The QUESO Library

User's Manual
Version 0.46.0

Quantification of Uncertainty for Estimation, Simulation, and Optimization (QUESO)

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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.

Disclaimer

Contents

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, since its first version, has been publicly released as open source under the GNU General Public License and is available for free download world-wide. See http://www.gnu.org/licenses/gpl.html for more information on the GPL software use agreement.

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Referencing the QUESO Library

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

```
@incollection{QUESO,
  author    = "Ernesto Prudencio and Karl W. Schulz",
  title     = {The Parallel C++ Statistical Library ‘QUESO’:
               Quantification of Uncertainty for Estimation,
               Simulation and Optimization},
  booktitle = {Euro-Par 2011: Parallel Processing Workshops},
  series    = {Lecture Notes in Computer Science},
  publisher = {Springer Berlin / Heidelberg},
  isbn      = {978-3-642-29736-6},
  keyword   = {Computer Science},
  pages     = {398-407},
  volume    = {7155},
  url       = {http://dx.doi.org/10.1007/978-3-642-29737-3_44},
  year      = {2012}
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   Institution = {Center for Predictive Engineering and Computational Sciences
                  (PECOS), at the Institute for Computational and Engineering
                  Sciences (ICES), The University of Texas at Austin},
   Note        = {in preparation},
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}
```

QUESO Development Team

The QUESO development team currently consists of Paul T. Bauman, Sai Hung Cheung, Kemelli C. Estacio-Hiroms, Damon McDougall, Kenji Miki, Todd A. Oliver, Ernesto E. Prudencio (lead developer), Karl W. Schulz, 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 <u>not</u> 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 [6, 7, 20];
2. Bayes' formula [4, 9, 21, 32];
3. Markov chain Monte Carlo (MCMC) methods [3, 10, 13, 14, 15, 23, 25, 28, 29];
4. Monte Carlo methods [33];
5. Kernel density estimation [34];
6. C++ [22, 26];
7. Message Passing Interface (MPI) [39, 37];
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 [5].

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 [23].

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 [28, 15]) as well as the DRAM [13] (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 [31].

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

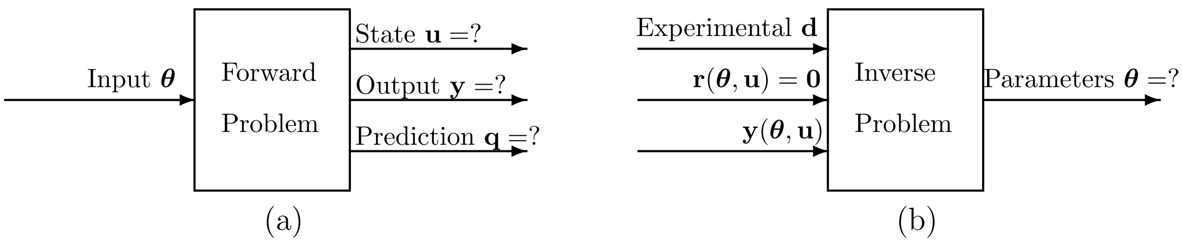


Figure 1.2.1: The representation of (a) a generic forward problem and (b) a generic inverse problem.

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.

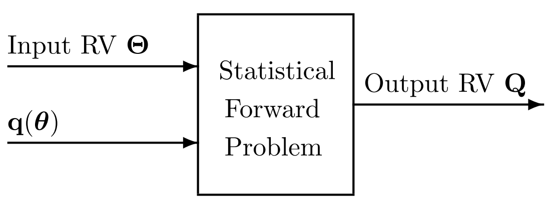


Figure 1.2.2: The representation of a statistical forward problem. $\boldsymbol{\Theta}$ denotes a random variable related to parameters, $\boldsymbol{\theta}$ denotes a realization of $\boldsymbol{\Theta}$ and $\mathbf{Q}$ denotes a random variable related to quantities of interest.

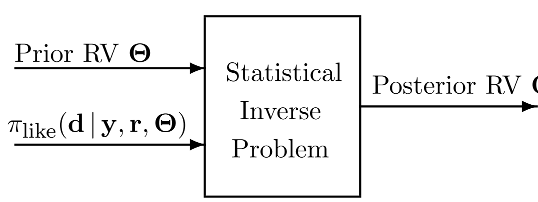


Figure 1.2.3: The representation of a statistical inverse problem. $\boldsymbol{\Theta}$ denotes a random variable related to parameters, $\boldsymbol{\theta}$ denotes a realization of $\boldsymbol{\Theta}$ and $\mathbf{r}$ denotes model equations, $\mathbf{y}$ denotes some model output data and $\mathbf{d}$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

QUESO adopts a Bayesian analysis [23, 32] 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

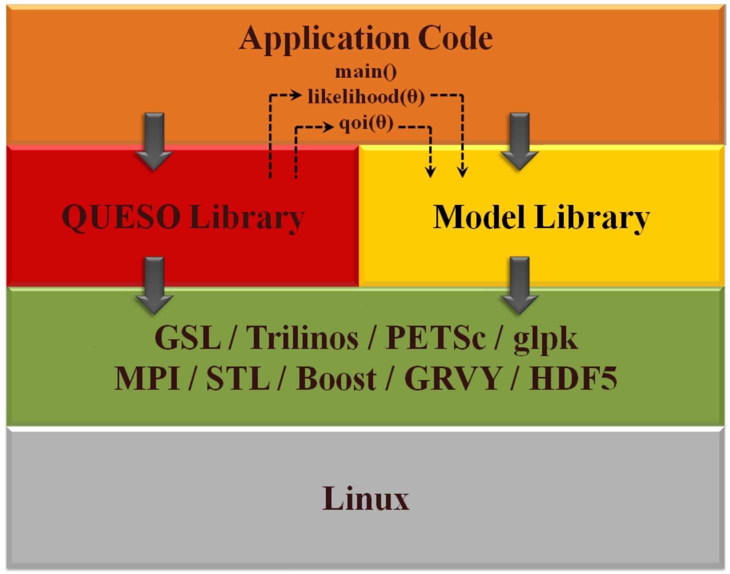


Figure 1.3.1: An application software stack. QUESO requires the input of a likelihood routine $\pi_{\text{like}} : \mathbb{R}^n \to \mathbb{R}_+$ for IPs and of a QoI routine $\mathbf{q} : \mathbb{R}^n \to \mathbb{R}^m$ for FPs. These application level routines provide the bridge between the statistical 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]The parallel capabilities of QUESO have been exercised on the Ranger system of the TACC [2] with up to 16k processors.

CHAPTER 2

Installation

This chapter covers the basic steps that a user will need follow when beginning to use QUESO: how to obtain, configure, 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 his/her application.

This manual is current at the time of printing; however, QUESO library is under active development.

2.1 Pre-QUESO Installation Steps

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

```
$HOME/LIBRARIES/
```

so that you will not need root 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 the QUESO Library: obtain and install QUESO dependencies, and define a number of environmental variables. 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. **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 [19].

2. **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 [8]. The lowest version of GSL required by QUESO is GSL 1.10.

3. **Boost**: Boost provides free peer-reviewed portable C++ source libraries, which can be used with the C++ Standard Library [35]. QUESO requires Boost 1.35.0 or newer.

4. **MPI**: The Message Passing Interface is a standard for parallel programming using the message passing model. E.g. Open MPI [39] or MPICH [37]. 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 [36]. 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 [11]. 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 [27]. 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 [17, 16]. QUESO requires Trilinos release to be newer than or equal to 8.0.7.

The majority of QUESO output files is MATLAB®/GNU Octave compatible [12, 38]. 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

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

For example, under the UNIX C shell (csh) a command of the form

```
$ setenv LD_LIBRARY_PATH \$LD_LIBRARY_PATH:
    $HOME/LIBRARIES/gsl-1.15/lib:
    $HOME/LIBRARIES/boost-1.53.0/lib:
    $HOME/LIBRARIES/grvy-0.32.0/lib
```

can be placed in the user's `.cshrc` or other startup file. Under UNIX bash shell, `.cshrc` is replaced with a startup file such as `.bashrc`, and the command `setenv` with `export`.

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

```
$ setenv CC gcc
$ setenv CXX g++
$ setenv MPICC mpicc
$ setenv MPICXX mpic++
$ setenv F77 f77
$ setenv FC gfortran
```

2.2 Obtaining a Copy of QUESO

The QUESO library is available in the form of a tarball (tar format compressed with gzip), for research collaborators, upon request to Ernesto E. Prudencio (prudenci@ices.utexas.edu).

Suppose you have copied the file '`queso-0.46.0.tar.gz`' into `$HOME/queso_download/`. Then just follow these commands to expand the tarball:

```
$ cd $HOME/queso_download/
$ tar xvf queso-0.46.0.tar.gz
$ cd queso-0.46.0     #enter the directory
```

Naturally, for versions of QUESO other than 0.46.0, 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 [17].

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.

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 a package that is not currently built by default, HDF5, 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, '`--prefix=$HOME/LIBRARIES`'.

The basic steps to configure QUESO using Boost, GSL and HDF5 for installation at '`$HOME/LIBRARIES/QUESO-0.46.0`' are:

```
$ ./configure --prefix=$HOME/LIBRARIES/QUESO-0.46.0 \
  --with-boost=$HOME/LIBRARIES/boost-1.53.0 \
  --with-gsl=$HOME/LIBRARIES/gsl-1.15 \
  --with-hdf5=$HOME/LIBRARIES/hdf5-1.8.10
```

Note: the directory '`$HOME/LIBRARIES/QUESO-0.46.0`' 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-0.46.0/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 [40], and can be regenerated by typing in the build tree:

```
$ make docs
```

A directory named `docs` will be created in `$HOME/queso_download/queso-0.46.0` (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-0.46.0.tar.gz` into `$HOME/queso_download/`. The basic steps to configure QUESO using Boost, GSL and HDF5 for installation at '`$HOME/LIBRARIES/QUESO-0.46.0`' are:

```
$ cd $HOME/queso_download/                    #enter source dir
$ gunzip < queso-0.46.0.tar.gz  | tar xf -
$ cd $HOME/queso_download/queso-0.46.0  #enter the build dir
$ ./configure --prefix=$HOME/LIBRARIES/QUESO-0.46.0 \
  --with-boost=$HOME/LIBRARIES/boost-1.53.0 \
  --with-gsl=$HOME/LIBRARIES/gsl-1.15 \
  --with-hdf5=$HOME/LIBRARIES/hdf5-1.8.10
$ make
$ make check
$ make install
$ make docs
$ ls $HOME/LIBRARIES/QUESO-0.46.0 #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`, with five subdirectories:
   (a) `src/basic/`: with `inc` and `src` subdirectories,
   (b) `src/core/`: with `inc` and `src` subdirectories,
   (c) `src/misc/`: with `inc` and `src` subdirectories,
   (d) `src/stats/`: with `inc` and `src` subdirectories, and
   (e) `src/contrib/`.

The `src` directory contains the QUESO library itself; thus it has an entire chapter dedicated to its description (see Chapter 3).

2. `examples` with six subdirectories:

    (a) `examples/gravity/`
    (b) `examples/infoTheoryProblem/`
    (c) `examples/statisticalForwardProblem/`
    (d) `examples/statisticalInverseProblem/`
    (e) `examples/validationCycle/`
    (f) `examples/validationCycle2/`

    The simplest examples under this directory are: `statisticalInverseProblem` and `statisticalForwardProblem`, which solve a SIP and a SFP, respectively (see Section 2.9). The examples `validationCycle` and `validationCycle2` present a combination of SIP and SFP to solve the same problem; however, the first has the majority of its code in `*.h` files, with templated routines, whereas the latter has the majority of its code in `*.C` files. The `gravity` example is also a combination of a SIP and a SFP, and it is presented in detail in Chapter 5.

    The build directory contains only the source codes. The executables are available under the QUESO installation directory, together with some Matlab files for visualization of the results.

3. `test` with ten subdirectories:

    (a) `test/gsl_tests`
    (b) `test/t01_valid_cycle/`
    (c) `test/t02_sip_sfp/`
    (d) `test/t03_sequence/`
    (e) `test/t04_bimodal/`
    (f) `test_Environment/`
    (g) `test_GaussianVectorRVClass/`
    (h) `test_GslMatrix/`
    (i) `test_GslVector/`
    (j) `test_uqEnvironmentOptions/`

    The executables under `tests` are 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. They 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 §2.1 through §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 the output of it:

```
kemelli@violeta:~/LIBRARIES/QUESO-0.46.0/bin$ ./queso_version
----------------------------------------------------------------
QUESO Library: Version = 0.46.0 (4600)

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
----------------------------------------------------------------
```

2. `lib`: contains the static and dynamic versions of the library. The full to path to this directory, e.g., `$HOME/LIBRARIES/QUESO-0.46.0/bin` should be added to the user's `LD_LIBRARY_PATH` environmental variable in order to use QUESO library with his/her application code.

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.

   The executables under `examples` are examples of application codes that use QUESO to solve either SIP or SFP, or both. Section 2.9 presents the steps for running two of them, `statisticalInverseProblem` and `statisticalForwardProblem`; the user is invited to run them and understand their purpose (the codes are well documented and self-explanatory). The examples `validationCycle` and `validationCycle2` present a combination of SIP and SFP to solve the same problem; the main difference between them is that the first has the majority of its code in `*.h` files, with templated routines, whereas the latter has the majority of its code in `*.C` files. The `gravity` example is also a combination of a SIP and a SFP, and it is presented in detail in Chapter 5.

2.9 Running QUESO Examples

This section assumes that you have successfully executed steps described in Sections 2.1 through 2.5 above. The codes listed in this section are quite self-explanatory and print messages during execution to make clearer which problem they are solving and how.

The two following subsections illustrate how to run the executables provided under the `examples/statisticalInverseProblem/` and `examples/statisticalForwardProblem/`. For the remaining three examples, the steps should be analogous, except for `infoTheoryProblem`, which requires QUESO to be compiled with the ANN library [30].

It is worth noting presence of an argument passed to the executable in the examples. 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.

A complete example of an application that uses QUESO to solve a combination of a SIP and a SFP is in presented in Chapter 5. The chapter presents the mathematical models for both the SIP and SFP, the application code, the options input file and the Makefile to link the code with QUESO library.

2.9.1 A Simple Statistical Inverse Problem

This example is located at `examples/statisticalInverseProblem` and consists of a set of three files to illustrate the use of QUESO library to solve a simple inverse problem with four parameters.

To run the executable provided, enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.46.0/
$ cd examples/statisticalInverseProblem
$ rm outputData/*
$ ./exStatisticalInverseProblem_gsl sip.inp
$ matlab
   $ sip_plot             # inside matlab
   # press the left button of the mouse at each picture displayed
   # by 'sip_plot.m', in order to display the next picture
   $ exit                 # inside matlab
$ ls -l outputData/*.png
>>  parameters_samples_plane.png  parameters_PDF.png
```

As a result, the user should have created a couple of PNG plots for both marginal posterior PDFs of all four parameters and samples of first two parameters on the plane.

2.9.2 A Simple Statistical Forward Problem

This example consists of a set of three files to illustrate the use of QUESO library to solve a simple forward problem and it is located at '`examples/statisticalForwardProblem/`'.

To run the executable provided, enter the following commands:

```
$ cd $HOME/LIBRARIES/QUESO-0.46.0/
$ cd examples/statisticalForwardProblem/
$ rm outputData/*
$ ./exStatisticalForwardProblem_gsl sfp.inp
$ matlab
   $ sfp_plot        # inside matlab
   # press the left button of the mouse at a picture displayed
   # by 'sfp_plot.m', in order to display the next picture
   $ exit            # inside matlab
$ ls -l outputData/*.png
>>  QoI_autocorrelation.png  QoI_CDF.png  QoI_PDF.png
```

In this case, the user should have created a few PNG plots for the QoI kernel density estimation, cumulative distribution function and autocorrelation.

2.10 Create your Application with the Installed QUESO

Prepare your environment by either running or saving the following command in your `.cshrc` file (or `.bashrc` file depending whether you have a C or a bash shell):

```
setenv LD_LIBRARY_PATH \$LD_LIBRARY_PATH:
       $HOME/LIBRARIES/QUESO-0.46.0/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-0.46.0/
BOOST_DIR = $HOME/LIBRARIES/boost-1.53.0/
GSL_DIR = $HOME/LIBRARIES/gsl-1.15/
GRVY_DIR = $HOME/LIBRARIES/grvy-0.32.0/
HDF5_DIR = $HOME/LIBRARIES//hdf5-1.8.10
TRILINOS_DIR = $HOME/LIBRARIES/trilinos-10.12.2
```

```
INC_PATHS = \
  -I. \
  -I$(QUESO_DIR)/include \
  -I$(BOOST_DIR)/include \
  -I$(GSL_DIR)/include \
  -I$(GRVY_DIR)/include \
  -I$(HDF5_DIR)/include \
  -I$(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$(HDF5_DIR)/lib \
  -lhdf5 \
  -L$(TRILINOS_DIR)/lib \
  -lepetra \
  -lteuchos

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 `uqEmptyEnvironmentClass` and `uqFullEnvironmentClass`. 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 `uqVectorSequenceClass` 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`'.

Figure 3.1.1 depicts class diagram for the environment class; and Figure 3.1.2 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: `uqGslVectorClass` and `uqTrilinosVectorClass`. `uqGslVectorClass` is based on the GSL vector structure; whereas `uqTrilinosVectorClass` is based on Trilinos Epetra vector structure.

A class diagram for `uqVectorClass` is presented in Figure 3.1.3; the reader may notice that the diagram also presents an extra class, `uqPetscVectorClass`, in order to show QUESO flexibility to the inclusion of other classes – this class has yet to be implemented.

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

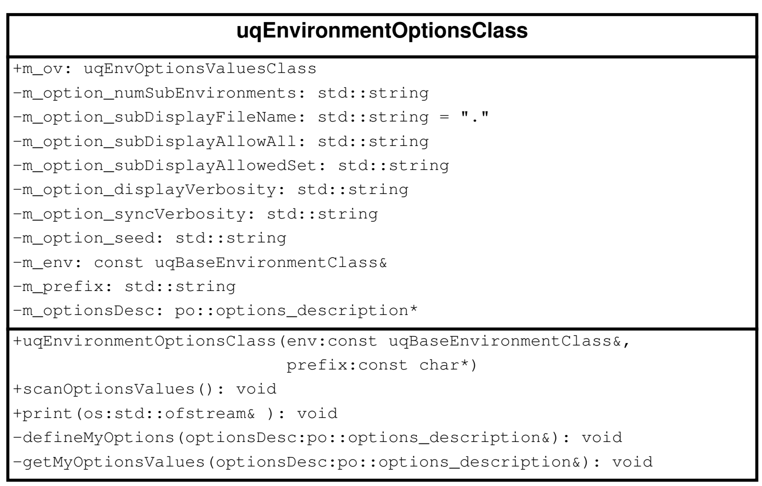


Figure 3.1.2: The environment options class.

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

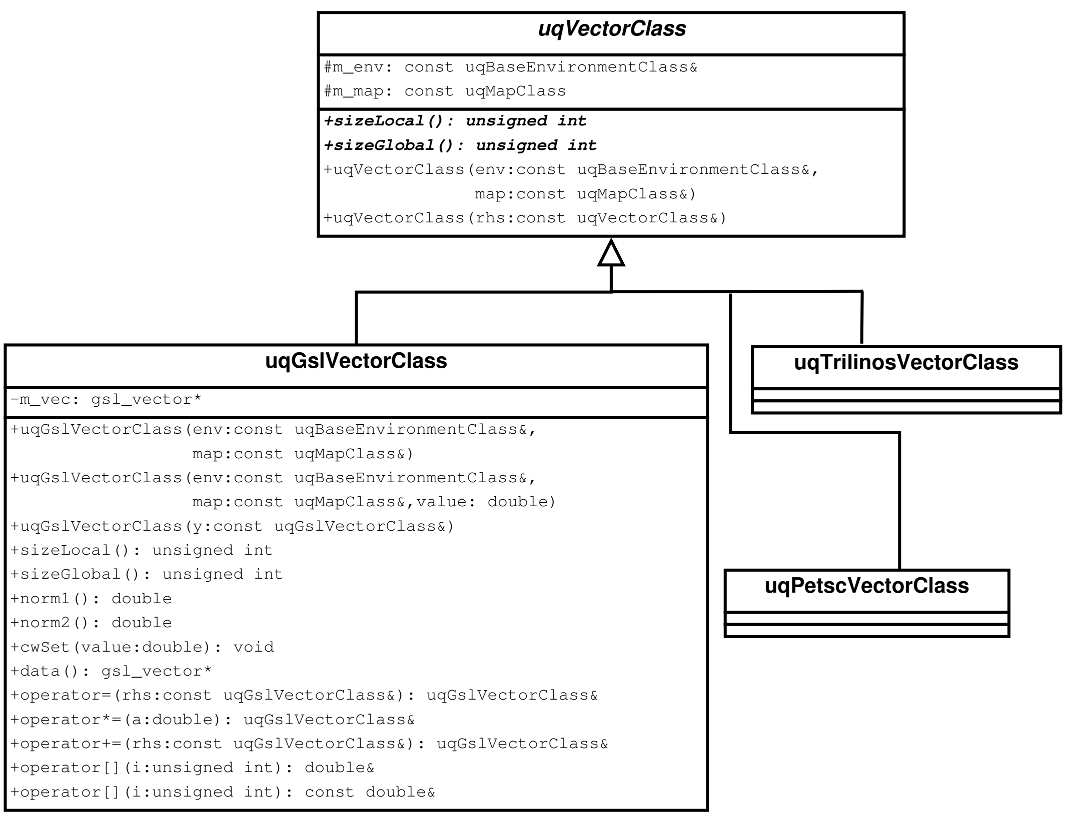


Figure 3.1.3: The class diagram for the vector class described in Section 3.1.2.

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

A class diagram for `uqMatrixClass` is presented in Figure 3.1.4; it displays some of its protected attributed together with some member functions. Again, the diagram displays in some detail the class `uqGslMatrixClass`, it shows without details the other inherited class, `uqTrilinosMatrixClass`, and indicated the possible inclusion of a third class, `uqPetscMatrixClass`.

Figure 3.1.4: The class diagram for the matrix class.

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 `uqVectorSetClass`; subsets, namely `uqVectorSubsetClass`; and vector spaces, namely `uqVectorSpaceClass` 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 `uqIntersectionSubsetClass` 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 `uqUniformJointPdfClass`, `uqGaussianJointPdfClass`, and `uqBayesianJointPdfClass`, respectively. The posterior PDF may be represented within QUESO by `uqGenericJointPdfClass`. 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 specification of the image vector space $\mathbb{R}^m$. The classes representing the vector function class `uqGenericVectorFunctionClass` and `uqConstantVectorFunctionClass` are derived from `uqBaseVectorFunctionClass` and are presented in Diagram 3.2.3

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

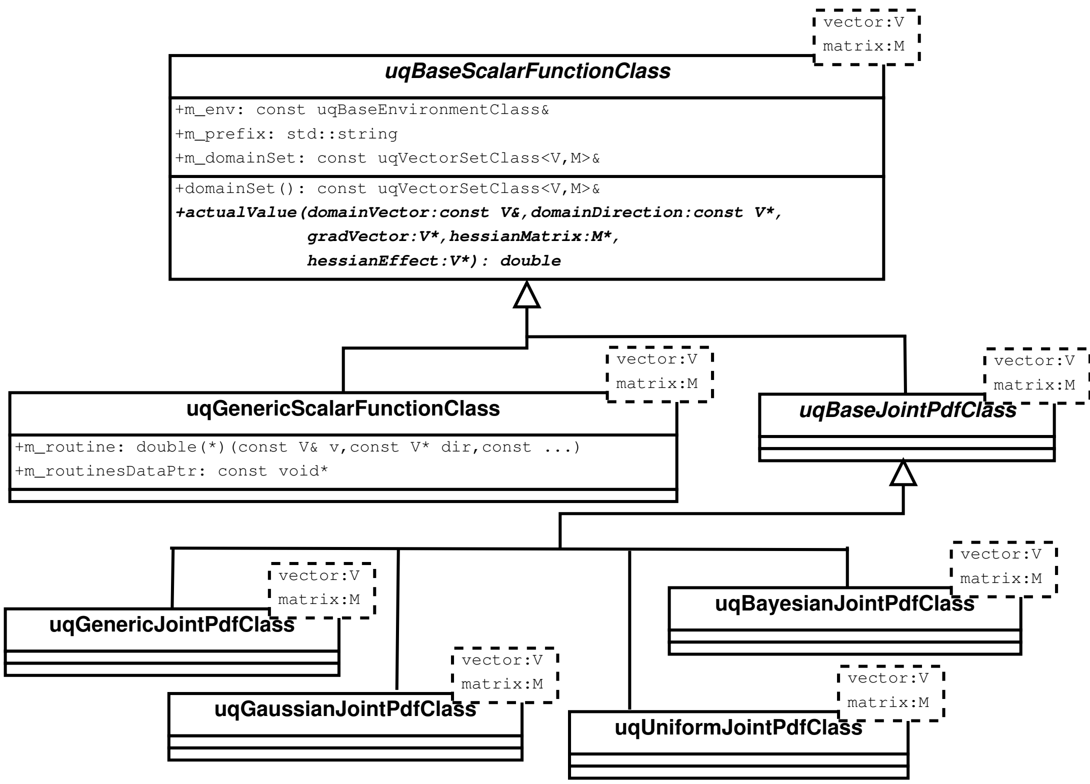


Figure 3.2.2: The class diagram for the scalar function class.

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

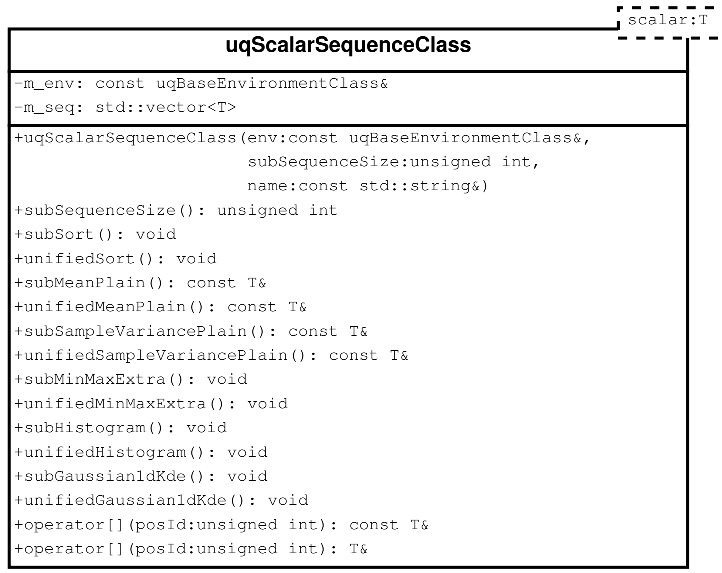


Figure 3.2.4: The class diagram for the scalar sequence class.

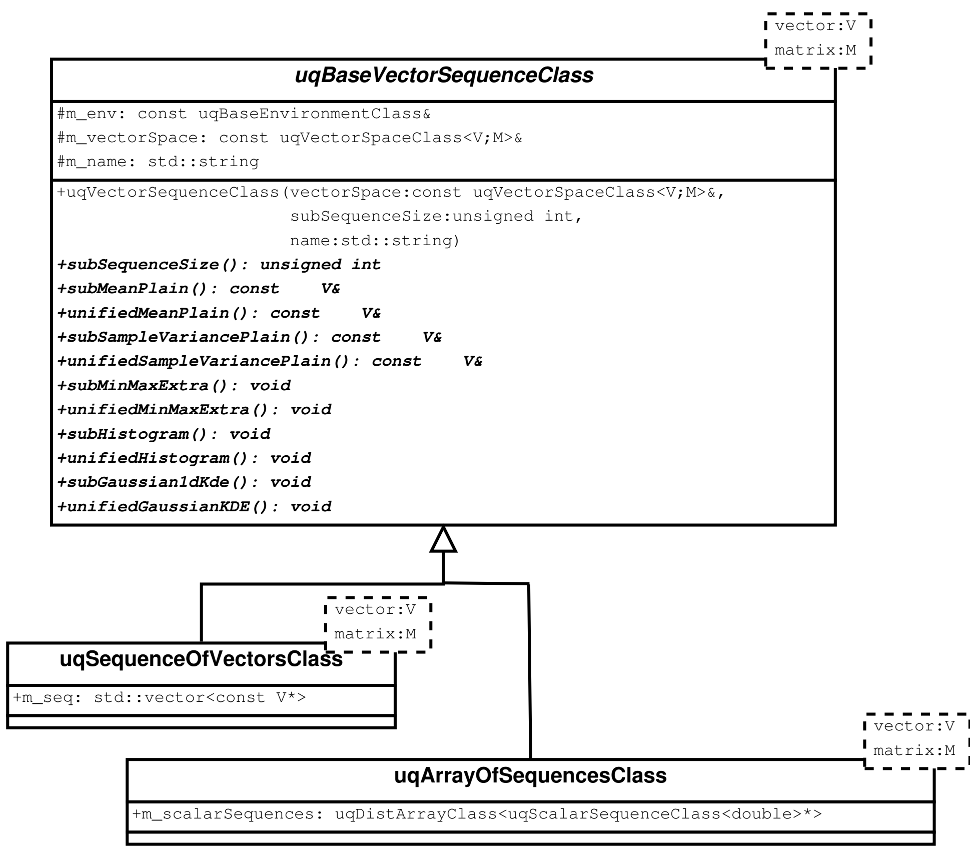


Figure 3.2.5: The class diagram for the vector sequence class.

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 `uqUniformVectorRealizerClass`), Gaussian (`uqGaussianVectorRealizerClass`), Log Normal (`uqLogNormalVectorRealizerClass`), Gamma (`uqGammaVectorRealizerClass`), Inverse Gamma (`uqInverseGammaVectorRealizerClass`) and Beta (`uqBetaVectorRealizerClass`), which are all derived from the base class `uqBaseVectorRealizerClass`.

QUESO conveniently provides the class `uqConcatenatedVectorRealizerClass`, 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 (`uqBaseJointPdfClass` and derived classes, see Section 3.2.2) and vector realizer (`uqBaseVectorRealizerClass` 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 `uqConcatenatedVectorRVClass`).

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.

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 `uqStatisticalInverseProblemClass<P_V,P_M>`, which is illustrated in Figure 3.3.2. One important characteristic of the QUESO design is that it

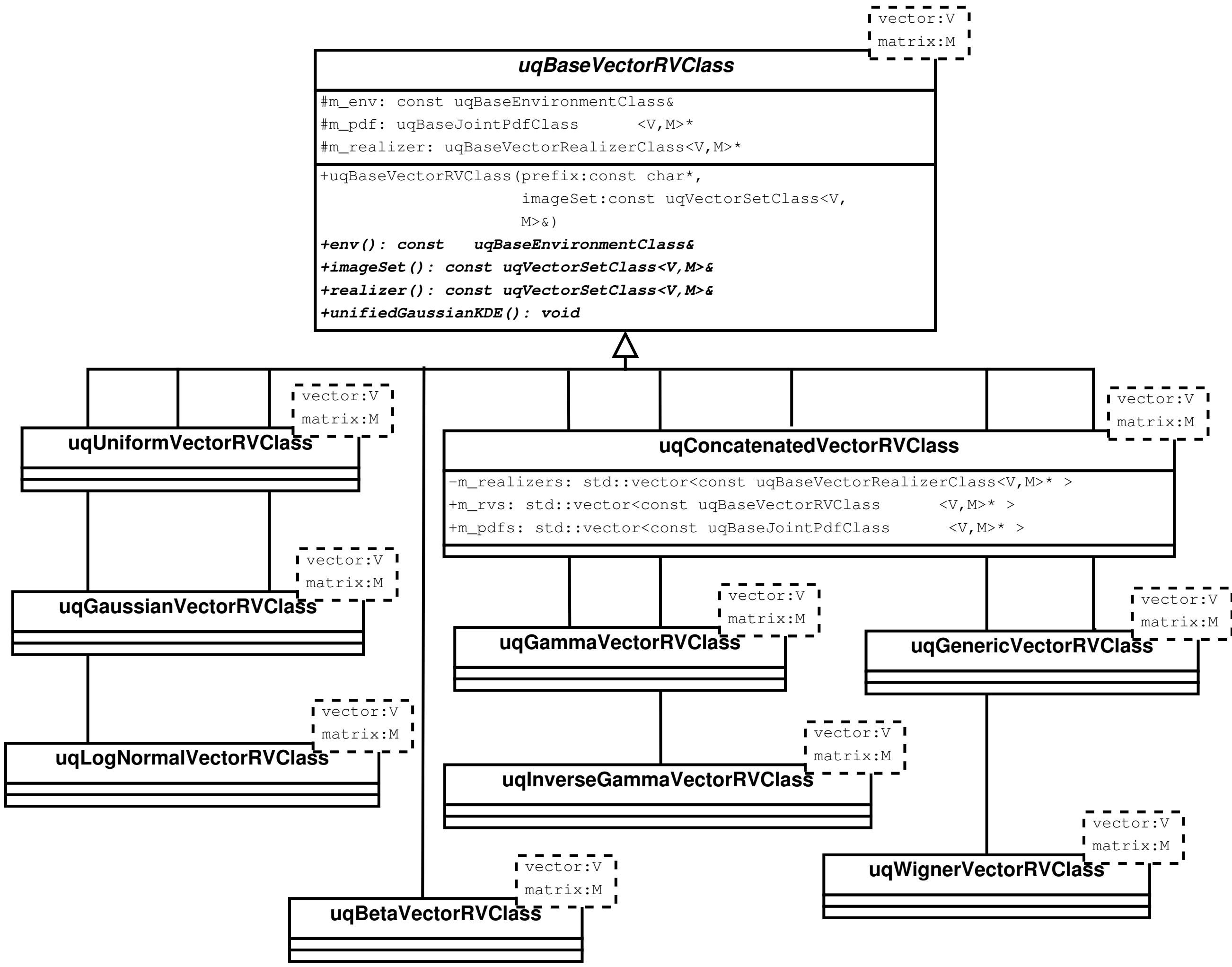


Figure 3.3.1: The class diagram for the vector random variable class.

separates 'what the problem is' from 'how the problem is solved'. The prior and the posterior RV are instances of the `uqBaseVectorRvClass<V,M>` class, while the likelihood function is an instance of the `uqBaseScalarFunctionClass<V,M>` class.

The solution of a SIP is computed by calling the `solveWithBayesMetropolisHastings()` member function of the `uqStatisticalInverseProblemClass<P_V,P_M>` class. Upon return from a solution operation, the posterior RV is available through the `postRv()` member function.

Figure 3.3.3 displays the statistical inverse problem options 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.

```
                                                              param vector:P_V
                                                              param matrix:P_M
uqStatisticalInverseProblemClass
-----------------------------------------------------------------------------
-m_env: const uqBaseEnvironmentClass&
-m_optionsObj: uqStatisticalInverseProblemOptionsClass*
-m_priorRv: const uqBaseVectorRVClass<P_V,P_M>&
-m_likelihoodFunction: const uqBaseScalarFunctionClass <P_V,P_M>&
-m_postRv: uqGenericVectorRVClass<P_V,P_M>&
-m_solutionDomain: uqVectorSetClass<P_V,P_M>*
-m_solutionPdf: uqBaseJointPdfClass<P_V,P_M>*
-m_solutionRealizer: uqBaseVectorRealizerClass<P_V,P_M>*
-m_mhSeqGenerator<P_V,P_M>*: uqMetropolisHastingsSGClass
-m_chain: uqBaseVectorSequenceClass<P_V,P_M>*
-----------------------------------------------------------------------------
+uqStatisticalInverseProblemClass(prefix:const char*,
                                  alternativeOptionsValues:const uqSipOptionsValuesClass*,
                                  priorRv:const uqBaseVectorRVClass<P_V;P_M>&,
                                  likelihoodFunction:const uqBaseScalarFunctionClass<P_V;P_M>&,
                                  postRv:uqGenericVectorRVClass&)
+computeSolutionFlag(): bool
+solveWithBayesMetropolisHastings(alternativeOptionsValues:const uqMhOptionsValuesClass*,
                                  initialValues:const P_V&,
                                  initialProposalCovMatrix:const P_M*): void
+priorRv(): const uqBaseVectorRVClass   <P_V;P_M>&
+postRv(): const uqGenericVectorRVClass<P_V;P_M>&
```

Figure 3.3.2: The statistical inverse problem class. It implements the representation in Figure 1.2.3.

```
uqBaseStatisticalInverseProblemOptionsClass
-----------------------------------------------------------------------------
+m_computeSolution: bool = 1
+m_dataOutputFileName: std::string = "."
+m_dataOutputAllowSet: std::set<unsigned int> = empty
+m_prefix: std::string
-m_env: const uqBaseEnvironmentClass&
-m_optionsDesc: po::options_description*
-----------------------------------------------------------------------------
+uqStatisticalInverseProblemOptionsClass(env:const uqBaseEnvironmentClass&,
                                         prefix:const char*)
+scanOptionsValues(): void
+print(std::ostream& os): void
-defineMyOptions(optionsDesc:po::options_description&): void
-getMyOptionsValues(optionsDesc:po::options_description&): void
```

Figure 3.3.3: The 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 `uqMetropolisHastingsSGClass<P_V,P_M>`, where SG stands for 'Sequence Generator'. This class implements the DRAM algorithm of Haario, Laine, Mira and Saksman [13] together with an operation based on the core routine at the MCMC toolbox for MATLAB [24]. In fact,, the reader may notice that the example available in the QUESO build tree directory `examples/statisticalInverseProblem` is closely related to the 'normal example' in the toolbox.

The Metropolis-Hastings sequence generator class is depicted in Figure 3.3.4; the Metropolis-Hastings sequence generator options class is depicted in Figure 3.3.5; whereas its options are presented in Table 3.3.2.

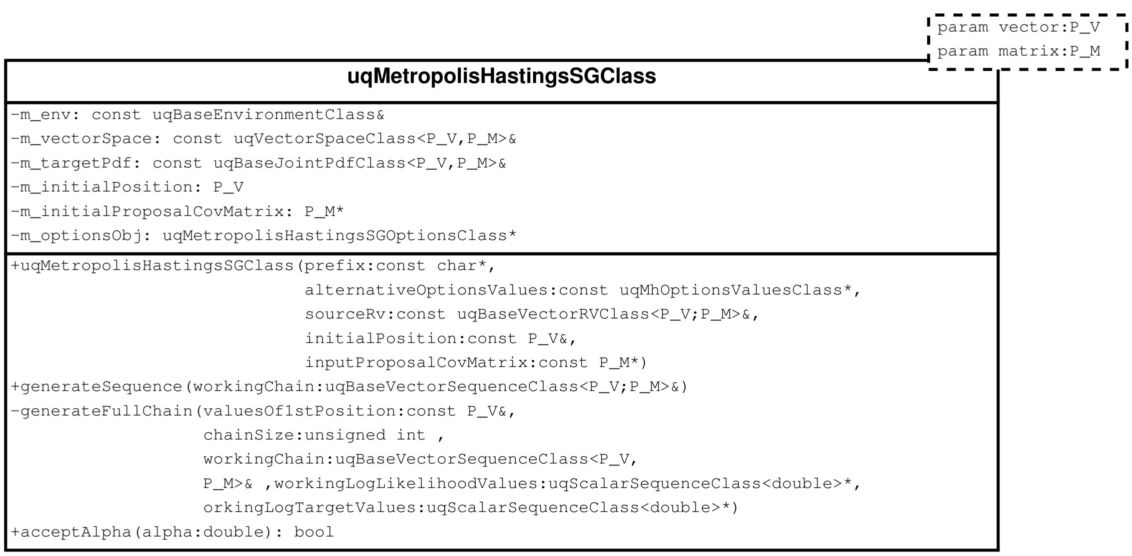


Figure 3.3.4: The Metropolis-Hastings sequence generator class.

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

```
uqMetropolisHastingsSGOptionsClass
-m_env: const uqBaseEnvironmentClass&
-m_optionsDesc: po::options_description*
-m_option_dataOutputFileName: std::string = "."
-m_option_dataOutputAllowedSet: std::string = empty
-m_option_rawChain_size: unsigned int = 100
- m_option_rawChain_displayPeriod: unsigned int = 500
-m_option_rawChain_dataOutputFileName: std::string
-m_option_rawChain_dataOutputAllowedSet: std::string = empty
-m_filteredChainGenerate: std::string
-m_option_filteredChain_discardedPortion: std::string
-m_option_filteredChain_lag: std::string
-m_option_filteredChain_dataOutputFileName: std::string = "."
-m_option_filteredChain_dataOutputAllowedSet: std::string
-m_option_dr_maxNumExtraStages: std::string
-m_option_dr_listOfScalesForExtraStages: std::string
-m_option_am_initialNonAdaptInterval: std::string
-m_option_am_adaptInterval: std::string
-m_option_am_eta: std::string
-m_option_am_epsilon: std::string
+m_prefix: std::string
+m_ov: uqMhOptionsValuesClass
+uqMetropolisHastingsSGOptionsClass(env:const uqBaseEnvironmentClass&,
                                    prefix:const char*)
+scanOptionsValues(): void
+print(os:std::ofstream& ): void
-defineMyOptions(optionsDesc:po::options_description&): void
-getMyOptionsValues(optionsDesc:po::options_description&): void
```

Figure 3.3.5: The Metropolis-Hastings sequence generator options class.

3.3.5 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 `uqStatisticalForwardProblemClass<P_V,P_M,Q_V,Q_M >`, which diagram is presented in Figure 3.3.6. 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 `uqBaseVectorRvClass<P_V,P_M>` class, while the QoI function is an instance of `uqBaseVectorFunctionClass<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 `uqStatisticalForwardProblemClass<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 `'uqBaseVectorRealizerClass<Q_V,Q_M>'`.

Figure 3.3.7 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 3.3.3. In the table, `p-q` stands for parameter–quantity of interest.

```
param vector:P_V
param matrix:P_M
qoi vector:Q_V
qoi matrix:Q_M

uqStatisticalForwardProblemClass
-m_env: const uqBaseEnvironmentClass&
-m_optionsObj: uqStatisticalForwardProblemOptionsClass*
-m_paramRv: const uqBaseVectorRVClass<P_V,P_M>&
-m_qoiFunction: const uqBaseVectorFunctionClass <P_V,P_M,Q_V,Q_M>&
-m_qoiRv: uqGenericVectorRVClass<Q_V,Q_M>&
-m_solutionPdf: uqBaseJointPdfClass<P_V,P_M>*
-m_solutionRealizer: uqBaseVectorRealizerClass<Q_V,Q_M>*
-m_mcSeqGenerator: uqMonteCarloSGClass <P_V,P_M,Q_V,Q_M>*
-m_paramChain: uqBaseVectorSequenceClass<Q_V,Q_M>*
-m_qoiChain: uqBaseVectorSequenceClass<Q_V,Q_M>*

+uqStatisticalForwardProblemClass(prefix:const char*,
                                  alternativeOptionsValues:const uqSfpOptionsValuesClass*,
                                  paramRv:const uqBaseVectorRVClass<P_V;P_M>&,
                                  qoiFunction:const uqBaseVectorFunctionClass<P_V;P_M;Q_V;Q_M>&,
                                  qoiRv:uqGenericVectorRVClass<Q_V;Q_M>&)
+computeSolutionFlag(): bool
+olveWithMonteCarlo(alternativeOptionsValues:const uqMcOptionsValuesClass*): void
+qoiRv(): const uqGenericVectorRVClass<Q_V;Q_M>&
```

Figure 3.3.6: The statistical forward problem class. It implements the representation in Figure 1.2.2.

```
uqStatisticalForwardProblemOptionsClass
+m_prefix: std::string
+m_ov: uqSfpOptionsValuesClass
-m_env: const uqBaseEnvironmentClass&
-m_option_computeSolution: std::string
-m_option_dataOutputFileName: std::string = "."
-m_option_dataOutputAllowedSet: std::string
-m_optionsDesc: po::options_description*

+uqStatisticalForwardProblemOptionsClass(env:const uqBaseEnvironmentClass&,
                                         prefix:const char*)
+scanOptionsValues(): void
+print(os:std::ostream& ): void
-defineMyOptions(optionsDesc:po::options_description&): void
-getMyOptionsValues(optionsDesc:po::options_description&): void
```

Figure 3.3.7: The statistical forward problem options class.

Table 3.3.3: 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

3.3.6 Monte Carlo Solver (and Options)

The templated class that implements a Monte Carlo generator of samples within QUESO is `uqMonteCarloSGClass<P_V,P_M,Q_V,Q_M>`, as illustrated in Figure 3.3.8. 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 3.3.4). Options reading is handled by class `uqMonteCarloOptionsClass`, which is illustrated in Figure 3.3.9.

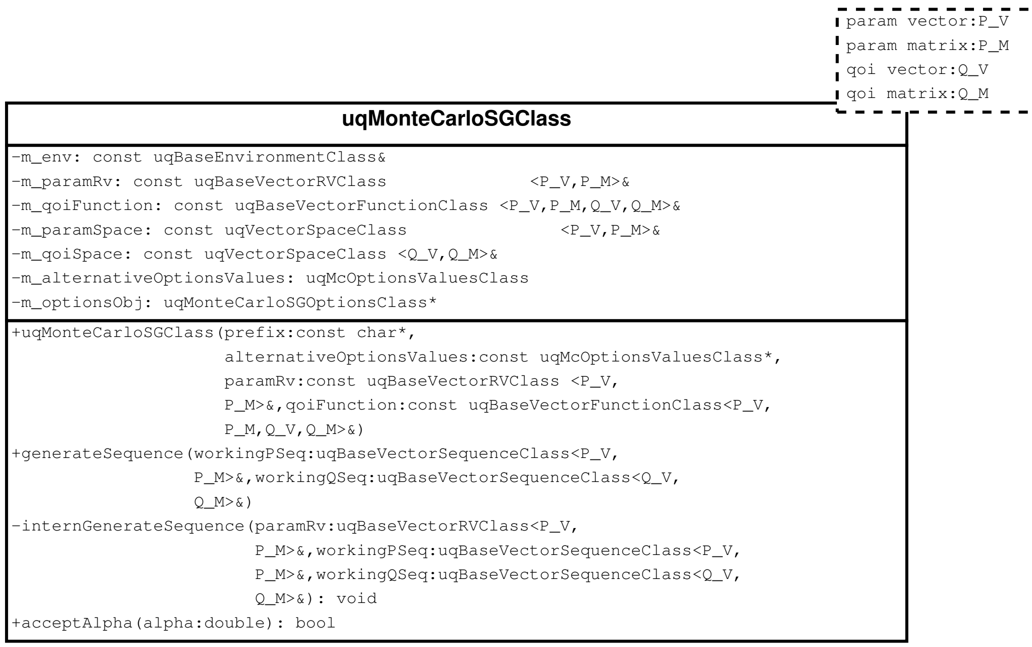


Figure 3.3.8: The Monte Carlo sequence generator class.

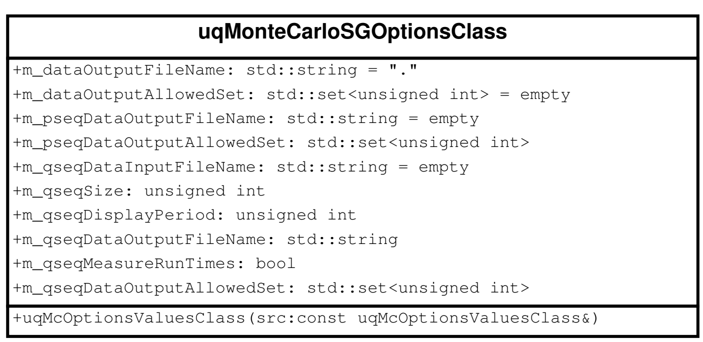


Figure 3.3.9: The Monte Carlo sequence generator options class.

Table 3.3.4: 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 `uqMiscReadDoublesFromString` is used for reading the options input files and assigning the values to the respective variables, in `uqMonteCarloSGOptionsClass::getMyOptionValues` and in `uqMetropolisHastingsSGOptionsClass::getMyOptionValues`.

QUESO class `uqBaseOneDGridClass` generates grids necessary for calculating the CDF of a RV; it is required by class `uqArrayOfOneDGridsClass`, which, in turn, is used in both classes: `uqStatisticalForwardProblemClass` and `uqStatisticalInverseProblemClass`.

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 – 3.3.4). 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` defines 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 [25, 13]. 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 5.4; 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 <u>covariance matrix</u> before calling the DRAM solver, `solveWithBayesMetropolisHastings(...)`, in his/her application code.

It is worth to note that this is rather a DRAM requirement [25], 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 5.3, Section 5.3.

CHAPTER 5

An Application Example

This chapter presents an example of how to use QUESO in order to develop an application that solves a statistical inverse problem and a statistical forward problem, where the solution of the former serves as input to the later.

Section 5.1 gives the mathematical formulation of the statistical inverse problem, and presents the required tools and approach for solving it (experimental data, Bayesian approach, and a short overview of DRAM algorithm). Section 5.2 gives the mathematical formulation of the statistical forward problem, its input RV and QoI function, and indicates the statistical method for its solution, the Monte Carlo algorithm.

Section 5.3 presents the codes that translate the mathematical language into C++ using the QUESO classes and algorithms; Section 5.4 shows the input file that contains a list of options for the Markov chain algorithm (SIP) and the Monte Carlo algorithm (SFP) which will be used by QUESO classes and algorithms. Instructions on how to compile and run the code are presented in Section 5.5. Finally, Section 5.6 shows how to plot figures using Matlab and the output data generated by the application. All the program examples provided in this document are compatible with QUESO 0.46.0.

5.1 A Statistical Inverse Problem

The example described in this section consists of a statistical inverse problem which infers the acceleration due to gravity for an object in free fall near the surface of the Earth. Later, the inferred acceleration of gravity will be used in a statistical forward problem to propagate uncertainty in the calculation the motion of an object in projectile movement.

5.1.1 Mathematical Model for the 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

$$h(t) = -\frac{1}{2}gt^2 + v_0 t + h_0. \tag{5.1.1}$$

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).

5.1.2 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 5.1.1). The data collected, e.g. $\mathbf{d}$, is displayed in Table 5.1.1; the standard deviations, σ's, refer to the uncertainties in the measured times during the experiment execution [1].

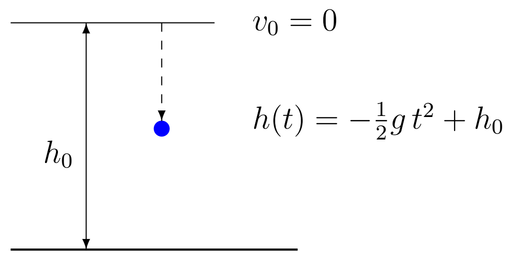


Figure 5.1.1: An object falls from altitude h_0 with zero initial velocity ($v_0 = 0$).

5.1.3 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:

$$\pi_{\text{prior}} = \mathcal{U}(8, 11). \tag{5.1.2}$$

We choose the usual likelihood function:

$$\pi_{\text{like}}(\mathbf{d}|\boldsymbol{\theta}) \propto \exp\left\{-\frac{1}{2}[\mathbf{y}(\boldsymbol{\theta}) - \mathbf{d}]^T [\mathbf{C}(\boldsymbol{\theta})]^{-1} [\mathbf{y}(\boldsymbol{\theta}) - \mathbf{d}]\right\}, \tag{5.1.3}$$

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

Table 5.1.1: 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

Recalling the deterministic model for the acceleration of gravity (5.1.1) with zero initial velocity, the information provided in Table 5.1.1, and Equation (5.1.3); and, additionally, invoking the nomenclature used in Section 1.2, we have:

$$\boldsymbol{\theta} \stackrel{\text{def.}}{=} g, \quad \mathbf{y}(\boldsymbol{\theta}) = \begin{bmatrix} \sqrt{\dfrac{2h_1}{g}} \\ \sqrt{\dfrac{2h_2}{g}} \\ \vdots \\ \sqrt{\dfrac{2h_{n_d}}{g}} \end{bmatrix}, \quad \mathbf{d} = \begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_{n_d} \end{bmatrix}, \quad \mathbf{C}(\boldsymbol{\theta}) = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & \sigma_{n_d}^2 \end{bmatrix}, \tag{5.1.4}$$

where $n_d = 14$ is the number of data points in Table 5.1.1.

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

$$\pi_{\text{post}}(\boldsymbol{\theta}|\mathbf{d}) \propto \pi_{\text{like}}(\mathbf{d}|\boldsymbol{\theta})\, \pi_{\text{prior}}(\boldsymbol{\theta}). \tag{5.1.5}$$

5.1.4 Algorithms for solving the Statistical Inverse Problem

The goal of inference is to characterize the posterior PDF, or to evaluate point or interval estimates based on the posterior [18]. 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 MCMC are: the Metropolis-Hastings (MH) algorithm [28, 15], the Delayed Rejection (DR) algorithm [10, 29], and Adaptive Metropolis (AM) [14] which are combined together in the DRAM algorithm [13].

DRAM, the Delayed Rejection Adaptive Metropolis algorithm, is implemented in QUESO and used to solve the gravity inference problem. There are six variables in the QUESO input file used to set available options for the DRAM algorithm; they are presented and explained in details in Section 5.4.

5.2 A Statistical Forward Problem

In this section we describe a statistical forward problem of predicting the distance traveled by a projectile launched at a given angle and altitude, and using a calibrated magnitude of the acceleration of gravity. This calibrated (inferred) gravity is the Bayesian solution (posterior PDF) of the inverse problem described in Section 5.1.

5.2.1 Mathematical Model for the 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

$$v_x = v_{0x} \tag{5.2.1}$$

$$v_y = v_{0y} - gt \tag{5.2.2}$$

$$x = v_{0x}t \tag{5.2.3}$$

$$h = h_0 + v_{0y}t - \frac{1}{2}gt^2 \tag{5.2.4}$$

where h_0 is the initial height, $x = x(t)$ is the distance traveled by the object, $\mathbf{v_0} = (v_{0x}, v_{0y})$ is the initial velocity, $v_{0x} = v_0 \cos(\alpha)$, $v_{0y} = v_0 \sin(\alpha)$, and $v_0 = \|\mathbf{v_0}\|^2$. Figure 5.2.1 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 5.1.

Since a PDF is assigned to parameter g; thus, the output of the mathematical model (5.2.1) becomes a random variable, thus we have a statistical forward problem.

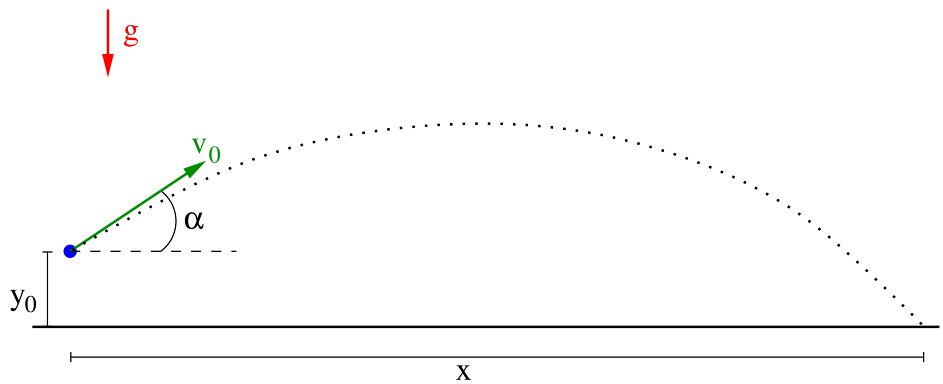


Figure 5.2.1: Object traveling with projectile motion.

5.2.2 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 5.1. 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 5.2.1 and rearranging them, we have that QoI function for x is:

$$x = \frac{v_0 \cos\alpha}{g}\left(v_0 \sin\alpha + \sqrt{(v_0 \sin\alpha)^2 + 2g\, y_0}\right). \tag{5.2.5}$$

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

5.2.3 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 [33].

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.

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.

5.3 Application 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 5.1, 5.2 and 5.3. Two of files specifically handle the SIP: `gravity_likelihood.h`, and `gravity_likelihood.C`, and are displayed in Listings 5.4 and 5.5. Finally, the files specific for the SFP are `gravity_qoi.h` and `gravity_qoi.C`, and they are presented in Listings 5.6 and 5.7.

```
/*------------------------------------------------------------------
 * 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
  MPI_Init(&argc,&argv);
  uqFullEnvironmentClass* env =
    new uqFullEnvironmentClass(MPI_COMM_WORLD,argv[1],"",NULL);

  // Call application
  computeGravityAndTraveledDistance(*env);

  // Finalize QUESO environment
```

```
  delete env;
  MPI_Finalize();

  return 0;
}
```

Listing 5.1: File gravity_main.C.

```
/*------------------------------------------------------------------
 * Brief description of this file:
 *
 * This is the header file for 'gravity_compute.C'.
 *-----------------------------------------------------------------*/

#ifndef __EX_COMPUTE_H__
#define __EX_COMPUTE_H__

#include <uqEnvironment.h>

void computeGravityAndTraveledDistance(const uqFullEnvironmentClass&
   env);

#endif
```

Listing 5.2: File gravity_compute.h.

```
/*------------------------------------------------------------------
 * Brief description of this file:
 *
 * 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.
 * See files 'gravity_likelihood.h' and 'gravity_likelihood.C'.
 *
 * The SFP definition requires a user defined qoi function.
 * See files 'gravity_qoi.h' and 'gravity_qoi.C'.
 *-----------------------------------------------------------------*/

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

```
#include <uqGslMatrix.h>
#include <uqStatisticalInverseProblem.h>
#include <uqStatisticalForwardProblem.h>
#include <sys/time.h>
#include <cmath>

//================================================================
// If PRIOR_IS_GAUSSIAN is defined, then:
// --> Gaussian prior for gravity.
// Otherwise:
// --> Uniform prior for gravity.
//================================================================

//#define PRIOR_IS_GAUSSIAN

void computeGravityAndTraveledDistance(const uqFullEnvironmentClass& 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
  //------------------------------------------------------
  uqVectorSpaceClass<uqGslVectorClass,uqGslMatrixClass> paramSpace(
     env, "param_", 1, NULL);

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

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

  uqBoxSubsetClass<uqGslVectorClass,uqGslMatrixClass>
    paramDomain("param_",
      paramSpace,
      paramMinValues,
      paramMaxValues);

  //------------------------------------------------------
  // SIP Step 3 of 6: Instantiate the likelihood function
  // object to be used by QUESO.
  //------------------------------------------------------
  likelihoodRoutine_DataClass likelihoodRoutine_Data(env);
  uqGenericScalarFunctionClass<uqGslVectorClass,uqGslMatrixClass>
    likelihoodFunctionObj("like_",
        paramDomain,
        likelihoodRoutine,
        (void *) &likelihoodRoutine_Data,
        true); // the routine computes [ln(function)]

  //------------------------------------------------------
  // SIP Step 4 of 6: Define the prior RV
  //------------------------------------------------------

#ifdef PRIOR_IS_GAUSSIAN
```

```
  uqGslVectorClass meanVector( paramSpace.zeroVector() );
  meanVector[0] = 9;

  uqGslMatrixClass covMatrix = uqGslMatrixClass(paramSpace.zeroVector());
  covMatrix(0,0) = 1.;

  // Create a Gaussian prior RV
  uqGaussianVectorRVClass<uqGslVectorClass,uqGslMatrixClass> priorRv("prior_",paramDomain,meanVector,covMatrix);

#else
  // Create an uniform prior RV
  uqUniformVectorRVClass<uqGslVectorClass,uqGslMatrixClass> priorRv("prior_",paramDomain);

#endif

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

  uqStatisticalInverseProblemClass<uqGslVectorClass,uqGslMatrixClass>
    ip("",           // No extra prefix before the default "ip_" prefix
       NULL,
       priorRv,
       likelihoodFunctionObj,
       postRv);

  //------------------------------------------------------
  // SIP Step 6 of 6: Solve the inverse problem, that is,
  // set the 'pdf' and the 'realizer' of the posterior RV
  //------------------------------------------------------
  std::cout << "Solving the SIP with Metropolis Hastings"
      << std::endl << std::endl;

  uqGslVectorClass paramInitials(paramSpace.zeroVector());
  priorRv.realizer().realization(paramInitials);

  uqGslMatrixClass proposalCovMatrix(paramSpace.zeroVector());
```

```
proposalCovMatrix(0,0) = std::pow( fabs(paramInitials[0])/20. , 2.
   );

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.
//================================================================
gettimeofday(&timevalNow, NULL);
std::cout << "Beginning 'SFP -> Projectile motion' at "
          << ctime(&timevalNow.tv_sec)
          << std::endl;

//------------------------------------------------------
// 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.
//------------------------------------------------------
uqVectorSpaceClass<uqGslVectorClass,uqGslMatrixClass> qoiSpace(env,
    "qoi_", 1, NULL);

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

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

//------------------------------------------------------
// SFP Step 3 of 6: Instantiate the qoi function object
// to be used by QUESO.
//------------------------------------------------------
qoiRoutine_DataClass qoiRoutine_Data;
qoiRoutine_Data.m_angle          = M_PI/4.0; //45 degrees (radians)
qoiRoutine_Data.m_initialVelocity= 5.;      //initial speed (m/s)
qoiRoutine_Data.m_initialHeight  = 0.;       //initial height (m)

uqGenericVectorFunctionClass<uqGslVectorClass,uqGslMatrixClass,
   uqGslVectorClass,uqGslMatrixClass>
  qoiFunctionObj("qoi_",
                 paramDomain,
                 qoiSpace,
```

```
                        qoiRoutine,
                        (void *) &qoiRoutine_Data);

  //--------------------------------------------------------
  // SFP Step 4 of 6: Define the input RV
  //--------------------------------------------------------

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

  //--------------------------------------------------------
  // SFP Step 5 of 6: Instantiate the forward problem
  //--------------------------------------------------------
  uqGenericVectorRVClass<uqGslVectorClass,uqGslMatrixClass> qoiRv("qoi_", qoiSpace);

  uqStatisticalForwardProblemClass<uqGslVectorClass,uqGslMatrixClass,
     uqGslVectorClass,uqGslMatrixClass>
    fp("",
       NULL,
       postRv,
       qoiFunctionObj,
       qoiRv);

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

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

```
  }

230   return;
}
```

Listing 5.3: File `gravity_compute.C`. The first part of the code (lines 37–113) handles the statistical forward problem, whereas the second part of the code (lines 115–163) handles the statistical forward problem.

```
 /*------------------------------------------------------------------
 * Brief description of this file:
 *
 * This is the header file for gravity_likelihood.C.
 *-----------------------------------------------------------------*/

#ifndef __GRAVITY_LIKELIHOOD_H__
#define __GRAVITY_LIKELIHOOD_H__

#include <uqGslMatrix.h>

struct likelihoodRoutine_DataClass // user defined class
{
  likelihoodRoutine_DataClass(const uqBaseEnvironmentClass& env);
 ~likelihoodRoutine_DataClass();

  std::vector<double> m_heights; // heights
  std::vector<double> m_times;   // times
  std::vector<double> m_stdDevs; // account for uncertainties in
         // time measurement: sigmas

  const uqBaseEnvironmentClass* m_env;
};

double likelihoodRoutine( // user defined routine
  const uqGslVectorClass& paramValues,
  const uqGslVectorClass* paramDirection,
  const void*             functionDataPtr,
  uqGslVectorClass*       gradVector,
  uqGslMatrixClass*       hessianMatrix,
  uqGslVectorClass*       hessianEffect);

#endif
```

Listing 5.4: File `gravity_likelihood.h`.

```
/*------------------------------------------------------------------
 * Brief description of this file:
 *
 * This file contains the code for the user defined likelihood data
 * class and the user defined likelihood routine.
 *------------------------------------------------------------------*/

#include <gravity_likelihood.h>
#include <cmath>
#include <stdio.h>
#include <fstream>

// Construtor
likelihoodRoutine_DataClass::likelihoodRoutine_DataClass(const
   uqBaseEnvironmentClass& env)
  :
  m_heights(0),
  m_times  (0),
  m_stdDevs(0),
  m_env    (&env)
{
  // 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);
}

// Destructor
likelihoodRoutine_DataClass::~likelihoodRoutine_DataClass()
{
}

//------------------------------------------------------
// The user defined likelihood routine
//------------------------------------------------------
```

```
double likelihoodRoutine(
  const uqGslVectorClass& paramValues,
  const uqGslVectorClass* paramDirection,
  const void*             functionDataPtr,
  uqGslVectorClass*       gradVector,
  uqGslMatrixClass*       hessianMatrix,
  uqGslVectorClass*       hessianEffect)
{
  const uqBaseEnvironmentClass& env = *(((likelihoodRoutine_DataClass
     *) functionDataPtr)->m_env);

  if (paramDirection && functionDataPtr && gradVector &&
     hessianMatrix && hessianEffect)
  {
    // Just to eliminate INTEL compiler warnings
  }

  env.subComm().Barrier();

  // The user, at the application level, should have set
  // the vector 'paramValues' to have size 1.
  UQ_FATAL_TEST_MACRO(paramValues.sizeGlobal() != 1,
                      env.fullRank(),
                      "likelihoodRoutine()",
                      "paramValues vector does not have size 1");

  // Compute likelihood
  double g = paramValues[0];
  const std::vector<double>& heights=((likelihoodRoutine_DataClass*)
     functionDataPtr)->m_heights;
  const std::vector<double>& times  =((likelihoodRoutine_DataClass*)
     functionDataPtr)->m_times;
  const std::vector<double>& stdDevs=((likelihoodRoutine_DataClass*)
     functionDataPtr)->m_stdDevs;

  double misfitValue = 0.;
  for (unsigned int i = 0; i < heights.size(); ++i) {
    double modelTime = sqrt(2.0 * heights[i]/g);
    double ratio = (modelTime - times[i])/stdDevs[i];
    misfitValue += ratio*ratio;
  }
  return (-0.5*misfitValue);
}
```

Listing 5.5: File gravity_likelihood.C.

```
/*------------------------------------------------------------------
 * Brief description of this file:
 *
 * This is the header file from gravity_qoi.C.
 *-----------------------------------------------------------------*/

#ifndef __GRAVITY_QOI_H__
#define __GRAVITY_QOI_H__

#include <uqGslMatrix.h>
#include <uqDistArray.h>

struct
qoiRoutine_DataClass
{
  double m_angle;
  double m_initialVelocity;
  double m_initialHeight;
};

void
qoiRoutine(
  const uqGslVectorClass&                     paramValues,
  const uqGslVectorClass*                     paramDirection,
  const void*                                 functionDataPtr,
        uqGslVectorClass&                     qoiValues,
        uqDistArrayClass<uqGslVectorClass* >* gradVectors,
        uqDistArrayClass<uqGslMatrixClass* >* hessianMatrices,
        uqDistArrayClass<uqGslVectorClass* >* hessianEffects);

#endif
```

Listing 5.6: File gravity_qoi.h.

```
/*------------------------------------------------------------------
 * Brief description of this file:
 *
 * This file contains the code for the user defined qoi routine.
 *-----------------------------------------------------------------*/

#include <gravity_qoi.h>
#include <cmath>

//-----------------------------------------------------
```

```
/// The actual (user-defined) qoi routine
//------------------------------------------------------
void
qoiRoutine(
  const uqGslVectorClass&                          paramValues,
  const uqGslVectorClass*                          paramDirection,
  const void*                                      functionDataPtr,
        uqGslVectorClass&                          qoiValues,
        uqDistArrayClass<uqGslVectorClass*>* gradVectors,
        uqDistArrayClass<uqGslMatrixClass*>* hessianMatrices,
        uqDistArrayClass<uqGslVectorClass*>* hessianEffects)
{
  const uqBaseEnvironmentClass& env = paramValues.env();

  if (paramDirection &&
      gradVectors    &&
      hessianEffects &&
      hessianMatrices) {
    // Logic just to avoid warnings from INTEL compiler
  }

  // The user, at the application level, should have set
  // the vector 'paramValues' to have size 1 and
  // the vector 'qoiValues' to have size 1.
  UQ_FATAL_TEST_MACRO(paramValues.sizeGlobal() != 1,
                      env.fullRank(),
                      "qoiRoutine()",
                      "paramValues vector does not have size 1");

  UQ_FATAL_TEST_MACRO(qoiValues.sizeGlobal() != 1,
                      env.fullRank(),
                      "qoiRoutine()",
                      "qoiValues vector does not have size 1");

  // Compute qoi(s)
  double g = paramValues[0]; // Sample of the RV 'gravity
     acceleration'
  double distanceTraveled = 0.;
  if (env.subRank() == 0) {
    double velocity = ((qoiRoutine_DataClass *) functionDataPtr)->
       m_initialVelocity;
    double heights  = ((qoiRoutine_DataClass *) functionDataPtr)->
       m_initialHeight;
    double alpha    = ((qoiRoutine_DataClass *) functionDataPtr)->
       m_angle;
```

```
    double aux        = velocity * sin(alpha);
    distanceTraveled = (velocity * cos(alpha) / g) * ( aux + sqrt(pow
       (aux,2) + 2.*g*heights) );
  }

  qoiValues[0] = distanceTraveled;

  return;
}
```

Listing 5.7: File `gravity_qoi.C`.

5.4 Application 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 most relevant options of an input file for the solution of a SIP using QUESO are displayed in Listing 5.8. 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`);

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.

```
###############################################
# UQ Environment
###############################################
env_numSubEnvironments   = 1 #or 8, if 8 processors can be used in a
   parallel run;  see Section 5.5.1
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 5.8: Some options for QUESO library used in application code (Listings 5.1-5.5).

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`).

5.5 Application Compilation and Run

Makefiles are special format files that together with the make utility will help one to compile and automatically build and manage projects (programs). Listing 5.9 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).

```
############################################################
# Using installed QUESO 0.46.0, from tarball, in 'violeta'
############################################################
```

```
QUESO_DIR = /home/kemelli/LIBRARIES/QUESO-0.46.0
BOOST_DIR = /home/kemelli/LIBRARIES/boost-1.53.0
GSL_DIR  =  /home/kemelli/LIBRARIES/gsl-1.15
HDF5_DIR  = /home/kemelli/LIBRARIES/hdf5-1.8.10

INC_PATHS = \
  -I. \
  -I$(QUESO_DIR)/include \
  -I$(BOOST_DIR)/include \
  -I$(GSL_DIR)/include \
  -I$(HDF5_DIR)/include

LIBS = \
  -L$(QUESO_DIR)/lib \
  -lqueso \
  -L$(BOOST_DIR)/lib \
  -lboost_program_options \
  -L$(GSL_DIR)/lib \
  -lgsl \
  -L$(HDF5_DIR)/lib \
  -lhdf5

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 5.9: Makefile for the application code in Listings 5.1-5.5

Suppose the user either does not needto modify the Makefile presented in Listings 5.9 or has already done so. Then, in order to compile, build and run the application code together with its input file `gravity_inv_fwd.inp`, presented in Listing 5.8, the user simply needs to enter following commands, under QUESO build tree:

```
cd $HOME/queso_download/queso-0.46.0/examples/gravity/src
make -f Makefile_example_violeta
cd ../tests/test_2013_01_22
../../src/gravity_gsl gravity_inv_fwd.inp
```

Alternatively, if the user is not interested in re-compiling and and building the code, he/she can simply run the executable created during QUESO installation, and, thus, located at QUESO installation tree:

```
cd $HOME/LIBRARIES/QUESO-0.46.0/examples/gravity
./gravity_gsl gravity_inv_fwd.inp
```

In either case, the console output of the program is:

```
kemelli@violeta:~/LIBRARIES/QUESO-0.46.0/examples/gravity$ ./
   gravity_gsl gravity_inv_fwd.inp
--------------------------------------------------------------------
QUESO Library: Version = 0.46.0 (4600)

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-0.46.0/examples/gravity$
```

Listing 5.10: Console output of program `gravity_gsl`

5.5.1 Application Run with Several Processors

Even though the application described in Section 5.3 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 5.8) and enter the following command lines:

```
cd $HOME/LIBRARIES/QUESO-0.46.0/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).

5.6 Application Results

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 5.3, and shows how to use Matlab for the post-processing of such results.

According to the specifications of the input file in Listing 5.8, both a folder named `outputData` and a the following files should be generated:

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

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 5.8, 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.

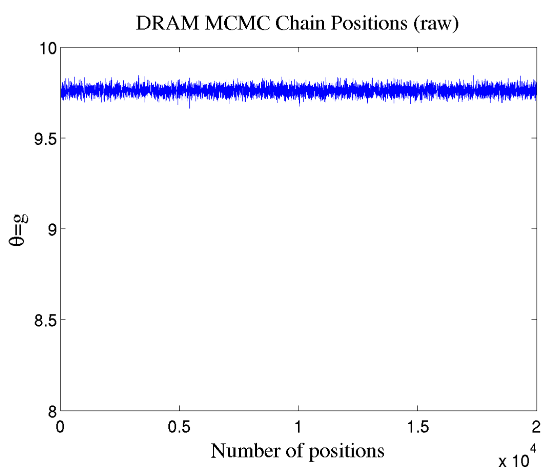
5.6.1 Statistical Inverse Problem

5.6.1.1 Chain Plots

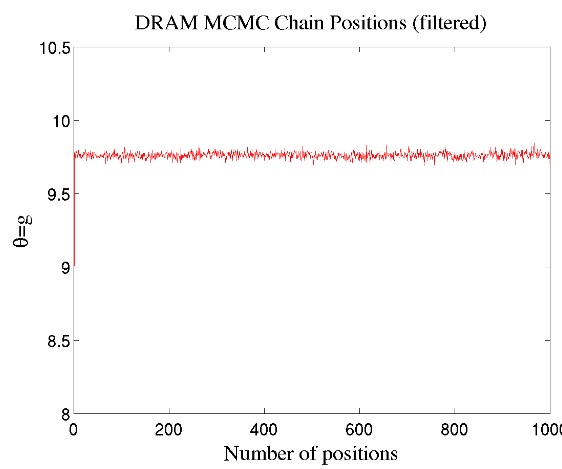
It is quite simple to plot, using Matlab, the chain of positions used in the DRAM algorithm implemented within QUESO. The sequence of Matlab commands presented in Listing 5.11 generates the graphic depicted in Figure 5.1(a). Figure 5.1(b) is obtained analogously.

```
% 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 5.11: Matlab code for the chain plot.



(a) Raw chain



(b) Filtered chain

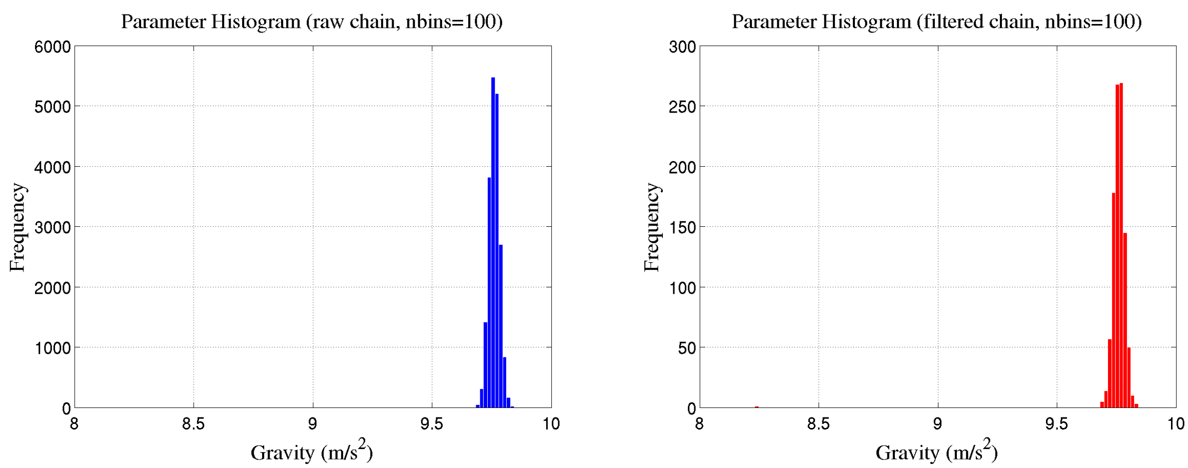
Figure 5.6.1: MCMC raw chain with 20000 positions and a filtered chain with lag of 20 positions.

5.6.1.2 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 5.12: Matlab code for the histogram plot.



(a) Raw chain (b) Filtered chain

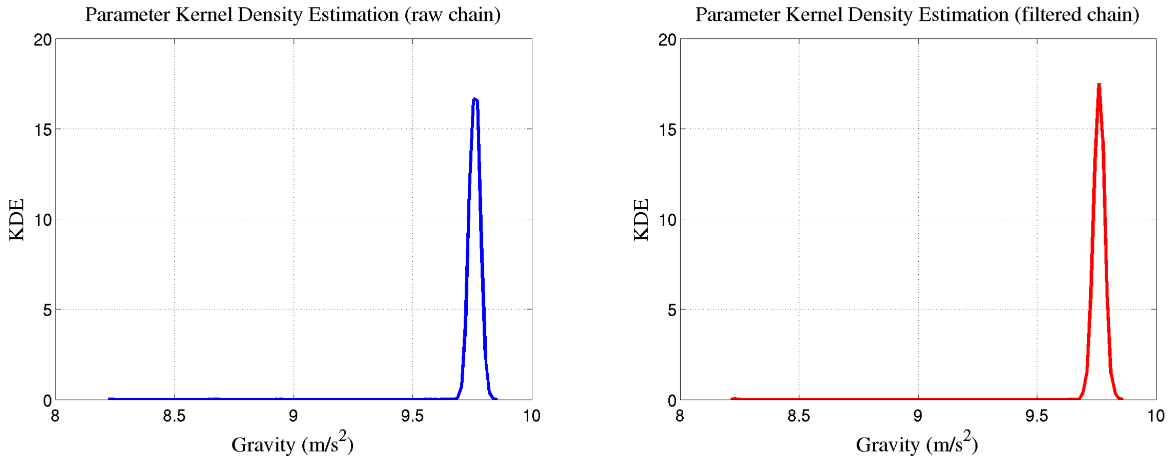
Figure 5.6.2: Histograms of parameter $\theta = g$.

5.6.1.3 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 5.13: Matlab code for the KDE plot.



(a) Raw chain

(b) Filtered chain

Figure 5.6.3: Kernel Density Estimation.

5.6.1.4 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.

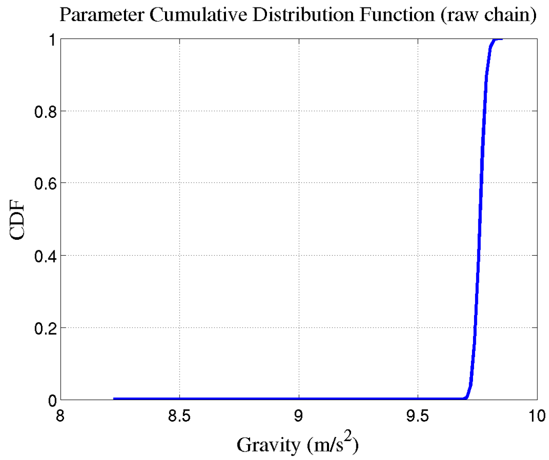
```
% inside Matlab
>> sip_gravity_raw_chain
>> [f,xi] = ksdensity(ip_mh_rawChain_unified,'function','cdf');
>> plot(xi,f,'-b','linewidth',3)
>> title('Parameter Cumulative Distribution Function','fontsize',20);
>> xlabel('Gravity (m/s^2)','fontsize',20);
>> ylabel('CDF','fontsize',20);
>> grid on;
```

Listing 5.14: Matlab code for the CDF plot.

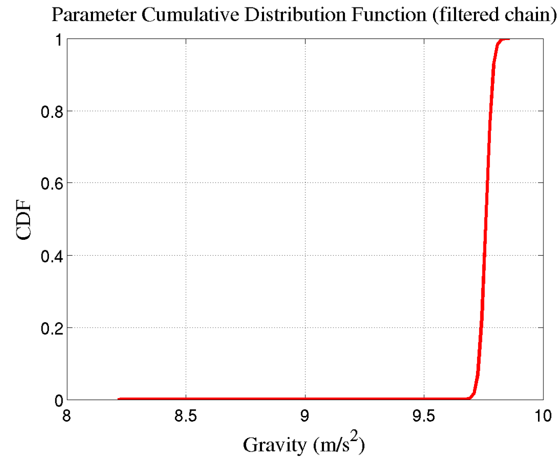
5.6.1.5 Autocorrelation Plots

The code presented in Listing 5.15 uses matlab function **autocorr** to generate Figure 5.6.5 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);
```



(a) Raw chain



(b) Filtered chain

Figure 5.6.4: Cumulative Distribution Function.

```
>> ylabel('Autocorrelation for \theta=g','fontsize',20);
>> xlabel('Lag','fontsize',20);
>> title('Parameter Autocorrelation','fontsize',20);
>> grid on;
>> h=legend('raw chain','filtered chain','location','northeast');
>> set(h,'fontsize',16);
```

Listing 5.15: Matlab code for the autocorrelation plots.

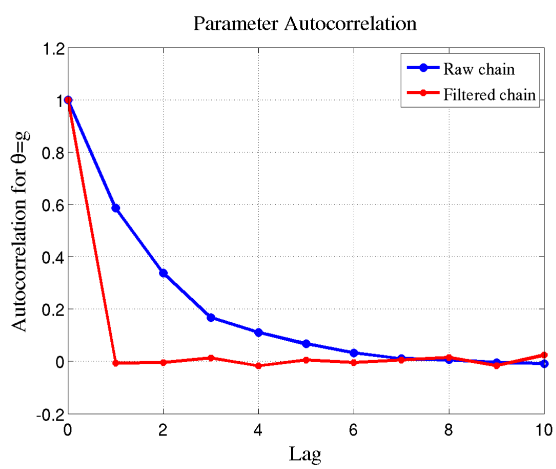


Figure 5.6.5: Autocorrelation plots.

5.6.1.6 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 5.16: Matlab code for finding the covariance matrix.

5.6.2 Statistical Forward Problem

5.6.2.1 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.

```
% 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 5.17: Matlab code for the chain plot.

5.6.2.2 Histogram Plots

In order to plot a histogram of the QoI, you may use the pre-defined Matlab function `hist`.

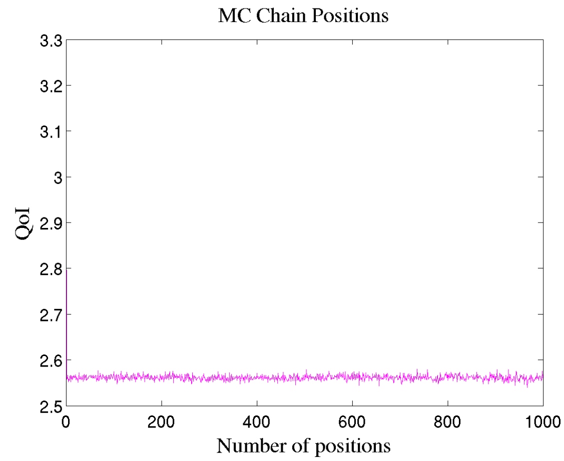


Figure 5.6.6: MC chain positions for the QoI.

```
>> 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 5.18: Matlab code for the QoI histogram plot.

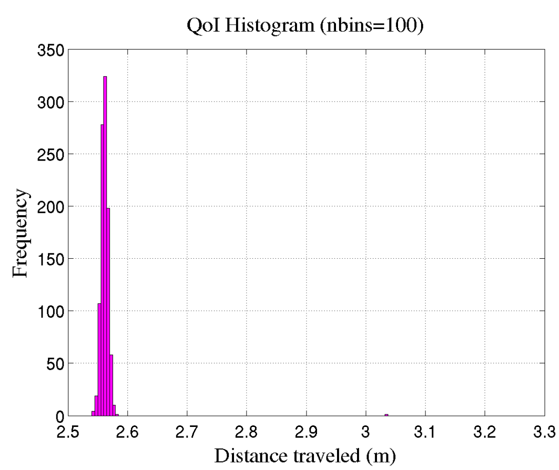


Figure 5.6.7: Histogram of QoI $= d$.

5.6.2.3 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.

```
% 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 5.19: Matlab code for the QoI KDE plot.

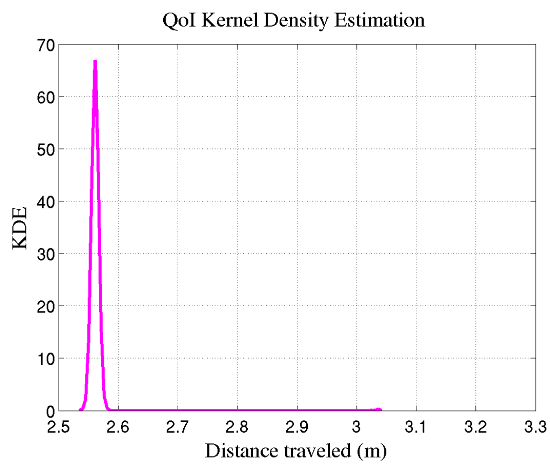


Figure 5.6.8: Kernel Density Estimation.

5.6.2.4 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.

```
% 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 5.20: Matlab code for the QoI CDF plot.

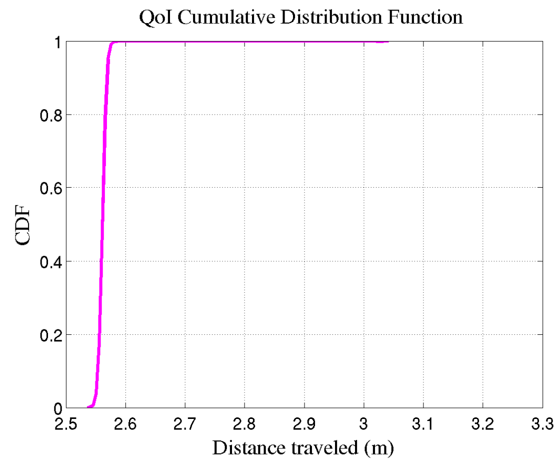


Figure 5.6.9: Cumulative Distribution Function.

5.6.2.5 Autocorrelation Plots

The code presented in Listing 5.21 uses Matlab function `autocorr` to generate Figure 5.6.10, 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 5.21: Matlab code for the QoI autocorrelation plot.

5.6.2.6 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 5.22 shows the usage of Matlab commands for finding such the matrix.

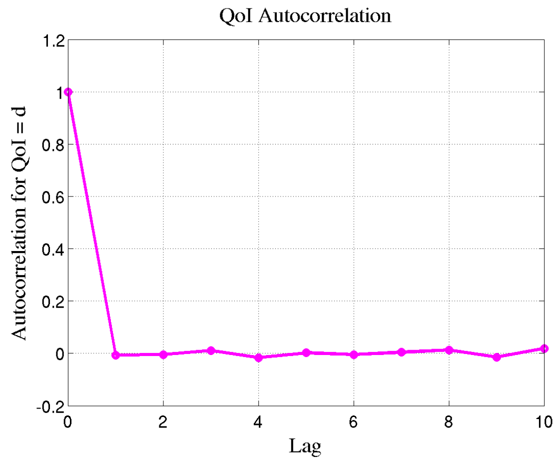


Figure 5.6.10: Autocorrelation plot.

```
% 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 5.22: 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 5.23: Matlab code for the matrix of correlation between parameter g and quantity of interest d.

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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.

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APPENDIX B

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Preamble

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Version 1.3, 3 November 2008

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