Bayesian Statistics Applied to Complex Models of Physical Systems

Bayesian Methods in Nuclear Physics INT 16-2A

Ian Vernon
Department of Mathematical Sciences
Durham University, UK

Work done in collaboration with Michael Goldstein (Dept. Mathematical Sciences); Richard Bower and Carlos Frenk's group at the Institute for Computational Cosmology, Durham University, UK. EPSRC funding.

Overview

- Remarks on the use of Bayesian statistics.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.
  - Choices within Bayesian Statistics.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.
  - Choices within Bayesian Statistics.
- Bayesian Statistics as applied to Complex Models of Physical Systems.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.
  - Choices within Bayesian Statistics.
- Bayesian Statistics as applied to Complex Models of Physical Systems.
  - Application to a Galaxy Formation Simulation.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.
  - Choices within Bayesian Statistics.
- Bayesian Statistics as applied to Complex Models of Physical Systems.
  - Application to a Galaxy Formation Simulation.
  - Bayesian Emulation.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.
  - Choices within Bayesian Statistics.
- Bayesian Statistics as applied to Complex Models of Physical Systems.
  - Application to a Galaxy Formation Simulation.
  - Bayesian Emulation.
  - Linking Model to Reality: a full Bayesian Uncertainty Analysis.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.
  - Choices within Bayesian Statistics.
- Bayesian Statistics as applied to Complex Models of Physical Systems.
  - Application to a Galaxy Formation Simulation.
  - Bayesian Emulation.
  - Linking Model to Reality: a full Bayesian Uncertainty Analysis.
  - Iterative History Matching via Implausibility: a pre-calibration method.

Overview

- Remarks on the use of Bayesian statistics.
  - Why it is the right thing to do.
  - Choices within Bayesian Statistics.
- Bayesian Statistics as applied to Complex Models of Physical Systems.
  - Application to a Galaxy Formation Simulation.
  - Bayesian Emulation.
  - Linking Model to Reality: a full Bayesian Uncertainty Analysis.
  - Iterative History Matching via Implausibility: a pre-calibration method.
  - Visualisation of results.

Why Bayesian Statistics is the right thing to do.

- There is a war going on within Statistics, between the traditional Frequentist statisticians and the more modern Bayesian statisticians.

Why Bayesian Statistics is the right thing to do.

- There is a war going on within Statistics, between the traditional Frequentist statisticians and the more modern Bayesian statisticians.
- This is currently turning in the Bayesian's favour, with Bayesian statistics now being employed across a wide range of applications.

Why Bayesian Statistics is the right thing to do.

- There is a war going on within Statistics, between the traditional Frequentist statisticians and the more modern Bayesian statisticians.
- This is currently turning in the Bayesian's favour, with Bayesian statistics now being employed across a wide range of applications.
- Part of this popularity is due to modern computer power: algorithms such as MCMC and its variants allow the solution to previously intractable Bayesian calculations.

Why Bayesian Statistics is the right thing to do.

- There is a war going on within Statistics, between the traditional Frequentist statisticians and the more modern Bayesian statisticians.

- This is currently turning in the Bayesian's favour, with Bayesian statistics now being employed across a wide range of applications.

- Part of this popularity is due to modern computer power: algorithms such as MCMC and its variants allow the solution to previously intractable Bayesian calculations.

- But why is the Bayesian approach actually better?

Why Bayesian Statistics is the right thing to do.

- There is a war going on within Statistics, between the traditional Frequentist statisticians and the more modern Bayesian statisticians.
- This is currently turning in the Bayesian's favour, with Bayesian statistics now being employed across a wide range of applications.
- Part of this popularity is due to modern computer power: algorithms such as MCMC and its variants allow the solution to previously intractable Bayesian calculations.
- But why is the Bayesian approach actually better?
- For many different reasons!

Why Bayesian Statistics is the right thing to do.

- There is a war going on within Statistics, between the traditional Frequentist statisticians and the more modern Bayesian statisticians.
- This is currently turning in the Bayesian's favour, with Bayesian statistics now being employed across a wide range of applications.
- Part of this popularity is due to modern computer power: algorithms such as MCMC and its variants allow the solution to previously intractable Bayesian calculations.
- But why is the Bayesian approach actually better?
- For many different reasons! Some are...

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:
  - Much study into the foundations of statistics and uncertainty itself.

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:
  - Much study into the foundations of statistics and uncertainty itself.
  - E.g. how to learn and/or make decisions in the face of uncertainty, and even what knowledge is in this context. (What does Random mean?)

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:
  - Much study into the foundations of statistics and uncertainty itself.
  - E.g. how to learn and/or make decisions in the face of uncertainty, and even what knowledge is in this context. (What does Random mean?)
  - The Bayesian paradigm gives a comprehensive and natural structure to represent and deal with uncertainty, which addresses these concerns.

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:
  - Much study into the foundations of statistics and uncertainty itself.
  - E.g. how to learn and/or make decisions in the face of uncertainty, and even what knowledge is in this context. (What does Random mean?)
  - The Bayesian paradigm gives a comprehensive and natural structure to represent and deal with uncertainty, which addresses these concerns.
- b) Allows the incorporation of many sources of information:

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:
  - Much study into the foundations of statistics and uncertainty itself.
  - E.g. how to learn and/or make decisions in the face of uncertainty, and even what knowledge is in this context. (What does Random mean?)
  - The Bayesian paradigm gives a comprehensive and natural structure to represent and deal with uncertainty, which addresses these concerns.
- b) Allows the incorporation of many sources of information:
  - Due to its comprehensive and appropriate representation of uncertainty, many sources of information can be amalgamated into one calculation.

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:
  - Much study into the foundations of statistics and uncertainty itself.
  - E.g. how to learn and/or make decisions in the face of uncertainty, and even what knowledge is in this context. (What does Random mean?)
  - The Bayesian paradigm gives a comprehensive and natural structure to represent and deal with uncertainty, which addresses these concerns.

- b) Allows the incorporation of many sources of information:
  - Due to its comprehensive and appropriate representation of uncertainty, many sources of information can be amalgamated into one calculation.
  - These can be from disparate data sources, expert knowledge or even logical argument.

Why Bayesian Statistics is the right thing to do.

- a) Philosophically well grounded:
  - Much study into the foundations of statistics and uncertainty itself.
  - E.g. how to learn and/or make decisions in the face of uncertainty, and even what knowledge is in this context. (What does Random mean?)
  - The Bayesian paradigm gives a comprehensive and natural structure to represent and deal with uncertainty, which addresses these concerns.

- b) Allows the incorporation of many sources of information:
  - Due to its comprehensive and appropriate representation of uncertainty, many sources of information can be amalgamated into one calculation.
  - These can be from disparate data sources, expert knowledge or even logical argument.
  - Bayesian statistics can be viewed as a natural extension to pure logic once uncertainty is introduced.

Why Bayesian Statistics is the right thing to do.

- c) Bayesian Statistics is just Extremely Useful!

Why Bayesian Statistics is the right thing to do.

- c) Bayesian Statistics is just Extremely Useful!
  - It provides exactly what scientists want: e.g. probability distributions on uncertain parameters of interest.

Why Bayesian Statistics is the right thing to do.

- c) Bayesian Statistics is just Extremely Useful!
  - It provides exactly what scientists want: e.g. probability distributions on uncertain parameters of interest.
  - Provides an actual probability of a Hypothesis being true $P(H_0|z)$, (and not the crap “fail to reject at α significance” of a frequentist approach ($P(z|H_0)$), that medical science is currently reeling from).

Why Bayesian Statistics is the right thing to do.

- c) Bayesian Statistics is just Extremely Useful!
  - It provides exactly what scientists want: e.g. probability distributions on uncertain parameters of interest.
  - Provides an actual probability of a Hypothesis being true $P(H_0|z)$, (and not the crap “fail to reject at α significance” of a frequentist approach ($P(z|H_0)$), that medical science is currently reeling from).
  - The results of Bayesian statistics, in terms of probabilities, can be directly inserted into Decision Theory, to advise on any possible decision: e.g. which experiment to perform to best learn about a particular scientific question.

Why Bayesian Statistics is the right thing to do.

- c) Bayesian Statistics is just Extremely Useful!
  - It provides exactly what scientists want: e.g. probability distributions on uncertain parameters of interest.
  - Provides an actual probability of a Hypothesis being true $P(H_0|z)$, (and not the crap "fail to reject at α significance" of a frequentist approach ($P(z|H_0)$), that medical science is currently reeling from).
  - The results of Bayesian statistics, in terms of probabilities, can be directly inserted into Decision Theory, to advise on any possible decision: e.g. which experiment to perform to best learn about a particular scientific question.
- Interestingly, Bayesian statistics tells us what we need to put in, in order to get what we want out.

Why Bayesian Statistics is the right thing to do.

- c) Bayesian Statistics is just Extremely Useful!
  - It provides exactly what scientists want: e.g. probability distributions on uncertain parameters of interest.
  - Provides an actual probability of a Hypothesis being true $P(H_0|z)$, (and not the crap "fail to reject at α significance" of a frequentist approach ($P(z|H_0)$), that medical science is currently reeling from).
  - The results of Bayesian statistics, in terms of probabilities, can be directly inserted into Decision Theory, to advise on any possible decision: e.g. which experiment to perform to best learn about a particular scientific question.
- Interestingly, Bayesian statistics tells us what we need to put in, in order to get what we want out.
- E.g. if you want posterior probabilities out, you have to put prior probabilities in. Prior requirement not a disadvantage.

Why Bayesian Statistics is the right thing to do.

- c) Bayesian Statistics is just Extremely Useful!
  - It provides exactly what scientists want: e.g. probability distributions on uncertain parameters of interest.
  - Provides an actual probability of a Hypothesis being true $P(H_0|z)$, (and not the crap "fail to reject at α significance" of a frequentist approach ($P(z|H_0)$), that medical science is currently reeling from).
  - The results of Bayesian statistics, in terms of probabilities, can be directly inserted into Decision Theory, to advise on any possible decision: e.g. which experiment to perform to best learn about a particular scientific question.
- Interestingly, Bayesian statistics tells us what we need to put in, in order to get what we want out.
- E.g. if you want posterior probabilities out, you have to put prior probabilities in. Prior requirement not a disadvantage.
- Subjective Bayesian statistics: the pure form!

Choices within Bayesian Statistics.

- If we are prepared to specify full probability distributions for the priors $\pi(y)$ and the likelihood $\pi(z|y)$, then we get everything we want from the posterior $\pi(y|z)$, found from Bayes theorem:

$$\pi(y|z) = \frac{\pi(z|y)\pi(y)}{\pi(z)}$$

Choices within Bayesian Statistics.

- If we are prepared to specify full probability distributions for the priors $\pi(y)$ and the likelihood $\pi(z|y)$, then we get everything we want from the posterior $\pi(y|z)$, found from Bayes theorem:

$$\pi(y|z) = \frac{\pi(z|y)\pi(y)}{\pi(z)}$$

- Can be fast for certain conjugate problems, but usually computationally demanding: requires MCMC or equivalent sampling algorithm.

Choices within Bayesian Statistics.

- If we are prepared to specify full probability distributions for the priors $\pi(y)$ and the likelihood $\pi(z|y)$, then we get everything we want from the posterior $\pi(y|z)$, found from Bayes theorem:

$$\pi(y|z) = \frac{\pi(z|y)\pi(y)}{\pi(z)}$$

- Can be fast for certain conjugate problems, but usually computationally demanding: requires MCMC or equivalent sampling algorithm.

- However if we are only prepared to specify prior means, variances and covariances, we can use Bayes Linear statistics to obtain:

$$\begin{aligned} \mathrm{E}_z(y) &= \mathrm{E}(y) + \mathrm{Cov}(y,z)\mathrm{Var}(z)^{-1}(z - \mathrm{E}(z)) \\ \mathrm{Var}_z(y) &= \mathrm{Var}(y) - \mathrm{Cov}(y,z)\mathrm{Var}(z)^{-1}\mathrm{Cov}(z,y) \end{aligned}$$

Choices within Bayesian Statistics.

- If we are prepared to specify full probability distributions for the priors $\pi(y)$ and the likelihood $\pi(z|y)$, then we get everything we want from the posterior $\pi(y|z)$, found from Bayes theorem:

$$\pi(y|z) = \frac{\pi(z|y)\pi(y)}{\pi(z)}$$

- Can be fast for certain conjugate problems, but usually computationally demanding: requires MCMC or equivalent sampling algorithm.

- However if we are only prepared to specify prior means, variances and covariances, we can use Bayes Linear statistics to obtain:

$$\begin{aligned} \mathrm{E}_z(y) &= \mathrm{E}(y) + \mathrm{Cov}(y,z)\mathrm{Var}(z)^{-1}(z - \mathrm{E}(z)) \\ \mathrm{Var}_z(y) &= \mathrm{Var}(y) - \mathrm{Cov}(y,z)\mathrm{Var}(z)^{-1}\mathrm{Cov}(z,y) \end{aligned}$$

- The adjusted mean $\mathrm{E}_z(y)$ and variance $\mathrm{Var}_z(y)$ are very fast to calculate as just uses matrix operations.

Bayesian Uncertainty Analysis of Complex Models

- In many scientific disciplines complex computer simulators are employed to help understand corresponding real world physical processes.

Bayesian Uncertainty Analysis of Complex Models

- In many scientific disciplines complex computer simulators are employed to help understand corresponding real world physical processes.
- For example oil reservoir simulators are used to analyse oil reservoirs, flood simulators to analyse floods etc.

Bayesian Uncertainty Analysis of Complex Models

- In many scientific disciplines complex computer simulators are employed to help understand corresponding real world physical processes.
- For example oil reservoir simulators are used to analyse oil reservoirs, flood simulators to analyse floods etc.
- These simulators, referred to as Computer Models, share many attributes, and also many problems.

Bayesian Uncertainty Analysis of Complex Models

- In many scientific disciplines complex computer simulators are employed to help understand corresponding real world physical processes.
- For example oil reservoir simulators are used to analyse oil reservoirs, flood simulators to analyse floods etc.
- These simulators, referred to as Computer Models, share many attributes, and also many problems.
- Often they take a long time to run, (minutes, hours, days or even weeks) and require the specification of a large number of input parameters that we represent as a vector x.

Bayesian Uncertainty Analysis of Complex Models

- In many scientific disciplines complex computer simulators are employed to help understand corresponding real world physical processes.
- For example oil reservoir simulators are used to analyse oil reservoirs, flood simulators to analyse floods etc.
- These simulators, referred to as Computer Models, share many attributes, and also many problems.
- Often they take a long time to run, (minutes, hours, days or even weeks) and require the specification of a large number of input parameters that we represent as a vector x.
- An area of (Bayesian) Statistics has arisen to deal with such models and the many problems they present.

Bayesian Uncertainty Analysis of Complex Models

- In many scientific disciplines complex computer simulators are employed to help understand corresponding real world physical processes.
- For example oil reservoir simulators are used to analyse oil reservoirs, flood simulators to analyse floods etc.
- These simulators, referred to as Computer Models, share many attributes, and also many problems.
- Often they take a long time to run, (minutes, hours, days or even weeks) and require the specification of a large number of input parameters that we represent as a vector x.
- An area of (Bayesian) Statistics has arisen to deal with such models and the many problems they present.
- This area is referred to as the study of Computer Models, or as Uncertainty Analysis (preferred) or Uncertainty Quantification (less preferred as sometimes used in a weaker sense).

Overview of Uncertainty Analysis of Complex Models

- The Bayesian uncertainty analysis of complex systems has led to the development of a large set of extremely general and powerful techniques.

Overview of Uncertainty Analysis of Complex Models

- The Bayesian uncertainty analysis of complex systems has led to the development of a large set of extremely general and powerful techniques.
- These have now been employed in a range of scientific disciplines:

Overview of Uncertainty Analysis of Complex Models

- The Bayesian uncertainty analysis of complex systems has led to the development of a large set of extremely general and powerful techniques.
- These have now been employed in a range of scientific disciplines:
  - Cosmology (galaxy formation simulations),
  - Climate science (climate models of global warming),
  - Environmental sciences (flood and rainfall runoff models),
  - Systems biology (genetic and metabolic network models),
  - Epidemiology (agent based stochastic HIV models).
  - Oil industry (oil reservoir models and geology models).
  - Many more...

Overview of Uncertainty Analysis of Complex Models

- The Bayesian uncertainty analysis of complex systems has led to the development of a large set of extremely general and powerful techniques.
- These have now been employed in a range of scientific disciplines:
  - Cosmology (galaxy formation simulations),
  - Climate science (climate models of global warming),
  - Environmental sciences (flood and rainfall runoff models),
  - Systems biology (genetic and metabolic network models),
  - Epidemiology (agent based stochastic HIV models).
  - Oil industry (oil reservoir models and geology models).
  - Many more...
- These techniques could be of substantial use to the Nuclear physics community.

Overview of Uncertainty Analysis of Complex Models

- All these areas share similar problems e.g.

Overview of Uncertainty Analysis of Complex Models

- All these areas share similar problems e.g.
  - history matching to learn about acceptable input parameters that ensure good matches between outputs and historical data,

Overview of Uncertainty Analysis of Complex Models

- All these areas share similar problems e.g.
  - history matching to learn about acceptable input parameters that ensure good matches between outputs and historical data,
  - forecasting/predicting future outputs with appropriate uncertainty,

Overview of Uncertainty Analysis of Complex Models

- All these areas share similar problems e.g.
  - history matching to learn about acceptable input parameters that ensure good matches between outputs and historical data,
  - forecasting/predicting future outputs with appropriate uncertainty,
  - Decision theory: deciding on which future experiments to perform (or data to pay for),

Overview of Uncertainty Analysis of Complex Models

- All these areas share similar problems e.g.
  - history matching to learn about acceptable input parameters that ensure good matches between outputs and historical data,
  - forecasting/predicting future outputs with appropriate uncertainty,
  - Decision theory: deciding on which future experiments to perform (or data to pay for),
  - and many others.

Overview of Uncertainty Analysis of Complex Models

- All these areas share similar problems e.g.
  - history matching to learn about acceptable input parameters that ensure good matches between outputs and historical data,
  - forecasting/predicting future outputs with appropriate uncertainty,
  - Decision theory: deciding on which future experiments to perform (or data to pay for),
  - and many others.
- All of these problems require a careful analysis of all relevant uncertainties.

Overview of Uncertainty Analysis of Complex Models

- All these areas share similar problems e.g.
  - history matching to learn about acceptable input parameters that ensure good matches between outputs and historical data,
  - forecasting/predicting future outputs with appropriate uncertainty,
  - Decision theory: deciding on which future experiments to perform (or data to pay for),
  - and many others.
- All of these problems require a careful analysis of all relevant uncertainties.
- Speed is always a problem for complex models so often we employ 'Emulators': fast stochastic approximations to the Computer Model.

Demonstration of a full Uncertainty Analysis: Galform

- Going to History Match a Galaxy formation simulation known as Galform.

Demonstration of a full Uncertainty Analysis: Galform

- Going to History Match a Galaxy formation simulation known as Galform.
- This involves learning about acceptable inputs x to the Galform model, using observed data z.

Demonstration of a full Uncertainty Analysis: Galform

- Going to History Match a Galaxy formation simulation known as Galform.
- This involves learning about acceptable inputs x to the Galform model, using observed data z.
- We use emulators and implausibility measures to cut out input space iteratively.

Demonstration of a full Uncertainty Analysis: Galform

- Going to History Match a Galaxy formation simulation known as Galform.
- This involves learning about acceptable inputs x to the Galform model, using observed data z.
- We use emulators and implausibility measures to cut out input space iteratively.
- We will discuss relevant uncertainties: model discrepancy, observational errors, function uncertainty etc.

Demonstration of a full Uncertainty Analysis: Galform

- Going to History Match a Galaxy formation simulation known as Galform.
- This involves learning about acceptable inputs x to the Galform model, using observed data z.
- We use emulators and implausibility measures to cut out input space iteratively.
- We will discuss relevant uncertainties: model discrepancy, observational errors, function uncertainty etc.
- The History Matching approach described is completely general, and can be used for any model that is relatively slow to run and has lots of inputs.

Demonstration of a full Uncertainty Analysis: Galform

- Going to History Match a Galaxy formation simulation known as Galform.
- This involves learning about acceptable inputs x to the Galform model, using observed data z.
- We use emulators and implausibility measures to cut out input space iteratively.
- We will discuss relevant uncertainties: model discrepancy, observational errors, function uncertainty etc.
- The History Matching approach described is completely general, and can be used for any model that is relatively slow to run and has lots of inputs.
- Vernon, I., Goldstein, M., Bower, R. G., Galaxy Formation: "Bayesian History Matching for the Observable Universe". *Statistical Science* 29 (2014), no. 1, 81–90.

Why History Match?

- History Matching is an efficient technique that seeks to identify the set $\mathcal{X}$ of all acceptable inputs x.

Why History Match?

- History Matching is an efficient technique that seeks to identify the set $\mathcal{X}$ of all acceptable inputs x.
- Often $\mathcal{X}$ only occupies a tiny fraction of the original input space.

Why History Match?

- History Matching is an efficient technique that seeks to identify the set $\mathcal{X}$ of all acceptable inputs x.
- Often $\mathcal{X}$ only occupies a tiny fraction of the original input space.
- This set $\mathcal{X}$ may be empty: we do not presuppose that any such inputs exist.

Why History Match?

- History Matching is an efficient technique that seeks to identify the set $\mathcal{X}$ of all acceptable inputs x.
- Often $\mathcal{X}$ only occupies a tiny fraction of the original input space.
- This set $\mathcal{X}$ may be empty: we do not presuppose that any such inputs exist.

- This is the main difference between History Matching and the related technique of Probabilistic Bayesian Calibration.

Why History Match?

- History Matching is an efficient technique that seeks to identify the set $\mathcal{X}$ of all acceptable inputs x.
- Often $\mathcal{X}$ only occupies a tiny fraction of the original input space.
- This set $\mathcal{X}$ may be empty: we do not presuppose that any such inputs exist.

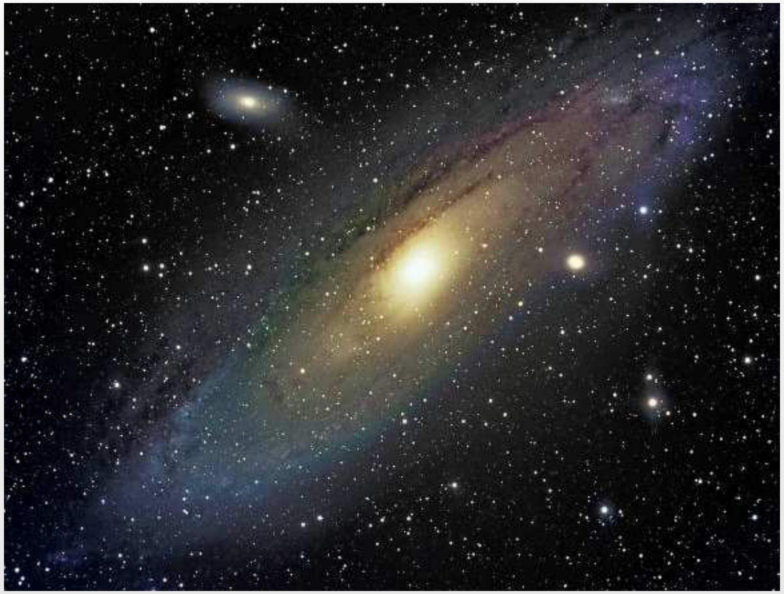
- This is the main difference between History Matching and the related technique of Probabilistic Bayesian Calibration.
- The later is a useful technique, but assumes a single 'best input' x^* and gives its posterior distribution $\pi(x^*|z)$, via the standard Bayesian update, using e.g. MCMC.

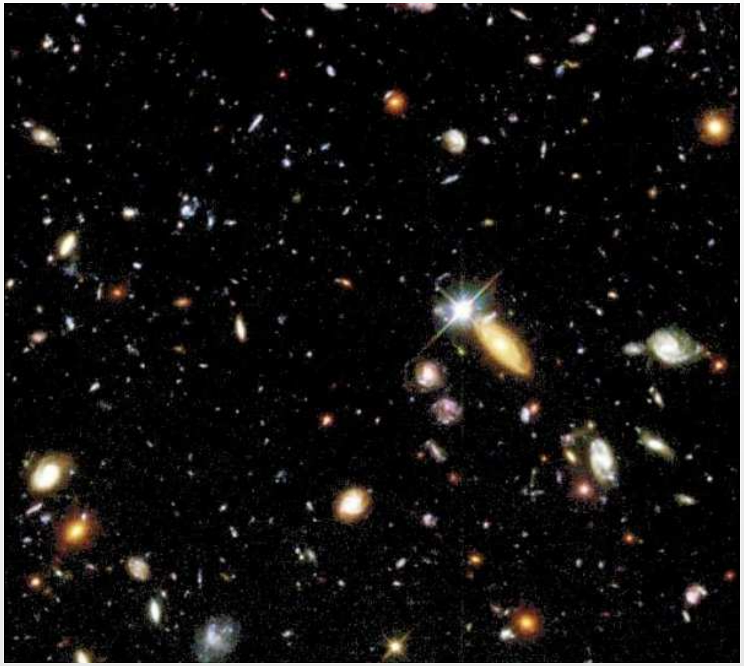
Why History Match?

- History Matching is an efficient technique that seeks to identify the set $\mathcal{X}$ of all acceptable inputs x.
- Often $\mathcal{X}$ only occupies a tiny fraction of the original input space.
- This set $\mathcal{X}$ may be empty: we do not presuppose that any such inputs exist.

- This is the main difference between History Matching and the related technique of Probabilistic Bayesian Calibration.
- The later is a useful technique, but assumes a single 'best input' x^* and gives its posterior distribution $\pi(x^*|z)$, via the standard Bayesian update, using e.g. MCMC.
- This involves the specification of many complex multivariate distributions related to all uncertain quantities of interest, which may or may not be warranted at this stage.

Andromeda Galaxy and Hubble Deep Field View





- Andromeda Galaxy: closest large galaxy to our own milky way.
- Hubble Deep Field: covers approximately 2 millionths of the sky but contains thousands of galaxies.

The Galform Model

- World leading cosmology group at the ICC are interested in modelling galaxy formation in the presence of Dark Matter.

The Galform Model

- World leading cosmology group at the ICC are interested in modelling galaxy formation in the presence of Dark Matter.
- First a Dark Matter simulation is performed over a volume of (1.63 billion light years$)^3$. This takes 3 months on a supercomputer.

The Galform Model

- World leading cosmology group at the ICC are interested in modelling galaxy formation in the presence of Dark Matter.
- First a Dark Matter simulation is performed over a volume of $(1.63$ billion light years$)^3$. This takes 3 months on a supercomputer.
- Galform takes the results of this simulation and models the evolution and attributes of approximately 1 million galaxies.

The Galform Model

- World leading cosmology group at the ICC are interested in modelling galaxy formation in the presence of Dark Matter.
- First a Dark Matter simulation is performed over a volume of (1.63 billion light years$)^3$. This takes 3 months on a supercomputer.
- Galform takes the results of this simulation and models the evolution and attributes of approximately 1 million galaxies.
- Galform requires the specification of 17 unknown inputs x in order to run.

The Galform Model

- World leading cosmology group at the ICC are interested in modelling galaxy formation in the presence of Dark Matter.
- First a Dark Matter simulation is performed over a volume of (1.63 billion light years$)^3$. This takes 3 months on a supercomputer.
- Galform takes the results of this simulation and models the evolution and attributes of approximately 1 million galaxies.
- Galform requires the specification of 17 unknown inputs x in order to run.
- It takes approximately 1 day to complete 1 run (using a single processor).

The Galform Model

- World leading cosmology group at the ICC are interested in modelling galaxy formation in the presence of Dark Matter.
- First a Dark Matter simulation is performed over a volume of (1.63 billion light years$)^3$. This takes 3 months on a supercomputer.
- Galform takes the results of this simulation and models the evolution and attributes of approximately 1 million galaxies.
- Galform requires the specification of 17 unknown inputs x in order to run.
- It takes approximately 1 day to complete 1 run (using a single processor).
- The Galform model produces lots of outputs $f(x)$, some of which can be compared to observed data z from the real Universe.

Galform: Which Inputs to Use?

- PROBLEM: We want to identify the set of all inputs $\mathcal{X}$ that lead to acceptable matches between model outputs $f(x)$ and observed data z.

Galform: Which Inputs to Use?

- PROBLEM: We want to identify the set of all inputs $\mathcal{X}$ that lead to acceptable matches between model outputs $f(x)$ and observed data z.
- 17-dimensional input space is large! If we did the simplest grid based search (setting each input to max or min), we would require 2^{17} runs.

Galform: Which Inputs to Use?

- PROBLEM: We want to identify the set of all inputs $\mathcal{X}$ that lead to acceptable matches between model outputs $f(x)$ and observed data z.

- 17-dimensional input space is large! If we did the simplest grid based search (setting each input to max or min), we would require 2^{17} runs.

- This would take approximately 180 years to complete (on one processor)!

Galform: Which Inputs to Use?

- PROBLEM: We want to identify the set of all inputs $\mathcal{X}$ that lead to acceptable matches between model outputs $f(x)$ and observed data z.

- 17-dimensional input space is large! If we did the simplest grid based search (setting each input to max or min), we would require 2^{17} runs.

- This would take approximately 180 years to complete (on one processor)!

- We would really want a higher definition, so would want say 10^{17} runs...

Galform: Which Inputs to Use?

- PROBLEM: We want to identify the set of all inputs $\mathcal{X}$ that lead to acceptable matches between model outputs $f(x)$ and observed data z.
- 17-dimensional input space is large! If we did the simplest grid based search (setting each input to max or min), we would require 2^{17} runs.
- This would take approximately 180 years to complete (on one processor)!
- We would really want a higher definition, so would want say 10^{17} runs... This would take far longer than the current age of the Universe.

Galform: Which Inputs to Use?

- PROBLEM: We want to identify the set of all inputs $\mathcal{X}$ that lead to acceptable matches between model outputs $f(x)$ and observed data z.

- 17-dimensional input space is large! If we did the simplest grid based search (setting each input to max or min), we would require 2^{17} runs.

- This would take approximately 180 years to complete (on one processor)!

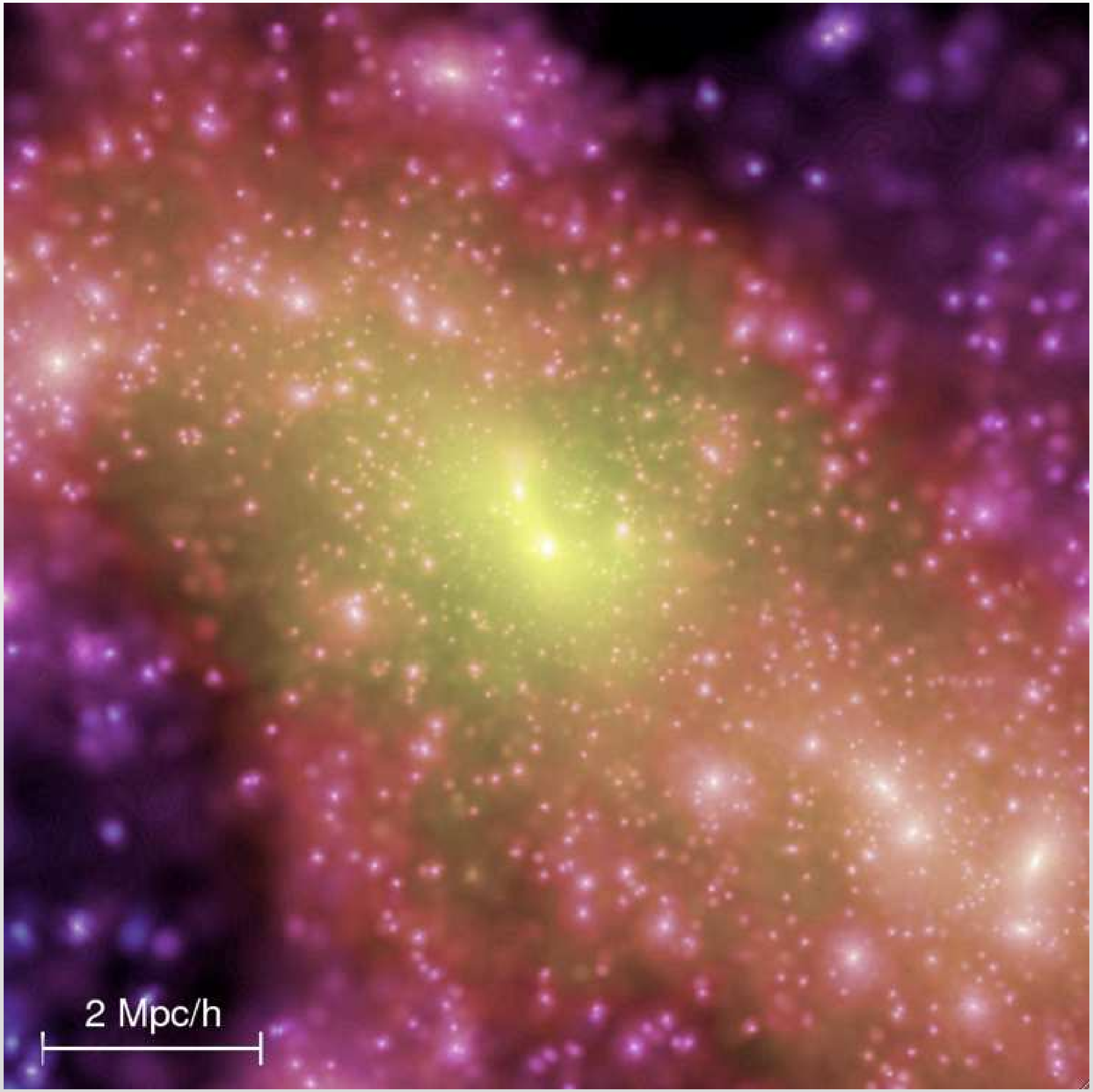
- We would really want a higher definition, so would want say 10^{17} runs... This would take far longer than the current age of the Universe.

- SOLUTION: Construct a Bayesian Emulator, which is a stochastic function that approximates the Galform model, and is fast to evaluate: our emulators were approximately 10^{7} times faster than Galform.

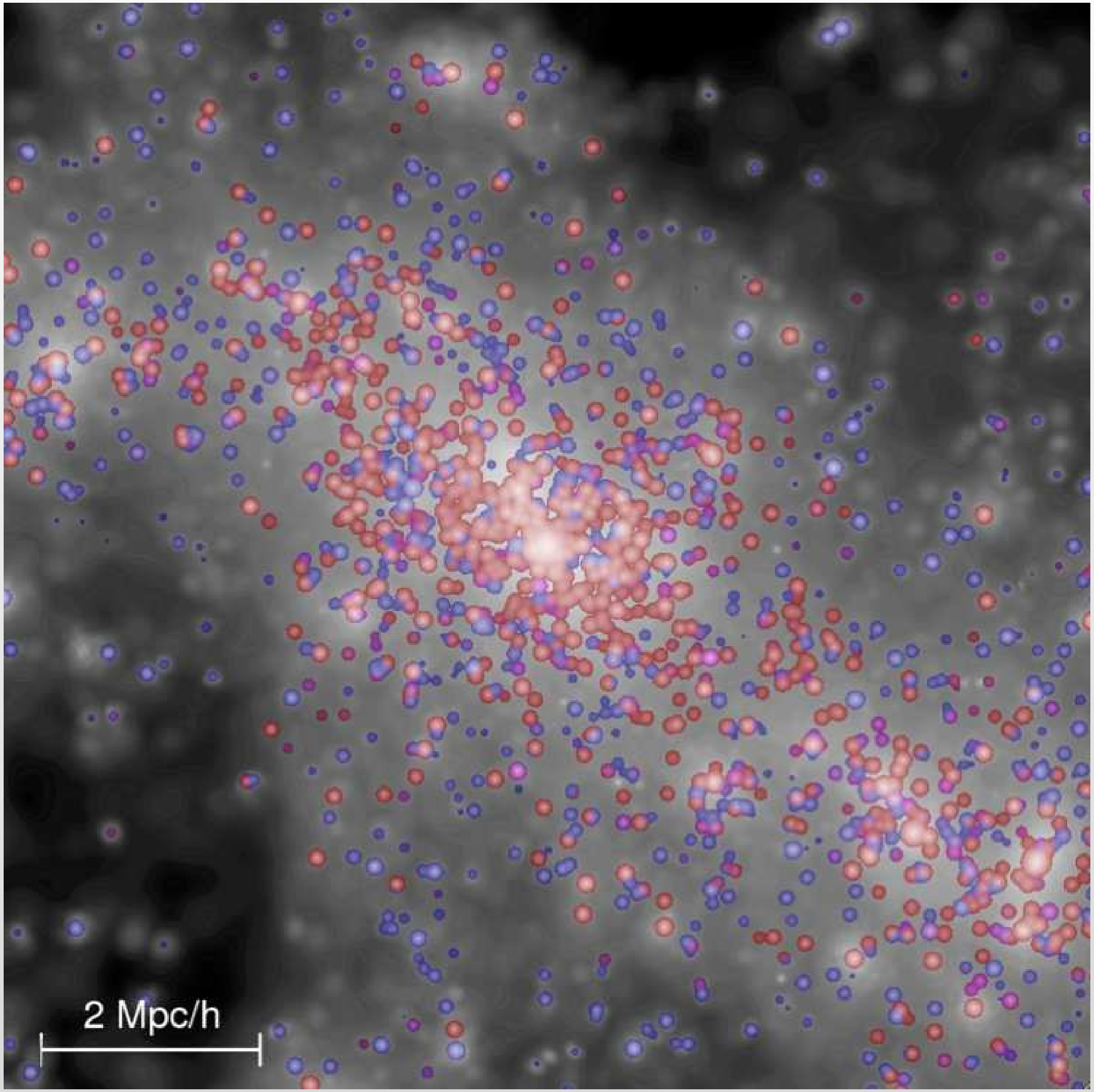
Galform: Which Inputs to Use?

- PROBLEM: We want to identify the set of all inputs $\mathcal{X}$ that lead to acceptable matches between model outputs $f(x)$ and observed data z.
- 17-dimensional input space is large! If we did the simplest grid based search (setting each input to max or min), we would require 2^{17} runs.
- This would take approximately 180 years to complete (on one processor)!
- We would really want a higher definition, so would want say 10^{17} runs... This would take far longer than the current age of the Universe.
- SOLUTION: Construct a Bayesian Emulator, which is a stochastic function that approximates the Galform model, and is fast to evaluate: our emulators were approximately 10^7 times faster than Galform.
- Use the Emulator to find the acceptable inputs.

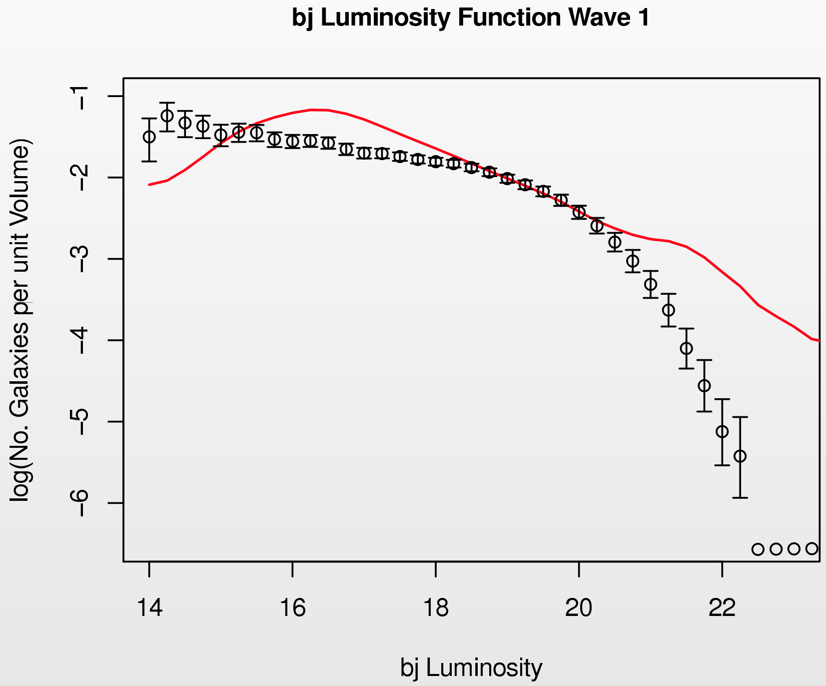
The Dark Matter Simulation: (thanks to VIRGO Consortium)

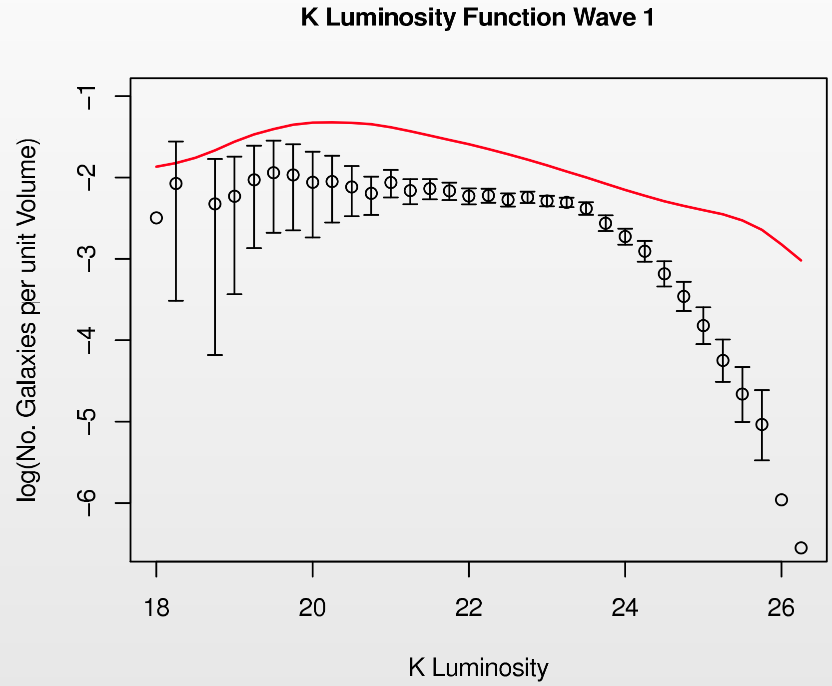


The Galform Model



Galform Outputs: The Luminosity Functions





- Galform provides multiple output data sets.
- Initially we analyse the luminosity functions which give the number of galaxies per unit volume, for each luminosity.
- Bj Luminosity: corresponds to density of young (blue) galaxies
- K Luminosity: corresponds to density of old (red) galaxies

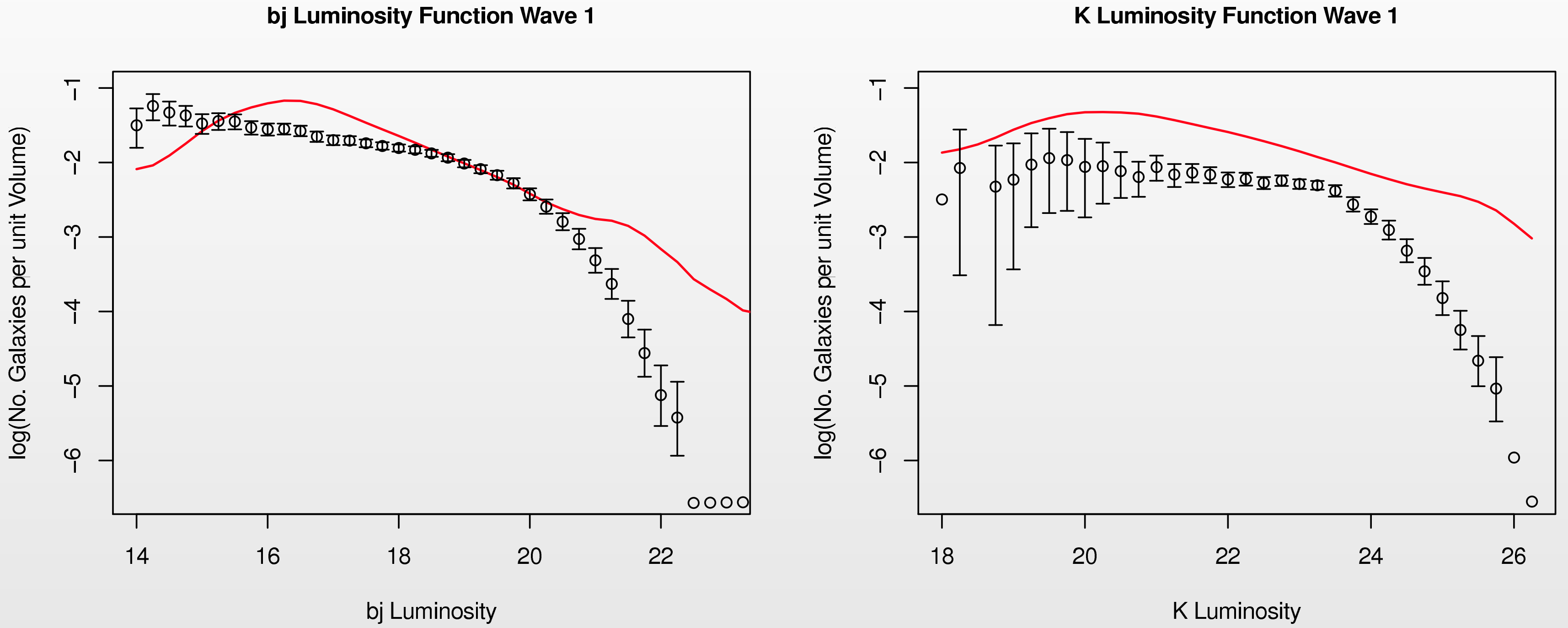
Input Parameters

- To perform one run, we need to specify numbers for each of the following 17 inputs:

vhotdisk:	100 - 550	**VCUT**:	20 - 50
aReheat:	0.2 - 1.2	**ZCUT**:	6 - 9
alphacool:	0.2 - 1.2	**alphastar**:	-3.2 - -0.3
vhotburst:	100 - 550	**tau0mrg**:	0.8 - 2.7
epsilonStar:	0.001 - 0.1	**fellip**:	0.1 - 0.35
stabledisk:	0.65 - 0.95	**fburst**:	0.01 - 0.15
alphahot:	2 - 3.7	**FSMBH**:	0.001 - 0.01
yield:	0.02 - 0.05	**eSMBH**:	0.004 - 0.05
tdisk:	0 - 1		

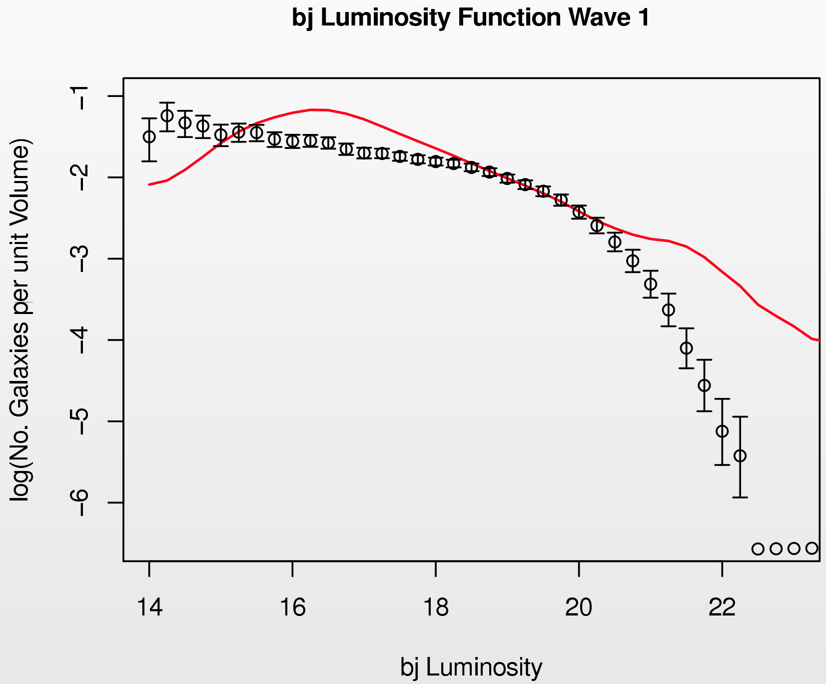
- What input values should we choose to get ‘acceptable’ outputs?

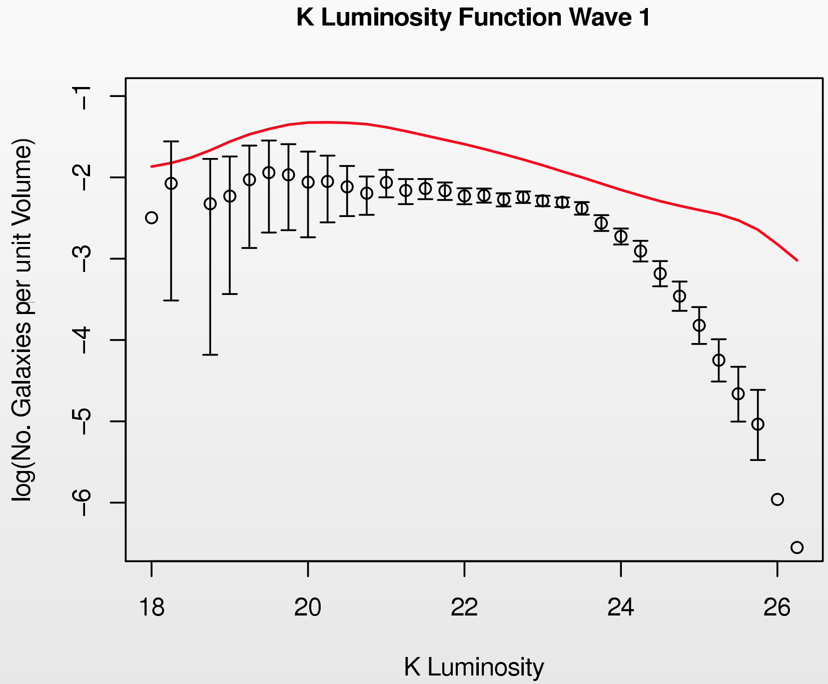
Galform Outputs: The Luminosity Functions



- Basic problem is that we pick inputs:
- vhotdisk $= 290.5$, aReheat $= 1.15$, alphacool $= 0.31$, ...
- And find that after 1 Day of Runtime:

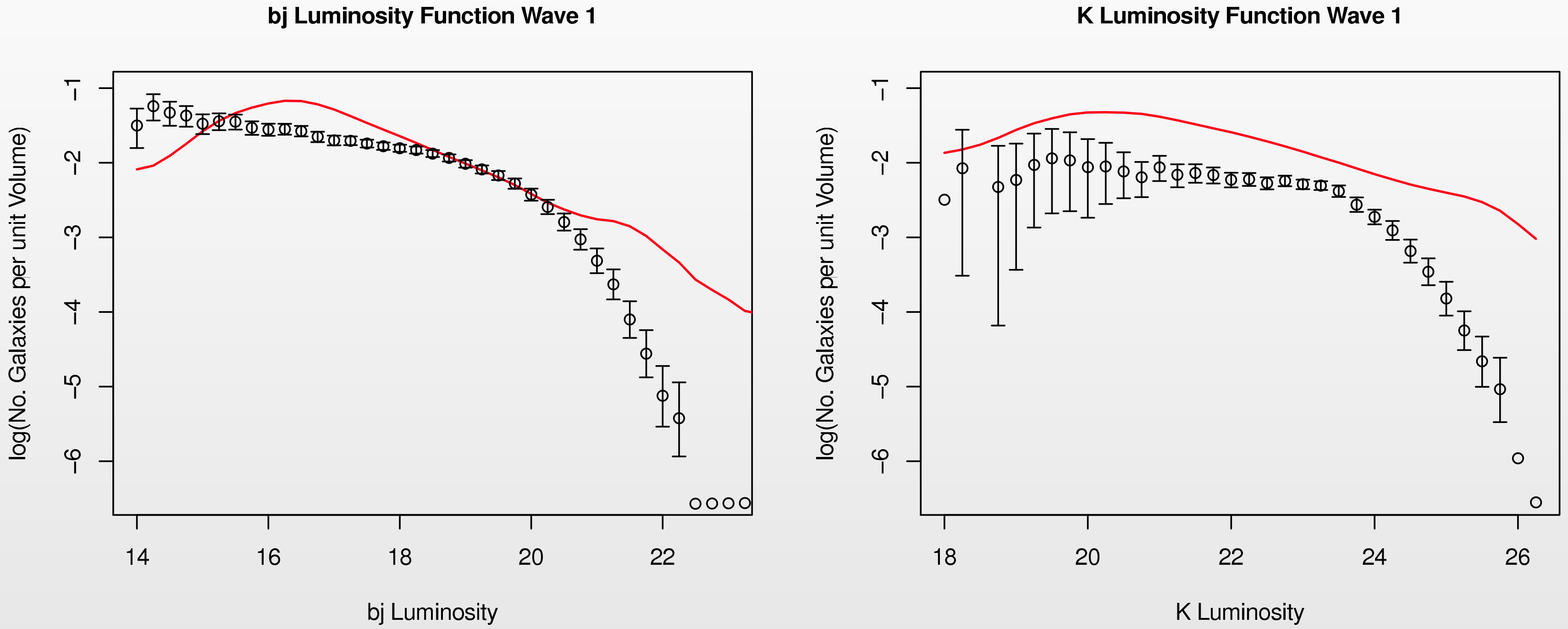
Galform Outputs: The Luminosity Functions





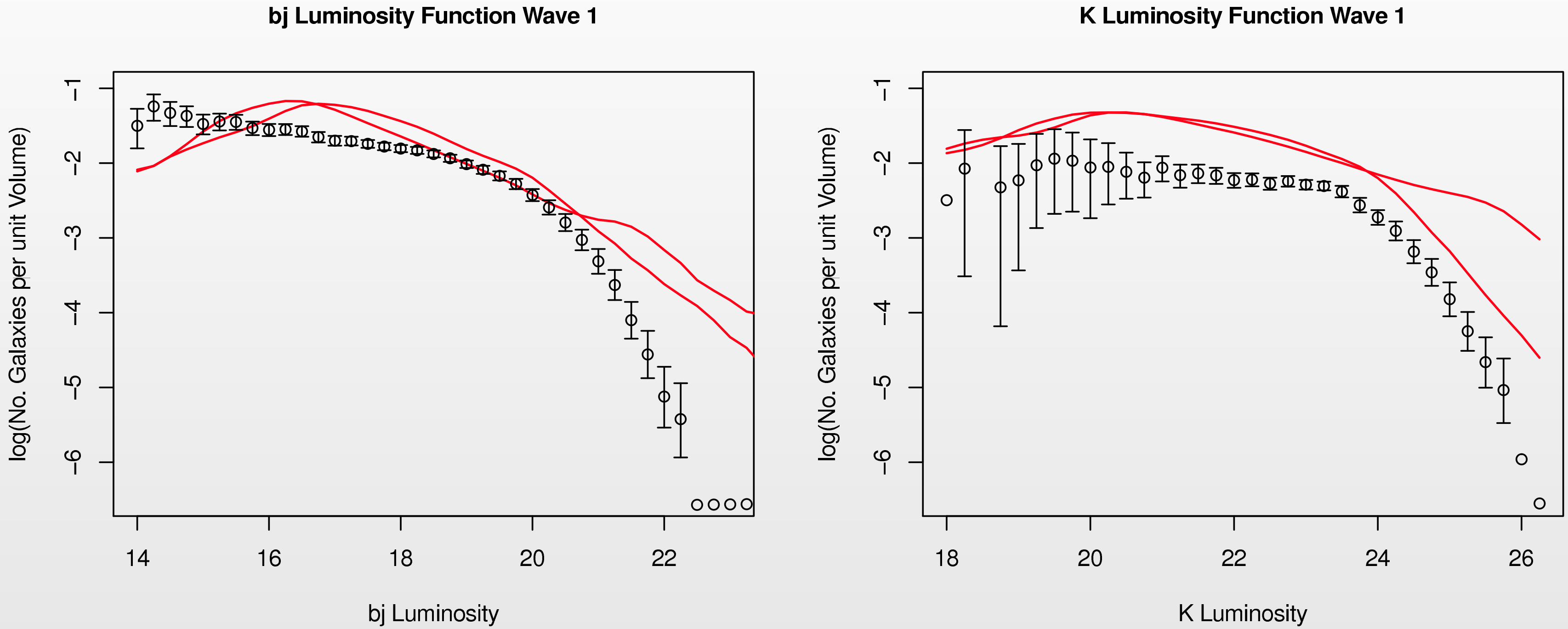
- Basic problem is that we pick inputs:
- vhotdisk $= 290.5$, aReheat $= 1.15$, alphacool $= 0.31$, ...
- And find that after 1 Day of Runtime:
- 1st run is rubbish.

Galform Outputs: The Luminosity Functions



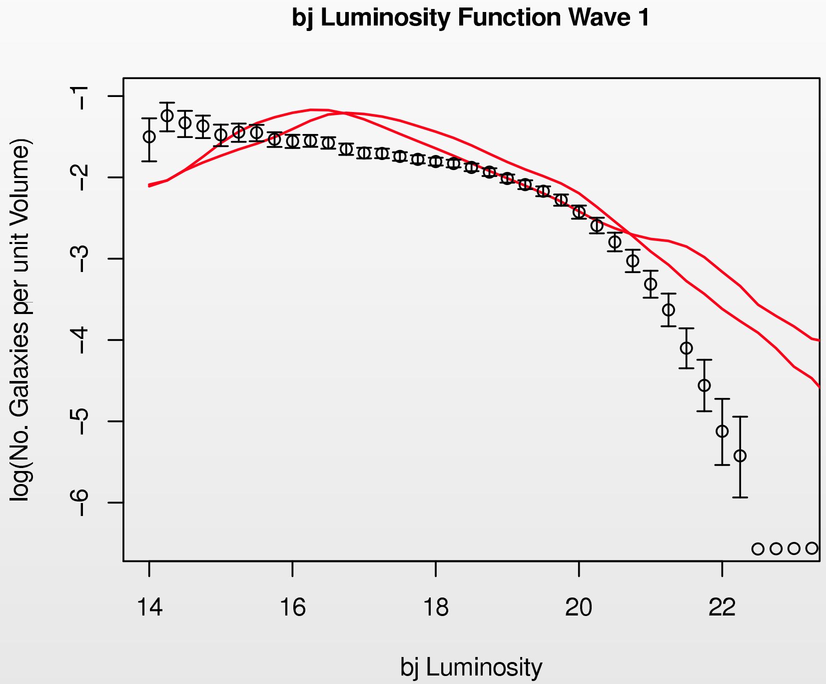
- Basic problem is that we pick inputs:
- vhotdisk $= 223.3$, aReheat $= 0.49$, alphacool $= 1.12$, ...
- And find that after 2 Days of Runtime:

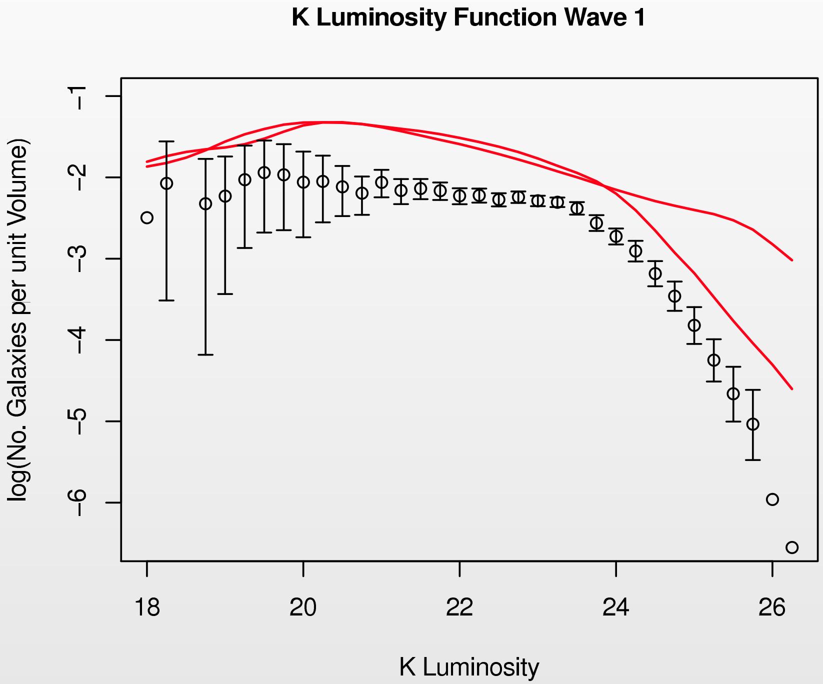
Galform Outputs: The Luminosity Functions



- Basic problem is that we pick inputs:
- vhotdisk $= 223.3$, aReheat $= 0.49$, alphacool $= 1.12$, ...
- And find that after 2 Days of Runtime:
- 2nd run is rubbish.

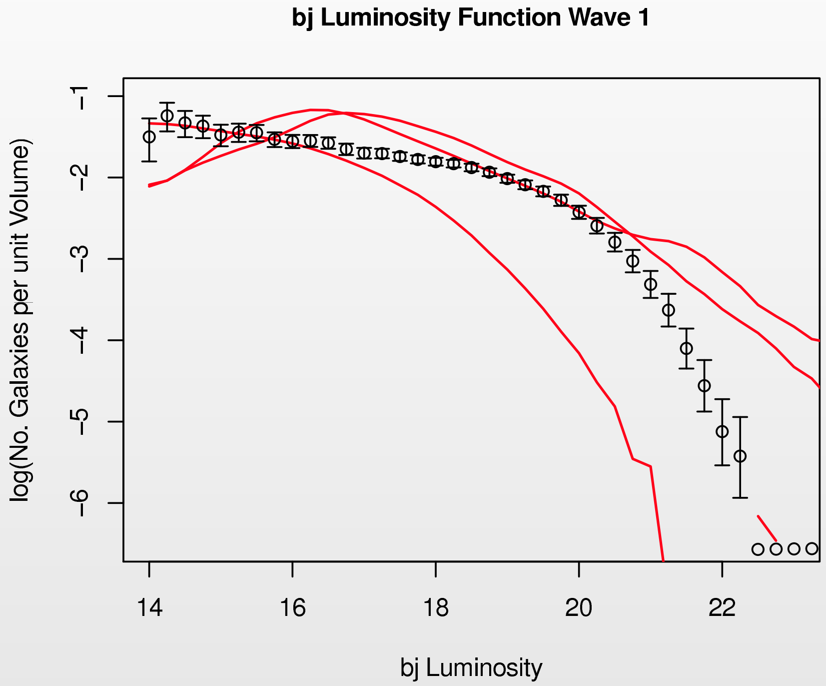
Galform Outputs: The Luminosity Functions

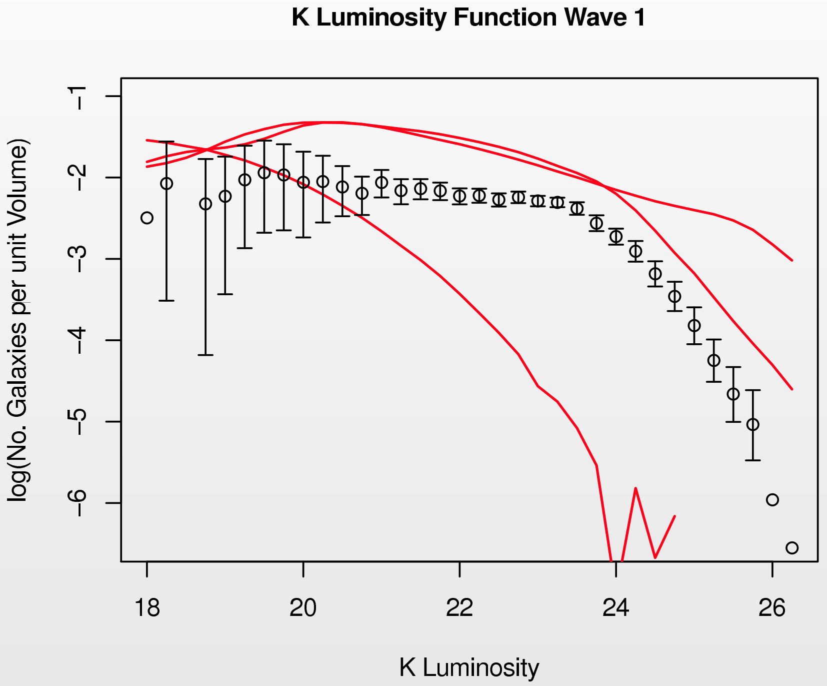




- Basic problem is that we pick inputs:
- vhotdisk $= 349.7$, aReheat $= 0.21$, alphacool $= 1.08$, ...
- And find that after 3 Days of Runtime:

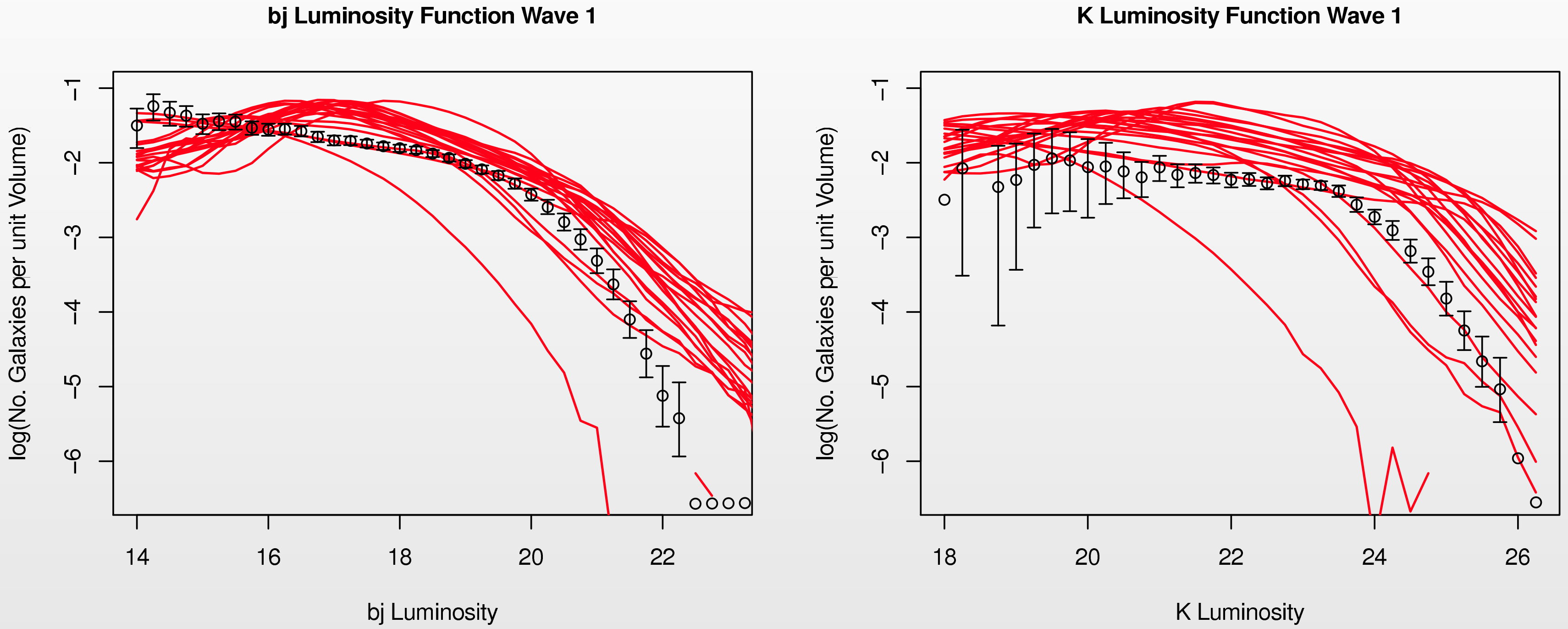
Galform Outputs: The Luminosity Functions





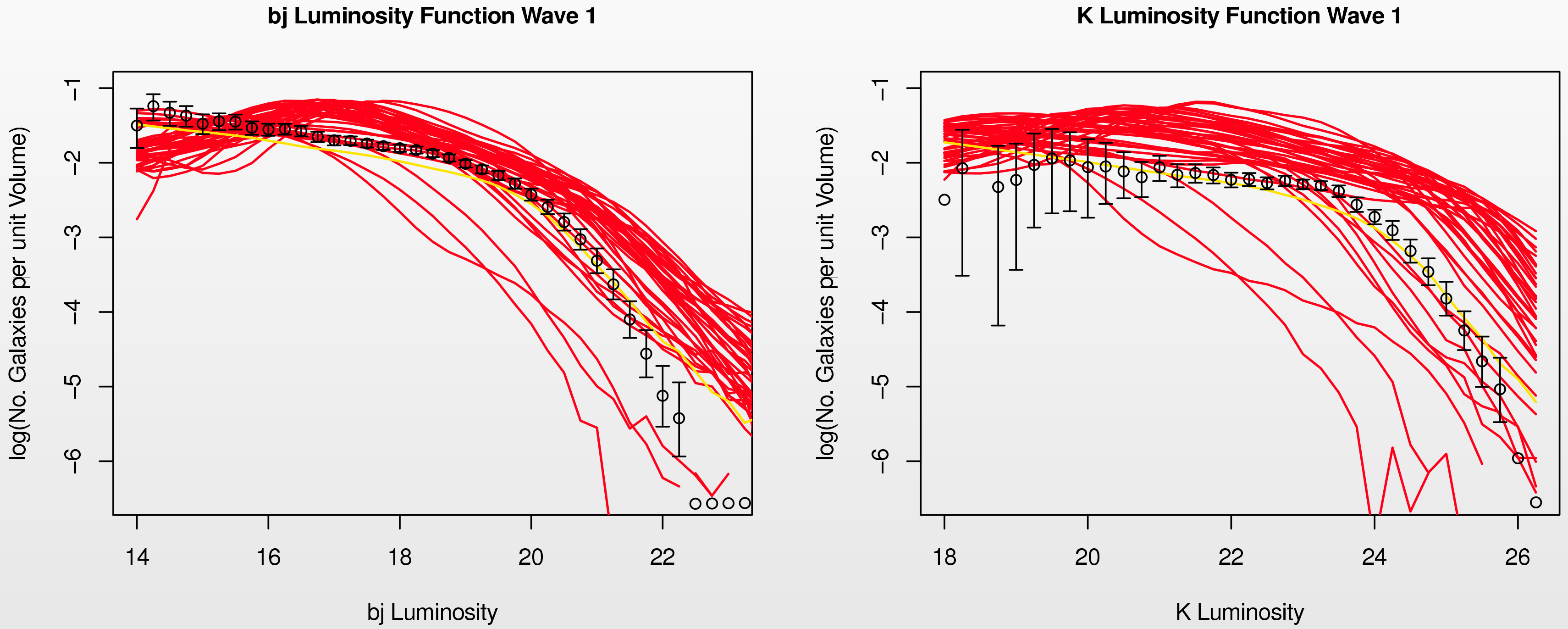
- Basic problem is that we pick inputs:
- vhotdisk $= 349.7$, aReheat $= 0.21$, alphacool $= 1.08$, ...
- And find that after 3 Days of Runtime:
- 3rd run is rubbish.

Galform Outputs: The Luminosity Functions



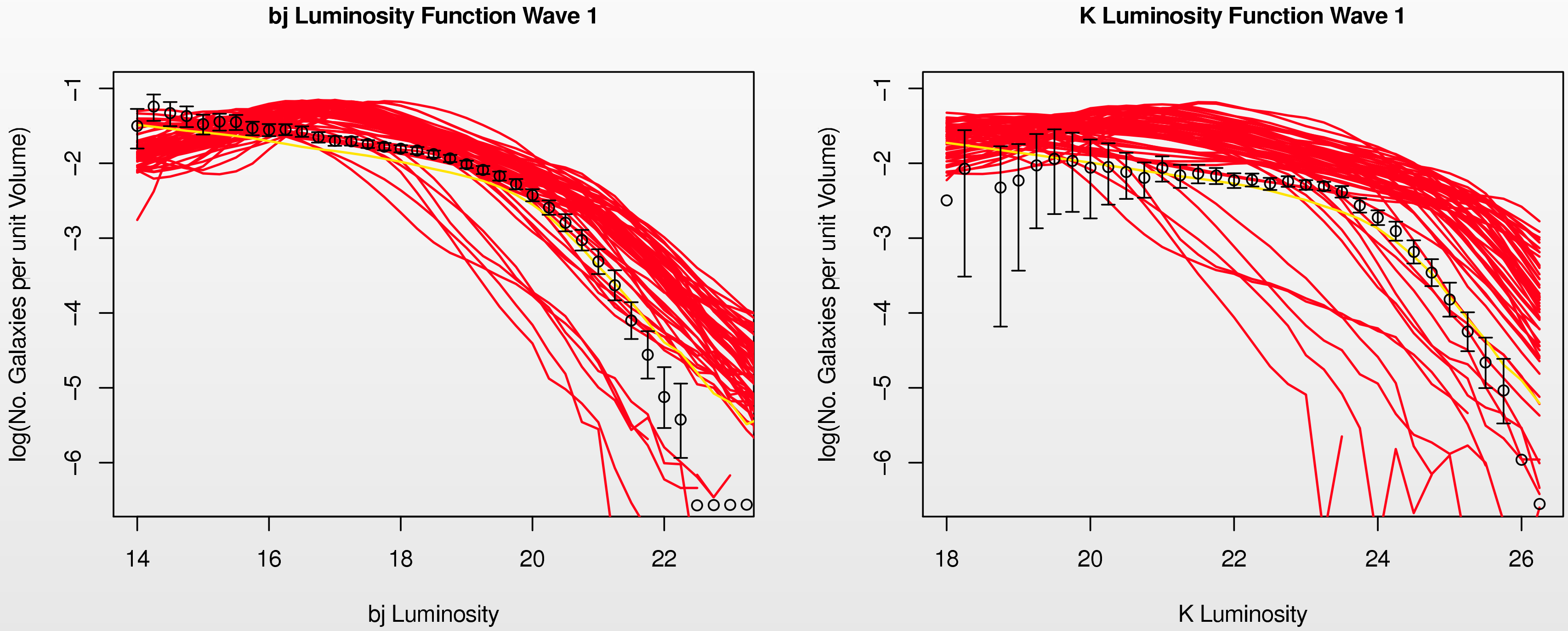
- Pick 20 inputs and find after 20 Days of Runtime:
- All runs are rubbish.

Galform Outputs: The Luminosity Functions



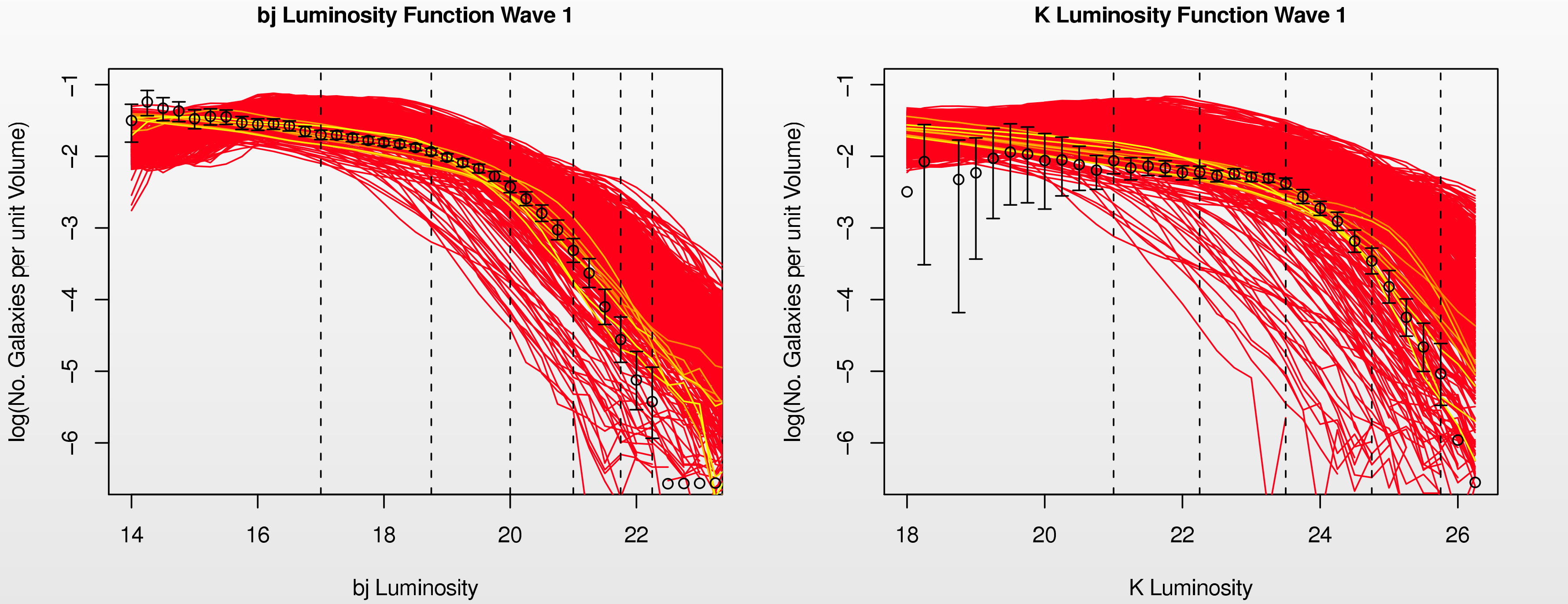
- Pick 40 inputs and find after 40 Days of Runtime:
- All runs are rubbish.

Galform Outputs: The Luminosity Functions



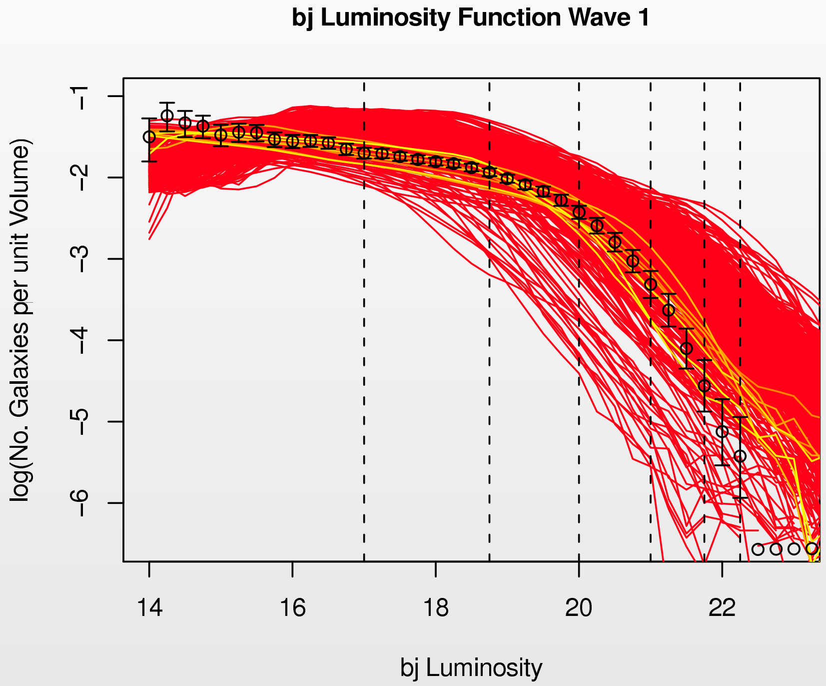
- Pick 60 inputs and find after 60 Days of Runtime:
- All runs are rubbish.

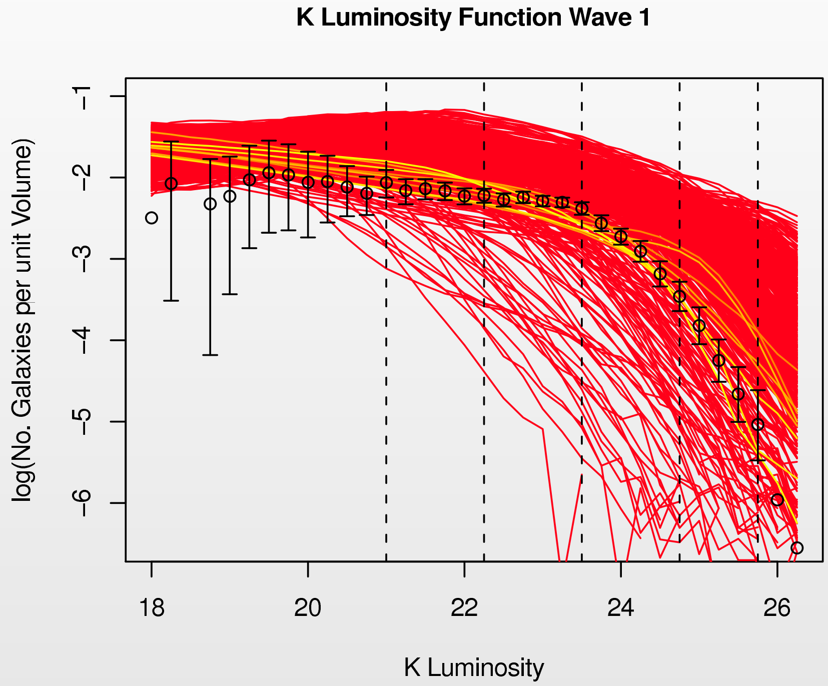
11 Outputs Chosen



- We do 1000 runs using carefully chosen inputs (a space-filling maximin latin hypercube design).
- (Again all runs are found to be unacceptable.)

11 Outputs Chosen

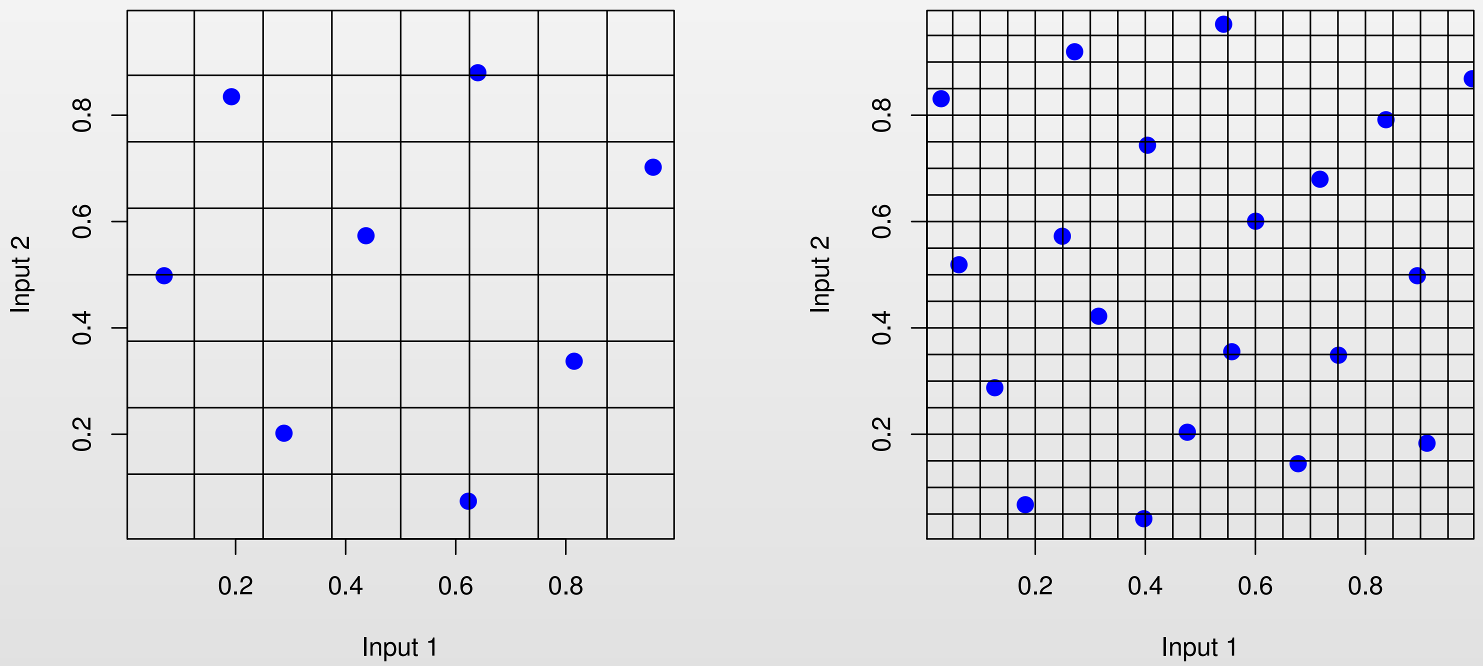




- We do 1000 runs using carefully chosen inputs (a space-filling maximin latin hypercube design).
- (Again all runs are found to be unacceptable.)
- We choose 11 outputs that are representative of the Luminosity functions and emulate these functions $f_i(x)$.

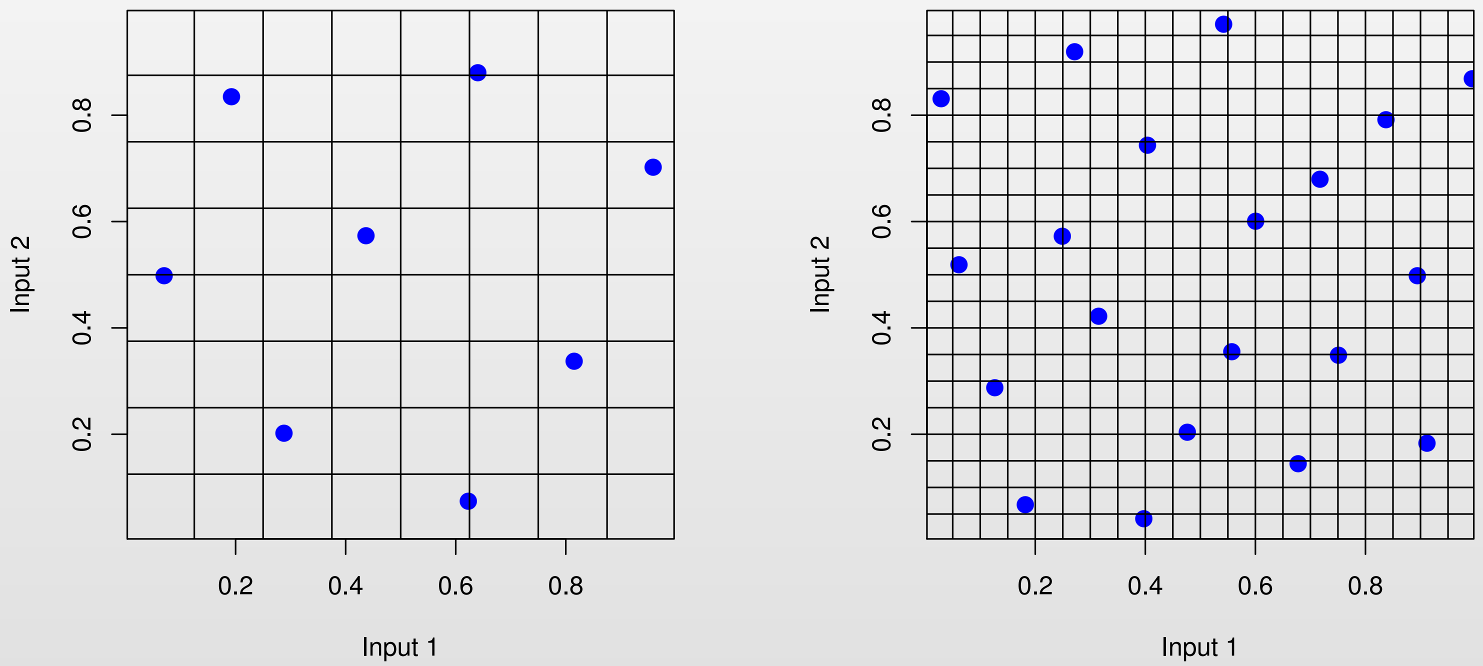
Design: Latin Hypercubes

- Design: Construct a batch of runs of the model using a space filling maximin Latin Hypercube design:



Design: Latin Hypercubes

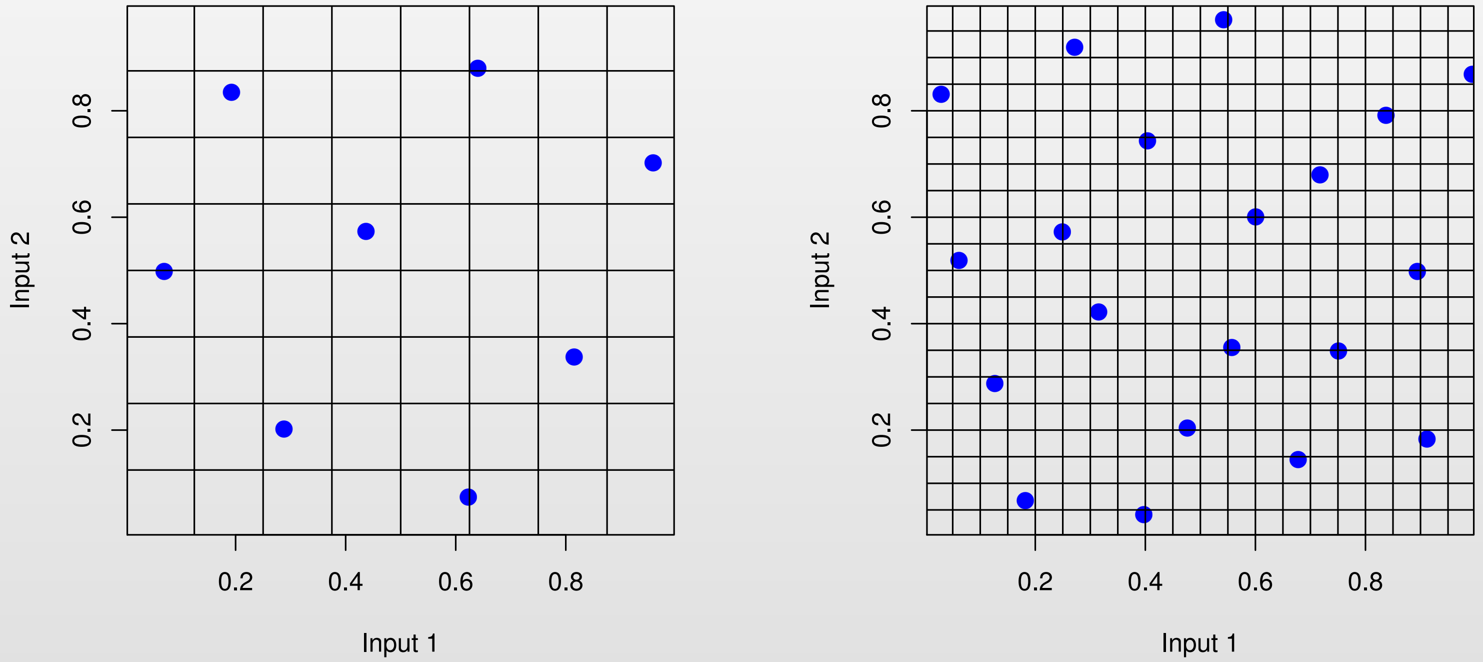
- Design: Construct a batch of runs of the model using a space filling maximin Latin Hypercube design:



- These designs are both space filling and approximately orthogonal, both desirable features for fitting emulators.

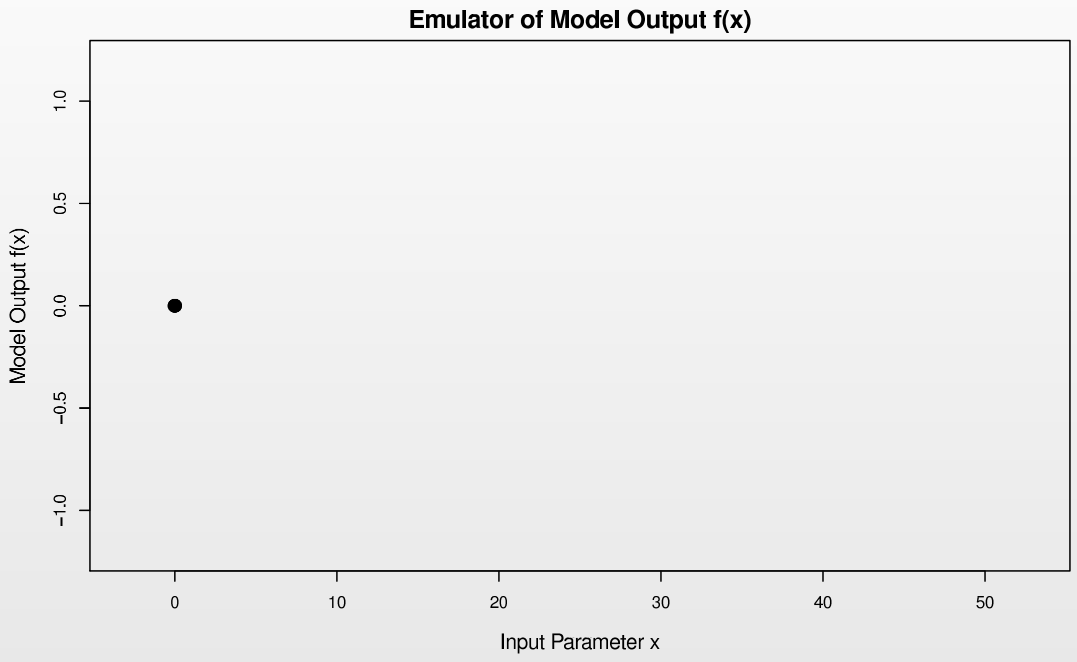
Design: Latin Hypercubes

- Design: Construct a batch of runs of the model using a space filling maximin Latin Hypercube design:

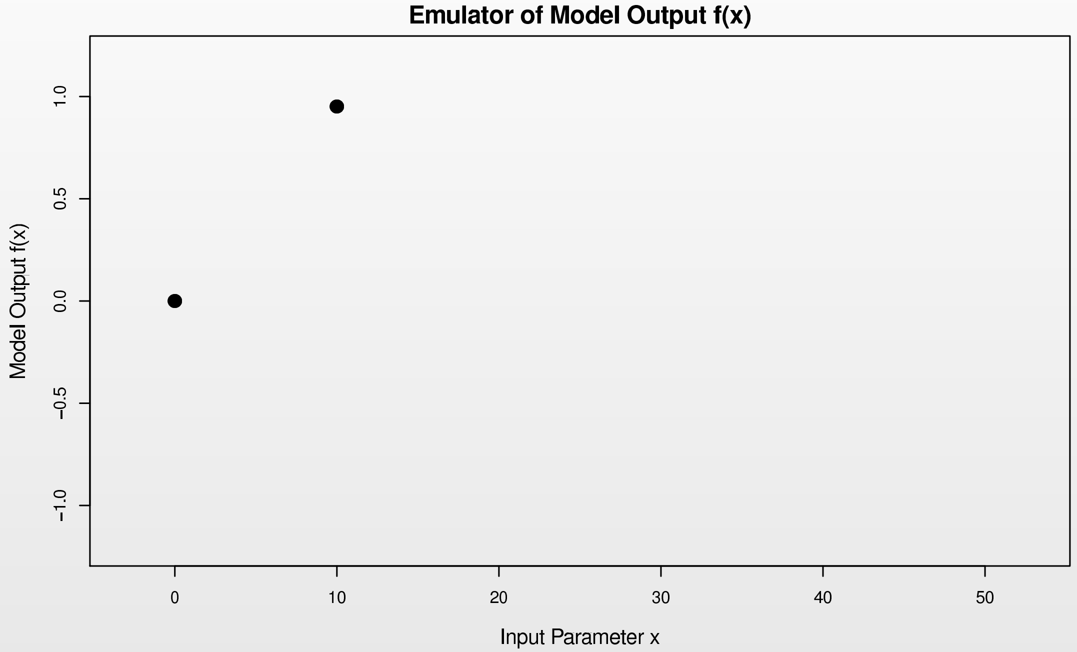


- These designs are both space filling and approximately orthogonal, both desirable features for fitting emulators.
- We evaluated 1000 runs of the model for the first Wave.

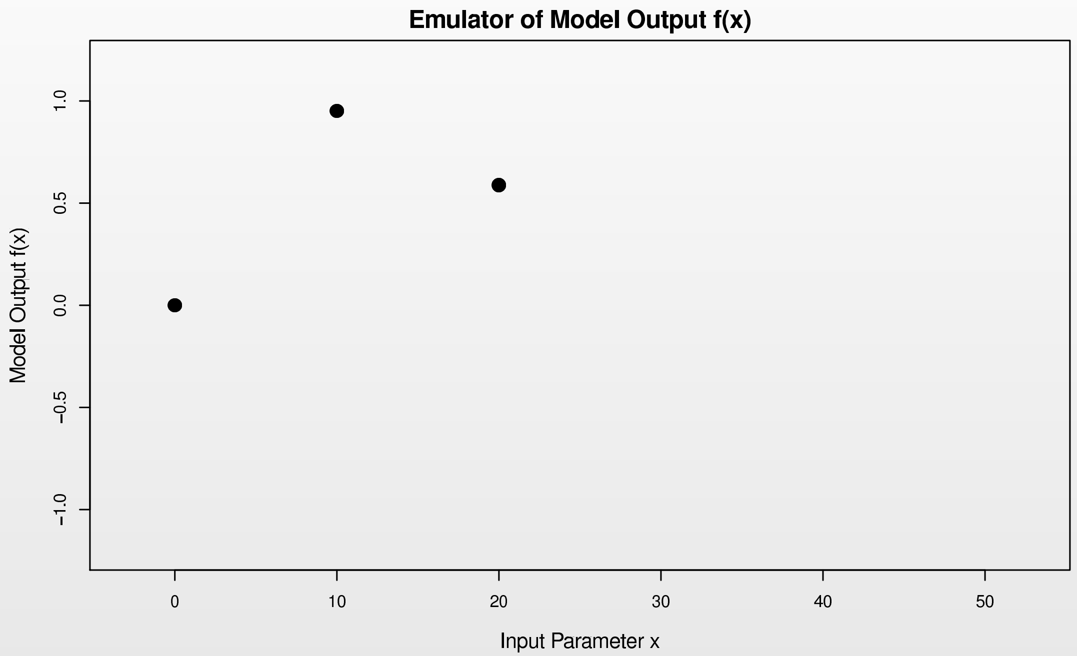
Emulation: a 1D Example



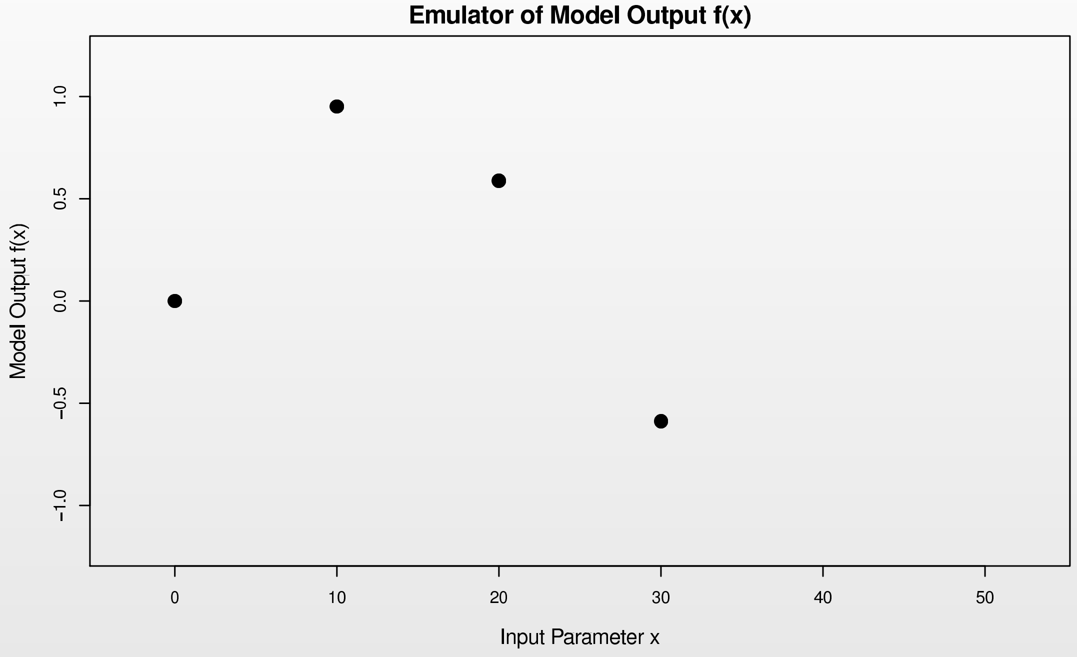
Emulation: a 1D Example



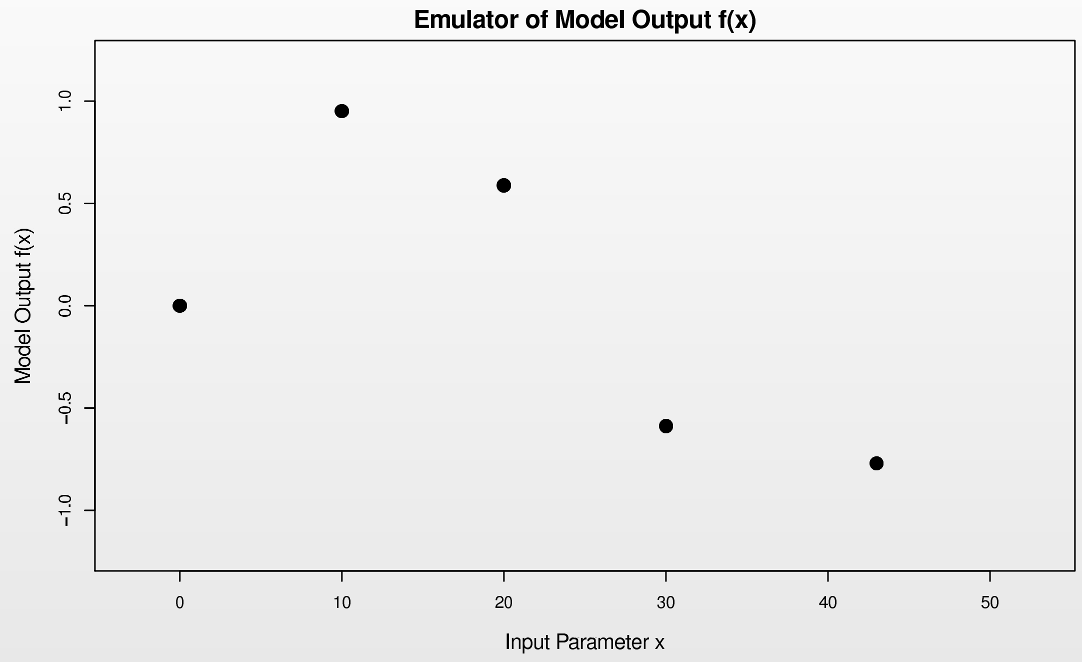
Emulation: a 1D Example



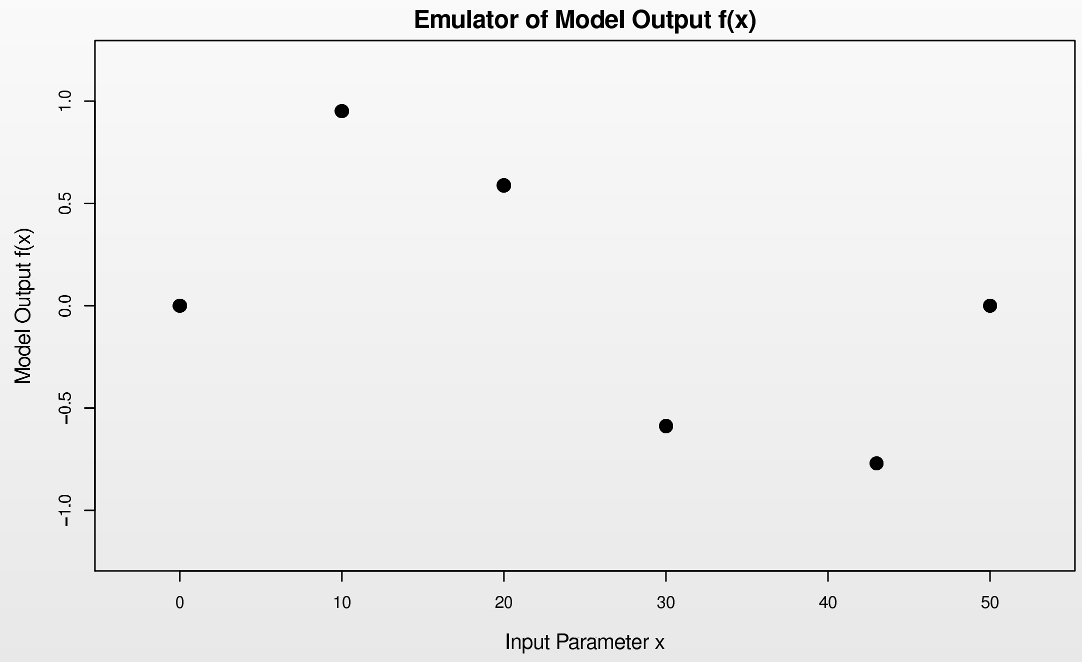
Emulation: a 1D Example



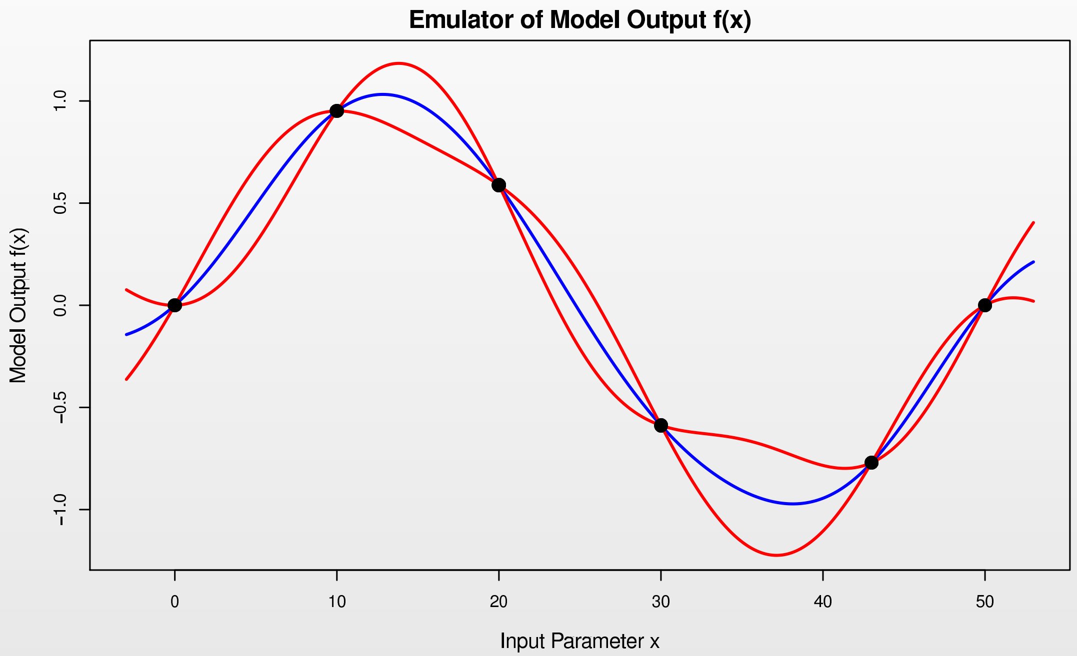
Emulation: a 1D Example



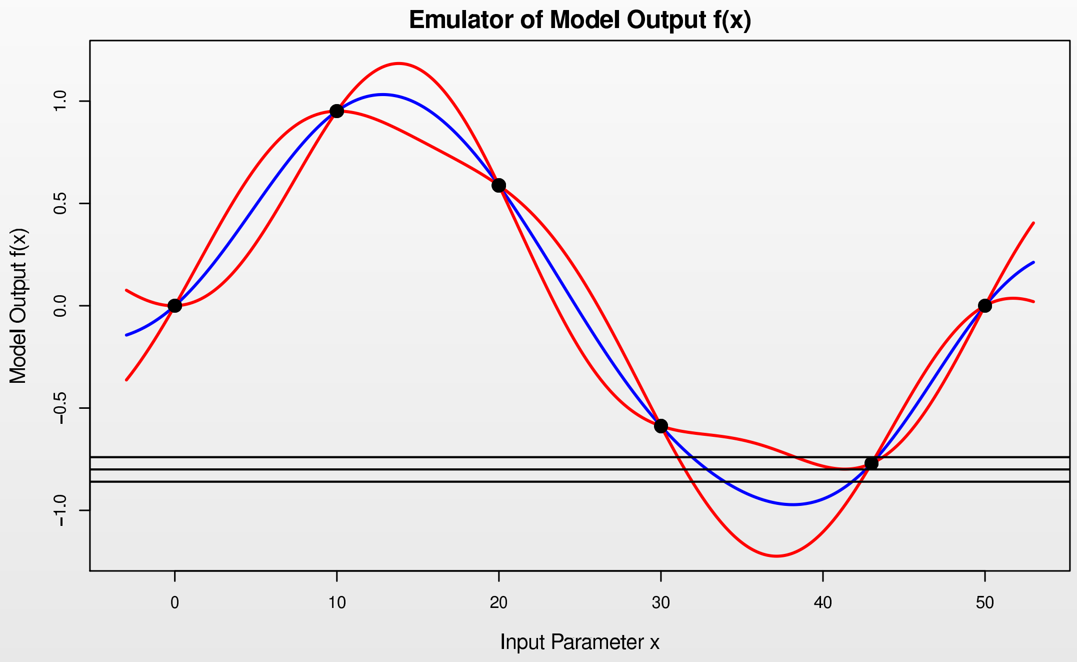
Emulation: a 1D Example



Emulation: a 1D Example



Emulation: a 1D Example



Linking Model to Reality

- We represent the model (Galform) as a function, which maps the 17 inputs x to the 11 outputs $f(x)$.

Linking Model to Reality

- We represent the model (Galform) as a function, which maps the 17 inputs x to the 11 outputs $f(x)$.
- We use the "Best Input Approach" to link the model $f(x)$ to the real system y (i.e. the real Universe) via:

$$y = f(x^*) + \epsilon$$

where we define ϵ to be the model discrepancy and assume that ϵ is independent of $f(x^*)$ and x^*.

Linking Model to Reality

- We represent the model (Galform) as a function, which maps the 17 inputs x to the 11 outputs $f(x)$.

- We use the "Best Input Approach" to link the model $f(x)$ to the real system y (i.e. the real Universe) via:

$$y = f(x^*) + \epsilon$$

  where we define ϵ to be the model discrepancy and assume that ϵ is independent of $f(x^*)$ and x^*.

- Finally, we relate the true system y to the observational data z by,

$$z = y + e$$

  where e represent the observational errors.

Linking Model to Reality

- We represent the model (Galform) as a function, which maps the 17 inputs x to the 11 outputs $f(x)$.

- We use the "Best Input Approach" to link the model $f(x)$ to the real system y (i.e. the real Universe) via:

$$y = f(x^*) + \epsilon$$

  where we define ϵ to be the model discrepancy and assume that ϵ is independent of $f(x^*)$ and x^*.

- Finally, we relate the true system y to the observational data z by,

$$z = y + e$$

  where e represent the observational errors.

- Often, scientists may be able to specify say $\mathrm{E}[\epsilon]$, $\mathrm{E}[e]$ (often zero), and $\mathrm{Var}[\epsilon]$, $\mathrm{Var}[e]$.

Galform: Emulation

- For each of the 11 outputs we pick active variables x^A then emulate univariately (at first) using:

$$f_i(x) = \sum_j \beta_{ij}\, g_{ij}(x^A) + u_i(x^A) + \delta_i(x)$$

Galform: Emulation

- For each of the 11 outputs we pick active variables x^A then emulate univariately (at first) using:

$$f_i(x) = \sum_j \beta_{ij}\, g_{ij}(x^A) + u_i(x^A) + \delta_i(x)$$

- The $\sum_j \beta_{ij}\, g_{ij}(x^A)$ is a 3rd order polynomial in the active inputs.

Galform: Emulation

- For each of the 11 outputs we pick active variables x^A then emulate univariately (at first) using:

$$f_i(x) = \sum_j \beta_{ij}\, g_{ij}(x^A) + u_i(x^A) + \delta_i(x)$$

- The $\sum_j \beta_{ij}\, g_{ij}(x^A)$ is a 3rd order polynomial in the active inputs.
- $u_i(x^A)$ is a Gaussian process.

Galform: Emulation

- For each of the 11 outputs we pick active variables x^A then emulate univariately (at first) using:

$$f_i(x) = \sum_j \beta_{ij}\, g_{ij}(x^A) + u_i(x^A) + \delta_i(x)$$

- The $\sum_j \beta_{ij}\, g_{ij}(x^A)$ is a 3rd order polynomial in the active inputs.
- $u_i(x^A)$ is a Gaussian process.
- The nugget $\delta_i(x)$ models the effects of inactive variables as random noise.

Galform: Emulation

- For each of the 11 outputs we pick active variables x^A then emulate univariately (at first) using:

$$f_i(x) = \sum_j \beta_{ij}\, g_{ij}(x^A) + u_i(x^A) + \delta_i(x)$$

- The $\sum_j \beta_{ij}\, g_{ij}(x^A)$ is a 3rd order polynomial in the active inputs.
- $u_i(x^A)$ is a Gaussian process.
- The nugget $\delta_i(x)$ models the effects of inactive variables as random noise.
- The $u_i(x^A)$ have covariance structure given by:

$$\mathrm{Cov}(u_i(x_1^A), u_i(x_2^A)) \quad = \quad \sigma_i^2 \exp[-|x_1^A - x_2^A|^2/\theta_i^2]$$

Galform: Emulation

- For each of the 11 outputs we pick active variables x^A then emulate univariately (at first) using:

$$f_i(x) = \sum_j \beta_{ij}\, g_{ij}(x^A) + u_i(x^A) + \delta_i(x)$$

- The $\sum_j \beta_{ij}\, g_{ij}(x^A)$ is a 3rd order polynomial in the active inputs.
- $u_i(x^A)$ is a Gaussian process.
- The nugget $\delta_i(x)$ models the effects of inactive variables as random noise.
- The $u_i(x^A)$ have covariance structure given by:

$$\mathrm{Cov}(u_i(x_1^A), u_i(x_2^A)) \quad = \quad \sigma_i^2 \exp[-|x_1^A - x_2^A|^2/\theta_i^2]$$

- The Emulators give the expectation $\mathsf{E}[f_i(x)]$ and variance $\mathsf{Var}(f_i(x))$ at point x for each output given by $i = 1, .., 11$, and are fast to evaluate.

Emulation Theory: Bayes Theorem

- We perform an initial wave 1 set of n runs at input locations $x^{(1)}, x^{(2)}, \ldots, x^{(n)}$ giving a column vector of model output values

$$D_i = (f_i(x^{(1)}), f_i(x^{(2)}), \ldots, f_i(x^{(n)}))^T$$

Emulation Theory: Bayes Theorem

- We perform an initial wave 1 set of n runs at input locations $x^{(1)}, x^{(2)}, \ldots, x^{(n)}$ giving a column vector of model output values

$$D_i = (f_i(x^{(1)}), f_i(x^{(2)}), \ldots, f_i(x^{(n)}))^T$$

- If we had provided prior distributions for each part of the emulator we could use Bayes Theorem to update our beliefs $\pi(f_i(x))$ about $f(x)$:

$$\pi(f_i(x)|D_i) = \frac{\pi(D_i|f_i(x))\pi(f_i(x))}{\pi(D_i)}$$

where $\pi(f_i(x))$ and $\pi(f_i(x)|D)$ are the prior and posterior pdfs for $f_i(x)$.

Emulation Theory: Bayes Theorem

- We perform an initial wave 1 set of n runs at input locations $x^{(1)}, x^{(2)}, \ldots, x^{(n)}$ giving a column vector of model output values

$$D_i = (f_i(x^{(1)}), f_i(x^{(2)}), \ldots, f_i(x^{(n)}))^T$$

- If we had provided prior distributions for each part of the emulator we could use Bayes Theorem to update our beliefs $\pi(f_i(x))$ about $f(x)$:

$$\pi(f_i(x)|D_i) = \frac{\pi(D_i|f_i(x))\pi(f_i(x))}{\pi(D_i)}$$

where $\pi(f_i(x))$ and $\pi(f_i(x)|D)$ are the prior and posterior pdfs for $f_i(x)$.

- This follows the standard Bayesian statistics paradigm, however this involves a detailed, full specification of the joint prior distribution: a complex and difficult task, and is hard to calculate.

Emulation Theory: Bayes Linear Methods

- There is a better way: if we are instead prepared to specify just the expectations, variances and covariances of the parts of the emulator, we can use Bayes Linear methodology.

Emulation Theory: Bayes Linear Methods

- There is a better way: if we are instead prepared to specify just the expectations, variances and covariances of the parts of the emulator, we can use Bayes Linear methodology.

- This is an alternative version of Bayesian statistics that is easier to specify and far easier to calculate with.

Emulation Theory: Bayes Linear Methods

- There is a better way: if we are instead prepared to specify just the expectations, variances and covariances of the parts of the emulator, we can use Bayes Linear methodology.

- This is an alternative version of Bayesian statistics that is easier to specify and far easier to calculate with.

- Instead of Bayes Theorem we use the Bayes linear update:

$$\begin{aligned} \mathrm{E}_{D_i}(f_i(x)) &= \mathrm{E}(f_i(x)) + \mathrm{Cov}(f_i(x), D_i)\mathrm{Var}(D_i)^{-1}(D_i - \mathrm{E}(D_i)) \\ \mathrm{Var}_{D_i}(f_i(x)) &= \mathrm{Var}(f_i(x)) - \mathrm{Cov}(f_i(x), D_i)\mathrm{Var}(D_i)^{-1}\mathrm{Cov}(D_i, f_i(x)) \end{aligned}$$

where $\mathrm{E}_{D_i}(f_i(x))$ and $\mathrm{Var}_{D_i}(f_i(x))$ are the Bayes Linear adjusted expectation and variance for $f_i(x)$ at new input point x, and are all that are needed for the subsequent implausibility measures and history match.

Model Discrepancy

Before calculating the implausibility we need to assess the Model Discrepancy and Measurement error.

Model Discrepancy $\text{Var}(\epsilon) = \Phi_{40} + \Phi_9 + \Phi_E$

- Φ_{40}: Discrepancy term due to choosing first 40 sub-volumes from full 512 sub-volumes. Assess this by repeating 100 runs but now choosing 40 random regions.

- Φ_9: As we have neglected 9 parameters (due to expert advice) we need to assess effect of this (by running latin hypercube design across all 17 parameters)

- Φ_E: Expert assessment of model discrepancy of full model with 17 parameters and using 512 sub-volumes

It is straightforward to find the multivariate expressions for Φ_{40} and Φ_9, but Φ_E requires more careful thought.

Model Discrepancy: Subjective Φ_E

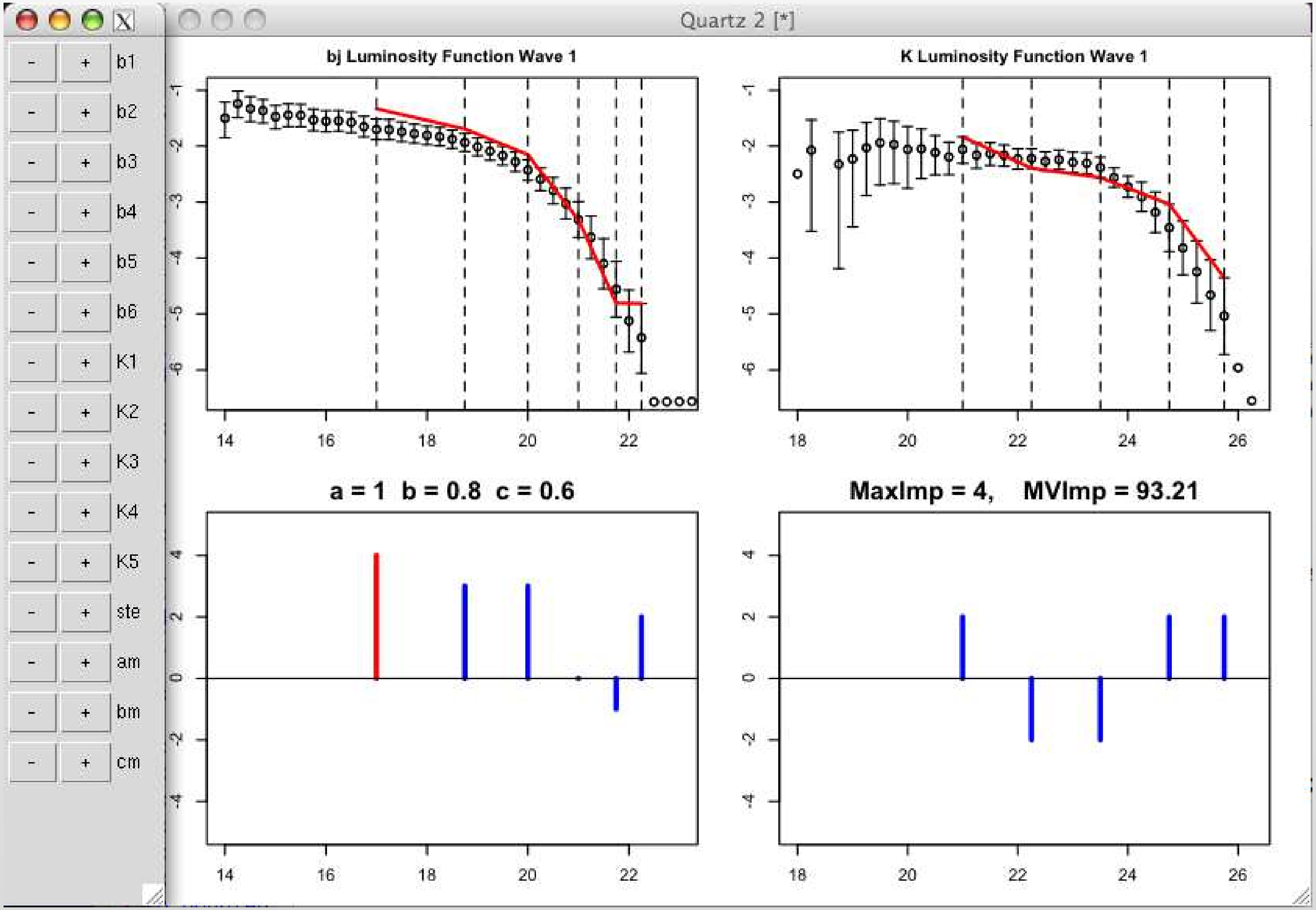
- Experts assert that there are clear ways that the model could be defective.
- Model predicts too many (or too few) galaxies. This would lead to a highly correlated model discrepancy across all outputs.
- Model systematically gets the colours of galaxies wrong: results in too few (too many) blue galaxies and too many (too few) red galaxies. Gives negatively correlated model discrepancy between outputs from different coloured (bj and K) luminosity graphs.
- We therefore assume the model discrepancy term Φ_E has the form:

$$\Phi_E = a \begin{pmatrix} 1 & b & .. & c & .. & c \\ b & 1 & .. & c & . & c \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ c & .. & c & 1 & b & .. \\ c & .. & c & b & 1 & .. \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

- Obtain values for a, b and c from expert assessment.

Expert Assessment of Φ_E: Elicitation Tool

- We obtain expert assessments of a, b and c using an elicitation tool.



Measurement Error

Observational Errors $\text{Var}(e)$ are composed of 4 parts:

- Normalisation Error: correlated vertical error on all luminosity output points
- Luminostiy Zero Point Error: correlated horizontal error on all luminosity points
- $k + e$ Correction Error: Outputs have to be corrected for the fact that galaxies are moving away from us at different speeds (light is red-shifted), and for the fact that galaxies are seen in the past (as light takes millions of years to reach us)
- Galaxy Production Error: assumed Poisson process to describe galaxy production

The multivariate form for each of these quantities is straightforward(!) to calculate.

Implausibility Measures (Univariate)

We can now calculate the Implausibility $I_{(i)}(x)$ at any input parameter point x for each of the $i = 1, .., 11$ outputs. This is given by:

$$I_{(i)}^2(x) = \frac{|\mathrm{E}_{D_i}(f_i(x)) - z_i|^2}{(\mathrm{Var}_{D_i}(f_i(x)) + \mathrm{Var}[\epsilon_i] + \mathrm{Var}[e_i])}$$

Implausibility Measures (Univariate)

We can now calculate the Implausibility $I_{(i)}(x)$ at any input parameter point x for each of the $i = 1, .., 11$ outputs. This is given by:

$$I_{(i)}^2(x) = \frac{|\mathrm{E}_{D_i}(f_i(x)) - z_i|^2}{(\mathrm{Var}_{D_i}(f_i(x)) + \mathrm{Var}[\epsilon_i] + \mathrm{Var}[e_i])}$$

- $\mathrm{E}_{D_i}(f_i(x))$ and $\mathrm{Var}_{D_i}(f_i(x))$ are the emulator expectation and variance.

Implausibility Measures (Univariate)

We can now calculate the Implausibility $I_{(i)}(x)$ at any input parameter point x for each of the $i = 1, .., 11$ outputs. This is given by:

$$I^2_{(i)}(x) = \frac{|\mathrm{E}_{D_i}(f_i(x)) - z_i|^2}{(\mathrm{Var}_{D_i}(f_i(x)) + \mathrm{Var}[\epsilon_i] + \mathrm{Var}[e_i])}$$

- $\mathrm{E}_{D_i}(f_i(x))$ and $\mathrm{Var}_{D_i}(f_i(x))$ are the emulator expectation and variance.
- z_i are the observed data and $\mathrm{Var}[\epsilon_i]$ and $\mathrm{Var}[e_i]$ are the (univariate) Model Discrepancy and Observational Error variances.

Implausibility Measures (Univariate)

We can now calculate the Implausibility $I_{(i)}(x)$ at any input parameter point x for each of the $i = 1, .., 11$ outputs. This is given by:

$$I^2_{(i)}(x) = \frac{|\mathrm{E}_{D_i}(f_i(x)) - z_i|^2}{(\mathrm{Var}_{D_i}(f_i(x)) + \mathrm{Var}[\epsilon_i] + \mathrm{Var}[e_i])}$$

- $\mathrm{E}_{D_i}(f_i(x))$ and $\mathrm{Var}_{D_i}(f_i(x))$ are the emulator expectation and variance.
- z_i are the observed data and $\mathrm{Var}[\epsilon_i]$ and $\mathrm{Var}[e_i]$ are the (univariate) Model Discrepancy and Observational Error variances.
- **Large values** of $I_{(i)}(x)$ imply that we are highly unlikely to obtain acceptable matches between model output and observed data at input x.

Implausibility Measures (Univariate)

We can now calculate the Implausibility $I_{(i)}(x)$ at any input parameter point x for each of the $i = 1, .., 11$ outputs. This is given by:

$$I_{(i)}^2(x) = \frac{|\mathrm{E}_{D_i}(f_i(x)) - z_i|^2}{(\mathrm{Var}_{D_i}(f_i(x)) + \mathrm{Var}[\epsilon_i] + \mathrm{Var}[e_i])}$$

- $\mathrm{E}_{D_i}(f_i(x))$ and $\mathrm{Var}_{D_i}(f_i(x))$ are the emulator expectation and variance.
- z_i are the observed data and $\mathrm{Var}[\epsilon_i]$ and $\mathrm{Var}[e_i]$ are the (univariate) Model Discrepancy and Observational Error variances.
- **Large values** of $I_{(i)}(x)$ imply that we are highly unlikely to obtain acceptable matches between model output and observed data at input x.
- Small values of $I_{(i)}(x)$ do not imply that x is good!

Implausibility Measures (Univariate)

- We can combine the univariate implausibilities across the 11 outputs by maximizing over the current outputs:

$$I_M(x) = \max_{i \in Q} I_{(i)}(x)$$

Implausibility Measures (Univariate)

- We can combine the univariate implausibilities across the 11 outputs by maximizing over the current outputs:

$$I_M(x) = \max_{i \in Q} I_{(i)}(x)$$

- We can then impose a cutoff

$$I_M(x) < c_M$$

in order to discard regions of input parameter space x that we now deem to be implausible.

Implausibility Measures (Univariate)

- We can combine the univariate implausibilities across the 11 outputs by maximizing over the current outputs:

$$I_M(x) = \max_{i \in Q} I_{(i)}(x)$$

- We can then impose a cutoff

$$I_M(x) < c_M$$

in order to discard regions of input parameter space x that we now deem to be implausible.

- The choice of cutoff c_M is often motivated by Pukelsheim's 3-sigma rule, which does not require precise distributions.

Implausibility Measures (Univariate)

- We can combine the univariate implausibilities across the 11 outputs by maximizing over the current outputs:

$$I_M(x) = \max_{i \in Q} I_{(i)}(x)$$

- We can then impose a cutoff

$$I_M(x) < c_M$$

in order to discard regions of input parameter space x that we now deem to be implausible.

- The choice of cutoff c_M is often motivated by Pukelsheim's 3-sigma rule, which does not require precise distributions.

- We may simultaneously employ other choices of implausibility measure: e.g. multivariate, second maximum etc.

Multivariate Implausibility Measure

- As we have constructed a multivariate model discrepancy, we can define a multivariate Implausibility measure:

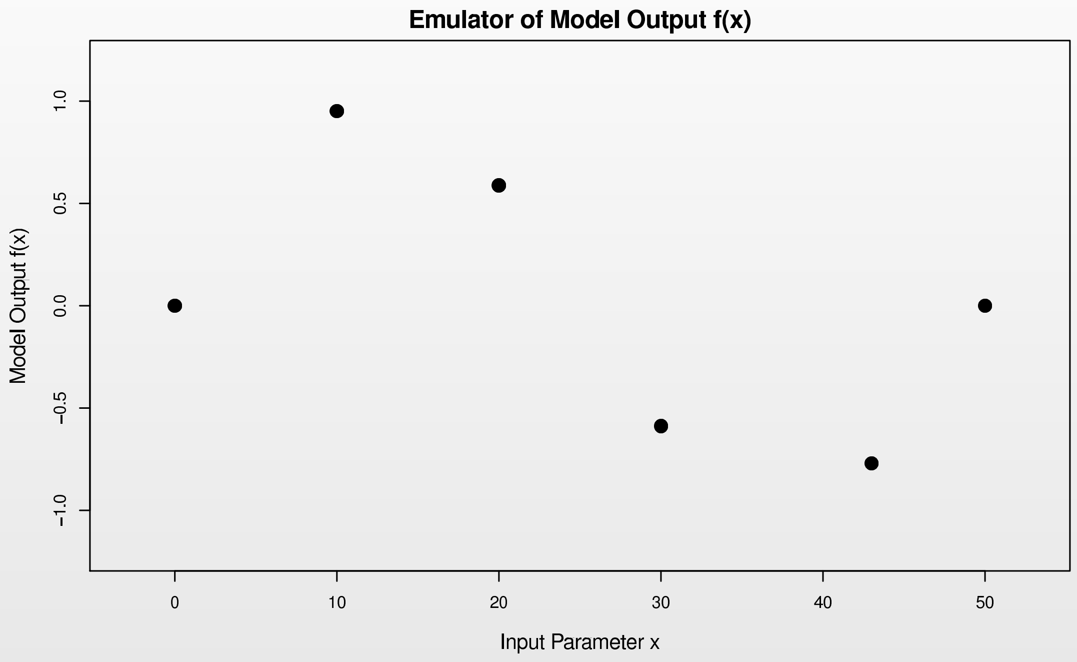
$$I^2(x) = (\mathrm{E}[f(x)] - z)^T \mathrm{Var}[f(x) - z]^{-1} (\mathrm{E}[f(x)] - z),$$

which becomes:

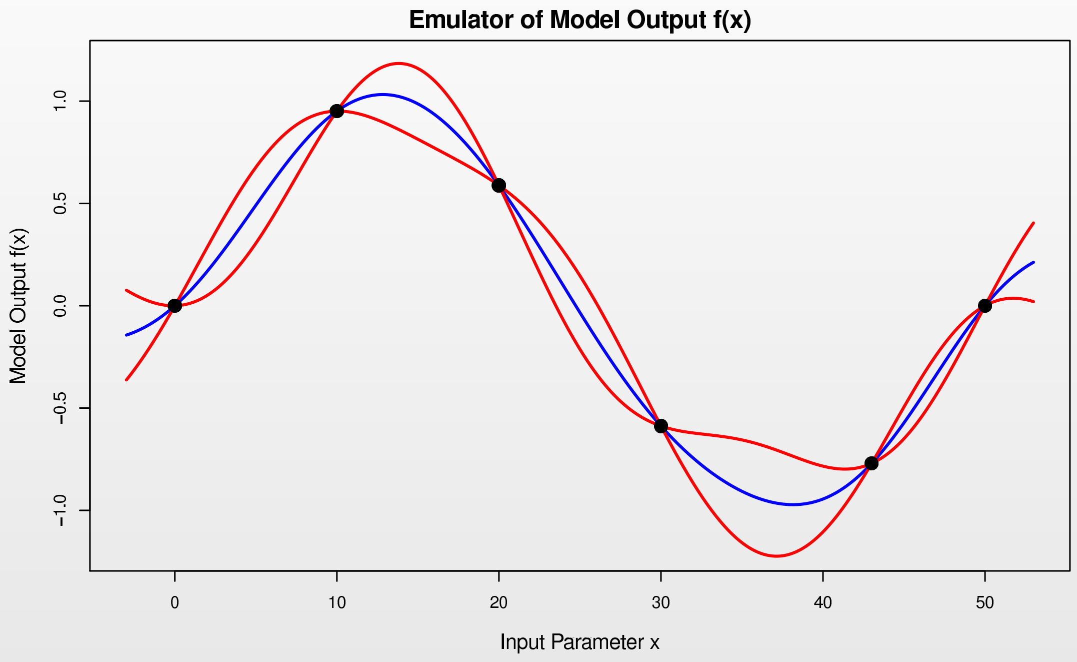
$$I^2(x) = (\mathrm{E}[f(x)] - z)^T (\mathrm{Var}[f(x)] + \mathrm{Var}[\epsilon] + \mathrm{Var}[e])^{-1} (\mathrm{E}[f(x)] - z)$$

- where $\mathrm{Var}[f(x)]$, $\mathrm{Var}[\epsilon]$ and $\mathrm{Var}[e]$ are now the multivariate emulator variance, multivariate model discrepancy and multivariate observational errors respectively (all 11$\times$11 matrices).
- We now have two implausibility measures $I_M(x)$ and $I(x)$ that we can use to reduce the input space.
- We impose suitable cutoffs on each measure to define a smaller set of non-implausible inputs.

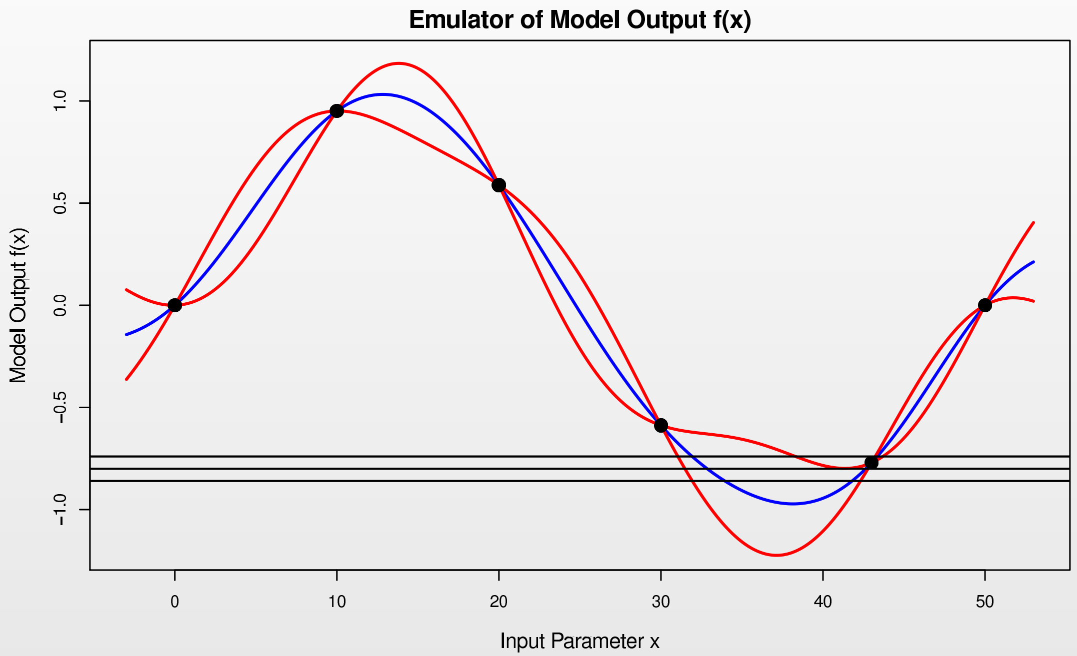
History Matching via Implausibility: a 1D Example



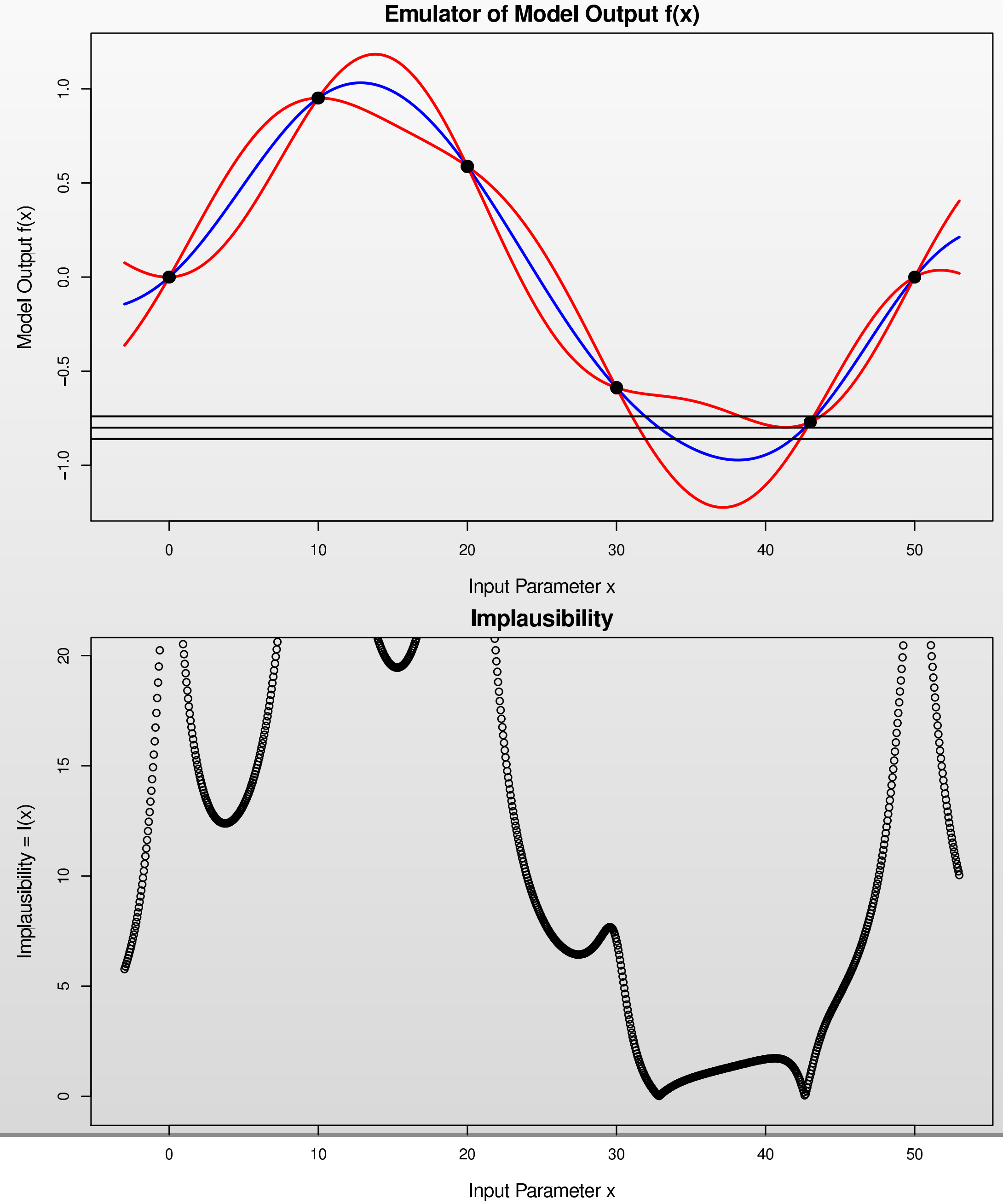
History Matching via Implausibility: a 1D Example



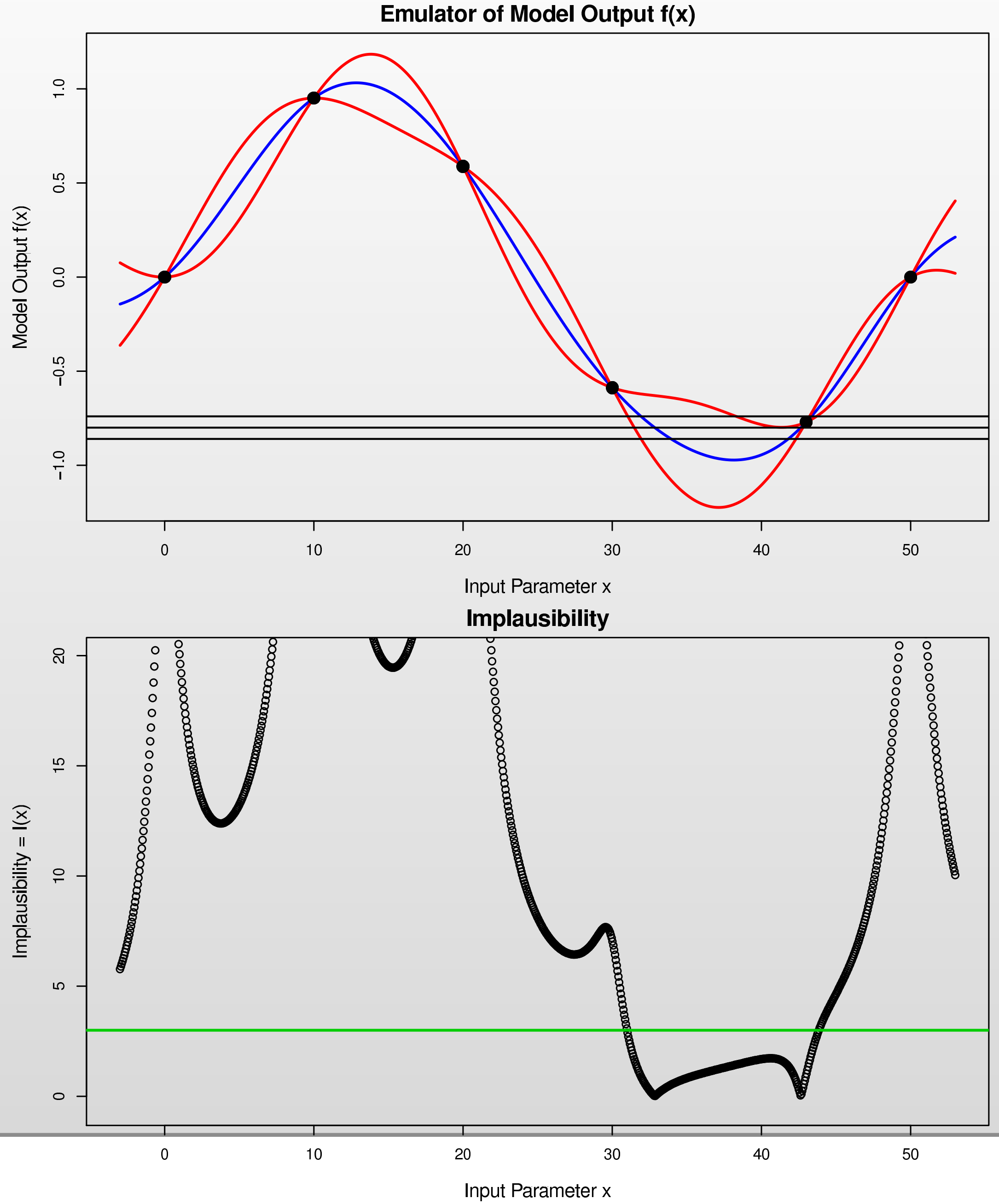
History Matching via Implausibility: a 1D Example



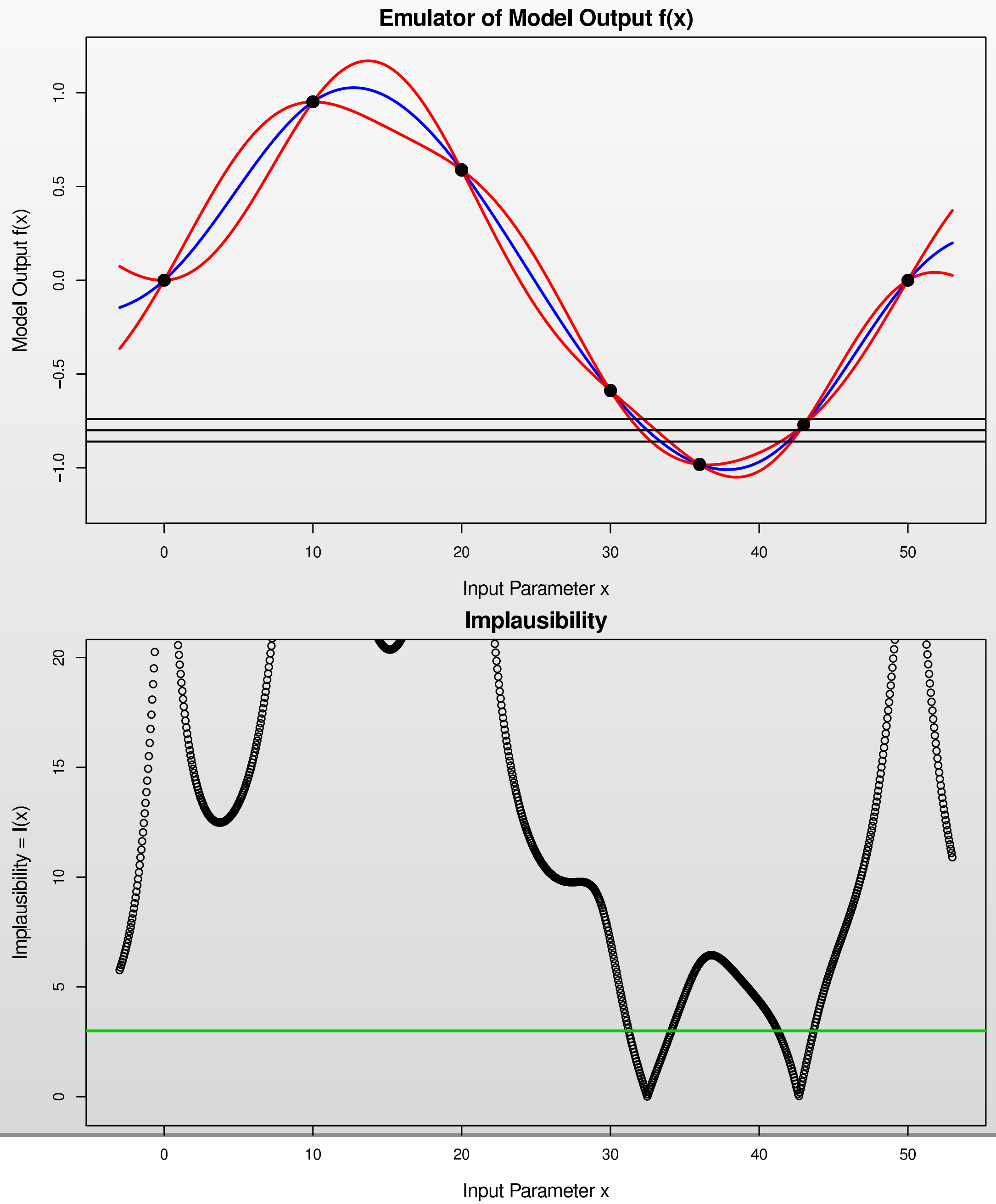
History Matching via Implausibility: a 1D Example



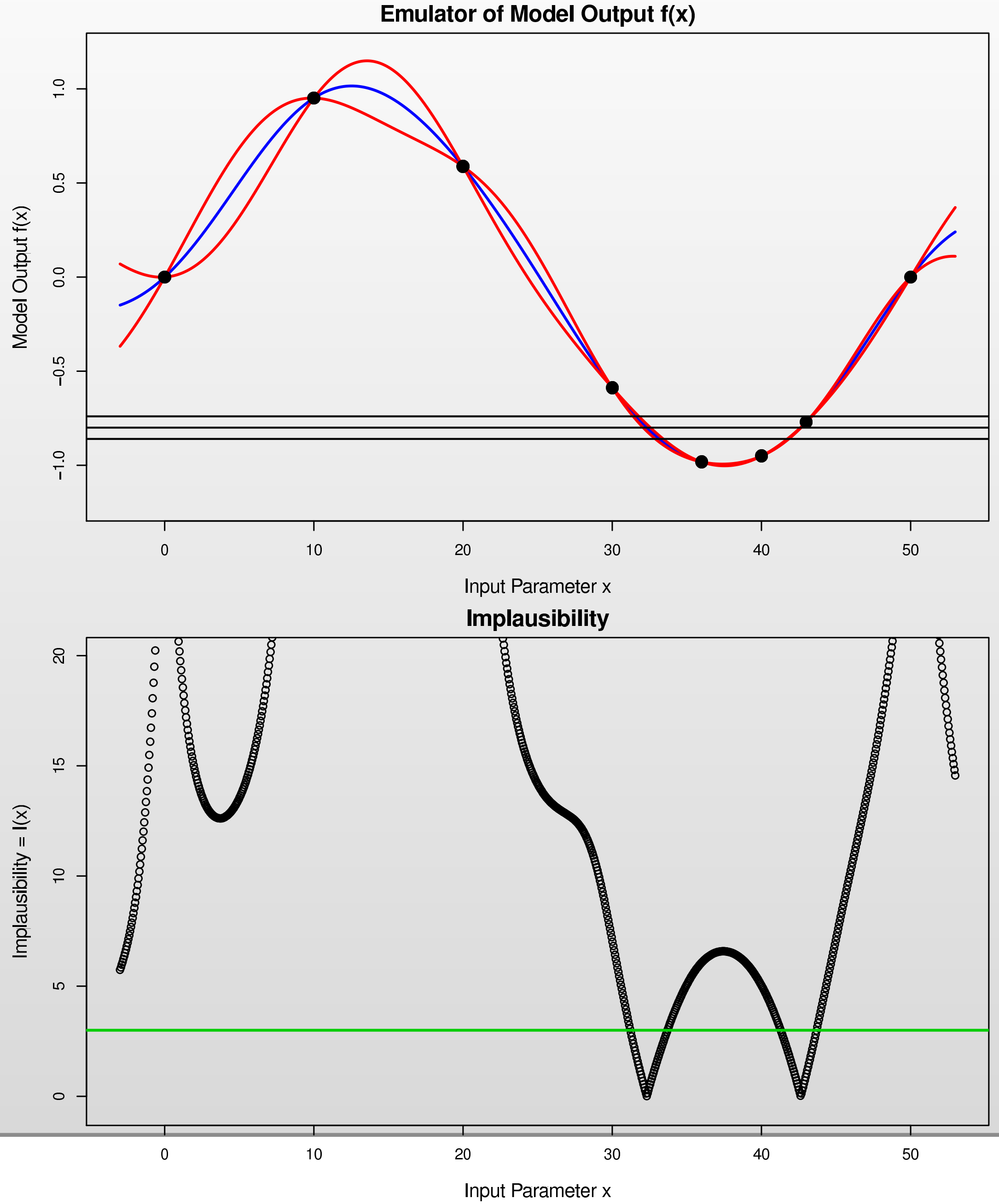
History Matching via Implausibility: a 1D Example



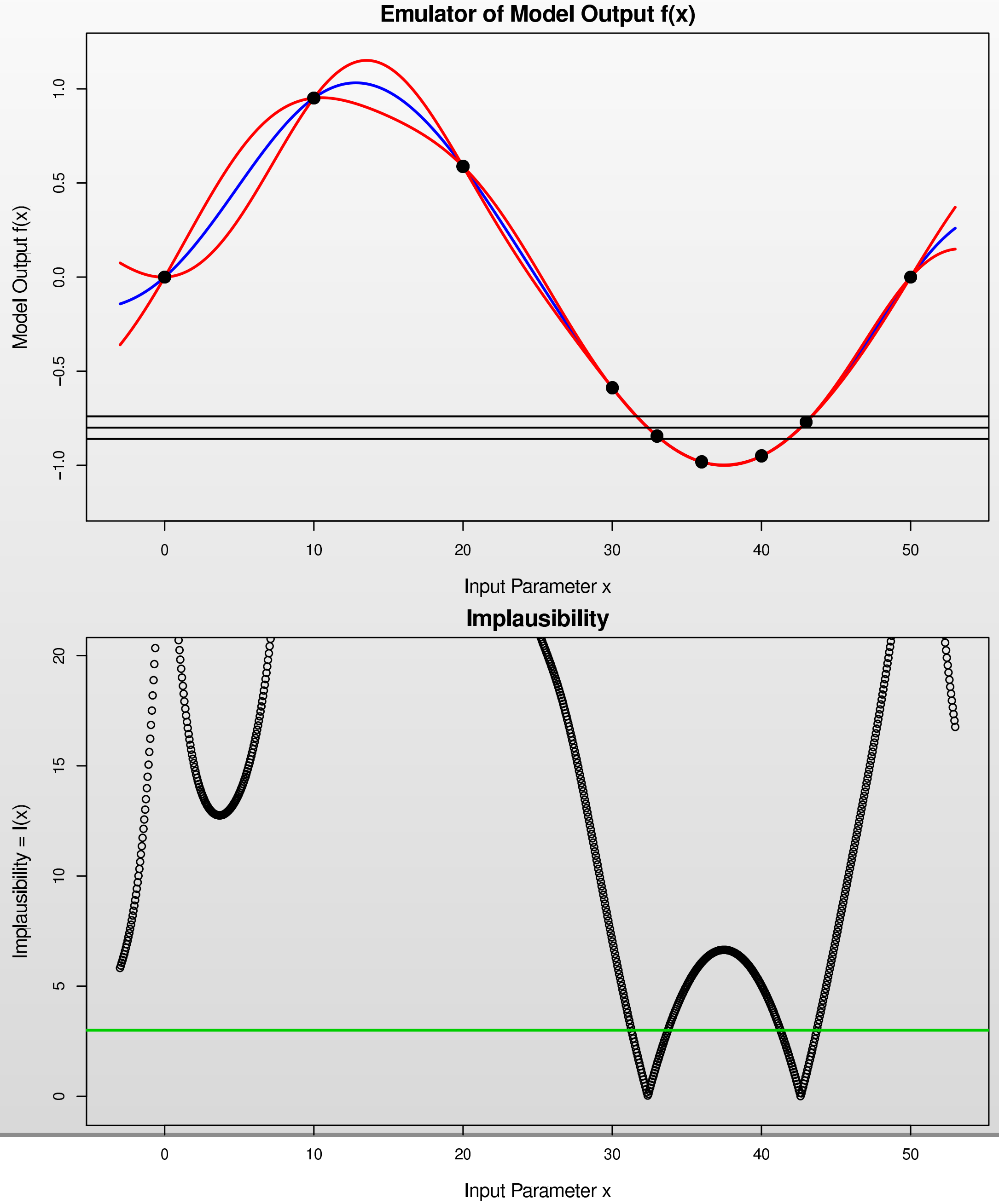
History Matching via Implausibility: a 1D Example



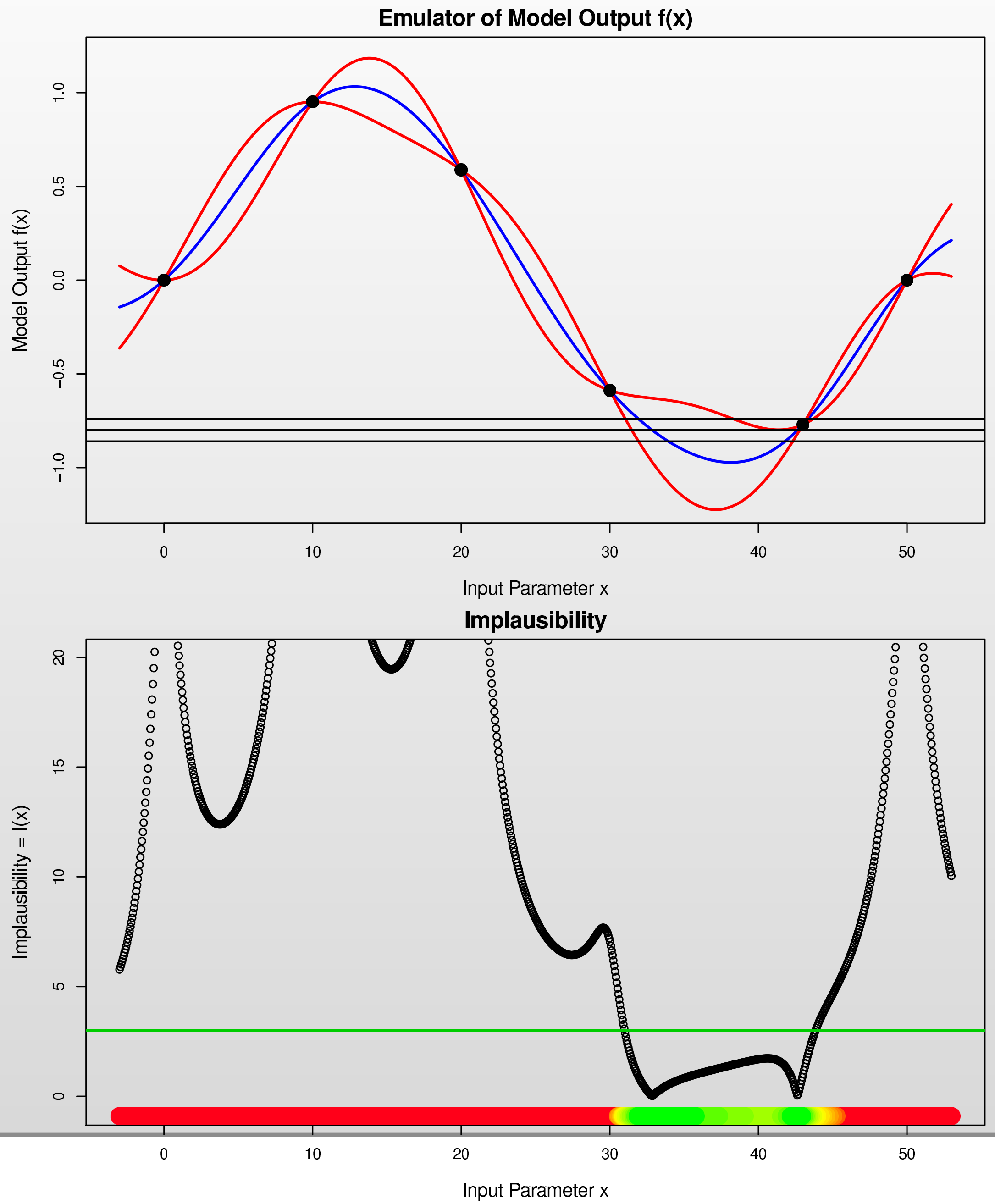
History Matching via Implausibility: a 1D Example



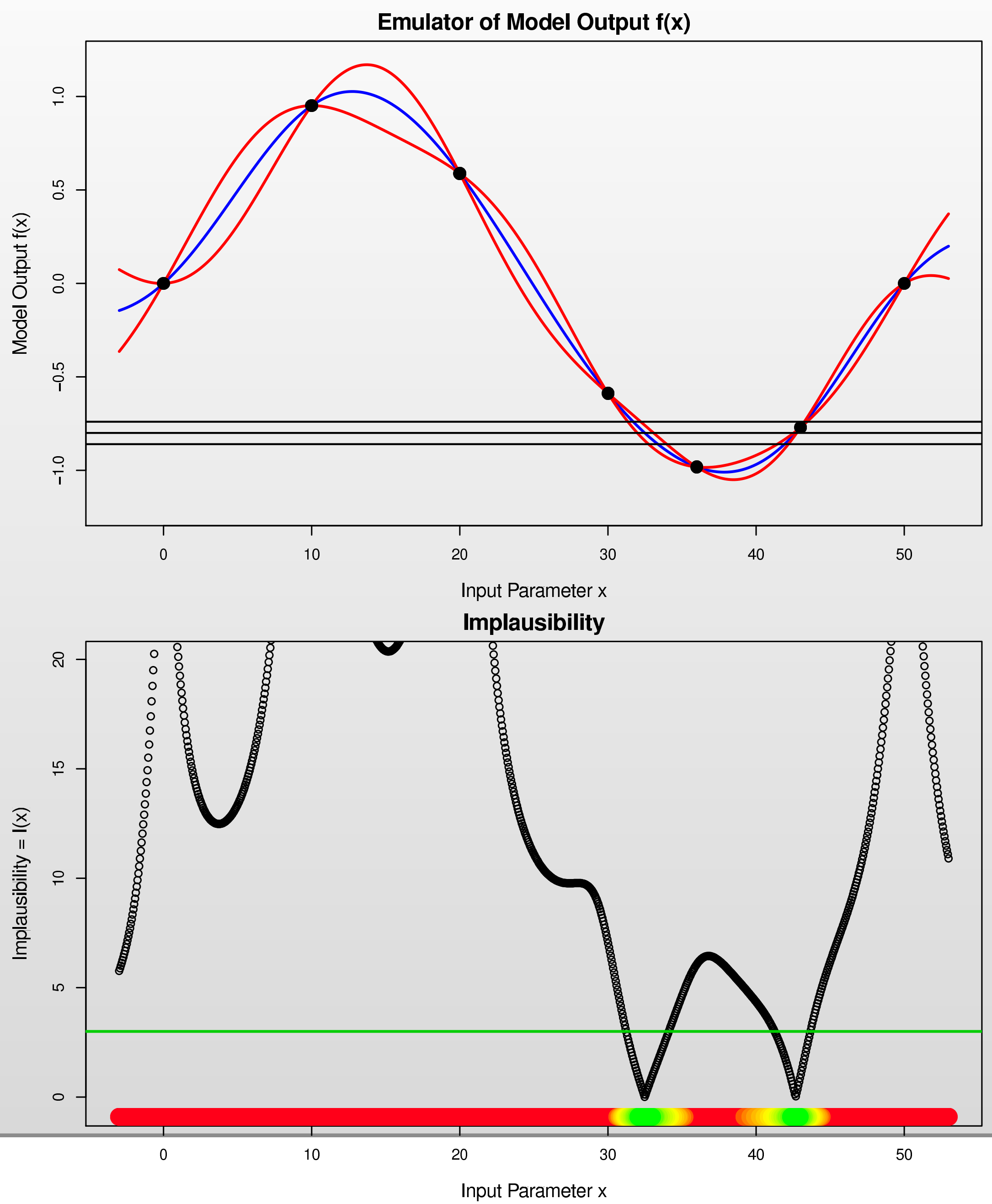
History Matching via Implausibility: a 1D Example



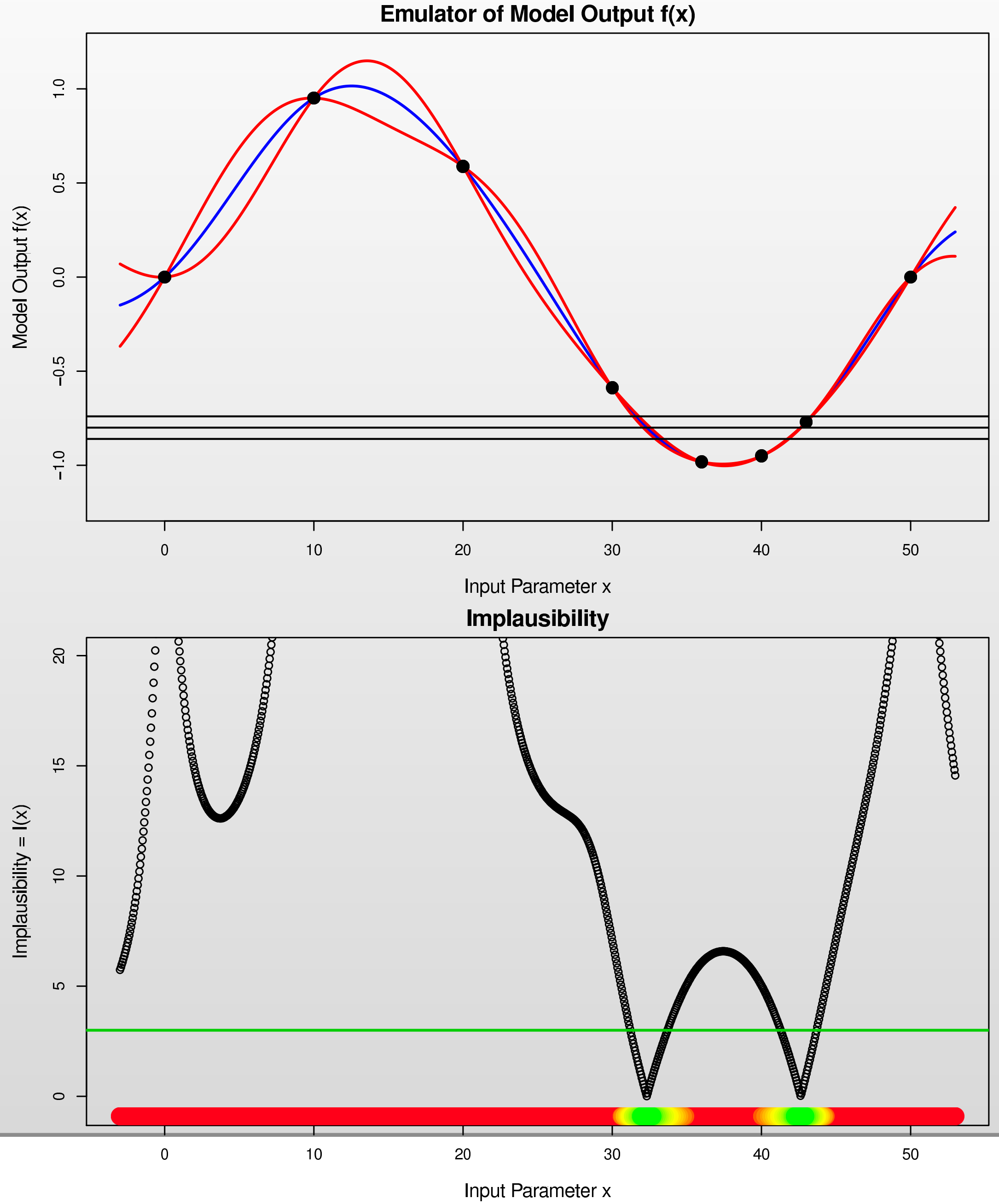
History Matching via Implausibility: a 1D Example



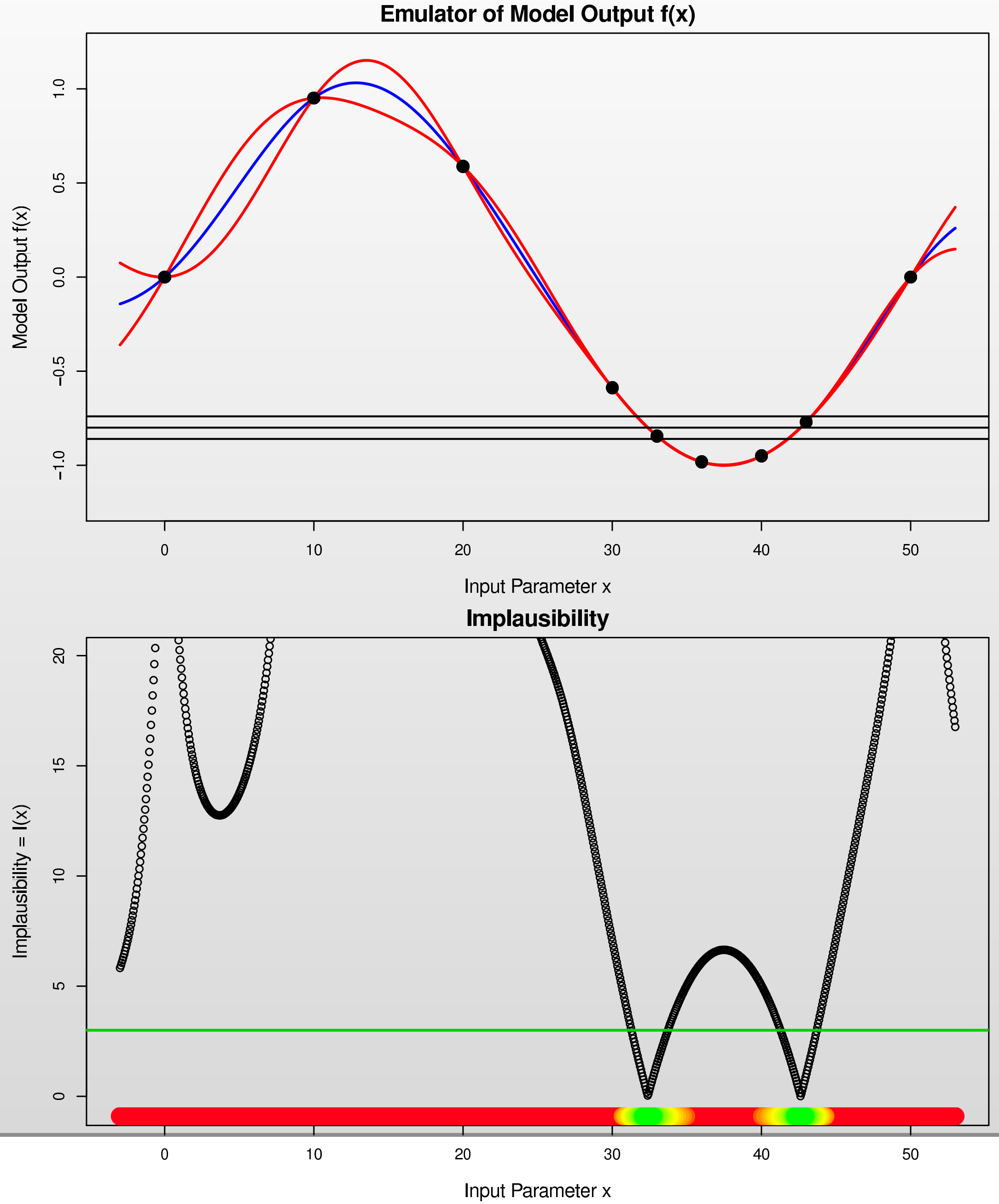
History Matching via Implausibility: a 1D Example



History Matching via Implausibility: a 1D Example



History Matching via Implausibility: a 1D Example



Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$

Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$
2. Identify the set Q_{j+1} of informative outputs that we can emulate easily

Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$
2. Identify the set Q_{j+1} of informative outputs that we can emulate easily
3. Construct new emulators for $f_i(x)$, where $i \in Q_{j+1}$ defined only over $\mathcal{X}_j$

Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$
2. Identify the set Q_{j+1} of informative outputs that we can emulate easily
3. Construct new emulators for $f_i(x)$, where $i \in Q_{j+1}$ defined only over $\mathcal{X}_j$
4. Evaluate the new implausibility functions $I_i(x), i \in Q_{j+1}$ only over $\mathcal{X}_j$

Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$
2. Identify the set Q_{j+1} of informative outputs that we can emulate easily
3. Construct new emulators for $f_i(x)$, where $i \in Q_{j+1}$ defined only over $\mathcal{X}_j$
4. Evaluate the new implausibility functions $I_i(x), i \in Q_{j+1}$ only over $\mathcal{X}_j$
5. Define a new (reduced) non-implausible region $\mathcal{X}_{j+1}$, by $I_M(x) < c_M$, which should satisfy $\mathcal{X} \subset \mathcal{X}_{j+1} \subset \mathcal{X}_j$

Iterative History Matching for Reducing Input Space.

We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

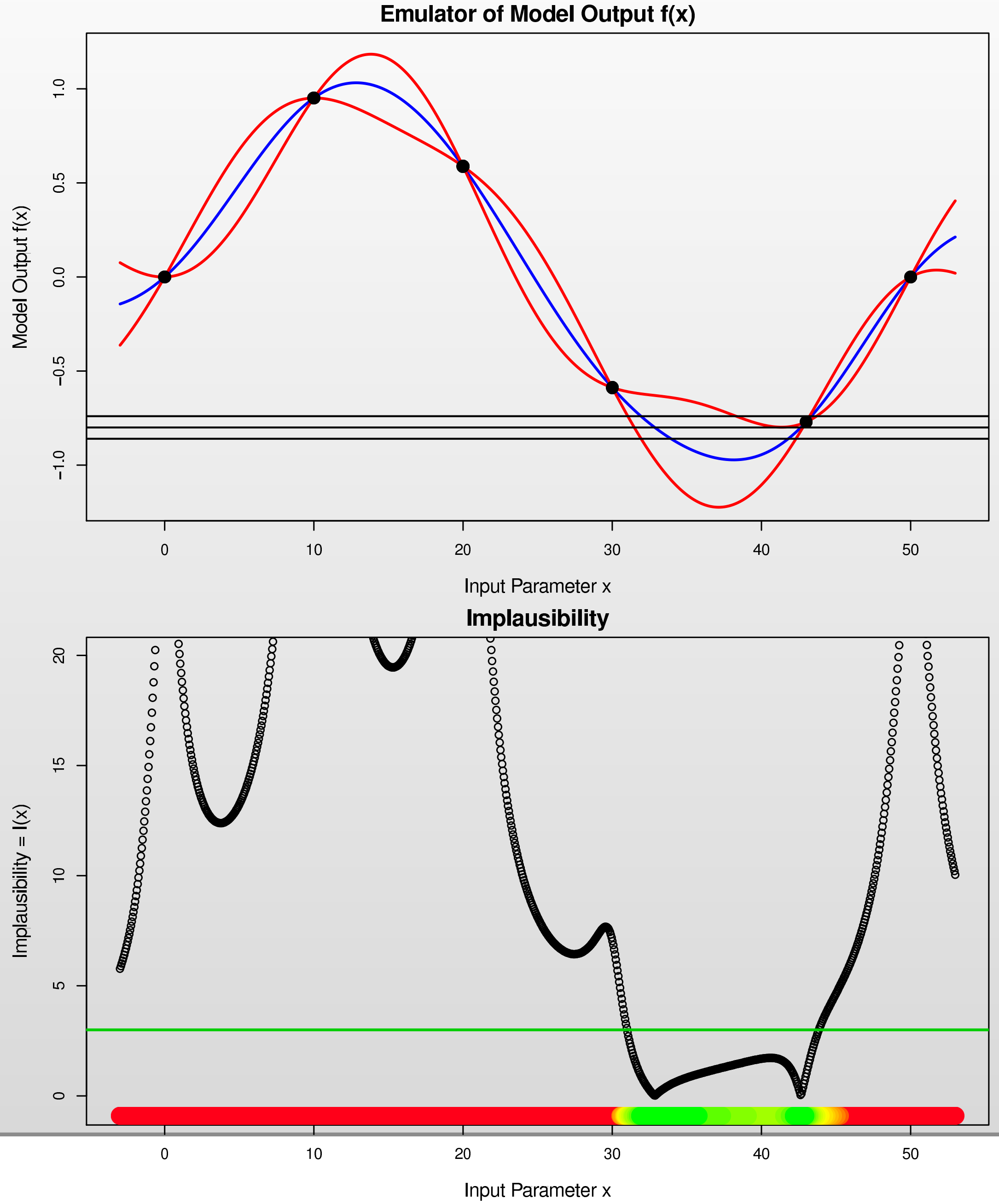
1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$
2. Identify the set Q_{j+1} of informative outputs that we can emulate easily
3. Construct new emulators for $f_i(x)$, where $i \in Q_{j+1}$ defined only over $\mathcal{X}_j$
4. Evaluate the new implausibility functions $I_i(x), i \in Q_{j+1}$ only over $\mathcal{X}_j$
5. Define a new (reduced) non-implausible region $\mathcal{X}_{j+1}$, by $I_M(x) < c_M$, which should satisfy $\mathcal{X} \subset \mathcal{X}_{j+1} \subset \mathcal{X}_j$
6. Unless (a) the emulator variances are now small in comparison to the other sources of uncertainty (model discrepancy and observation errors) or (b) computational resources are exhausted or (c) all the input space is deemed implausible, return to step 1

Iterative History Matching for Reducing Input Space.

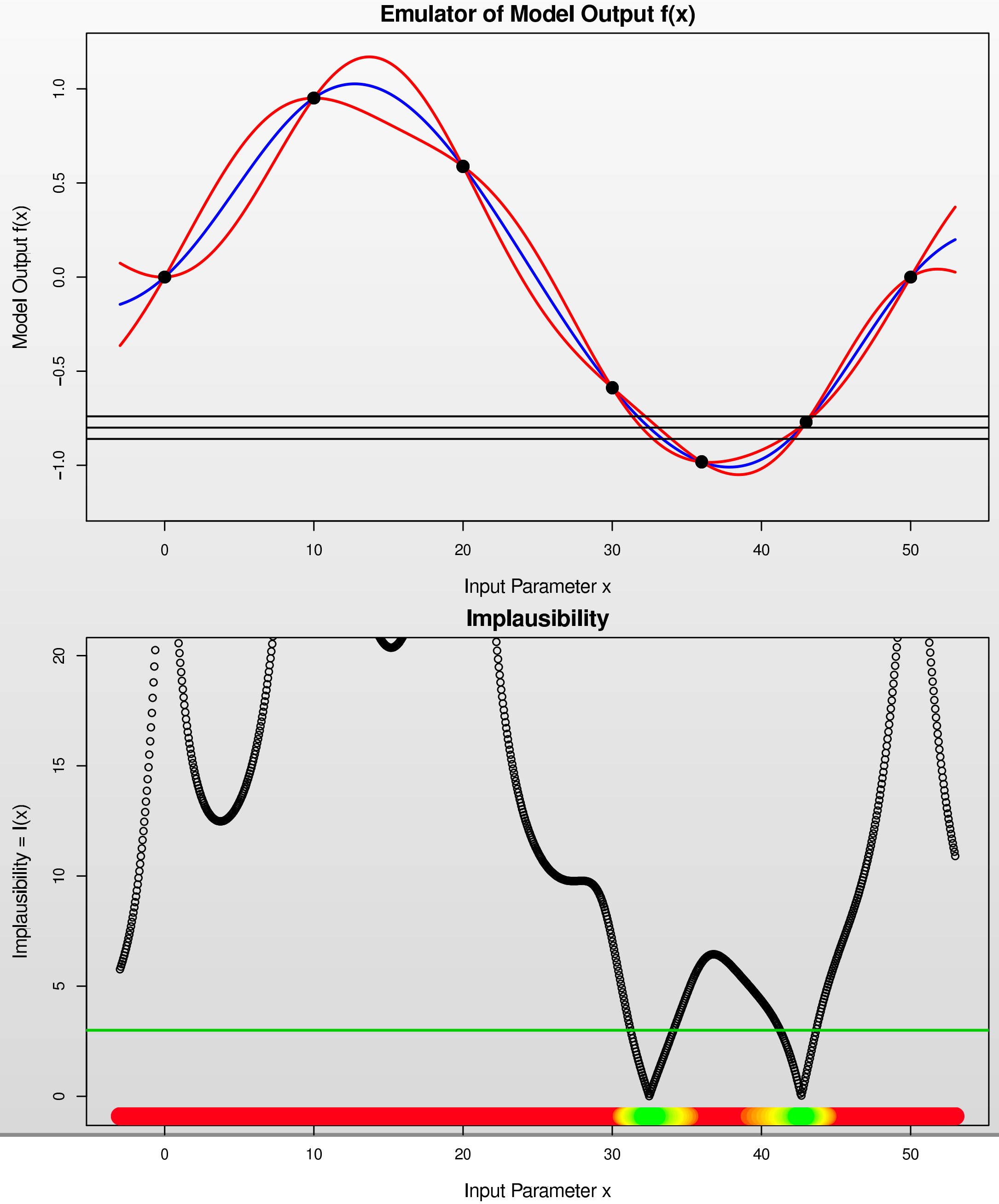
We use an iterative strategy to reduce the input parameter space. Denoting the current non-implausible volume by $\mathcal{X}_j$, at each stage or wave we:

1. Design and perform a set of runs over the non-implausible input region $\mathcal{X}_j$
2. Identify the set Q_{j+1} of informative outputs that we can emulate easily
3. Construct new emulators for $f_i(x)$, where $i \in Q_{j+1}$ defined only over $\mathcal{X}_j$
4. Evaluate the new implausibility functions $I_i(x), i \in Q_{j+1}$ only over $\mathcal{X}_j$
5. Define a new (reduced) non-implausible region $\mathcal{X}_{j+1}$, by $I_M(x) < c_M$, which should satisfy $\mathcal{X} \subset \mathcal{X}_{j+1} \subset \mathcal{X}_j$
6. Unless (a) the emulator variances are now small in comparison to the other sources of uncertainty (model discrepancy and observation errors) or (b) computational resources are exhausted or (c) all the input space is deemed implausible, return to step 1
7. If 6(a) true, generate a large number of acceptable runs from the final non-implausible volume $\mathcal{X}$, with appropriate sampling.

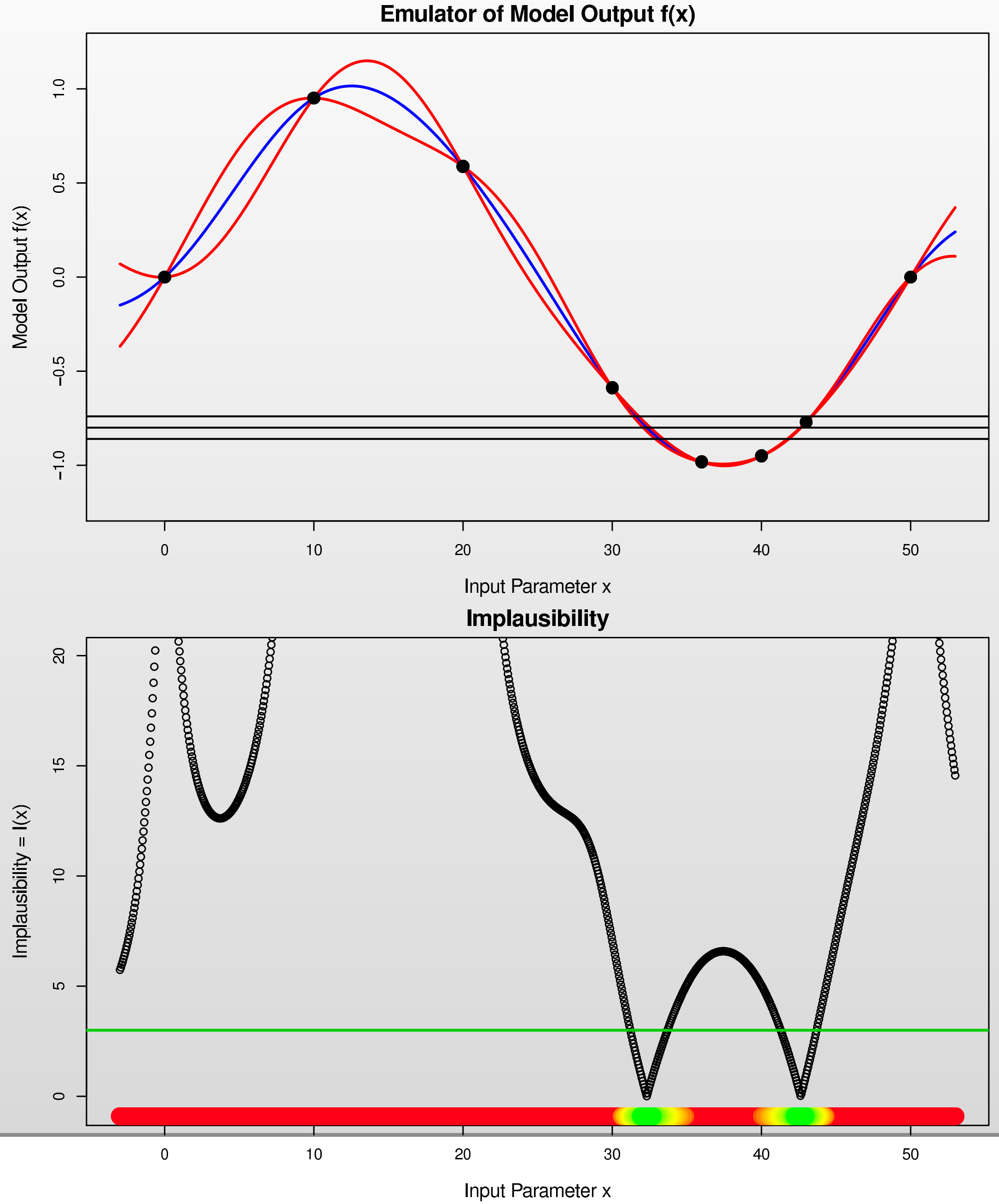
History Matching via Implausibility: a 1D Example



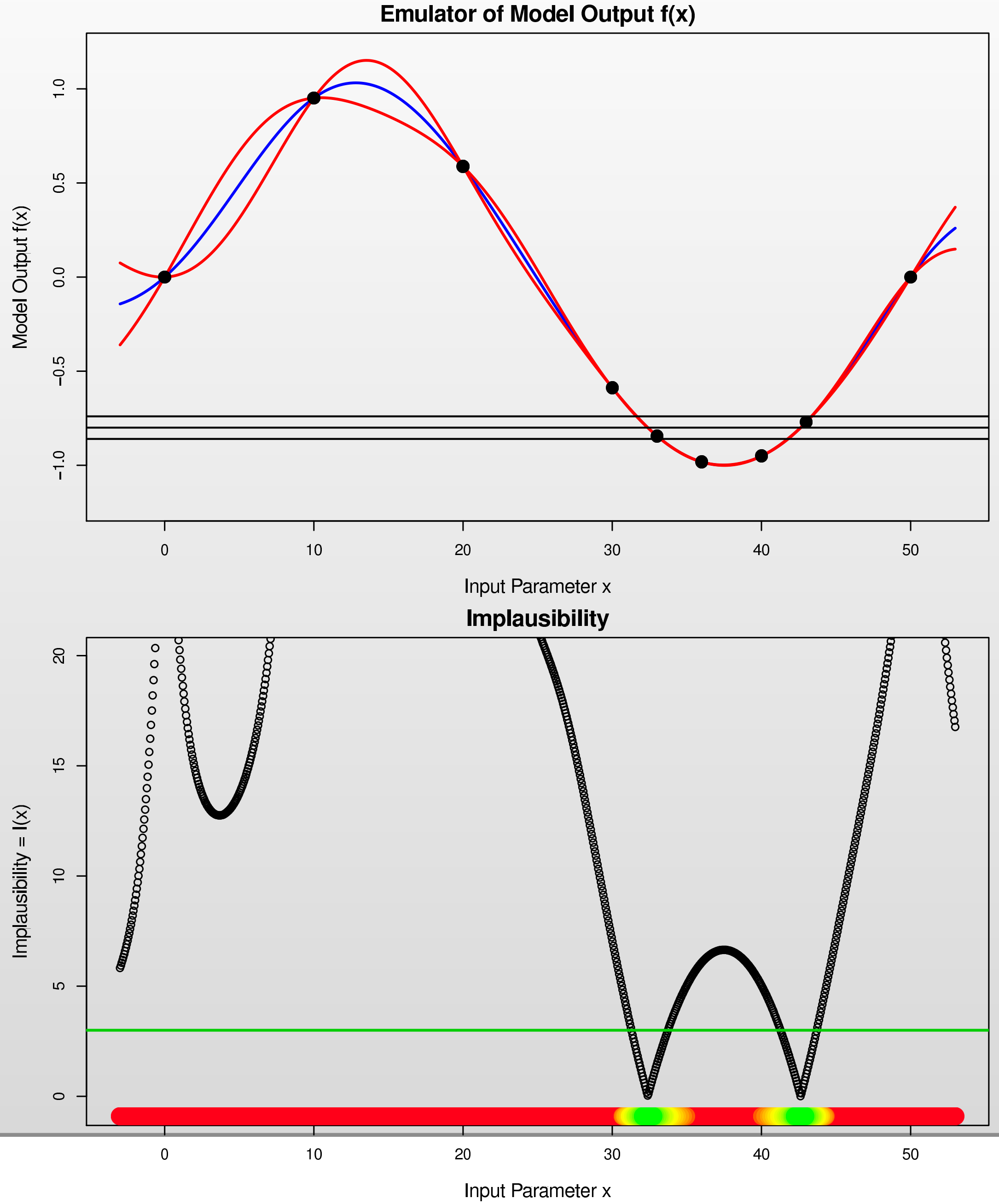
History Matching via Implausibility: a 1D Example



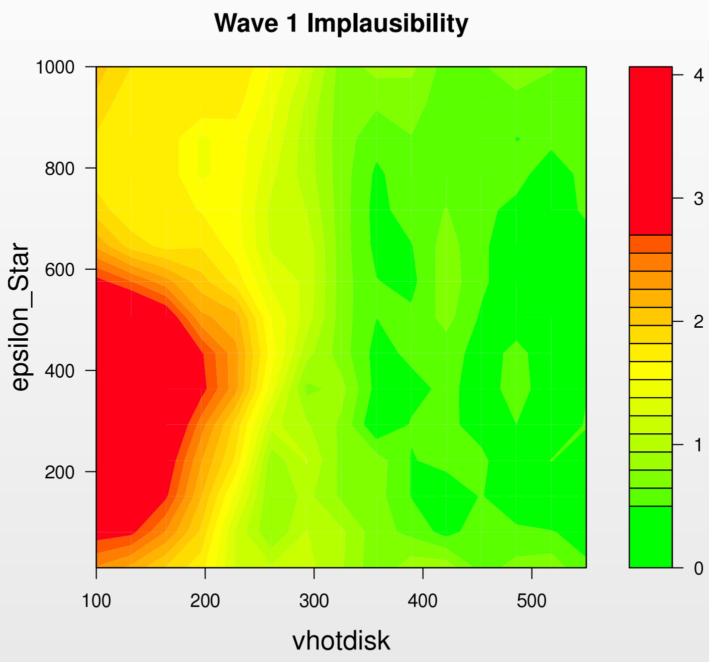
History Matching via Implausibility: a 1D Example



History Matching via Implausibility: a 1D Example

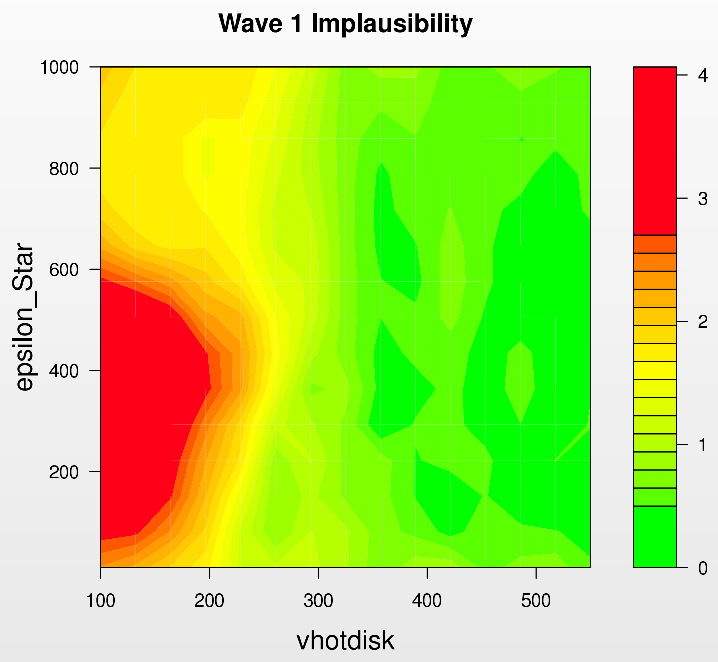


2D Minimised Implausibility Projections: Wave 1



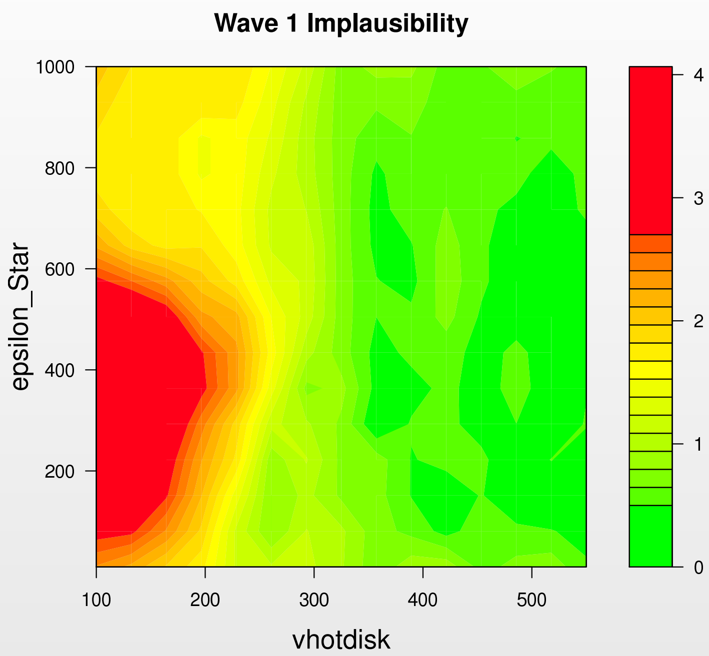
- Minimised Implausibility Projections: at each 2D grid point, minimise the implausibility $I_M(x)$ over the 15D hypercube.

2D Minimised Implausibility Projections: Wave 1



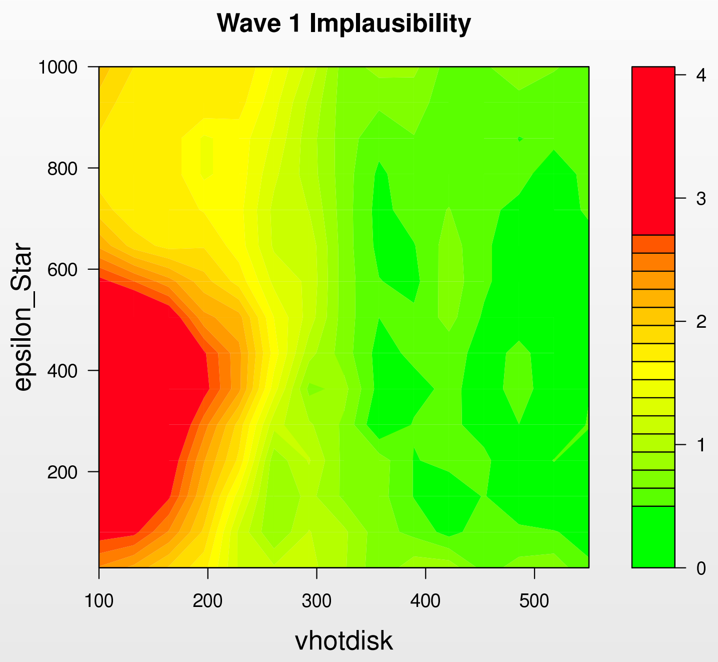
- Minimised Implausibility Projections: at each 2D grid point, minimise the implausibility $I_M(x)$ over the 15D hypercube.
- If a point on these plots is implausible (coloured red), then it will be implausible for any choice of the 15 other inputs.

2D Minimised Implausibility Projections: Wave 1

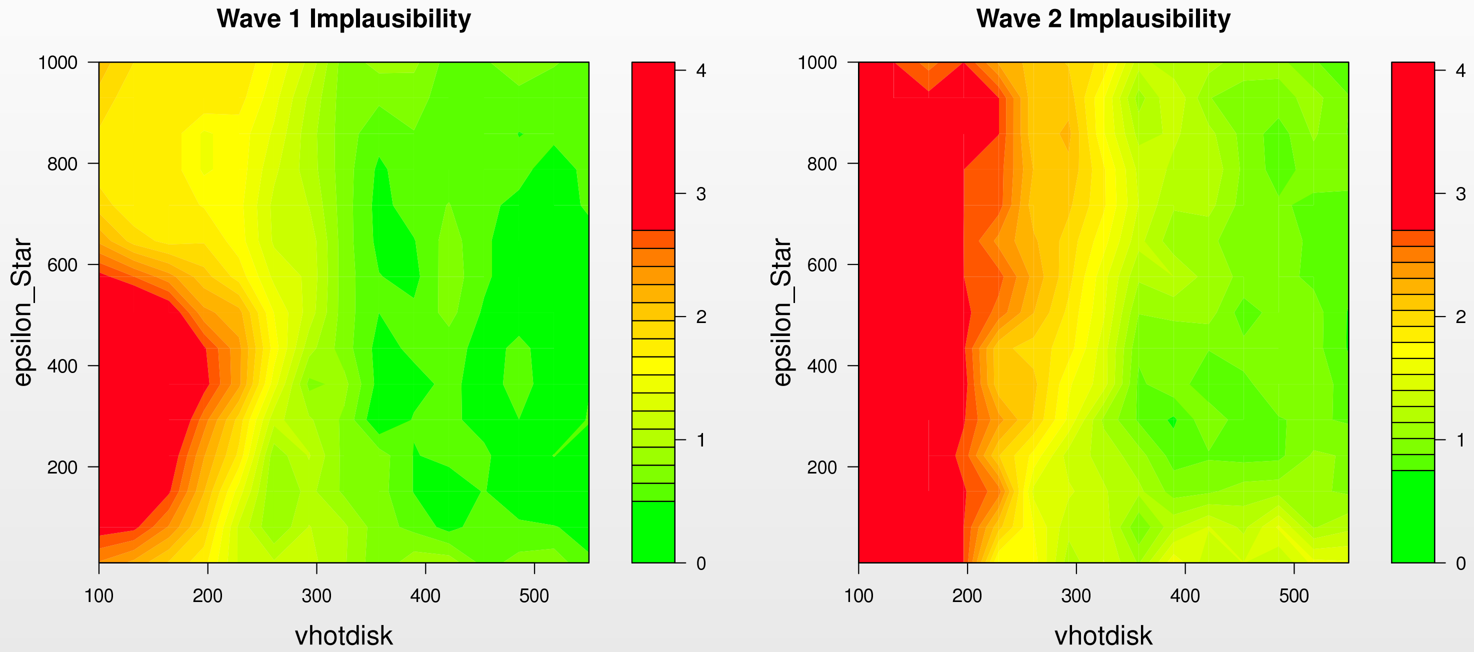


- Minimised Implausibility Projections: at each 2D grid point, minimise the implausibility $I_M(x)$ over the 15D hypercube.
- If a point on these plots is implausible (coloured red), then it will be implausible for any choice of the 15 other inputs.
- If a point is green, it may or may not prove to be an acceptable input.

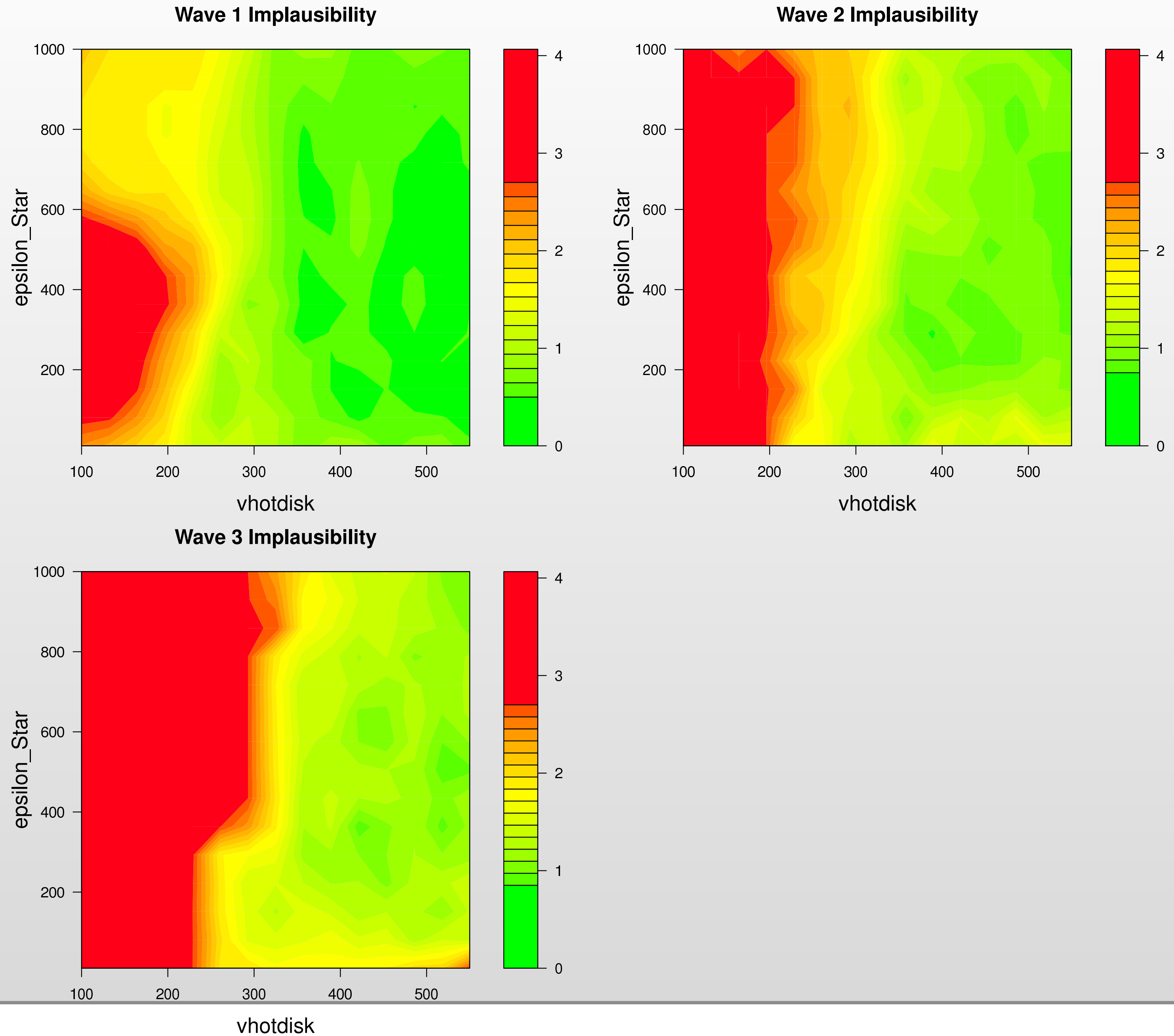
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



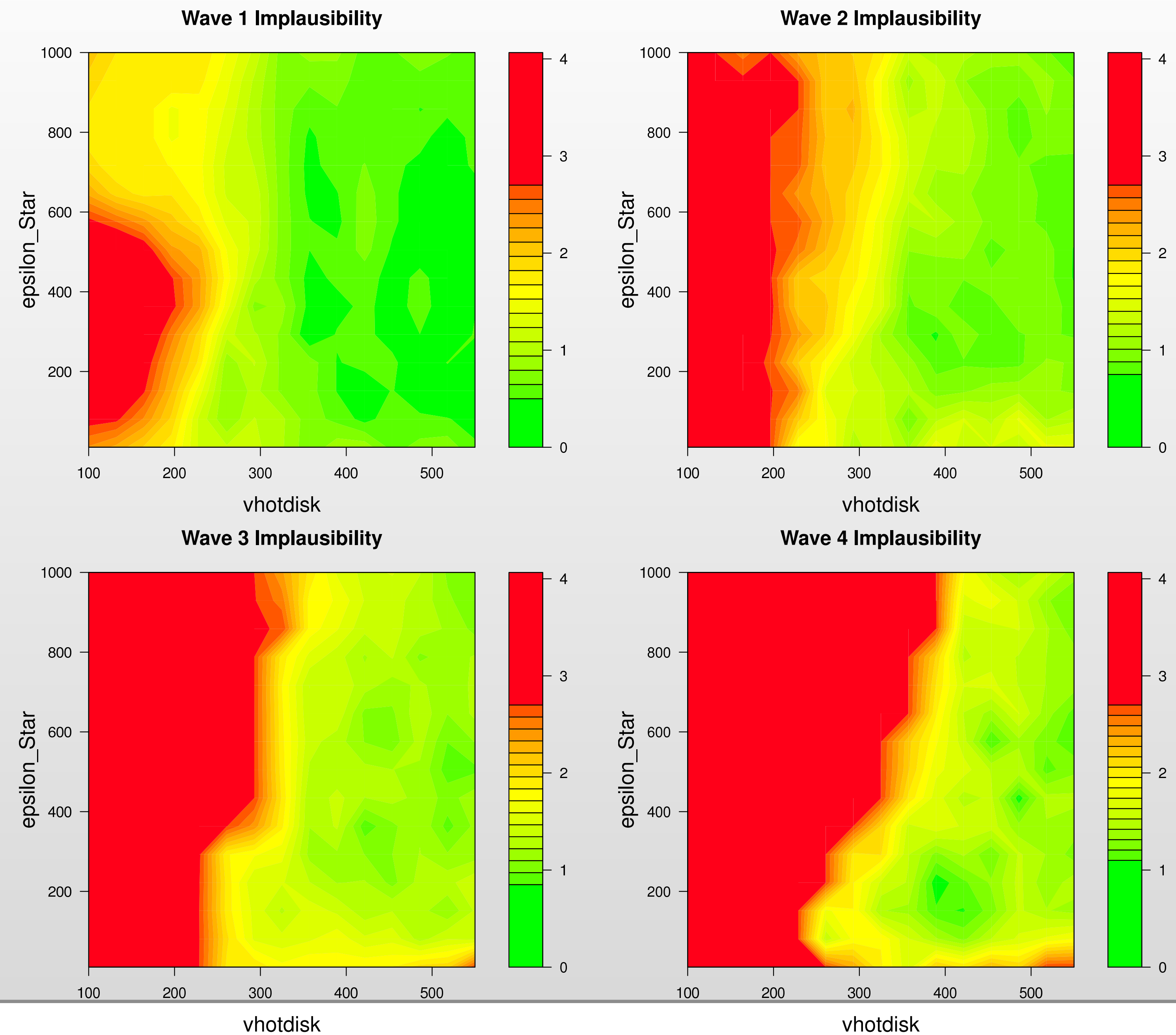
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



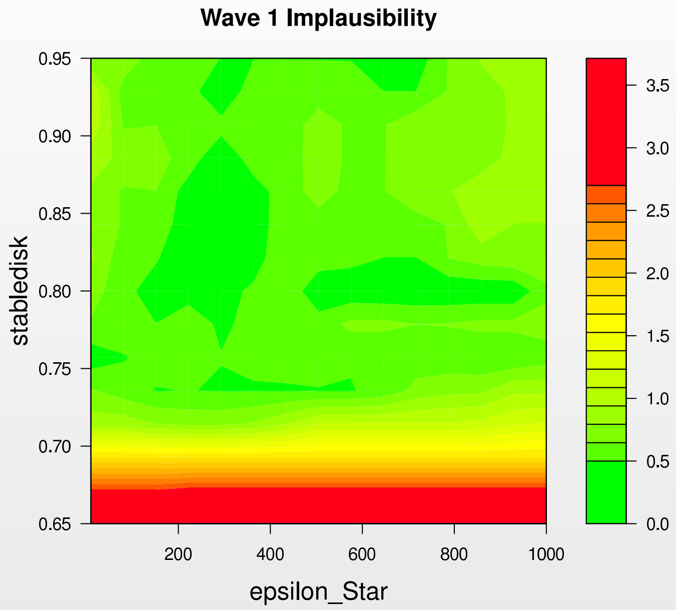
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



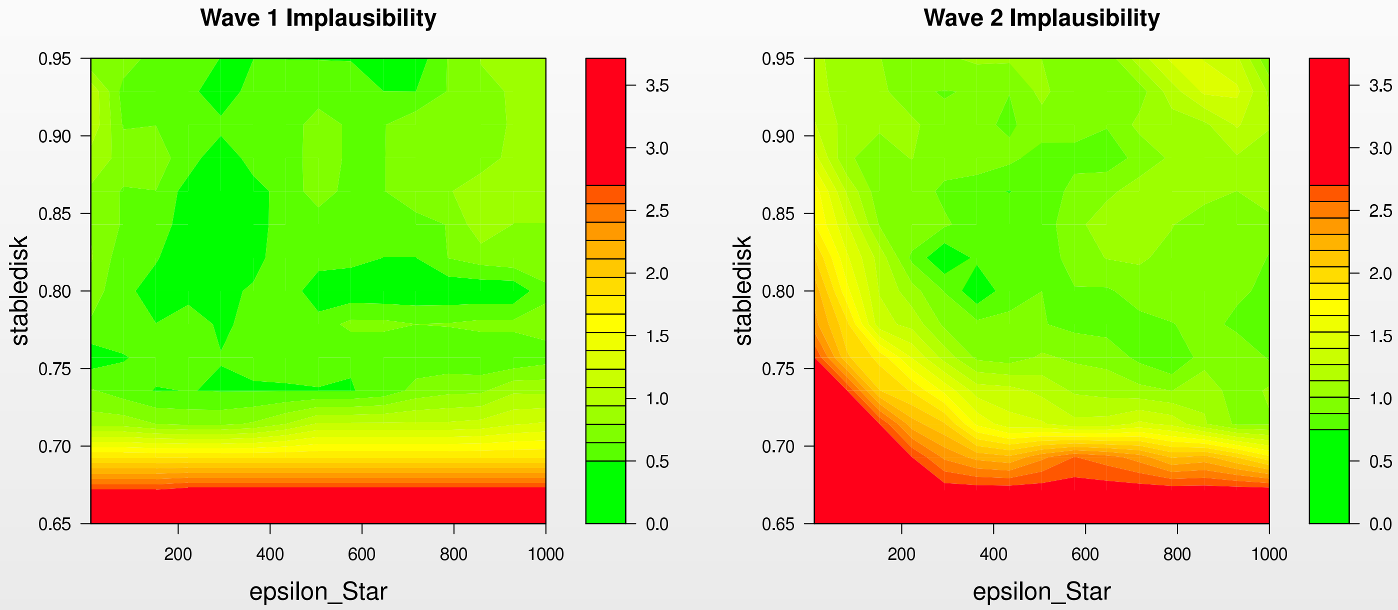
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



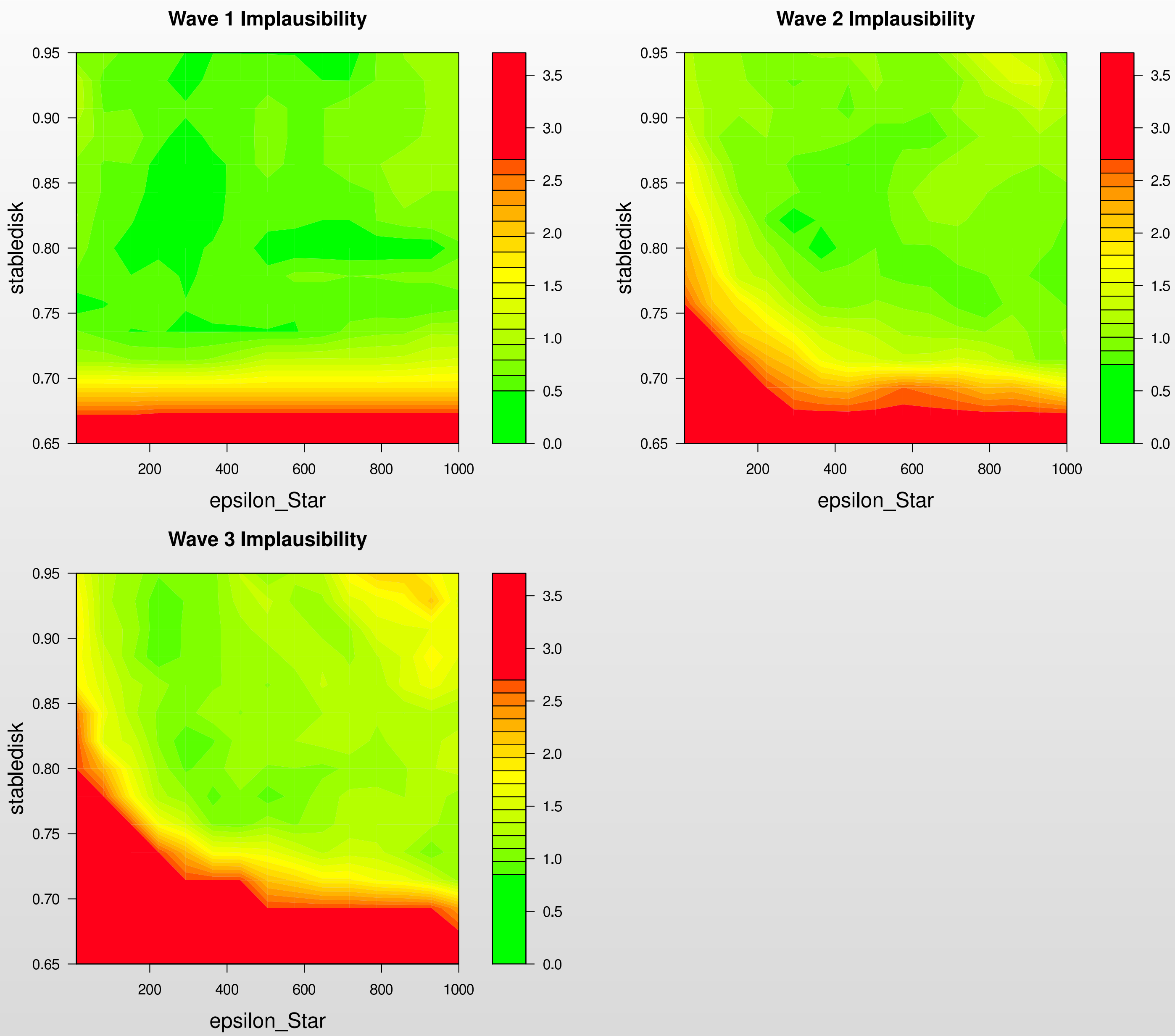
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



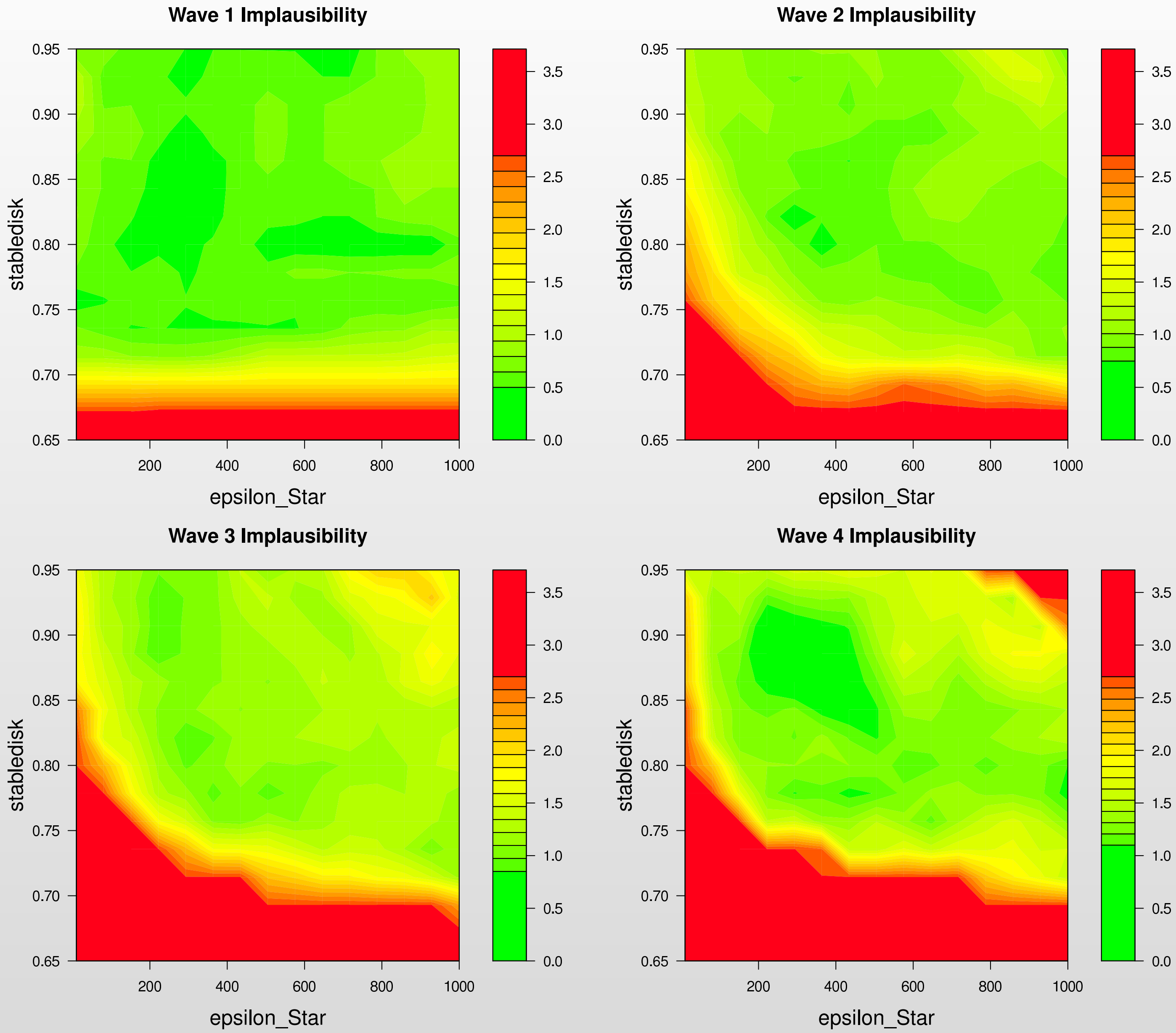
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



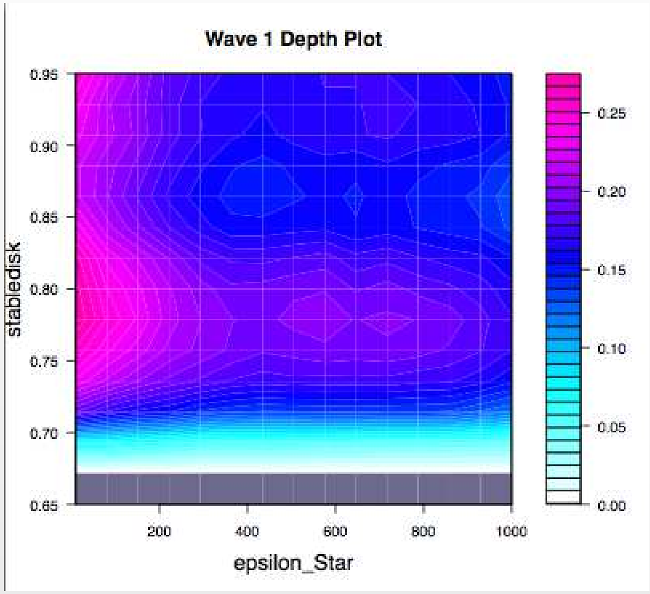
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)

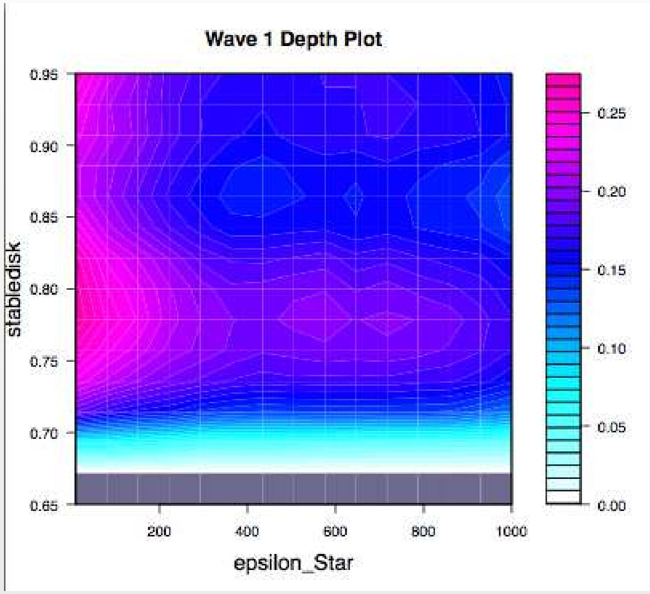


2D Optical Depth Plots: Wave 2



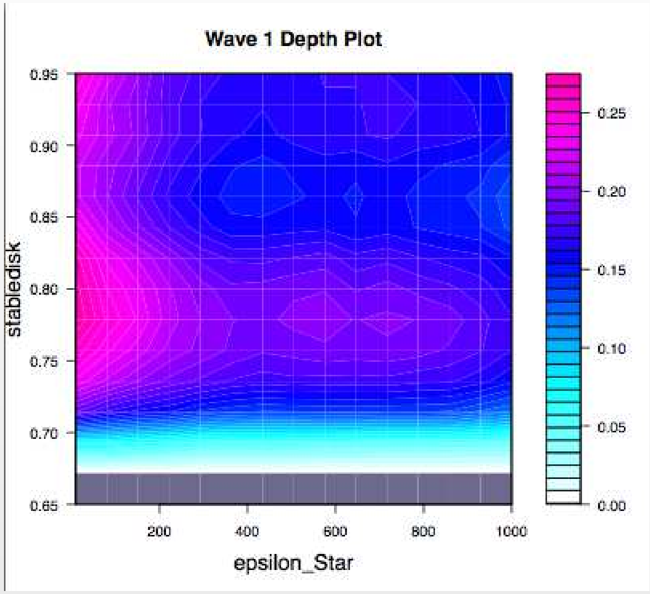
- Optical Depth Plots: at each 2D grid point plot the proportion of the 15D latin hypercube points that survive the cutoff $I_M(x) < c_M$.

2D Optical Depth Plots: Wave 2



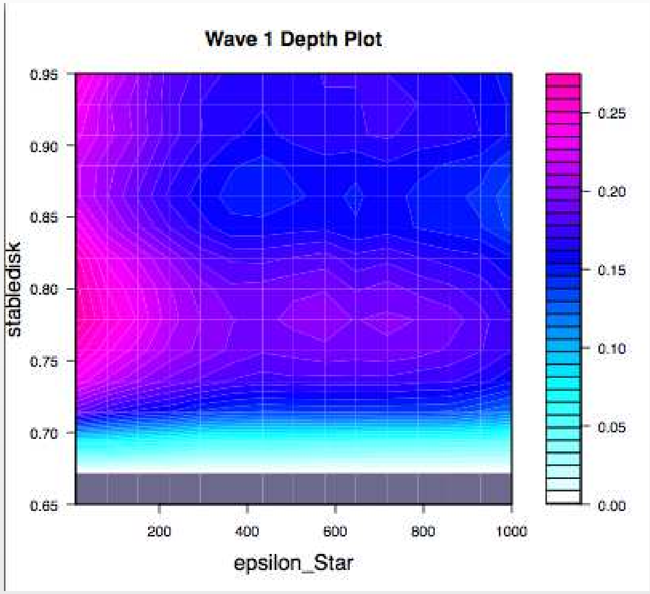
- Optical Depth Plots: at each 2D grid point plot the proportion of the 15D latin hypercube points that survive the cutoff $I_M(x) < c_M$.
- These plots show the ‘depth’ of the non-implausible volume $\mathcal{X}_j$ for wave j, at each grid point.

2D Optical Depth Plots: Wave 2

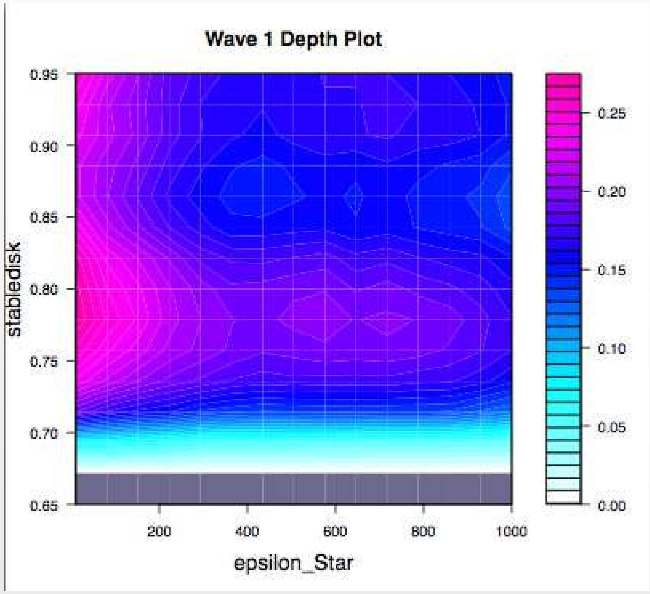


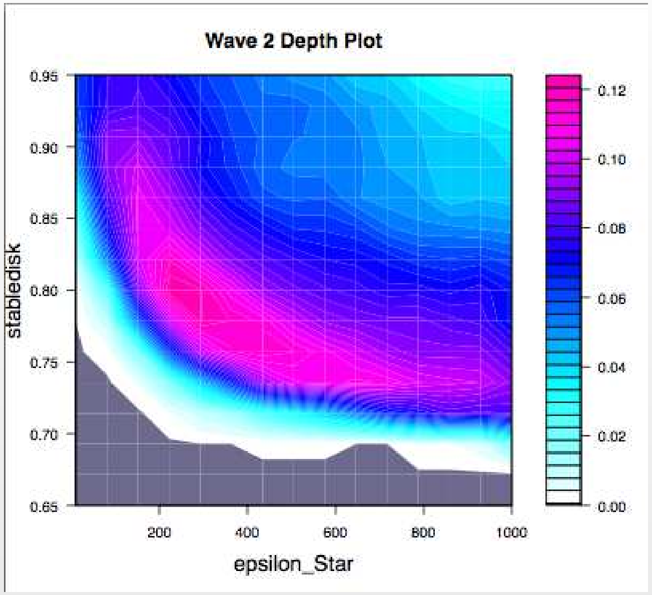
- Optical Depth Plots: at each 2D grid point plot the proportion of the 15D latin hypercube points that survive the cutoff $I_M(x) < c_M$.
- These plots show the 'depth' of the non-implausible volume $\mathcal{X}_j$ for wave j, at each grid point.
- Shows where the majority of non-implausible points can be found, but not necessarily where the best matches are.

2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)

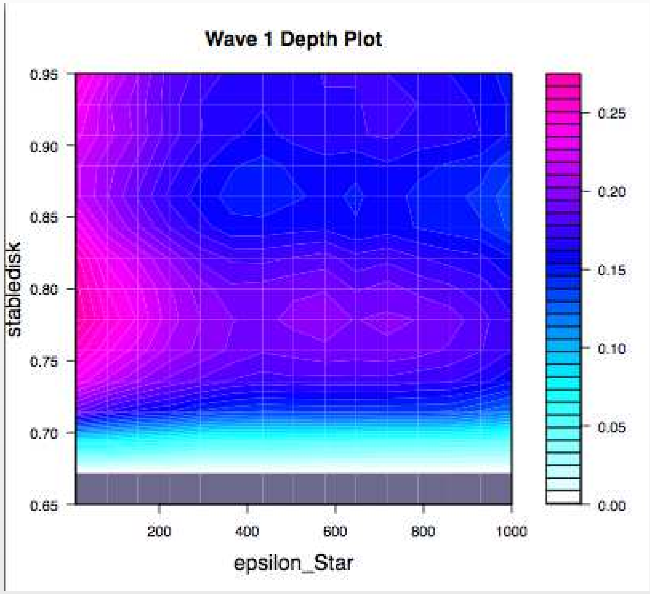


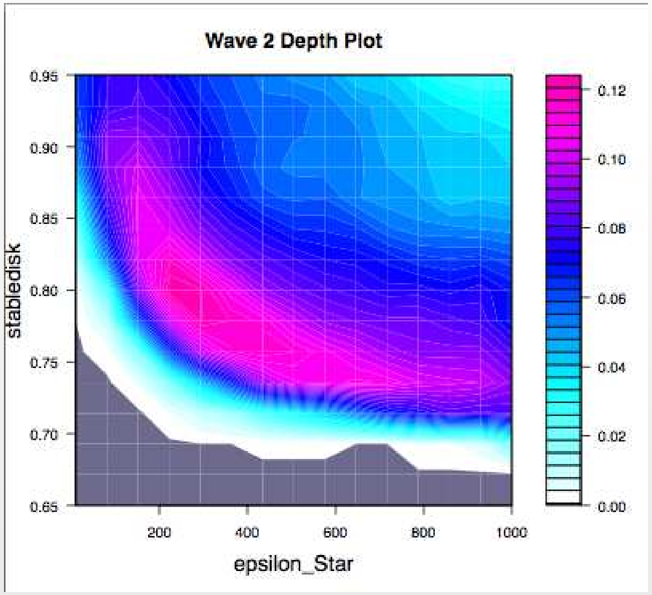
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)

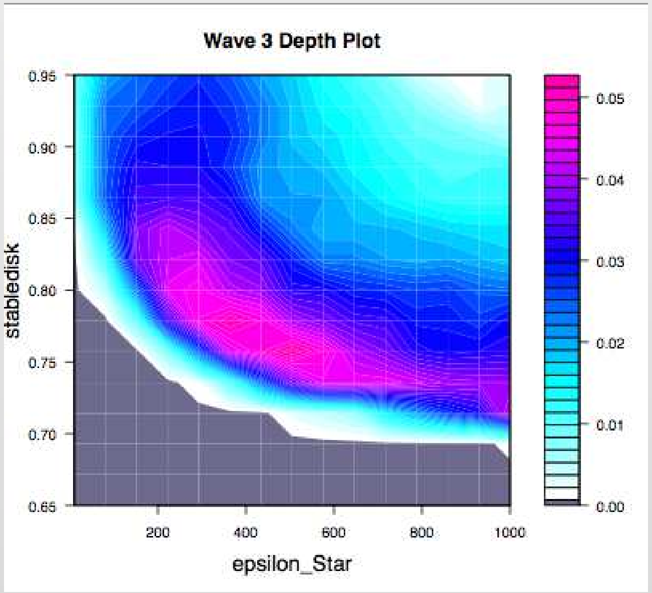




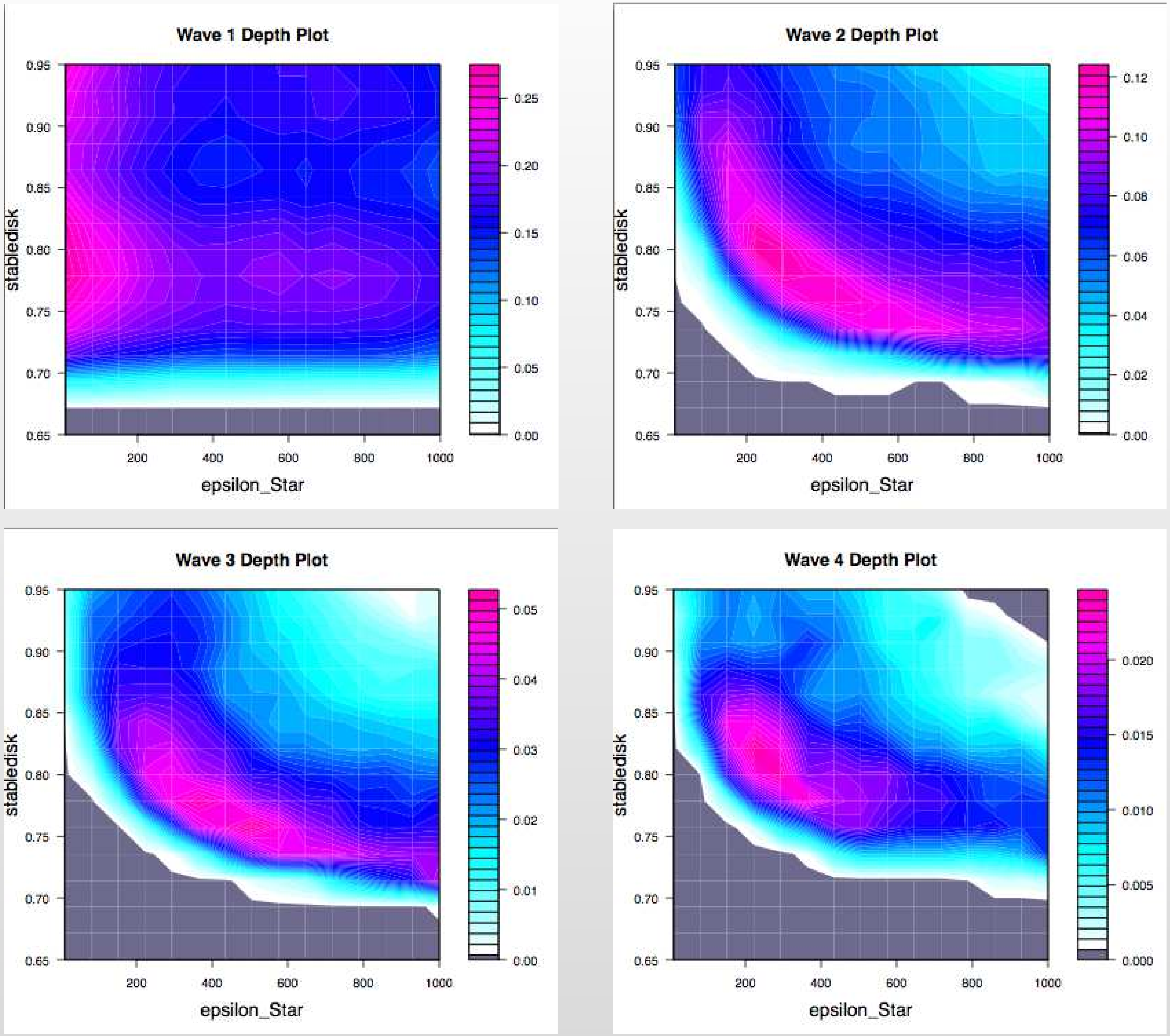
2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)







2D Implausibility Projections: Wave 1 to Wave 4 (0.12%)



Why Does Iterative Refocussing Work?

Why do we reduce space in waves? Why not attempt to do it all at once?

Why Does Iterative Refocussing Work?

Why do we reduce space in waves? Why not attempt to do it all at once?

Because this requires an accurate emulator valid over whole input space.

- In contrast, the iterative approach is far more efficient.

Why Does Iterative Refocussing Work?

Why do we reduce space in waves? Why not attempt to do it all at once? Because this requires an accurate emulator valid over whole input space.

- In contrast, the iterative approach is far more efficient.
- At each wave the emulators are found to be significantly more accurate (in that $\mathrm{Var}[f(x)]$ becomes smaller). This is expected as:

  1. We have 'zoomed in' on a smaller part of the function, it will be smoother and most likely easier to fit with low order polynomials.

Why Does Iterative Refocussing Work?

Why do we reduce space in waves? Why not attempt to do it all at once? Because this requires an accurate emulator valid over whole input space.

- In contrast, the iterative approach is far more efficient.
- At each wave the emulators are found to be significantly more accurate (in that $\mathrm{Var}[f(x)]$ becomes smaller). This is expected as:

    1. We have ‘zoomed in’ on a smaller part of the function, it will be smoother and most likely easier to fit with low order polynomials.
    2. We have a much higher density of runs in the new volume, and hence the Gaussian process part of the emulator will do more work.

Why Does Iterative Refocussing Work?

Why do we reduce space in waves? Why not attempt to do it all at once? Because this requires an accurate emulator valid over whole input space.

- In contrast, the iterative approach is far more efficient.
- At each wave the emulators are found to be significantly more accurate (in that $\mathrm{Var}[f(x)]$ becomes smaller). This is expected as:

  1. We have ‘zoomed in’ on a smaller part of the function, it will be smoother and most likely easier to fit with low order polynomials.
  2. We have a much higher density of runs in the new volume, and hence the Gaussian process part of the emulator will do more work.
  3. We can identify more active variables, leading to more detailed polynomial and Gaussian process parts of the emulator, as previously dominant variables are now somewhat suppressed.

Why Does Iterative Refocussing Work?

Why do we reduce space in waves? Why not attempt to do it all at once? Because this requires an accurate emulator valid over whole input space.

- In contrast, the iterative approach is far more efficient.
- At each wave the emulators are found to be significantly more accurate (in that $\mathrm{Var}[f(x)]$ becomes smaller). This is expected as:

  1. We have 'zoomed in' on a smaller part of the function, it will be smoother and most likely easier to fit with low order polynomials.
  2. We have a much higher density of runs in the new volume, and hence the Gaussian process part of the emulator will do more work.
  3. We can identify more active variables, leading to more detailed polynomial and Gaussian process parts of the emulator, as previously dominant variables are now somewhat suppressed.
  4. We can hence add more outputs to the set of informative and easy to emulate outputs Q_k.

Why Does Iterative Refocussing Work?

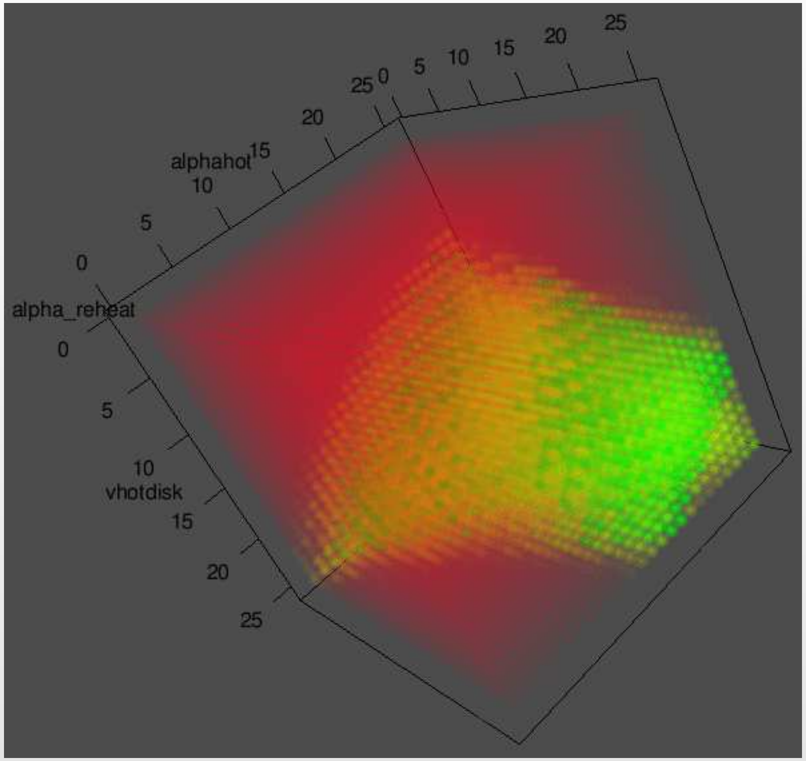
Why do we reduce space in waves? Why not attempt to do it all at once? Because this requires an accurate emulator valid over whole input space.

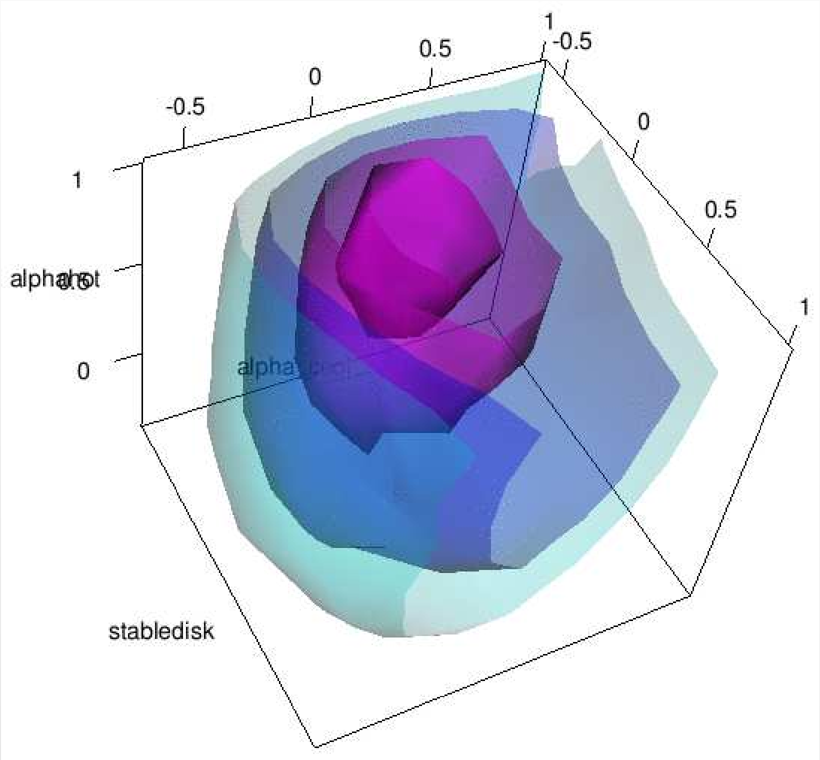
- In contrast, the iterative approach is far more efficient.
- At each wave the emulators are found to be significantly more accurate (in that $\mathrm{Var}[f(x)]$ becomes smaller). This is expected as:

  1. We have ‘zoomed in’ on a smaller part of the function, it will be smoother and most likely easier to fit with low order polynomials.
  2. We have a much higher density of runs in the new volume, and hence the Gaussian process part of the emulator will do more work.
  3. We can identify more active variables, leading to more detailed polynomial and Gaussian process parts of the emulator, as previously dominant variables are now somewhat suppressed.
  4. We can hence add more outputs to the set of informative and easy to emulate outputs Q_k.

- This is a major strength of the History Matching approach.

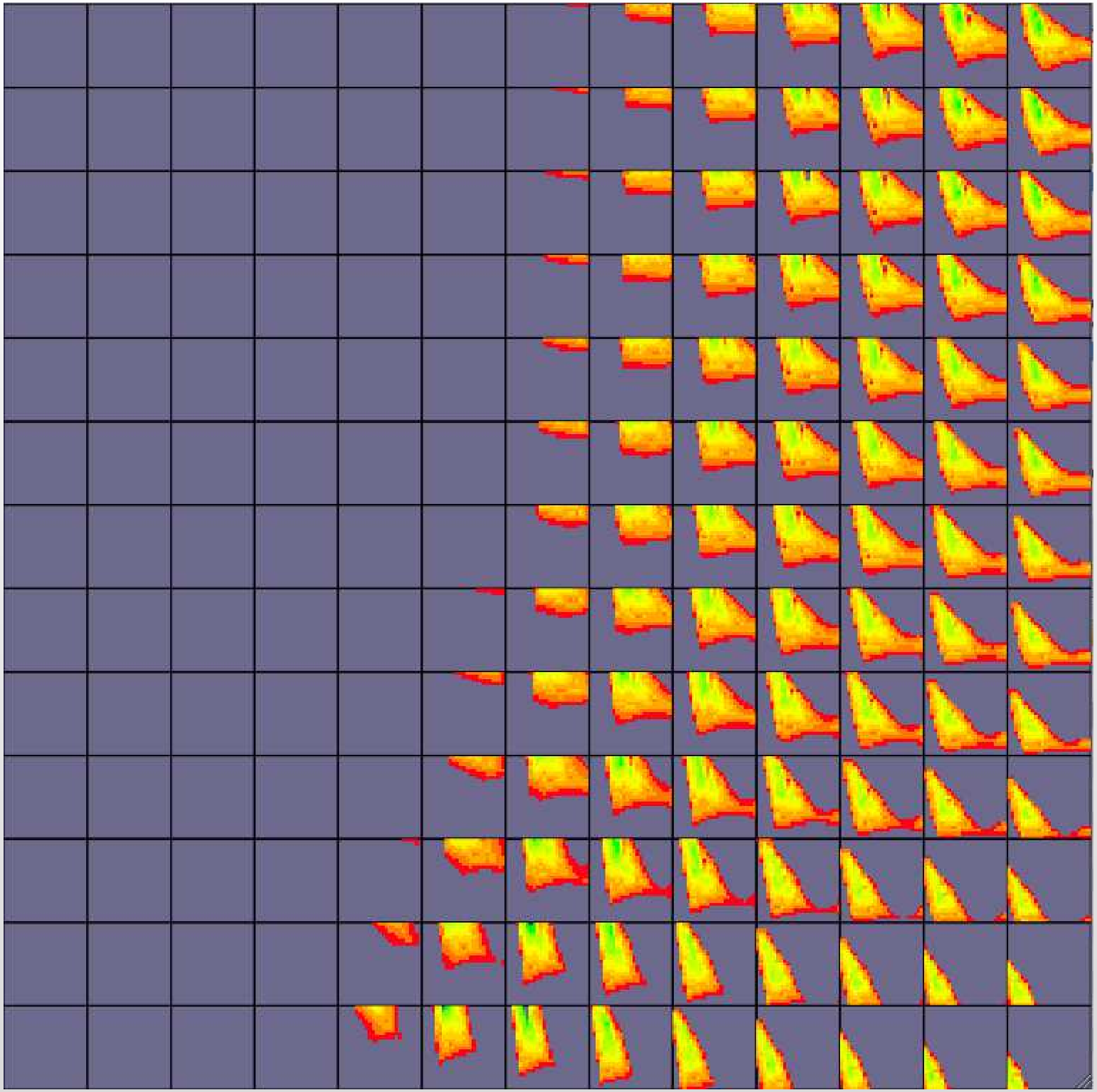
3D Minimised Implausibility and Optical Depth Plots



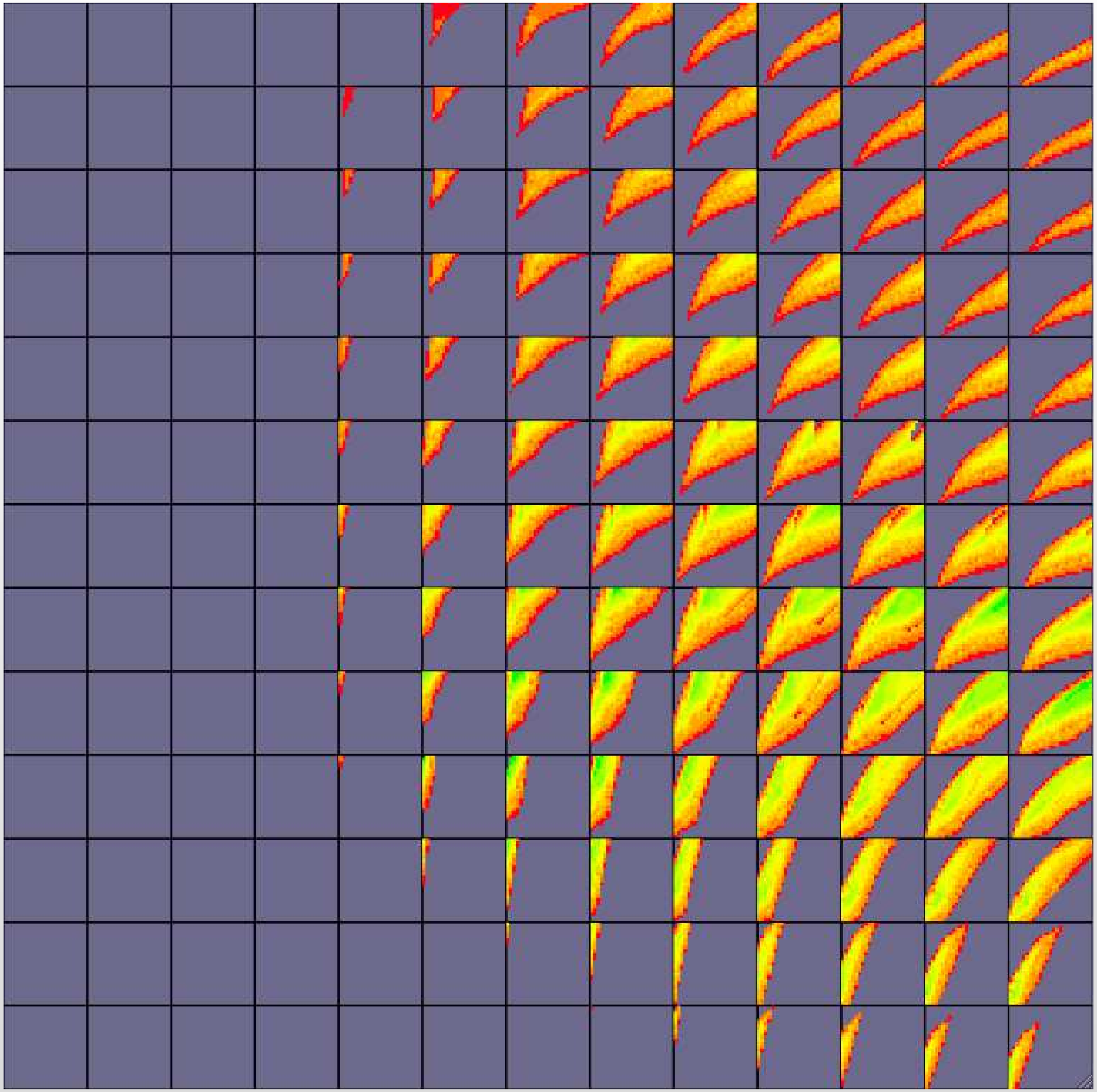


- 3D projections created using the **Fast Approximate Emulator** approach.

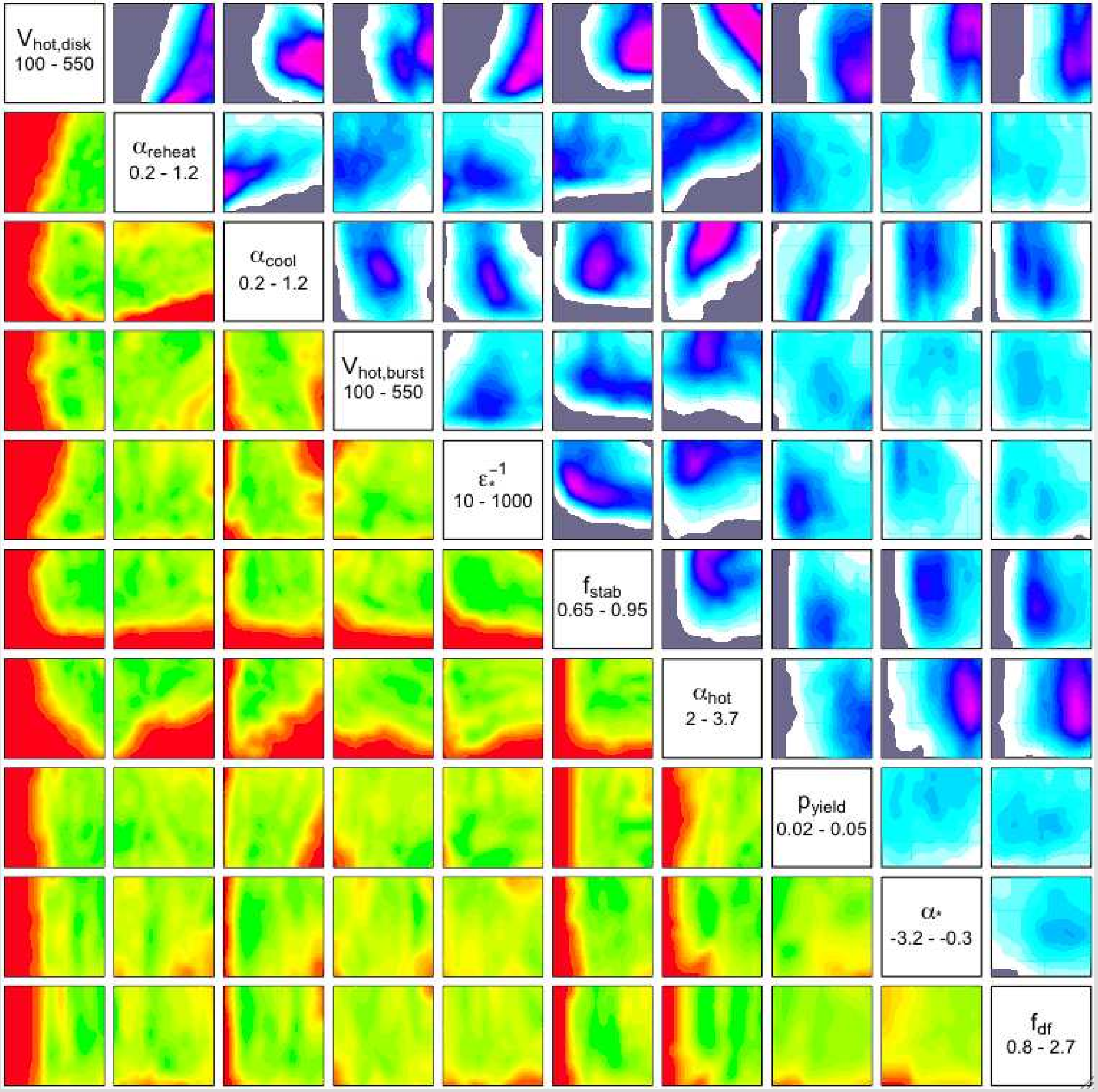
4-Dimensional Implausibility Plots: Anyone?



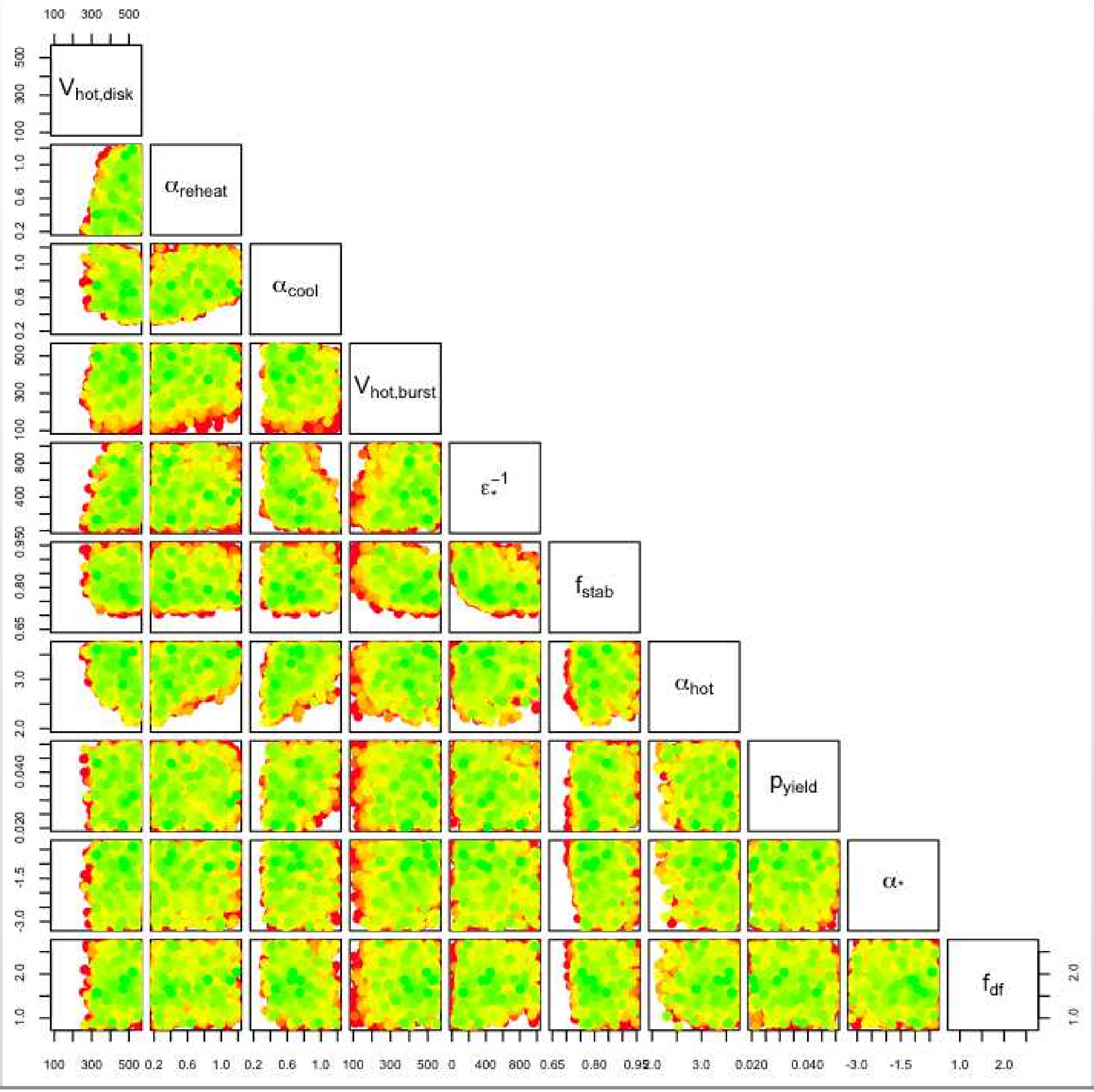
4-Dimensional Implausibility Plots: Anyone?



2D Implausibility Projections: Stage 4 (0.12%)

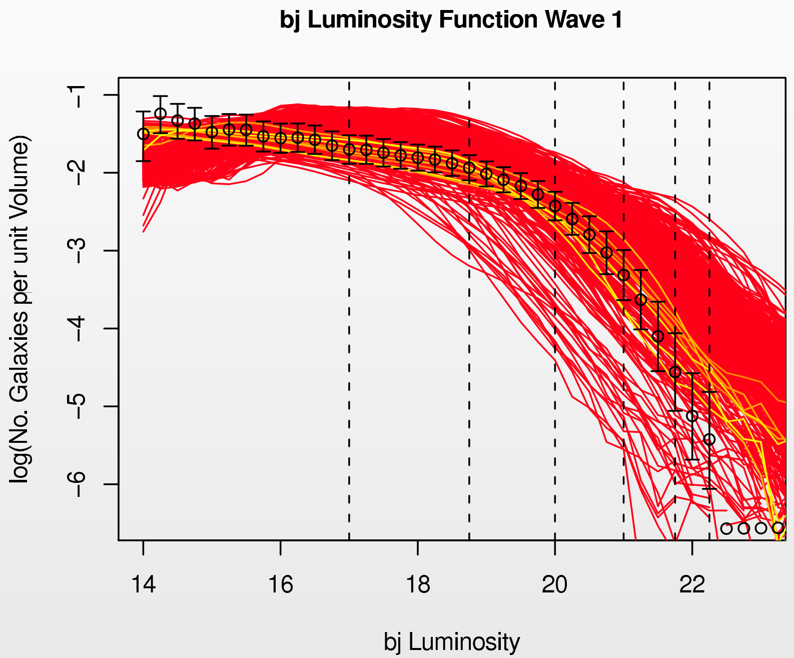


Wave 5 runs

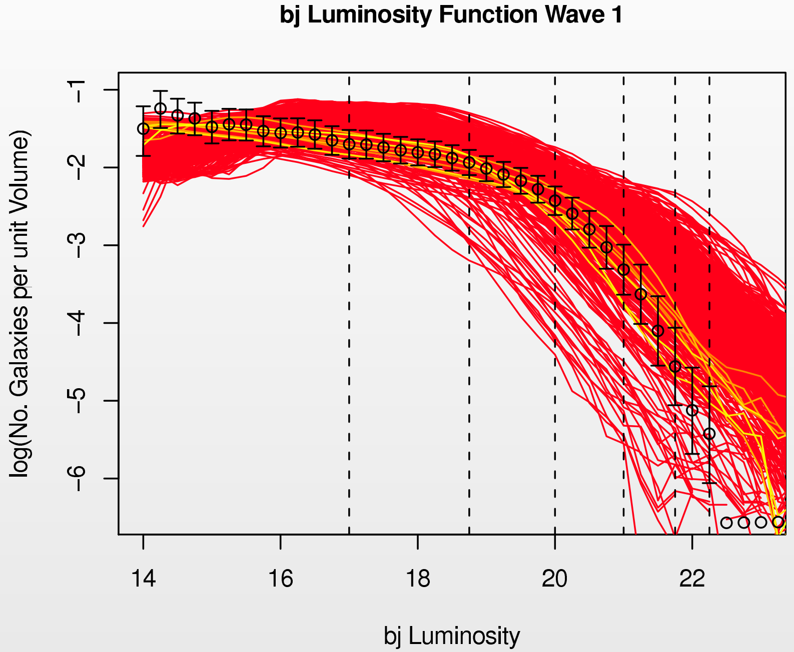


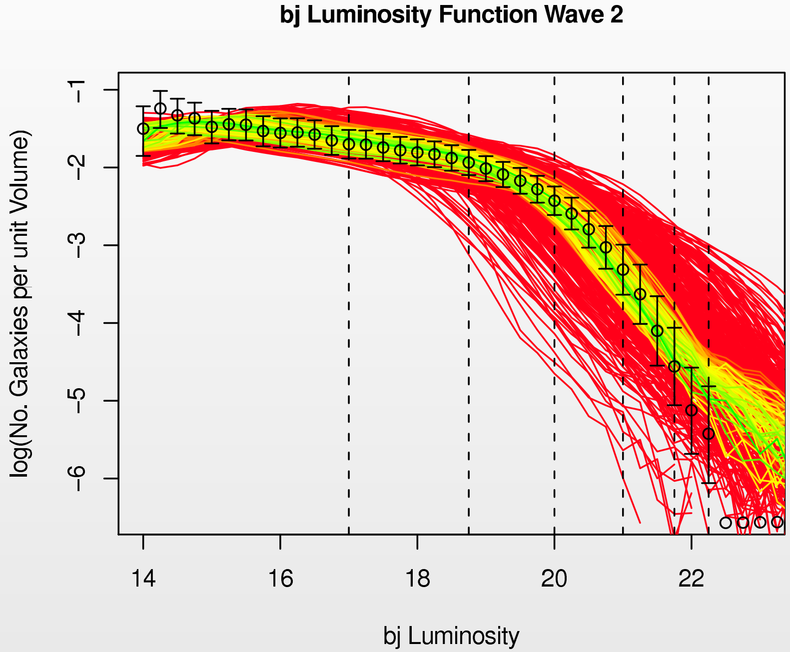
$V_{hot,disk}$
α_{reheat}
α_{cool}
$V_{hot,burst}$
ε_*^{-1}
f_{stab}
α_{hot}
p_{yield}
α_*
f_{df}
100 300 500
0.2 0.6 1.0
0 400 800
0.65 0.80 0.95
2.0 3.0
0.020 0.040
-3.0 -1.5
1.0 2.0

bj Luminosity Output of Waves 1,2,3 and 5

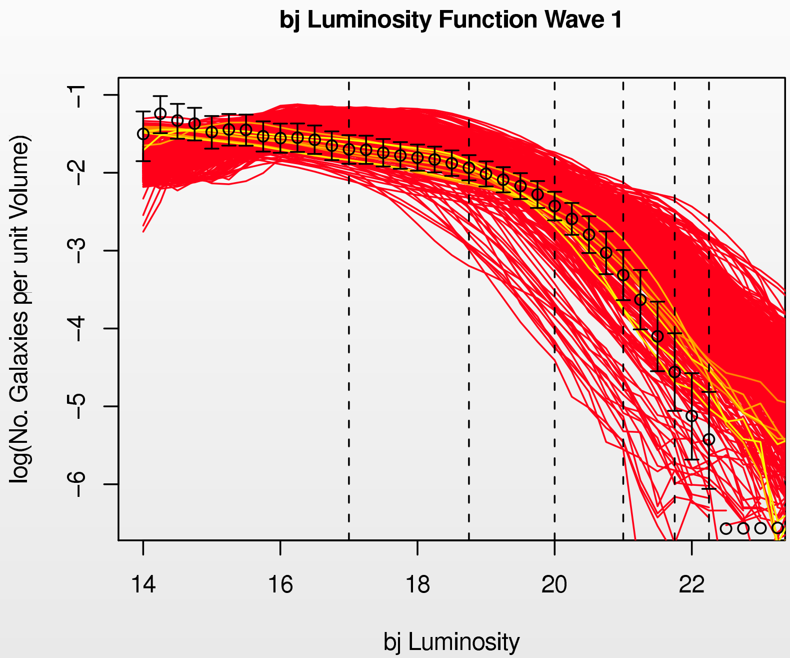


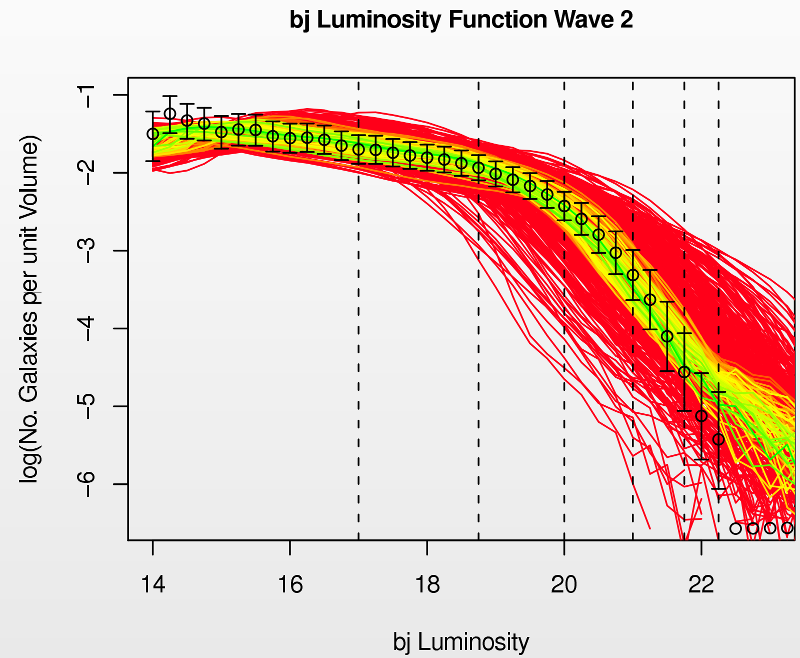
bj Luminosity Output of Waves 1,2,3 and 5

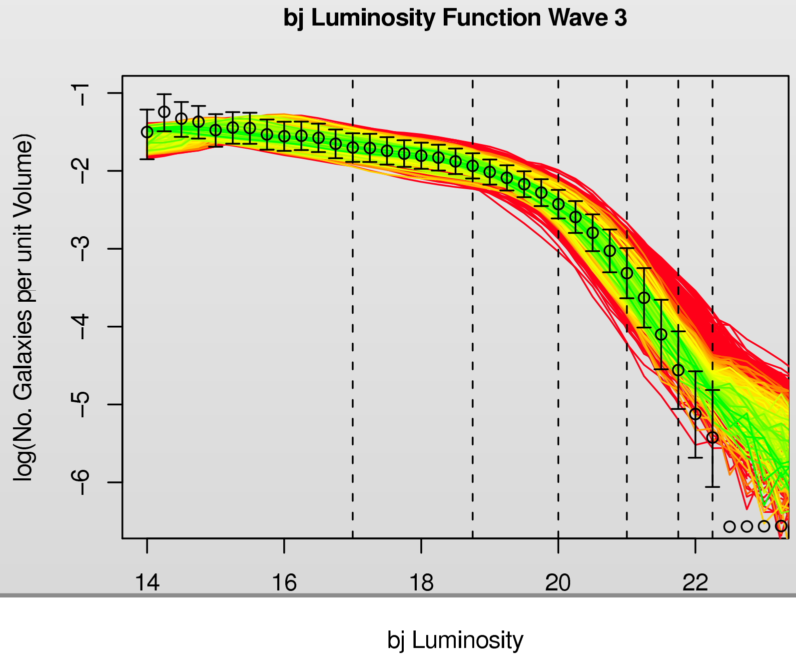




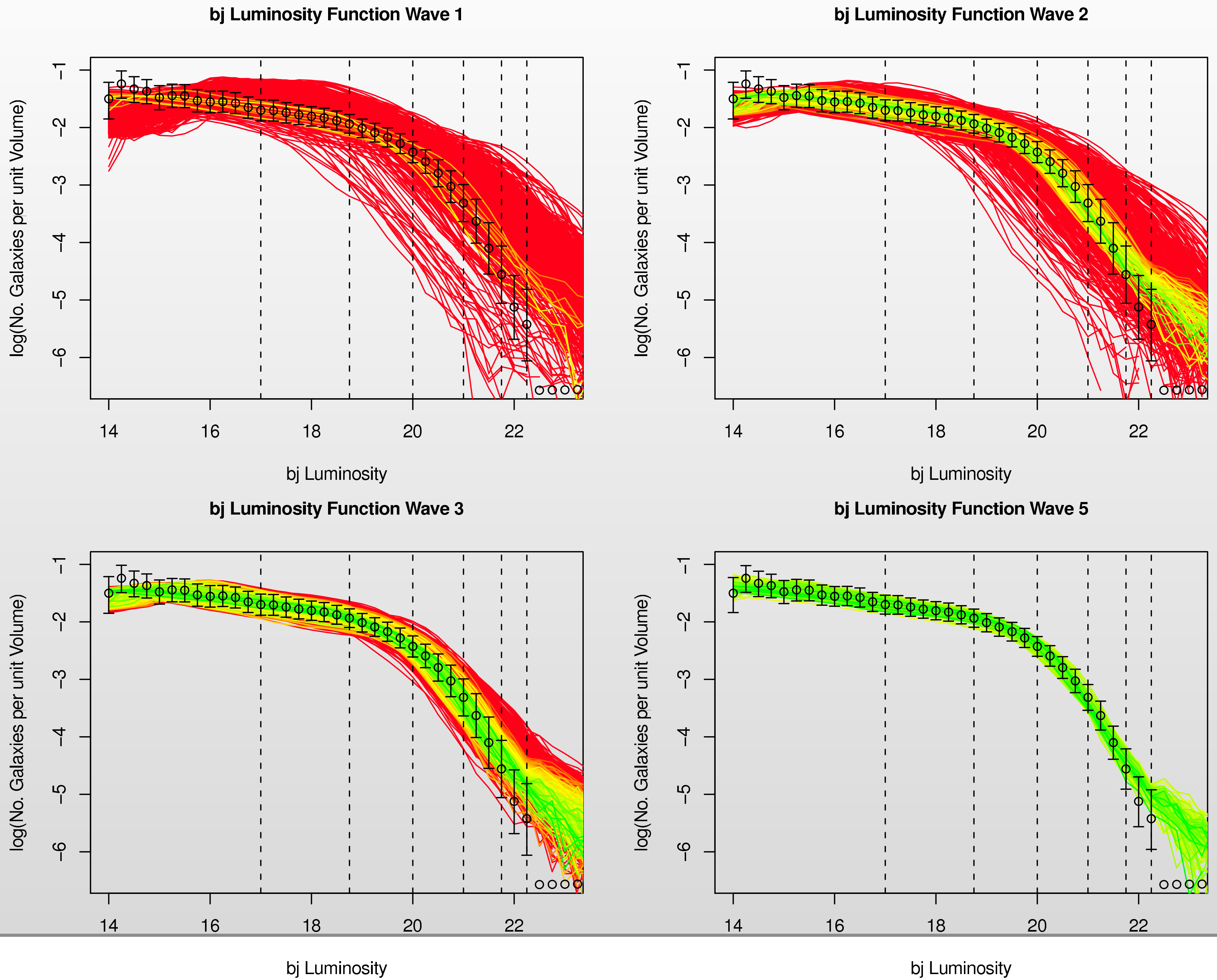
bj Luminosity Output of Waves 1,2,3 and 5



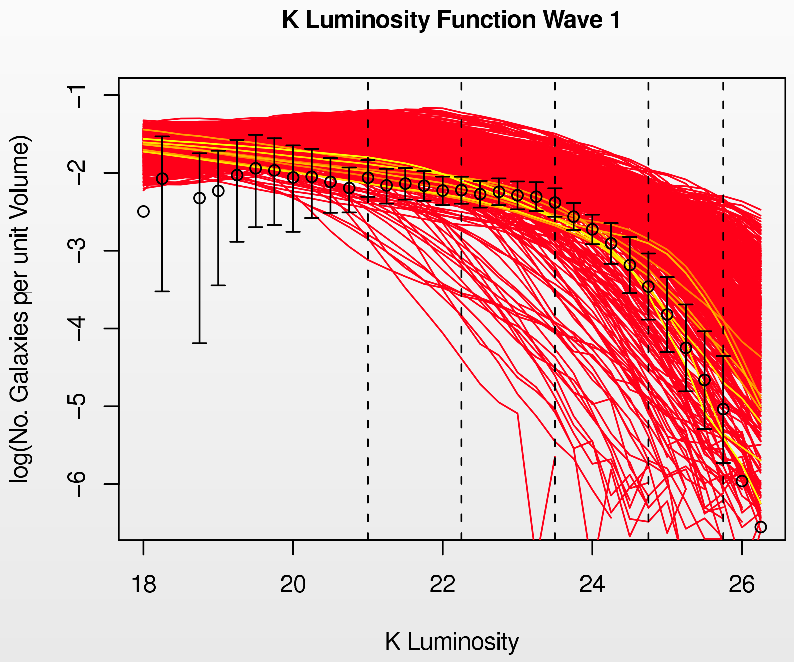




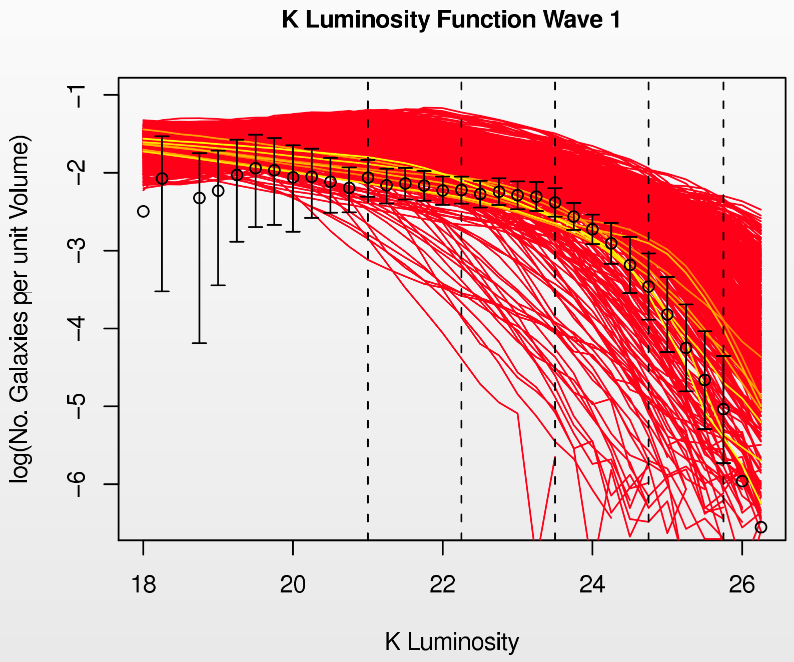
bj Luminosity Output of Waves 1,2,3 and 5

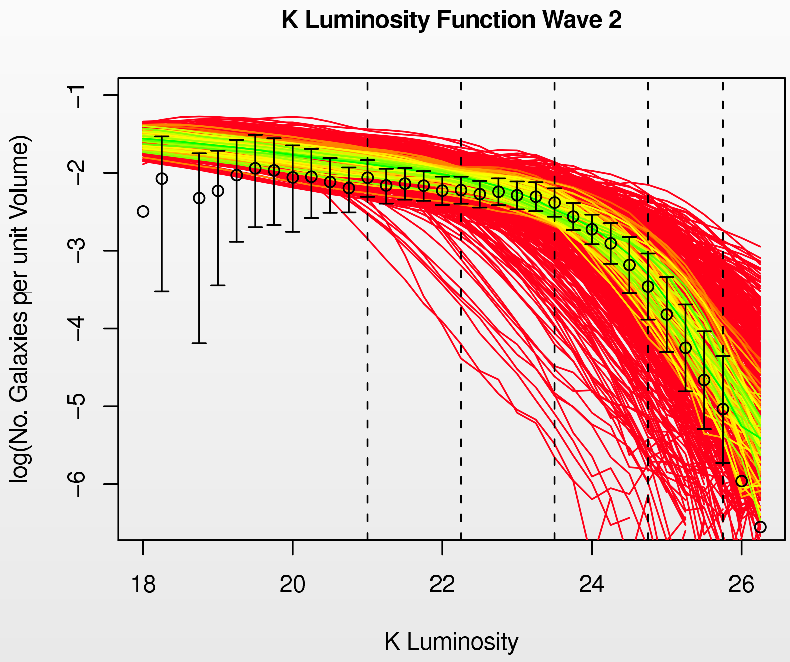


bj Luminosity Output of Waves 1,2,3 and 5

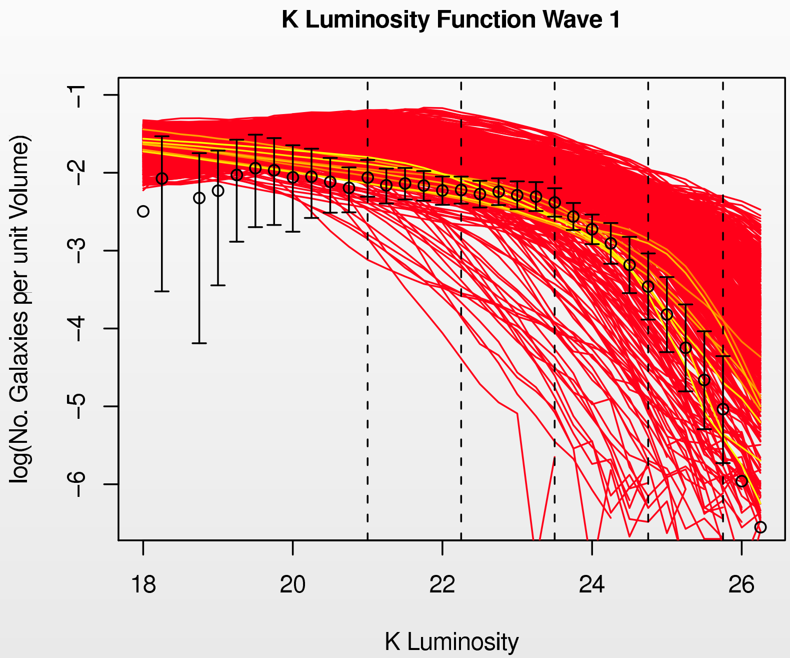


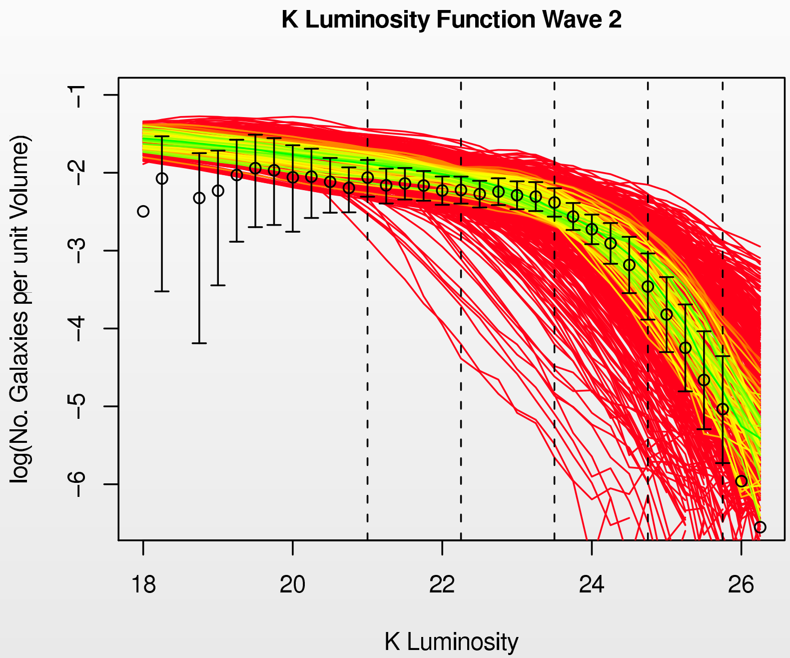
bj Luminosity Output of Waves 1,2,3 and 5

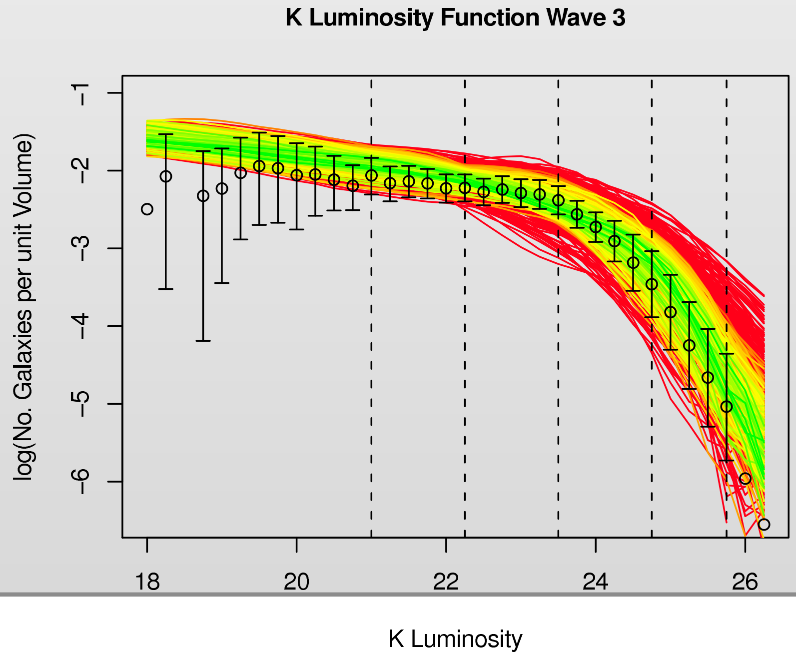




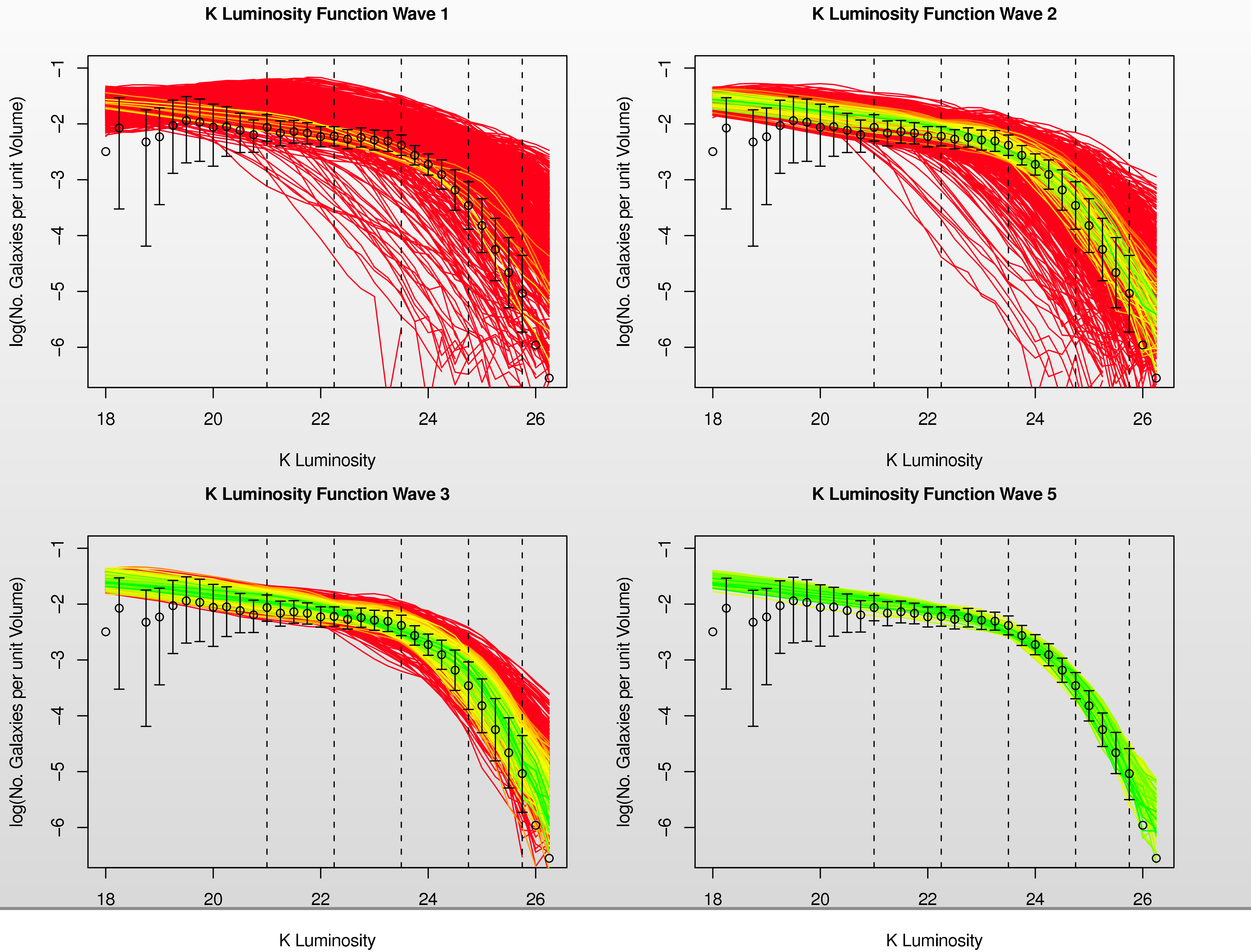
bj Luminosity Output of Waves 1,2,3 and 5







bj Luminosity Output of Waves 1,2,3 and 5



Conclusions

- Bayesian Statistics: the right thing to do!

Conclusions

- Bayesian Statistics: the right thing to do!
- Bayesian analysis of complex models: many techniques of possible use to the nuclear physics community.

Conclusions

- Bayesian Statistics: the right thing to do!
- Bayesian analysis of complex models: many techniques of possible use to the nuclear physics community.
- Iterative History Matching via implausibility: very efficient technique for learning about the set of acceptable inputs $\mathcal{X}$.

Conclusions

- Bayesian Statistics: the right thing to do!
- Bayesian analysis of complex models: many techniques of possible use to the nuclear physics community.
- Iterative History Matching via implausibility: very efficient technique for learning about the set of acceptable inputs $\mathcal{X}$.
- Relies upon Bayesian emulation and a careful analysis of all relevant uncertainties present in the problem: function uncertainty, structural model discrepancy, observed errors etc.

Conclusions

- Bayesian Statistics: the right thing to do!
- Bayesian analysis of complex models: many techniques of possible use to the nuclear physics community.
- Iterative History Matching via implausibility: very efficient technique for learning about the set of acceptable inputs $\mathcal{X}$.
- Relies upon Bayesian emulation and a careful analysis of all relevant uncertainties present in the problem: function uncertainty, structural model discrepancy, observed errors etc.
- Often appropriate to check model performance and analyse model structure. Can be a useful precursor to a fully Bayesian analysis over the whole input space, if such an analysis is deemed worthwhile.

Conclusions

- Bayesian Statistics: the right thing to do!
- Bayesian analysis of complex models: many techniques of possible use to the nuclear physics community.
- Iterative History Matching via implausibility: very efficient technique for learning about the set of acceptable inputs $\mathcal{X}$.
- Relies upon Bayesian emulation and a careful analysis of all relevant uncertainties present in the problem: function uncertainty, structural model discrepancy, observed errors etc.
- Often appropriate to check model performance and analyse model structure. Can be a useful precursor to a fully Bayesian analysis over the whole input space, if such an analysis is deemed worthwhile.
- We now have a large set of acceptable (Wave 5) runs that can be analysed by the Cosmologists, and used to explore other features of Galform.

References

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: “Bayesian History Matching for the Observable Universe”. *Statistical Science* 29 (2014), no. 1, 81–90.

References

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: “Bayesian History Matching for the Observable Universe”. *Statistical Science* 29 (2014), no. 1, 81–90.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in uganda. PLoS Comput Biol. 11(1), 1003968 (2015)

References

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: “Bayesian History Matching for the Observable Universe”. *Statistical Science* 29 (2014), no. 1, 81–90.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in uganda. PLoS Comput Biol. 11(1), 1003968 (2015)

Vernon, I., Goldstein, M., and Bower, R. G. (2010), “*Galaxy Formation: a Bayesian Uncertainty Analysis*”, *Bayesian Analysis*, 5(4): 619–670, with rejoinder. Invited discussion paper. Awarded Mitchell Prize.

References

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: “Bayesian History Matching for the Observable Universe”. *Statistical Science* 29 (2014), no. 1, 81–90.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in uganda. PLoS Comput Biol. 11(1), 1003968 (2015)

Vernon, I., Goldstein, M., and Bower, R. G. (2010), “*Galaxy Formation: a Bayesian Uncertainty Analysis*”, *Bayesian Analysis*, 5(4): 619–670, with rejoinder. Invited discussion paper. Awarded Mitchell Prize.

Bower, R., Vernon, I., Goldstein, M., et al. (2010), “*The Parameter Space of Galaxy Formation*”, *Mon.Not.Roy.Astron.Soc.*, 407: 2017–2045.

References

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: “Bayesian History Matching for the Observable Universe”. *Statistical Science* 29 (2014), no. 1, 81–90.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in uganda. PLoS Comput Biol. 11(1), 1003968 (2015)

Vernon, I., Goldstein, M., and Bower, R. G. (2010), “*Galaxy Formation: a Bayesian Uncertainty Analysis*”, *Bayesian Analysis*, 5(4): 619–670, with rejoinder. Invited discussion paper. Awarded Mitchell Prize.

Bower, R., Vernon, I., Goldstein, M., et al. (2010), “*The Parameter Space of Galaxy Formation*”, *Mon.Not.Roy.Astron.Soc.*, 407: 2017–2045.

Goldstein, M., Seheult, A., Vernon, I.: Assessing Model Adequacy. In: Wainwright, J., Mulligan, M. (eds.) Environmental Modelling: Finding Simplicity in Complexity, 2nd edn. John Wiley & Sons, Ltd, Chichester, UK (2013)

References

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: “Bayesian History Matching for the Observable Universe”. *Statistical Science* 29 (2014), no. 1, 81–90.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in uganda. PLoS Comput Biol. 11(1), 1003968 (2015)

Vernon, I., Goldstein, M., and Bower, R. G. (2010), “*Galaxy Formation: a Bayesian Uncertainty Analysis*”, *Bayesian Analysis*, 5(4): 619–670, with rejoinder. Invited discussion paper. Awarded Mitchell Prize.

Bower, R., Vernon, I., Goldstein, M., et al. (2010), “*The Parameter Space of Galaxy Formation*”, *Mon.Not.Roy.Astron.Soc.*, 407: 2017–2045.

Goldstein, M., Seheult, A., Vernon, I.: Assessing Model Adequacy. In: Wainwright, J., Mulligan, M. (eds.) Environmental Modelling: Finding Simplicity in Complexity, 2nd edn. John Wiley & Sons, Ltd, Chichester, UK (2013)

”Bayesian uncertainty analysis for complex systems biology models: emulation, global parameter searches and evaluation of gene functions.”, Vernon, I, Goldstein, M, Rowe, J, Liu, J and Lindsey, K, *in prep for BMC Systems Biology*. On arXiv soon.

References

Vernon, I.; Goldstein, M.; Bower, R. G.; Galaxy Formation: “Bayesian History Matching for the Observable Universe”. *Statistical Science* 29 (2014), no. 1, 81–90.

Andrianakis, I., Vernon, I., McCreesh, N., McKinley, T.J., Oakley, J.E., Nsubuga, R., Goldstein, M., White, R.G.: Bayesian history matching of complex infectious disease models using emulation: A tutorial and a case study on HIV in uganda. PLoS Comput Biol. 11(1), 1003968 (2015)

Vernon, I., Goldstein, M., and Bower, R. G. (2010), “*Galaxy Formation: a Bayesian Uncertainty Analysis*”, *Bayesian Analysis*, 5(4): 619–670, with rejoinder. Invited discussion paper. Awarded Mitchell Prize.

Bower, R., Vernon, I., Goldstein, M., et al. (2010), “*The Parameter Space of Galaxy Formation*”, *Mon.Not.Roy.Astron.Soc.*, 407: 2017–2045.

Goldstein, M., Seheult, A., Vernon, I.: Assessing Model Adequacy. In: Wainwright, J., Mulligan, M. (eds.) Environmental Modelling: Finding Simplicity in Complexity, 2nd edn. John Wiley & Sons, Ltd, Chichester, UK (2013)

”Bayesian uncertainty analysis for complex systems biology models: emulation, global parameter searches and evaluation of gene functions.”, Vernon, I, Goldstein, M, Rowe, J, Liu, J and Lindsey, K, *in prep for BMC Systems Biology*. On arXiv soon.

Rodrigues, L.F.S., Vernon, I., Bower, R.G.: Constraints to galaxy formation models using the galaxy stellar mass function, stronger feedback during starbursts? *in prep for Mon.Not.Roy.Astron.Soc.*. On arXiv soon.