Numerical Computation, Statistical analysis and Visualization Using MATLAB and Tools
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Agenda

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- Problem Statement
- Methodology
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- References
Simulation and modelling is the best approach for analyzing the physical system where the experiments become difficult and requires repeatable tests and analysis. Mathematical Models are designed and implemented which requires complex numerical computations and are widely used in all areas of science and technology to represent complex real-world phenomena.

To design, implement, and analyse the models, MATLAB has wide range of algorithms and toolboxes for numerical computation, statistical analysis, optimization, computation of multidimensional matrices, Data Visualization.
Problem Statement

Statistical analysis of Computer Simulations

- Any physical system behavior cannot always be analyzed by experiments due to inaccessible inputs and outputs, Cost, difficulty and sometimes time consuming. Therefore computer models also known as simulators are widely used in all areas of science and technology to represent complex real-world phenomena.

- Complex numerical computations are to be implemented for mathematical representations of a physical system in a computer.

- Visualization for better understanding of the simulation results with user interaction is required.

- Highly complex stochastic model calculation and iterative process are to be implemented for prediction modelling, variance based sensitivity analysis.

But modeling and implementation of numerical algorithms is not handy to implement and is time consuming.
Methodology

- Gaussian process is one of the most widely used stochastic processes for modeling dependent data observed over time, or space, or time and space.
- Gaussian Process Modeling involves building a relationship between the simulation inputs and outputs and also a difference model between the simulation results and the experimental results, which calibrate simulation parameters. MATLAB has extensive library of built-in function from basic to complex functions for calculation of the model and obtaining predictions from the model.
- Sensitivity analysis and prediction modules are developed using MATLAB statistical functions.
- Data analysis and visualization is implemented with graphical user interface.
- MATLAB scripts are developed to generate customized comprehensive statistical plots using MATLAB graphics and control charts.
- Optimization toolbox and search algorithms are used to replicate the IMSL Numerical Libraries.
- Legacy code like FORTRAN, C and C++ is integrated to the MATLAB application using MATLAB external programming language interface. This MATLAB application is freely distributed to the end users by building standalone executable using MATLAB compiler.
Observed $y_{obs}$ corresponds to measured variables $x$ and simulated $y_{sim}$ is generated from input variables $(z \ t)$, the $y$ responses will be modeled as

$$K_w = y_{sim}$$

$$K_u + D_v = y_{obs}$$

Parameter modeling using *Markov Chain Monte Carlo – mcmc* using MATLAB routines

Calibration, prediction and analysis
Predictive modeling

Process to create a statistical model to best predict the probability of an outcome or future behavior.

Given a dataset \((X,Y)\), where \(X=(x_1,\ldots, x_n)\), each \(x\) possible vectors and \(Y=(y_1,\ldots, Y_n)\) determine an accurate model \(y=f(x)\) so that for a new data set \(X^*\), one can determine \(Y^*=f(X^*)\).

Statistics toolbox -

- supports a wide range of common statistical tasks, to curve fitting, to design of experiments and statistical process control.
- A quick implementation of interactive GUI
- Statistical Plots such as Box plots, Quantile-Quantile Plots, scatter plots, normal
Variance based Sensitivity analysis

Sensitivity Analysis:
Sensitivity analysis is the study of how the variation (uncertainty) in the output of a mathematical model can be apportioned, qualitatively or quantitatively, to different source of variation in the input of a model.

- It helps to build confidence in the model by studying the uncertainties that are often associated with the parameters in models.
- SA methods use the decomposition of \( y = f(x) \) into main effects and interaction effects:

  \[
  f(x) = f_0 + f_1(x_1) + f_2(x_2) + f_{12}(x_1, x_2)
  \]

- The Statistics Toolbox supports various methods in multivariate statistics, including principal components analysis, factor analysis, one-way multivariate analysis of variance, cluster analysis, and classical multidimensional scaling.
- The Statistics Toolbox helps to quickly implement control charts such as Xbar, MA, S Charts.
Variance based Sensitivity analysis cont…

- Variance based sensitivity analysis and uses the covariance of the emulator inputs as a multivariate input control and uses the emulator outputs tracked in time order as physical response control both in the sense of Univariate Shewhart control charts (I-MR or Xbar-R) with the options of all the control rules that are currently programmed in Minitab and as compared to a specification requirement considering the uncertainty in the emulator prediction. The responses are compared to both control limits and specification limits.

- It is useful in statistical process control when there is more than one variable and when the effects of multiple variables is not independent or parameters are measure of some other parameters (correlation).

- Multivariate charts are used to detect shifts in the means or the relation ship (covariance) between several related parameters.

- Uses the process principal components instead of the raw process variables.
Conclusion

- MATLAB is a high-level technical computing language with extensive toolboxes for computation and for visualization that made the implementation of numerical methods much easier.
- Research and development time and cost is reduced significantly due to MATLAB standard predefined commands.
- MATLAB matrix manipulations, numerical calculations and developing customized tools, GUIs are greatly simplified without complicated programming.
- MATLAB external programming language interface for legacy code like FORTRAN, C and C++ increased performance during run time.
- MATLAB language with extensive tools and built-in math functions enabled to explore multiple approaches and reach the solution faster.
References

- MATLAB, The Mathworks Inc. MATLAB is a software tool for doing mathematical computations
  Mathworks website: [http://www.mathworks.in/products/matlab/?s_cid=wiki_matlab_15](http://www.mathworks.in/products/matlab/?s_cid=wiki_matlab_15)

- Statistical Toolbox product page on the Mathworks website.

- Optimization Toolbox product page on the Mathworks website.

- Signal processing Toolbox product page on the Mathworks website.

- IMSL® Numerical Libraries

- GPM/SA Code Operation: Brian Williams, CCS-6, Jim Gattiker, CCS-6

- Univariate and Multivariate Sensitivity Analysis Using GPMSA: Brian Williams and Thomas Santner
Thank You

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