Bayesian Statistics Applied to Complex Models of Physical Systems

ISNET-5

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  - Iterative History Matching via Implausibility: a pre-calibration method.
  - Visualisation of results.

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  - Bayesian statistics can be viewed as a natural extension to pure logic once uncertainty is introduced.

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- Subjective Bayesian statistics: the pure form!

Choices within Bayesian Statistics.

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

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- 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).

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- These techniques could be of substantial use to the Nuclear physics community.

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- 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.

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

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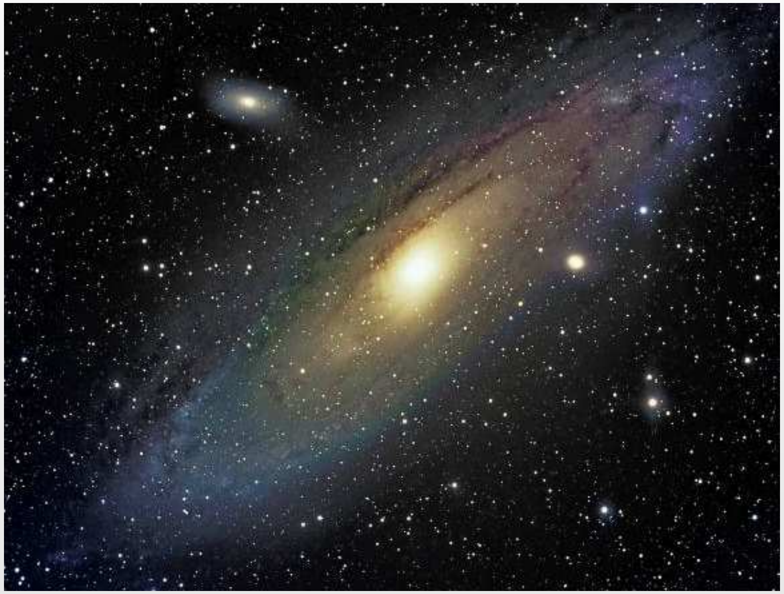
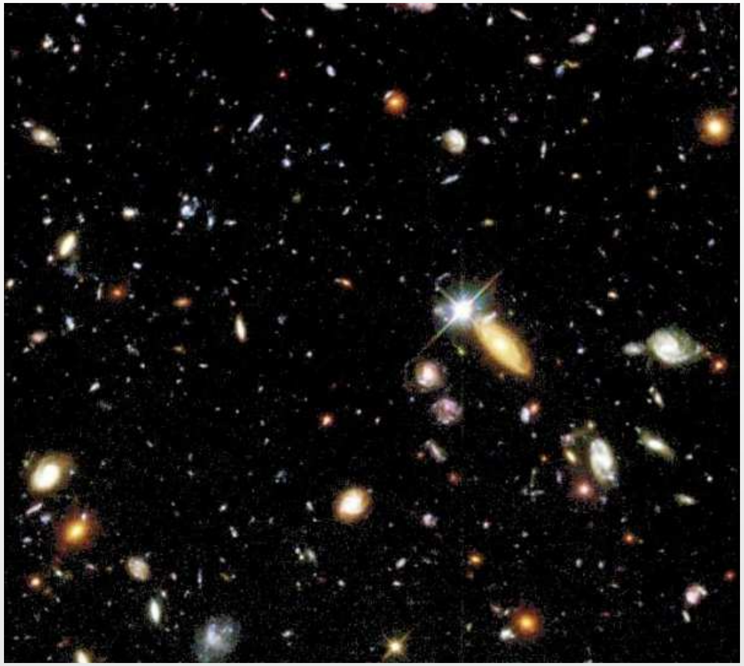
- This involves the specification of many complex multivariate distributions related to all uncertain quantities of interest, which may or may not be warranted at this stage.

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.

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- 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.

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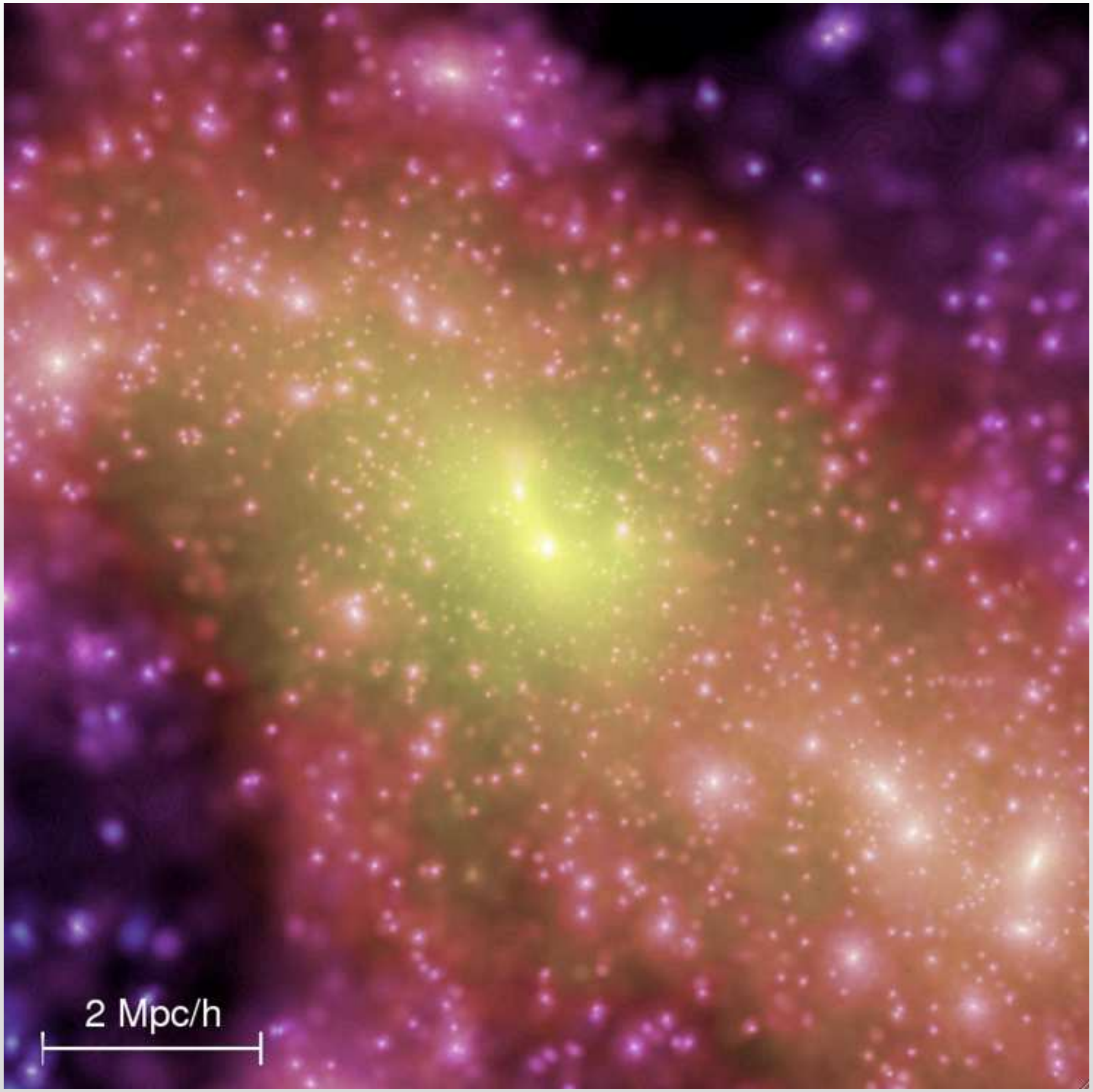
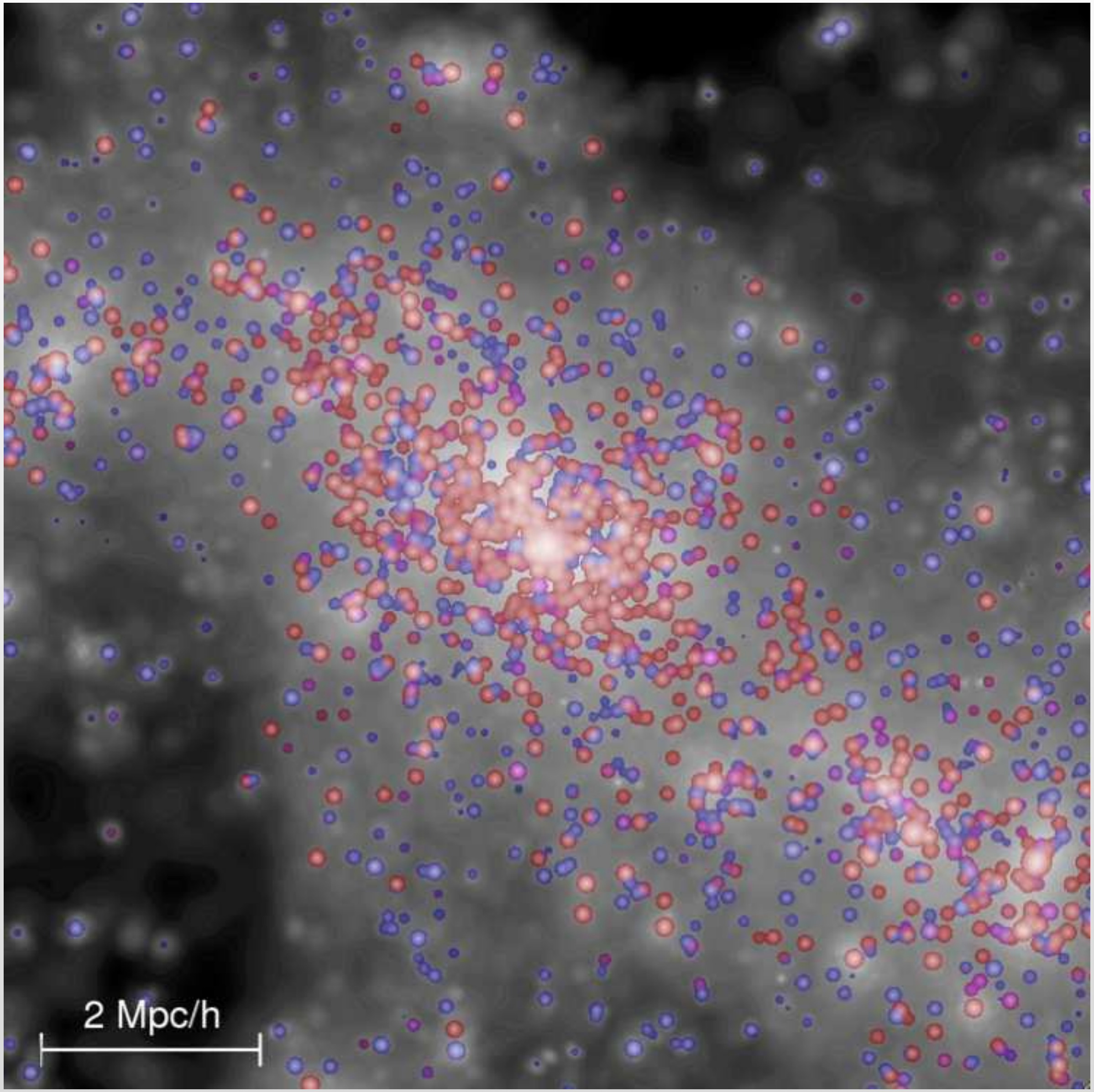
- Use the Emulator to find the acceptable inputs.

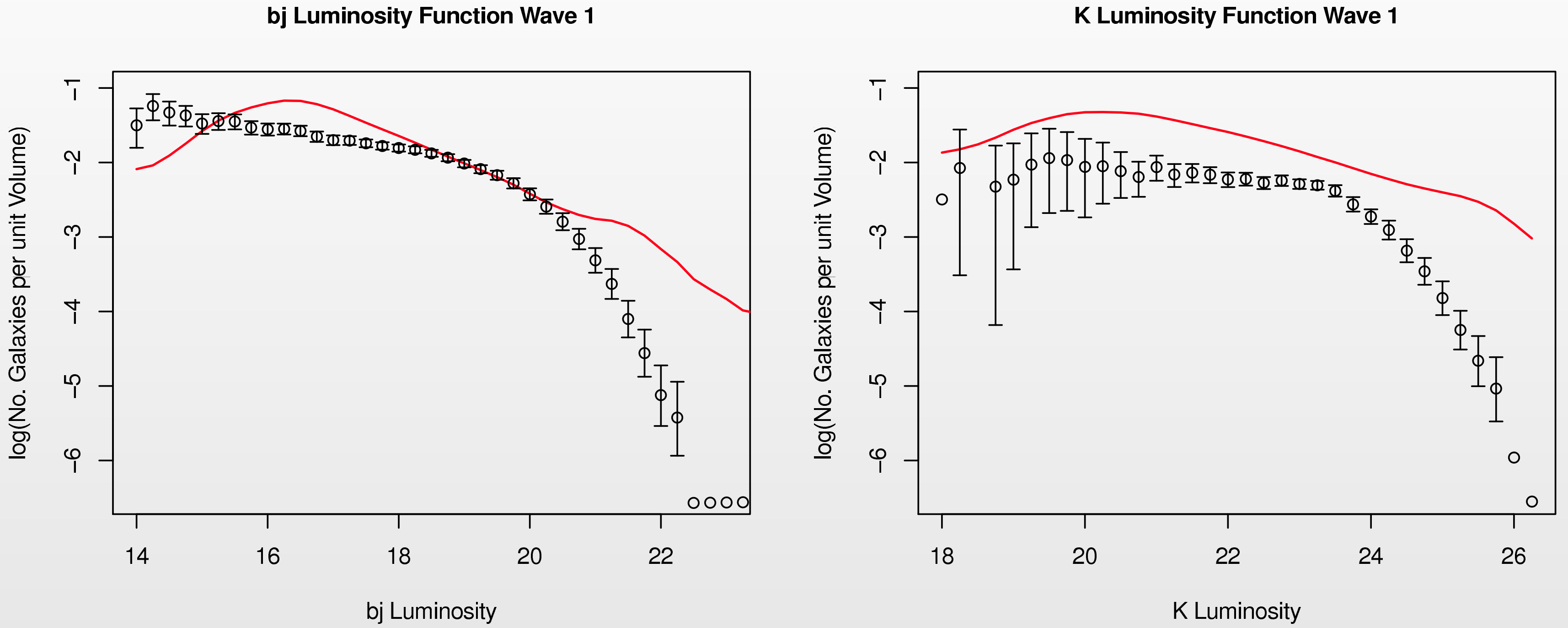
The Dark Matter Simulation: (thanks to VIRGO Consortium)



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

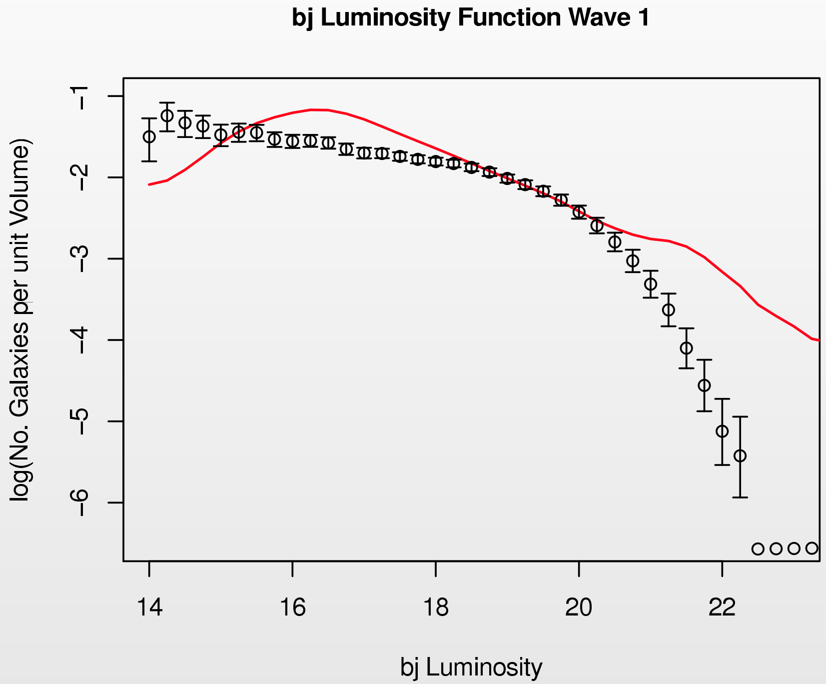
Input Parameters

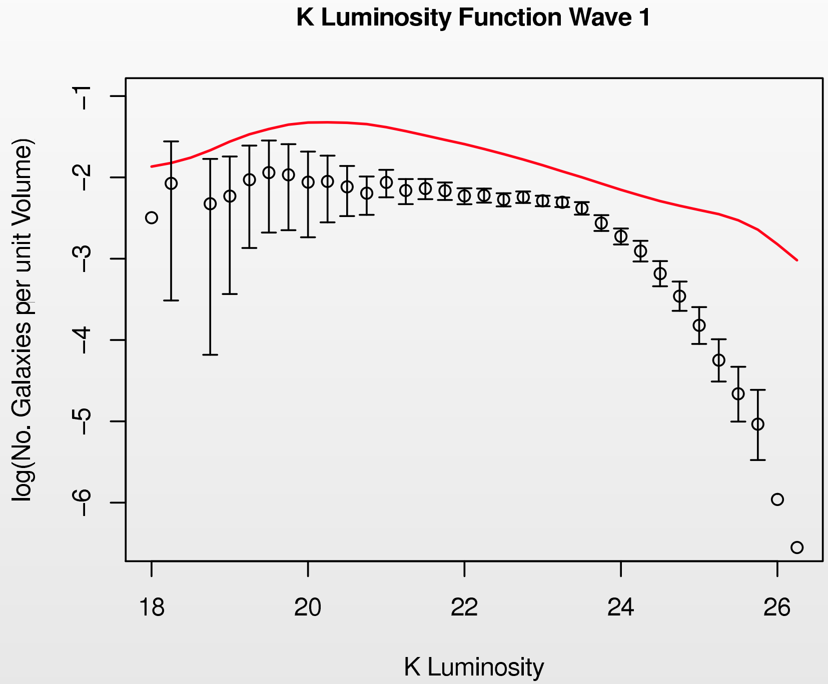
- To perform one run, we need to specify numbers for each of the following 17 inputs:

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?

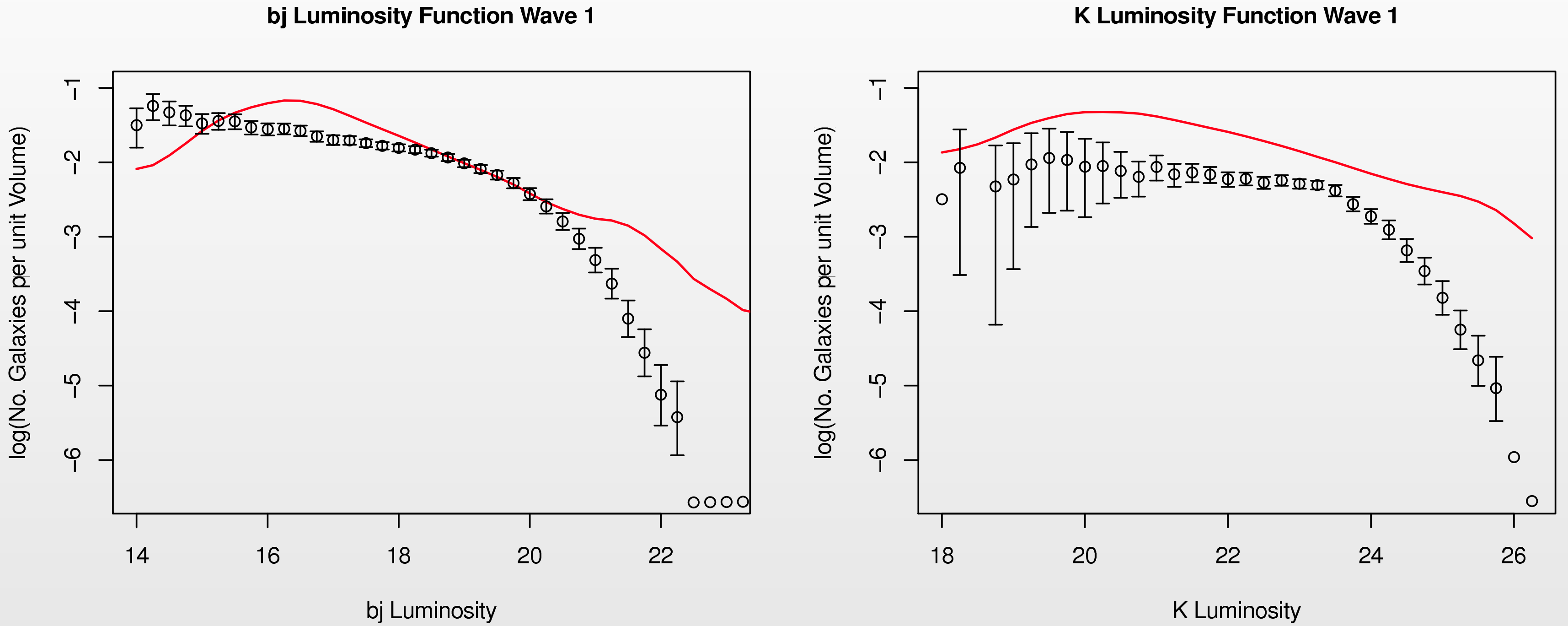
Galform Outputs: The Luminosity Functions





- 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.

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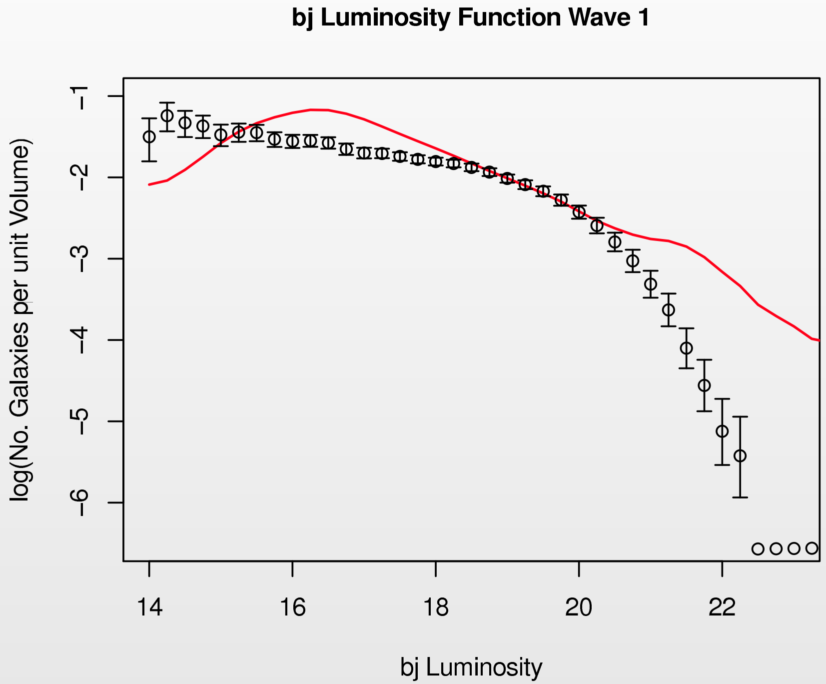
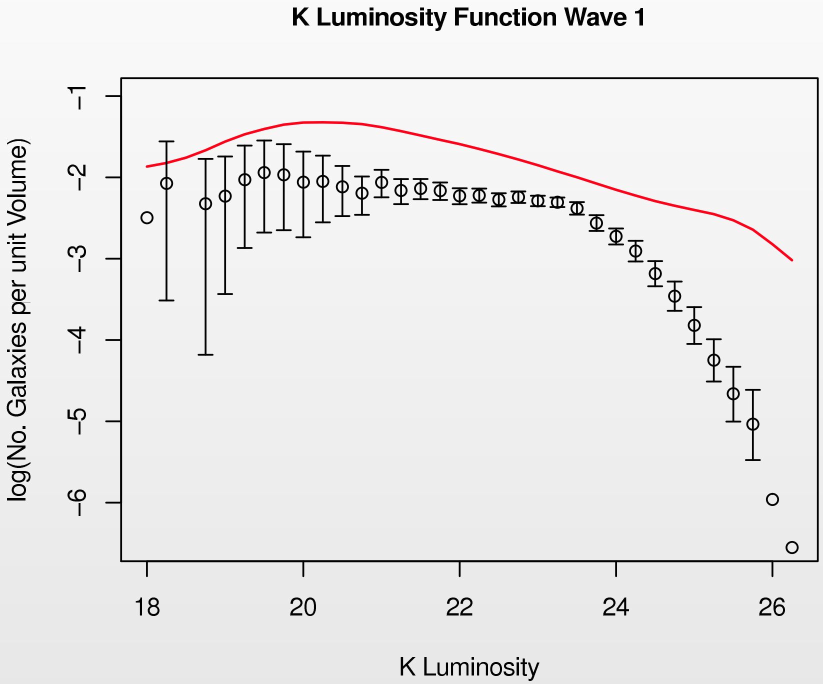
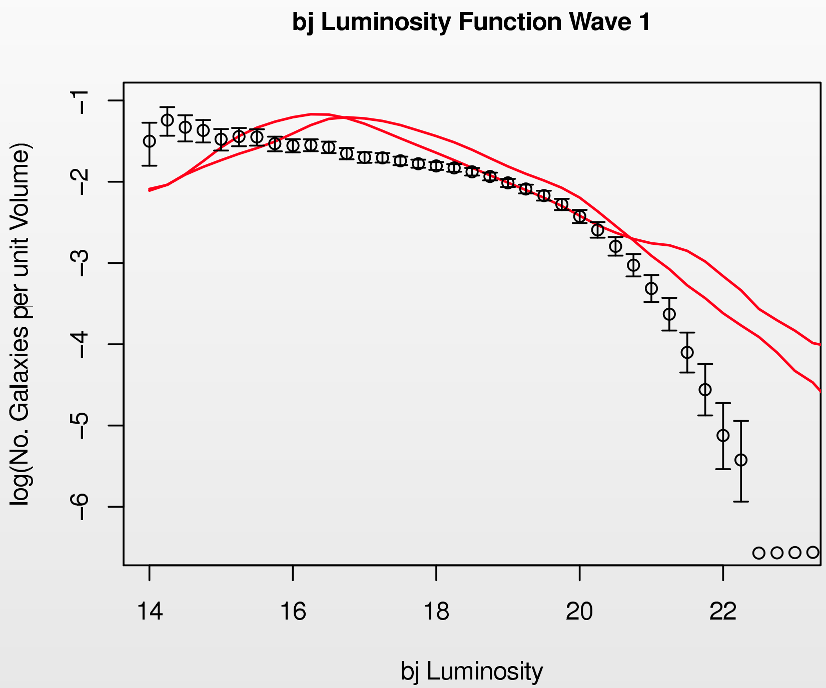
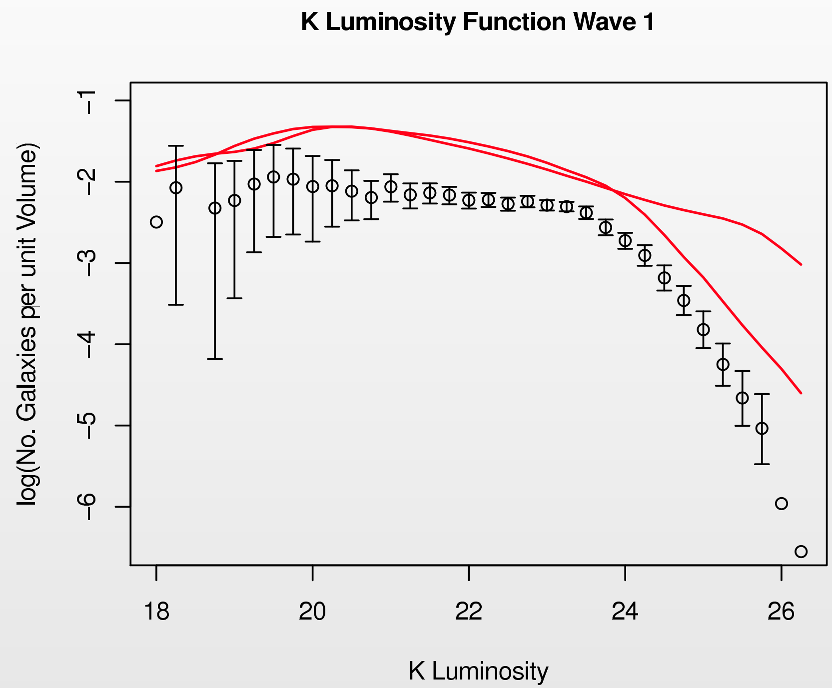




- Basic problem is that we pick inputs:
- vhotdisk $= 223.3$, aReheat $= 0.49$, alphacool $= 1.12$, ...
- And find that after 2 Days of Runtime:

Galform Outputs: The Luminosity Functions





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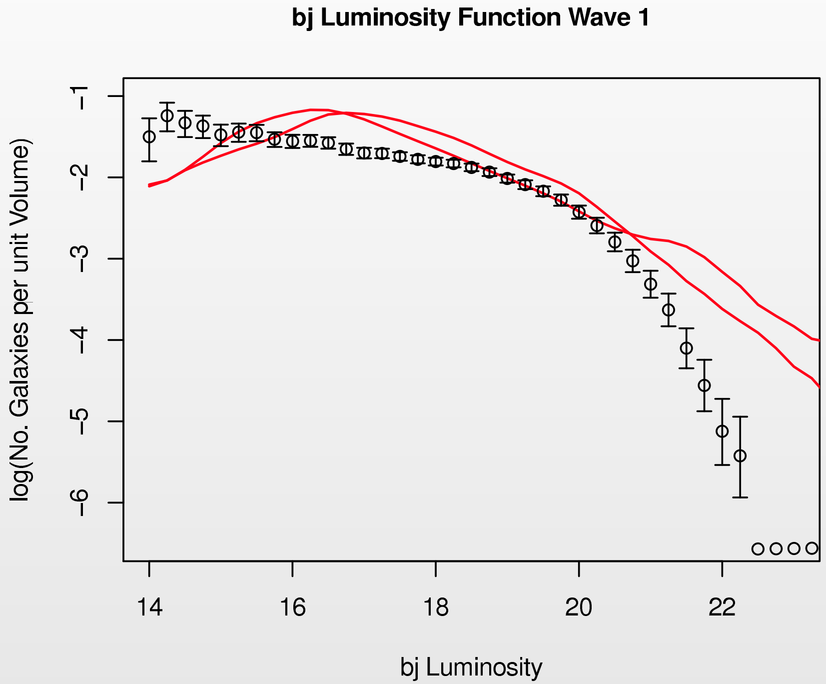
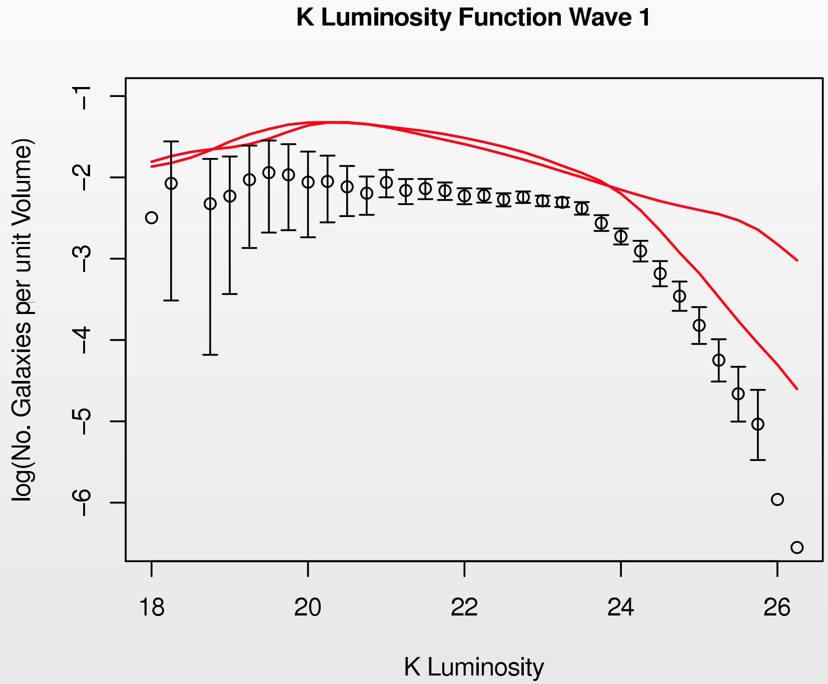
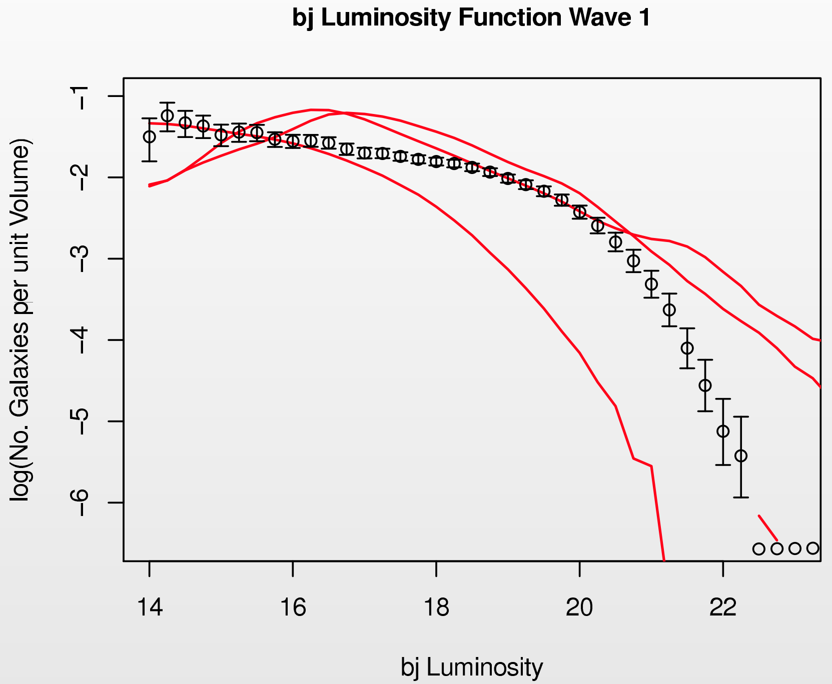
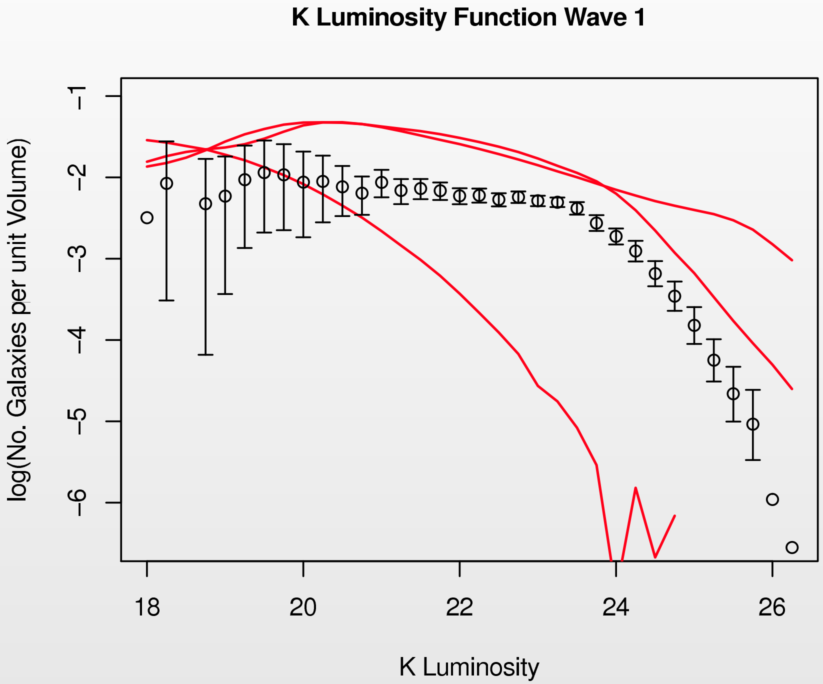




- Basic problem is that we pick inputs:
- vhotdisk $= 349.7$, aReheat $= 0.21$, alphacool $= 1.08$, ...
- And find that after 3 Days of Runtime:

Galform Outputs: The Luminosity Functions





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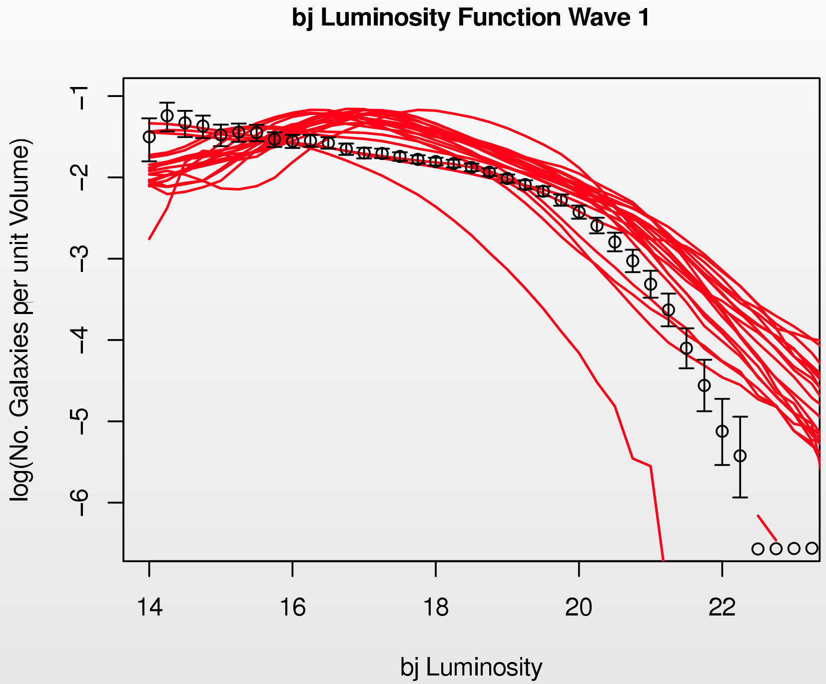
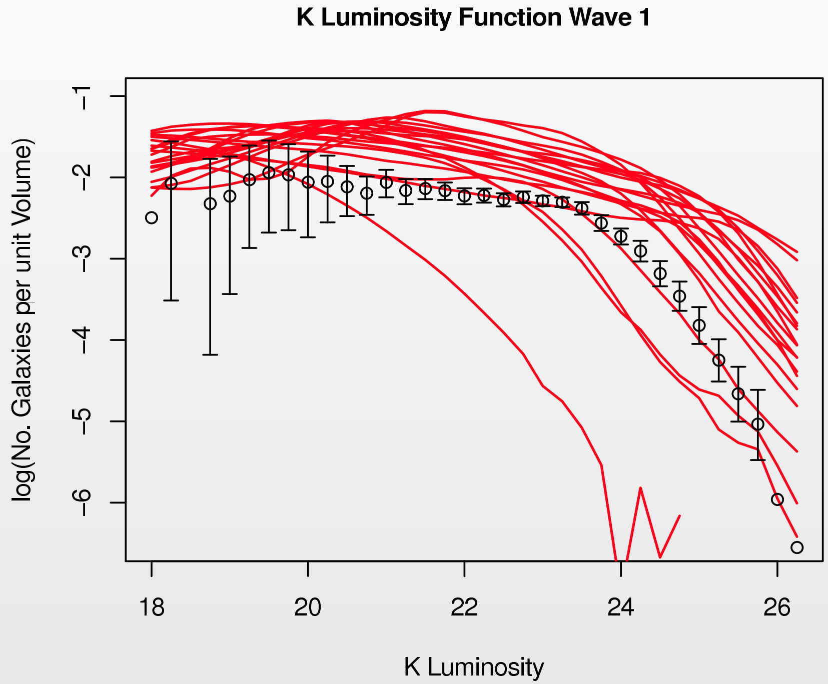
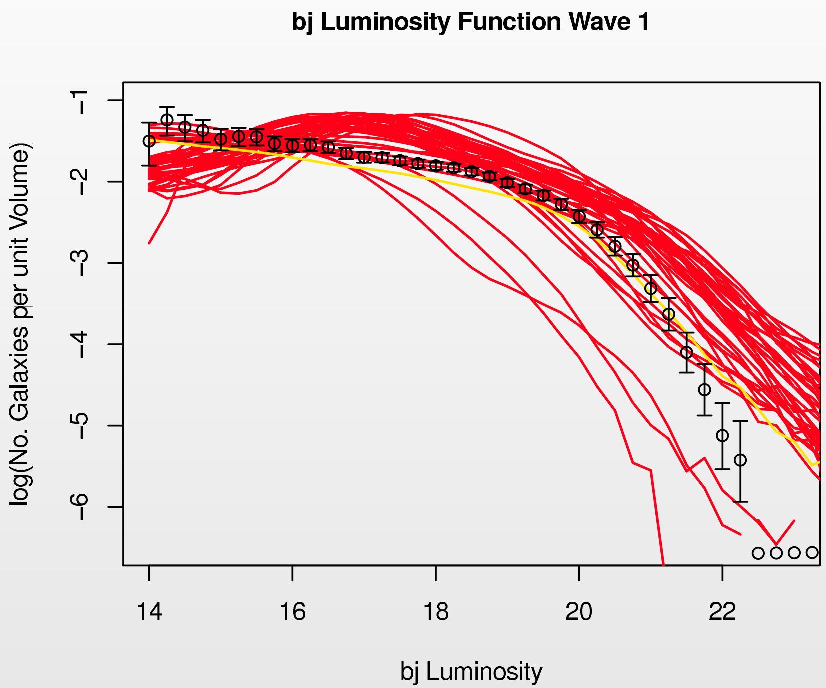
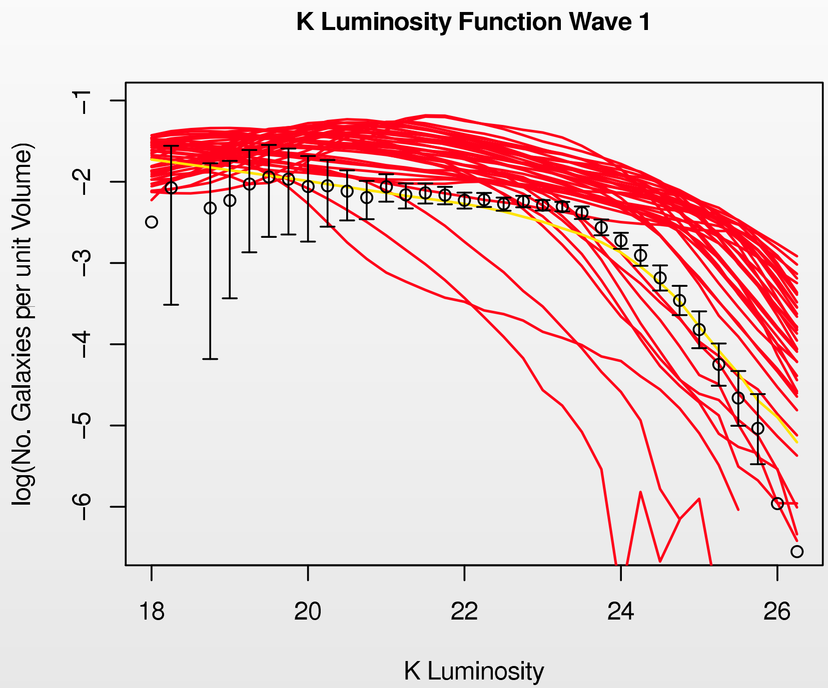




- Pick 20 inputs and find after 20 Days of Runtime:
- All runs are rubbish.

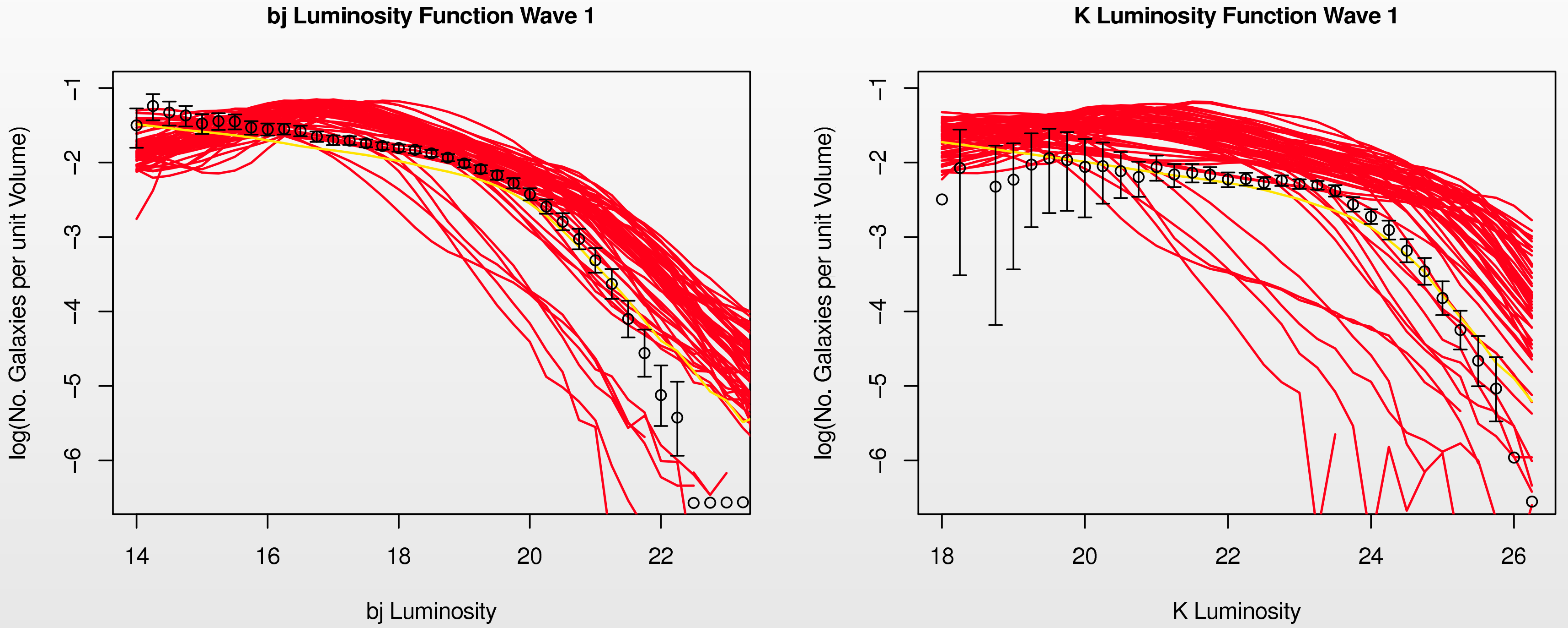
Galform Outputs: The Luminosity Functions





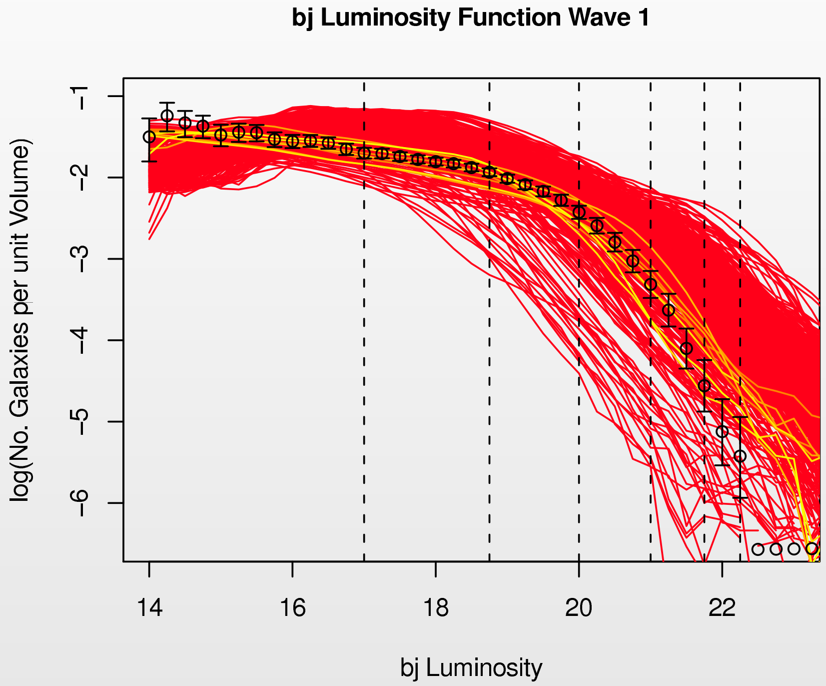
- Pick 40 inputs and find after 40 Days of Runtime:
- All runs are rubbish.

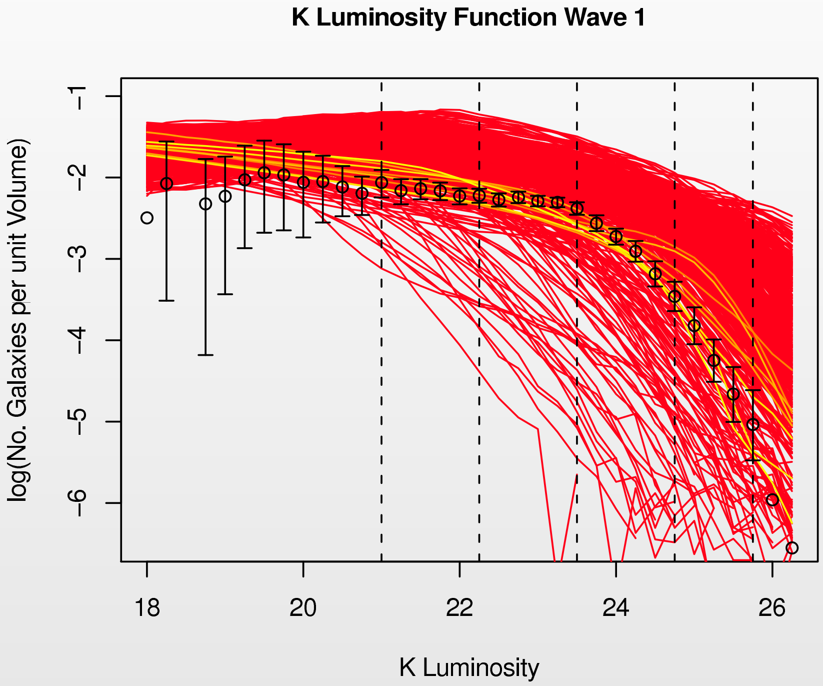
Galform Outputs: The Luminosity Functions



- 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.)

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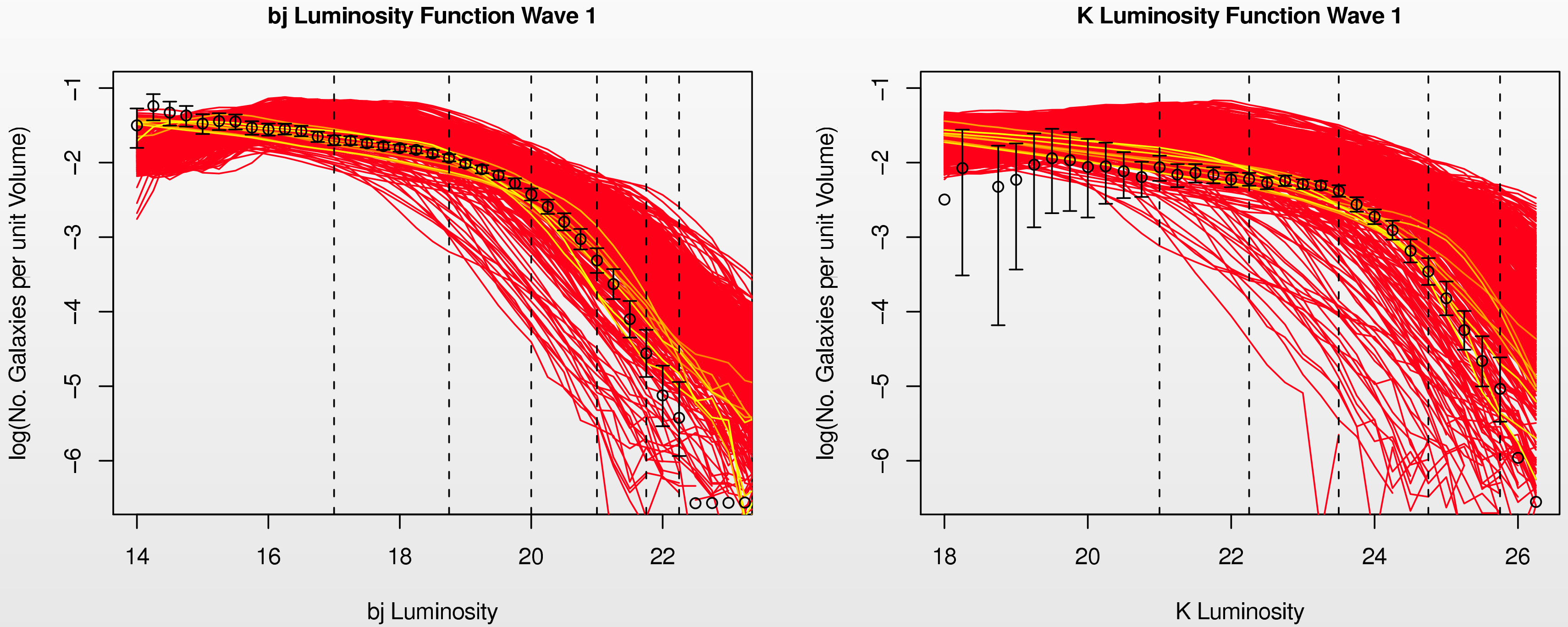
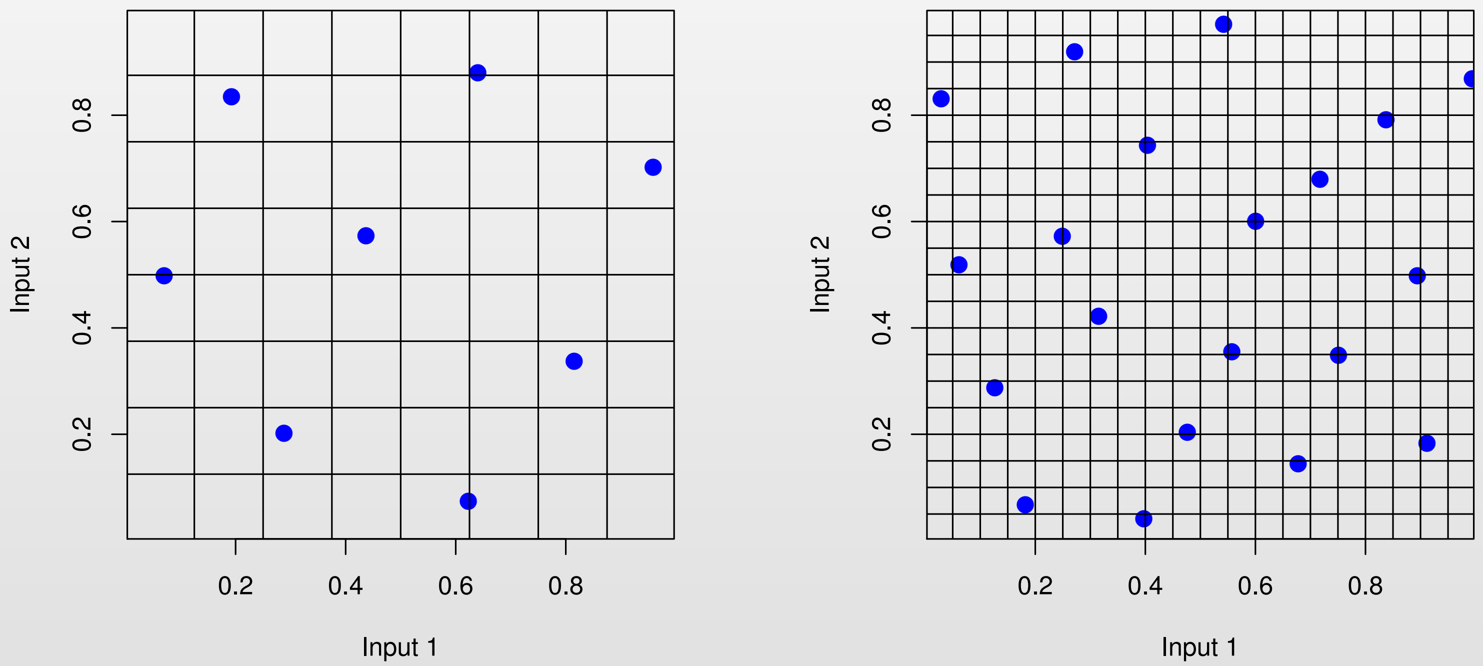


- We do 1000 runs using carefully chosen inputs (a space-filling maximin latin hypercube design).
- (Again all runs are found to be unacceptable.)
- We choose 11 outputs that are representative of the Luminosity functions and emulate these functions $f_i(x)$.

Design: Latin Hypercubes

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



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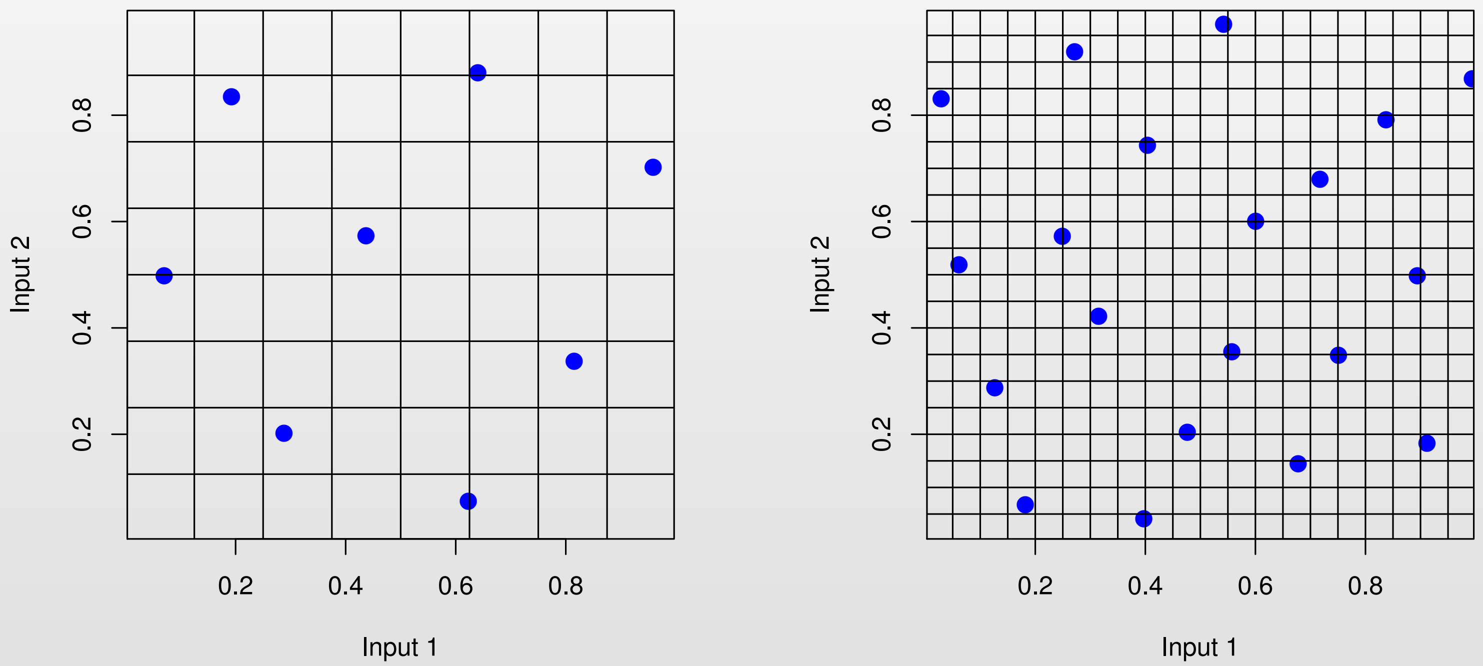

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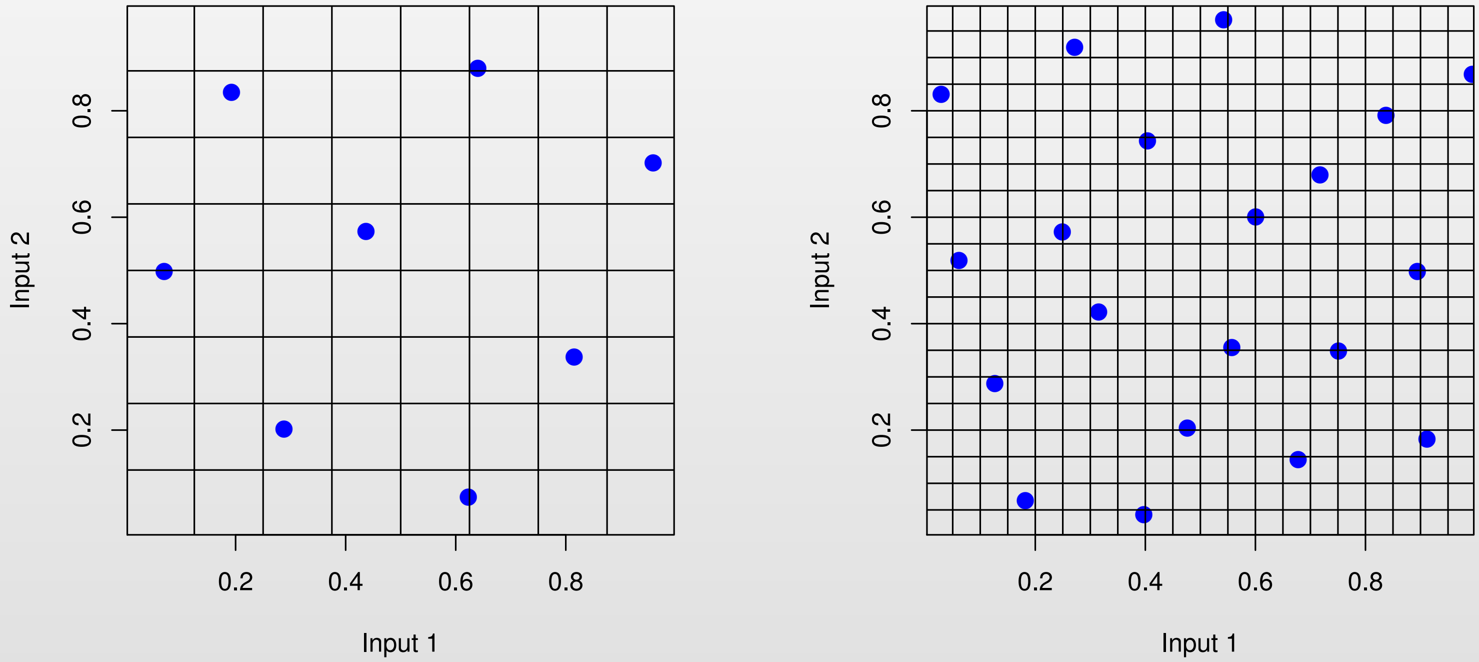
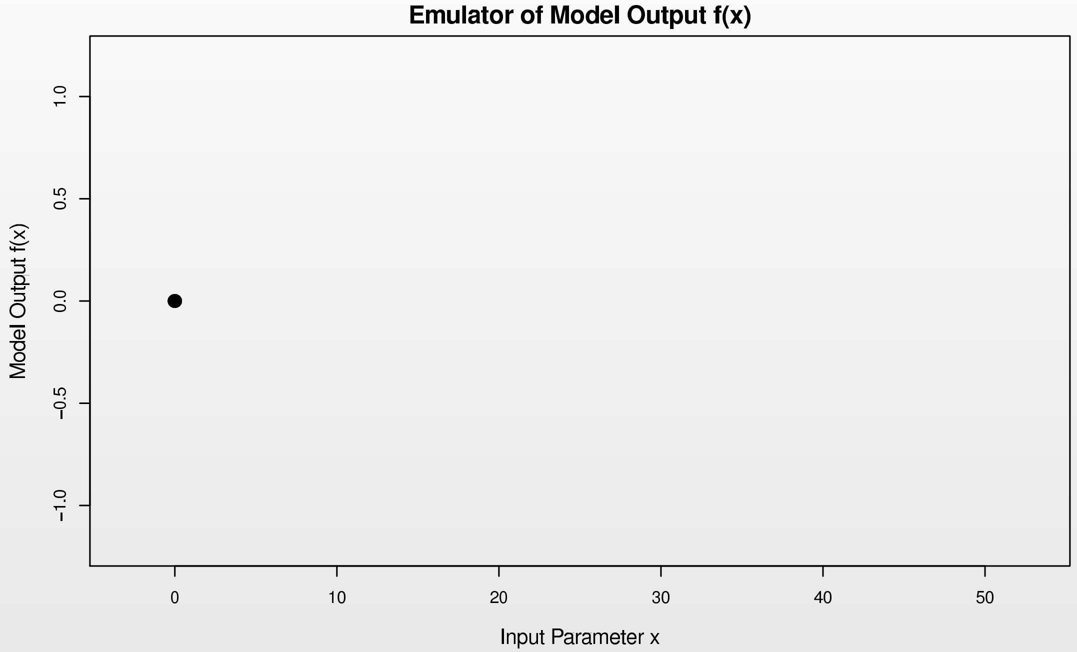


- These designs are both space filling and approximately orthogonal, both desirable features for fitting emulators.
- We evaluated 1000 runs of the model for the first Wave.

Emulation: a 1D Example



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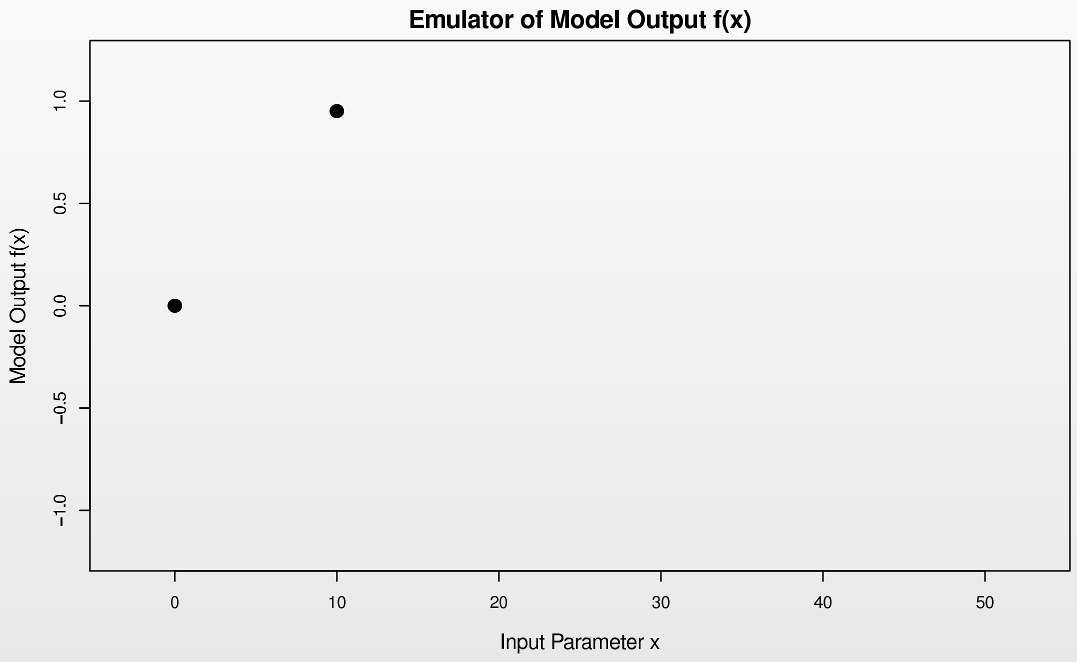

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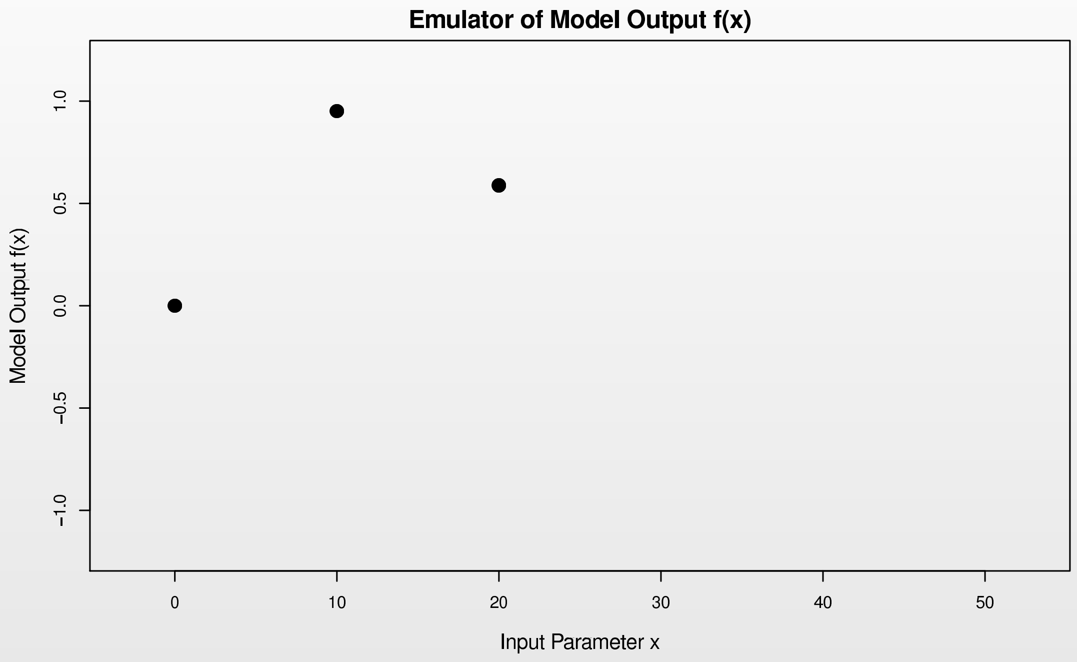

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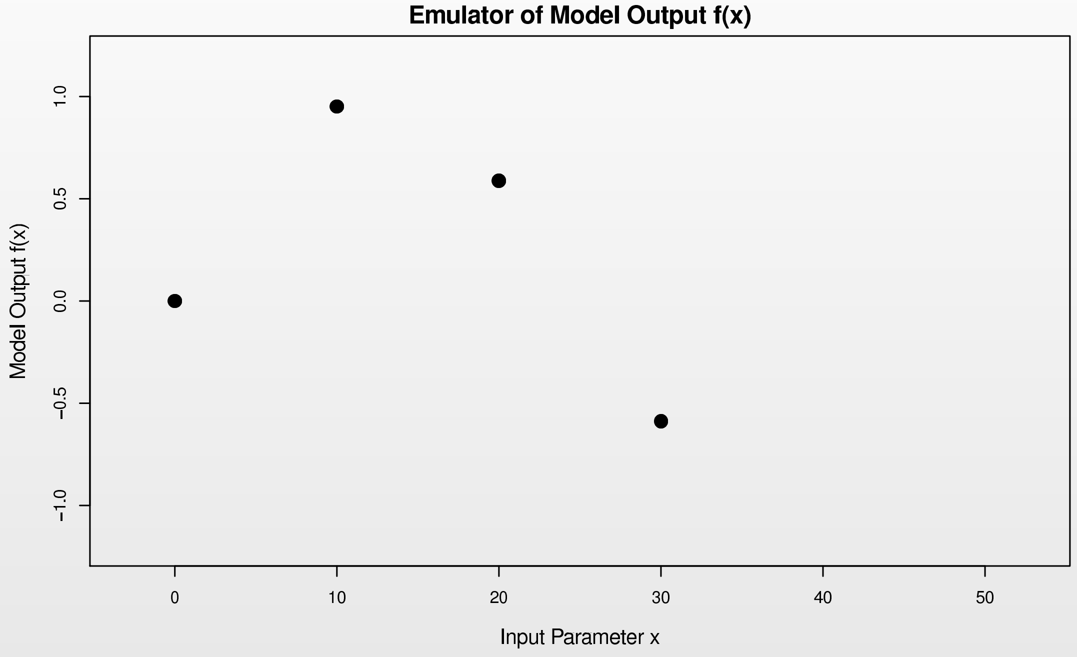

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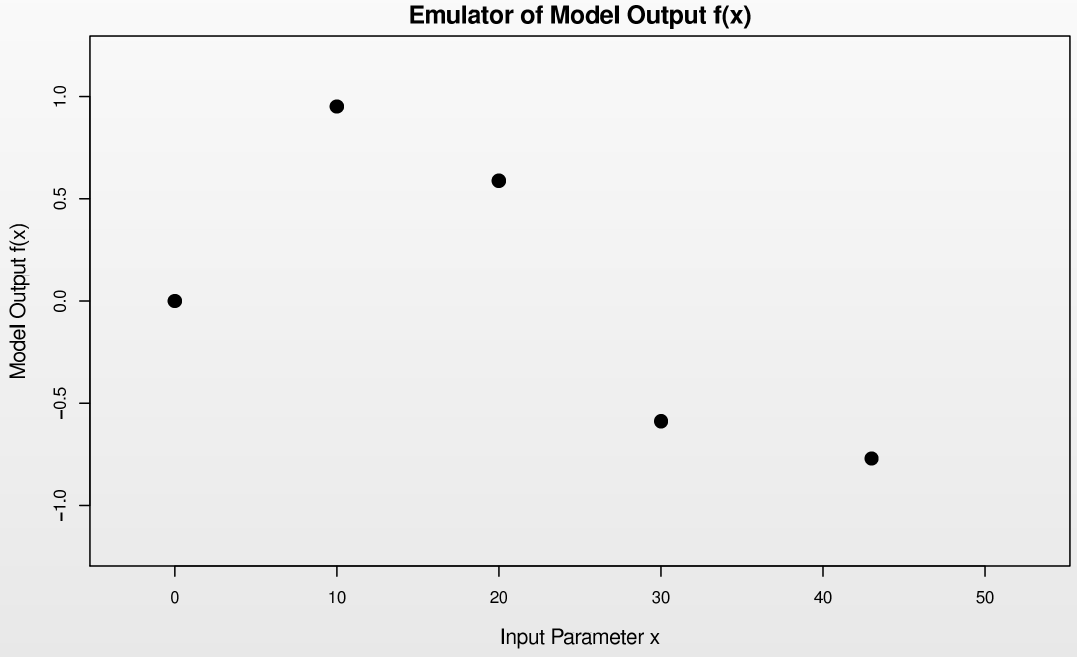

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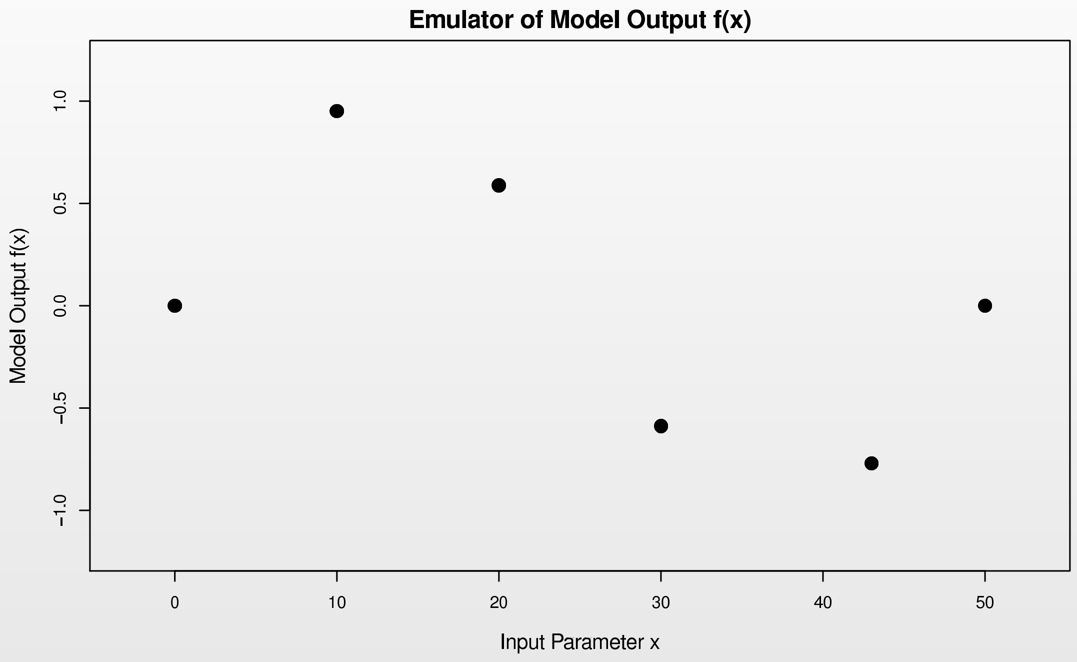

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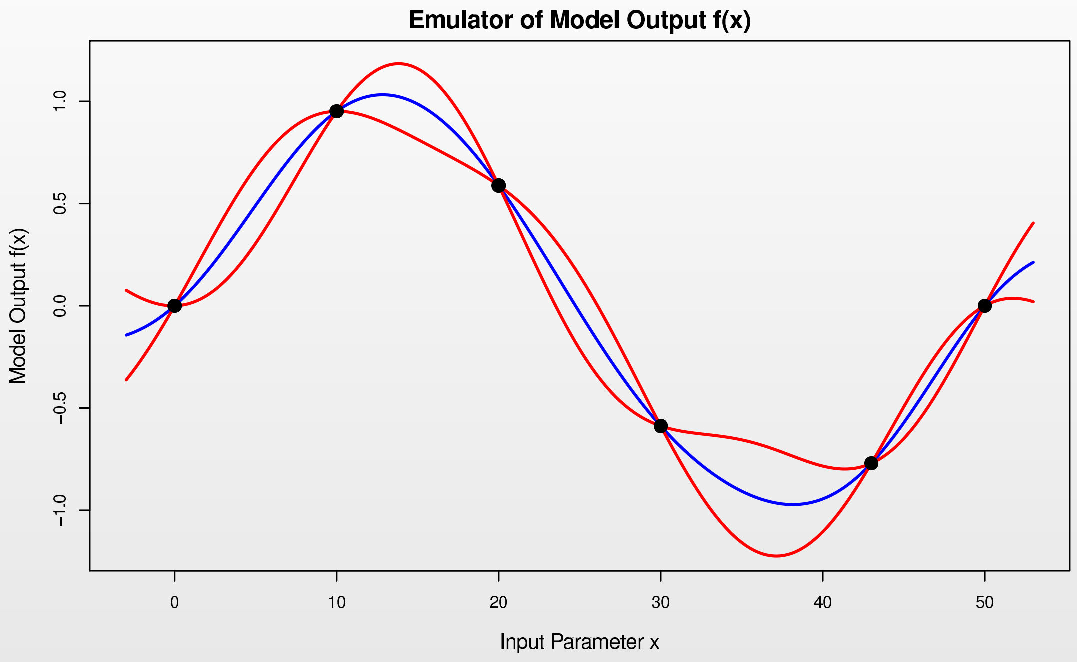

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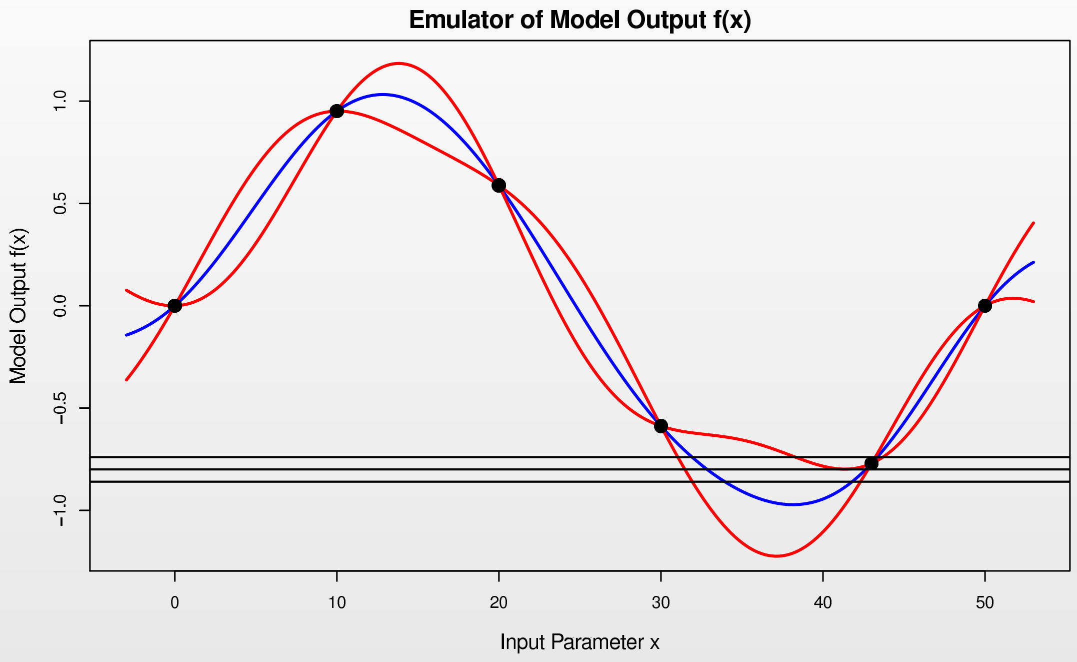

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- Finally, we relate the true system y to the observational data z by,

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  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:

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

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- The $u_i(x^A)$ have covariance structure given by:

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- 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

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

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- 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 $f_i(x)$.

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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

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- 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 $\mathsf{Var}(\epsilon) = \Phi_{40} + \Phi_9 + \Phi_E$

- 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

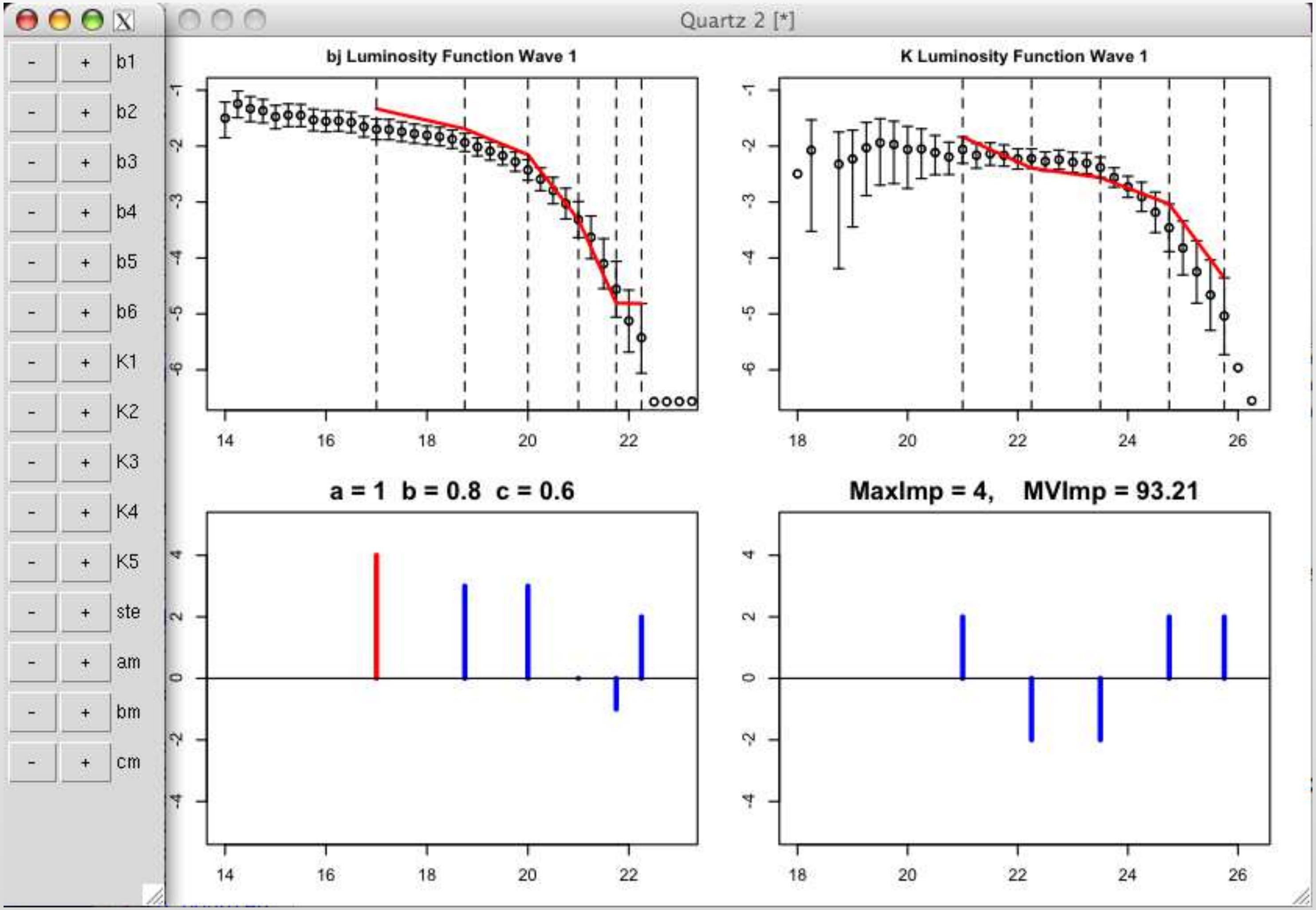
- Experts assert that there are clear ways that the model could be defective.
- Model predicts too many (or too few) galaxies. This would lead to a highly correlated model discrepancy across all outputs.
- Model systematically gets the colours of galaxies wrong: results in too few (too many) blue galaxies 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:

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

- 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:

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

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- Small values of $I_{(i)}(x)$ do not imply that x is good!

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- 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:

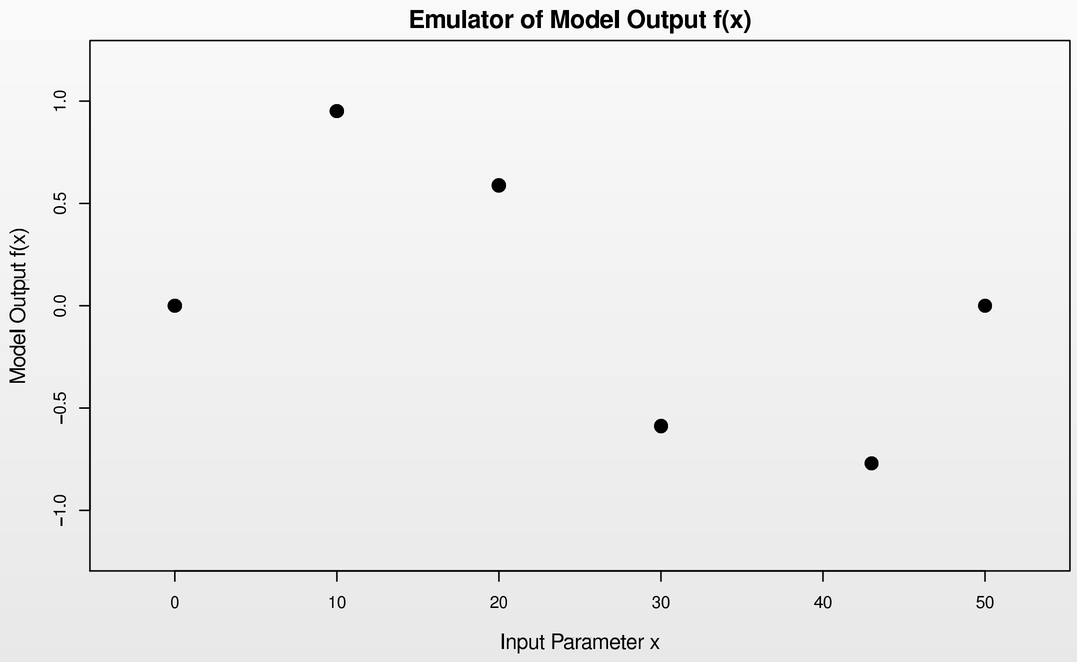
$$I^2(x) = (\mathrm{E}[f(x)] - z)^T \mathrm{Var}[f(x) - z]^{-1} (\mathrm{E}[f(x)] - z),$$

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 11×11 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



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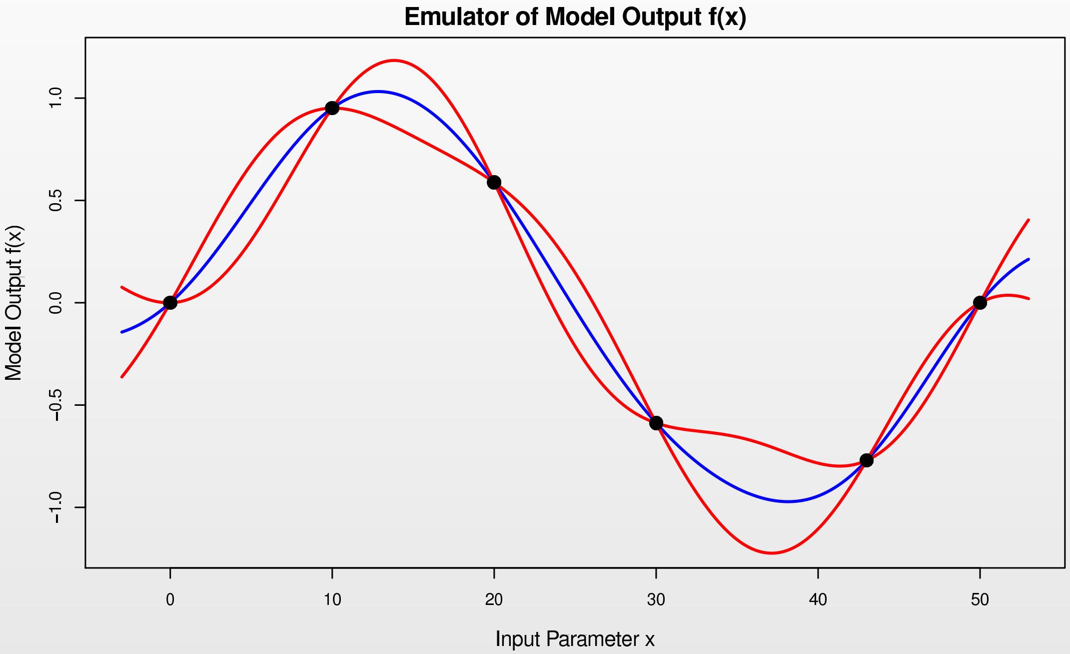

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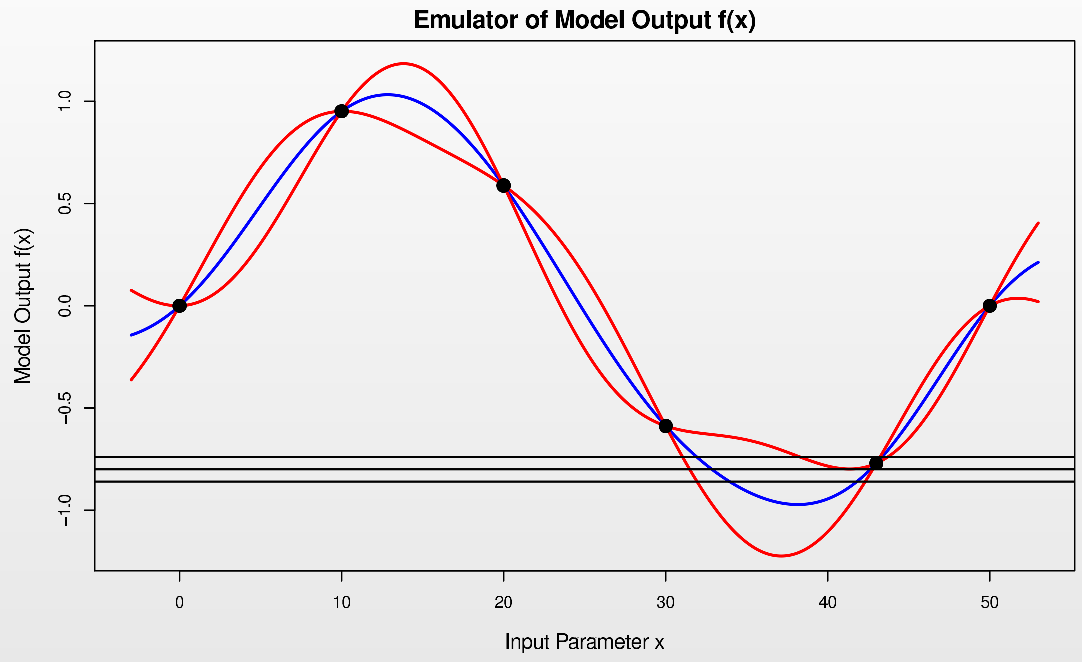

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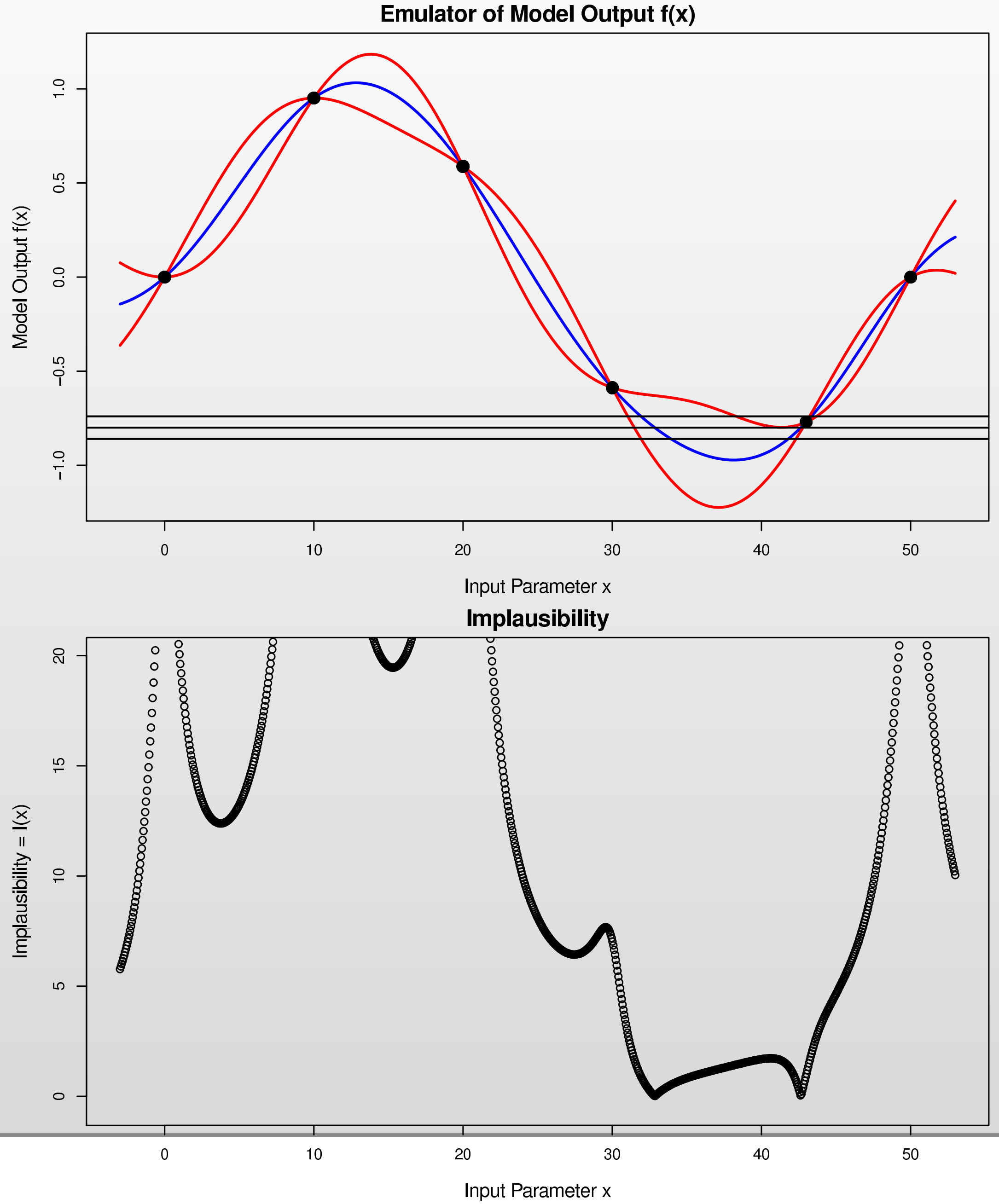

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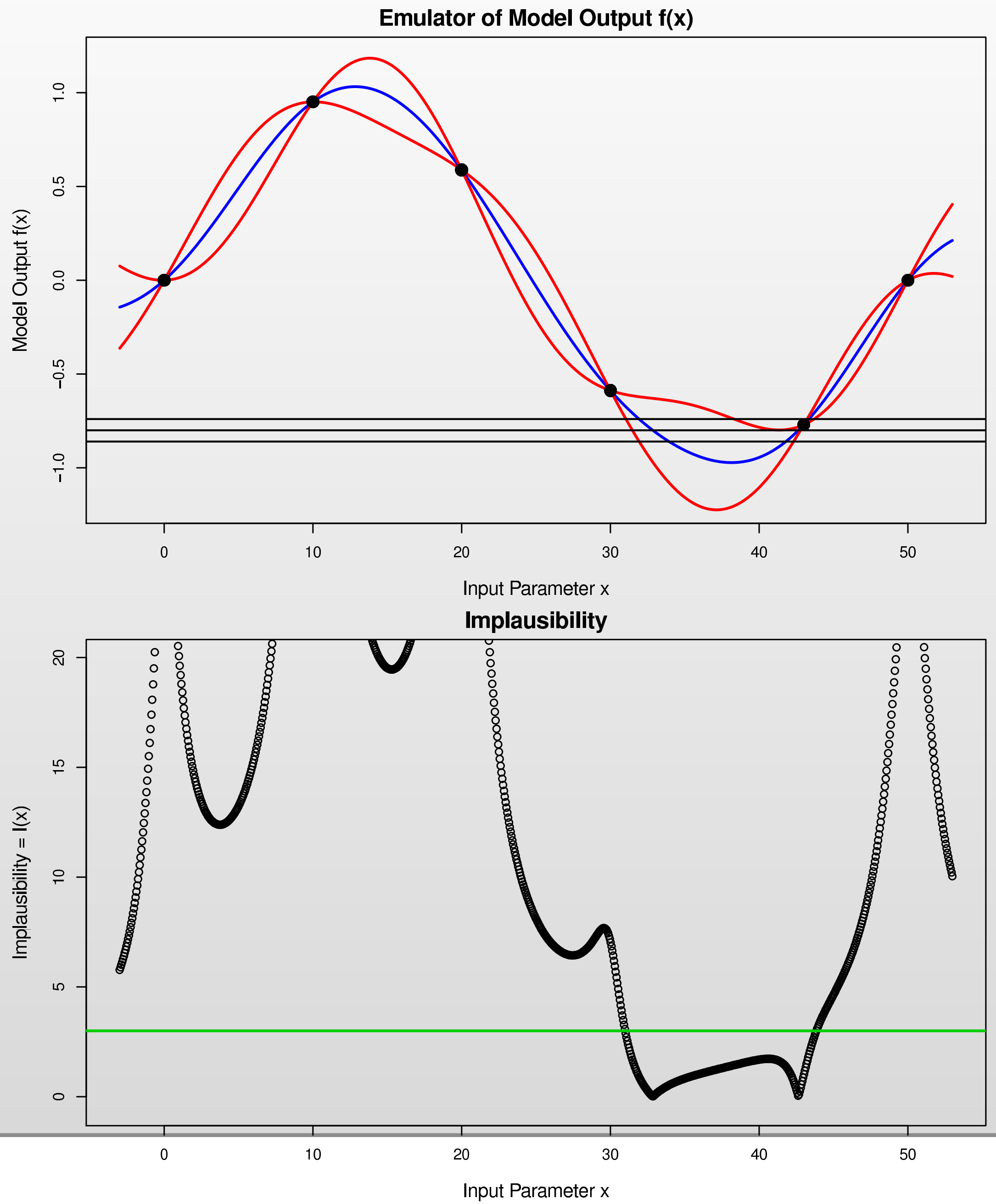

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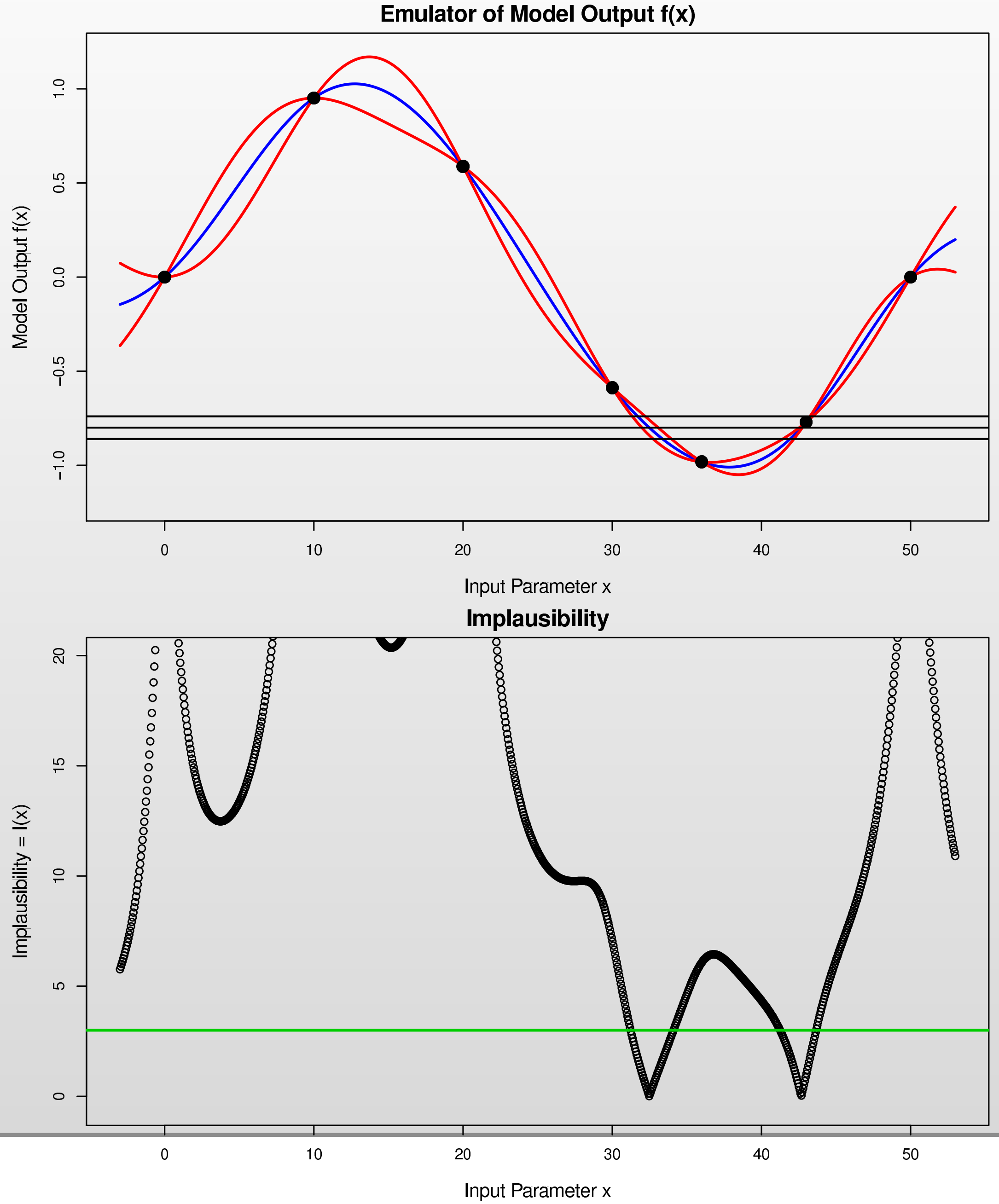

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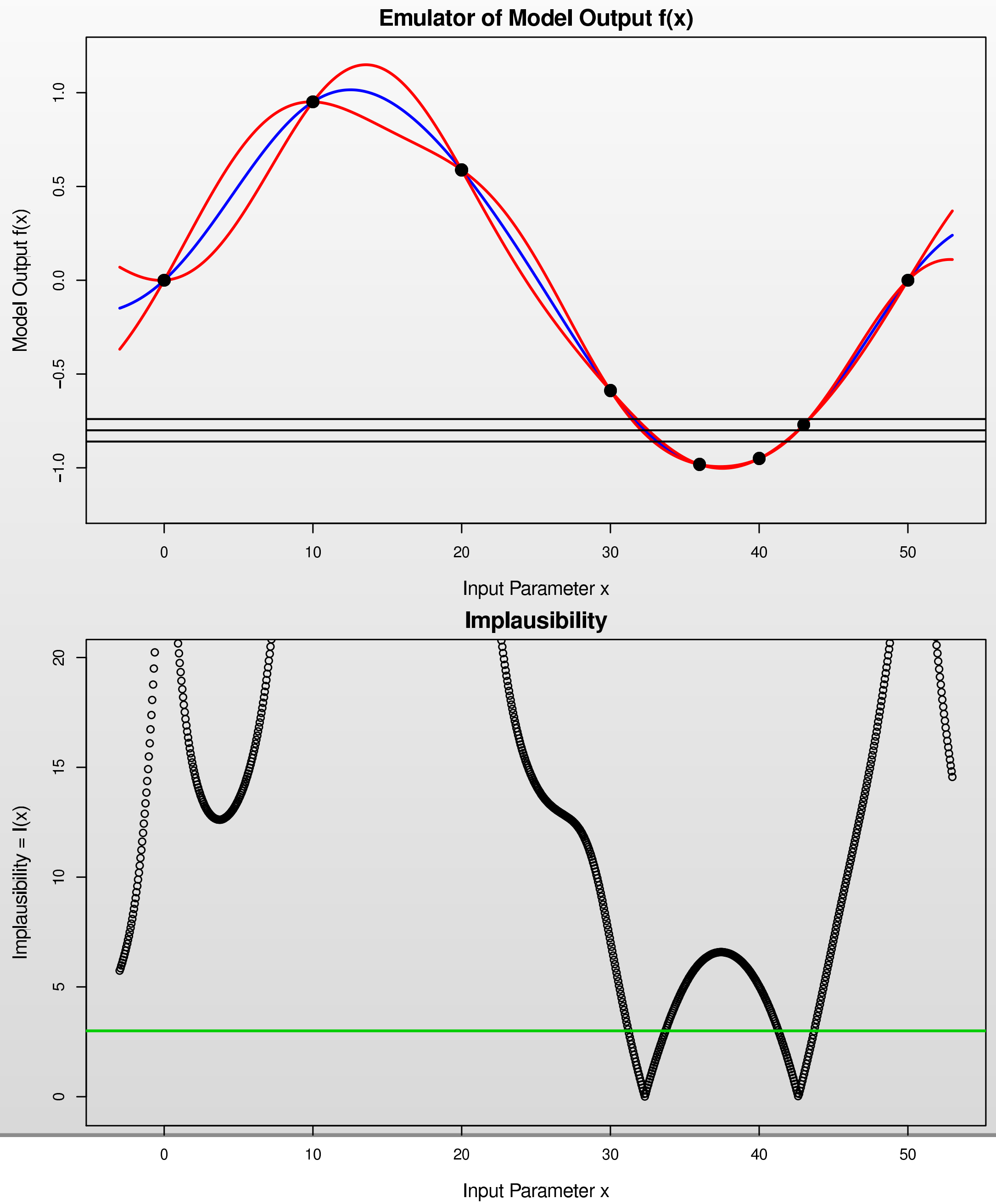

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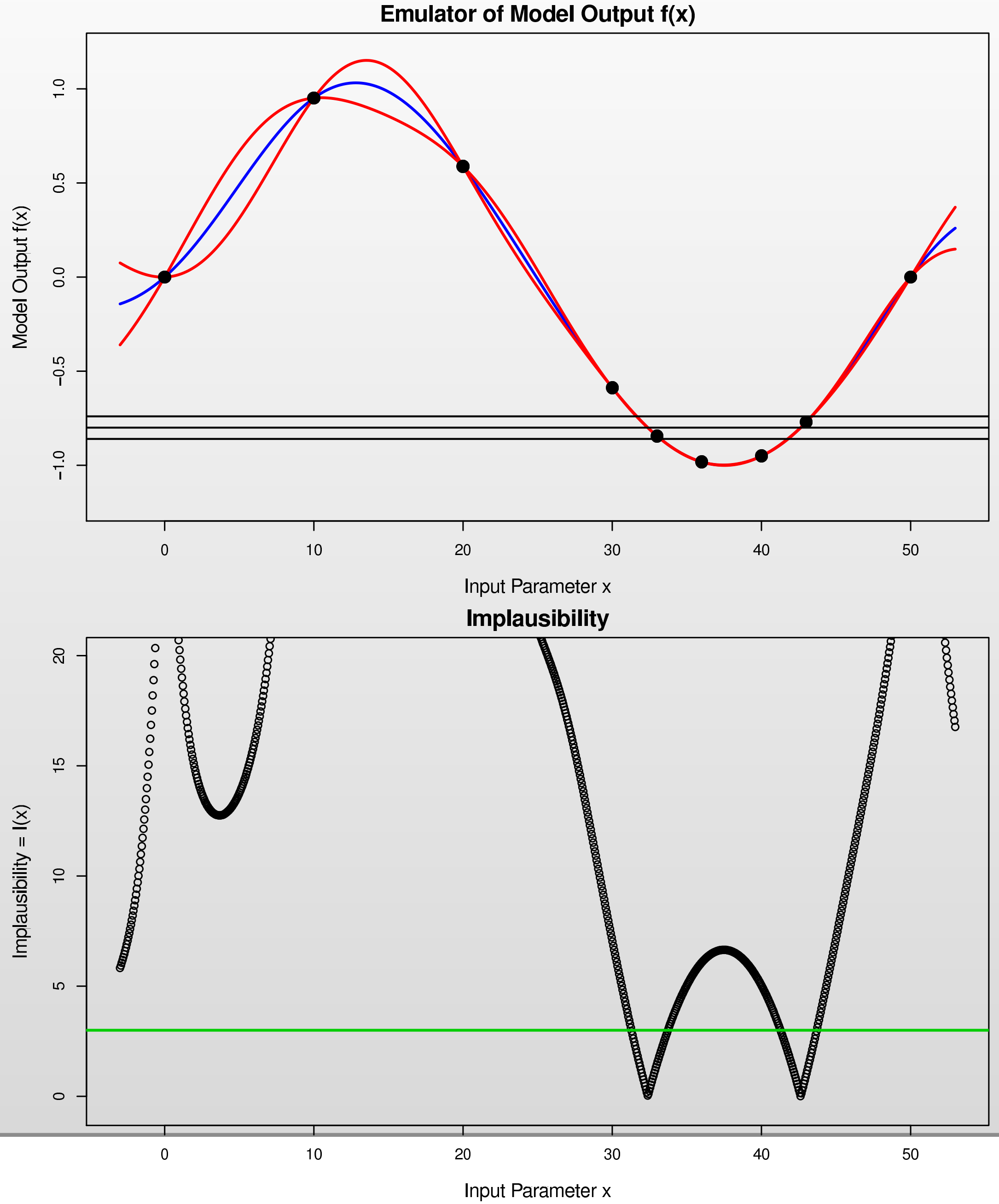

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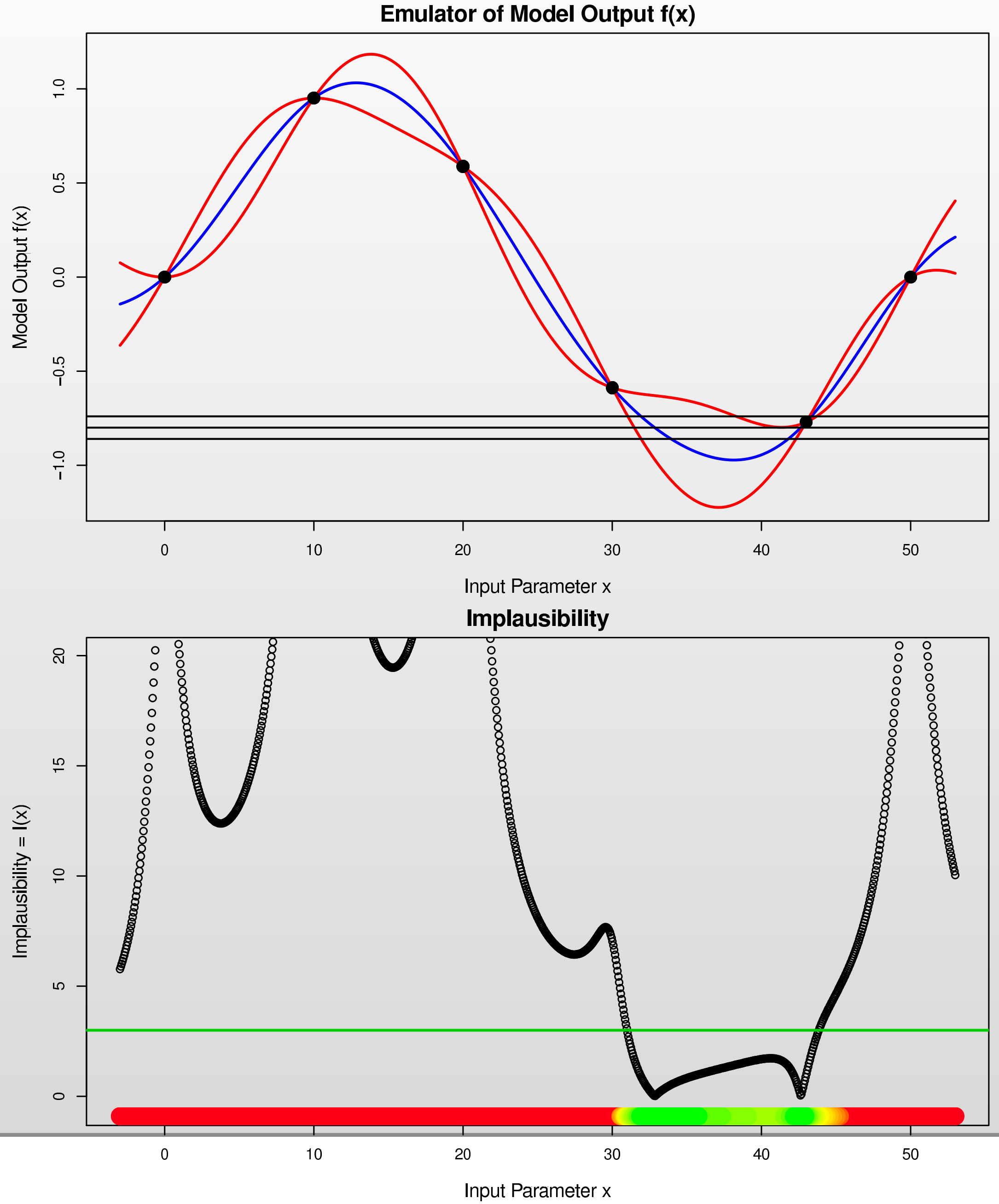

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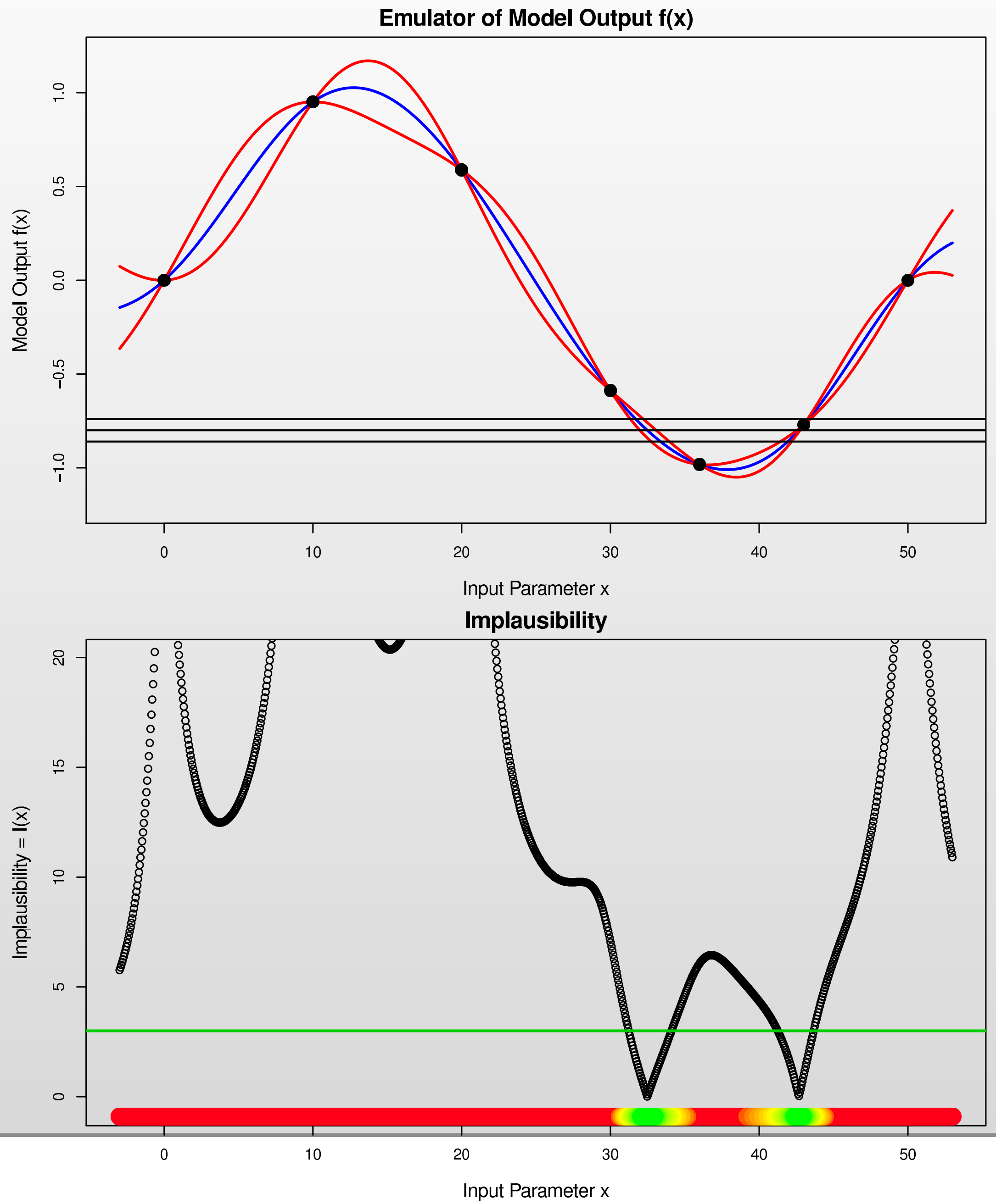

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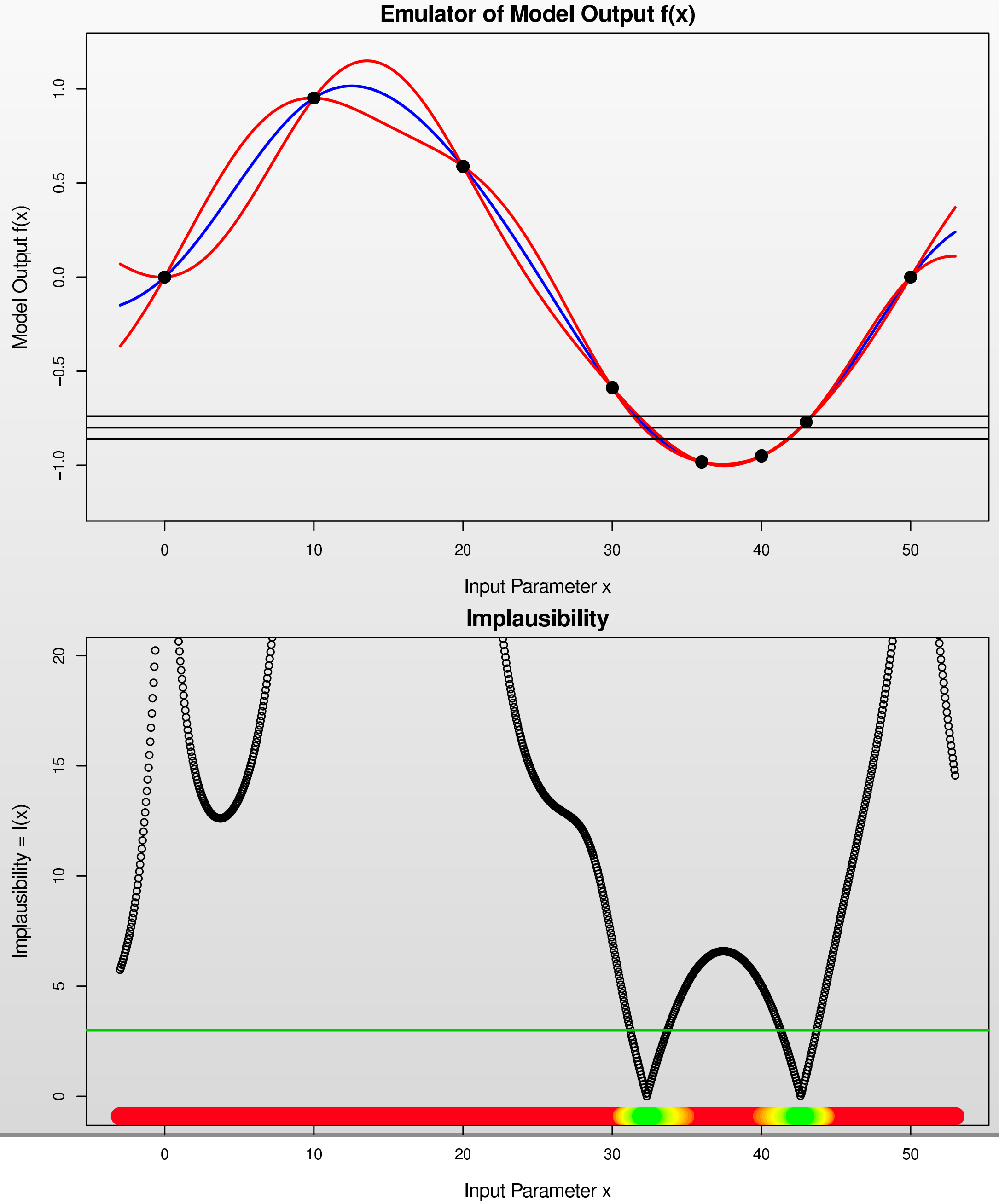

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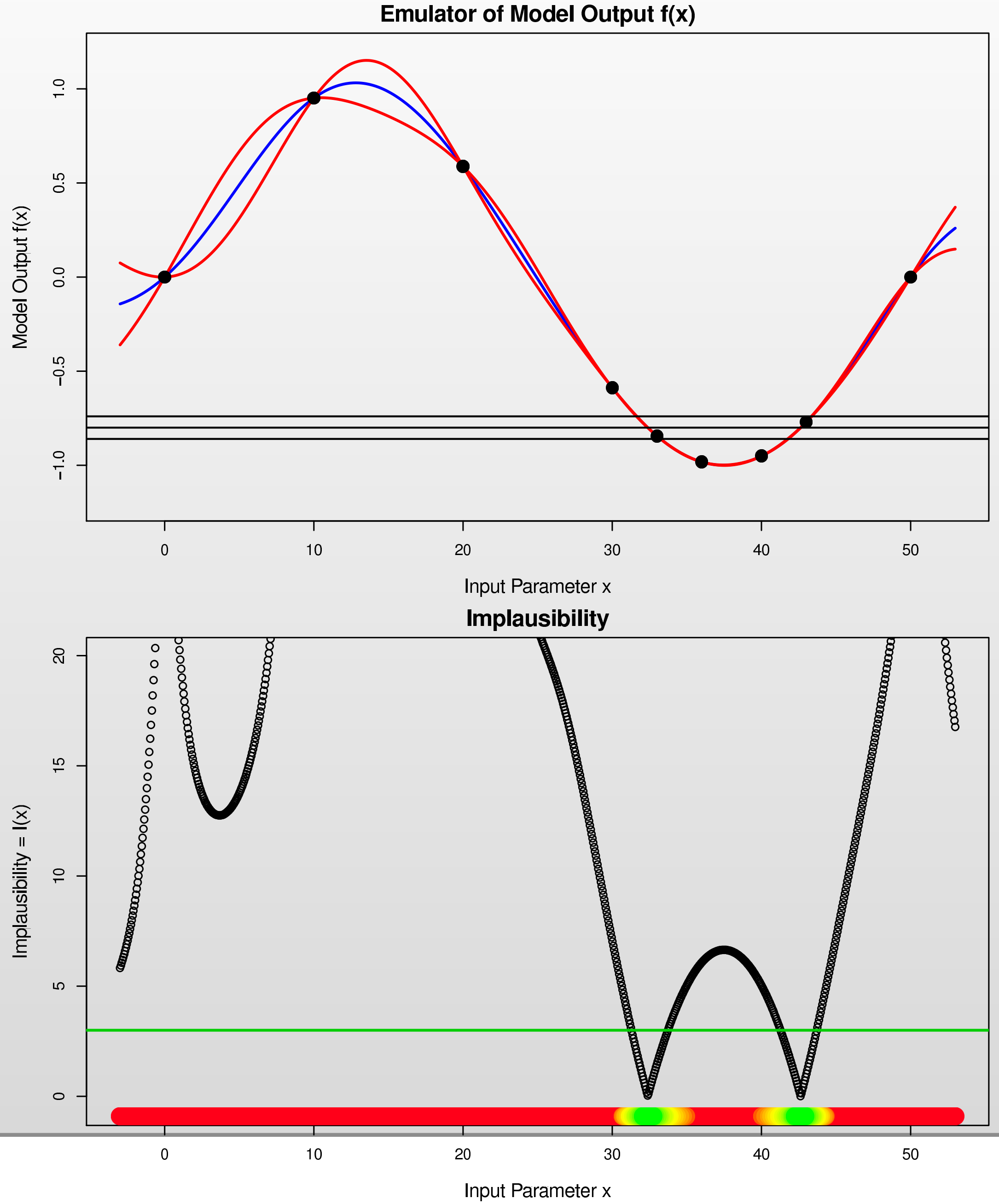

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7. If 6(a) true, generate a large number of acceptable runs from the final non-implausible volume $\mathcal{X}$, with appropriate sampling.

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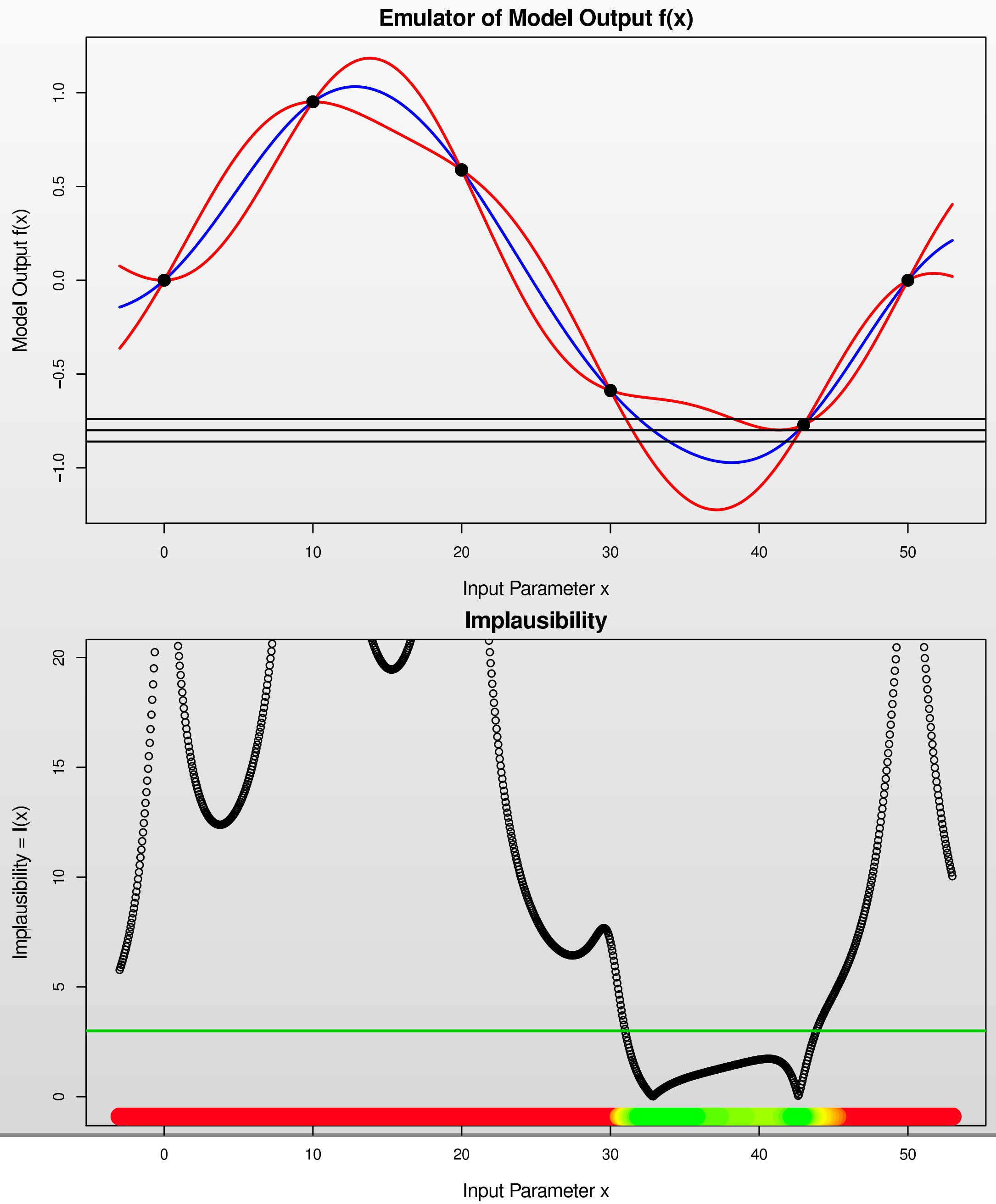

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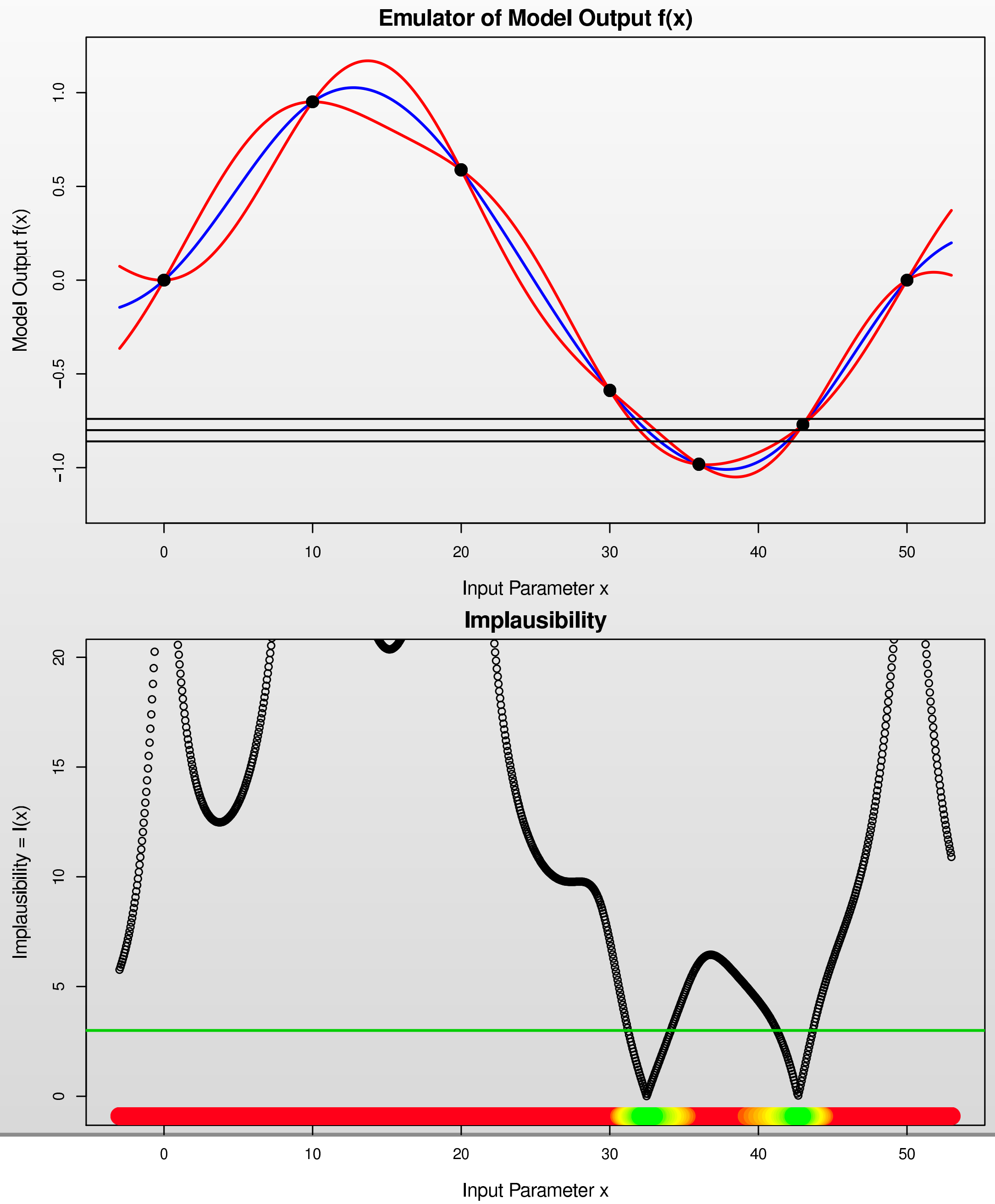

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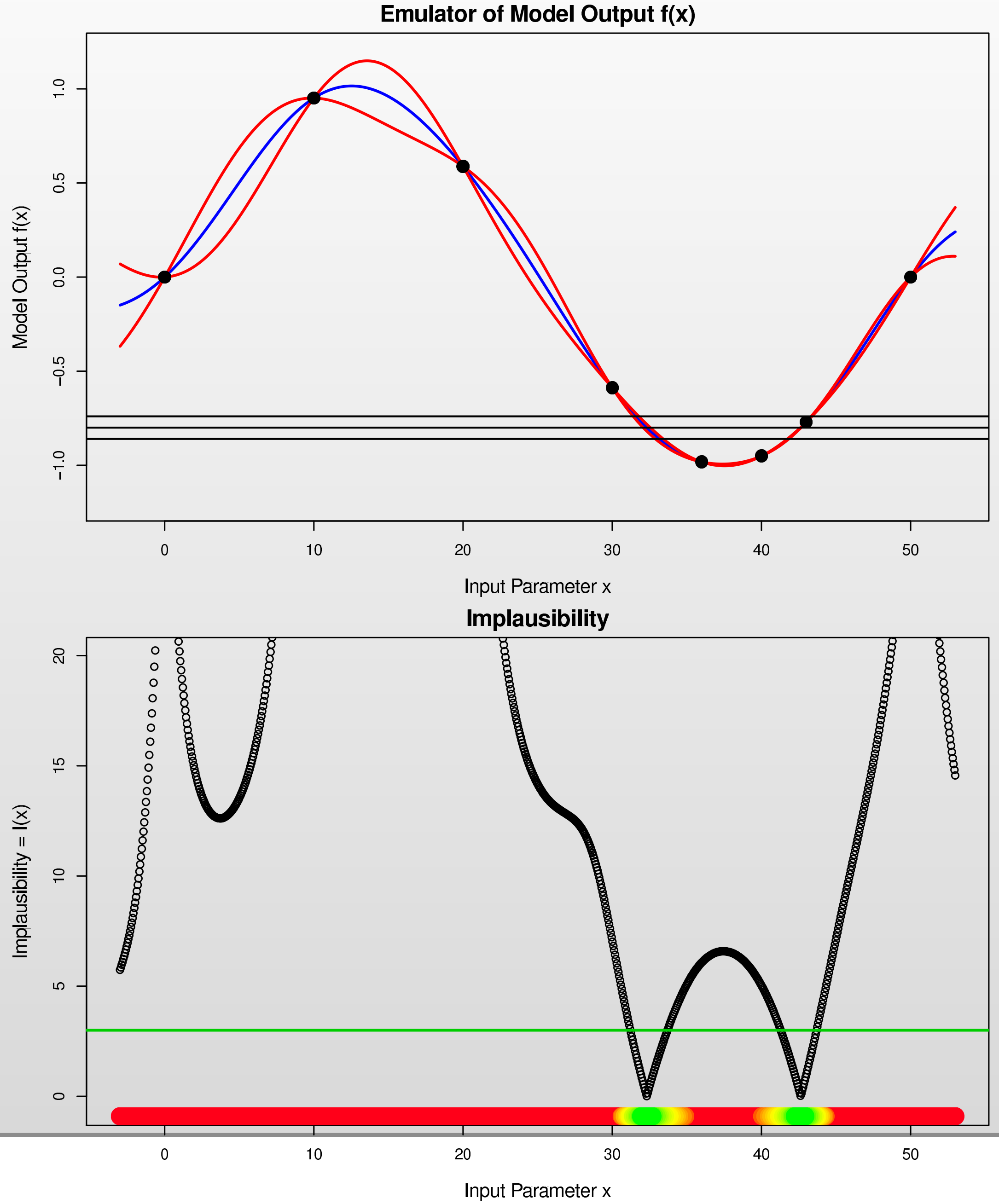

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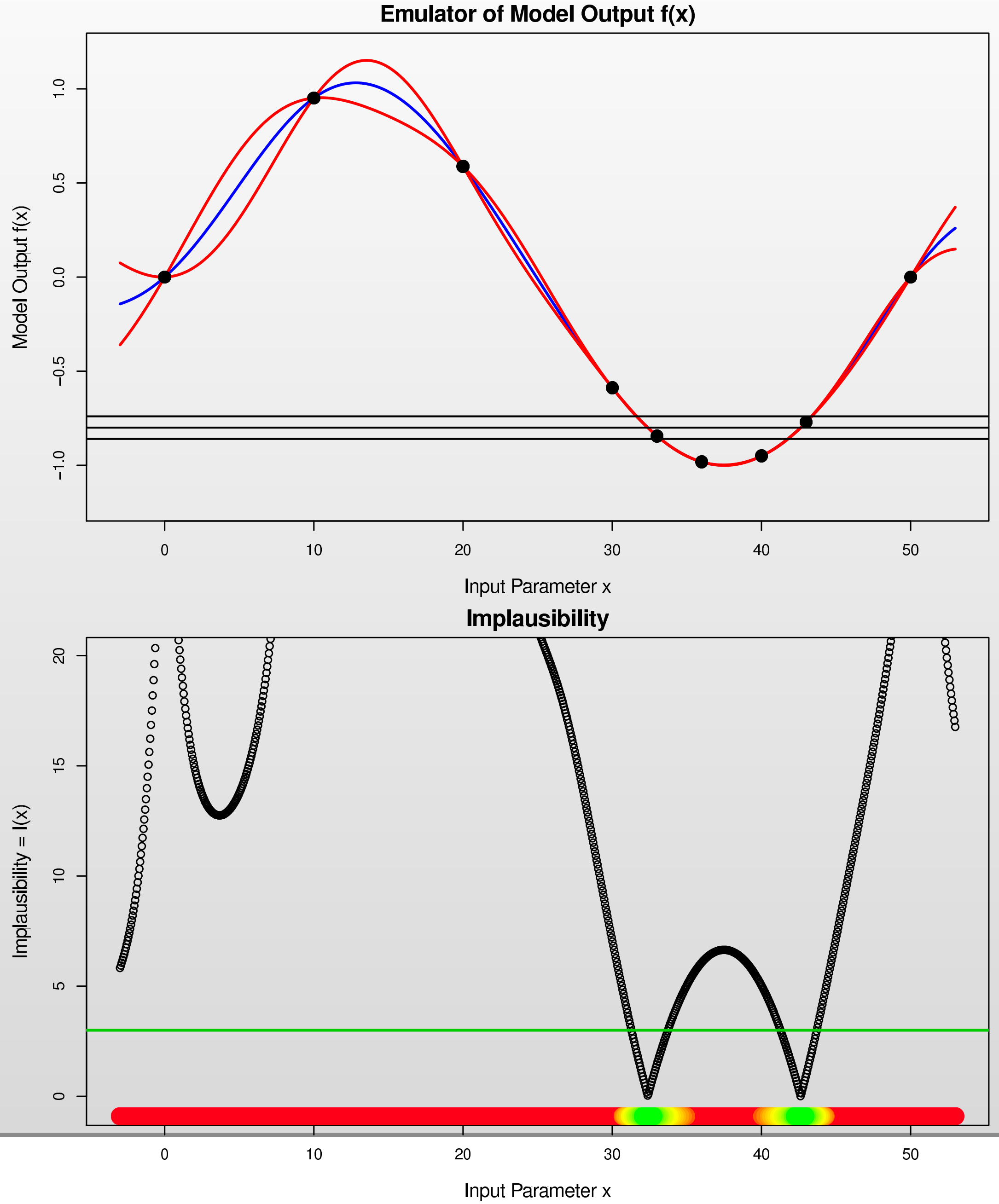
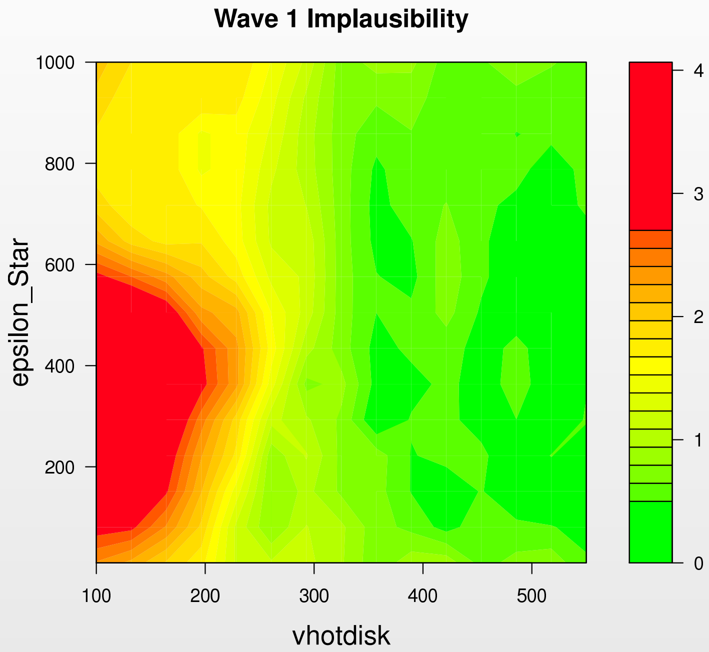


2D Minimised Implausibility Projections: Wave 1



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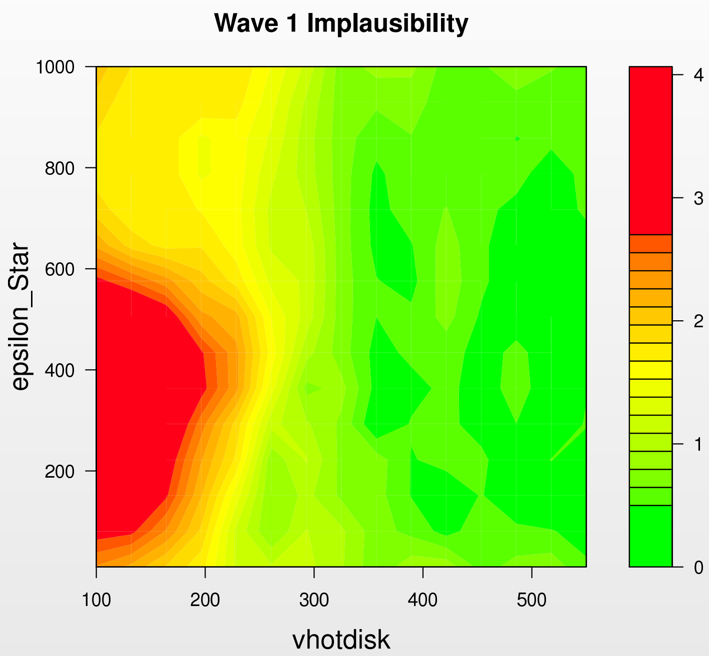

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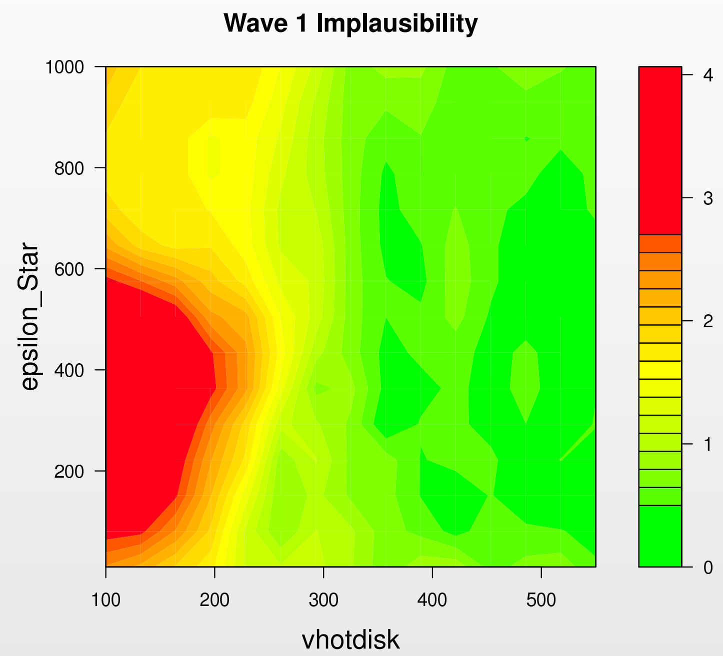

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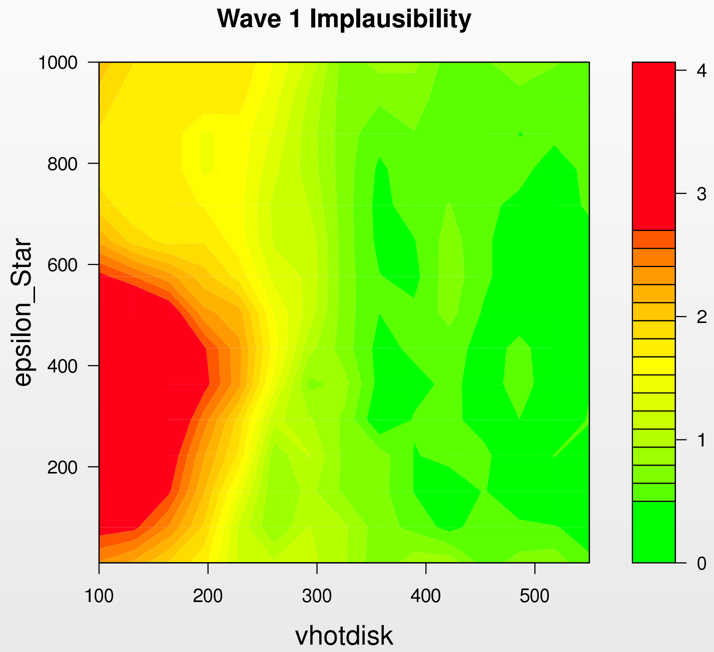
- If a point is green, it may or may not prove to be an acceptable input.

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



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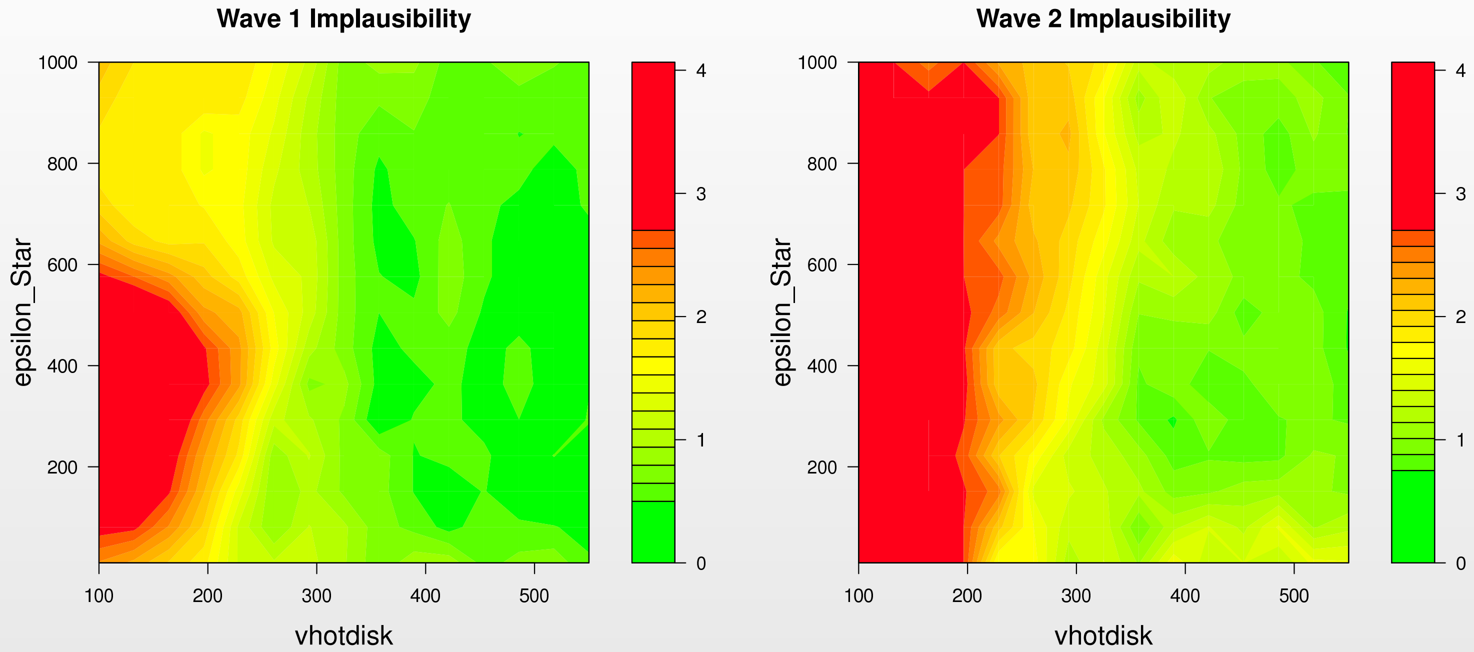

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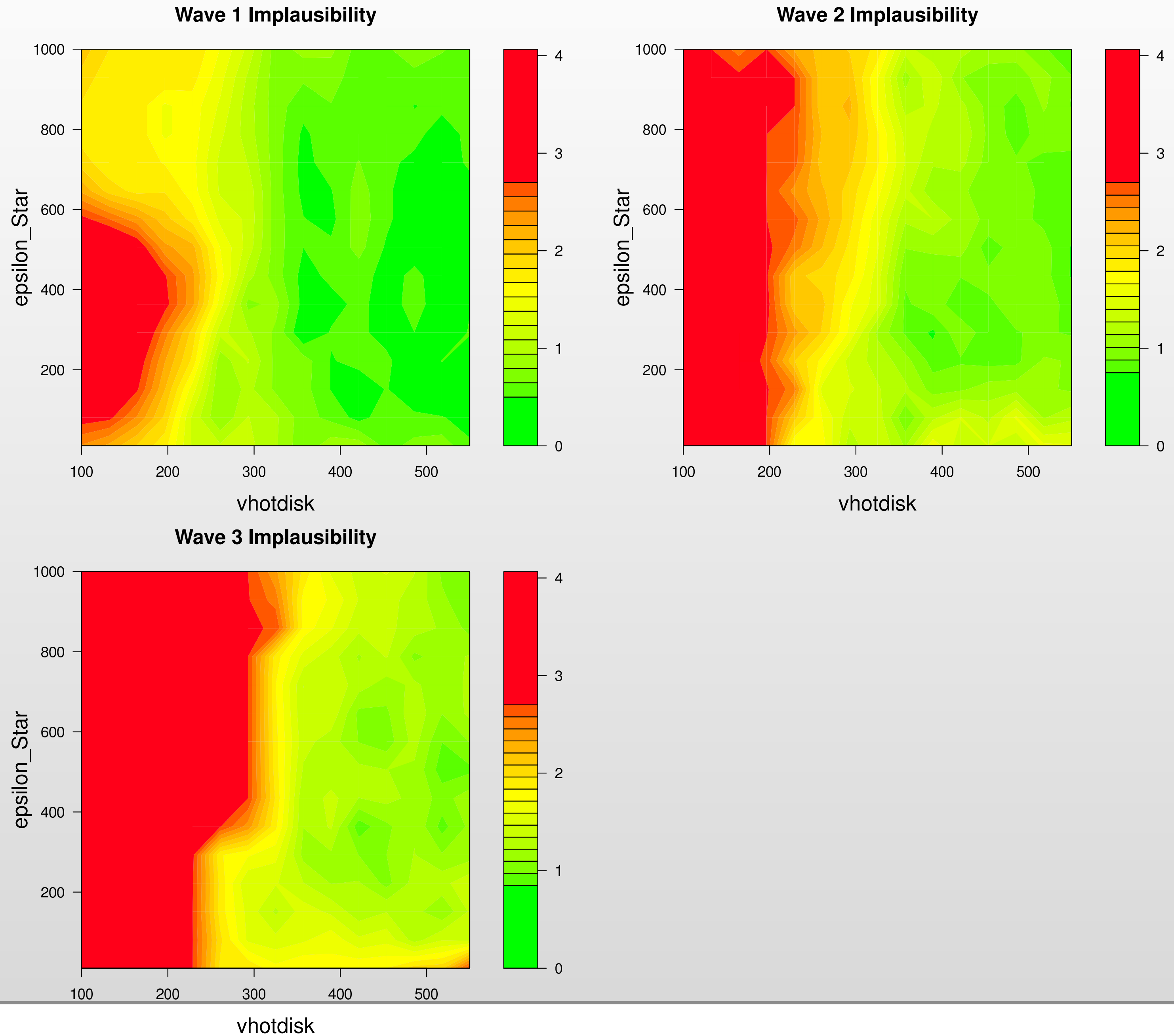

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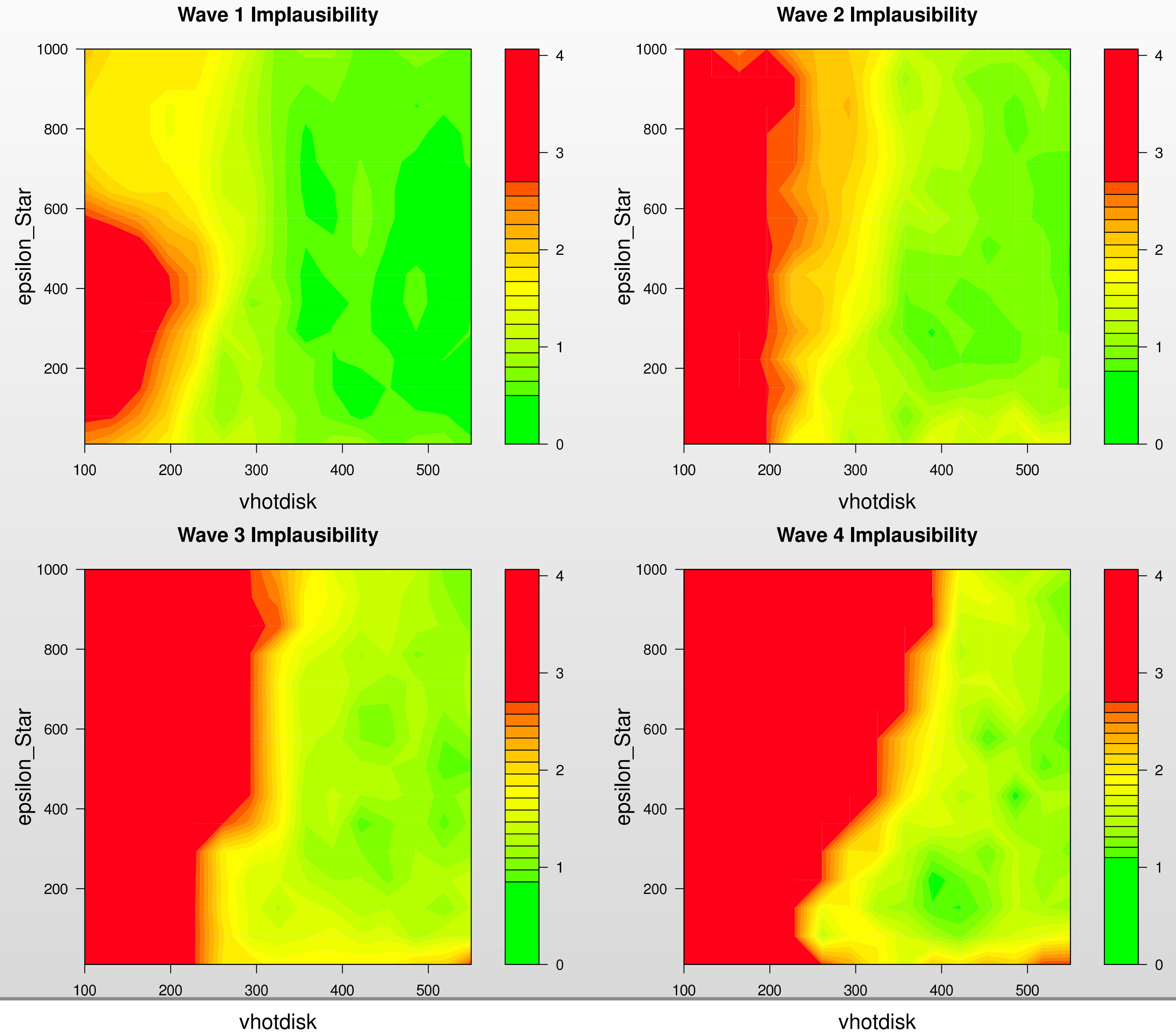

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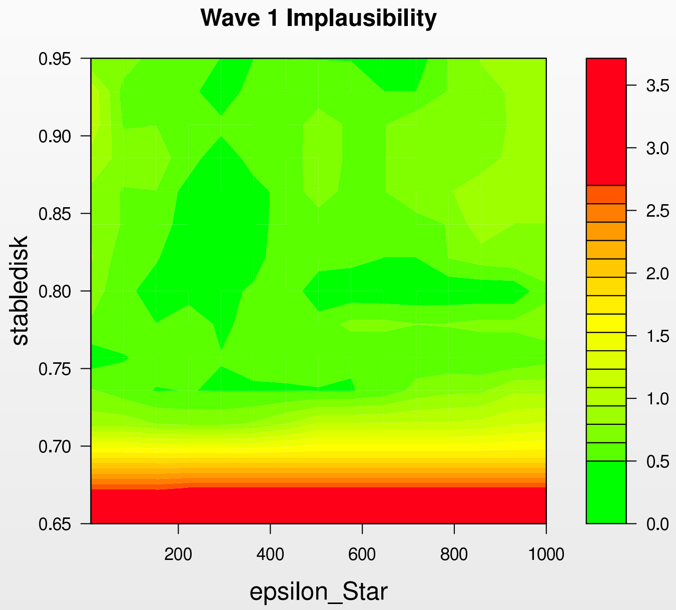

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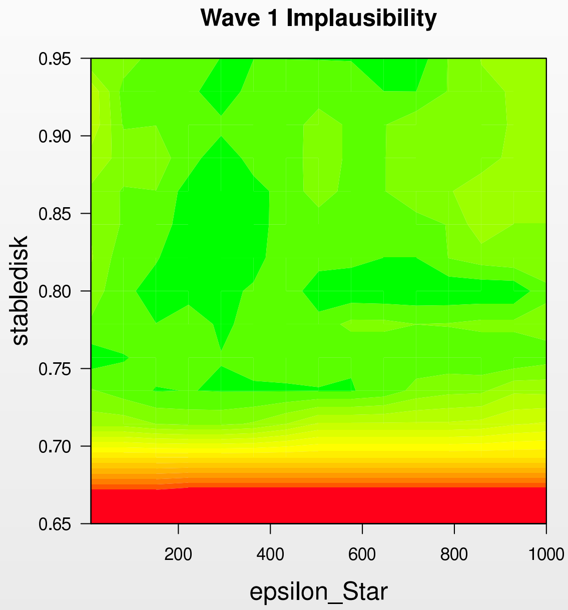

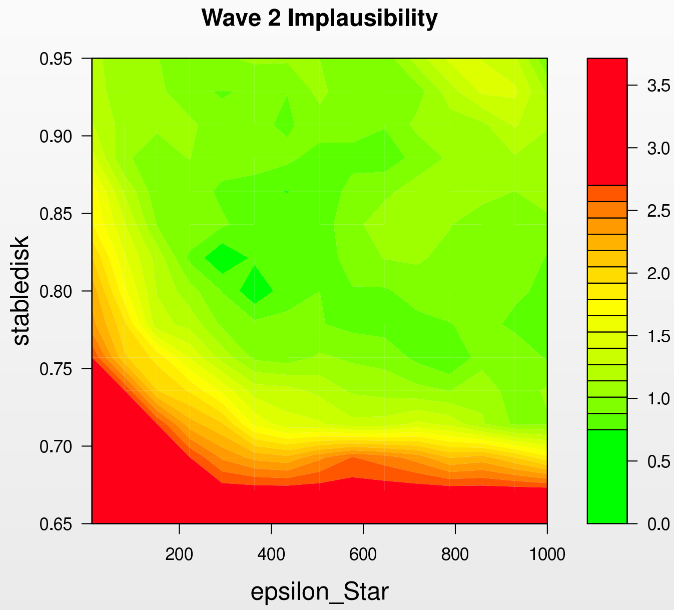

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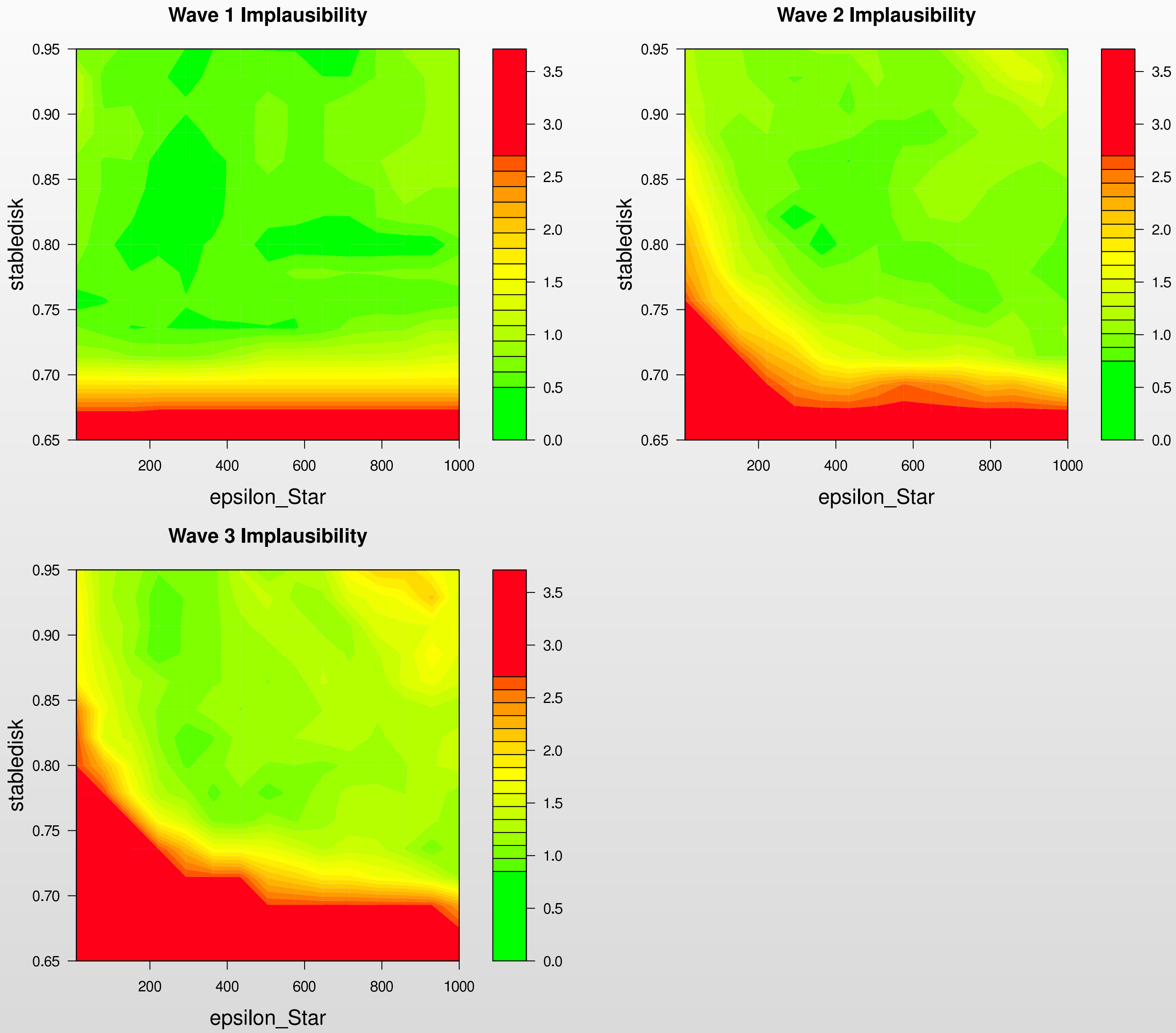

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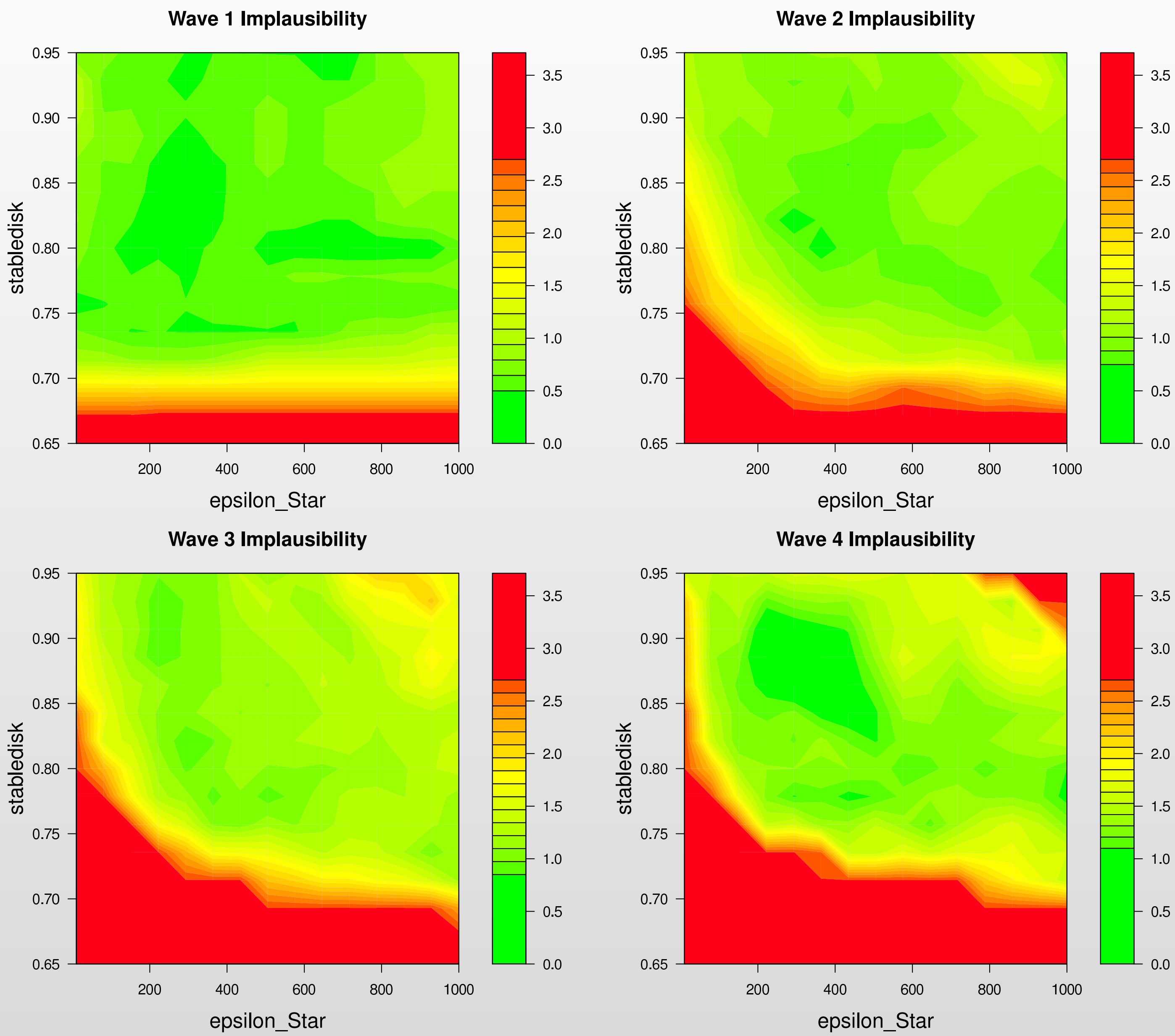
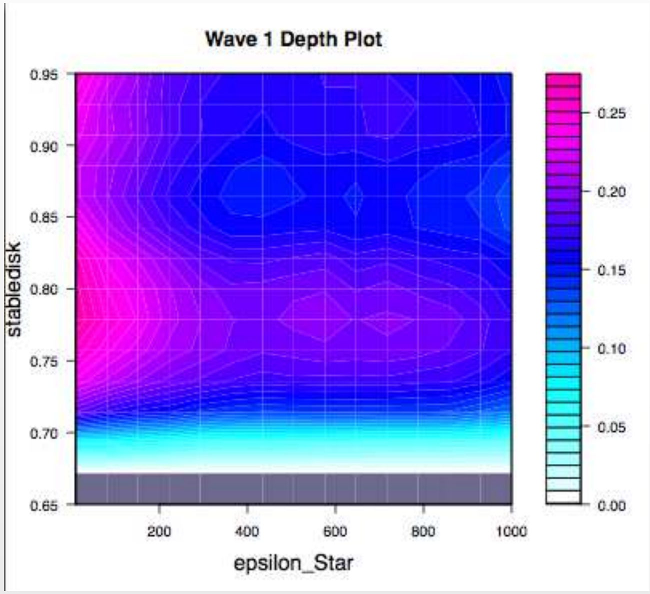


2D Optical Depth Plots: Wave 2



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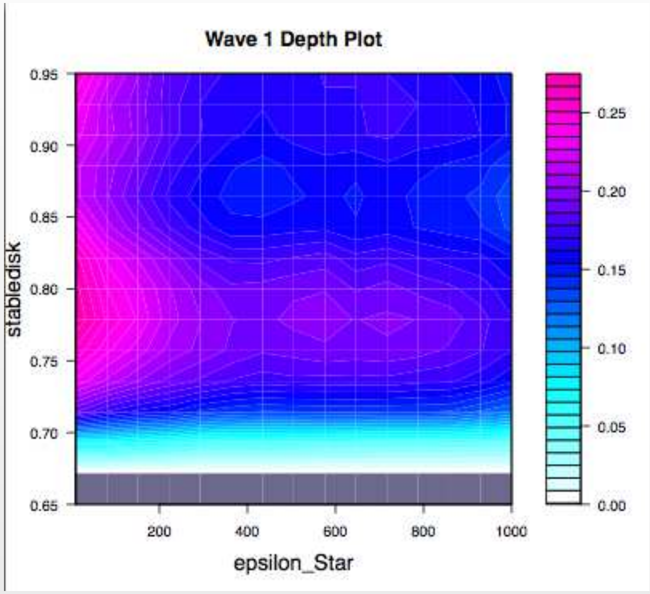

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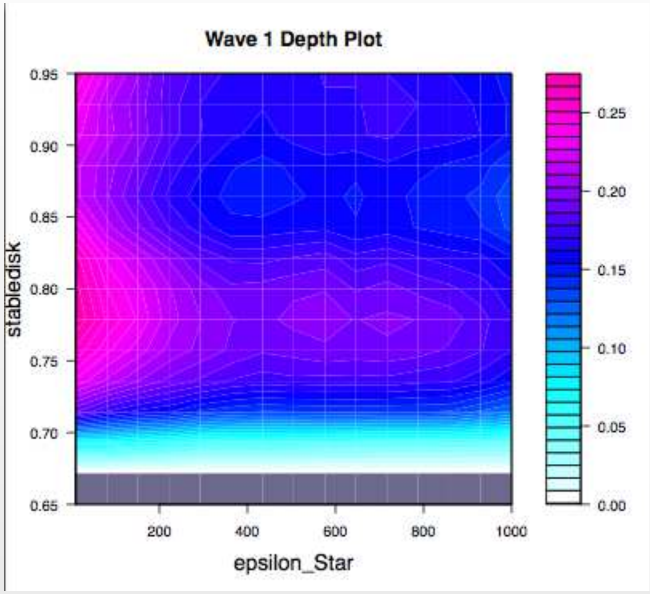

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- Shows where the majority of non-implausible points can be found, but not necessarily where the best matches are.

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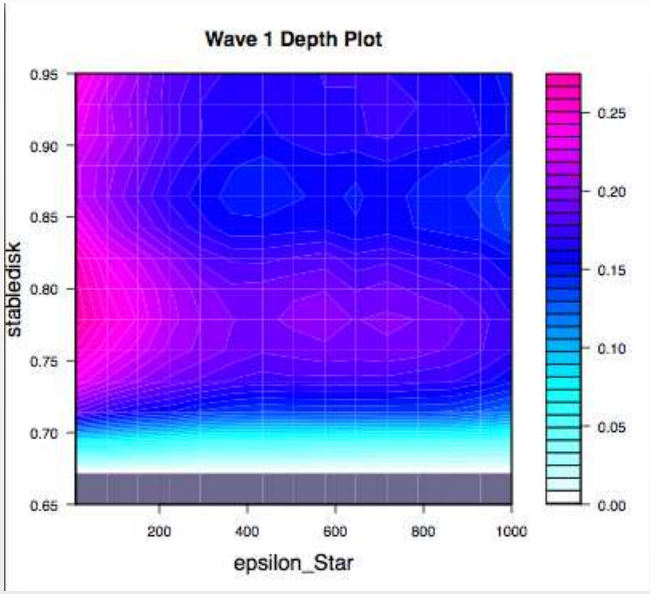

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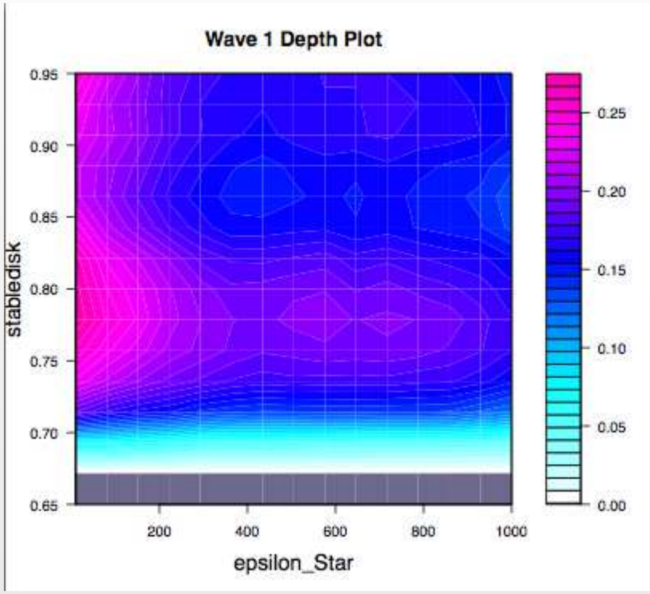

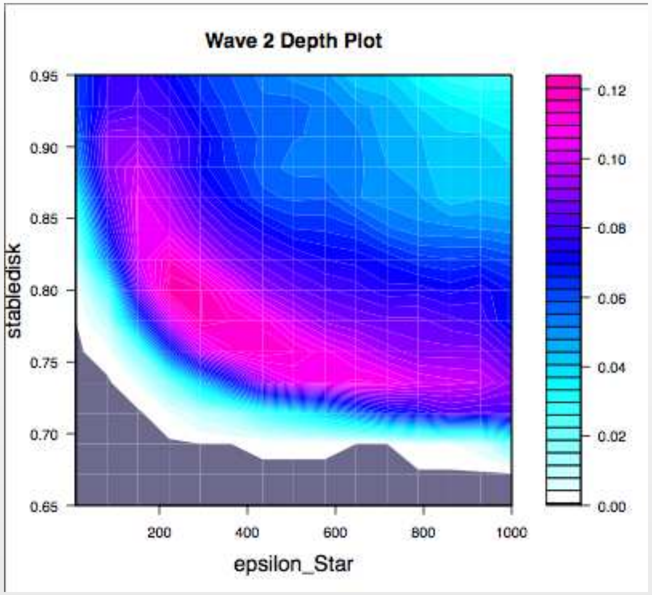

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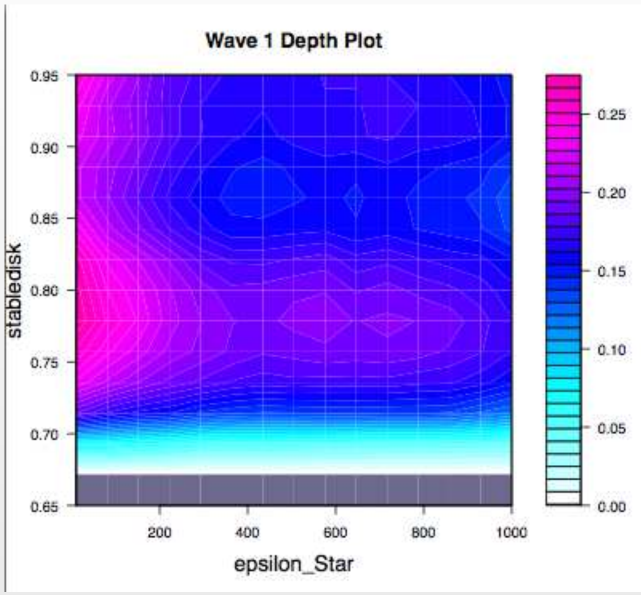

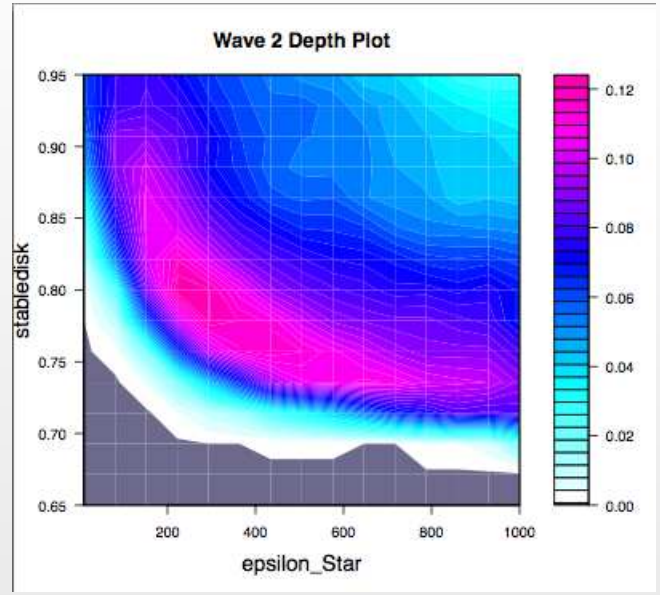

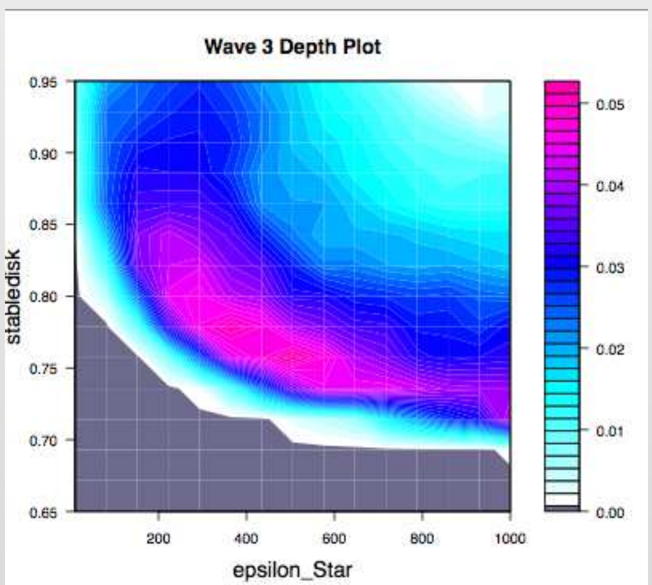

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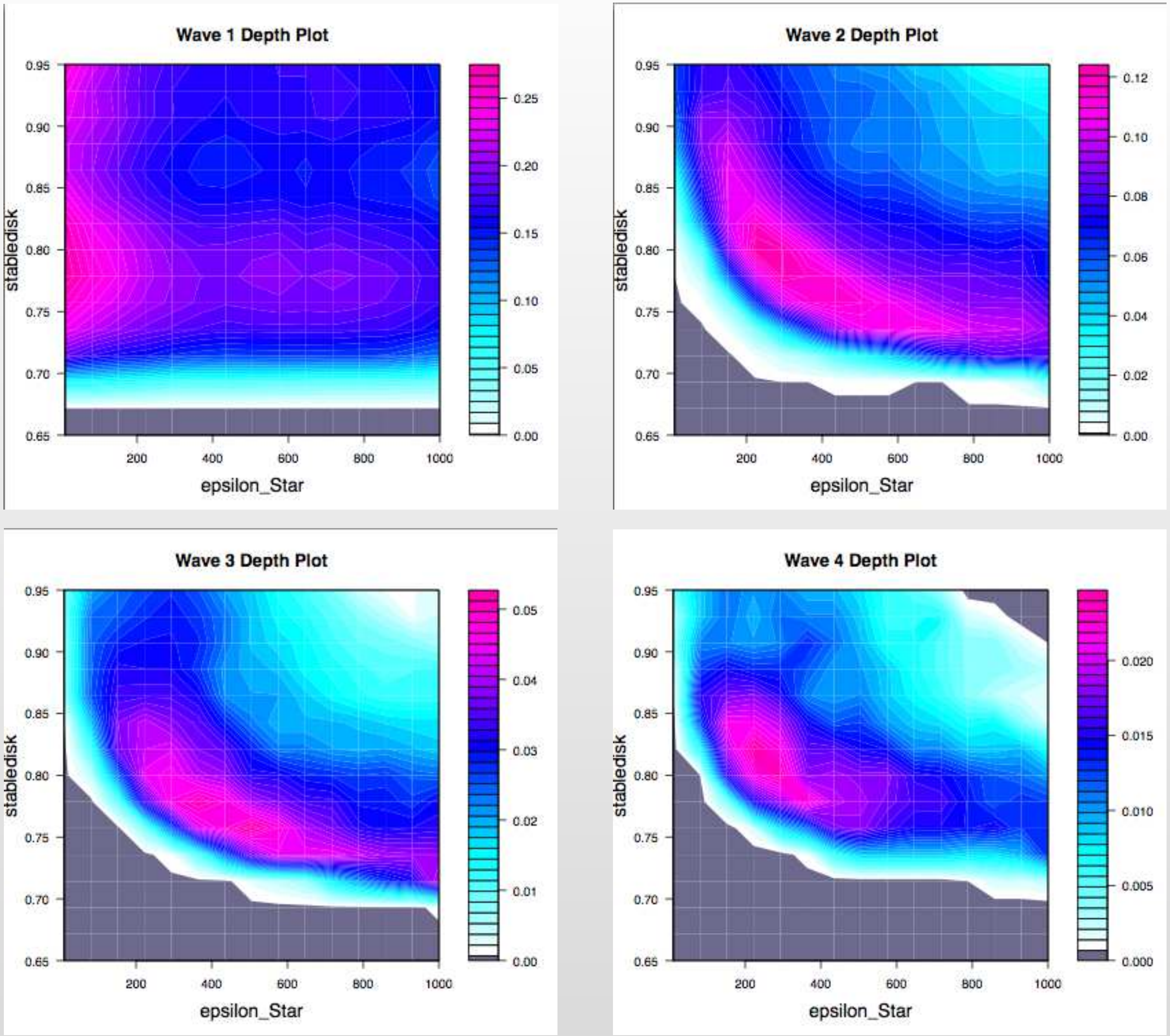

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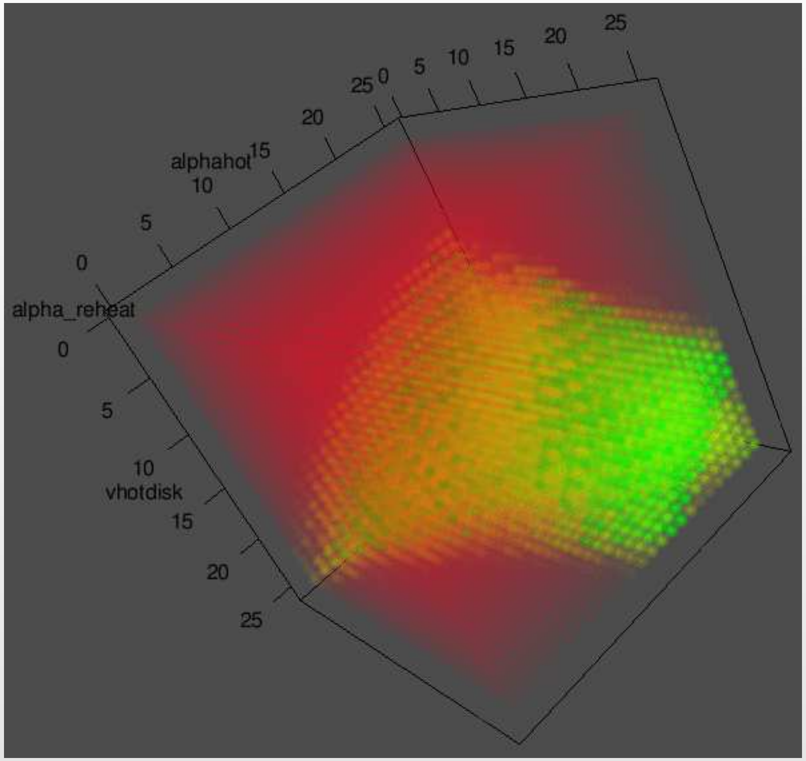
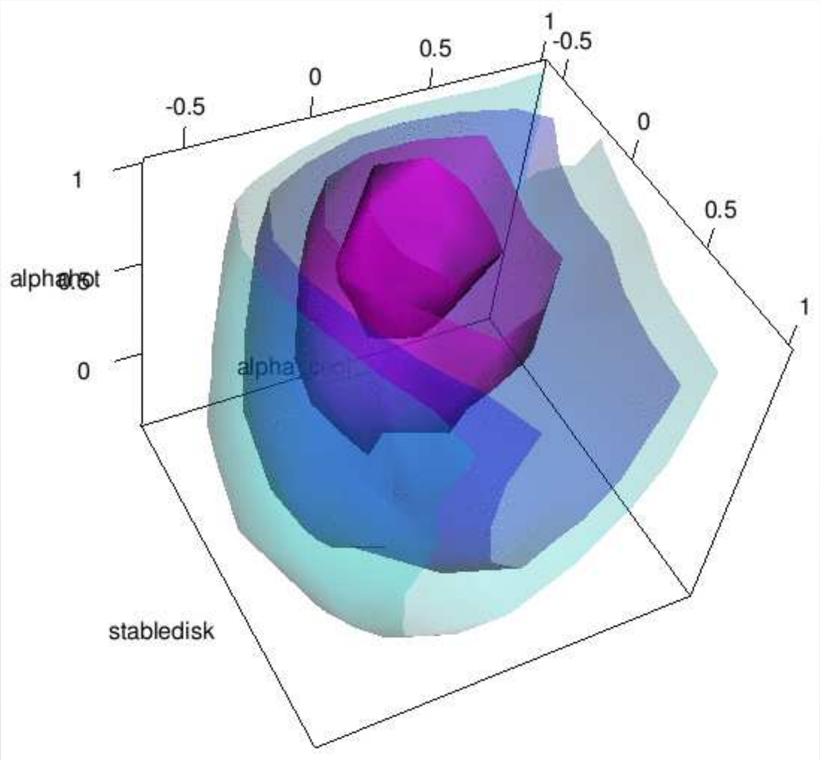
- This is a major strength of the History Matching approach.

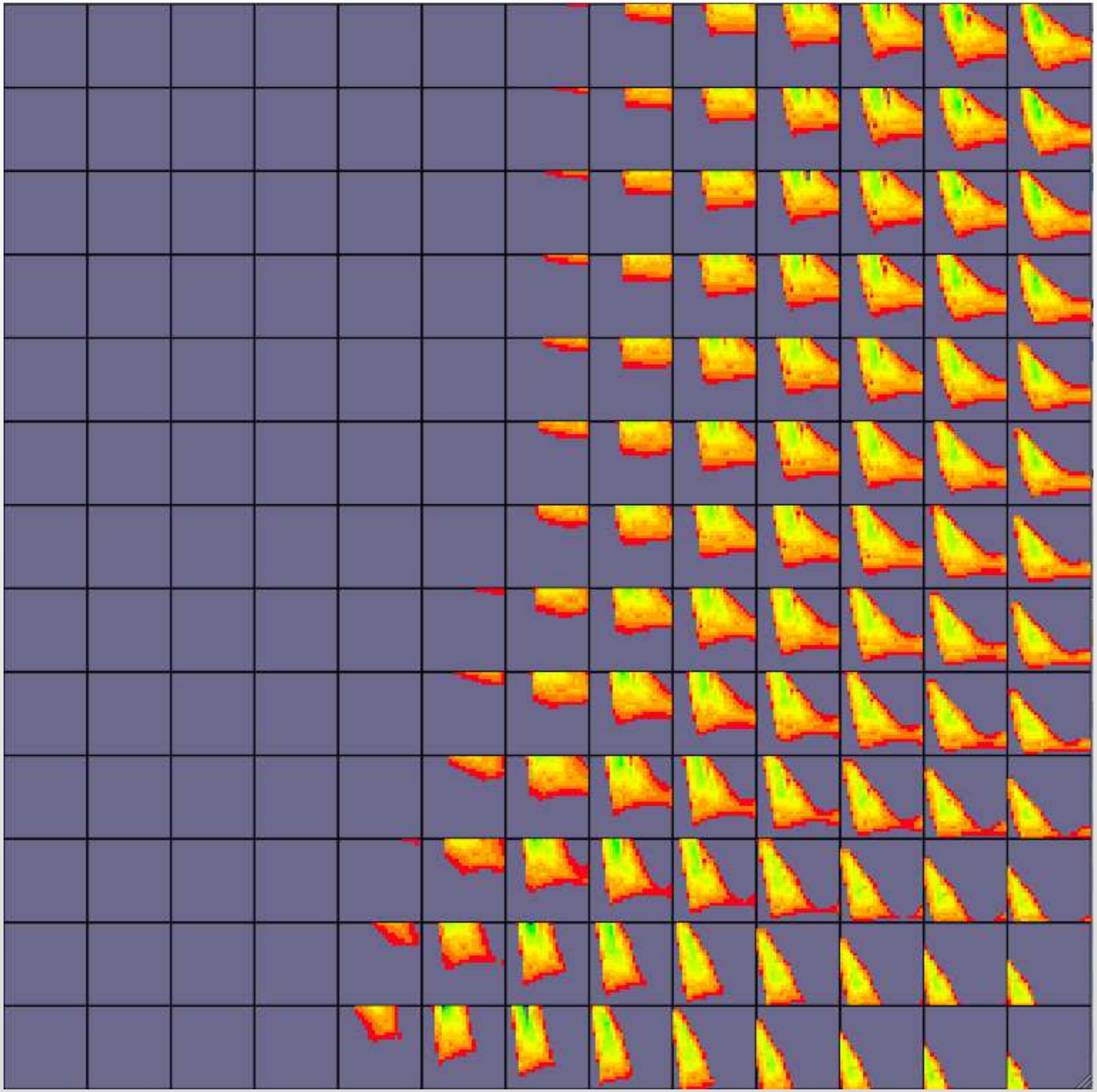
3D Minimised Implausibility and Optical Depth Plots





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

4-Dimensional Implausibility Plots: Anyone?



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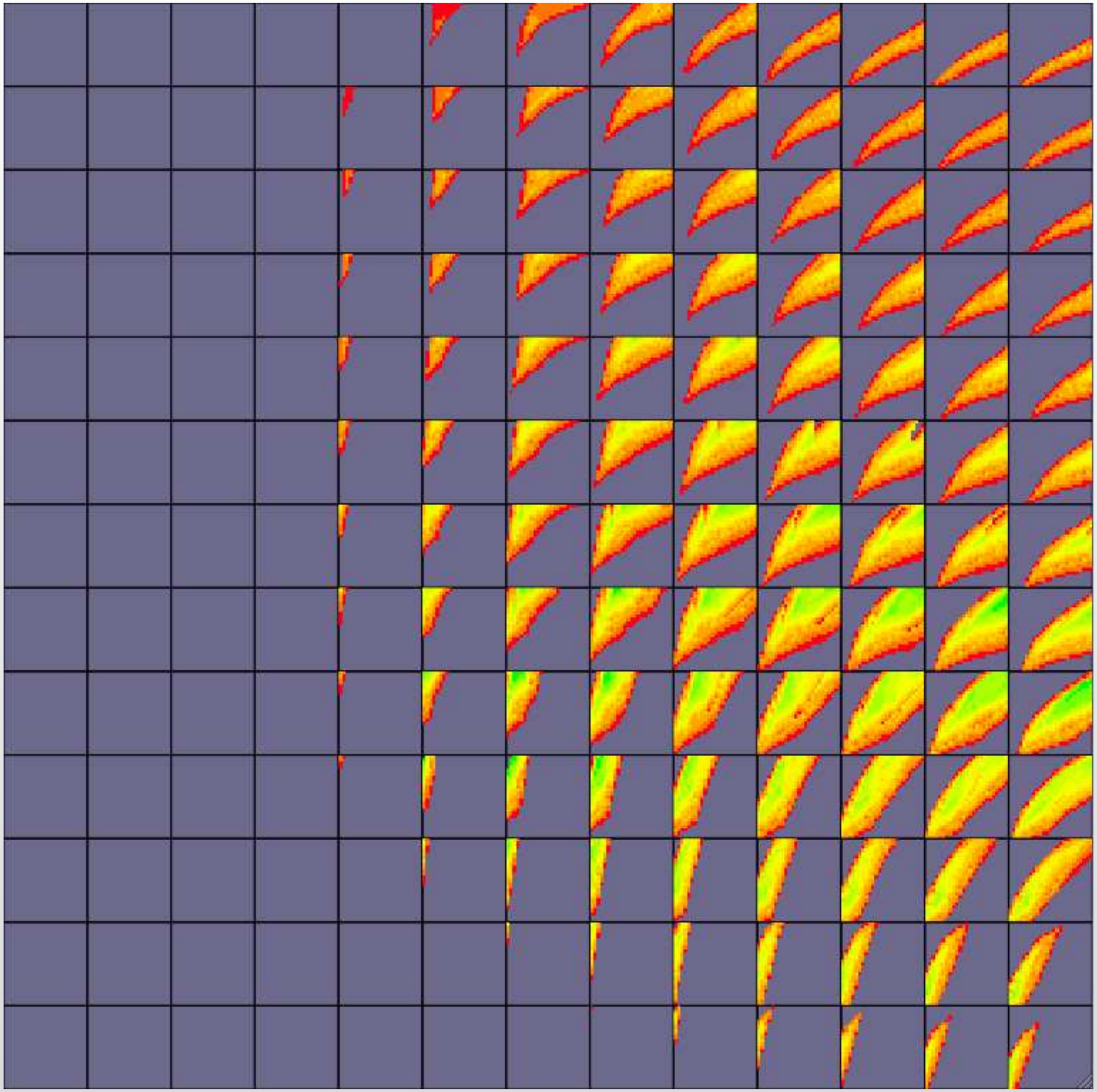
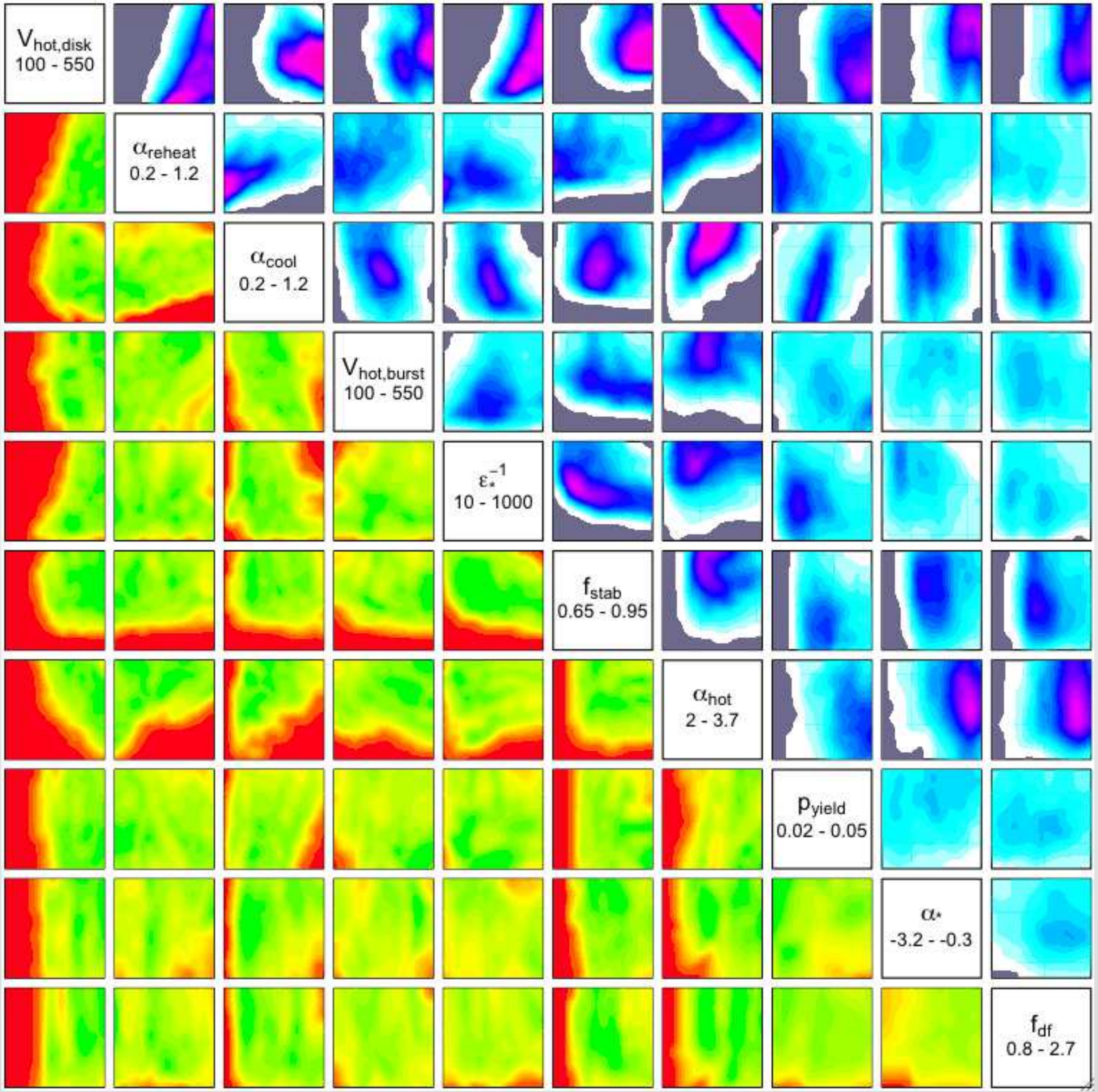
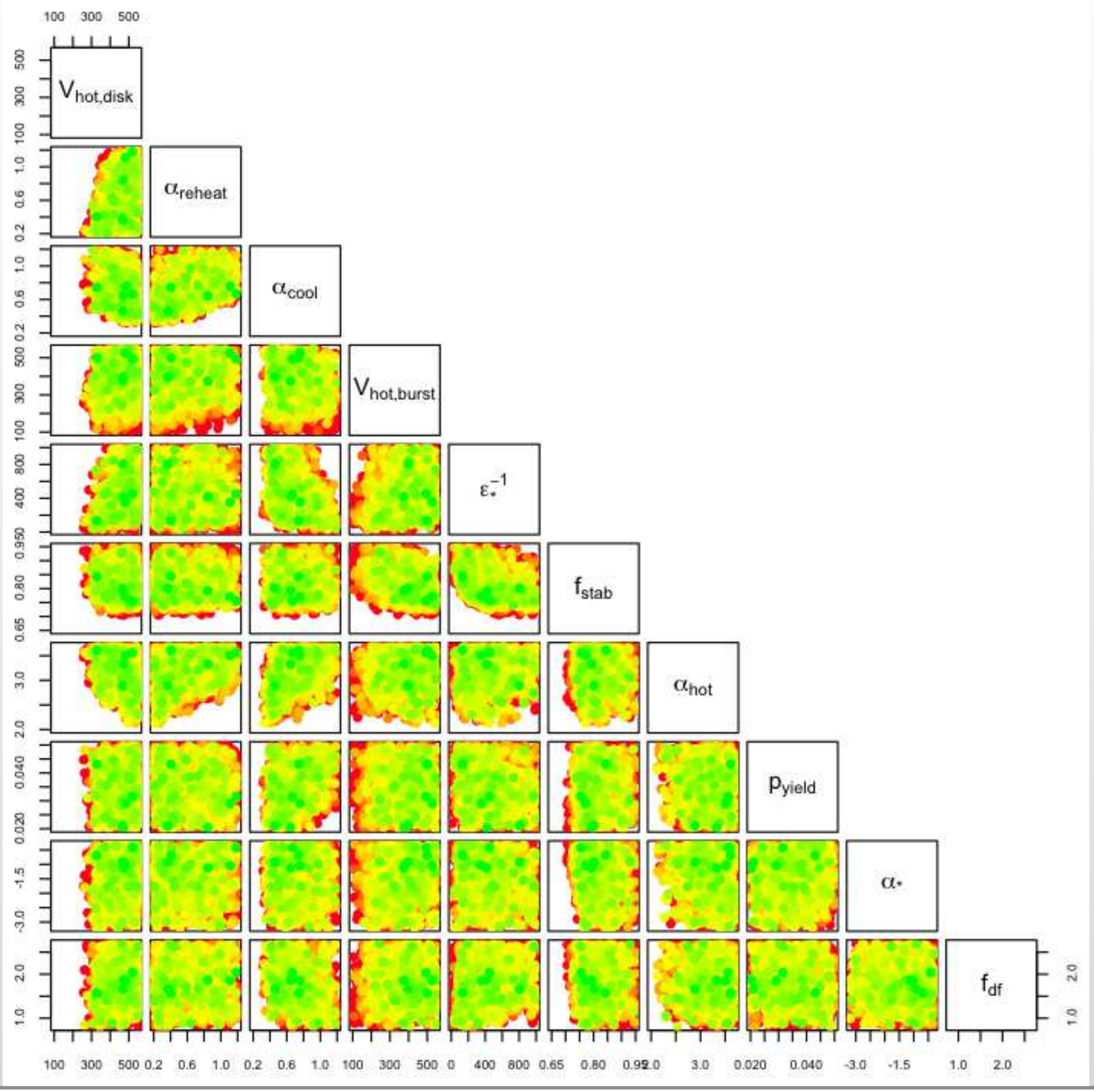


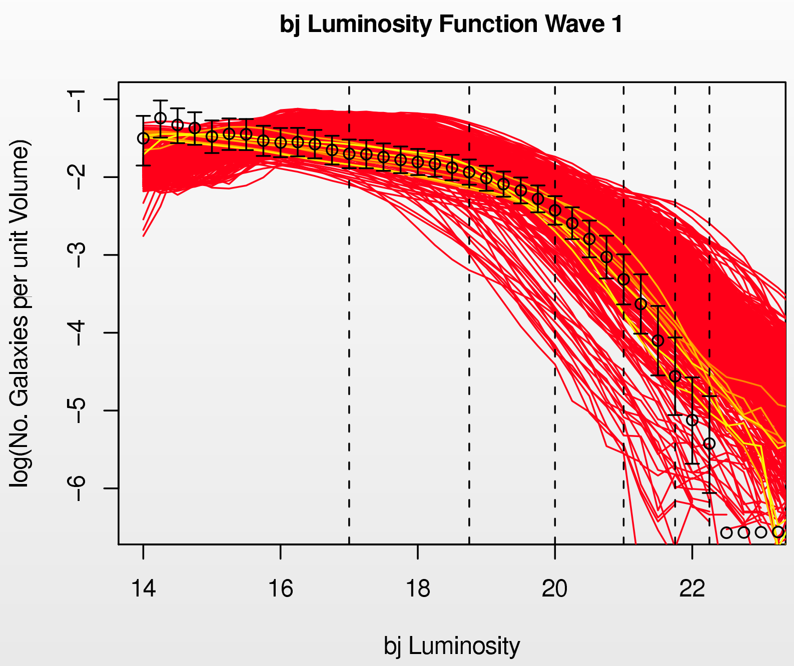
2D Implausibility Projections: Stage 4 (0.12%)



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
0.2 0.6 1.0
100 300 500
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



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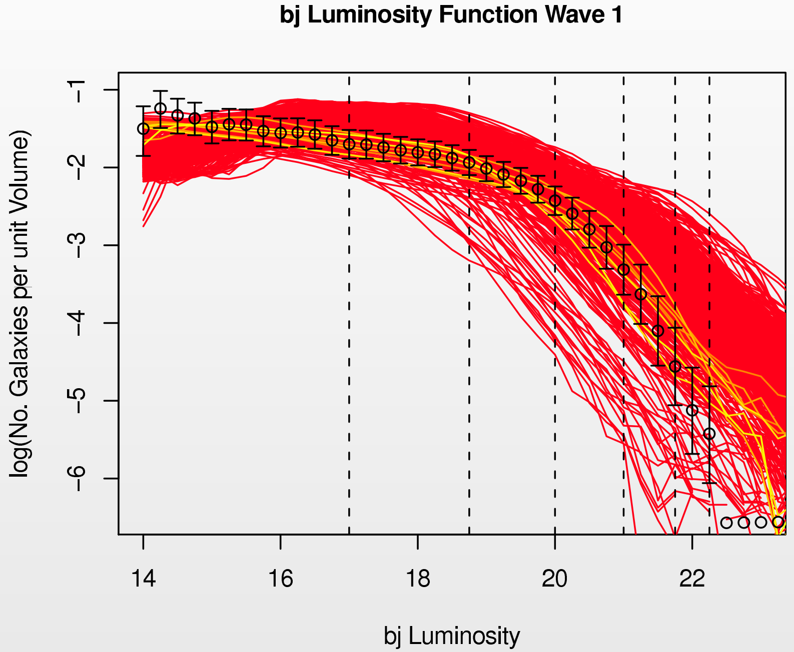

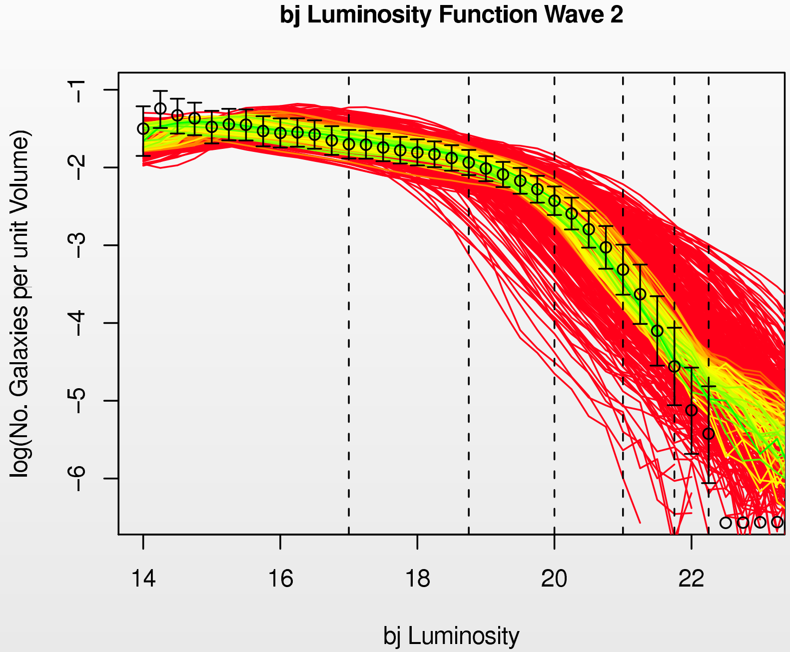

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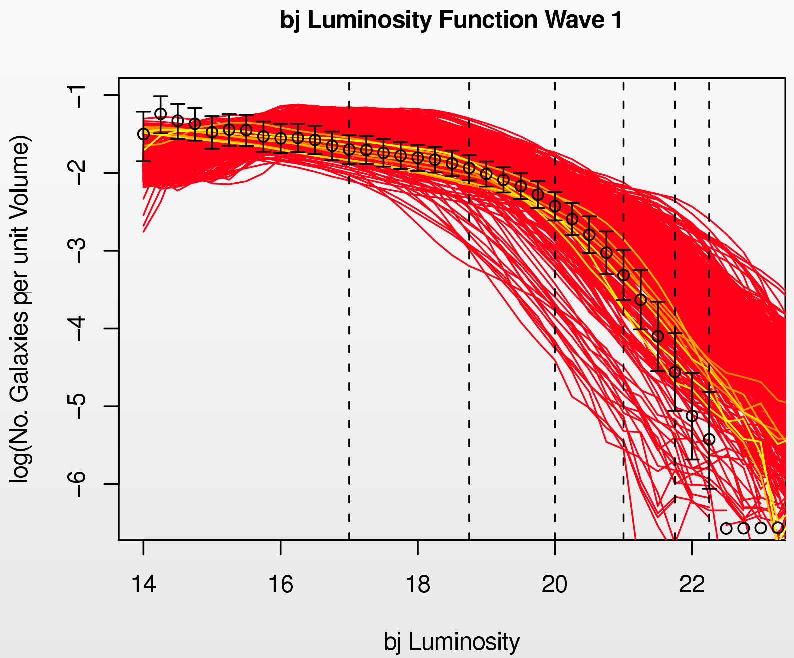

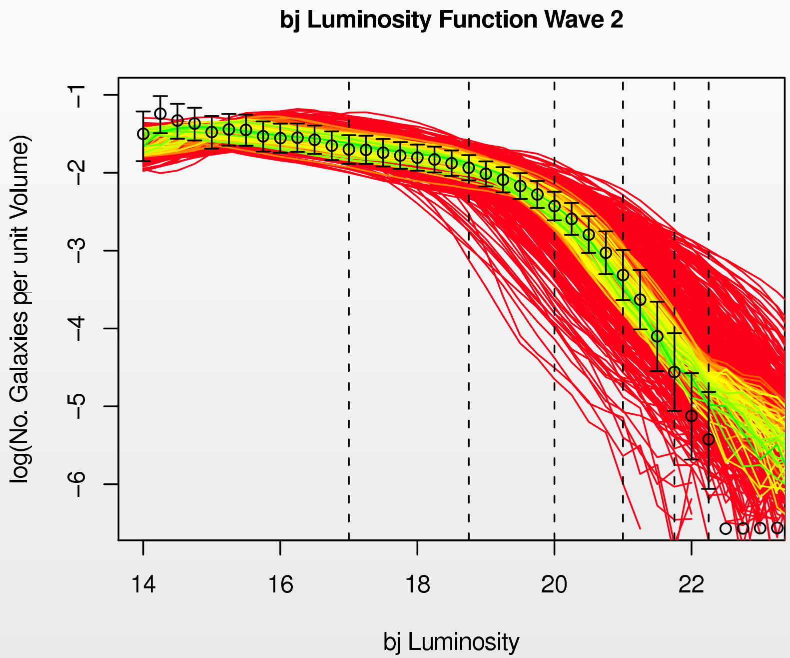

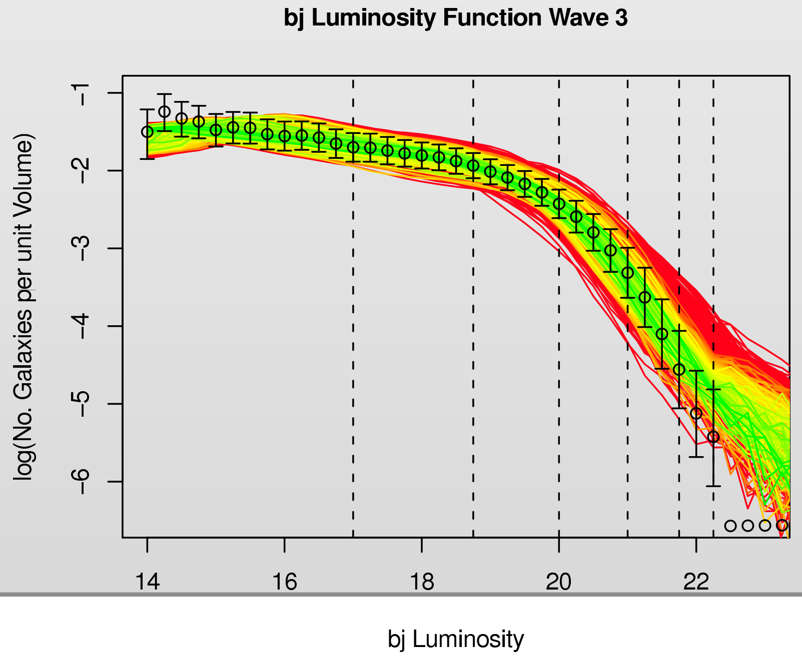

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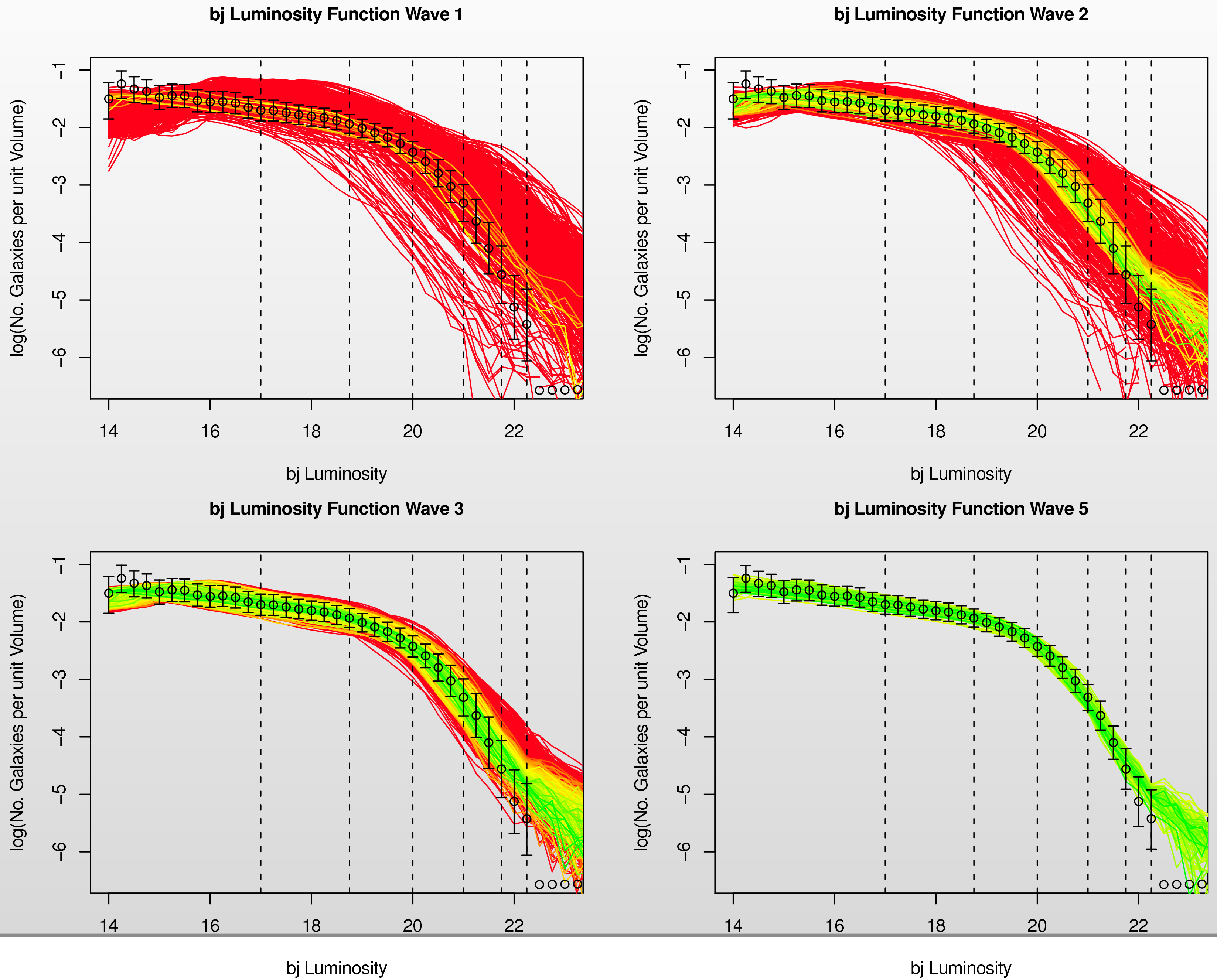

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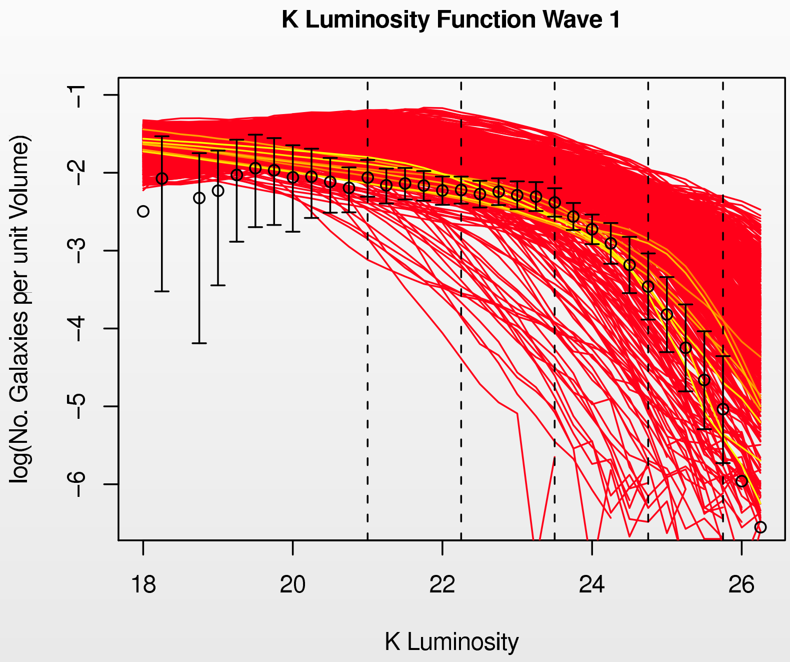

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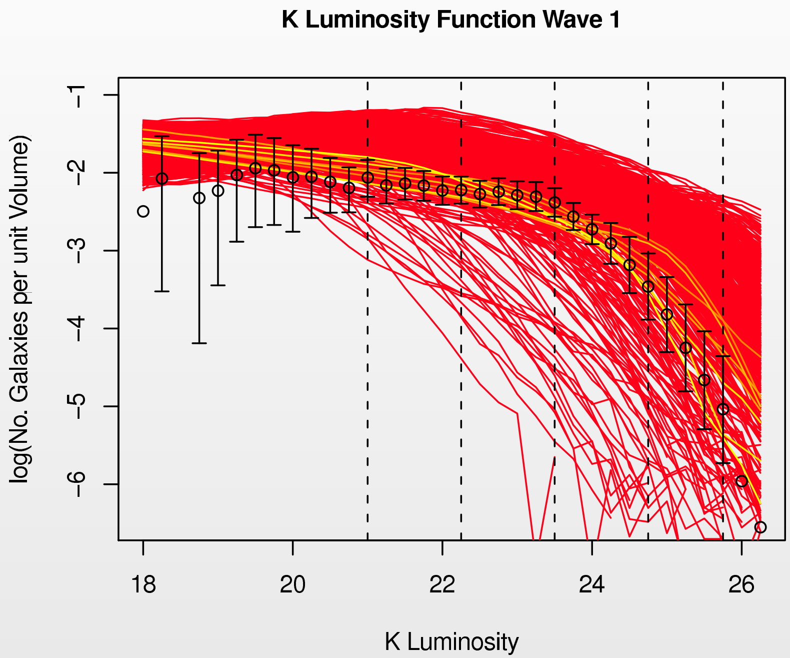

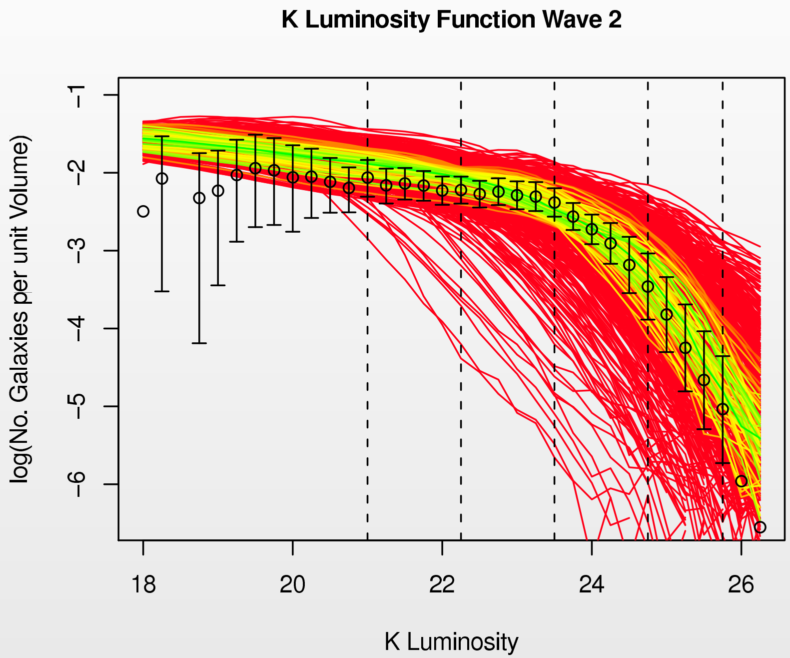

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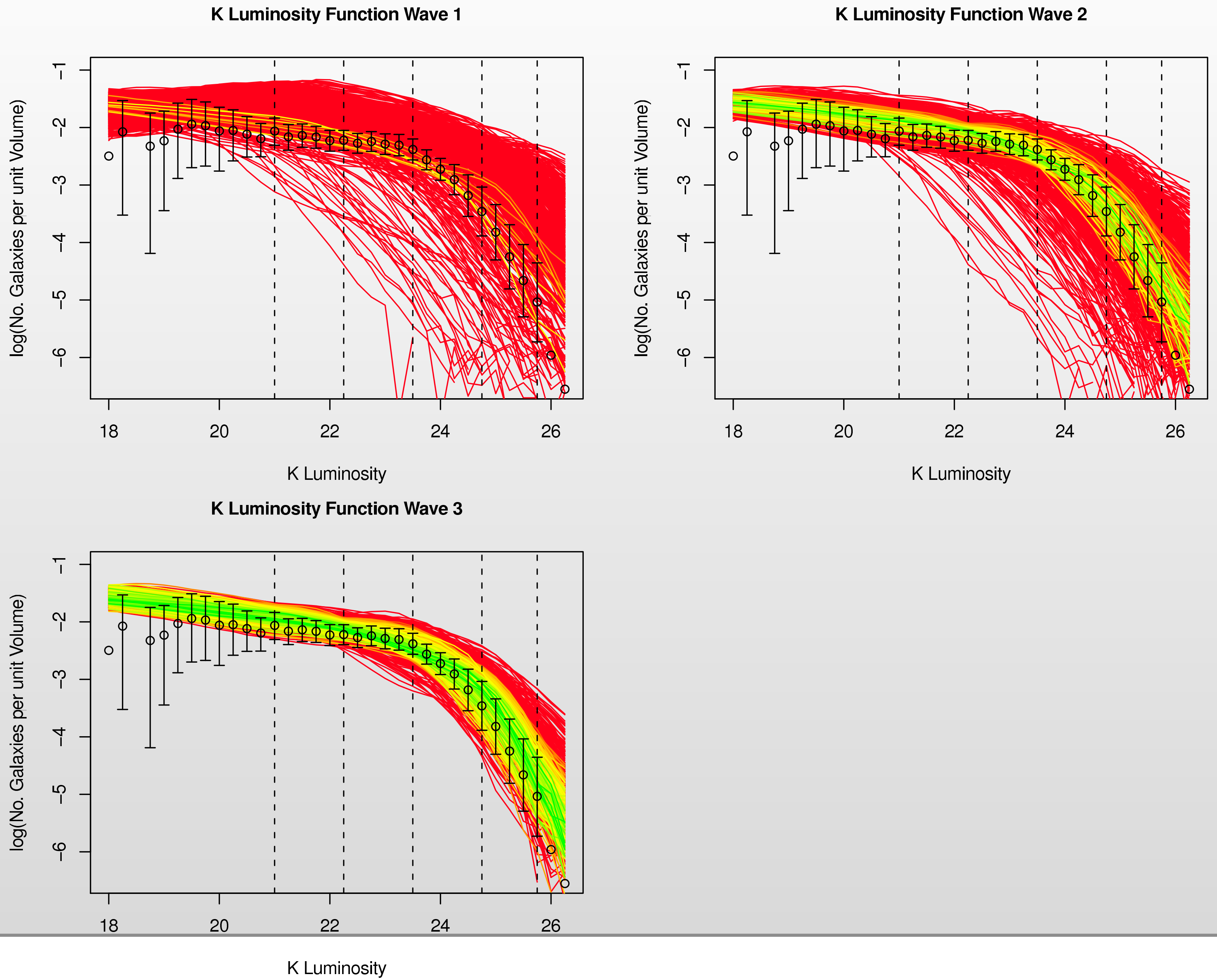

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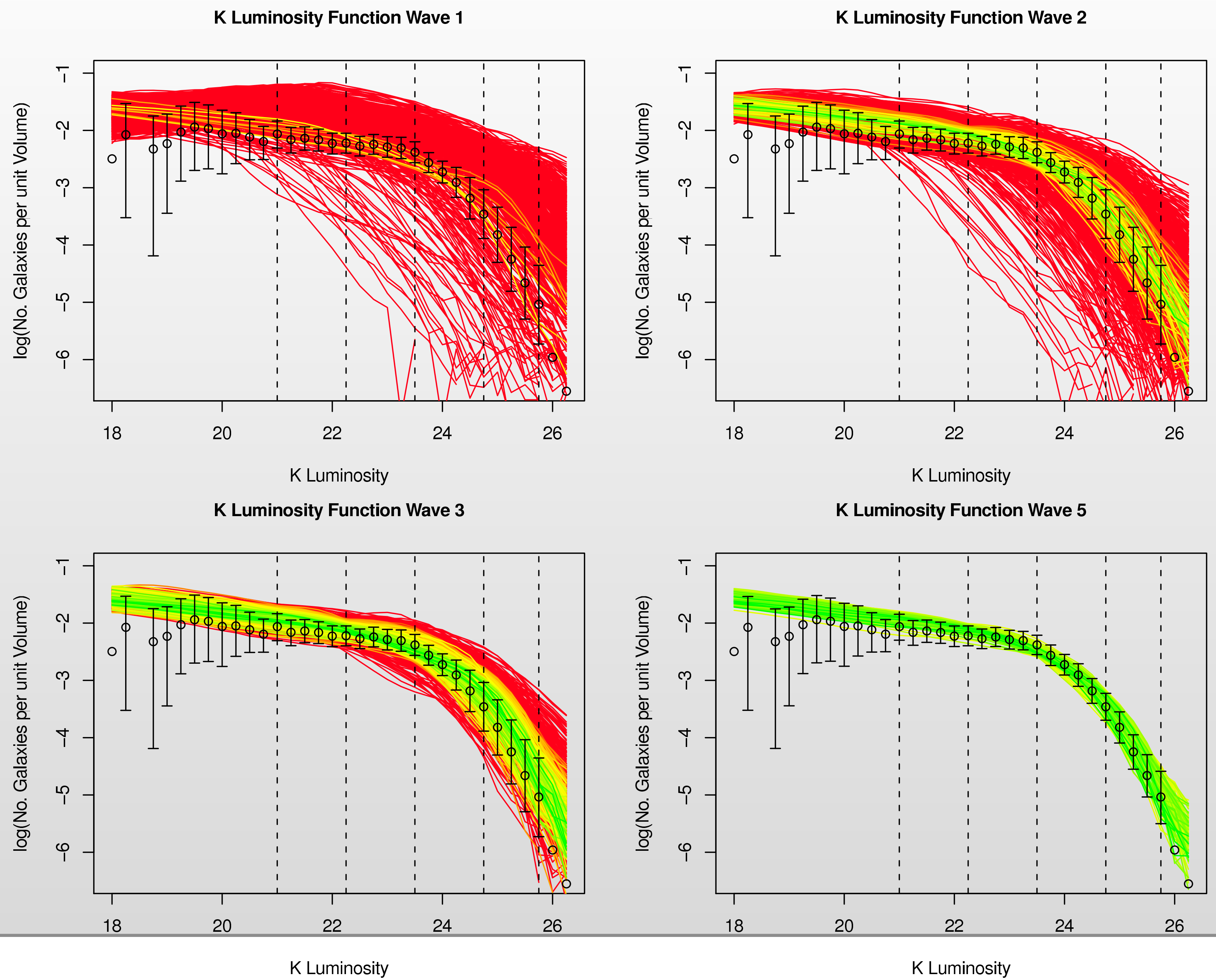

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- We now have a large set of acceptable (Wave 5) runs that can be analysed by the Cosmologists, and used to explore other features of Galform.

References

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