg]. \end{aligned} \tag{6.5.2}$$

6.5.2.1 Running the Two-Mode Example

To run the executable provided considering a two-modes distribution, enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/
$ cd examples/modal
$ rm outputData/*
```

```
$ ./modal_gsl example.inp 2          # two modes!
$ matlab
   $  plot_modal_all_levels_2modes  # inside matlab
   $ exit                           # inside matlab
$ ls -l outputData/*.png
modal_2_modes_kde_target.png  modal_2_modes_level_1.png  modal_2_modes_level_5.png
modal_2_modes_kde_theta1.png  modal_2_modes_level_2.png  modal_2_modes_level_6.png
modal_2_modes_kde_theta2.png  modal_2_modes_level_3.png  modal_2_modes_level_7.png
modal_2_modes_kde_theta3.png  modal_2_modes_level_4.png  modal_2_modes_level_8.png
```

Listing 6.53: Running the example with a two-mode distribution.

As a result, the user should have created several of PNG figures scatter plots of each one of the levels and the kernel density estimation of the parameters, for each level in the Multilevel method. The name of the figure files have been chosen to be informative, as shown in the Listing above.

6.5.3 Example Code

The source code for the example is composed of 5 files: `example_main.C` (Listing 6.54), `example_likelihood.h` and `example_likelihood.C` (Listings 6.55 and 6.56), `example_compute.h` and `example_compute.C` (Listings 6.57 and 6.58).

```
#include <example_compute.h>

int main(int argc, char* argv[])
{
  // Initialize environment
  MPI_Init(&argc,&argv);

  UQ_FATAL_TEST_MACRO(argc != 3,
                      QUESO::UQ_UNAVAILABLE_RANK,
                      "main()",
                      "after executable argv[0], input file must be specified in command line
                           as argv[1], then numModes (1 or 2) must be specified as argv[2]");

  QUESO::FullEnvironment* env =
    new QUESO::FullEnvironment(MPI_COMM_WORLD,argv[1],"",NULL);

  // Compute
  unsigned int numModes = (unsigned int) atoi(argv[2]);

  compute(*env,numModes);

  // Finalize environment
  delete env;
  MPI_Finalize();

  std::cout << std::endl << "FIM!" << std::endl << std::endl;

  return 0;
}
```

Listing 6.54: File `example_main.C`.

```
#ifndef __EX_LIKELIHOOD_H__
#define __EX_LIKELIHOOD_H__

#include <queso/GslMatrix.h>

struct
likelihoodRoutine_DataType
{
  unsigned int numModes;
};

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect);

#endif
```

Listing 6.55: File `example_likelihood.h`.

```
#include <example_likelihood.h>

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect)
{
  double theta1  = paramValues[0];
  double theta2  = paramValues[1];
  double sigmaSq = paramValues[2];

  unsigned int numModes = ((likelihoodRoutine_DataType *) functionDataPtr)->numModes;

  double aux1 = theta1 + 2.*theta2;
  double aux2 = sqrt(theta1*theta1+4.*theta2*theta2);

  double w1 = 10.*sqrt(10.*(aux1+aux2));
  double w2 = 10.*sqrt(10.*(aux1-aux2));

  double sum1 = 0.;
  double sum2 = 0.;

  double aux = (w1 - 72.0470);
  sum1 += aux*aux;
  aux = (w1 - 71.8995);
  sum1 += aux*aux;
  aux = (w1 - 72.2801);
  sum1 += aux*aux;
  aux = (w1 - 71.9421);
  sum1 += aux*aux;
  aux = (w1 - 72.3578);
  sum1 += aux*aux;

  if (numModes == 1) {
    // Ok, do nothing
  }
```

```
  else if (numModes == 2) {
    aux = (w2 - 28.0292);
    sum2 += aux*aux;
    aux = (w2 - 27.3726);
    sum2 += aux*aux;
    aux = (w2 - 27.5388);
    sum2 += aux*aux;
    aux = (w2 - 27.0357);
    sum2 += aux*aux;
    aux = (w2 - 27.1588);
    sum2 += aux*aux;
  }
  else {
    UQ_FATAL_TEST_MACRO(true,
                        paramValues.env().fullRank(),
                        "example_likelihood()",
                        "invalid 'numModes'");
  }

  double result = -0.5*((double) numModes)*5.*log(2.*M_PI*sigmaSq) - 0.5*(sum1+sum2)/sigmaSq;


  return result;
}
```

Listing 6.56: File `example_likelihood.C`.

```
#ifndef __EX_COMPUTE_H__
#define __EX_COMPUTE_H__

#include <queso/Environment.h>

void compute(const QUESO::FullEnvironment& env, unsigned int numModes);

#endif
```

Listing 6.57: File `example_compute.h`.

Note that in line 12 of Listings 6.58 the `#define` directive creates the macro `APPLS_MODAL_USES_CONCATENATION`. Such macro, together with the directives `#ifdef`, `#else`, and `#endif`, tells the compiler that the application will use concatenated priors, by controlling compilation of portions of file `example_compute.C`. Commenting line 12 of Listings 6.58 will make the application to use uniform priors only:

```
1  #include <example_compute.h>
   #include <example_likelihood.h>
   #include <queso/GslMatrix.h>
   #include <queso/StatisticalInverseProblem.h>
   #include <queso/GenericScalarFunction.h>
6  #include <queso/GenericVectorRV.h>
   #include <queso/UniformVectorRV.h>
   #include <queso/ConcatenatedVectorRV.h>
   #include <queso/InverseGammaVectorRV.h>
   #include <queso/ConcatenationSubset.h>
11
   #define APPLS_MODAL_USES_CONCATENATION

   void compute(const QUESO::FullEnvironment& env, unsigned int numModes) {
     //////////////////////////////////////////////////////
```

```
  // Step 1 of 5: Instantiate the parameter space
  /////////////////////////////////////////////////////


#ifdef APPLS_MODAL_USES_CONCATENATION
  QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix>
    paramSpaceA(env, "paramA_", 2, NULL);
  QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix>
    paramSpaceB(env, "paramB_", 1, NULL);
#endif
  QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix>
    paramSpace(env, "param_", 3, NULL);

  /////////////////////////////////////////////////////
  // Step 2 of 5: Instantiate the parameter domain
  /////////////////////////////////////////////////////
#ifdef APPLS_MODAL_USES_CONCATENATION
  QUESO::GslVector paramMinsA(paramSpaceA.zeroVector());
  paramMinsA[0] = 0.;
  paramMinsA[1] = 0.;
  QUESO::GslVector paramMaxsA(paramSpaceA.zeroVector());
  paramMaxsA[0] = 3.;
  paramMaxsA[1] = 3.;
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>

  paramDomainA("paramA_",paramSpaceA,paramMinsA,paramMaxsA);

  QUESO::GslVector paramMinsB(paramSpaceB.zeroVector());
  paramMinsB[0] = 0.;
  QUESO::GslVector paramMaxsB(paramSpaceB.zeroVector());
  paramMaxsB[0] = INFINITY;
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomainB("paramB_",paramSpaceB,paramMinsB,paramMaxsB);

  QUESO::ConcatenationSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomain("",paramSpace,paramDomainA,paramDomainB);
#else
  QUESO::GslVector paramMins(paramSpace.zeroVector());
  paramMins[0] = 0.;
  paramMins[1] = 0.;
  paramMins[2] = 0.;
  QUESO::GslVector paramMaxs(paramSpace.zeroVector());
  paramMaxs[0] = 3.;
  paramMaxs[1] = 3.;
  paramMaxs[2] = .3;
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomain("param_",paramSpace,paramMins,paramMaxs);
#endif

  /////////////////////////////////////////////////////
  // Step 3 of 5: Instantiate the likelihood function object
  /////////////////////////////////////////////////////
  likelihoodRoutine_DataType likelihoodRoutine_Data;

  likelihoodRoutine_Data.numModes = numModes;
  QUESO::GenericScalarFunction<QUESO::GslVector,QUESO::GslMatrix>
    likelihoodFunctionObj("like_",
                          paramDomain,
                          likelihoodRoutine,
                          (void *) &likelihoodRoutine_Data,
                          true); // routine computes [-2.*ln(function)]

    /////////////////////////////////////////////////////
  // Step 4 of 5: Instantiate the inverse problem
  /////////////////////////////////////////////////////
```

```
#ifdef APPLS_MODAL_USES_CONCATENATION
  QUESO::UniformVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    priorRvA("priorA_", paramDomainA);

  QUESO::GslVector alpha(paramSpaceB.zeroVector());
  alpha[0] = 3.;
  QUESO::GslVector beta(paramSpaceB.zeroVector());
  if (numModes == 1) {
    beta[0] = 0.09709133373799;
  }
  else {
    beta[0] = 0.08335837191688;
  }
  QUESO::InverseGammaVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    priorRvB("priorB_", paramDomainB,alpha,beta);

  QUESO::ConcatenatedVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    priorRv("prior_", priorRvA, priorRvB, paramDomain);
#else
  QUESO::UniformVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    priorRv("prior_", paramDomain);
#endif

  QUESO::GenericVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    postRv("post_", paramSpace);

  QUESO::StatisticalInverseProblem<QUESO::GslVector,QUESO::GslMatrix>
    ip("", NULL, priorRv, likelihoodFunctionObj, postRv);

  /////////////////////////////////////////////////////
  // Step 5 of 5: Solve the inverse problem
  /////////////////////////////////////////////////////
  ip.solveWithBayesMLSampling();

  /////////////////////////////////////////////////////
  // Print some statistics
  /////////////////////////////////////////////////////
  unsigned int numPosTotal = postRv.realizer().subPeriod();
  if (env.subDisplayFile()) {
    *env.subDisplayFile() << "numPosTotal = " << numPosTotal
                          << std::endl;
  }

  QUESO::GslVector auxVec(paramSpace.zeroVector());
  unsigned int numPosTheta1SmallerThan1dot5 = 0;
  for (unsigned int i = 0; i < numPosTotal; ++i) {
    postRv.realizer().realization(auxVec);
    if (auxVec[0] < 1.5) numPosTheta1SmallerThan1dot5++;
  }

  if (env.subDisplayFile()) {
    *env.subDisplayFile() << "numPosTheta1SmallerThan1dot5 = " <<
        numPosTheta1SmallerThan1dot5
                          << ", ratio = " << ((double) numPosTheta1SmallerThan1dot5)/((double
                              ) numPosTotal)
                          << std::endl;
  }

  return;
}
```

Listing 6.58: File `example_compute.C`.

6.5.4 Input File

QUESO reads an input file for solving statistical problems, which provides options for the Multilevel or MCMC method. In this example, the Multilevel method is chosen to sample from the distribution. Many variables are common to both MCMC and Multilevel method, especially because the Multilevel method also has the option of delaying the rejection of a candidate. The names of the variables have been designed to be informative in this case as well:

`env:` refers to QUESO environment;

`ip:` refers to inverse problem;

`ml:` refers to Multilevel;

`dr:` refers to delayed rejection;

`rawChain:` refers to the raw, entire chain;

`filteredChain:` refers to a filtered chain (related to a specified `lag`);

`last:` refers to instructions specific for the last level of the Multilevel algorithm.

The user may select options for a specific level by naming its number, i.e., in case the user wants to write the raw chain of the level 3 in a separate file, say `'rawChain_ml_level3.m'`, he/she may include the line:

```
ip_ml_3_rawChain_dataOutputFileName = outputData/rawChain_ml_level3
```

in the input file.

The options used for solving this example are displayed in Listing 6.59.

```
###############################################
# UQ Environment
###############################################
#env_help                  = anything
env_numSubEnvironments    = 1
env_subDisplayFileName    = outputData/display
env_subDisplayAllowAll    = 0
env_subDisplayAllowedSet  = 0
env_displayVerbosity      = 0
env_syncVerbosity         = 0
env_seed                  = 0

###############################################
# Statistical inverse problem (ip)
###############################################
#ip_help                  = anything
ip_computeSolution       = 1
ip_dataOutputFileName    = outputData/sipOutput
ip_dataOutputAllowedSet  = 0

###############################################
# 'ip_': information for Multilevel algorithm
###############################################
#ip_ml_help                  = anything
ip_ml_dataOutputFileName    = outputData/sipOutput_ml
ip_ml_dataOutputAllowedSet  = 0
```

```
###############################################
# All levels, unless otherwise specified
###############################################
ip_ml_default_minEffectiveSizeRatio = 0.49
ip_ml_default_maxEffectiveSizeRatio = 0.51
ip_ml_default_rawChain_size = 10000
ip_ml_default_rawChain_dataOutputFileName = outputData/rawChain_ml
ip_ml_default_scaleCovMatrix                    = 1
ip_ml_default_dr_maxNumExtraStages              = 2
ip_ml_default_dr_listOfScalesForExtraStages     = 10. 25.

###############################################
# Last level (level 7 or 8 for 'example_gsl' executable)
###############################################
ip_ml_last_dataOutputFileName                 = outputData/sipOutput_ml
ip_ml_last_dataOutputAllowedSet               = 0 1
ip_ml_last_rawChain_size                      = 10000
ip_ml_last_rawChain_computeStats              = 1
ip_ml_last_rawChain_dataOutputFileName        = outputData/rawChain_ml
```

Listing 6.59: Options for QUESO library used in application code (Listings 6.54-6.58).

6.5.5 Create your own Makefile

Makefiles are special format files that together with the make utility will help one to compile and automatically build and manage projects (programs). Listing 6.60 presents a Makefile, named '`Makefile_modal_example_violeta`', that may be used to compile the code and create the executable `modal_gsl`. Naturally, it must be adapted to the user's settings, i.e., it has to have the correct paths for the user's libraries that have actually been used to compile and install QUESO (see Sections 2.1–2.4).

```
QUESO_DIR = /path/to/queso
BOOST_DIR = /path/to/boost
GSL_DIR   = /path/to/gsl

INC_PATHS = \
   -I. \
   -I$(QUESO_DIR)/include \
   -I$(BOOST_DIR)/include \
   -I$(GSL_DIR)/include

LIBS = \
   -L$(QUESO_DIR)/lib -lqueso \
   -L$(BOOST_DIR)/lib -lboost_program_options \
   -L$(GSL_DIR)/lib -lgsl

CXX = mpic++
CXXFLAGS += -g -Wall -c

default: all

.SUFFIXES: .o .C

all:       modal_example_gsl

clean:
   rm -f *~
```

```
    rm -f *.o
    rm -f modal_gsl

modal_example_gsl: example_main.o example_likelihood.o example_compute.o
    $(CXX) example_main.o \
           example_likelihood.o \
           example_compute.o \
           -o modal_gsl $(LIBS)

%.o: %.C
    $(CXX) $(INC_PATHS) $(CXXFLAGS) $<
```

Listing 6.60: Makefile for the application code in Listings 6.54-6.58

Thus, to compile, build and execute the code, the user just needs to run the following commands in the same directory where the files are:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/examples/modal/
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
  $HOME/LIBRARIES/gsl-1.15/lib/:\
  $HOME/LIBRARIES/boost-1.53.0/lib/:\
  $HOME/LIBRARIES/hdf5-1.8.10/lib:\
  $HOME/LIBRARIES/QUESO-0.56.0/lib
$ make -f Makefile_modal_violeta
$ ./modal_gsl example.inp <num_modes>
```

The '`export`' instruction above is only necessary if the user has not saved it in his/her `.bashrc` file.

6.5.6 Data Post-Processing and Visualization

According to the specifications of the input file in Listing 6.59, both a folder named `outputData` and a the following files should be generated:

`rawChain_ml.m`
`display_sub0.txt`

The sequence of Matlab commands is identical to the ones presented in Sections 6.1.5, 6.2.5, 6.3.8 and 6.4.7; therefore, are omitted here. The reader is invited to explore the Matlab files `plot_modal_all_levels_1mode.m` and/or `plot_modal_all_levels_2modes.m` for details of how the figures have been generated.

6.5.6.1 Scatter Plots

The code presented in Listing 6.61 uses Matlab function `plotmatrix` to generate Figures 6.5.1 and 6.5.2 which presents the scatter plots and histograms of the parameters θ_1 and θ_2, based on the generated raw chains.

```
fprintf(1,'Scatter plots and histograms of raw chains - Level 1 <press any key>\n');
plotmatrix(ip_ml_1_rawChain_unified, '+b')
set(gca,'fontsize',20);
```

```
xlabel('\theta_1                    \theta_2                    \theta_3','fontsize',16);
ylabel('\theta_3                    \theta_2                    \theta_1','fontsize',16);
title('Scatter plots and histograms, Level 1 - 1 mode')
```

Listing 6.61: Matlab code for the scatter plots depicted in Figures 6.5.1 and 6.5.2.

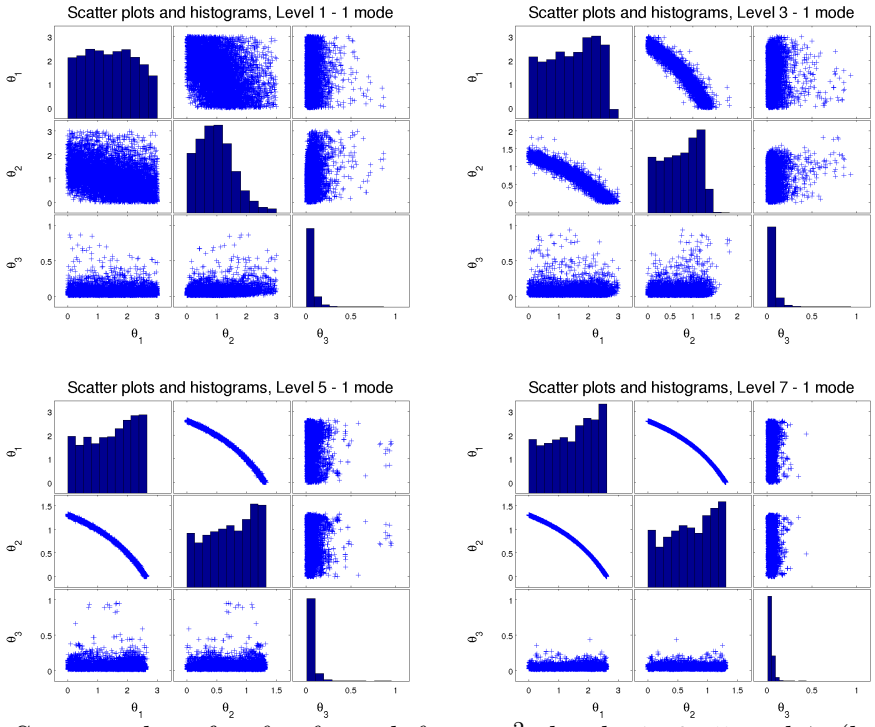


Figure 6.5.1: Scatter plots for θ_1, θ_2 and $\theta_3 = \sigma^2$, levels 1, 3, 5 and 7 (last). One mode distribution.

6.5.6.2 KDE Plots

Figures 6.5.3 and 6.5.4 present the KDE plots of the parameters θ_1, θ_2, θ_3 and target PDF in both cases: one-mode and two-modes distribution.

6.5.6.3 Autocorrelation Plots

Figures 6.5.5 and 6.5.6 present the autocorrelation of the parameters θ_1, θ_2 and θ_3 in both cases: one-mode and two-modes distribution.

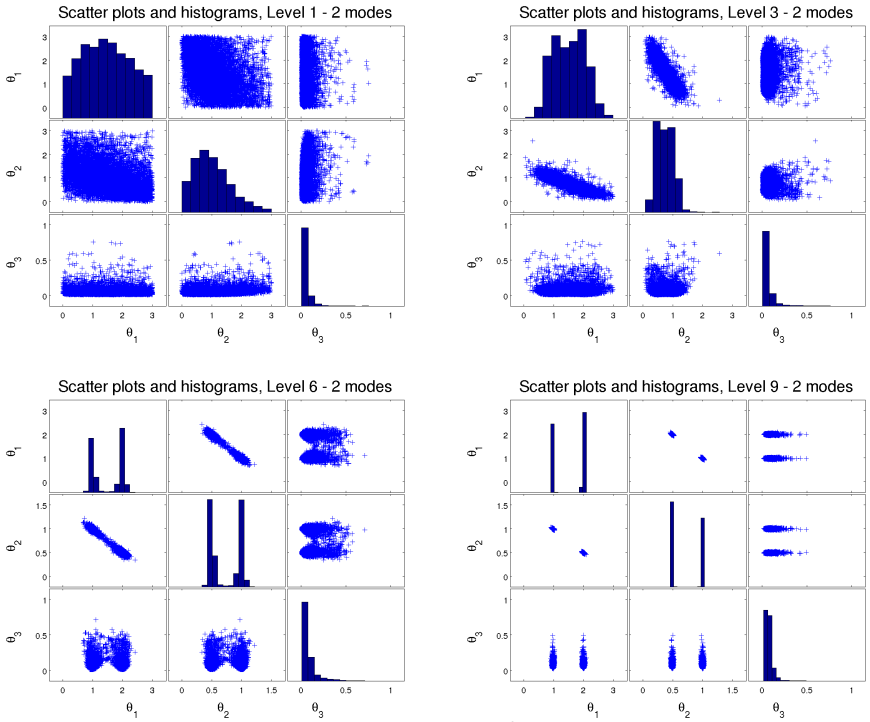


Figure 6.5.2: Scatter plots for θ_1, θ_2 and $\theta_3 = \sigma^2$, levels 1, 3, 6 and 9 (last). Two-mode distribution.

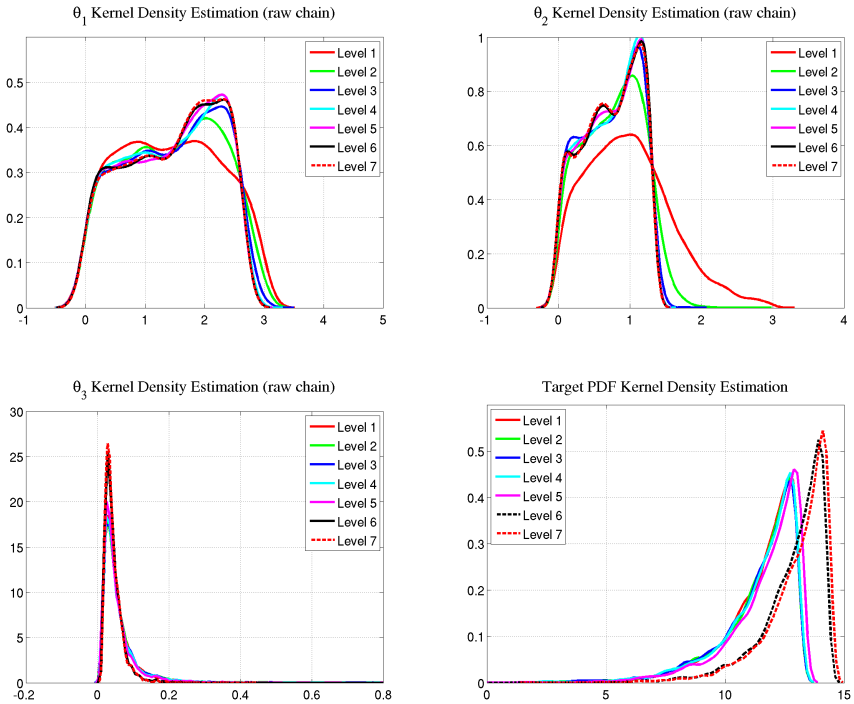


Figure 6.5.3: KDE plots for θ_1, θ_2, $\theta_3 = \sigma^2$, and the target PDF. One mode distribution.

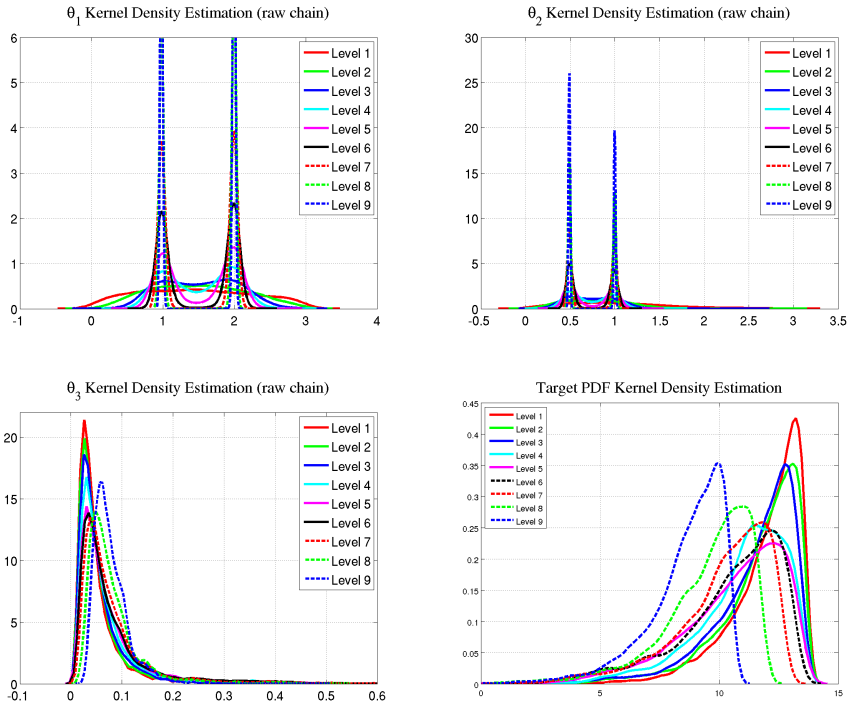


Figure 6.5.4: KDE plots for θ_1, θ_2, $\theta_3 = \sigma^2$, and the target PDF. Two-mode distribution.

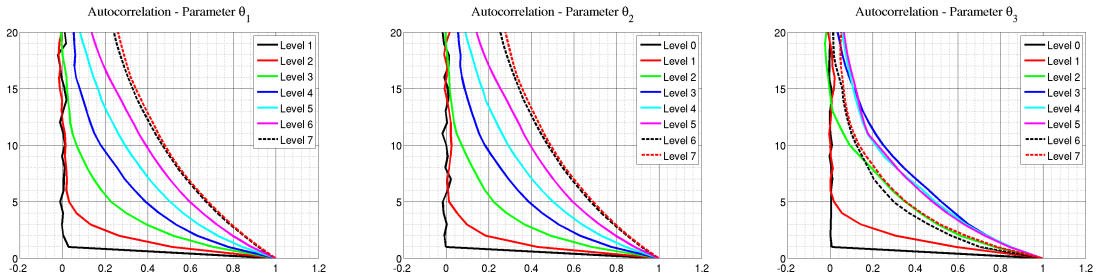


Figure 6.5.5: Autocorrelation plots for θ_1, θ_2 and $\theta_3 = \sigma^2$. One-mode distribution.

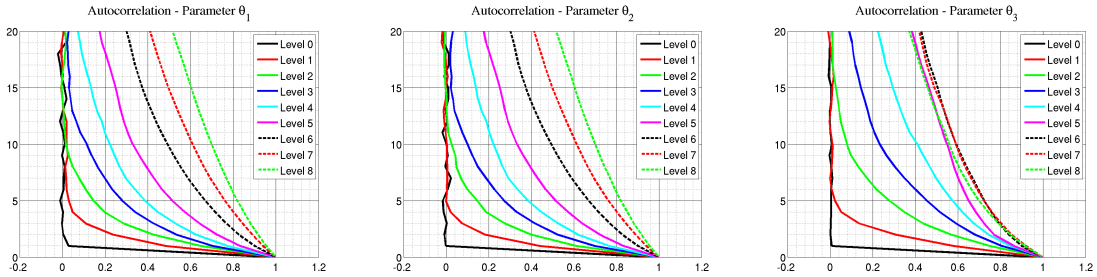


Figure 6.5.6: Autocorrelation plots for θ_1, θ_2 and $\theta_3 = \sigma^2$. Two-mode distribution.

6.6 bimodal

This example replicates the problem in "Section 4.1 A 1D Problem" of [8]: it presents how to use QUESO and the Multilevel method for sampling from a posterior PDF composed of the sum of two Gaussian distributions.

Let's define $D = [-250, 250]$ and the three distributions $\pi_{\text{prior}} : D \to \mathbb{R}_+$, $f_1 : \mathbb{R} \to \mathbb{R}_+$ and $f_2 : \mathbb{R} \to \mathbb{R}_+$ by:

$$\begin{aligned} \pi_{\text{prior}} &= \frac{1}{|D|} = \frac{1}{500}, \quad \forall\, \theta \in D \\ f_1(\theta) &= \frac{1}{(2\pi)^{1/2}\sqrt{|V_1|}} \exp\left(-\frac{1}{2}(\theta-\mu_1)^T V_1^{-1}(\theta-\mu_1)\right), \quad \forall\, \theta \in \mathbb{R} \\ f_2(\theta) &= \frac{1}{(2\pi)^{1/2}\sqrt{|V_2|}} \exp\left(-\frac{1}{2}(\theta-\mu_2)^T V_2^{-1}(\theta-\mu_2)\right), \quad \forall\, \theta \in \mathbb{R}, \end{aligned} \tag{6.6.1}$$

where

$$\mu_1 = 10, \quad V_1 = 1^2, \quad \mu_2 = 100, \quad V_2 = 5^2.$$

In this example, we want to sample the posterior PDF given by:

$$\pi_{\text{posterior}}(\theta) \propto \left[\frac{1}{2}f_1(\theta) + \frac{1}{2}f_2(\theta)\right] \cdot \pi_{\text{prior}} = f(\theta) \cdot \pi_{\text{prior}} \tag{6.6.2}$$

where $f(\theta) = \frac{1}{2}f_1(\theta) + \frac{1}{2}f_2(\theta)$ is the likelihood function, which is depicted in Figure 6.6.1.

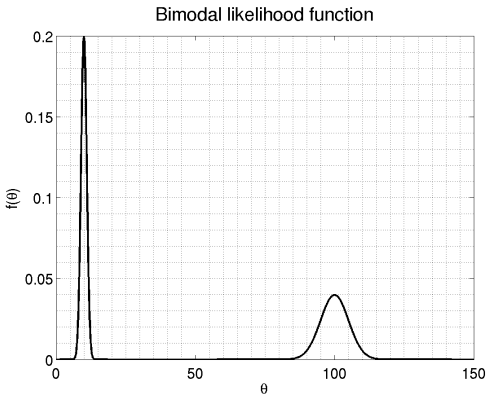


Figure 6.6.1: Likelihood function given by $f = f_1/2 + f_2/2$, where f_1 and f_2 are defined in Equation (6.6.1).

6.6.1 Running the Example

To run the executable provided (available after QUESO installation), and generate figures for the chains, PDFs, CDFs, etc., enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/examples/bimodal
$ rm outputData/*
$ ./bimodal_gsl bimodal_1chain.inp
$ matlab
   $ plot_all.m                              # inside matlab
   $ plot_likelihood_normalized_taus.m       # inside matlab
   $ plot_likelihood_unnormalized_taus.m     # inside matlab
   $ exit                                    # inside matlab
$ ls -l outputData/*.png
bimodal_autocorrelation_rawchain.png  bimodal_likelihood.png
bimodal_cdf_rawchain.png              bimodal_likelihood_taus_normalized.png
bimodal_kde_rawchain.png              bimodal_likelihood_taus.png
```

As a result, the user should have created several of PNG figures containing marginal posterior PDF, cumulative density distribution and autocorrelation. The name of the figure files have been chosen to be informative, as shown in the Listing above.

6.6.2 Example Code

The source code for the example is composed of 5 files: `bimodal_main.C` (Listing 6.62), `bimodal_likelihood.h` and `bimodal_likelihood.C` (Listings 6.63 and 6.64), `bimodal_compute.h` and `bimodal_compute.C` (Listings 6.65 and 6.66).

```
#include <bimodal_compute.h>

int main(int argc, char* argv[])
{
  // Initialize environment
#ifdef QUESO_HAS_MPI
  MPI_Init(&argc,&argv);
  QUESO::FullEnvironment* env = new QUESO::FullEnvironment(MPI_COMM_WORLD,argv[1],"",NULL);
#else
  QUESO::FullEnvironment* env = new QUESO::FullEnvironment(argv[1],"",NULL);
#endif

  // Compute
  compute(*env);

  // Finalize environment
  delete env;
#ifdef QUESO_HAS_MPI
  MPI_Finalize();
#endif
  return 0;
}
```

Listing 6.62: File `bimodal_main.C`.

```
#ifndef EX_LIKELIHOOD_H
#define EX_LIKELIHOOD_H

#include <queso/GslMatrix.h>

struct
likelihoodRoutine_DataType
{
```

```
  const QUESO::GslVector* meanVector;
  const QUESO::GslMatrix* covMatrix;
};

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect);

#endif
```

Listing 6.63: File `bimodal_likelihood.h`.

```
#include <bimodal_likelihood.h>
#include <cmath>

static unsigned int likelihoodCounter = 0;

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect)
{
  likelihoodCounter++;

  if (paramDirection  ||
      functionDataPtr ||
      gradVector      ||
      hessianMatrix   ||
      hessianEffect) {}; // just to remove compiler warning

    double returnValue = 0.;
    double x = paramValues[0];
    double mean1  = 10.;
    double sigma1 = 1.;
    double y1 = (x-mean1)*(x-mean1)/(2.*sigma1*sigma1);
    double z1 = (1./sigma1/sqrt(2*M_PI))*exp(-y1);

    double mean2  = 100.;
    double sigma2 = 5.;
    double y2 = (x-mean2)*(x-mean2)/(2.*sigma2*sigma2);
    double z2 = (1./sigma2/sqrt(2*M_PI))*exp(-y2);

    double resultValue = -2*log((z1+2.*z2)/3.);

    if (resultValue == INFINITY) {
      //std::cerr << "WARNING In likelihoodRoutine"
      //          << ", fullRank "       << paramValues.env().fullRank()
      //          << ", subEnvironment " << paramValues.env().subId()
      //          << ", subRank "        << paramValues.env().subRank()
      //          << ", inter0Rank "     << paramValues.env().inter0Rank()
      //          << ": x = "            << x
      //          << ", z1 = "           << z1
      //          << ", z2 = "           << z2
      //          << ", resultValue = "  << resultValue
      //          << std::endl;
```

```
      resultValue = 1040.;
    }

    returnValue = -.5*resultValue;


  if (paramValues.env().exceptionalCircumstance()) {
    if ((paramValues.env().subDisplayFile()       ) &&
        (paramValues.env().displayVerbosity() > 0)) { // detailed output debug
      *paramValues.env().subDisplayFile() << "Leaving likelihood function"
                                          << ": paramValues = " << paramValues
                                          << ", returnValue = " << returnValue
                                          << std::endl;
    }
  }

  return returnValue;
}
```

Listing 6.64: File `bimodal_likelihood.C`.

```
#ifndef EX_COMPUTE_H
#define EX_COMPUTE_H

#include <queso/Environment.h>

void compute(const QUESO::FullEnvironment& env);

#endif
```

Listing 6.65: File `bimodal_compute.h`.

Note that in line 57 of Listings 6.66 the '`#if 0`' directive tells the compiler that the application will not use DRAM algorithm, but rather the Multilevel solver (line 65). Naturally, the user may chose to use the DRAM algorithm by changing the directive in line 57 to '`#if 1`'.

```
#include <bimodal_compute.h>
#include <bimodal_likelihood.h>
#include <queso/GslMatrix.h>
#include <queso/StatisticalInverseProblem.h>
#include <queso/1D1DFunction.h>
#include <queso/GenericScalarFunction.h>
#include <queso/GenericVectorRV.h>
#include <queso/UniformVectorRV.h>

void compute(const QUESO::FullEnvironment& env) {
  //-----------------------------------------------------
  // Step 1 of 5: Instantiate the parameter space
  //-----------------------------------------------------
  QUESO::VectorSpace<QUESO::GslVector,QUESO::GslMatrix>
    paramSpace(env, "param_", 1, NULL);

  //-----------------------------------------------------
  // Step 2 of 5: Instantiate the parameter domain
  //-----------------------------------------------------
  QUESO::GslVector paramMins(paramSpace.zeroVector());
  paramMins.cwSet(-250.);
  QUESO::GslVector paramMaxs(paramSpace.zeroVector());
  paramMaxs.cwSet( 250.);
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>
```

```
    paramDomain("param_",paramSpace,paramMins,paramMaxs);

  //--------------------------------------------------
  // Step 3 of 5: Instantiate the likelihood function object
  //--------------------------------------------------
  QUESO::GslVector meanVector(paramSpace.zeroVector());
  meanVector[0] = 10.;
  QUESO::GslMatrix* covMatrix = paramSpace.newMatrix();
  (*covMatrix)(0,0) = 1.;
  likelihoodRoutine_DataType likelihoodRoutine_Data;
  likelihoodRoutine_Data.meanVector = &meanVector;
  likelihoodRoutine_Data.covMatrix  = covMatrix;
  QUESO::GenericScalarFunction<QUESO::GslVector,QUESO::GslMatrix>
    likelihoodFunctionObj("like_",
                          paramDomain,
                          likelihoodRoutine,
                          (void *) &likelihoodRoutine_Data,
                          true); // routine computes [-2.*ln(function)]

  //--------------------------------------------------
  // Step 4 of 5: Instantiate the inverse problem
  //--------------------------------------------------
  QUESO::UniformVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    priorRv("prior_", paramDomain);
  QUESO::GenericVectorRV<QUESO::GslVector,QUESO::GslMatrix>
    postRv("post_", paramSpace);
  QUESO::StatisticalInverseProblem<QUESO::GslVector,QUESO::GslMatrix>
    ip("", NULL, priorRv, likelihoodFunctionObj, postRv);

  //--------------------------------------------------
  // Step 5 of 5: Solve the inverse problem
  //--------------------------------------------------
#if 0
  uqGslVector paramInitials(paramSpace.zeroVector());
  paramInitials[0] = 45.;
  uqGslMatrix* proposalCovMatrix = paramSpace.newMatrix();
  (*proposalCovMatrix)(0,0) = 1600.;
  ip.solveWithBayesMetropolisHastings(NULL, paramInitials, proposalCovMatrix);
  delete proposalCovMatrix;
#else
  ip.solveWithBayesMLSampling();
#endif

  //--------------------------------------------------
  // Print some statistics in the file 'display_sub0.txt'
  // They will be in the last part of the file.
  //--------------------------------------------------
  unsigned int numPosTotal = postRv.realizer().subPeriod();
  if (env.subDisplayFile()) {
    *env.subDisplayFile() << "numPosTotal = " << numPosTotal
                          << std::endl;
  }

  QUESO::GslVector auxVec(paramSpace.zeroVector());
  unsigned int numPosSmallerThan40 = 0;
  for (unsigned int i = 0; i < numPosTotal; ++i) {
    postRv.realizer().realization(auxVec);
    if (auxVec[0] < 40.) numPosSmallerThan40++;
  }
  if (env.subDisplayFile()) {
    *env.subDisplayFile() << "numPosSmallerThan40 = " << numPosSmallerThan40
                          << ", ratio = " << ((double) numPosSmallerThan40)/((double)
                              numPosTotal)
                          << std::endl;
  }
```

```
  QUESO::ScalarSequence<double> seq1  (env,numPosSmallerThan40,"");
  QUESO::ScalarSequence<double> seq2  (env,numPosTotal - numPosSmallerThan40,"");
  QUESO::ScalarSequence<double> seqAll(env,numPosTotal,"");
93  unsigned int i1 = 0;
  unsigned int i2 = 0;
  for (unsigned int i = 0; i < numPosTotal; ++i) {
    postRv.realizer().realization(auxVec);
    if (auxVec[0] < 40.) seq1[i1++] = auxVec[0];
98  else                 seq2[i2++] = auxVec[0];
    seqAll[i] = auxVec[0];
  }

  double mean1 = seq1.subMeanExtra(0,seq1.subSequenceSize());
103 if (env.subDisplayFile()) {
    *env.subDisplayFile() << "seq1.size() = "    << seq1.subSequenceSize()
                          << "\n seq1.mean() = " << mean1
                          << "\n seq1.std() = "  << sqrt(seq1.subSampleVarianceExtra(0,seq1.
                              subSequenceSize(),mean1))
                          << std::endl;
108 }

  double mean2 = seq2.subMeanExtra(0,seq2.subSequenceSize());
  if (env.subDisplayFile()) {
    *env.subDisplayFile() << "seq2.size() = "    << seq2.subSequenceSize()
113                       << "\n seq2.mean() = " << mean2
                          << "\n seq2.std() = "  << sqrt(seq2.subSampleVarianceExtra(0,seq2.
                              subSequenceSize(),mean2))
                          << std::endl;
  }

118 double meanAll = seqAll.subMeanExtra(0,seqAll.subSequenceSize());
  if (env.subDisplayFile()) {
    *env.subDisplayFile() << "seqAll.size() = "    << seqAll.subSequenceSize()
                          << "\n seqAll.mean() = " << meanAll
                          << "\n seqAll.std() = "  << sqrt(seqAll.subSampleVarianceExtra(0,
                              seqAll.subSequenceSize(),meanAll))
123                       << std::endl;
  }

  //-----------------------------------------------------
  // Test if likelihood is normalized
128 //-----------------------------------------------------
  unsigned int numGridPoints = 1000001;
  double xMin = paramDomain.minValues()[0];
  double xMax = paramDomain.maxValues()[0];
  double intervalSize = (xMax-xMin)/((double) numGridPoints - 1);
133 double integral = 0.;
  for (unsigned int i = 0; i < numGridPoints; ++i) {
    auxVec[0] = xMin + i*intervalSize;
    integral += likelihoodFunctionObj.actualValue(auxVec,NULL,NULL,NULL,NULL);
  }
138 integral *= intervalSize;
  if (env.subDisplayFile()) {
    *env.subDisplayFile() << "integral = " << integral
                          << std::endl;
  }
143
  // Return
  delete covMatrix;

  return;
148 }
```

Listing 6.66: File `bimodal_compute.C`.

6.6.3 Input File

QUESO reads an input file for solving statistical problems, which provides options for the Multilevel or MCMC method. In this example, the Multilevel method is chosen to sample from the distribution. Many variables are common to both MCMC and Multilevel method, especially because the Multilevel method also has the option of delaying the rejection of a candidate. The names of the variables have been designed to be informative in this case as well:

`env:` refers to QUESO environment;

`ip:` refers to inverse problem;

`ml:` refers to Multilevel;

`dr:` refers to delayed rejection;

`rawChain:` refers to the raw, entire chain;

`filteredChain:` refers to a filtered chain (related to a specified `lag`);

`last:` refers to instructions specific for the last level of the Multilevel algorithm.

The user may select options for a specific level by naming its number, i.e., in case the user wants to define a different number of extra stages together with the scales for each stage (in the DRAM part of the ML algorithm) for the level 3, he/she may include the following instructions:

```
ip_ml_3_dr_maxNumExtraStages          = 1
ip_ml_3_dr_listOfScalesForExtraStages = 3.333
```

in the input file.

The options used for solving this example are displayed in Listing 6.67.

```
###############################################
# UQ Environment
###############################################
env_numSubEnvironments   = 1
env_subDisplayFileName   = outputData/display
env_subDisplayAllowAll   = 0
env_subDisplayAllowedSet = 0 1
env_displayVerbosity     = 2
env_syncVerbosity        = 0
env_seed                 = -1

###############################################
# Statistical inverse problem (ip)
###############################################
ip_computeSolution      = 1
ip_dataOutputFileName   = outputData/sipOutput
ip_dataOutputAllowedSet = 0
```

```
###############################################
# 'ip_': information for Multilevel algorithm
###############################################
ip_ml_dataOutputFileName    = outputData/sipOutput_ml
ip_ml_dataOutputAllowedSet = 0 1

###############################################
# All levels, unless otherwise specified
###############################################
#ip_ml_default_loadBalance = 0
ip_ml_default_rawChain_size = 10000
ip_ml_default_rawChain_dataOutputFileName = outputData/rawChain_ml #data from all levels will
    be written
ip_ml_default_minEffectiveSizeRatio = 0.49
ip_ml_default_maxEffectiveSizeRatio = 0.51
ip_ml_default_minRejectionRate      = 0.24
ip_ml_default_maxRejectionRate      = 0.4
ip_ml_default_putOutOfBoundsInChain = 0

###############################################
# Level 3
###############################################
#ip_ml_3_dr_maxNumExtraStages          = 1
#ip_ml_3_dr_listOfScalesForExtraStages = 3.333

###############################################
# Last level (level 4 for 'bimodal_gsl' executable)
###############################################
ip_ml_last_dataOutputFileName                  = outputData/sipOutput_ml
ip_ml_last_dataOutputAllowedSet                = 0 1

#ip_ml_last_loadBalance                         = 0
ip_ml_last_rawChain_size                       = 10000
ip_ml_last_rawChain_dataOutputFileName         = outputData/rawChain_ml
ip_ml_last_rawChain_dataOutputAllowedSet       = 0
ip_ml_last_rawChain_computeStats               = 1
ip_ml_last_rawChain_stats_kde_compute          = 1
ip_ml_last_rawChain_stats_kde_numEvalPositions = 200
ip_ml_last_rawChain_stats_covMatrix_compute    = 1
ip_ml_last_rawChain_stats_corrMatrix_compute   = 1

ip_ml_last_filteredChain_generate                    = 1
ip_ml_last_filteredChain_lag                         = 2
ip_ml_last_filteredChain_dataOutputFileName          = outputData/filtChain_ml
ip_ml_last_filteredChain_dataOutputAllowedSet        = 0
ip_ml_last_filteredChain_computeStats                = 1
ip_ml_last_filteredChain_stats_kde_compute           = 1
ip_ml_last_filteredChain_stats_kde_numEvalPositions = 200
ip_ml_last_filteredChain_stats_covMatrix_compute     = 1
ip_ml_last_filteredChain_stats_corrMatrix_compute    = 1

ip_ml_last_dr_maxNumExtraStages                = 1
ip_ml_last_dr_listOfScalesForExtraStages       = 5.

ip_ml_last_minEffectiveSizeRatio = 0.49
ip_ml_last_maxEffectiveSizeRatio = 0.51
ip_ml_last_minRejectionRate      = 0.24
ip_ml_last_maxRejectionRate      = 0.4
ip_ml_last_putOutOfBoundsInChain = 0
```

Listing 6.67: Options for QUESO library used in application code (Listings 6.62-6.66).

6.6.4 Create your own Makefile

Similarly to the other examples presented in this user's manual and also available with QUESO distribution, a user-created makefile is available: '`Makefile_bimodal_violeta`'. When adapted to the user's settings, namely paths for QUESO required libraries, it may be used to compile the code and create the executable `bimodal_gsl`.

Thus, to compile, build and execute the code, the user just needs to run the following commands in the same directory where the files are:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/examples/bimodal/
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
  $HOME/LIBRARIES/gsl-1.15/lib/:\
  $HOME/LIBRARIES/boost-1.53.0/lib/:\
  $HOME/LIBRARIES/hdf5-1.8.10/lib:\
  $HOME/LIBRARIES/QUESO-0.56.0/lib
$ make -f Makefile_bimodal_violeta
$ ./bimodal_gsl example.inp
```

Again, the '`export`' instruction above is only necessary if the user has not saved it in his/her `.bashrc` file.

6.6.5 Data Post-Processing and Visualization

According to the specifications of the input file in Listing 6.67, both a folder named `outputData` and a the following files should be generated:

`rawChain_ml.m`
`display_sub0.txt`

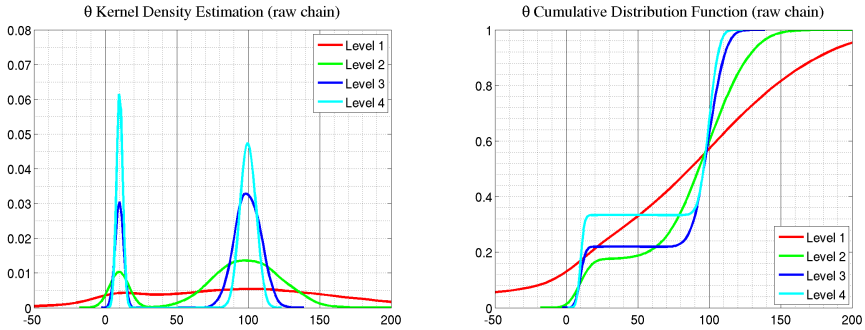
The sequence of Matlab commands is identical to the ones presented in Sections 6.1.5, 6.2.5, 6.3.8 and 6.4.7; therefore, are omitted here. The reader is invited to explore the Matlab files `plot_likelihood_normalized_taus.m`, `plot_likelihood_unnormalized_taus.m` and/or `plot_all.m`, for details of how the figures have been generated.

6.6.5.1 KDE and CDF Plots

Figure 6.6.2 presents the KDE and CDF plots of the parameter θ.

6.6.5.2 Autocorrelation Plots

Figure 6.6.3 presents the autocorrelation of the parameter θ, in each one of the intermediate levels.



(a) KDE (b) CDF

Figure 6.6.2: KDE and CDF plots of parameter θ, for all fours levels.

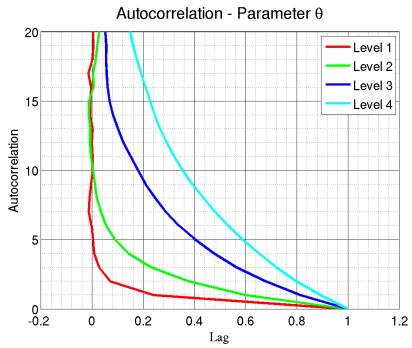
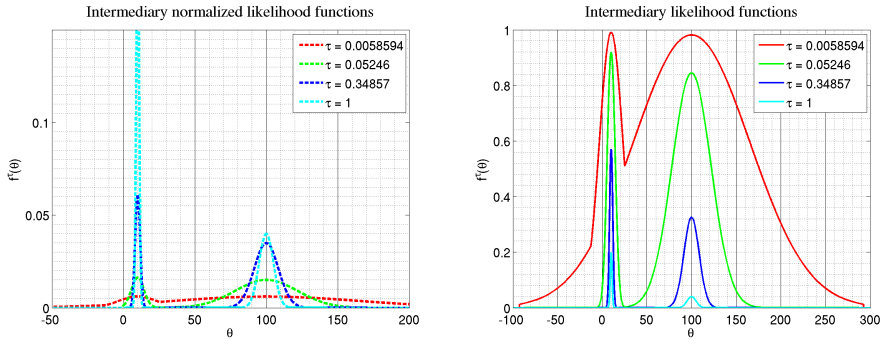


Figure 6.6.3: Autocorrelation plots for θ, all four levels.



(a) normalized (b) unnormalized

Figure 6.6.4: Intermediary likelihood functions $f(\theta)^\tau$, where τ_i is the exponent computed at the i-th level of Multilevel algorithm. In this simple problem, only four levels are needed, i.e. $i = 1 \ldots 4$. The cyan-colored curve (exponent $\tau = 1$) is the same curve as in Figure 6.6.1.

6.6.5.3 Intermediary Likelihood Plots

6.7 hysteretic

This example replicates the problem in "Section 4.3 A Hysteretic Model Class " of [8], and which is also discussed in [6]. In this example we consider the nonlinear seismic response of a four-story building. This response is modeled with an inelastic shear building model with some linear viscous damping and hysteretic bilinear interstory restoring forces [6]. More specifically, let $t \geq 0$ denote time, let $a_g(t)$ be a given total acceleration at the base (Fig. 13), and for the i-th floor [degree of freedom (dof)], $1 \leq i \leq N_o \equiv 4$, let us denote:

$$\begin{aligned} m_i &= \text{lumped mass}, \\ q_i(t) &= \text{horizontal displacement}, \\ F_i(t) &= \text{hysteretic restoring force} \end{aligned} \tag{6.7.1}$$

The hysteretic restoring force is illustrated in Figure 6.7.1 and the horizontal base (ground) acceleration (input data) used in [8] is illustrated in 6.7.2.

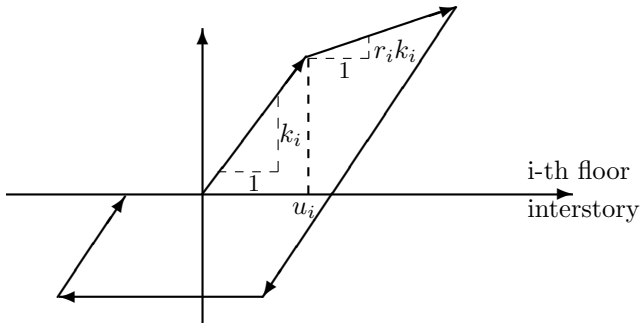


Figure 6.7.1: Illustration of the hysteretic restoring force [see Eq. (6.7.2)] used in our hysteretic test problem. The terms r_i, k_i, and u_i denote model parameters.

We also define the mass matrix $\boldsymbol{M}$ and the stiffness matrix $\boldsymbol{K}$:

$$\boldsymbol{M} = \begin{bmatrix} m_1 & 0 & 0 & 0 \\ 0 & m_2 & 0 & 0 \\ 0 & 0 & m_3 & 0 \\ 0 & 0 & 0 & m_4 \end{bmatrix} \quad \text{and} \quad \boldsymbol{K} = \begin{bmatrix} k_1 + k_2 & -k_2 & 0 & 0 \\ -k_2 & k_2 + k_3 & -k_3 & 0 \\ 0 & -k_3 & k_3 + k_4 & -k4 \\ 0 & 0 & -k_4 & k_4 \end{bmatrix}$$

and the Rayleigh damping matrix

$$\boldsymbol{C} = \rho \boldsymbol{M} + \gamma \boldsymbol{K}$$

for given positive scalar parameters ρ and γ. The response $\boldsymbol{q}(t) \equiv [q_1(t), q_2(t), q_3(t), q_4(t)]$ is modeled as satisfying the equation of motion:

$$\boldsymbol{M}\ddot{\boldsymbol{q}}(t) + \boldsymbol{C}\dot{\boldsymbol{q}}(t) + \boldsymbol{F}(t) = -\boldsymbol{M} \cdot \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}_{4\times 1} \cdot a_g(t), \tag{6.7.2}$$

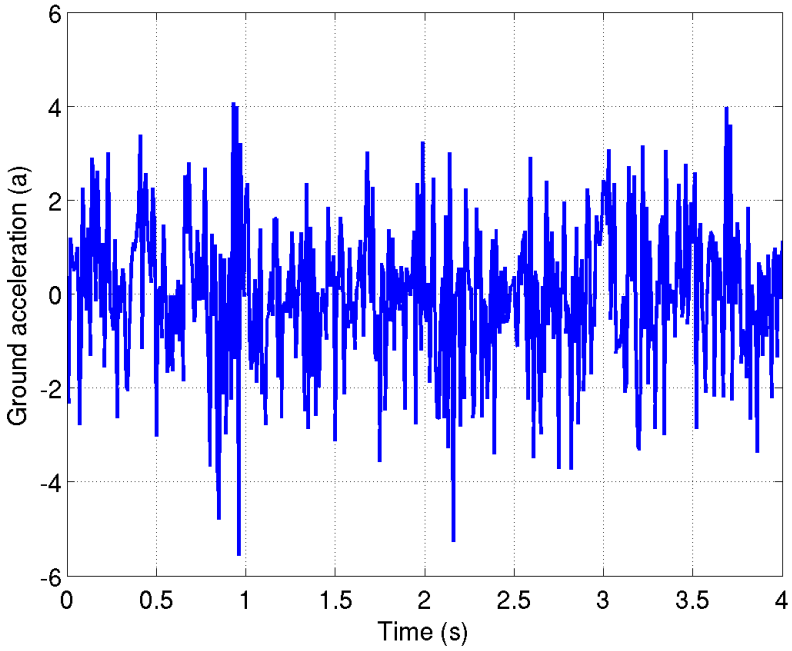


Figure 6.7.2: Horizontal base acceleration (input data) used in the hysteretic test problem [8].

where $\boldsymbol{F}(t) \equiv [F_1(t), F_2(t), F_3(t), F_4(t)]$. In this model, the hysteretic restoring force $\boldsymbol{F}(t)$ depends on the whole time history $[\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t)]$ of responses from the initial instant until time t.

The (noisy) measured data $y = (y_1, y_2, y_3, y_4)$ available for model calibration consists of 4 s of accelerometer data at each floor (refer to Fig. 6.7.3), with a sample interval $\Delta t = 0.01$ s. The simulated dynamic data was obtained by adding Gaussian white noise to the output simulation of the hysteretic model with the following input values:

$$
\begin{aligned}
m_1 &= m_2 = m_3 = m_4 = 2 \times 10^4\, kg, \\
k_1 &= 2.2 \times 10^7\, Nm^{-1}, \\
k_2 &= 2.0 \times 10^7\, Nm^{-1}, \\
k_3 &= 1.7 \times 10^7\, Nm^{-1}, \\
k_4 &= 1.45 \times 10^7\, Nm^{-1}, \\
r_1 &= r_2 = r_3 = r_4 = 0.1, \\
u_1 &= u_2 = 8 \times 10^{-3}\, m, \\
u_3 &= u_4 = 7 \times 10^{-3}\, m, \\
\rho &= 7.959 \times 10^{-1}, \\
\gamma &= 2.5 \times 10^{-3}, \\
\sigma^2 &= 0.6^2,
\end{aligned}
$$

where for $i = 1, 2, 3, 4$, k_i is the initial stiffness, r_i is the post-yield stiffness reduction factor, and u_i is yield displacement.

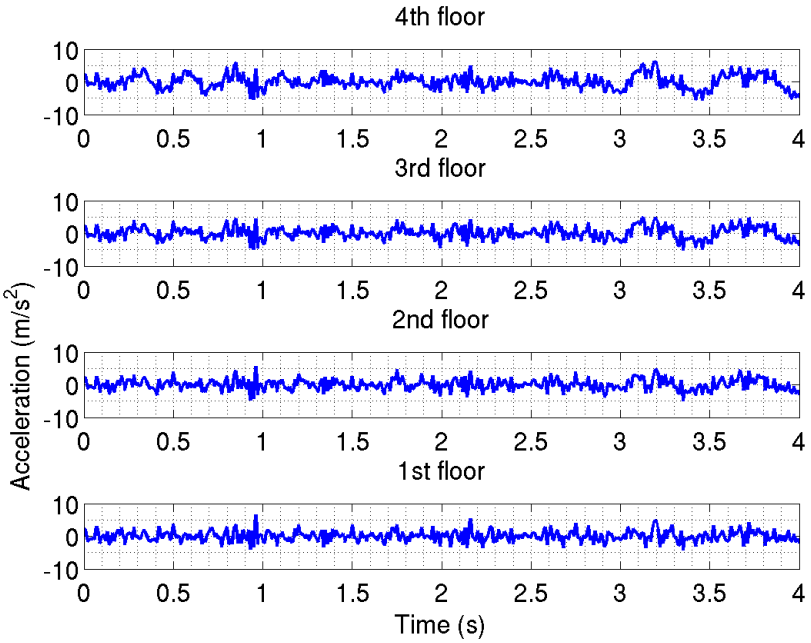


Figure 6.7.3: Horizontal acceleration of each of the four floors (measured data aimed for calibration) used in our hysteretic test problem.

According to Cheung and Prudencio [8], these input values were chosen deliberately so that the excitation a_g did not cause some of the upper floors to enter the nonlinear regime; that is, so that our test inverse problem did not become globally identifiable.

In this section, 400 time-steps are used, as the data is available at instants

$$t_n = (n-1) \times \Delta t, \quad 1 \leq n \leq N_T \equiv 401, \quad \Delta t = 0.01$$

however, Cheung and Prudencio used only 250 time steps [8].

An additive noise is assumed to be present in the measurements; i.e.,

$$y_i(n) = q_i(n) + \varepsilon_i(n), \quad 1 \leq i \leq N_o, \quad 1 \leq n \leq N_T \equiv 401,$$

where $q_i(n; \theta_2, ..., \theta_{15})$ denotes the output at time $t_n = n\Delta t\,(\Delta t = 0.01s)$ at the i-th observed degree of freedom predicted by the proposed structural model, and $y_i(n)$ denotes the corresponding measured output.

They considered a total of 15 unknown parameters $\boldsymbol{\theta} = (\theta_1, ..., \theta_{15})$ and modeled the variables ε_i as independently and identically distributed Gaussian variables with mean zero and some unknown prediction-error variance σ^2. The variance σ^2 is assumed to be the same for all $N_o = 4$ floors. The first component θ_1 is equal to the prediction error variance σ^2 and the other 14 parameters are related to the four triples (k_i, r_i, u_i), $1 \leq i \leq N_o$ (see Fig. 6.7.1), to ρ, and to γ. The likelihood function is given by:

$$f(\boldsymbol{y}|\boldsymbol{\theta}) = \frac{1}{(2\pi\sigma^2)^{N_o N_T/2}} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^{N_o} \sum_{n=1}^{N_T} [y_i(t_n) - q_i(t_n; \theta_2, \ldots, \theta_{15})]^2\right). \tag{6.7.3}$$

An inverse gamma prior was used for $\theta_1 = \sigma^2$, and a 14-dimensional Gaussian prior was used for $\theta_2, ..., \theta_{15}$ with zero mean and diagonal covariance matrix equal to a scaled identity matrix.

6.7.1 Running the Example

To run the executable provided (available after QUESO installation), and generate figures for the chains, KDEs, CDFs, autocorrelation and scatter plots, enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/examples/example
$ rm outputData/*
$ ./example_gsl example_1chain.inp
$ matlab
   $ plot_all.m                          # inside matlab
$ ls -l outputData/*.png
hysteretic_autocorr_thetas.png  hysteretic_kde_theta8.png
hysteretic_cdf_thetas.png       hysteretic_kde_theta9.png
hysteretic_kde_theta1.png       hysteretic_kde_theta10.png
hysteretic_kde_theta2.png       hysteretic_kde_theta11.png
hysteretic_kde_theta3.png       hysteretic_kde_theta12.png
hysteretic_kde_theta4.png       hysteretic_kde_theta13.png
hysteretic_kde_theta5.png       hysteretic_kde_theta14.png
hysteretic_kde_theta6.png       hysteretic_kde_theta15.png
hysteretic_kde_theta7.png       hysteretic_scatter_thetas.png
```

As a result, the user should have created several of PNG figures containing kernel density estimate of the 15 parameters, cumulative density distribution, autocorrelation and scatter plots. The name of the figure files have been chosen to be informative, as shown in the Listing above.

Additional figures may be generated if the user allows the procedure `debug_hyst(` be called by the compiler in Line 11 of file `example_main.C`; in that case, call the function `cpp_gen.m` inside Matlab/Octave.

6.7.2 Example Code

The source code for the example is composed of 5 files: `example_main.C` (Listing 6.68), `example_likelihood.h` and `example_likelihood.C` (Listings 6.69 and 6.70), `example_compute.h` and `example_compute.C` (Listings 6.71 and 6.72), and finally `example_hyst.h` and `example_hyst.C`, which contain the Hysteretic model properly said.

Note that in line 11 of Listings 6.68 the '`#if 1`' directive tells the compiler that the application will call `compute()`, which internally uses QUESO and the Multilevel algorithm. On the contrary, the user may calculate the hysteretic force without uncertainty by changing the directive to '`#if 0`', which can assist the analysis of the resulting data.

```
#include <example_compute.h>

int main(int argc, char* argv[])
{
5  // Initialize environment
#ifdef QUESO_HAS_MPI
  MPI_Init(&argc,&argv);
```

```
  QUESO::FullEnvironment* env =
    new QUESO::FullEnvironment(MPI_COMM_WORLD,argv[1],"",NULL);
#else
  QUESO::FullEnvironment* env =
    new QUESO::FullEnvironment(argv[1],"",NULL);
#endif

  // Compute
#if 1
  compute(*env);
#else
  debug_hyst(*env);
#endif

  // Finalize environment
  delete env;
#ifdef QUESO_HAS_MPI
  MPI_Finalize();
#endif

  return 0;
}
```

Listing 6.68: File `example_main.C`.

```
#ifndef __EX_LIKELIHOOD_H__
#define __EX_LIKELIHOOD_H__

#include <queso/GslMatrix.h>

struct
likelihoodRoutine_DataType
{
  std::vector<std::vector<double>* > floor;
              std::vector<double>    accel;
};

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect);

#endif
```

Listing 6.69: File `example_likelihood.h`.

```
#include <example_likelihood.h>
#include <example_hyst.h>

double likelihoodRoutine(
  const QUESO::GslVector& paramValues,
  const QUESO::GslVector* paramDirection,
  const void*             functionDataPtr,
  QUESO::GslVector*       gradVector,
  QUESO::GslMatrix*       hessianMatrix,
  QUESO::GslVector*       hessianEffect)
{
```

```
const QUESO::BaseEnvironment& env = paramValues.env();
UQ_FATAL_TEST_MACRO(paramValues.sizeLocal() != 15,
                    env.fullRank(),
                    "example_likelihood()",
                    "invalid parameter size");

const std::vector<std::vector<double>* >&
  floor = ((likelihoodRoutine_DataType *) functionDataPtr)->floor;
const std::vector<double>&
  accel = ((likelihoodRoutine_DataType *) functionDataPtr)->accel;

unsigned int numFloors    = floor.size();
unsigned int numTimeSteps = accel.size();

UQ_FATAL_TEST_MACRO((numFloors != 4),
                    env.fullRank(),
                    "example_likelihood()",
                    "invalid 'numFloors'");

UQ_FATAL_TEST_MACRO((numTimeSteps != 401),
                    env.fullRank(),
                    "example_likelihood()",
                    "invalid 'numTimeSteps'");

for (unsigned int i = 0; i < numFloors; ++i) {
  UQ_FATAL_TEST_MACRO(floor[i]->size() != numTimeSteps,
                      env.fullRank(),
                      "example_likelihood()",
                      "invalid number of steps");
}

QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix> floorSpace(env, "floor_", numFloors,
     NULL);

double sigmaSq = paramValues[0];

QUESO::GslVector kVec(floorSpace.zeroVector());
kVec[0] = 2.20e+7 * exp(paramValues[1]);
kVec[1] = 2.00e+7 * exp(paramValues[2]);
kVec[2] = 1.70e+7 * exp(paramValues[3]);
kVec[3] = 1.45e+7 * exp(paramValues[4]);

QUESO::GslVector rVec(floorSpace.zeroVector());
rVec[0] = 1.0e-1 * exp(paramValues[5]);
rVec[1] = 1.0e-1 * exp(paramValues[6]);
rVec[2] = 1.0e-1 * exp(paramValues[7]);
rVec[3] = 1.0e-1 * exp(paramValues[8]);

QUESO::GslVector uVec(floorSpace.zeroVector());
uVec[0] = 8.0e-3 * exp(paramValues[9]);
uVec[1] = 8.0e-3 * exp(paramValues[10]);
uVec[2] = 7.0e-3 * exp(paramValues[11]);
uVec[3] = 7.0e-3 * exp(paramValues[12]);

double rho   = 7.959e-1 * exp(paramValues[13]);

double gamma = 2.500e-3 * exp(paramValues[14]);

std::vector<double> t(numTimeSteps,0.);
QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> u     (floorSpace,numTimeSteps,
    ""); // absolute displacement
QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> ud    (floorSpace,numTimeSteps,
    ""); // velocity
QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> udd   (floorSpace,numTimeSteps,
    ""); // acceleration
```

```
  QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> resfor(floorSpace,numTimeSteps,
      ""); // restoring force
  QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> ru    (floorSpace,numTimeSteps,
      ""); // relative displacement

  QUESO::GslVector massVec(floorSpace.zeroVector());
  massVec.cwSet(2.0e+4);

  hystereticModel(env,
                  massVec,
                  kVec,
                  rVec,
                  uVec,
                  rho,
                  gamma,
                  accel,
                  t, // output
                  u,
                  ud,
                  udd,
                  resfor,
                  ru);

  QUESO::GslVector auxVec(floorSpace.zeroVector());

  double sum = 0.;
  for (unsigned int i = 0; i < numFloors; ++i) {
    for (unsigned int j = 0; j < numTimeSteps; ++j) {
    udd.getPositionValues(j,auxVec);
    sum += ((*floor[i])[j]-auxVec[i]-accel[j])*((*floor[i])[j]-auxVec[i]-accel[j]);
    }
  }

  double result = -0.5*((double) numFloors)*((double) numTimeSteps)*log(2.*M_PI*sigmaSq) -
      0.5*sum/sigmaSq;
  return result;
}
```

Listing 6.70: File `example_likelihood.C`.

```
#ifndef __EX_COMPUTE_H__
#define __EX_COMPUTE_H__

#include <queso/Environment.h>

void compute   (const QUESO::FullEnvironment& env);
void debug_hyst(const QUESO::FullEnvironment& env);

#endif
```

Listing 6.71: File `example_compute.h`.

```
#include <example_compute.h>
#include <example_likelihood.h>
#include <queso/GslMatrix.h>
#include <queso/StatisticalInverseProblem.h>
#include <queso/ConcatenationSubset.h>
#include <queso/ConcatenatedVectorRV.h>
#include <queso/GenericScalarFunction.h>
#include <queso/UniformVectorRV.h>
```

```
#include <sys/time.h>
#include <example_hyst.h>

void compute(const QUESO::FullEnvironment& env) {

  struct timeval timevalNow;
  gettimeofday(&timevalNow, NULL);
  std::cout << std::endl << "Beginning run of 'Hysteretic' example at "
            << ctime(&timevalNow.tv_sec);

  //-----------------------------------------------------
  // Step 1 of 5: Instantiate the parameter space
  //-----------------------------------------------------
  QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix>
    paramSpaceA(env, "paramA_", 1, NULL);
  QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix>
    paramSpaceB(env, "paramB_", 14, NULL);
  QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix>
    paramSpace (env, "param_", 15, NULL);

  //-----------------------------------------------------
  // Step 2 of 5: Instantiate the parameter domain
  //-----------------------------------------------------
  QUESO::GslVector paramMinsA(paramSpaceA.zeroVector());
  paramMinsA.cwSet(0);
  QUESO::GslVector paramMaxsA(paramSpaceA.zeroVector());
  paramMaxsA.cwSet(5);
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomainA("paramA_",paramSpaceA,paramMinsA,paramMaxsA);

  QUESO::GslVector paramMinsB(paramSpaceB.zeroVector());
  paramMinsB.cwSet(-INFINITY);
  QUESO::GslVector paramMaxsB(paramSpaceB.zeroVector());
  paramMaxsB.cwSet( INFINITY);
  QUESO::BoxSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomainB("paramB_",paramSpaceB,paramMinsB,paramMaxsB);

  QUESO::ConcatenationSubset<QUESO::GslVector,QUESO::GslMatrix>
    paramDomain("",paramSpace,paramDomainA,paramDomainB);

  //-----------------------------------------------------
  // Step 3 of 5: Instantiate the likelihood function object
  //-----------------------------------------------------
  std::cout << "\tInstantiating the Likelihood; calling internally the hysteretic model"
      << std::endl;

  likelihoodRoutine_DataType likelihoodRoutine_Data;
  likelihoodRoutine_Data.floor.resize(4,NULL);
  unsigned int numTimeSteps = 401;
  for (unsigned int i = 0; i < 4; ++i) {
    likelihoodRoutine_Data.floor[i] = new std::vector<double>(numTimeSteps,0.);
  }
  likelihoodRoutine_Data.accel.resize(numTimeSteps,0.);
  FILE *inp;
  inp = fopen("an.txt","r");
  unsigned int numObservations = 0;
  double tmpA;
  while (fscanf(inp,"%lf",&tmpA) != EOF) {
    likelihoodRoutine_Data.accel[numObservations] = tmpA;
    numObservations++;
  }

  numObservations=0;
  FILE *inp1_1;
  inp1_1=fopen("measured_data1_1.txt","r");
```

```
while (fscanf(inp1_1,"%lf",&tmpA) != EOF) {
  (*likelihoodRoutine_Data.floor[0])[numObservations]=tmpA;
   numObservations++;
}

numObservations=0;
FILE *inp1_2;
inp1_2=fopen("measured_data1_2.txt","r");
while (fscanf(inp1_2,"%lf",&tmpA) != EOF) {
  (*likelihoodRoutine_Data.floor[1])[numObservations]=tmpA;
  numObservations++;
}

numObservations=0;
FILE *inp1_3;
inp1_3=fopen("measured_data1_3.txt","r");
while (fscanf(inp1_3,"%lf",&tmpA) != EOF) {
  (*likelihoodRoutine_Data.floor[2])[numObservations]=tmpA;
  numObservations++;
}

numObservations=0;
FILE *inp1_4;
inp1_4=fopen("measured_data1_4.txt","r");
while (fscanf(inp1_4,"%lf",&tmpA) != EOF) {
  (*likelihoodRoutine_Data.floor[3])[numObservations]=tmpA;
  numObservations++;
}

QUESO::GenericScalarFunction<QUESO::GslVector,QUESO::GslMatrix>
  likelihoodFunctionObj("like_",
                        paramDomain,
                        likelihoodRoutine,
                        (void *) &likelihoodRoutine_Data,
                        true); // routine computes [ln(function)]

//--------------------------------------------------
// Step 4 of 5: Instantiate the inverse problem
//--------------------------------------------------
std::cout << "\tInstantiating the SIP" << std::endl;

QUESO::UniformVectorRV<QUESO::GslVector,QUESO::GslMatrix>
  priorRvA("priorA_", paramDomainA);

QUESO::GslVector meanVec(paramSpaceB.zeroVector());
QUESO::GslVector diagVec(paramSpaceB.zeroVector());

diagVec.cwSet(0.6*0.6);

QUESO::GslMatrix covMatrix(diagVec);

QUESO::GaussianVectorRV<QUESO::GslVector,QUESO::GslMatrix>
  priorRvB("priorB_", paramDomainB,meanVec,covMatrix);

QUESO::ConcatenatedVectorRV<QUESO::GslVector,QUESO::GslMatrix>
  priorRv("prior_", priorRvA, priorRvB, paramDomain);

QUESO::GenericVectorRV<QUESO::GslVector,QUESO::GslMatrix>
  postRv("post_", paramSpace);

QUESO::StatisticalInverseProblem<QUESO::GslVector,QUESO::GslMatrix>
  ip("", NULL, priorRv, likelihoodFunctionObj, postRv);

//--------------------------------------------------
// Step 5 of 5: Solve the inverse problem
```

```
  //-----------------------------------------------------
  std::cout << "\tSolving the SIP with Multilevel method" << std::endl;

  ip.solveWithBayesMLSampling();

  gettimeofday(&timevalNow, NULL);
  std::cout << "Ending run of 'Hysteretic' example at "
            << ctime(&timevalNow.tv_sec) << std::endl;
  return;
}

//-----------------------------------------------------
//-----------------------------------------------------
//-----------------------------------------------------
void debug_hyst(const QUESO::FullEnvironment& env) {
  unsigned int numFloors = 4;
  unsigned int numTimeSteps = 401;

  std::vector<double> accel(numTimeSteps,0.);
  FILE *inp;
  inp = fopen("an.txt","r");
  unsigned int numObservations = 0;
  double tmpA;
  while (fscanf(inp,"%lf",&tmpA) != EOF) {
    UQ_FATAL_TEST_MACRO((numObservations >= accel.size()),
                        env.fullRank(),
                        "debug_hyst()",
                        "input file has too many lines");
    accel[numObservations] = tmpA;
    numObservations++;
  }
  UQ_FATAL_TEST_MACRO((numObservations != accel.size()),
                      env.fullRank(),
                      "debug_hyst()",
                      "input file has a smaller number of observations than expected");

  QUESO::VectorSpace<QUESO::GslVector, QUESO::GslMatrix> floorSpace(env, "floor_", numFloors,
       NULL);

  QUESO::GslVector kVec(floorSpace.zeroVector());
  kVec[0] = 2.20e+7;
  kVec[1] = 2.00e+7;
  kVec[2] = 1.70e+7;
  kVec[3] = 1.45e+7;

  QUESO::GslVector rVec(floorSpace.zeroVector());
  rVec[0] = 0.1;
  rVec[1] = 0.1;
  rVec[2] = 0.1;
  rVec[3] = 0.1;

  QUESO::GslVector uVec(floorSpace.zeroVector());
  uVec[0] = 0.008;
  uVec[1] = 0.008;
  uVec[2] = 0.007;
  uVec[3] = 0.007;

  double rho   = 7.959e-1 ;//0.1976;
  double gamma = 2.500e-3 ; //0.0038;

  std::vector<double> t(numTimeSteps,0.);
  QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> u     (floorSpace,numTimeSteps,
      ""); // absolute displacement
  QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> ud    (floorSpace,numTimeSteps,
      ""); // velocity
```

```
QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> udd   (floorSpace,numTimeSteps,
    ""); // acceleration
QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> resfor(floorSpace,numTimeSteps,
    ""); // restoring force
QUESO::SequenceOfVectors<QUESO::GslVector,QUESO::GslMatrix> ru    (floorSpace,numTimeSteps,
    ""); // relative displacement

u.setPositionValues     (0,floorSpace.zeroVector());
ud.setPositionValues    (0,floorSpace.zeroVector());
udd.setPositionValues   (0,floorSpace.zeroVector());
resfor.setPositionValues(0,floorSpace.zeroVector());
ru.setPositionValues    (0,floorSpace.zeroVector());

QUESO::GslVector massVec(floorSpace.zeroVector());
massVec.cwSet(2.0e+4);

hystereticModel(env,
                massVec,
                kVec,
                rVec,
                uVec,
                rho,
                gamma,
                accel,
                t, // output
                u,
                ud,
                udd,
                resfor,
                ru);

std::set<unsigned int> auxSet;
auxSet.insert(0);

// Writing some data to the file 'outputData/cpp_output.m'
std::ofstream myFile;
myFile.open ("outputData/cpp_output.m");

// Write 't_cpp'
myFile << "t_cpp = zeros(" << 1 << "," << numTimeSteps << ");\n"
       << "t_cpp = [";
for (unsigned int j = 0; j < numTimeSteps; ++j) {
  myFile << t[j] << " ";
}
myFile << "];" << std::endl;

// Write 'a_cpp'
myFile << "a_cpp = zeros(" << 1 << "," << numTimeSteps << ");\n"
       << "a_cpp = [";
for (unsigned int j = 0; j < numTimeSteps; ++j) {
  myFile << accel[j] << " ";
}
myFile << "];" << std::endl;

QUESO::GslVector auxVec(floorSpace.zeroVector());

// Write 'u_cpp'
myFile << "u_cpp = zeros(" << numFloors << "," << numTimeSteps << ");\n"
       << "u_cpp = [";
for (unsigned int i = 0; i < numFloors; ++i) {
  for (unsigned int j = 0; j < numTimeSteps; ++j) {
    u.getPositionValues(j,auxVec);
    myFile << auxVec[i] << " ";
  }
  myFile << std::endl;
```

```
  }
  myFile << "];" << std::endl;

  // Write 'ud_cpp'
  myFile << "ud_cpp = zeros(" << numFloors << "," << numTimeSteps << ");\n"
         << "ud_cpp = [";
  for (unsigned int i = 0; i < numFloors; ++i) {
    for (unsigned int j = 0; j < numTimeSteps; ++j) {
      ud.getPositionValues(j,auxVec);
      myFile << auxVec[i] << " ";
    }
    myFile << std::endl;
  }
  myFile << "];" << std::endl;

  // Write 'udd_cpp'
  myFile << "udd_cpp = zeros(" << numFloors << "," << numTimeSteps << ");\n"
         << "udd_cpp = [";
  for (unsigned int i = 0; i < numFloors; ++i) {
    for (unsigned int j = 0; j < numTimeSteps; ++j) {
      udd.getPositionValues(j,auxVec);
      myFile << auxVec[i] << " ";
    }
    myFile << std::endl;
  }
  myFile << "];" << std::endl;

  // Write 'resfor_cpp'
  myFile << "resfor_cpp = zeros(" << numFloors << "," << numTimeSteps << ");\n"
         << "resfor_cpp = [";
  for (unsigned int i = 0; i < numFloors; ++i) {
    for (unsigned int j = 0; j < numTimeSteps; ++j) {
      resfor.getPositionValues(j,auxVec);
      myFile << auxVec[i] << " ";
    }
    myFile << std::endl;
  }
  myFile << "];" << std::endl;

  // Write 'ru_cpp'
  myFile << "ru_cpp = zeros(" << numFloors << "," << numTimeSteps << ");\n"
         << "ru_cpp = [";
  for (unsigned int i = 0; i < numFloors; ++i) {
    for (unsigned int j = 0; j < numTimeSteps; ++j) {
      ru.getPositionValues(j,auxVec);
      myFile << auxVec[i] << " ";
    }
    myFile << std::endl;
  }
  myFile << "];" << std::endl;

  myFile.close();

  return;
}
```

Listing 6.72: File `example_compute.C`.

6.7.3 Input File

The options used for solving this example are displayed in Listing 6.73.

```
###############################################
# UQ Environment
###############################################
#env_help                  = anything
env_numSubEnvironments   = 1
env_subDisplayFileName   = outputData/display
env_subDisplayAllowAll   = 0
env_subDisplayAllowedSet = 0
env_displayVerbosity     = 0
env_syncVerbosity        = 0
env_seed                 = 0

###############################################
# Statistical inverse problem (ip)
###############################################
#ip_help                  = anything
ip_computeSolution      = 1
ip_dataOutputFileName   = outputData/sipOutput
ip_dataOutputAllowedSet = 0

###############################################
# 'ip_': information for Multilevel algorithm
###############################################
#ip_ml_help                   = anything
ip_ml_dataOutputFileName   = outputData/sipOutput_ml
ip_ml_dataOutputAllowedSet = 0 1

###############################################
# All levels, unless otherwise specified
###############################################
ip_ml_default_minEffectiveSizeRatio = 0.49
ip_ml_default_maxEffectiveSizeRatio = 0.51
ip_ml_default_rawChain_size = 1000
#ip_ml_default_rawChain_dataOutputFileName = outputData/rawChain_ml
#ip_ml_0_rawChain_dataOutputFileName = outputData/rawChain_ml

#ip_ml_default_scaleCovMatrix                    = 0
#ip_ml_default_dr_maxNumExtraStages              = 2
#ip_ml_default_dr_listOfScalesForExtraStages     = 10. 25.

###############################################
# Last level (level 4 for 'example_gsl' executable)
###############################################
ip_ml_last_dataOutputFileName                 = outputData/sipOutput_ml
ip_ml_last_dataOutputAllowedSet               = 0 1
ip_ml_last_rawChain_size                      = 5000
ip_ml_last_rawChain_computeStats              = 1
ip_ml_last_rawChain_dataOutputFileName        = outputData/rawChain_ml

#ip_ml_last_scaleCovMatrix                     = 0
#ip_ml_last_dr_maxNumExtraStages               = 2
#ip_ml_last_dr_listOfScalesForExtraStages      = 10. 25.

ip_ml_last_rawChain_stats_kde_compute         = 1
ip_ml_last_rawChain_stats_kde_numEvalPositions = 250
ip_ml_last_rawChain_stats_covMatrix_compute   = 1
ip_ml_last_rawChain_stats_corrMatrix_compute  = 1
```

Listing 6.73: Options for QUESO library used in application code (Listings 6.68-6.72).

6.7.4 Create your own Makefile

Similarly to the other examples presented in this user's manual and also available with QUESO distribution, a user-created makefile is available: '`Makefile_hysteretic_violeta`' which may personalized to each user's computer settings and used to compile the code and create the executable `hysteretic_gsl`.

Thus to compile, build and execute the code, commands similar to the following should be entered:

```
$ cd $HOME/LIBRARIES/QUESO-0.56.0/examples/hysteretic/
$ export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:\
  $HOME/LIBRARIES/gsl-1.15/lib/:\
  $HOME/LIBRARIES/boost-1.53.0/lib/:\
  $HOME/LIBRARIES/hdf5-1.8.10/lib:\
  $HOME/LIBRARIES/QUESO-0.56.0/lib
$ make -f Makefile_hysteretic_violeta
$ ./hysteretic_gsl example.inp
```

Again, the '`export`' instruction above is only necessary if the user has not saved the path for the libraries used during QUESO installation in his/her `.bashrc` file.

6.7.5 Data Post-Processing and Visualization

According to the specifications of the input file in Listing 6.73, both a folder named `outputData` and a the following files should be generated:

`rawChain_ml.m`
`display_sub0.txt`

Note that in this hysteretic problem a total of 13 levels are required for the Multilevel method (e.g. see the contents of file `rawChain_ml.m`).

The sequence of Matlab commands is identical to the ones presented in Sections 6.1.5, 6.2.5, 6.3.8 and 6.4.7; therefore, are omitted here. The reader is invited to explore the Matlab files `plot_all.m` and/or `cpp_gen.m`, for details of how the figures have been generated.

6.7.5.1 KDE Plots

Figure 6.7.4 presents the KDE plots of each parameter θ_i, $i = 1, \ldots, 15$. The Multilevel method also provides data about the logarithm of the likelihood function as well as of the target PDF. Figure 6.7.5 presents the KDE plots of both the likelihood function and of its logarithm.

6.7.5.2 Autocorrelation and CDF Plots

Figure 6.7.6a combines the CDF of all parameters θ_i, $i = 1, \ldots, 15$ into a single plot. Figure 6.7.6b presents their autocorrelations.

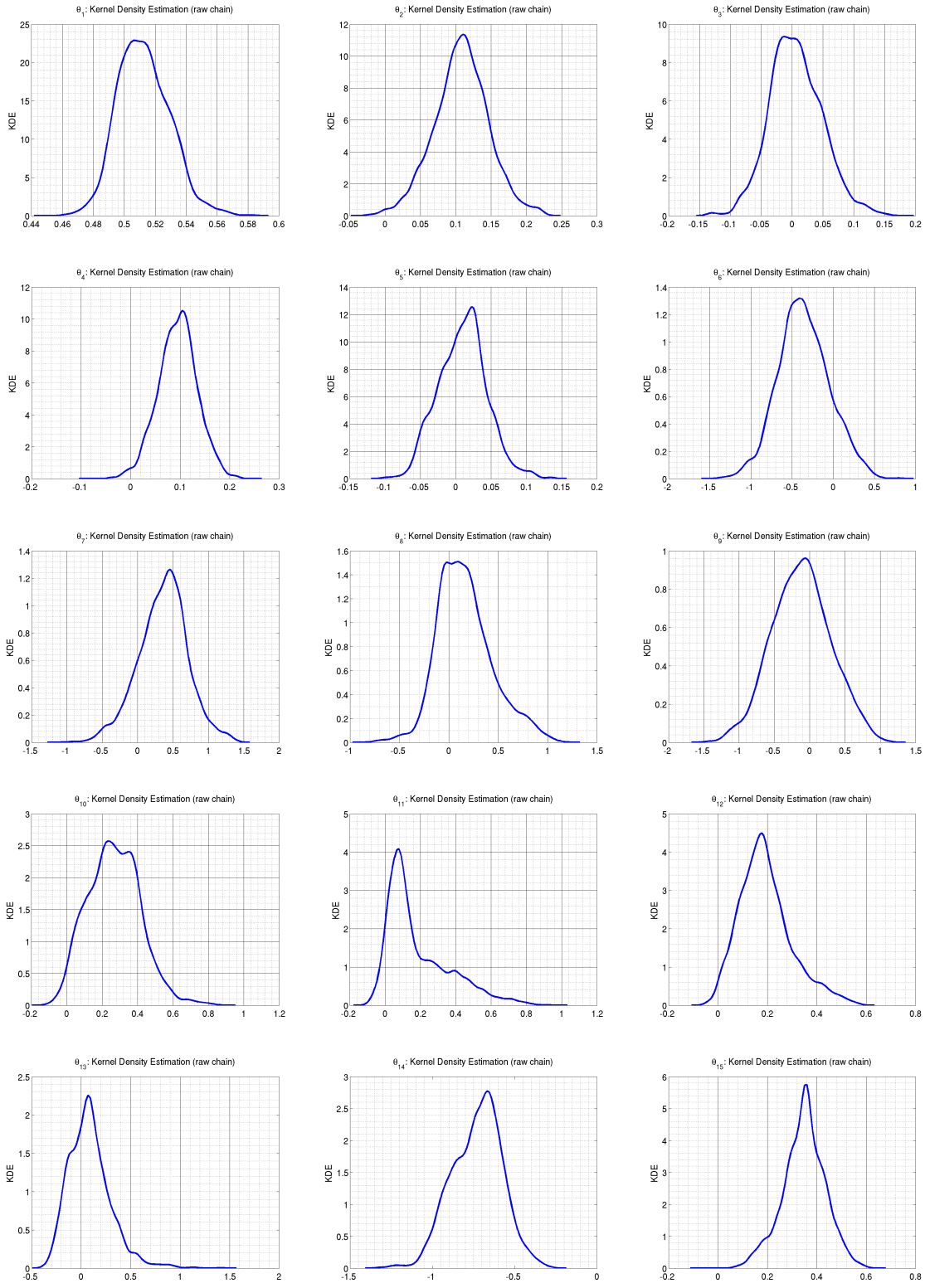
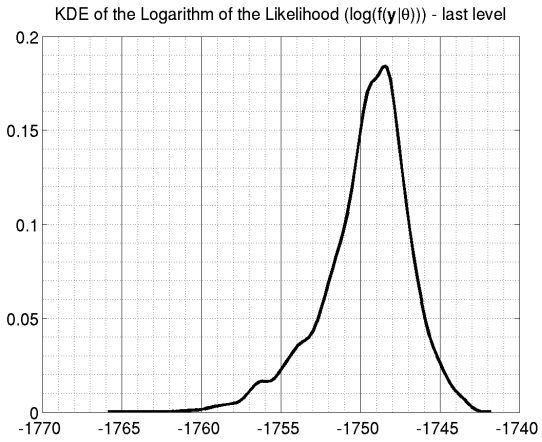
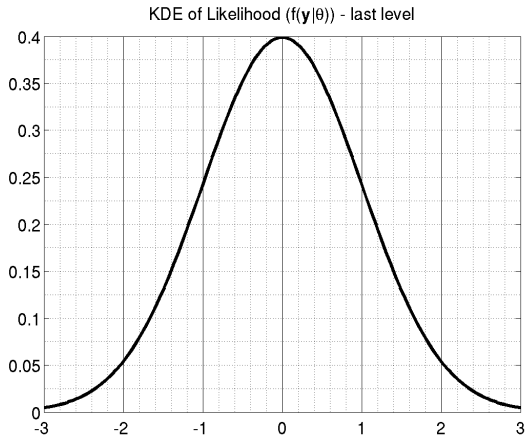


Figure 6.7.4: KDE plots of parameter $\boldsymbol{\theta}$ at the last level.

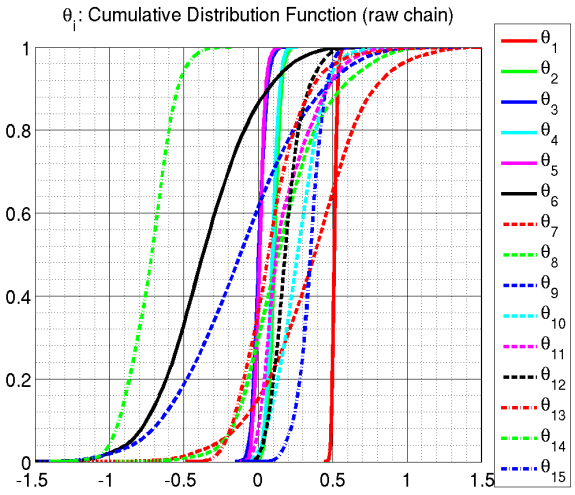


(a) $\log(f(\boldsymbol{y}|\boldsymbol{\theta}))$

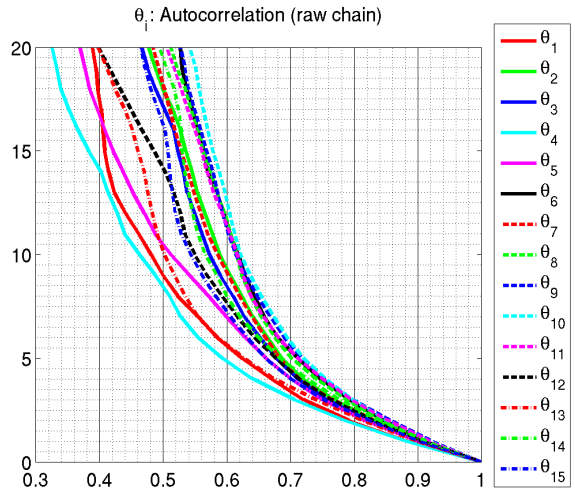


(b) $f(\boldsymbol{y}|\boldsymbol{\theta})$

Figure 6.7.5: KDE plots of the likelihood function, given by Eq. (6.7.3), and of its logarithm, at the last level.



(a) CDF



(b) Autocorrelation

Figure 6.7.6: CDF and autocorrelation plots of parameter $\boldsymbol{\theta}$ at the last level.

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APPENDIX A

Free Software Needs Free Documentation

The following article was written by Richard Stallman, founder of the GNU Project.

The biggest deficiency in the free software community today is not in the software—it is the lack of good free documentation that we can include with the free software. Many of our most important programs do not come with free reference manuals and free introductory texts. Documentation is an essential part of any software package; when an important free software package does not come with a free manual and a free tutorial, that is a major gap. We have many such gaps today.

Consider Perl, for instance. The tutorial manuals that people normally use are non-free. How did this come about? Because the authors of those manuals published them with restrictive terms—no copying, no modification, source files not available—which exclude them from the free software world.

That wasn't the first time this sort of thing happened, and it was far from the last. Many times we have heard a GNU user eagerly describe a manual that he is writing, his intended contribution to the community, only to learn that he had ruined everything by signing a publication contract to make it non-free.

Free documentation, like free software, is a matter of freedom, not price. The problem with the non-free manual is not that publishers charge a price for printed copies—that in itself is fine. (The Free Software Foundation sells printed copies of manuals, too.) The problem is the restrictions on the use of the manual. Free manuals are available in source code form, and give you permission to copy and modify. Non-free manuals do not allow this.

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APPENDIX B

GNU General Public License

Preamble

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For example, on rare occasions, there may be a special need to encourage the widest possible use of a certain library, so that it becomes a de-facto standard. To achieve this, non-free programs must be allowed to use the library. A more frequent case is that a free library does the same job as widely used non-free libraries. In this case, there is little to gain by limiting the free library to free software only, so we use the Lesser General Public License.

In other cases, permission to use a particular library in non-free programs enables a greater number of people to use a large body of free software. For example, permission to use the GNU C Library in non-free programs enables many more people to use the whole GNU operating system, as well as its variant, the GNU/Linux operating system.

Although the Lesser General Public License is Less protective of the users' freedom, it does ensure that the user of a program that is linked with the Library has the freedom and

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