A Guide to Emulation, Implausibility and History Matching, and an Introduction to Designing Future Experiments.

Tuesday Session 2

UNICAMP Workshop on Bayesian Uncertainty Analysis
of Complex Models

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Work done in collaboration with Michael Goldstein (Dept. Mathematical Sciences), Junli Liu and Keith Lindsey (Biological Sciences), Durham University, UK.

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- Hence Emulators are essential for any serious analysis.
- We will now build a simple emulator.

Full Emulator Equation

- For each output $f_i(x)$ we pick active variables x^A then emulate 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:

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

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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.

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- To really simplify things, lets set this polynomial to a constant β_0 (we will return to the polynomial later). Therefore we have:

$$f(x) = \beta_0 + u(x)$$

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- As we are going to use Bayes Linear methods to build our emulator, we need to specify a priori the $\mathrm{E}(\beta_0), \mathrm{Var}(\beta_0), \mathrm{E}(u(x))$ and the covariance structure of $u(x)$ which simply means the $\mathrm{Cov}(u(x), u(x'))$.

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- We then choose an appropriate covariance structure depending what we suspect the behaviour of the computer model $f(x)$ to be: if it is pretty smooth as a function of x we may choose the Gaussian form:

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- In this case we specify $\mathrm{E}(\beta_0)$ corresponding to our beliefs about the mean of $f(x)$, with $\mathrm{Var}(\beta_0)$ representing how unsure we are.

Simple 1-dimensional Sine Example

- Remember that $f(x)$ could represent any output of a complex model, so for a reservoir model, it could be the BHP or oil production at 1000 days, while x would be a vector of inputs e.g. porosities, permeabilities, fault multipliers.

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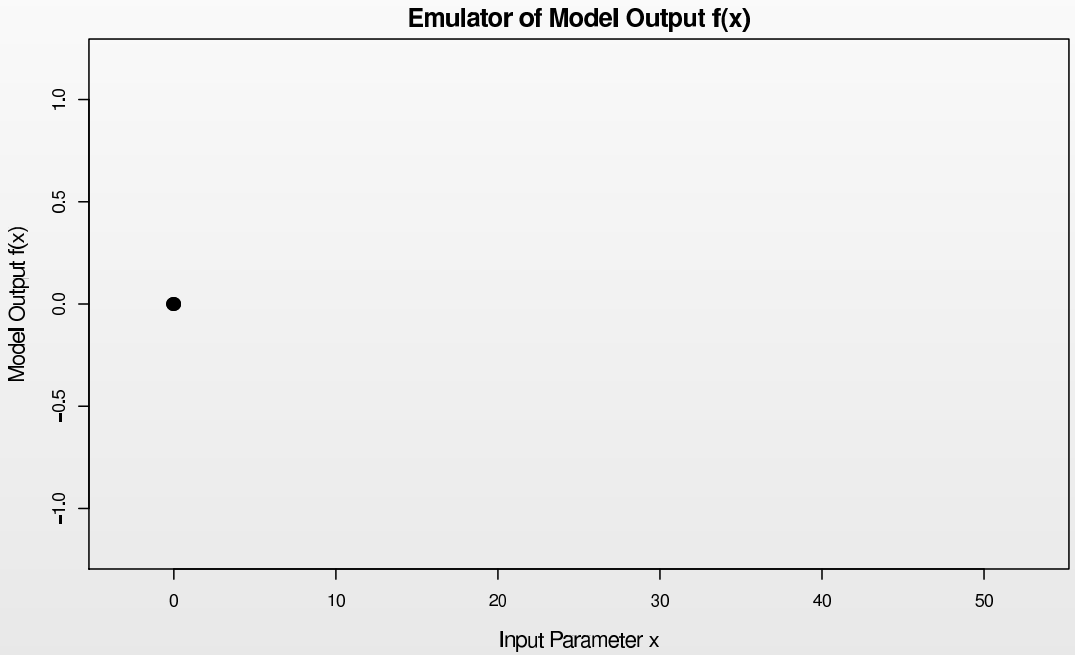
- We evaluate $f(x^{(j)})$ for $j = 1$ to 6, and gather the results into vector D:

$$\begin{aligned} D \;&= (f(x^{(1)}), f(x^{(2)}), \ldots, f(x^{(6)}))^T \\ &= \left(\sin\left(\frac{2\pi \times 0}{50}\right), \sin\left(\frac{2\pi \times 10}{50}\right), \ldots, \sin\left(\frac{2\pi \times 50}{50}\right)\right)^T \end{aligned}$$

Emulation: a 1D Example



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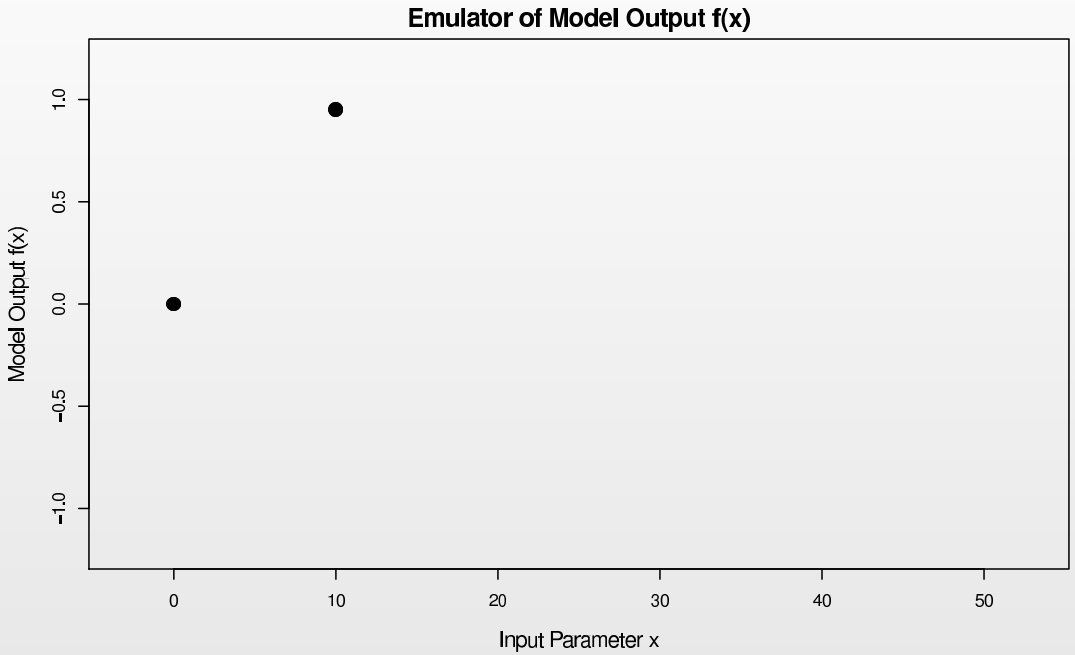

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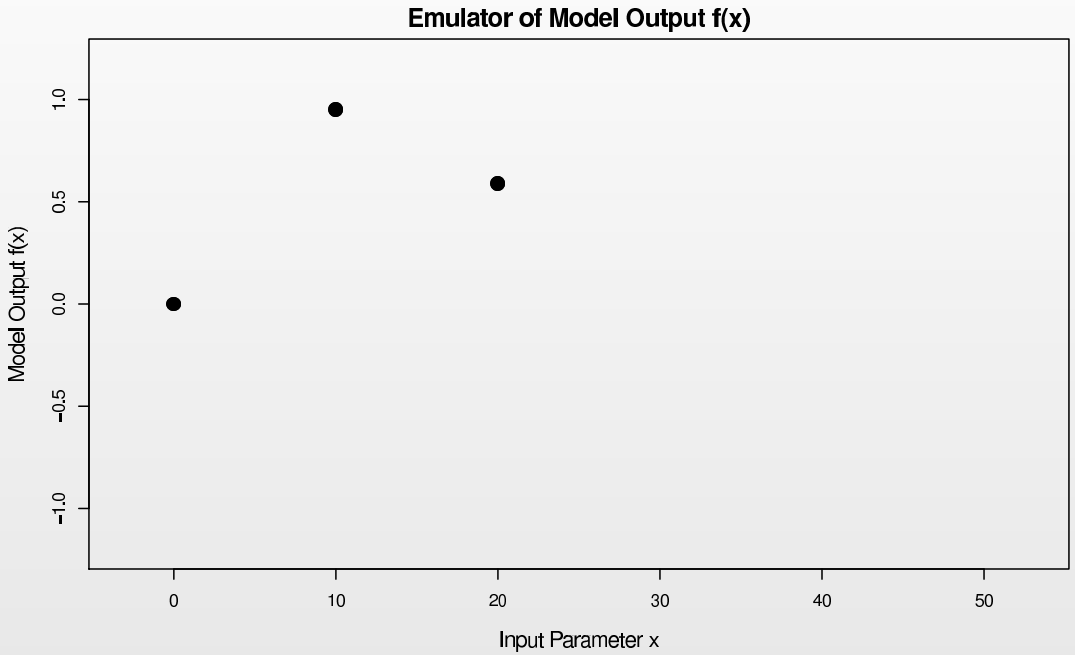

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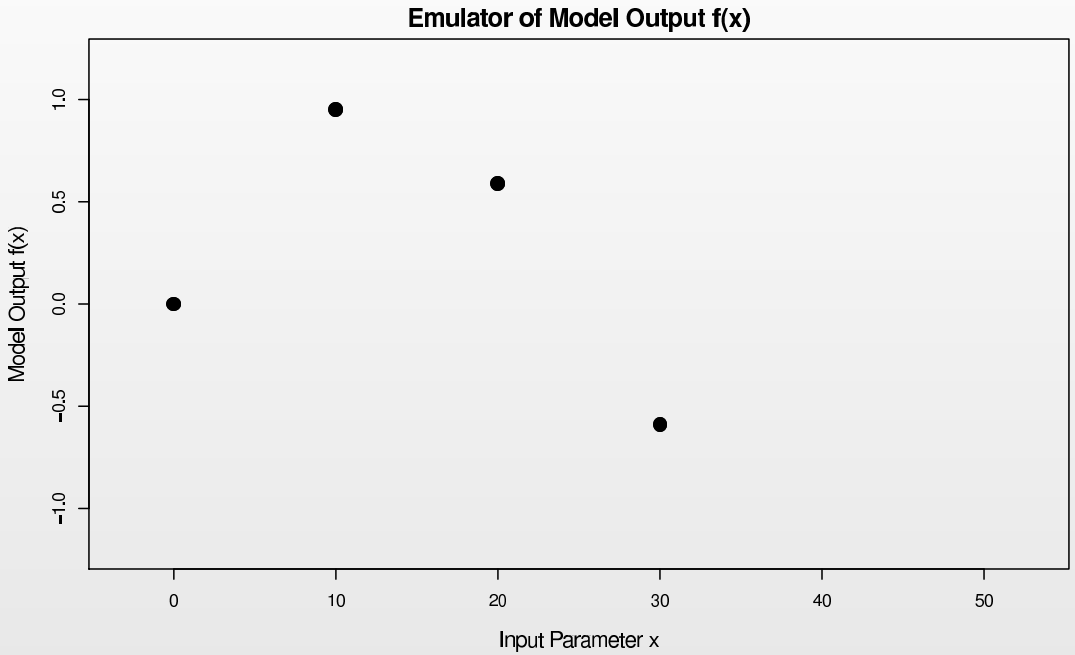

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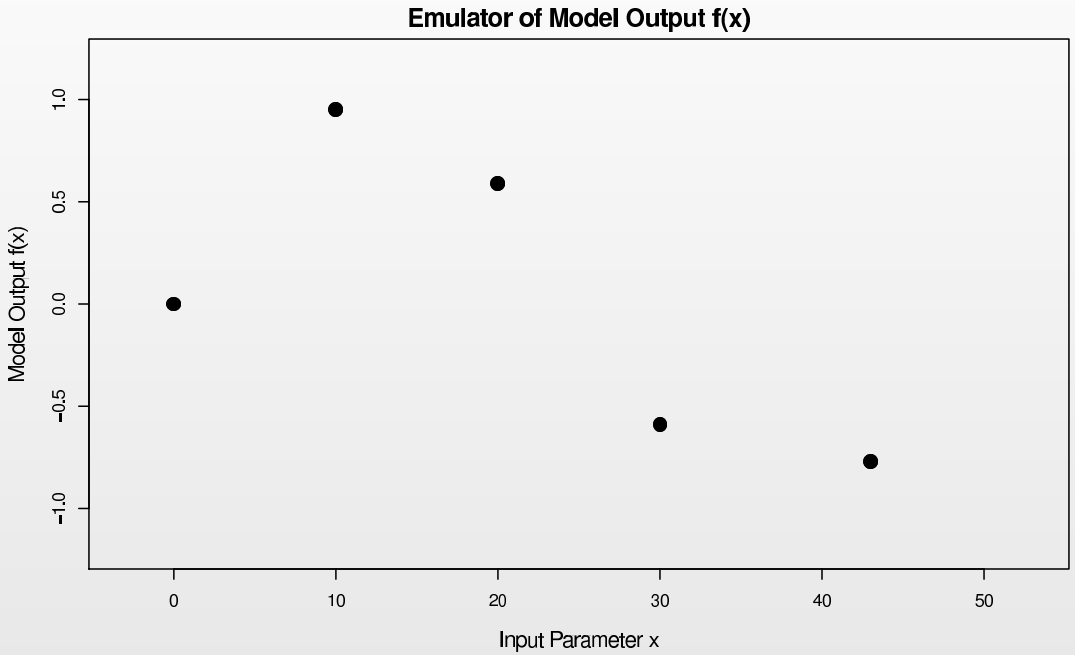

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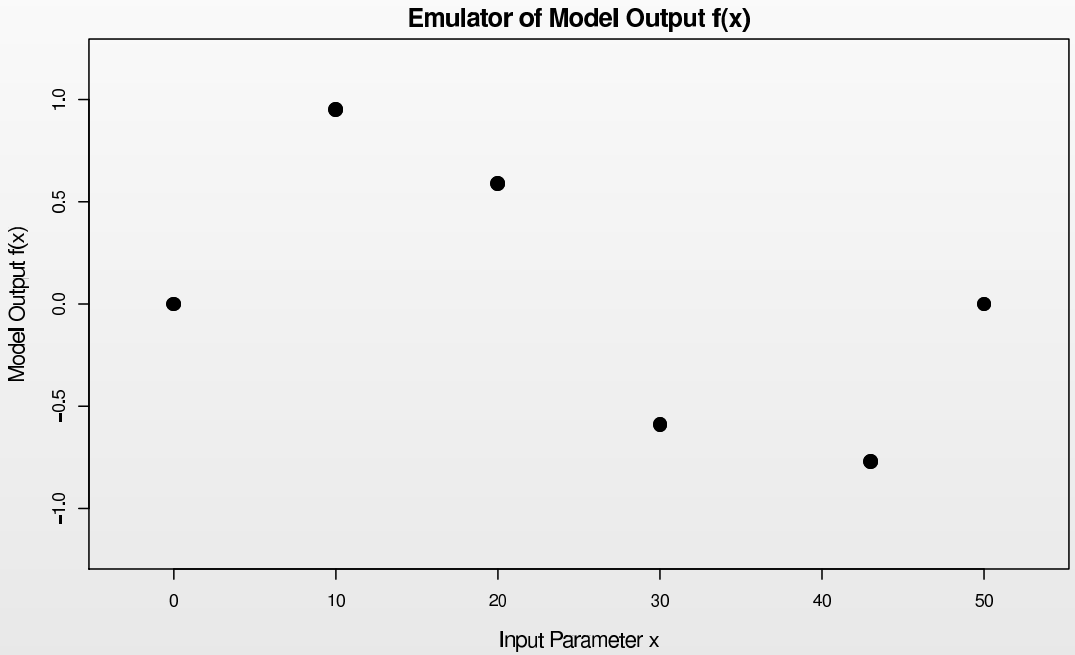

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- We now have all we need to use the Bayes Linear equations to update our prior beliefs $\mathrm{E}(f(x))$ and $\mathrm{Var}(f(x))$ about the behaviour of $f(x)$ given new run data D, to obtain adjusted beliefs $\mathrm{E}_D(f(x))$ and $\mathrm{Var}_D(f(x))$:

$$\mathrm{E}_D(f(x)) = \mathrm{E}(f(x)) + \mathrm{Cov}(f(x), D)\mathrm{Var}(D)^{-1}(D - \mathrm{E}(D))$$
$$\mathrm{Var}_D(f(x)) = \mathrm{Var}(f(x)) - \mathrm{Cov}(f(x), D)\mathrm{Var}(D)^{-1}\mathrm{Cov}(D, f(x))$$

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- Everything on the right hand side of the BL update equations has been specified: as $f(x) = \beta_0 + u(x)$, $\beta_0 = 0$, $\sigma = 1$ and $\theta = 15$, we have:

$$\mathrm{E}(f(x)) = \beta_0, \qquad \mathrm{Var}(f(x)) = \sigma^2$$
$$\mathrm{E}(D) = (\beta_0, \ldots, \beta_0)^T$$

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- $\mathrm{Cov}(f(x), D)$ is a row vector of length $n = 6$ with jth component

$$\begin{aligned} \mathrm{Cov}(f(x), D)_j &= \mathrm{Cov}(f(x), f(x^{(j)})) \\ &= \sigma^2 \exp\left\{ -\frac{\|x - x^{(j)}\|^2}{\theta^2} \right\} \end{aligned}$$

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- Similarly $\mathrm{Var}(D)$ is an $n \times n$ matrix with (j, k) element

$$\begin{aligned} \mathrm{Var}(D)_{jk} &= \mathrm{Cov}(f(x^{(j)}), f(x^{(k)})) \\ &= \sigma^2 \exp\left\{ -\frac{\|x^{(j)} - x^{(k)}\|^2}{\theta^2} \right\} \end{aligned}$$

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- Now $f(x)$ is a column vector of length m.
- In this case we use the same BL equations, but use $\mathrm{Cov}(f(x), D)$ which is now an $m \times n$ matrix, $\mathrm{Var}(f(x))$ is an $m \times m$ matrix, and $\mathrm{E}(f(x))$ is a column vector of length m.

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- We can now plot $\mathrm{E}_D(f(x))$ as a function of x (in blue), and plot credible intervals (in red) as $\mathrm{E}_D(f(x)) \pm 3\sqrt{\mathrm{Var}_D(f(x))}$.

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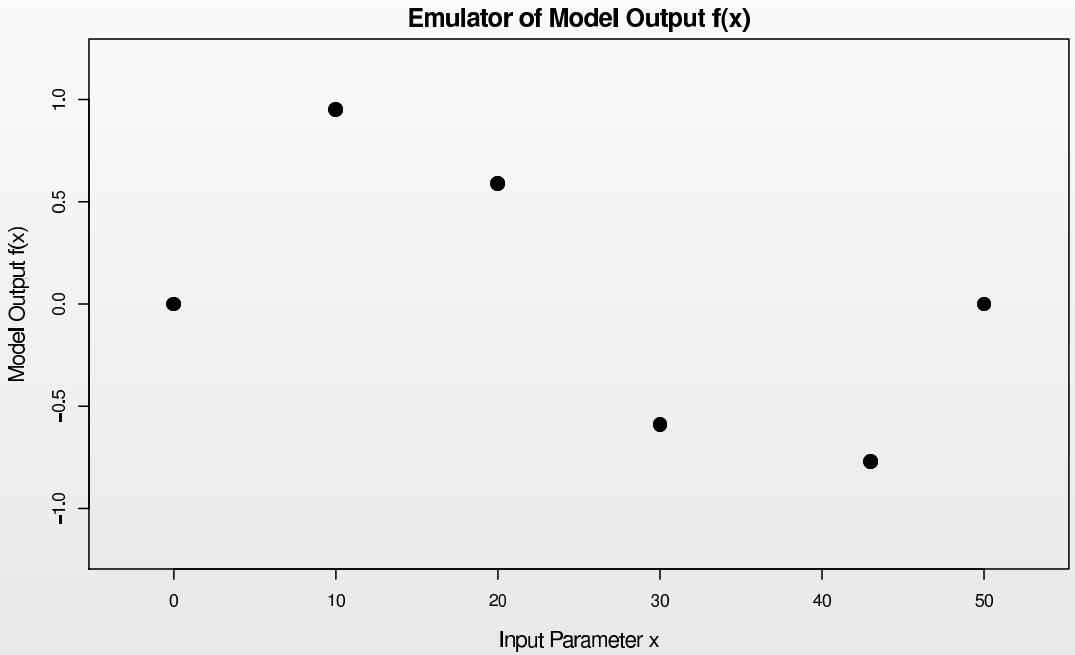

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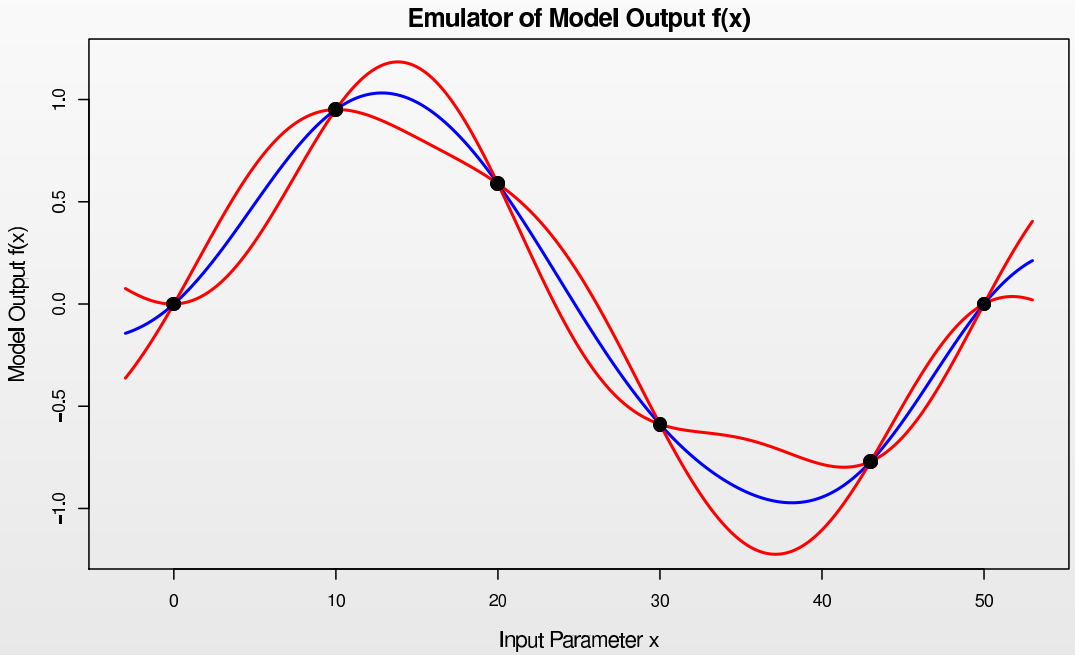

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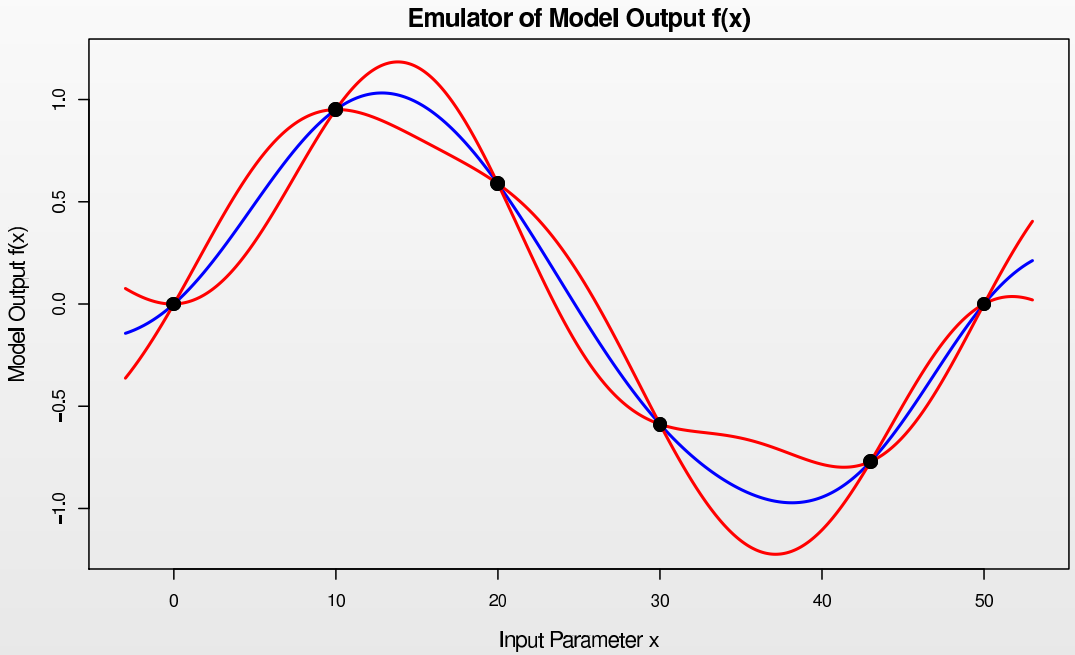

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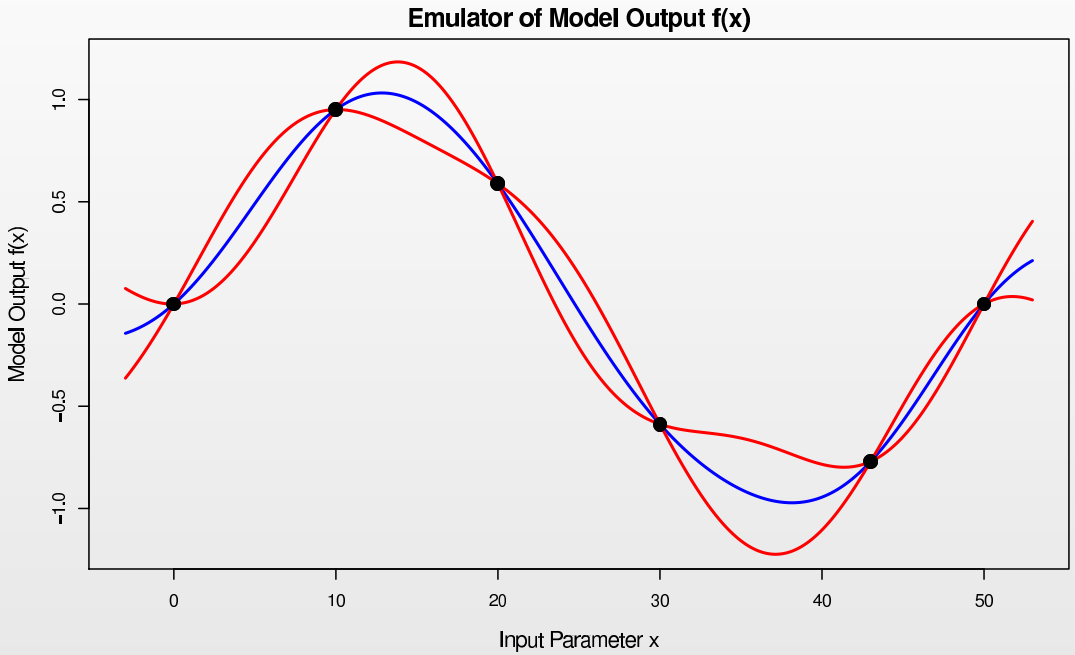

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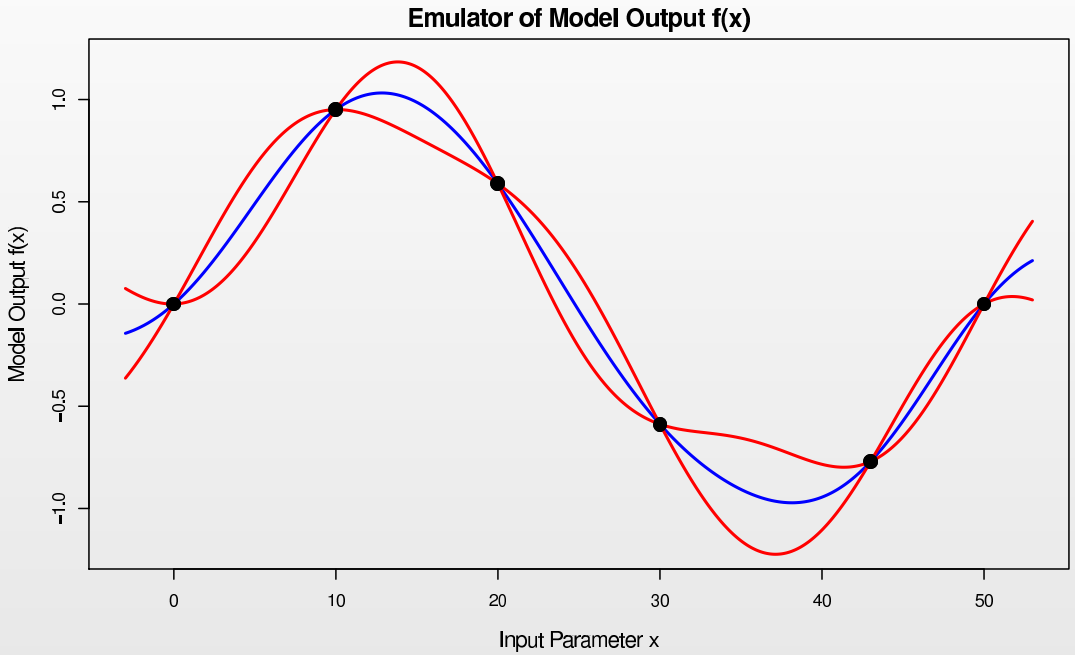

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- Today you will work with R code that does the above, and you will be able to play with β_0, σ, θ, D, $x^{(j)}$ and the function $f(x)$.

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- For our example we take $z = -0.8$ and $\sigma_e^2 + \sigma_\epsilon^2 = 0.02^2$ and plot $I(x)$.

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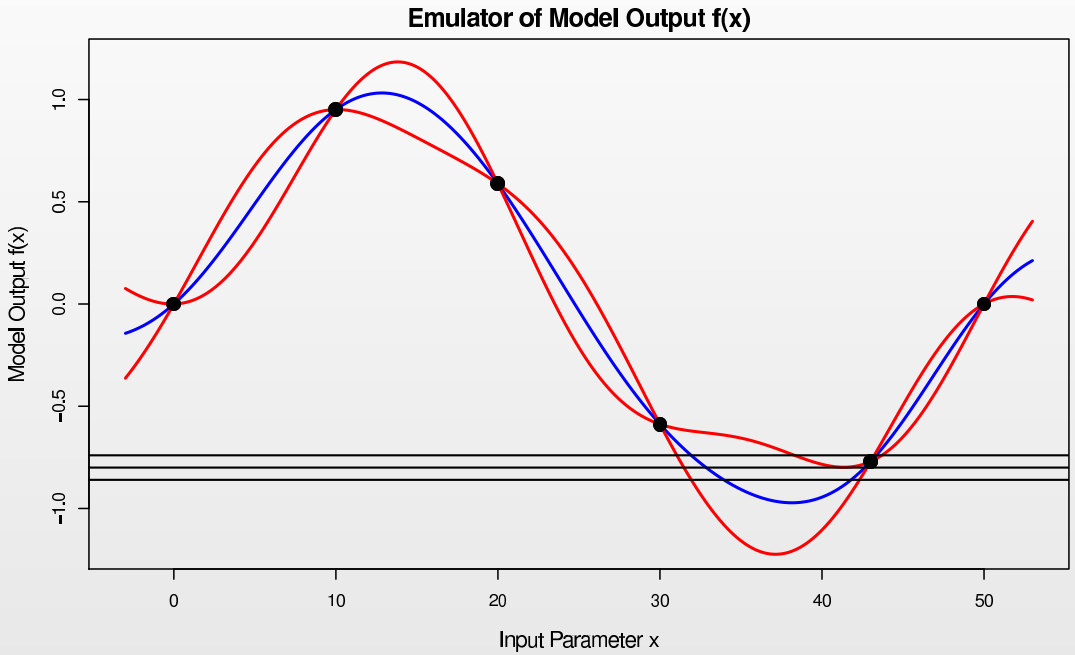

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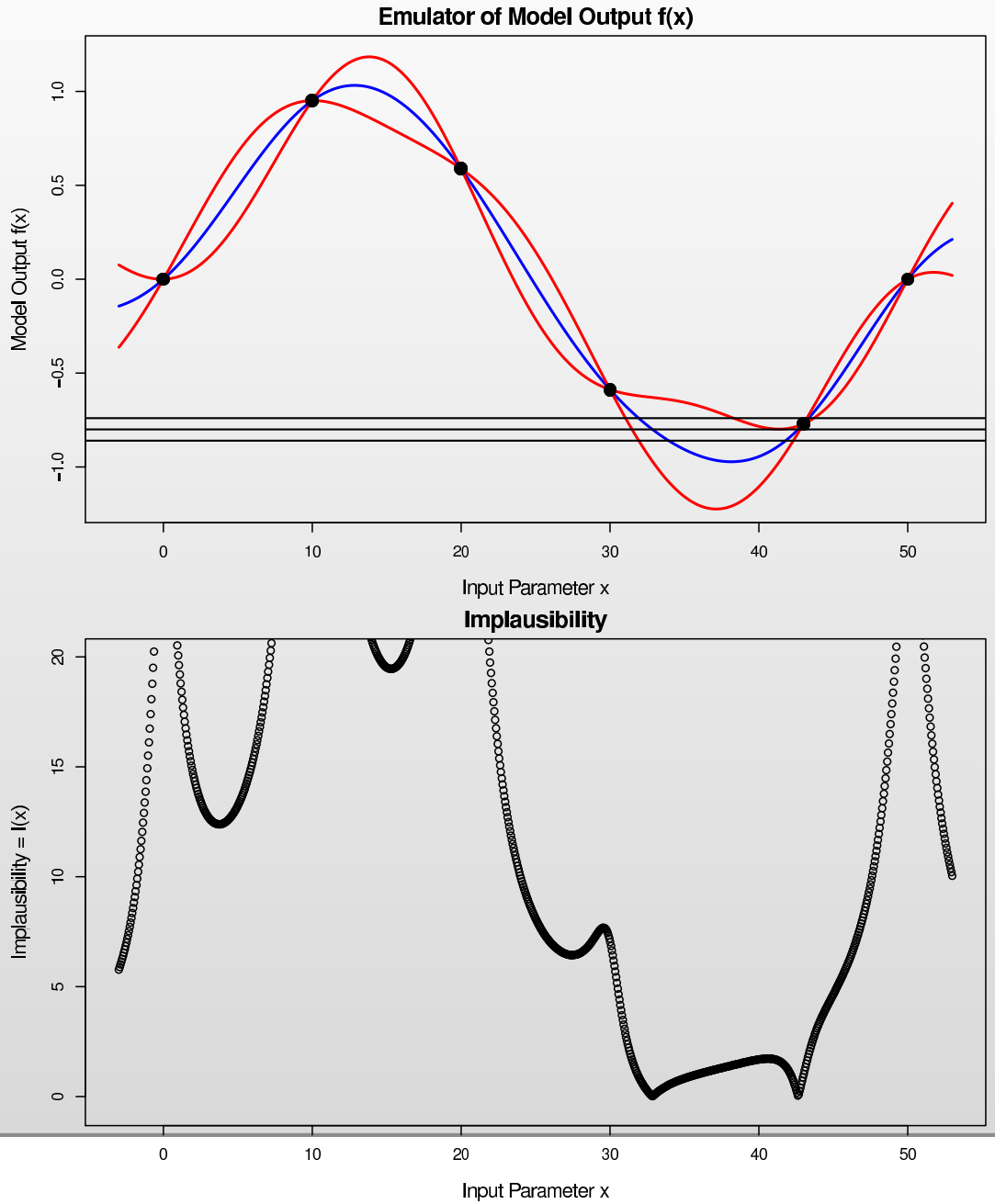

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- (This is a slight simplification, often we may create a new emulator from the $x^{(j)}_{wave2}$ points alone, perhaps using the wave 1 emulator as prior).

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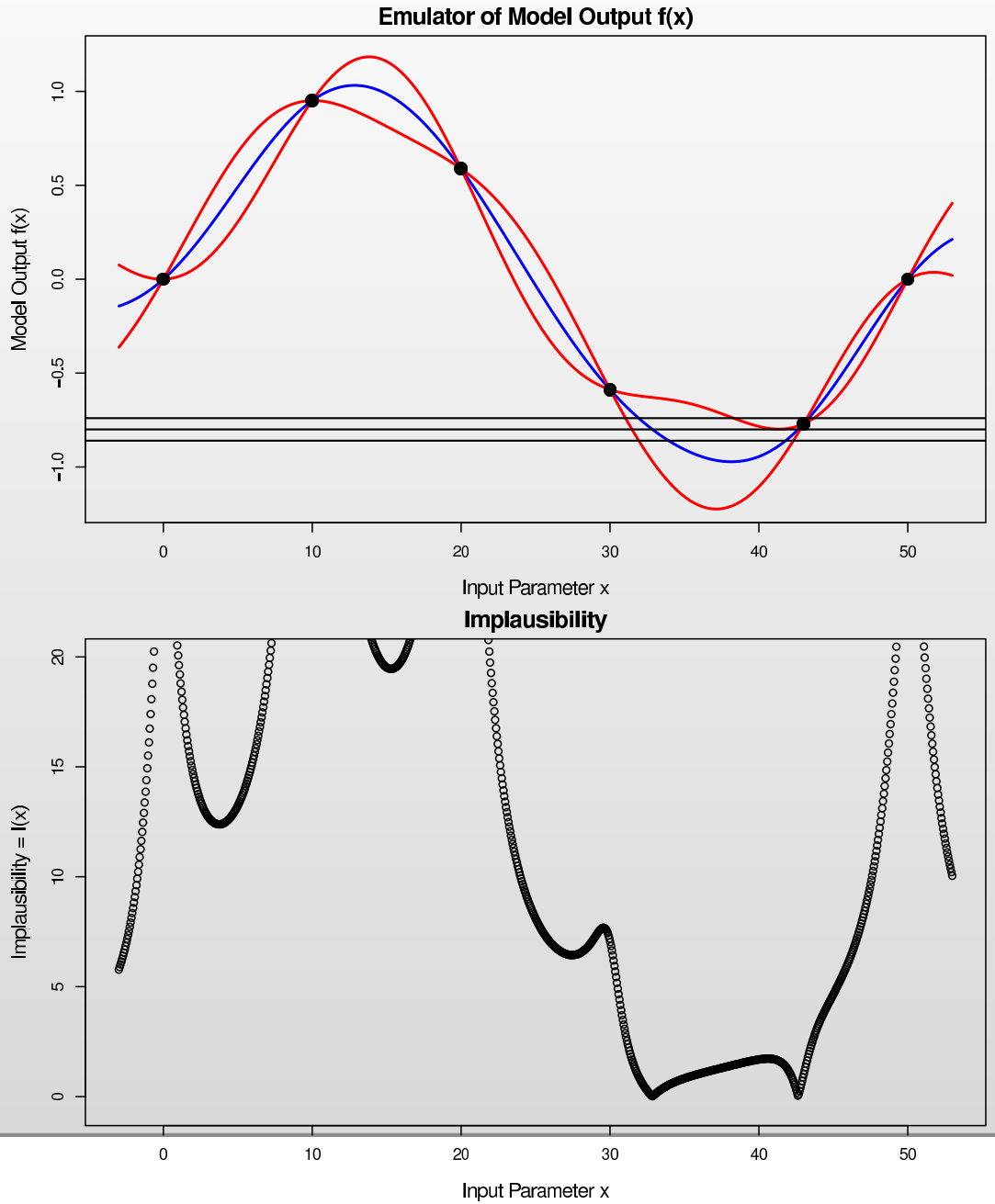

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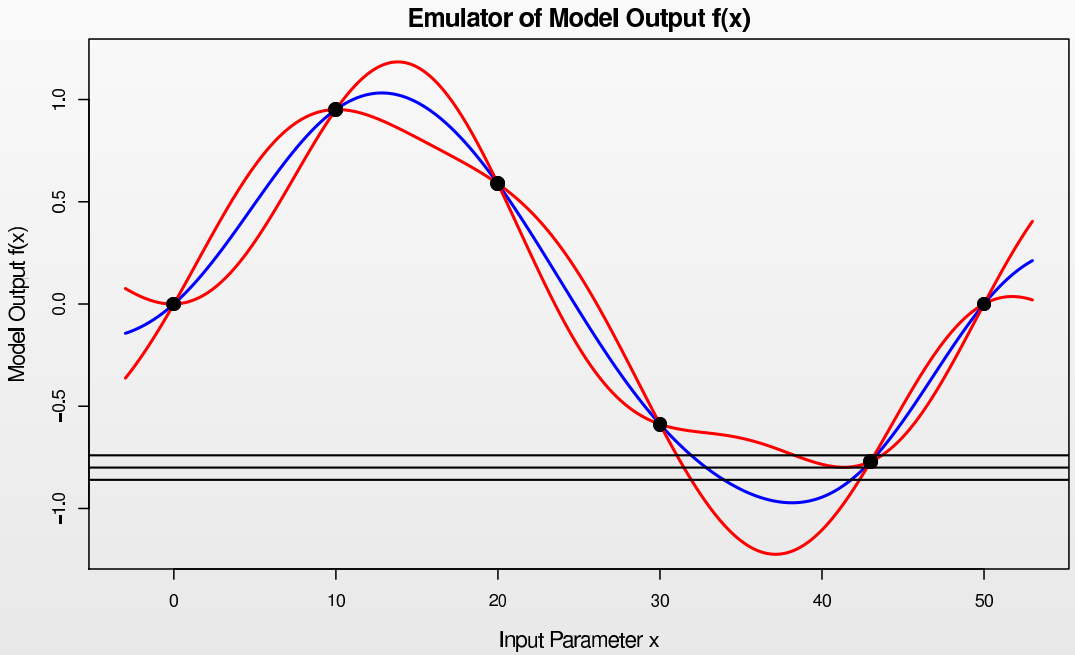

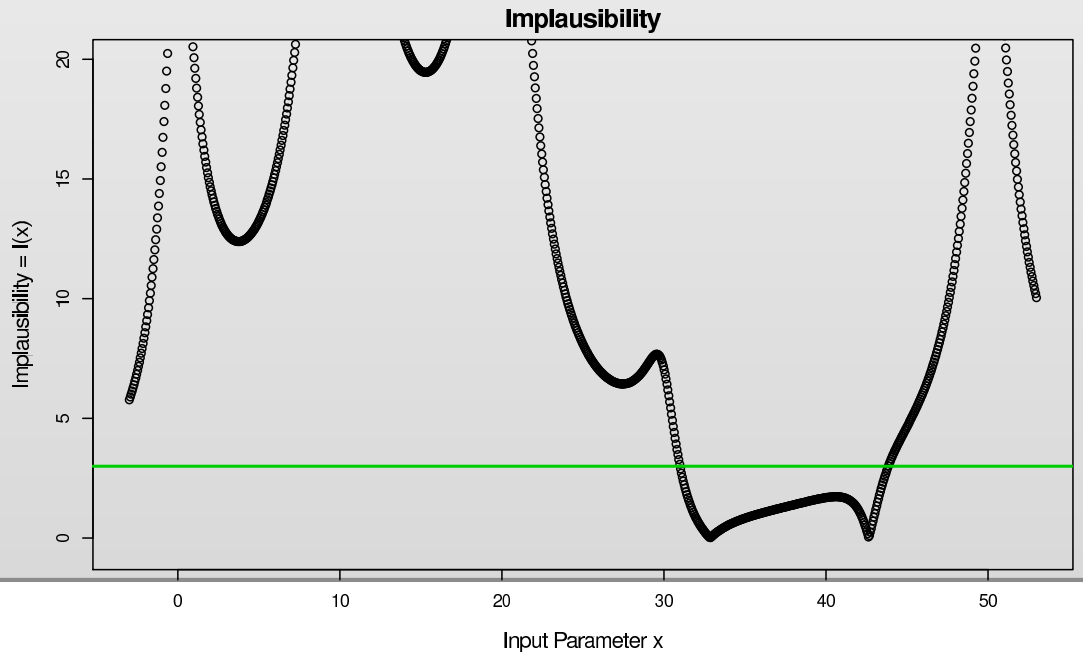

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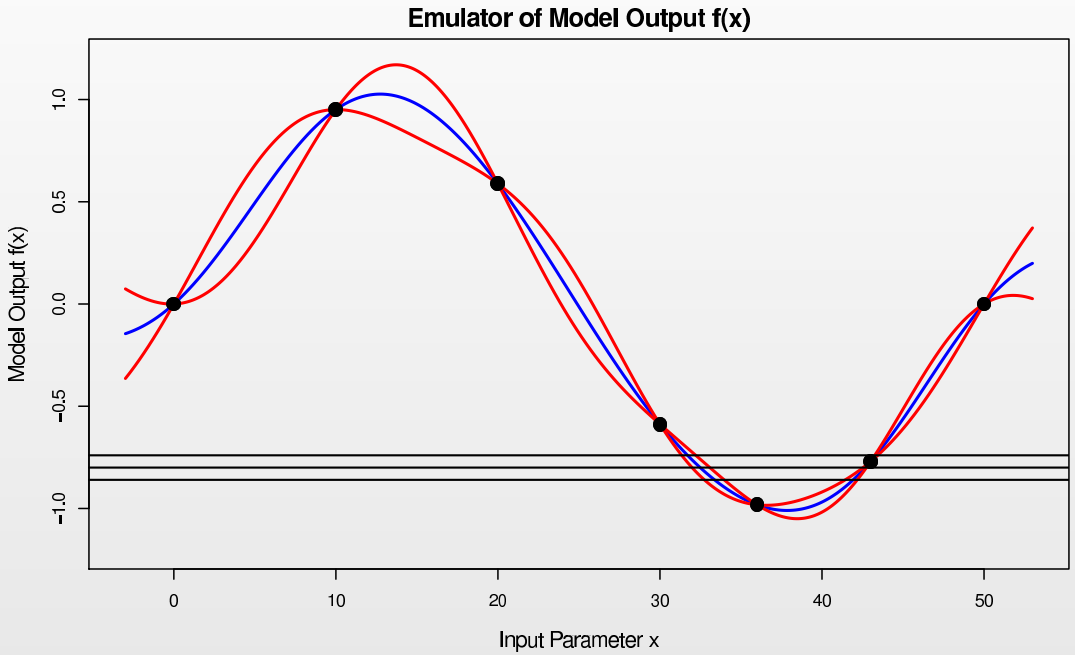

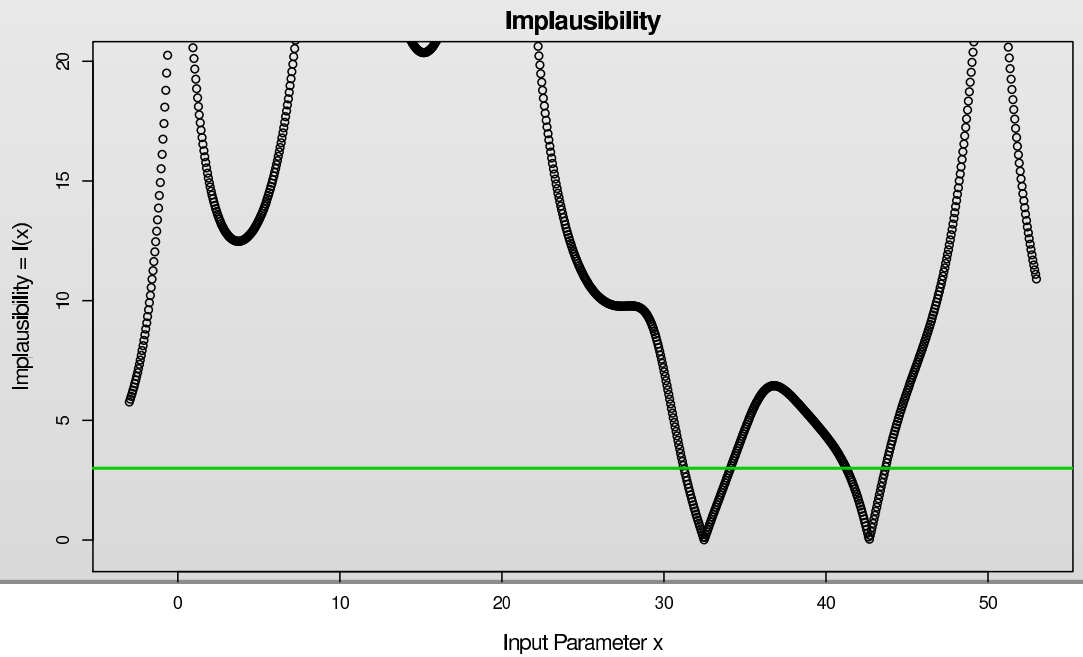

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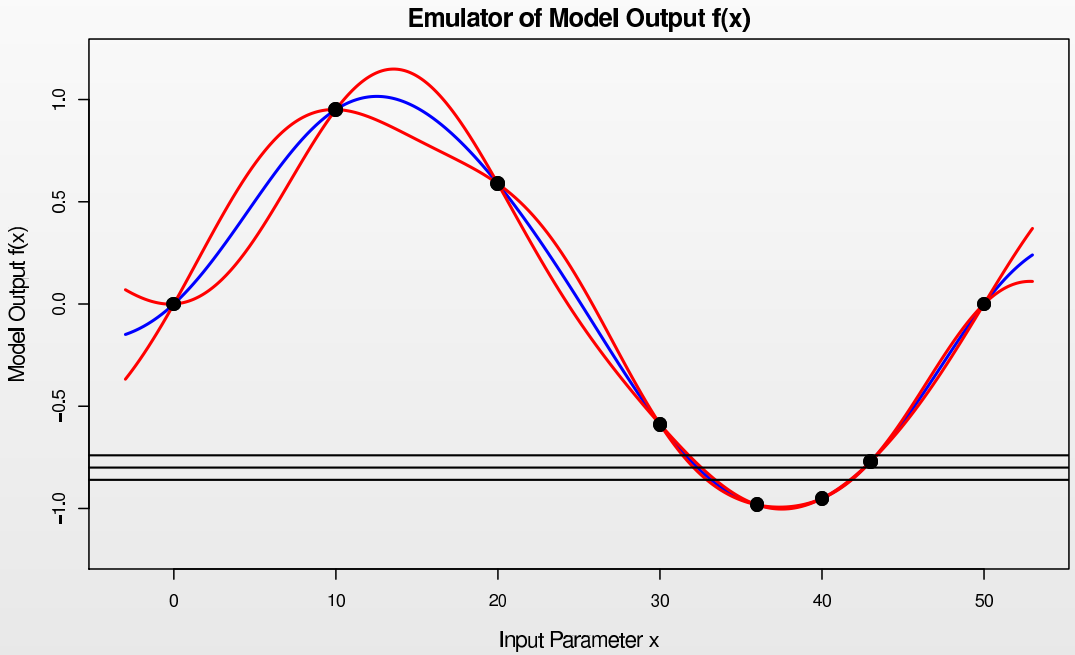

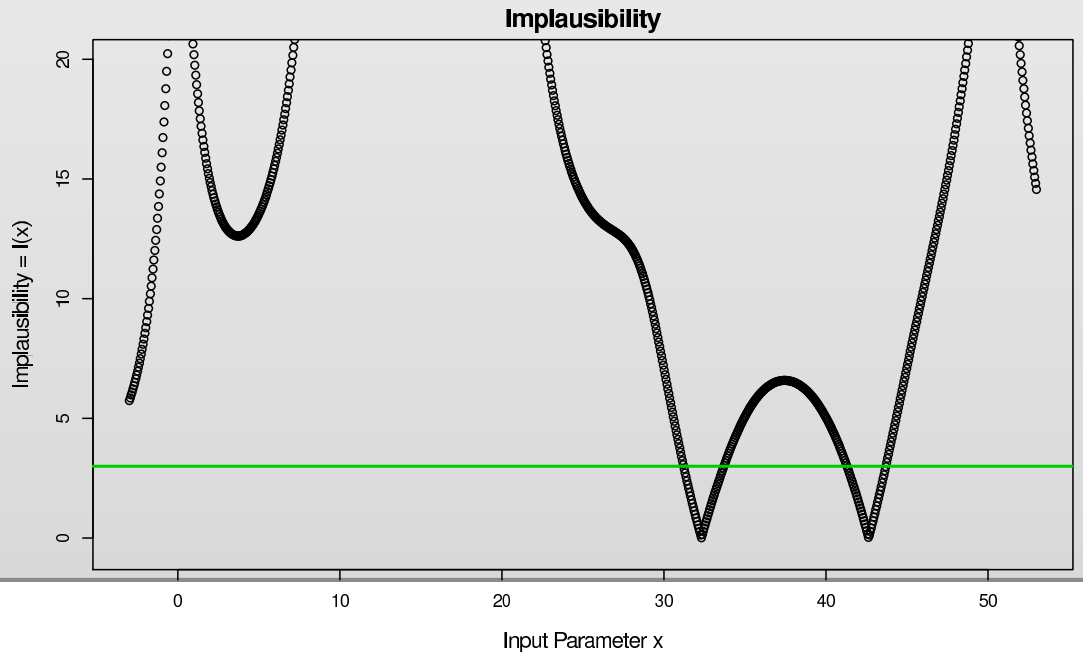

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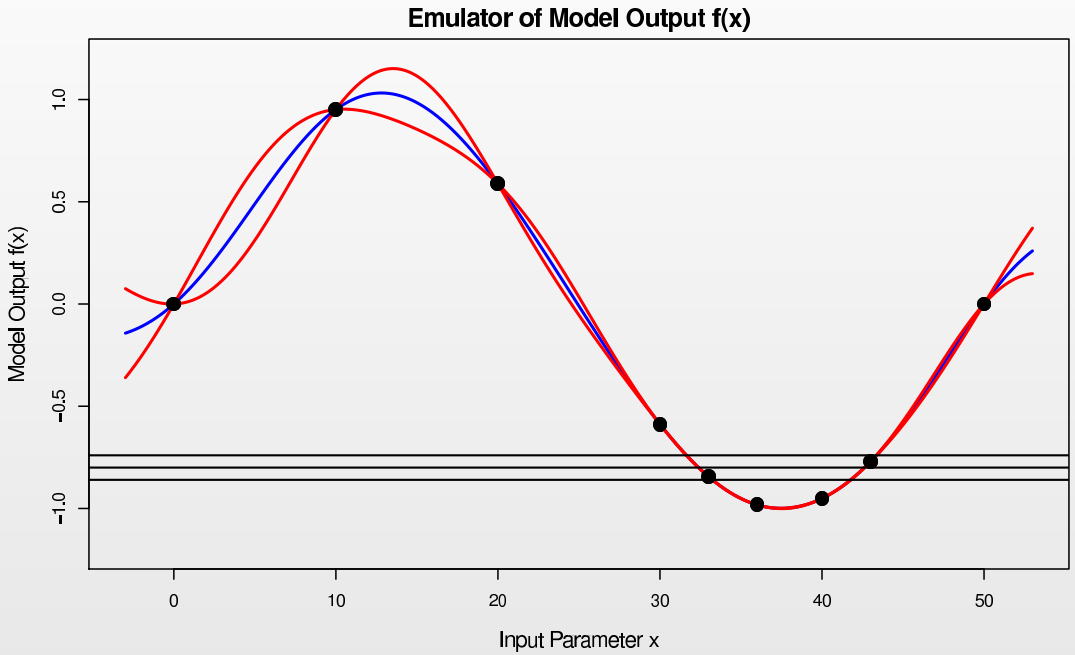

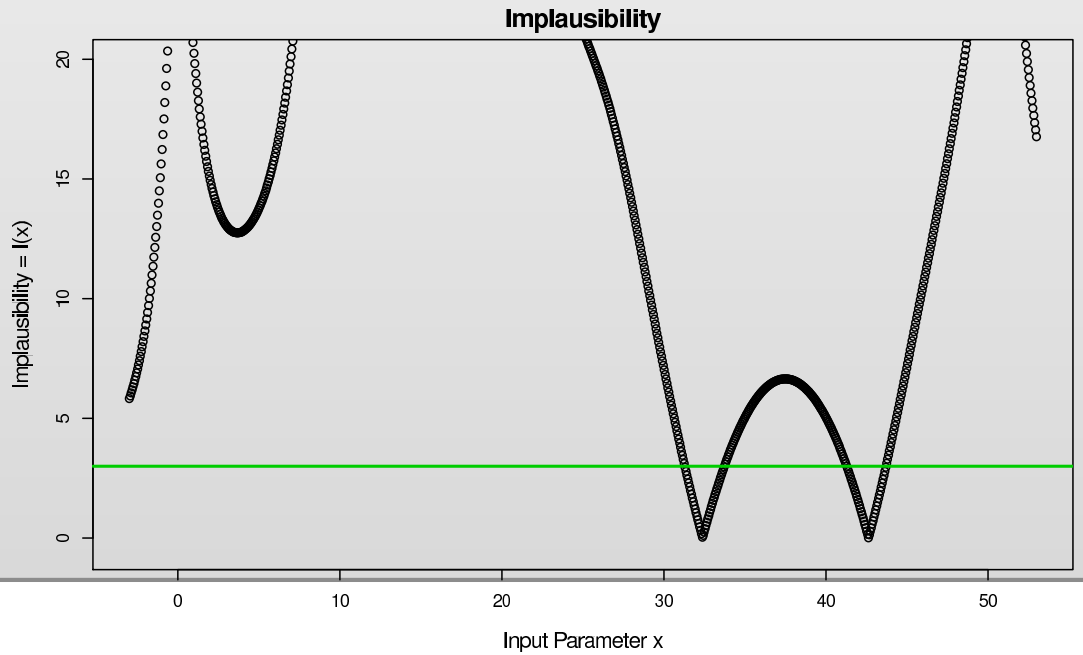

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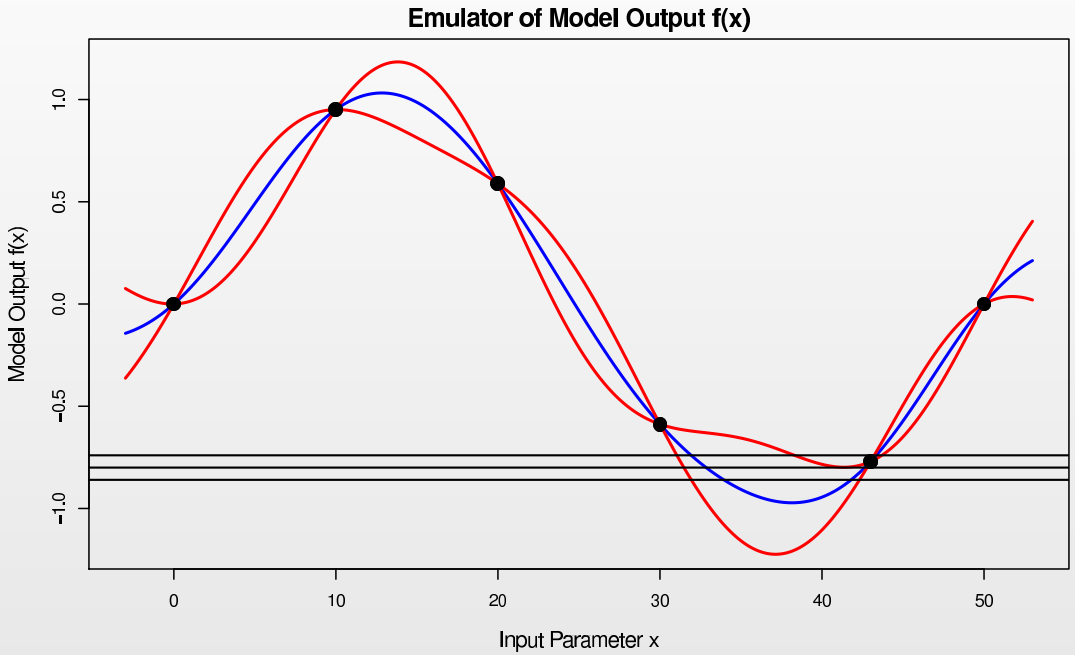

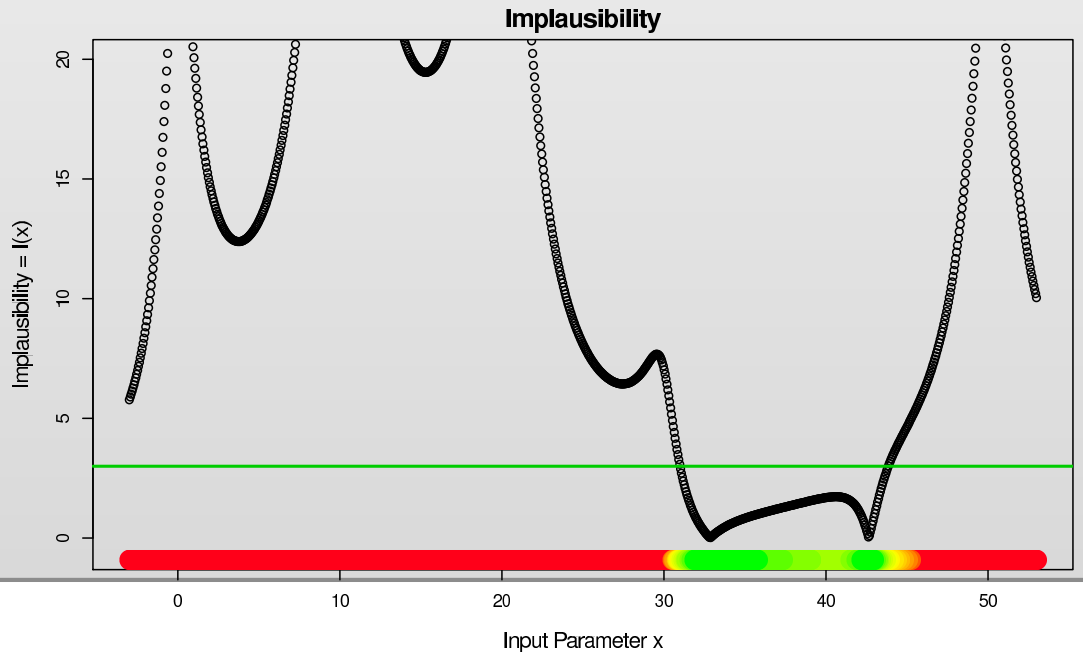

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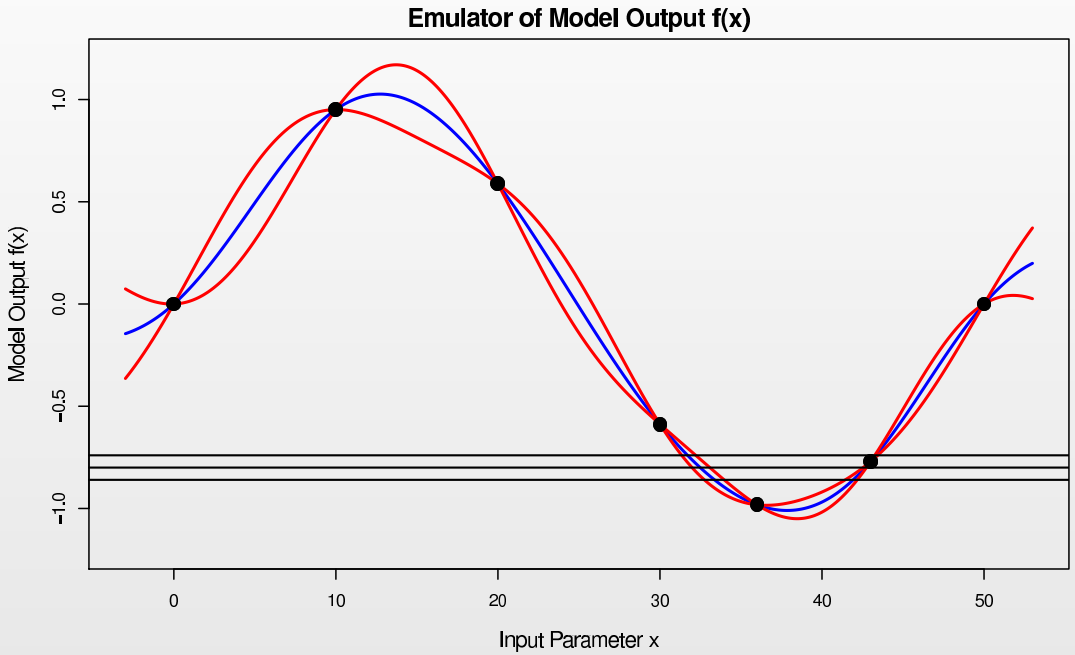

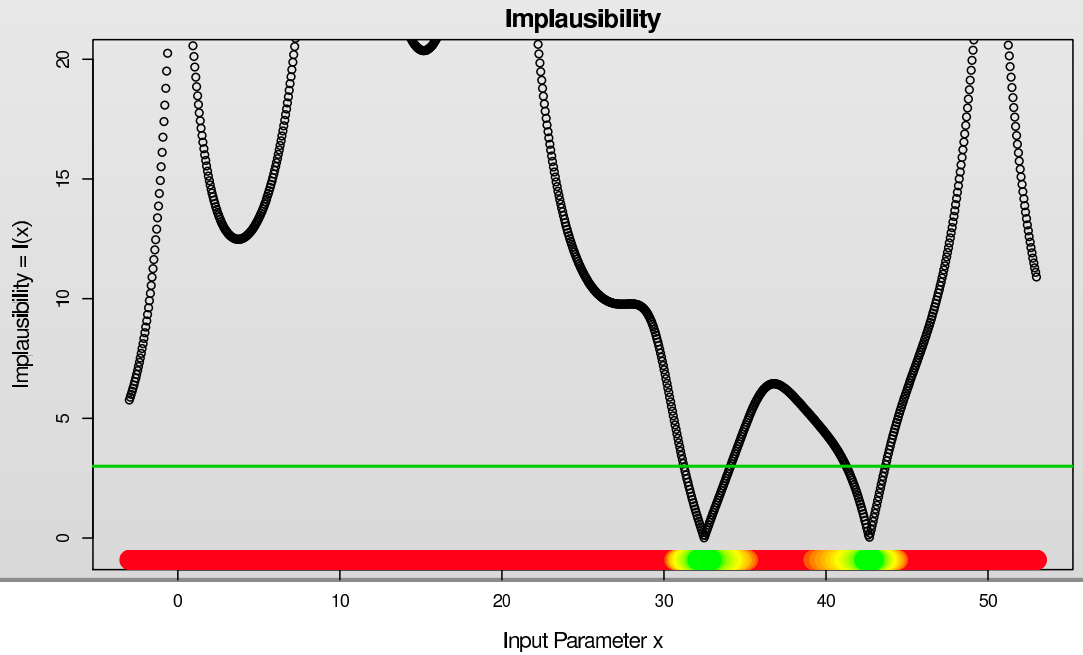

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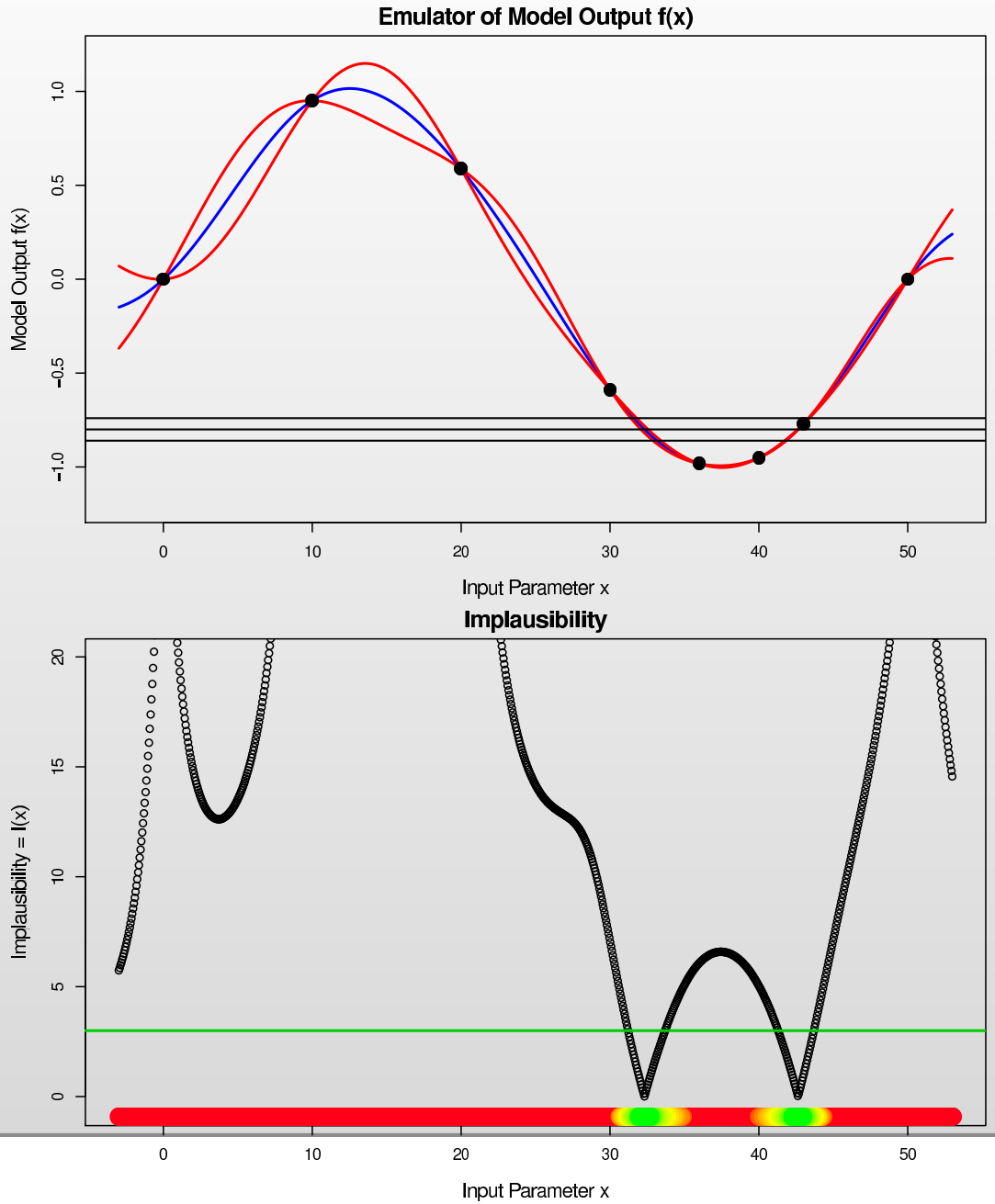

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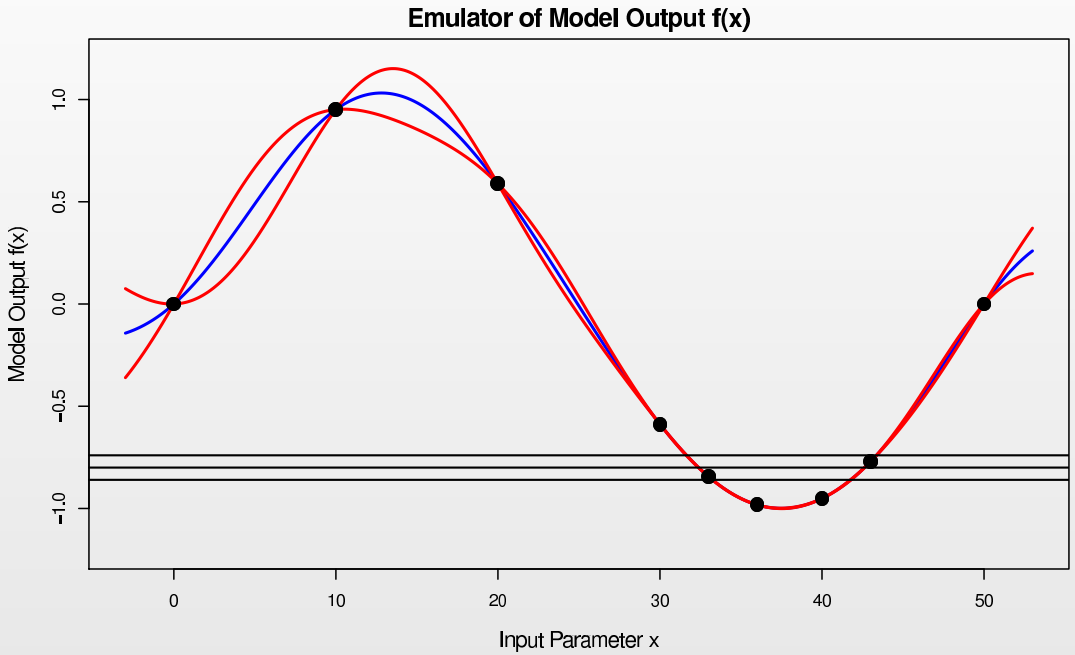

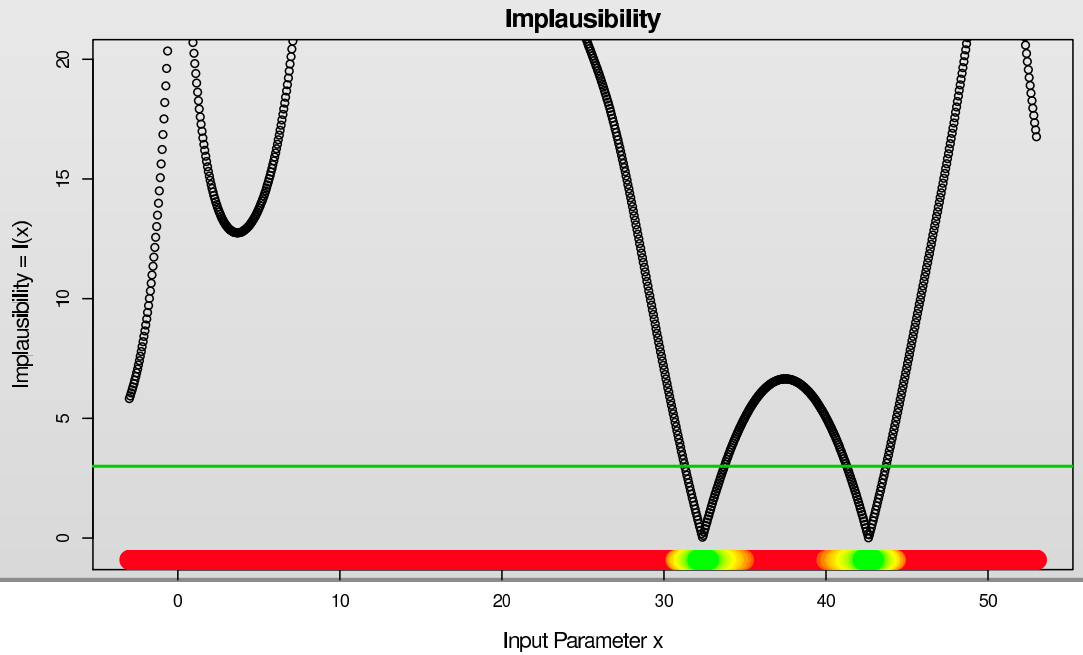

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- We can in principle specify prior expectations, variances and covariances for all the β_j terms: $\mathrm{E}(\beta_j)$ and $\mathrm{Cov}(\beta_j, \beta_k)$, if we have informed beliefs about them.

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- As this is actually corresponds to using a Maximum Likelihood Estimate (MLE), it can be used to approximate the full Bayesian posterior for the β's, in the large run number limit, as described yesterday.

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- For example, if we have access to a fast version of the model (e.g. a coarse or lower resolution version of a reservoir model) that we can run many times, we can use this to obtain highly informed priors for β_j.
- This is a powerful technique that is noticably under used in the oil industry.
- Alternatively, if we have performed a reasonable number of runs that are well spaced in the input space, the correlation between the $u(x^{(j)})$ terms will be small and our emulator will tend toward a standard regression model (or linear model).
- Hence we can approximate the β_j terms by their Ordinary Least Squares (OLS) estimate, (and use a corresponding estimate for σ^2 too).
- As this is actually corresponds to using a Maximum Likelihood Estimate (MLE), it can be used to approximate the full Bayesian posterior for the β's, in the large run number limit, as described yesterday.
- We can obtain all the OLS estimates we need from the R function "lm()" (see later this afternoon).

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- $\delta(x)$ an uncorrelated nugget that has $\mathrm{E}(\delta(x)) = 0$ and $\mathrm{Var}(\delta(x)) = \sigma_\delta^2$.

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- The identification of active inputs is also vital to the whole emulation process: it can greatly simplify a very complex and high dimensional function.

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- For an explicit demonstration of this, see our Galaxy papers.

Introduction to Designing future experiments

- We will now have a brief introduction to Designing future experiments or: what data should I pay for?
- Often we want to use a complex model to predict the future, with appropriate uncertainty.
- We would then want to use such predictions to inform us about decision we have to make.
- For example, we may wish to choose the best experiment from a list of possible experiments, to achieve some scientific goal.
- Similarly we may have the choice of paying for extra data, e.g. 4D seismic data, and wondered whether it is worth it.
- We do this by History Matching first, then employing Decision Theory.
- In the examples I show, we are going to judge future experiments based on how good we think they will be at reducing the size of the input space in a future history match: therefore our Utility will be linked to space reduction.

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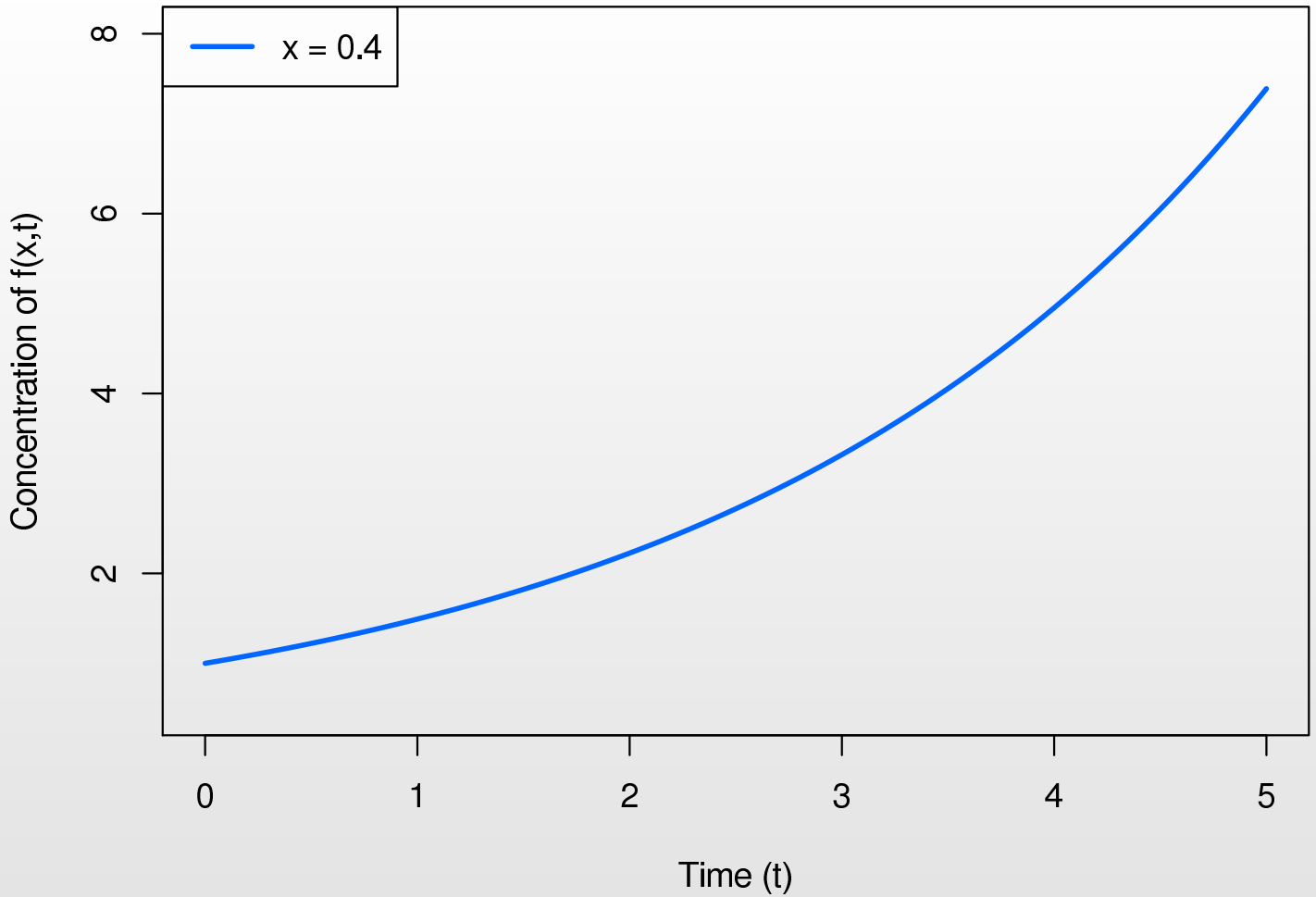
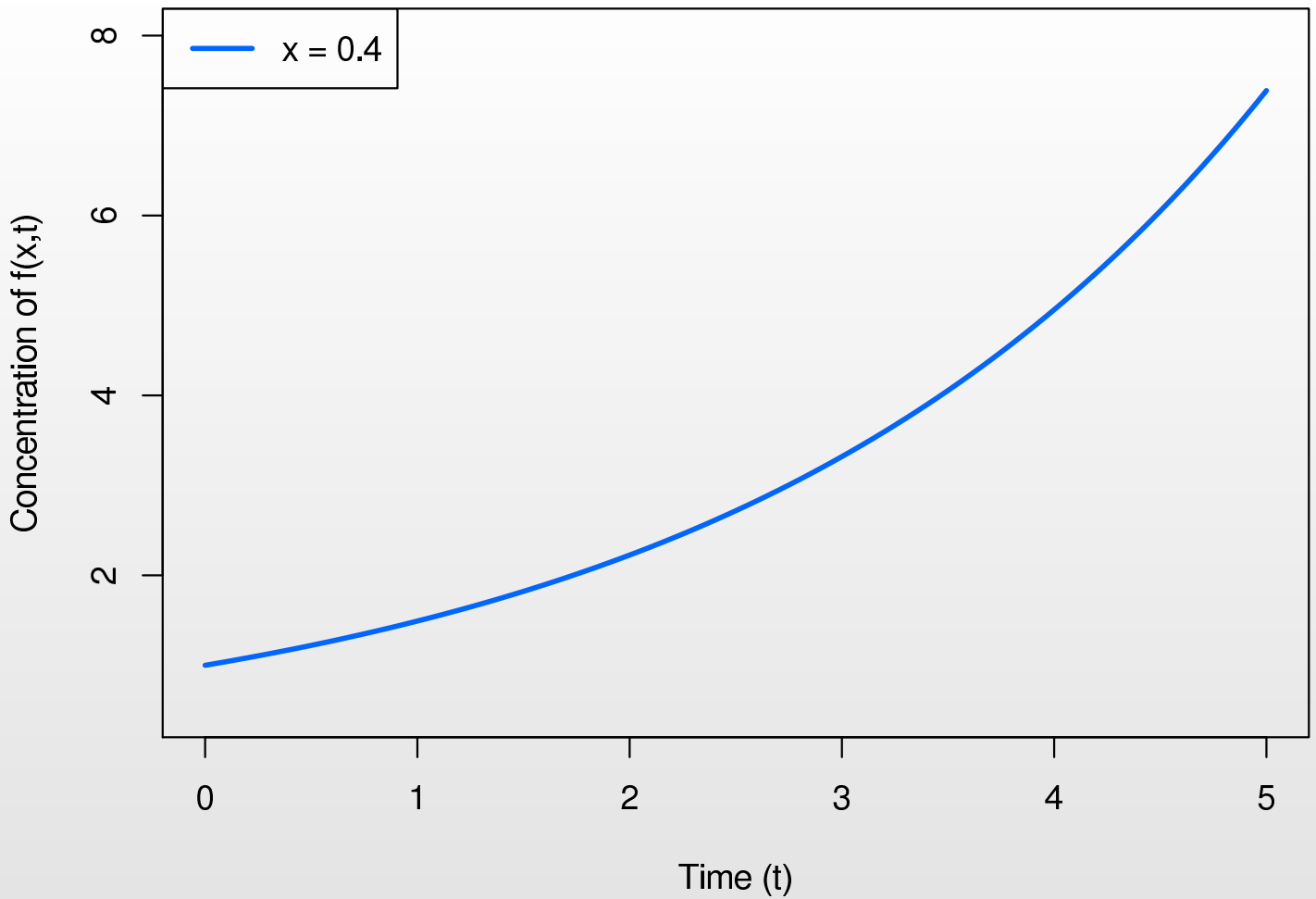
- Model features an input parameter x which we want to learn about.
- Note that normally we would not have the analytic solution for $f(x,t)$.



- One “model run” with the input parameter $x = 0.4$



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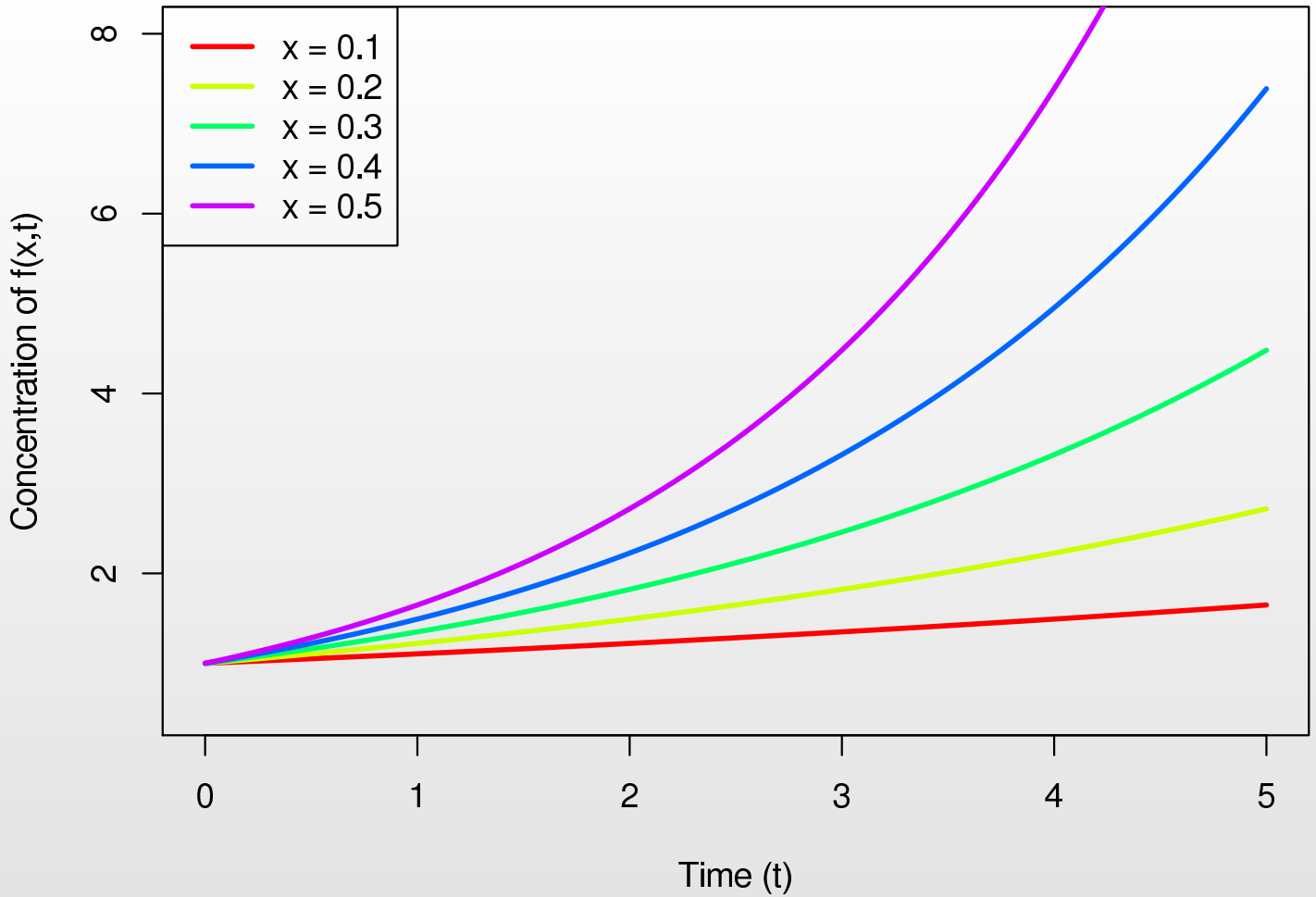
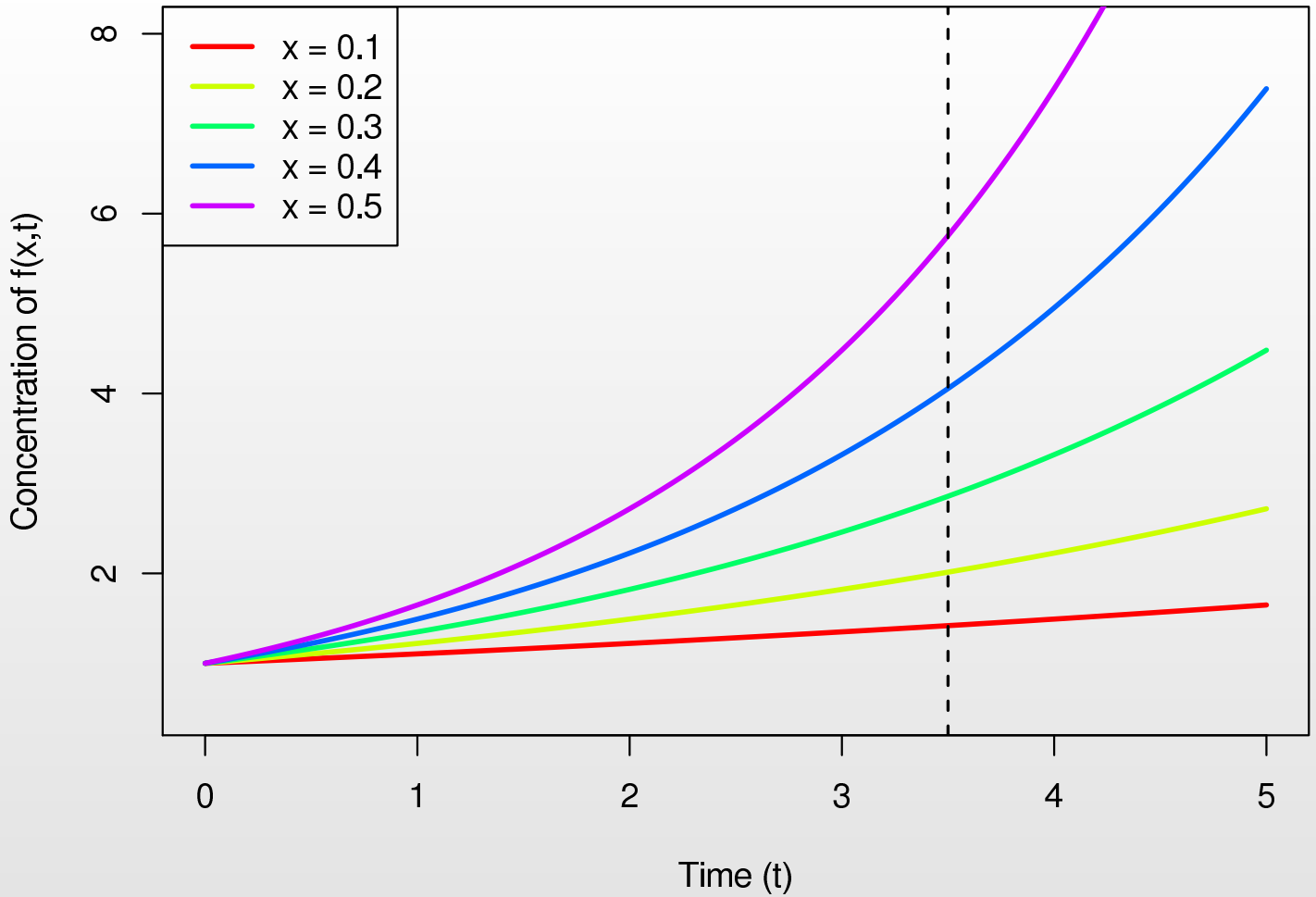
- If we did not know the analytic solution for $f(x, t)$ this would be generated by numerically solving the differential equation.



- Five model runs with the input parameter varying from $x = 0.1$ to $x = 0.5$



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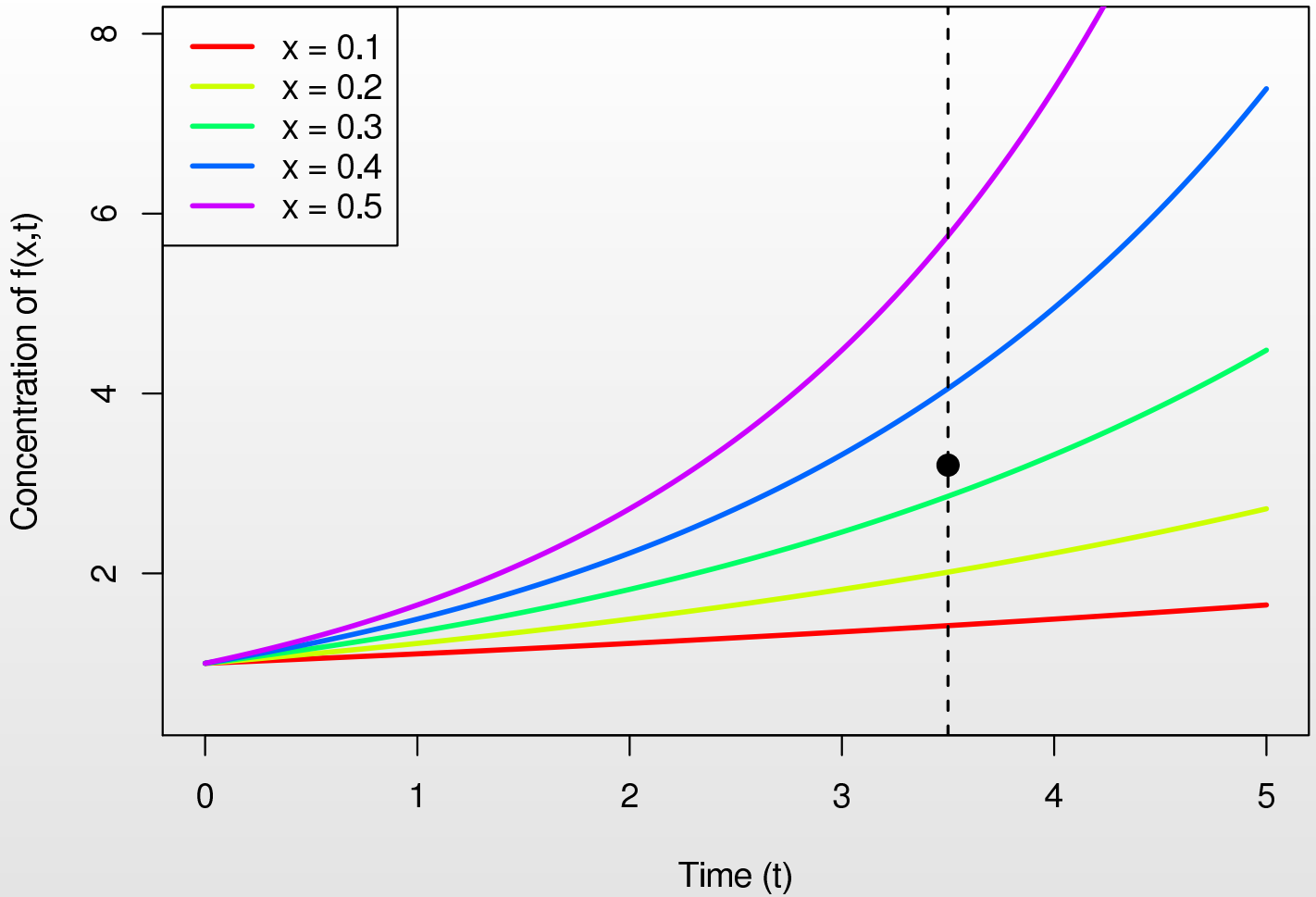

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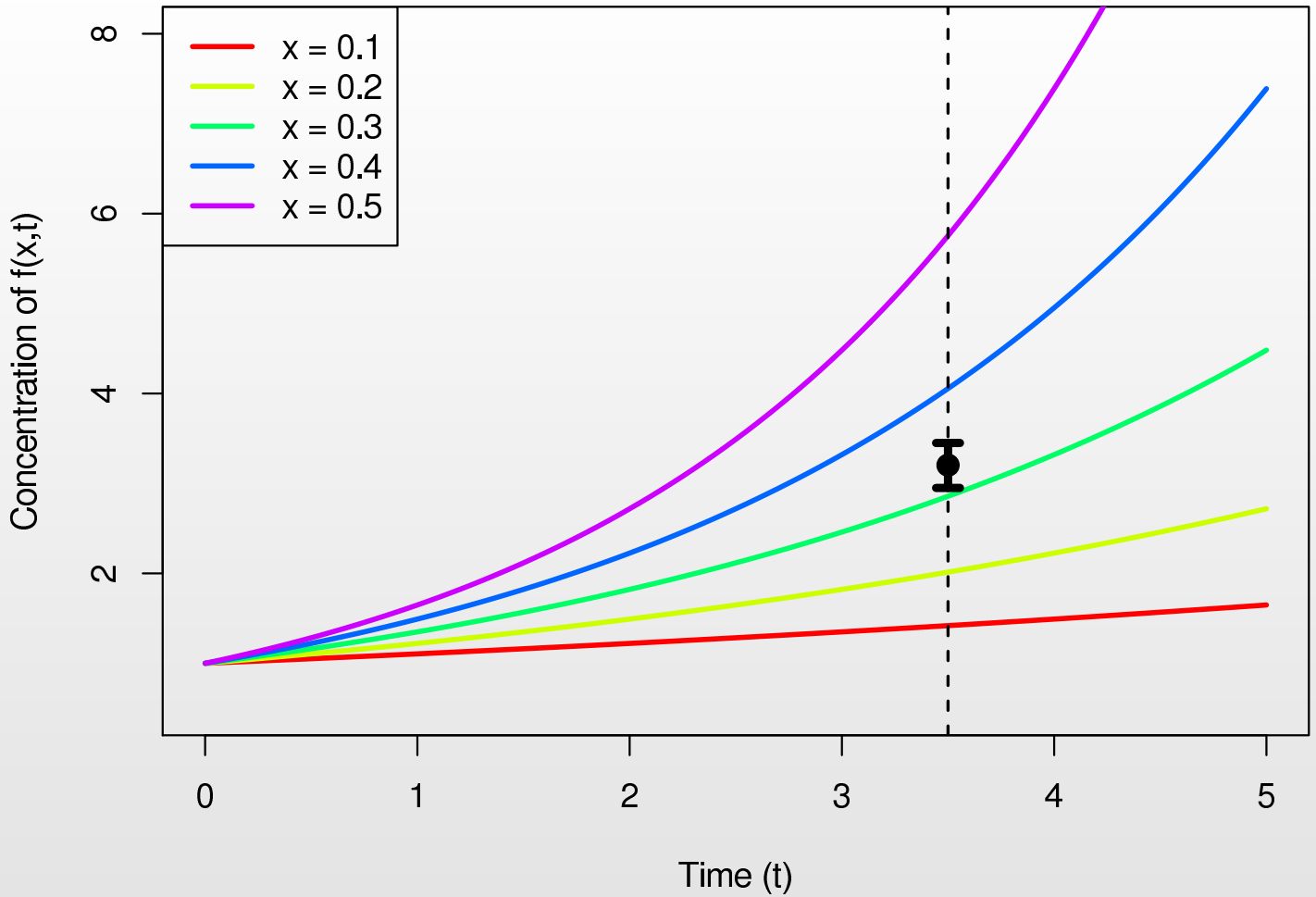

- Five model runs with the input parameter varying from $x = 0.1$ to $x = 0.5$
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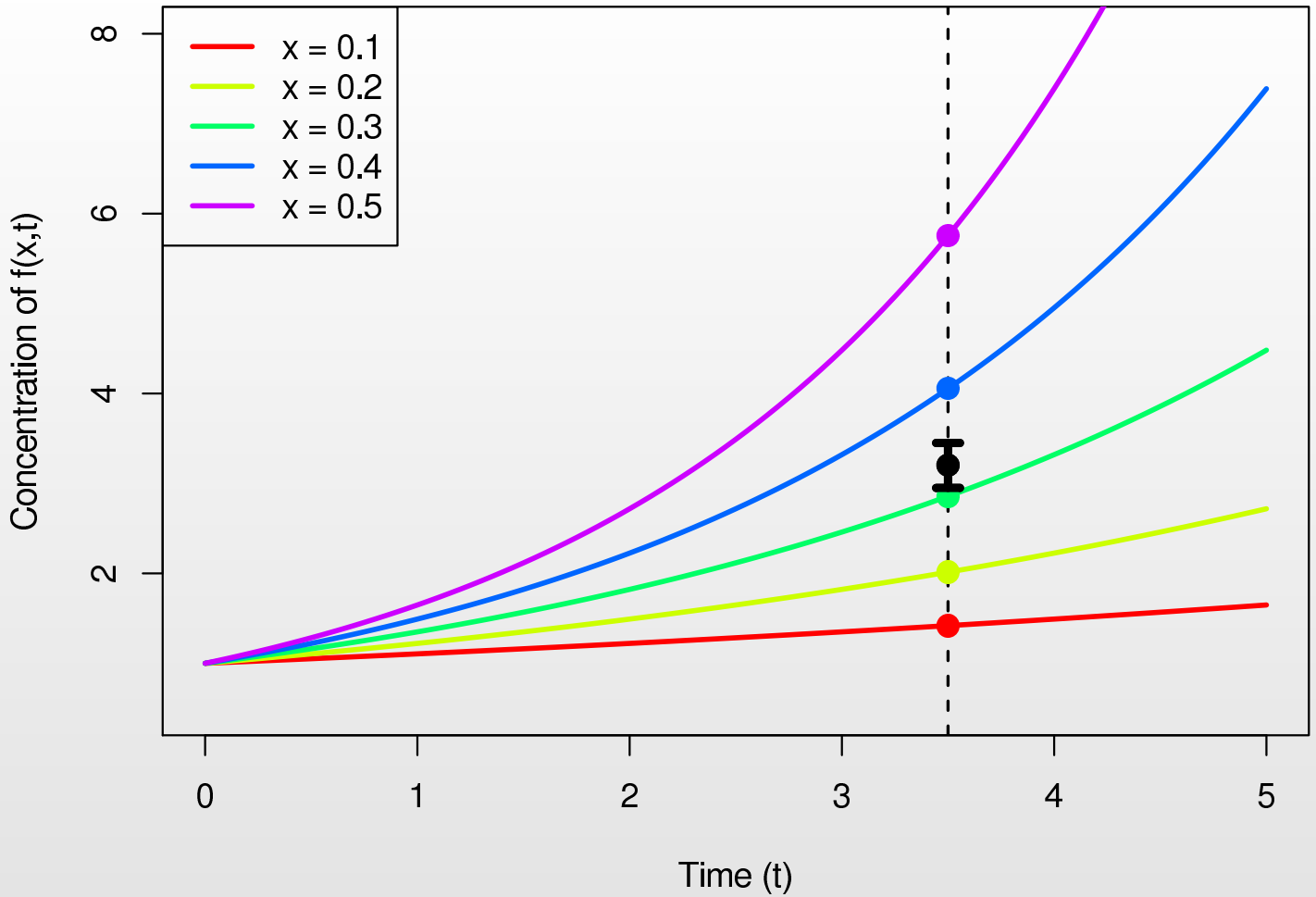
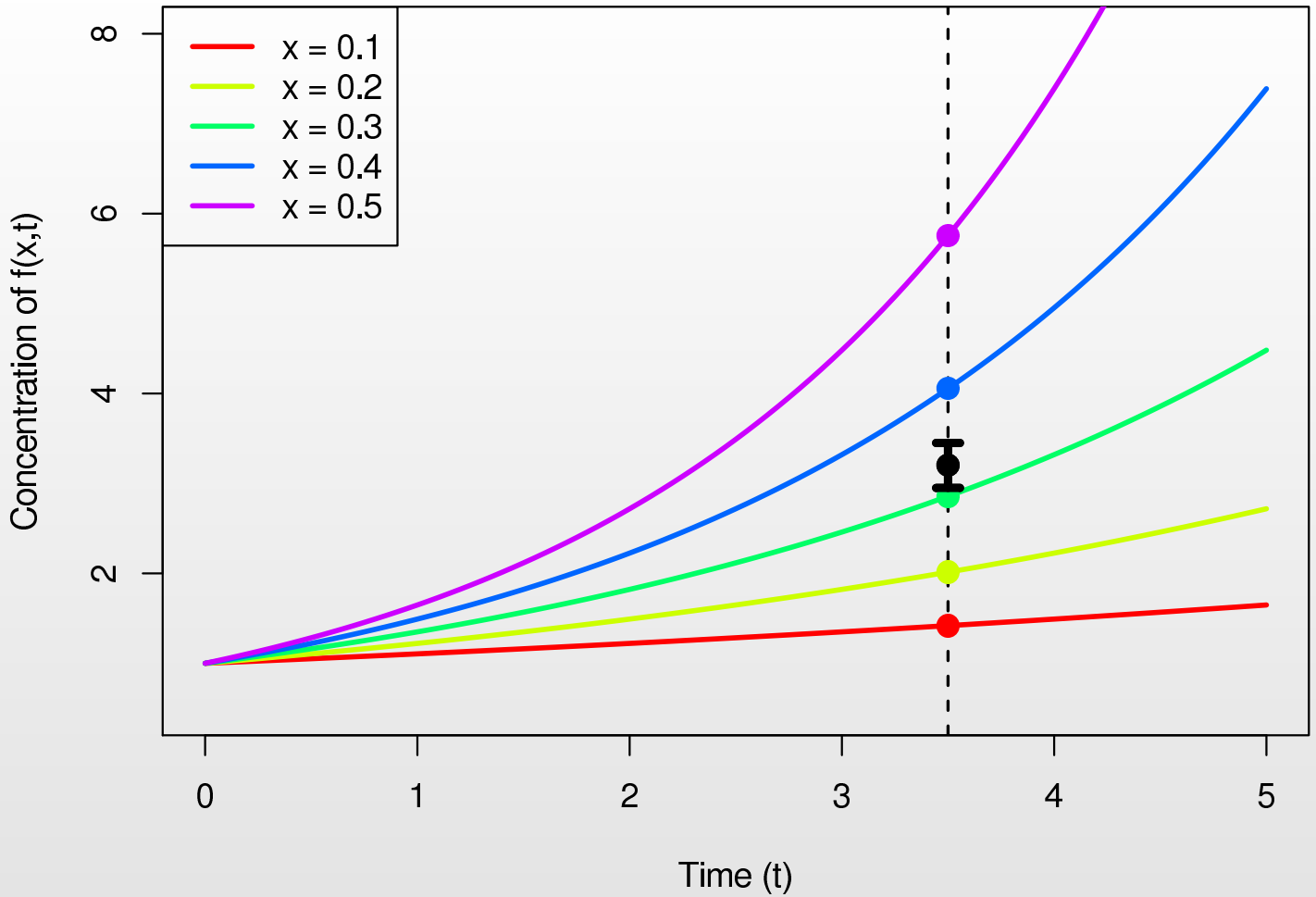
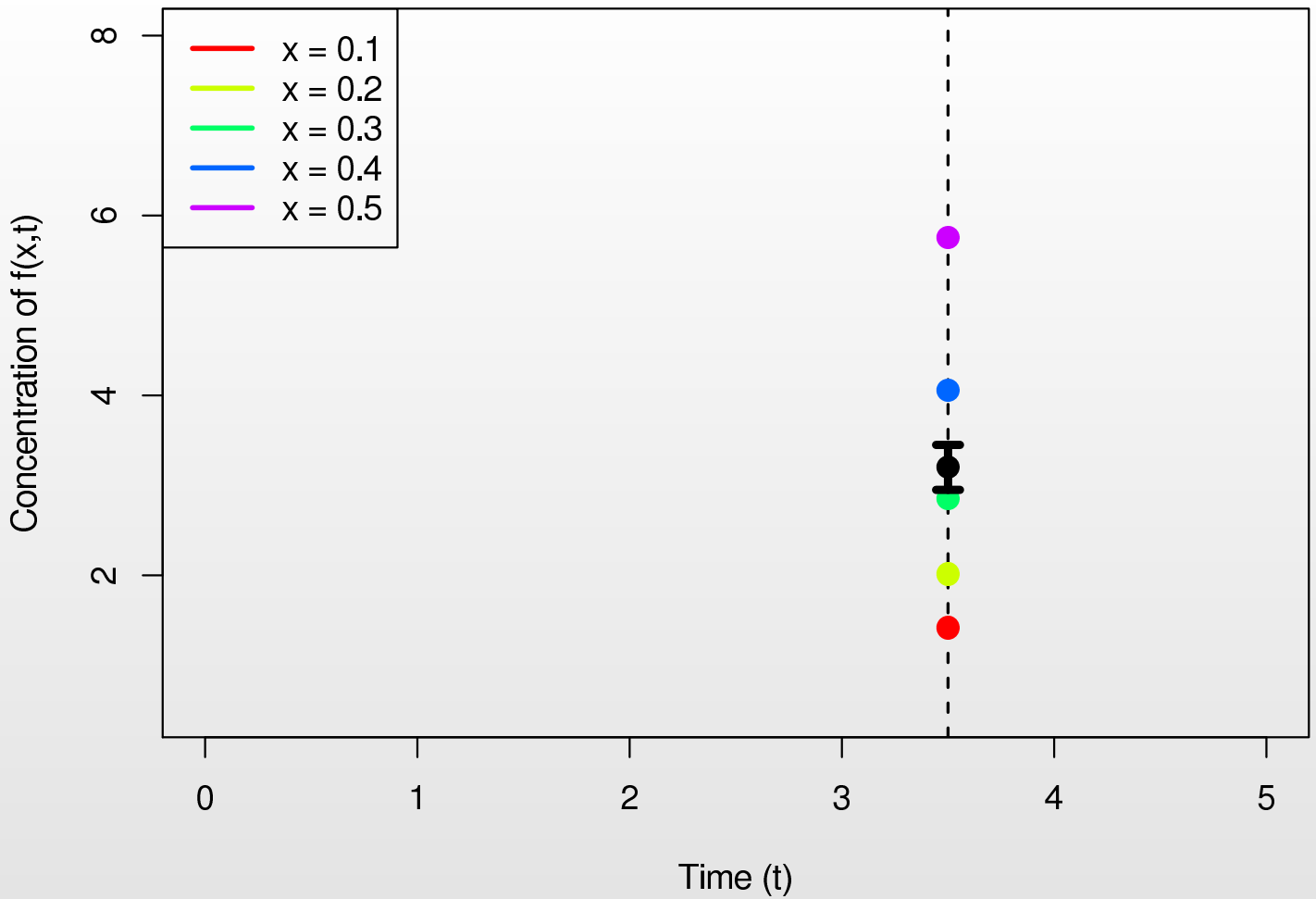


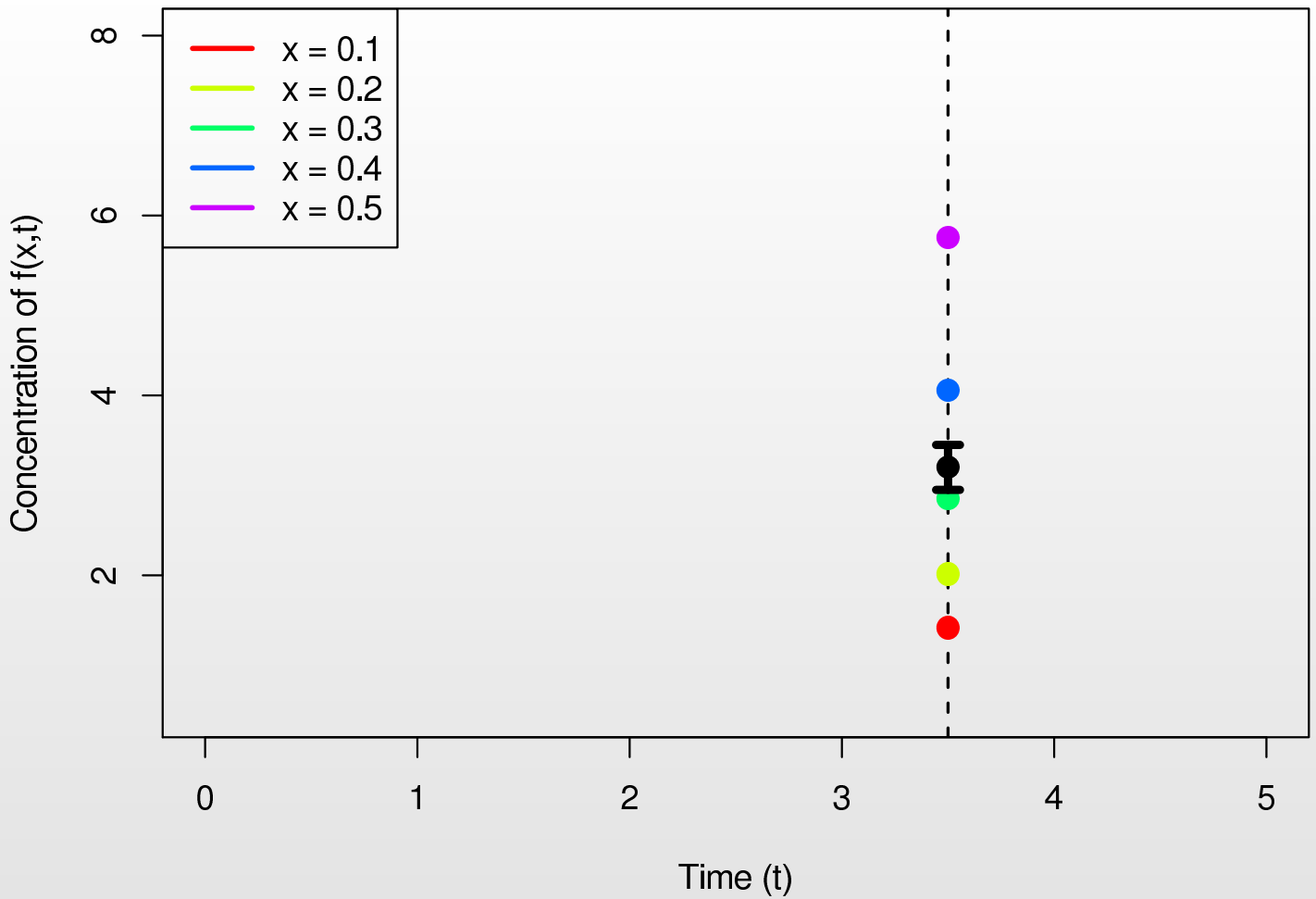
- Major question: which values of x ensure the output $f(x, t = 3.5)$ is consistent with the observations?



- Major question: which values of x ensure the output $f(x, t = 3.5)$ is consistent with the observations?
- It would seem that x has to be at least between 0.3 and 0.4.



- To answer this, we can now discard other values of $f(x,t)$ and think of $f(x, t = 3.5)$ as a function of x only.



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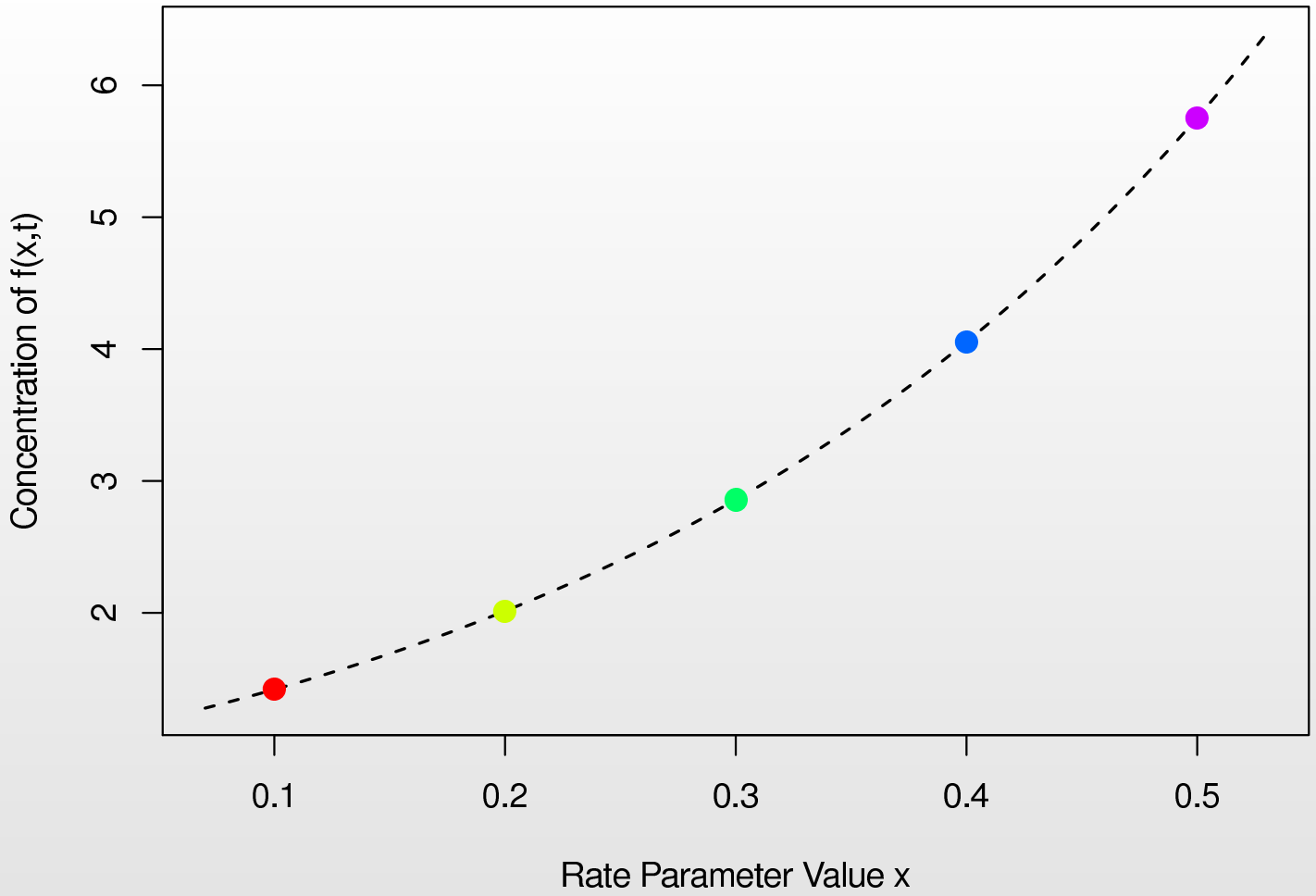
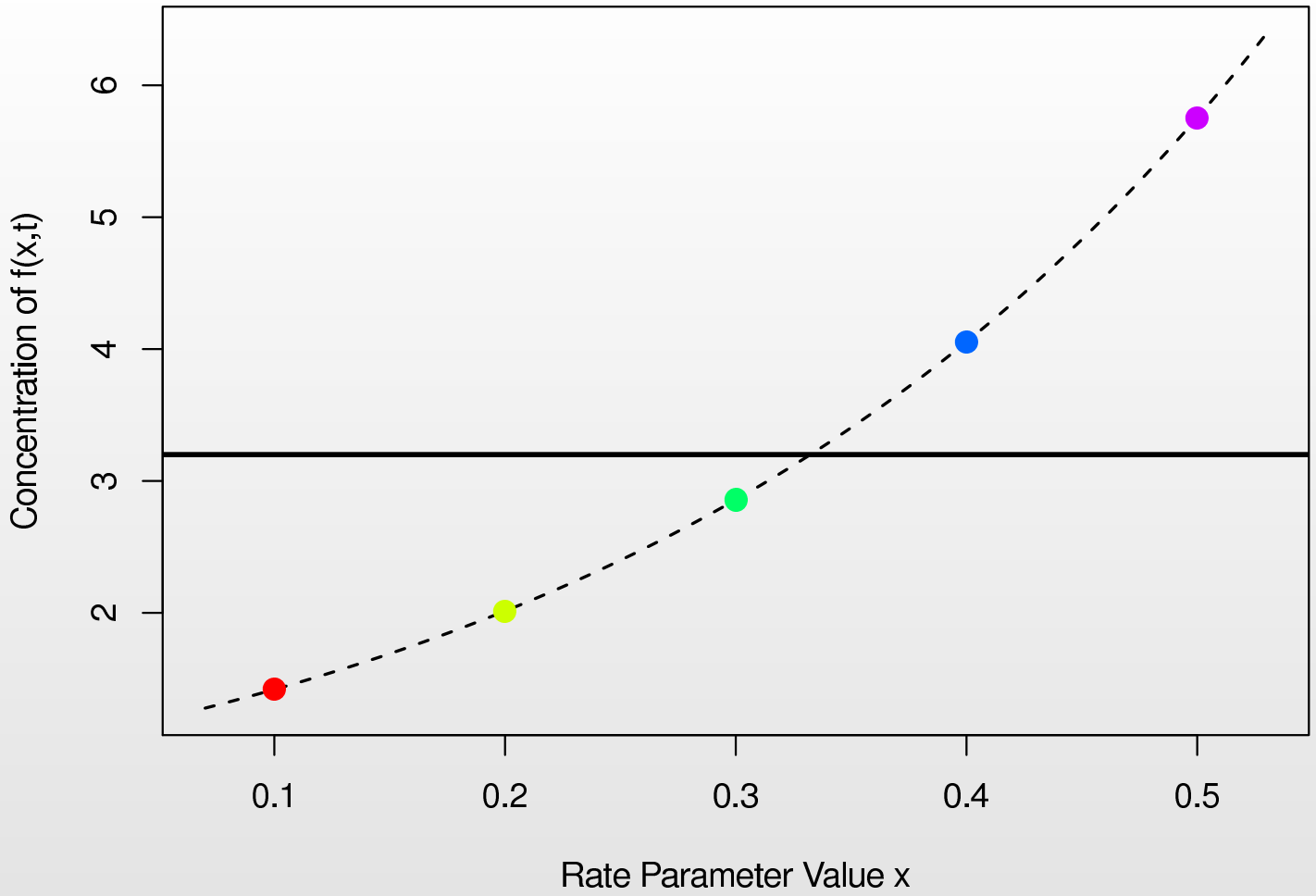
- That is take $f(x) \equiv f(x, t = 3.5)$



- We can now plot the concentration $f(x)$ as a function of the input parameter x.



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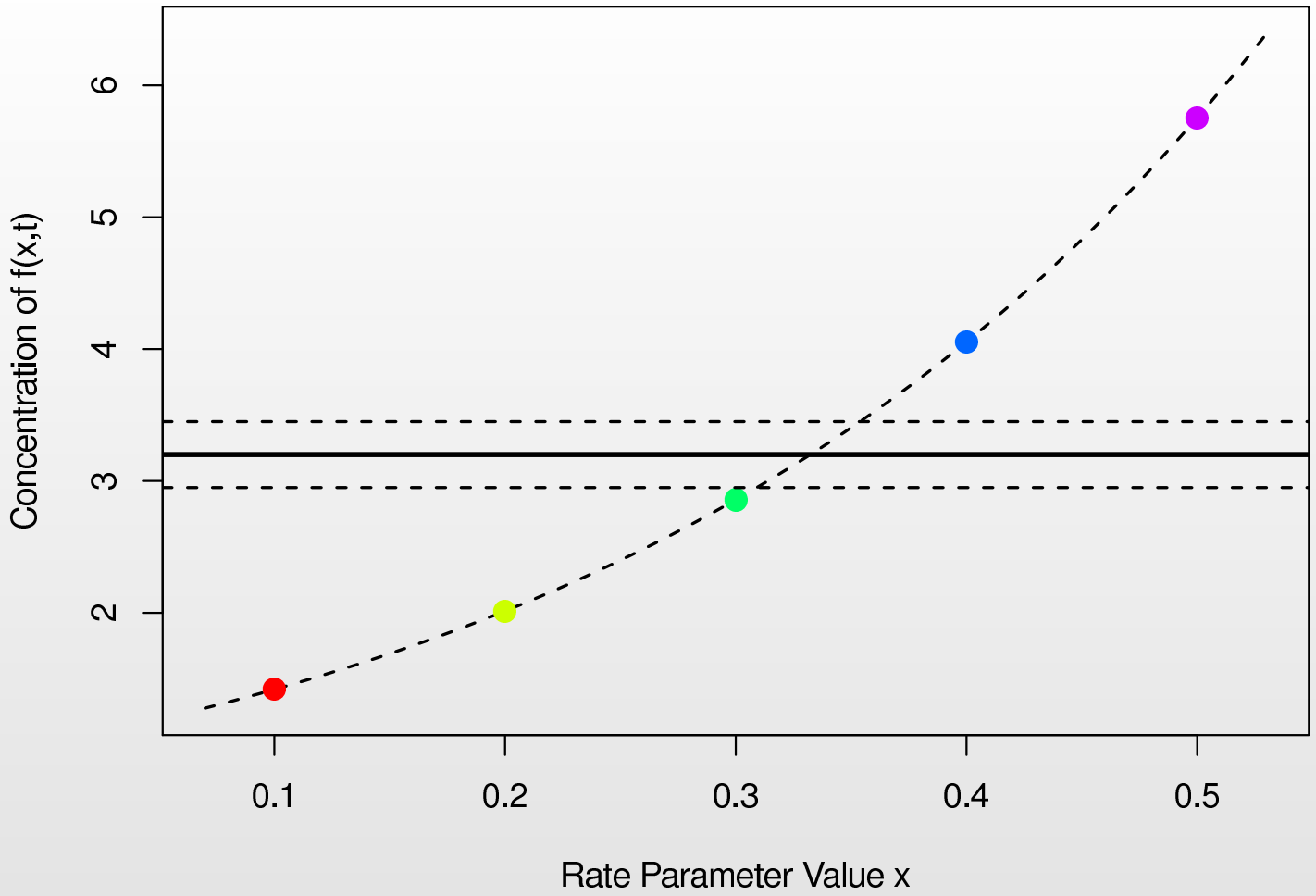
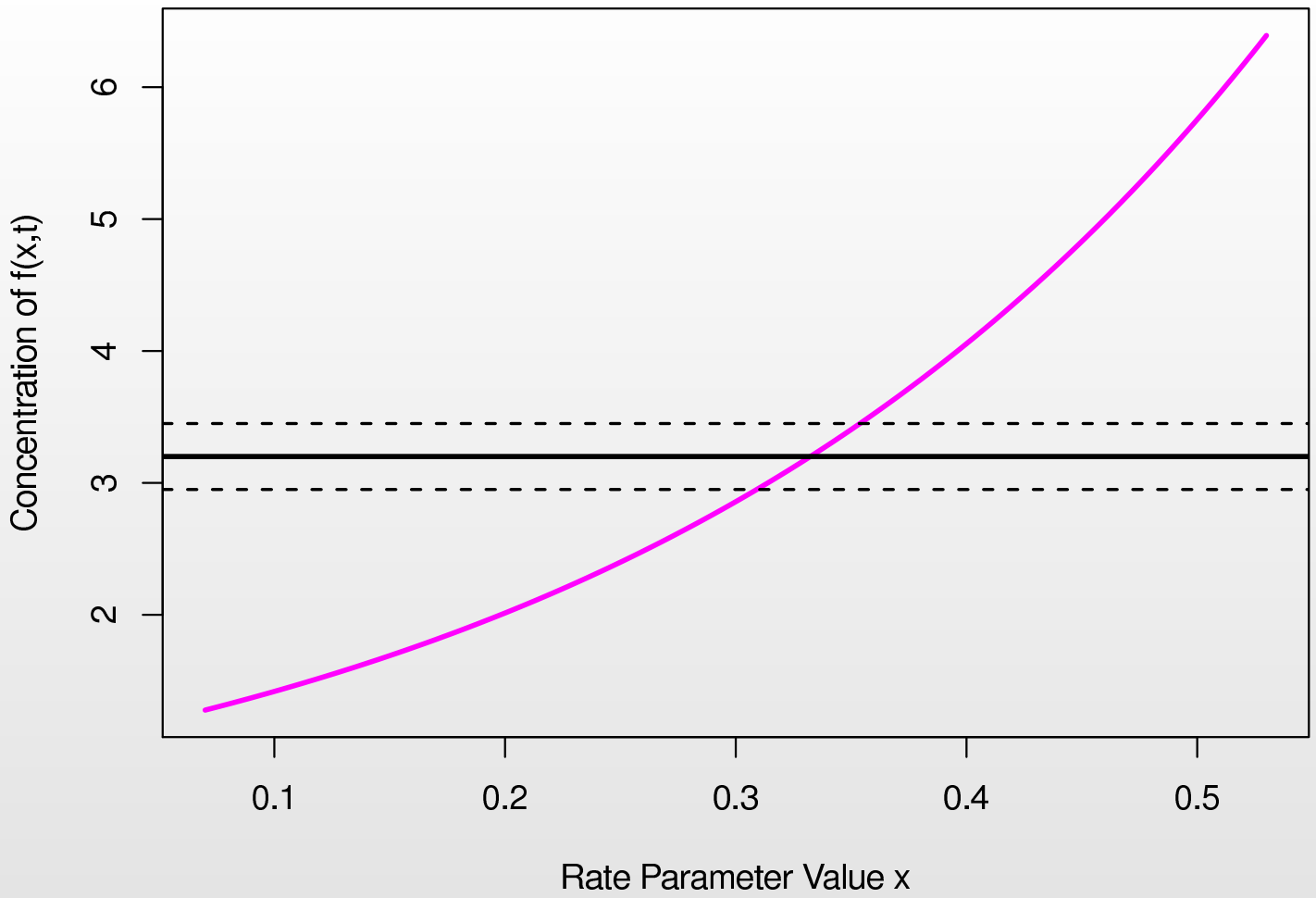
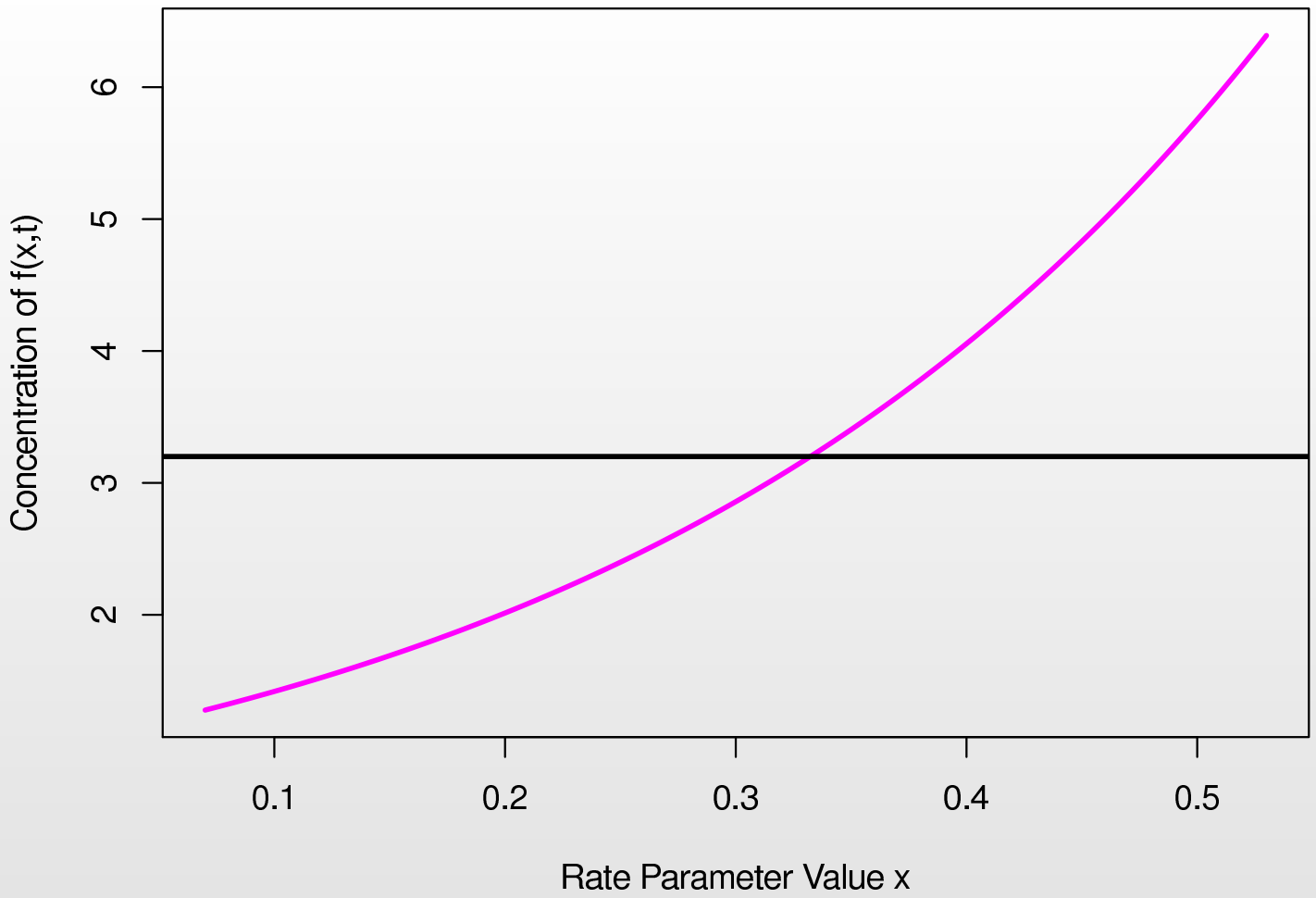


- We can now plot the concentration $f(x)$ as a function of the input parameter x.
- Black horizontal line: the observed measurement of f
- Dashed horizontal lines: the measurement errors



- If we know the analytical expression for $f(x) = \exp(3.5x)$, then we can identify the values of x of interest.



- If we know the analytical expression for $f(x) = \exp(3.5x)$, then we can identify the values of x of interest.
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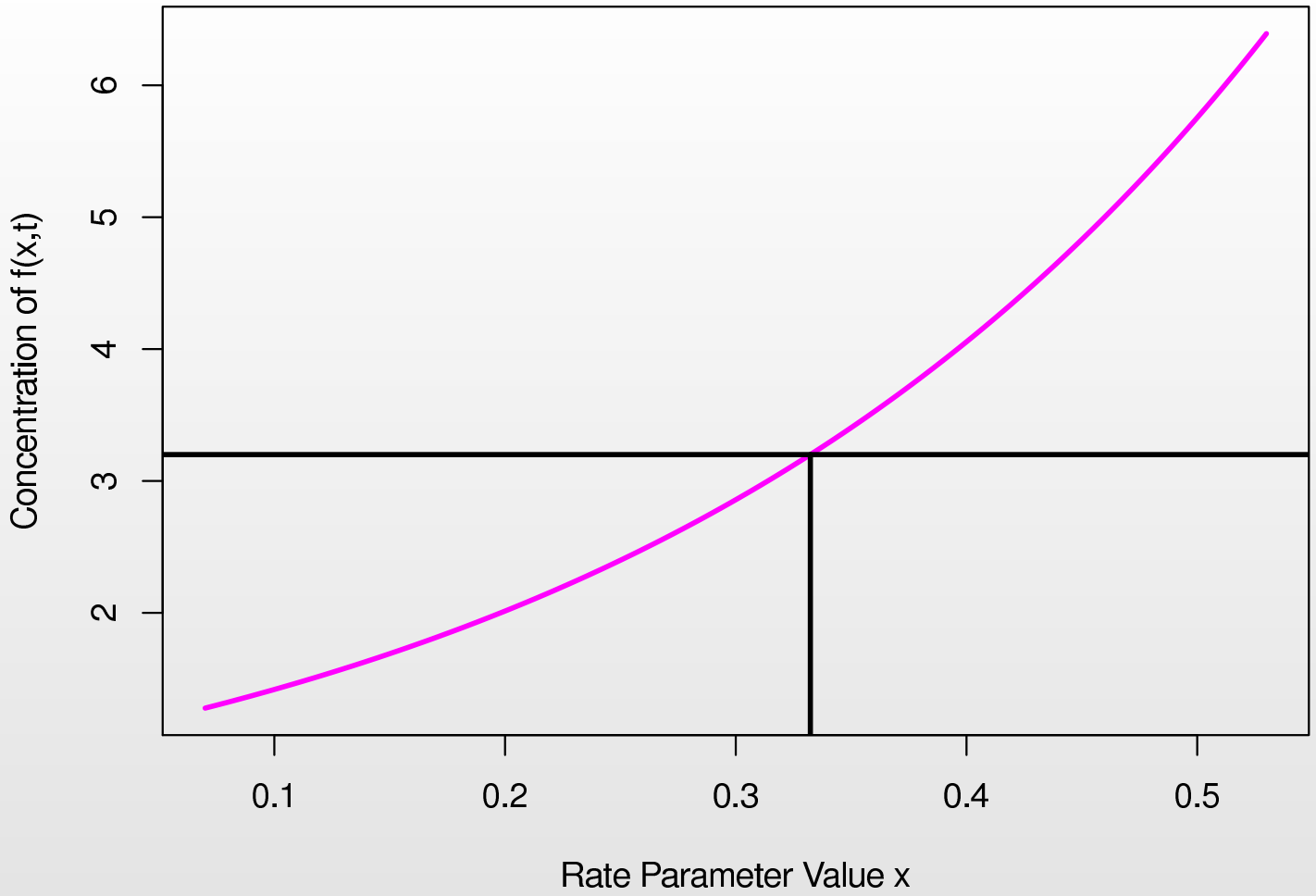

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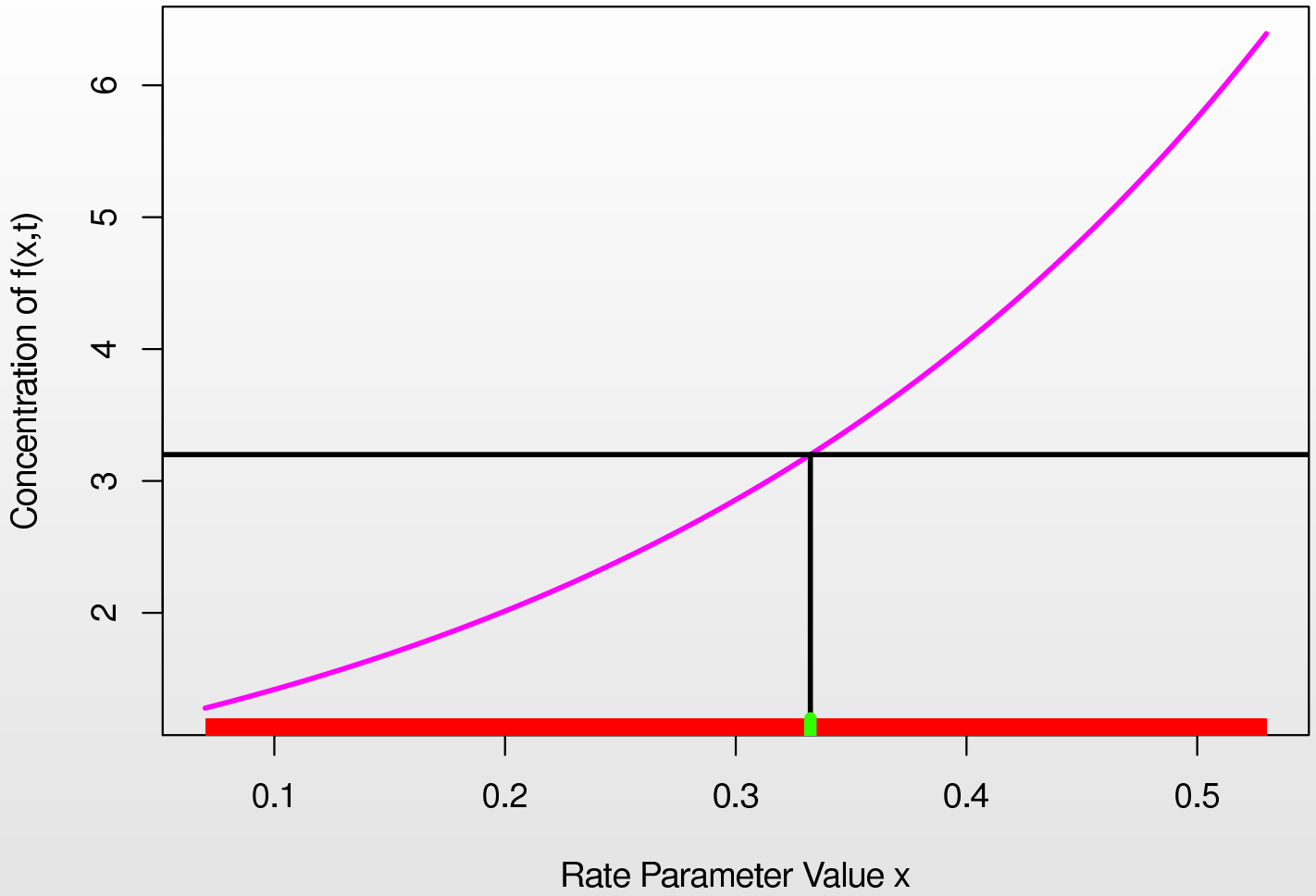

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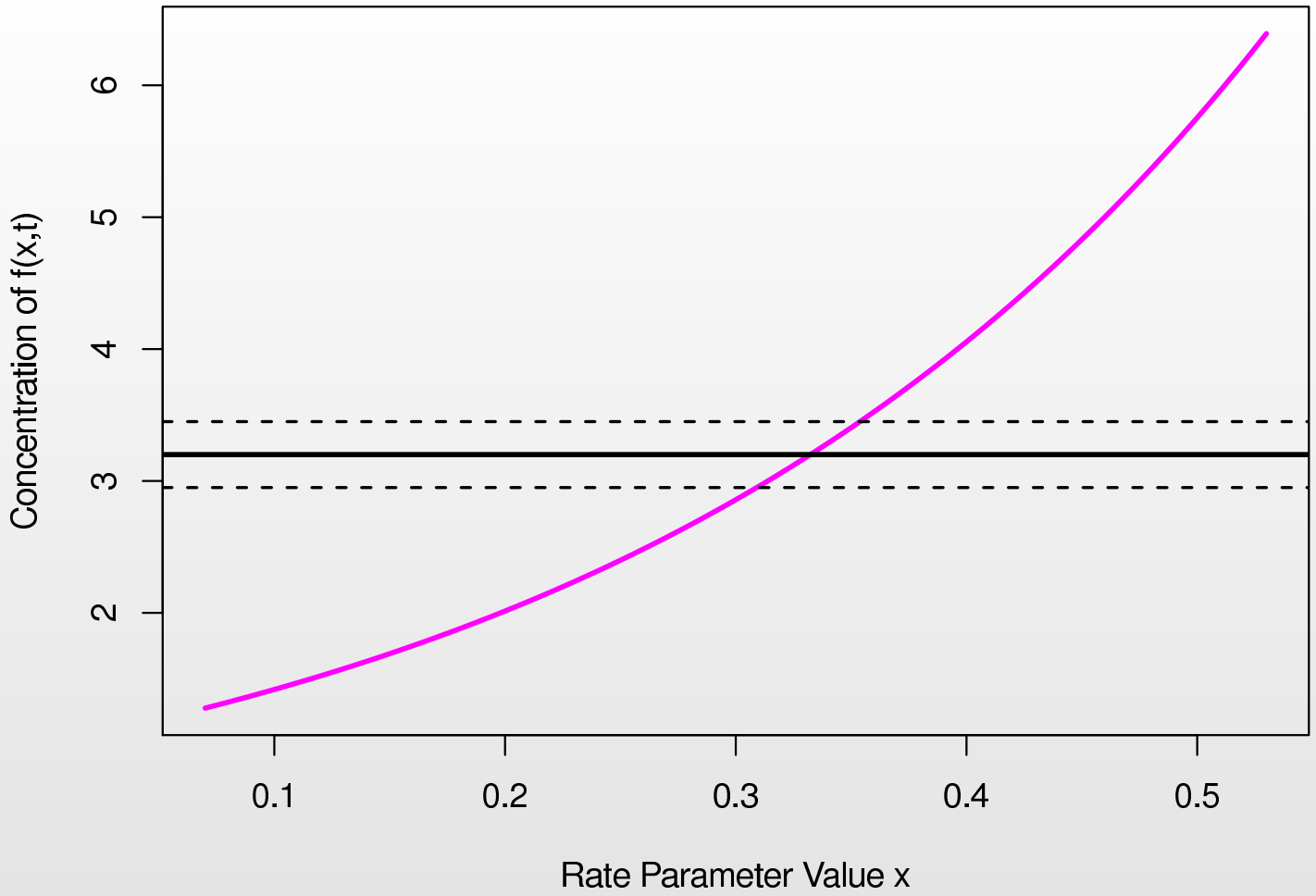
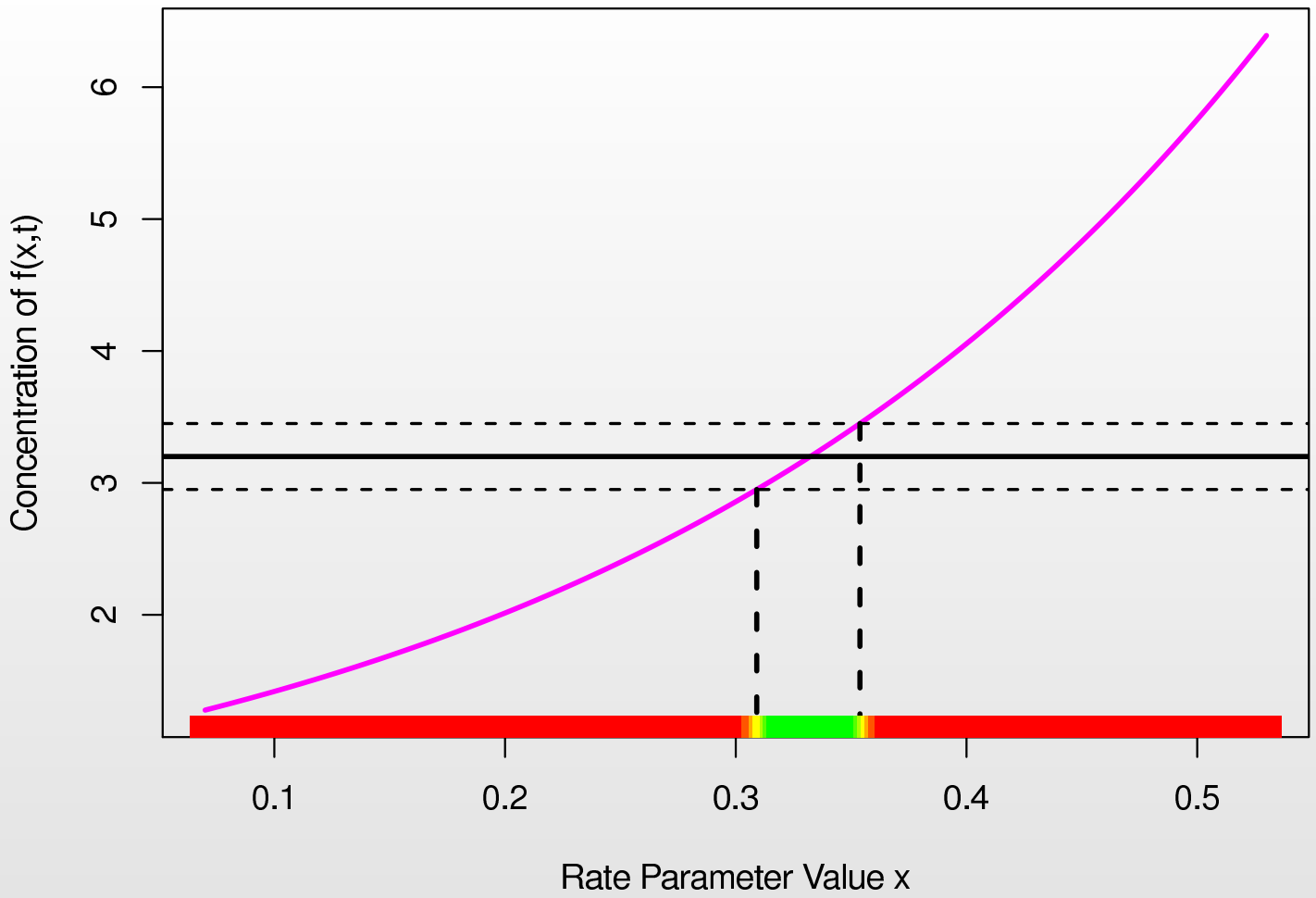
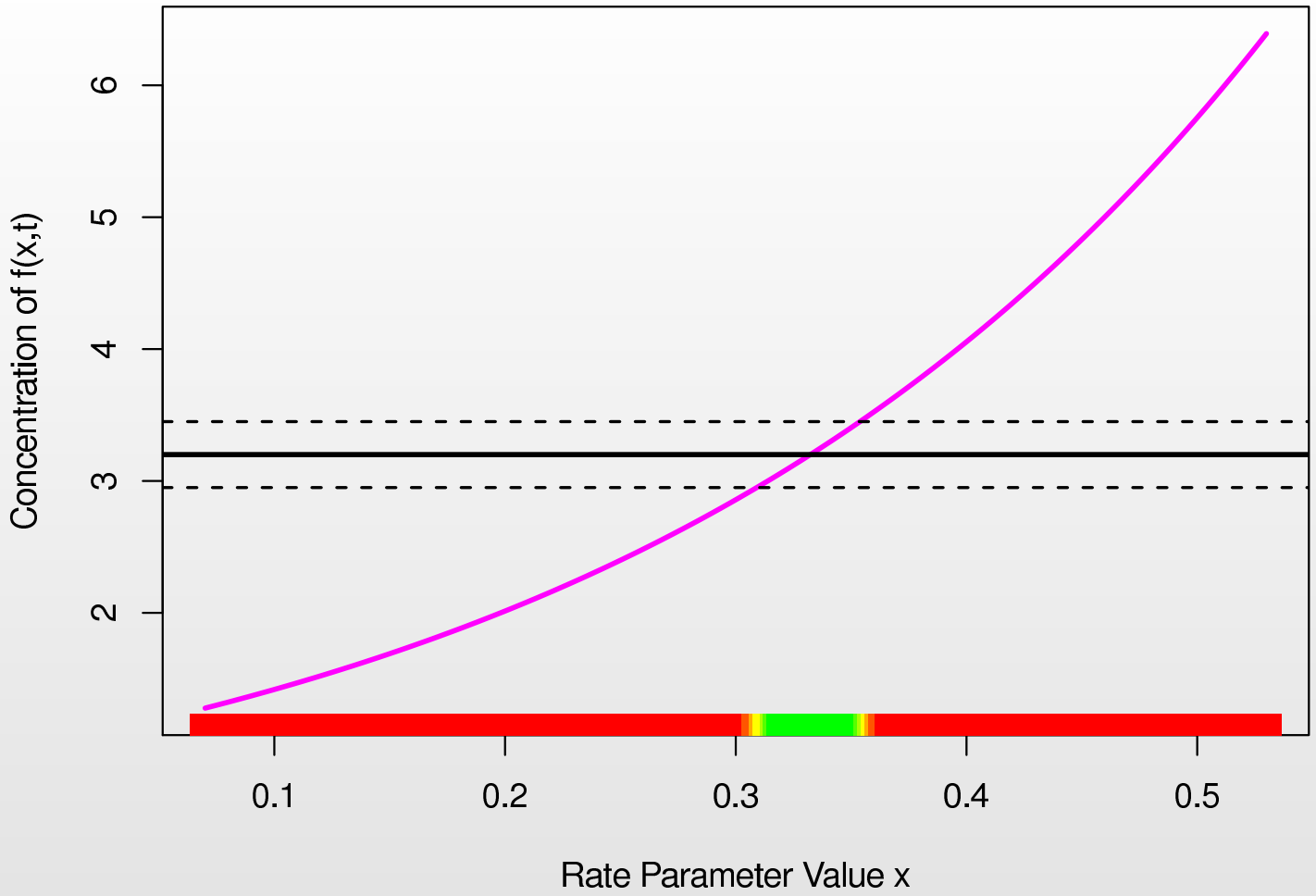


- Uncertainty in the measurement of $f(x, t = 3.5)$ leads to uncertainty in the inferred values of x.



- Uncertainty in the measurement of $f(x, t = 3.5)$ leads to uncertainty in the inferred values of x.
- Hence we see a range (green/yellow) of possible values of x consistent with the measurements, with all the implausible values of x in red.



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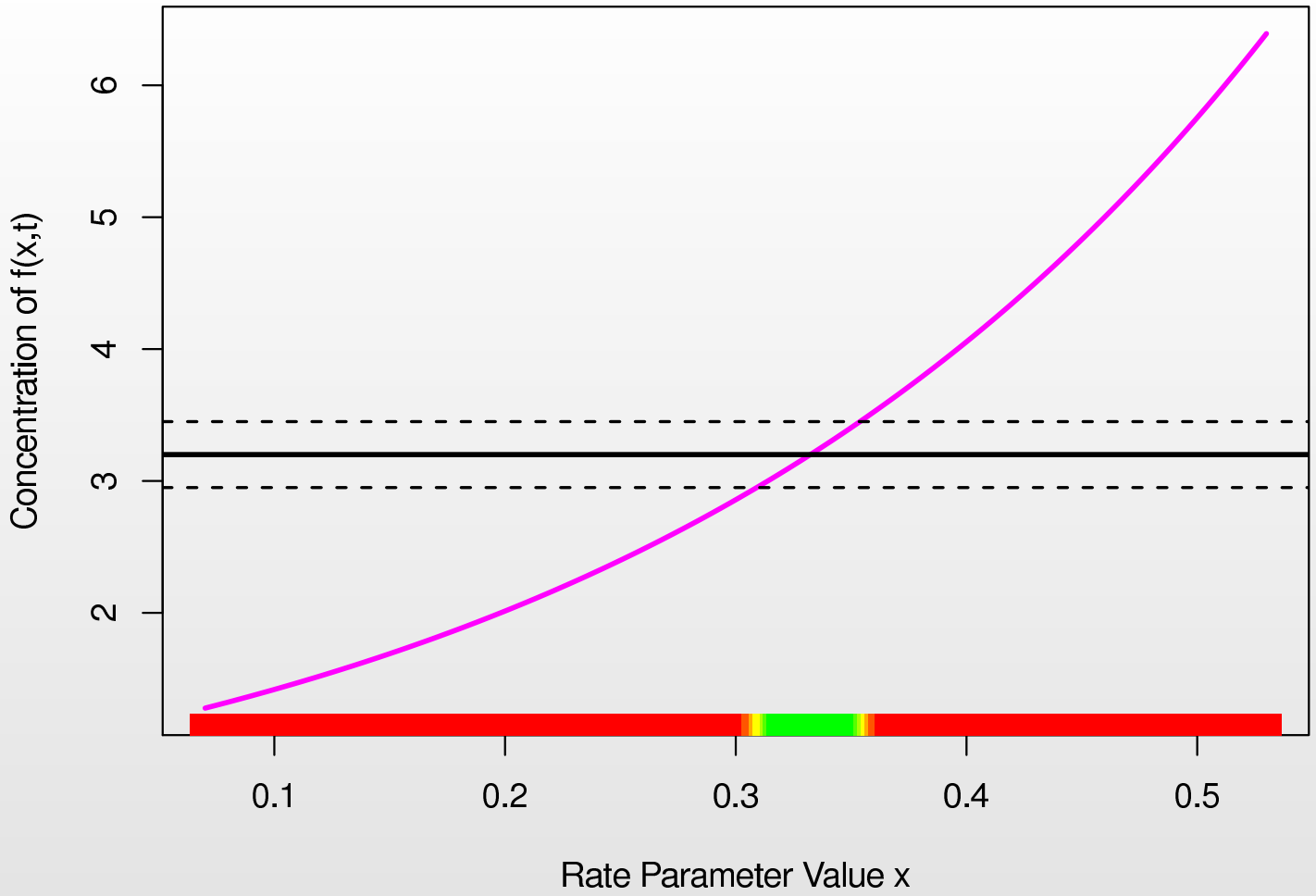

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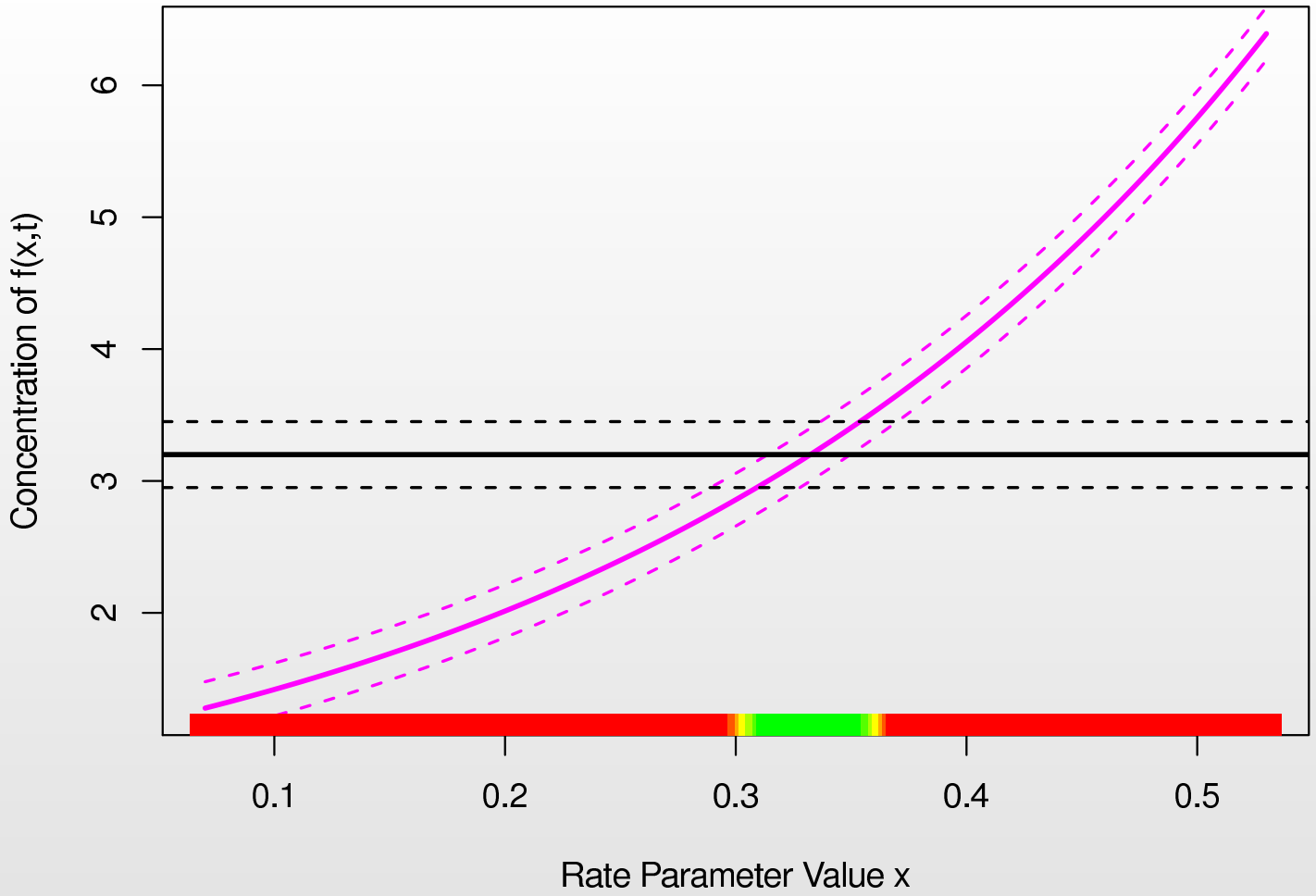
- This uncertainty arises from many issues e.g. is the form of the model (the differential equation) appropriate, is the model a simplified description of a more complex system, is there uncertainty in the initial conditions etc?



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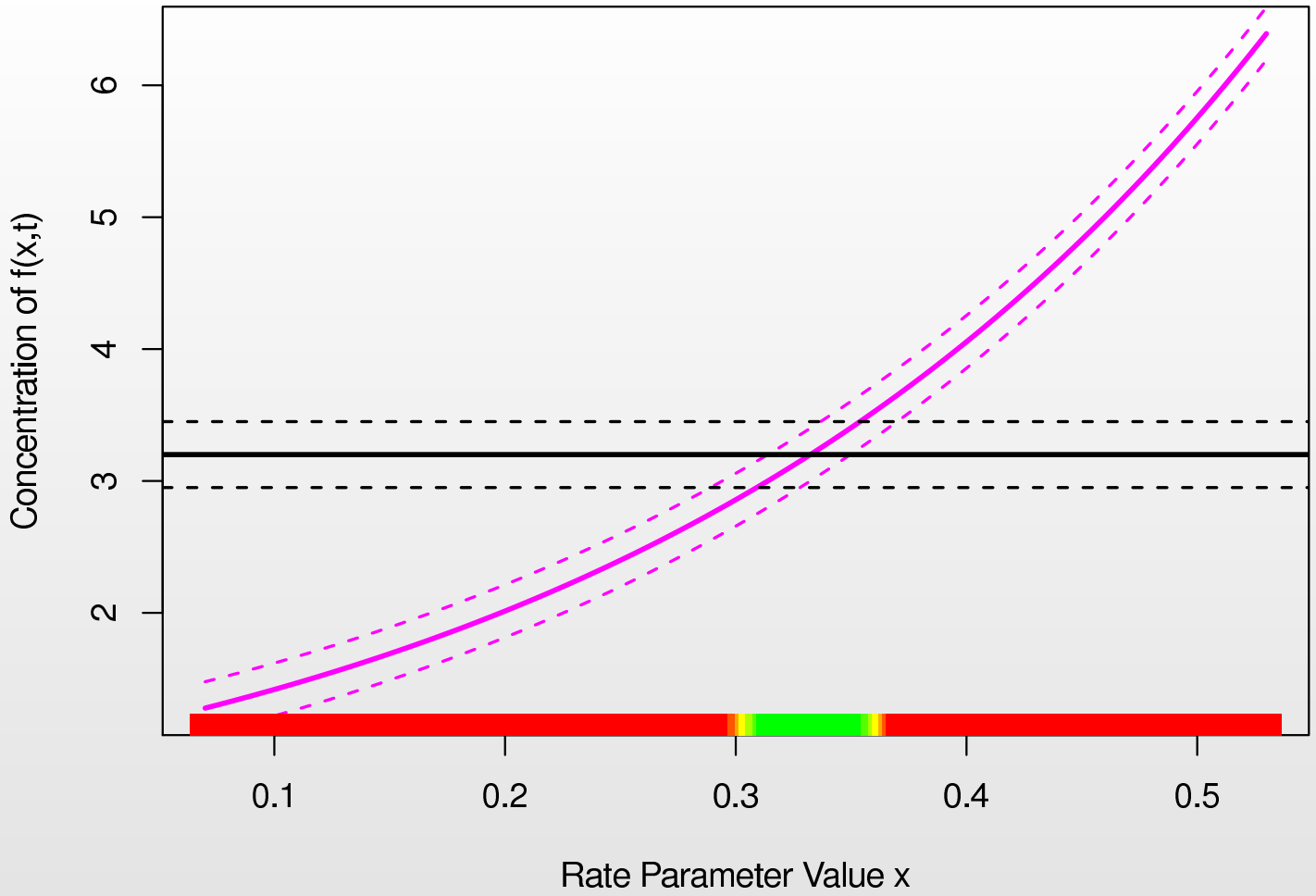

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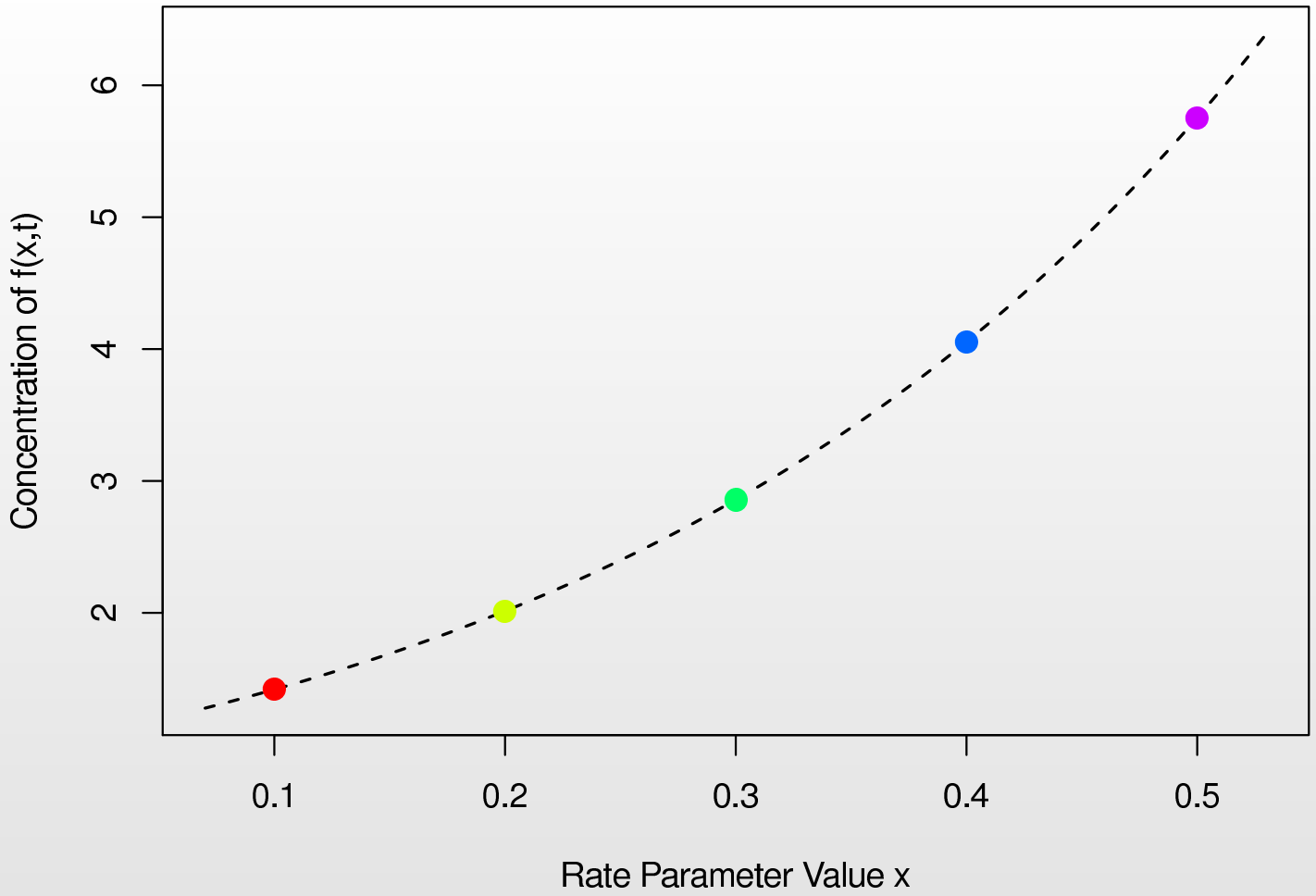
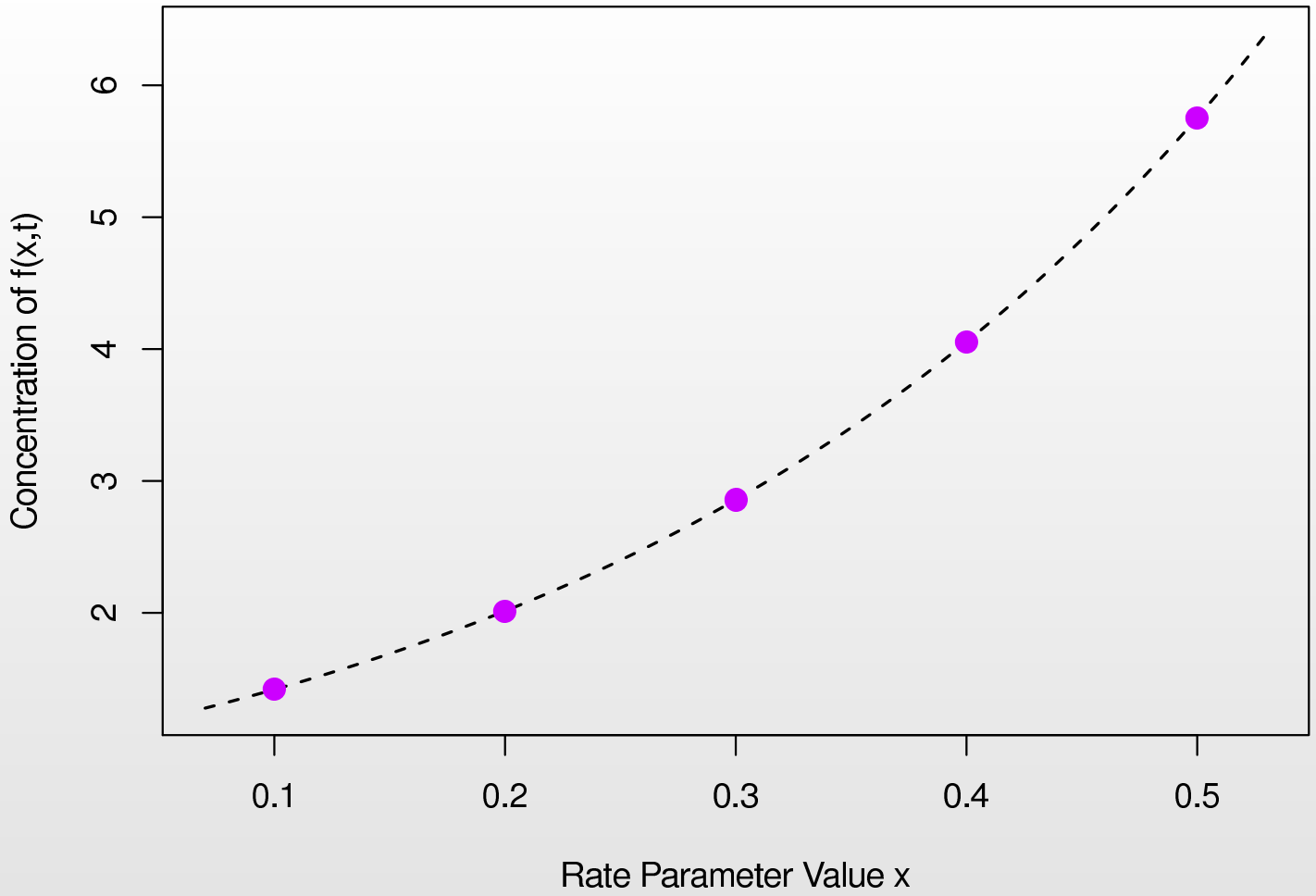
- This results in more uncertainty in x, and hence a larger range of x values.



- Consider the graph of $f(x)$: in general we do not have the analytic solution of $f(x)$, here given by the dashed line.



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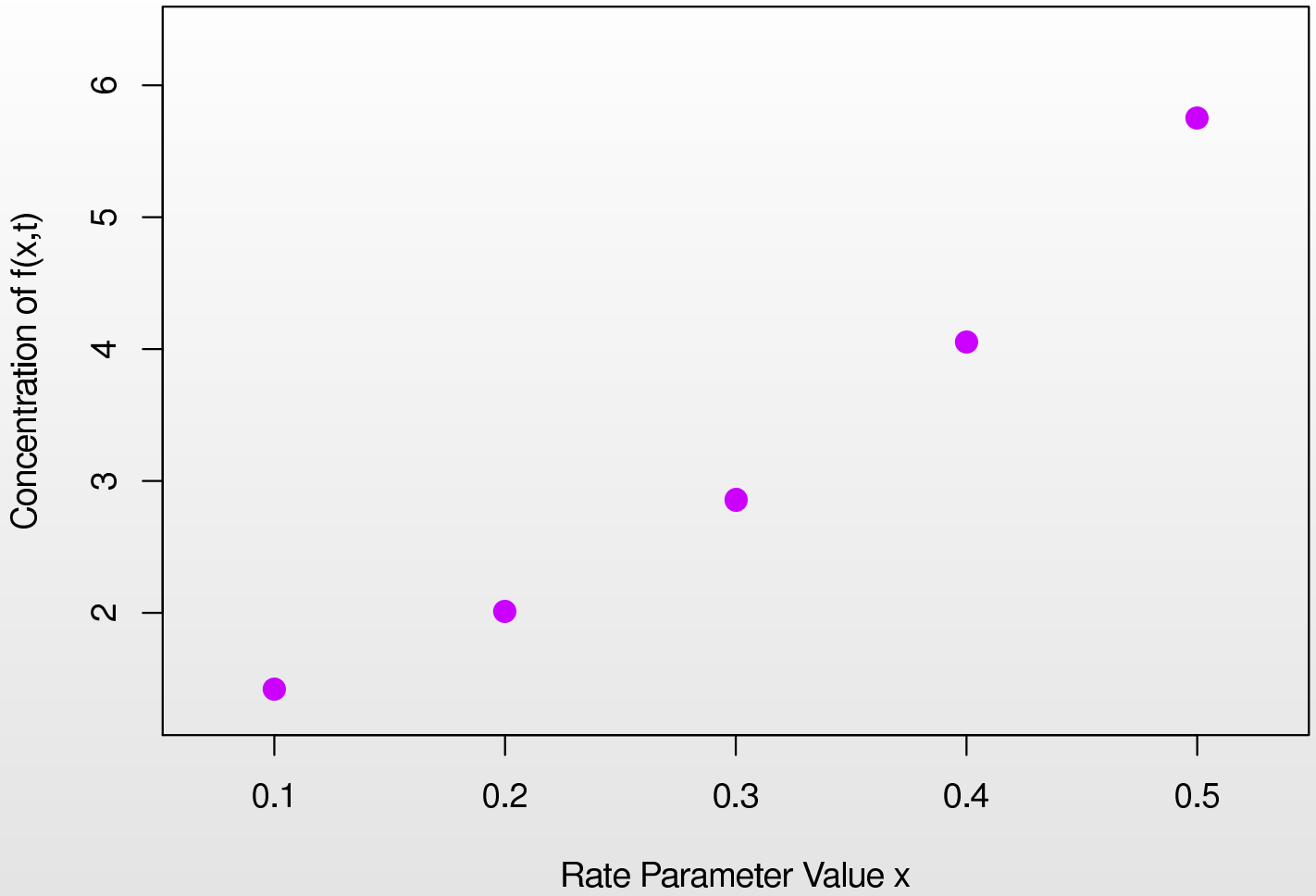

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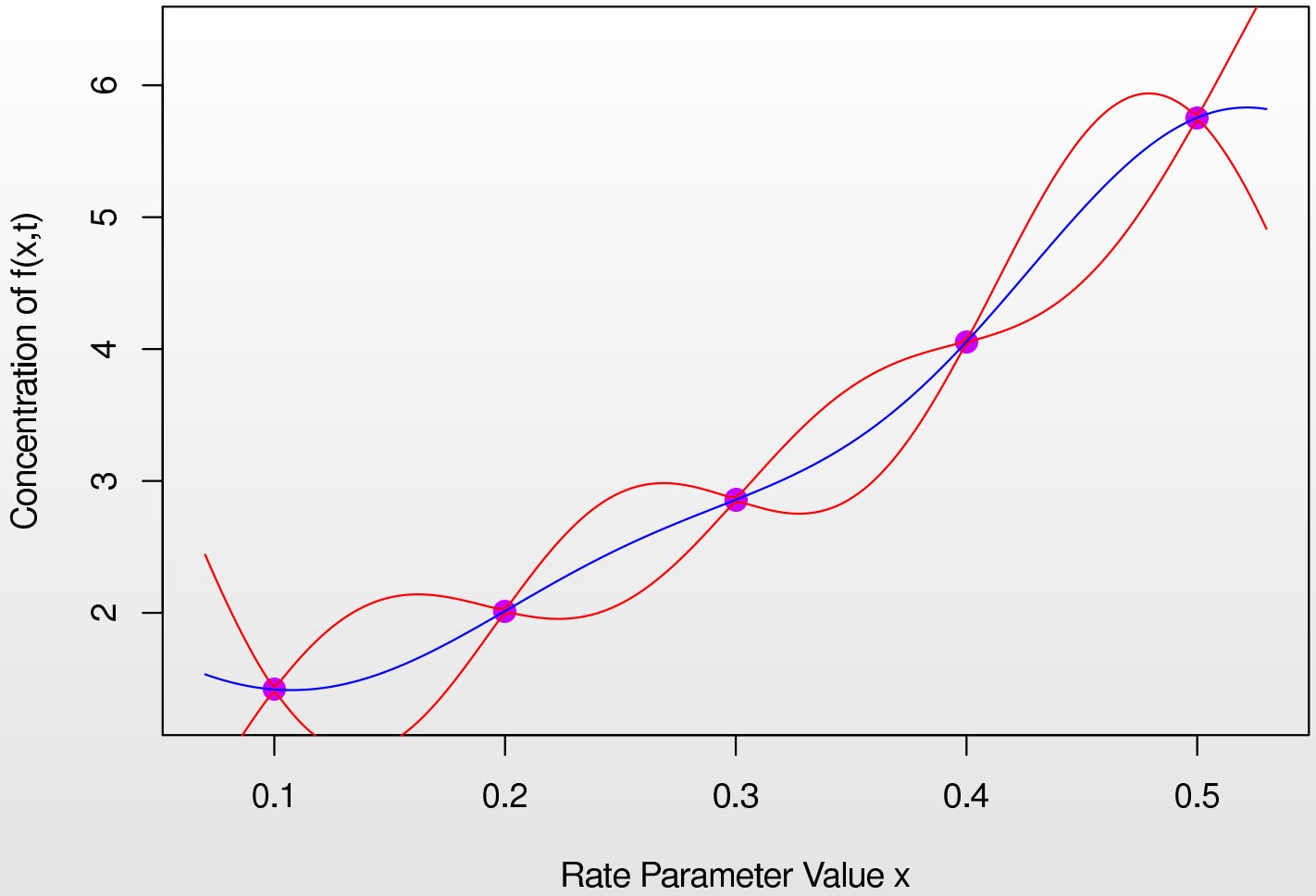
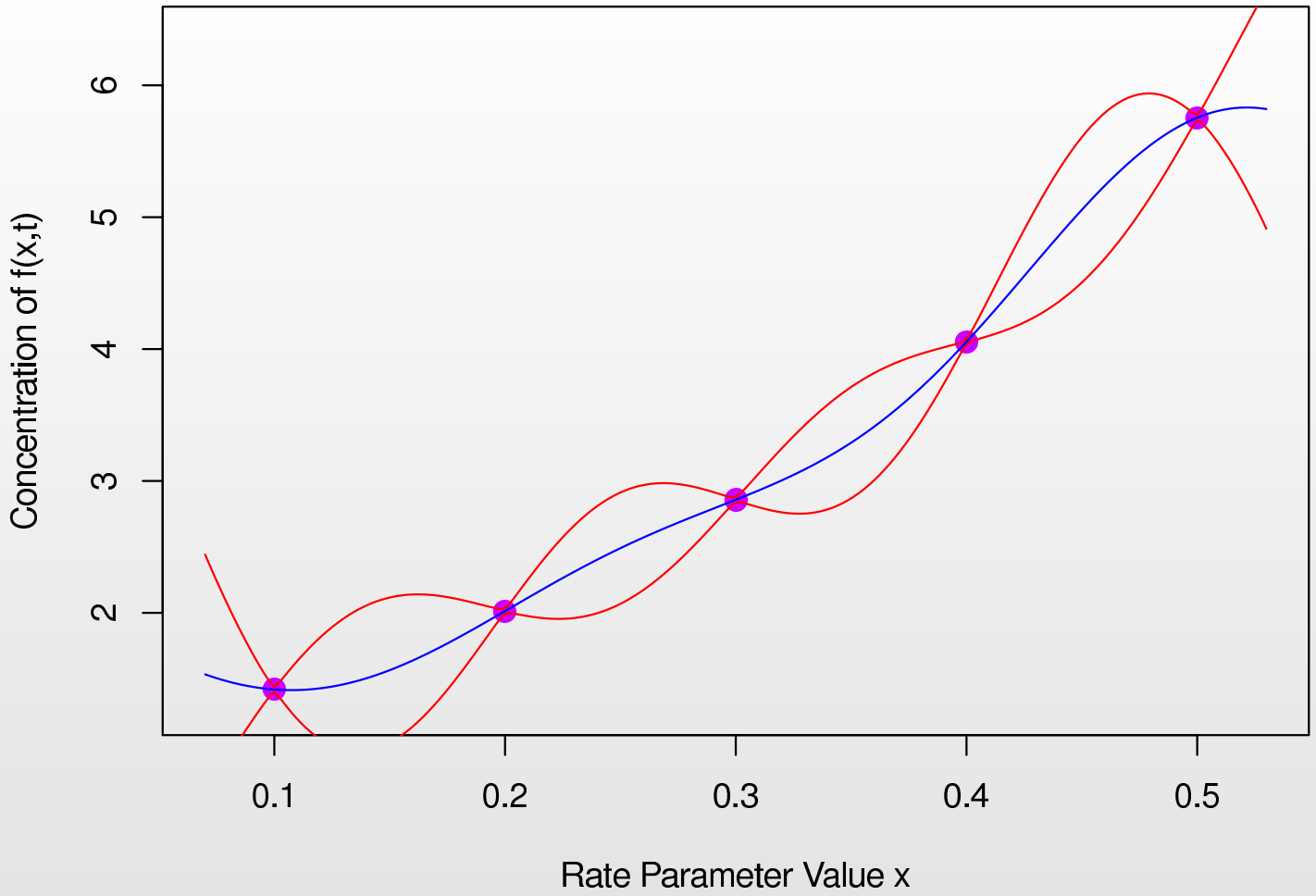
- Instead we only have a finite number of runs of the model, in this case five.



- The emulator can be used to represent our beliefs about the behaviour of the model at untested values of x, and is fast to evaluate.



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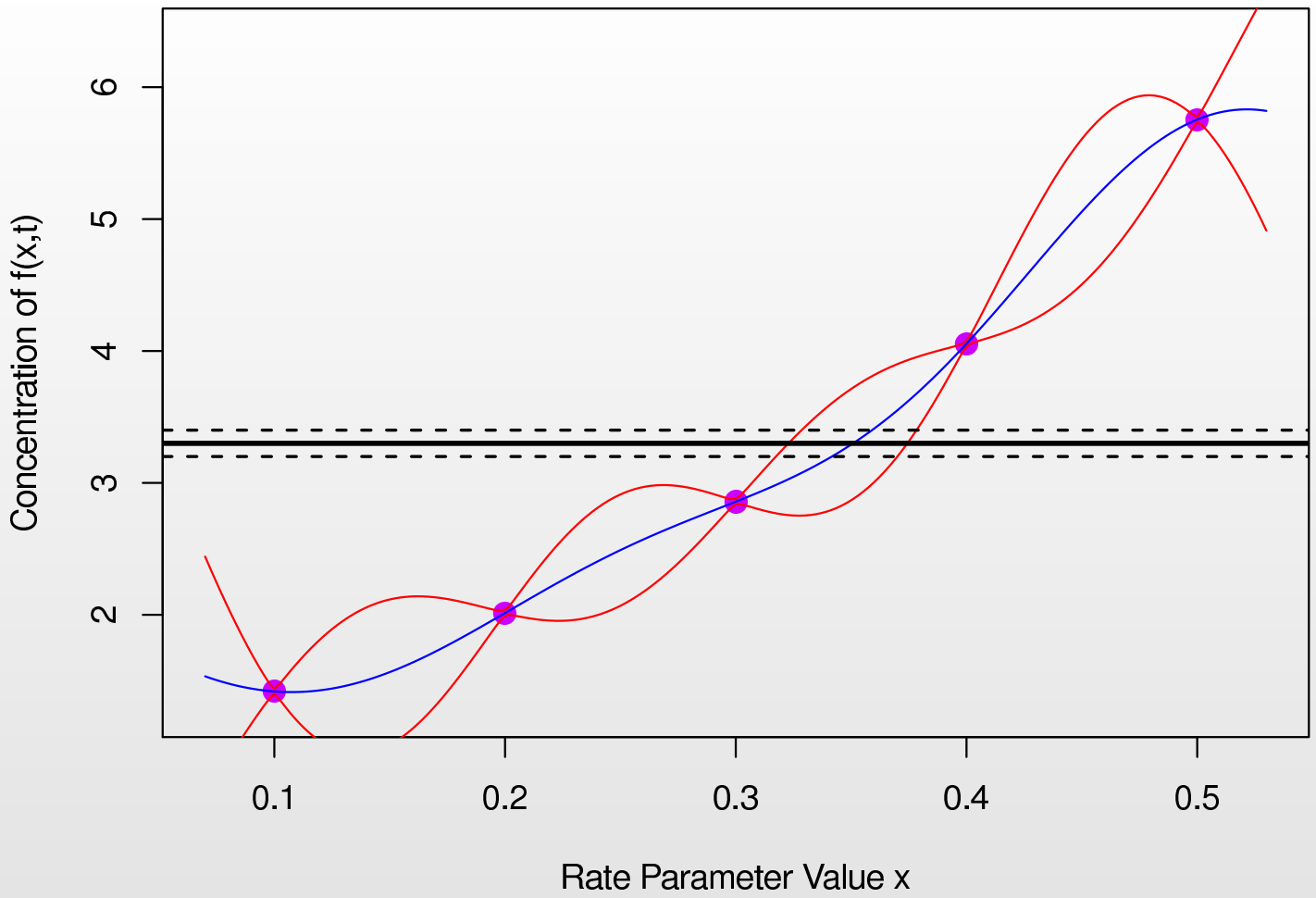

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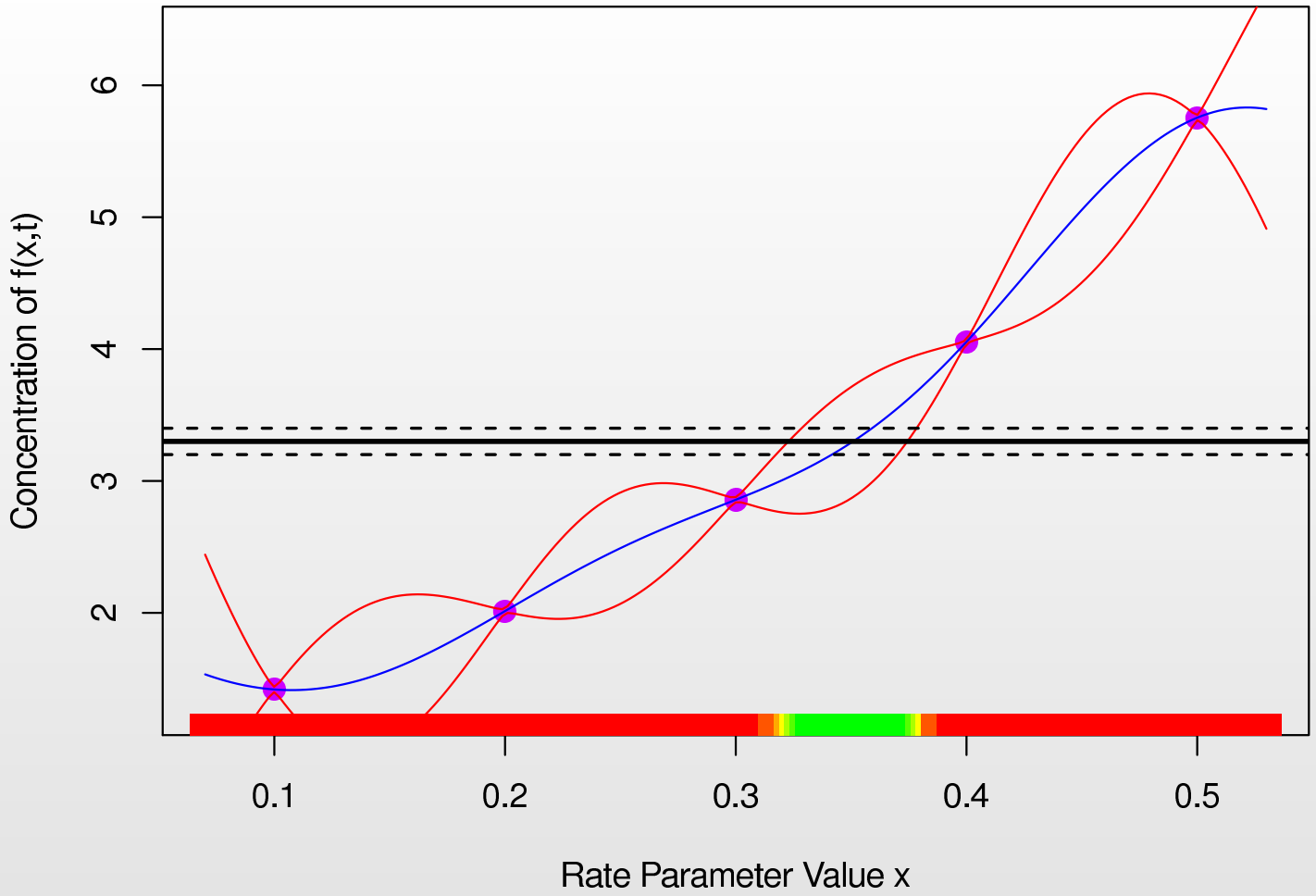

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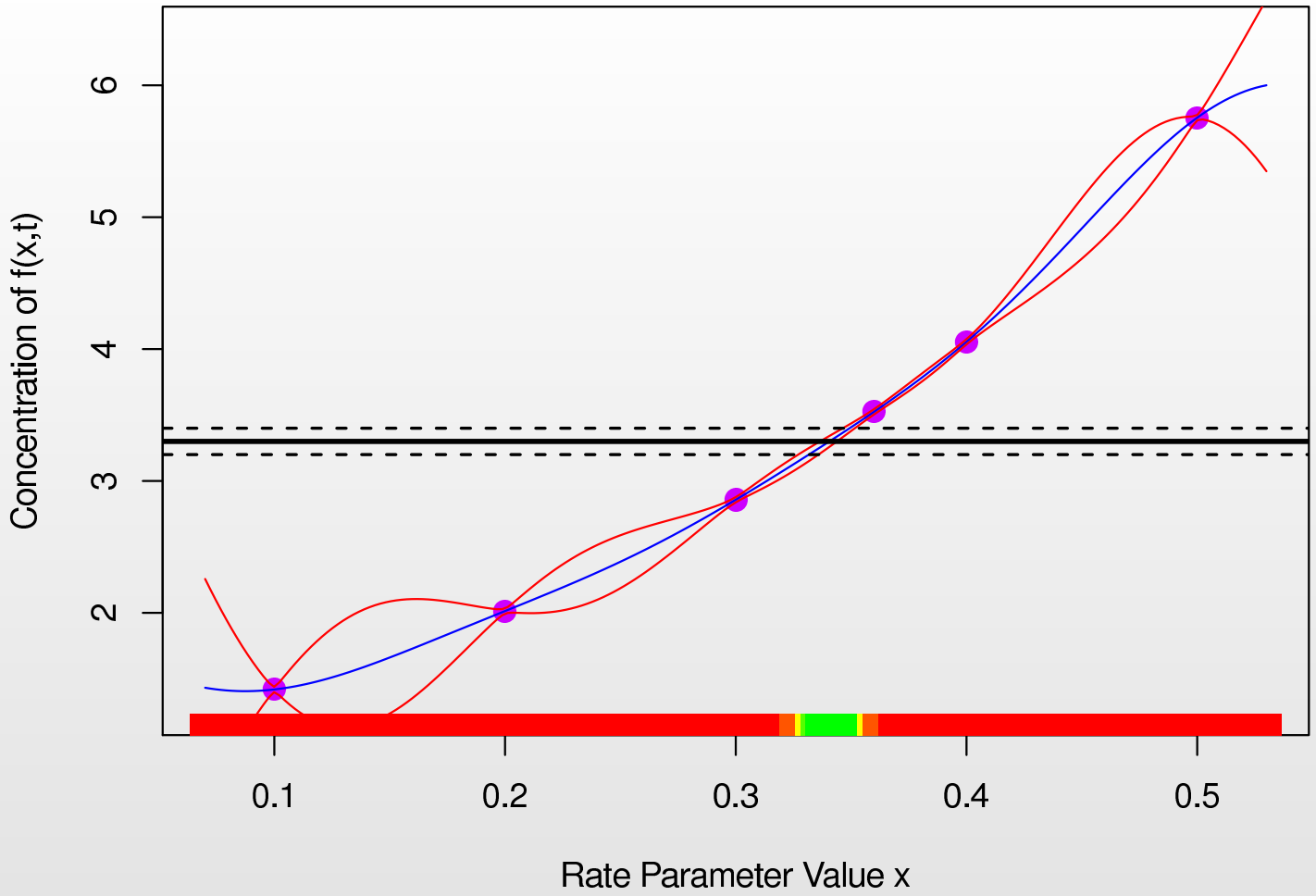
- Note the uncertainty on x now includes uncertainty coming from the emulator.



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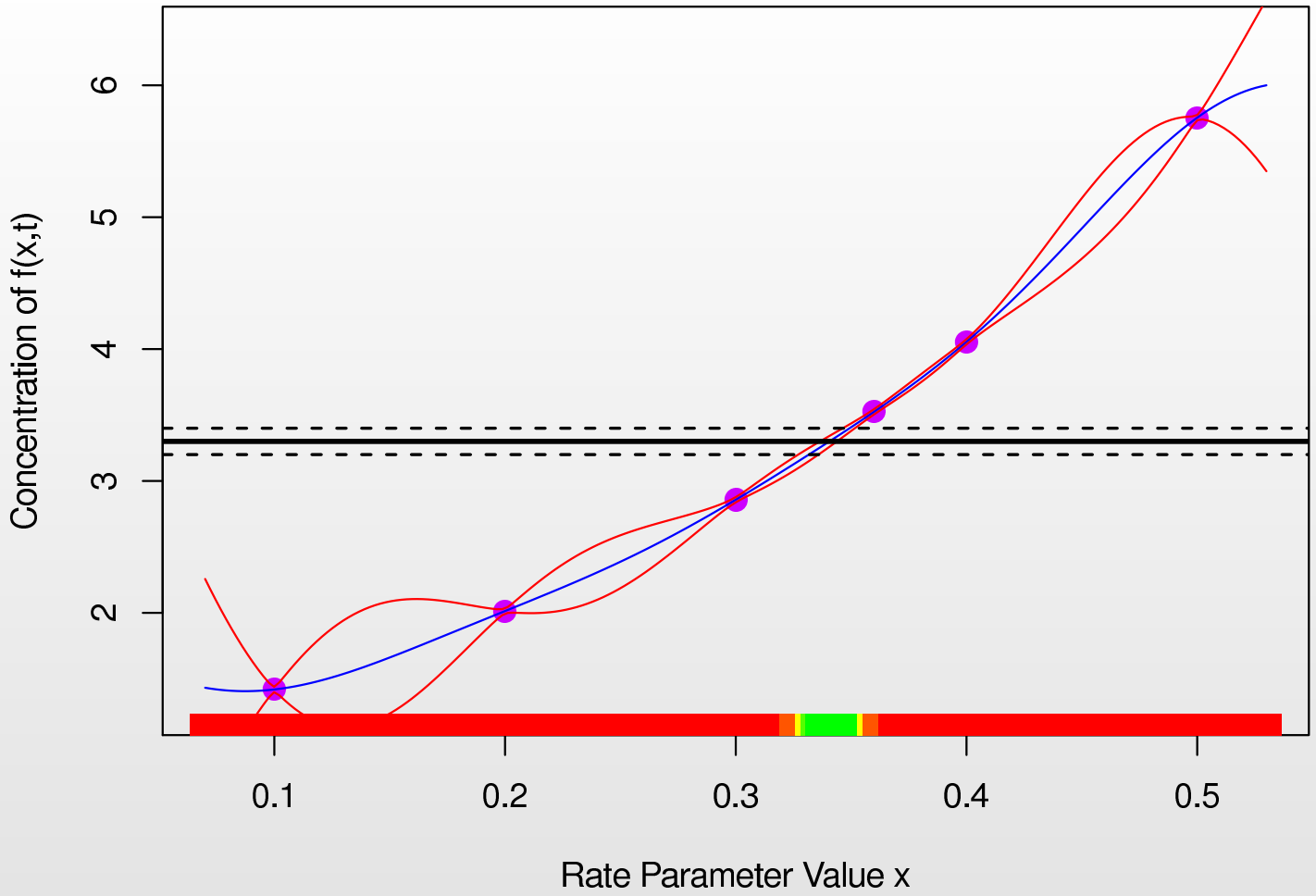

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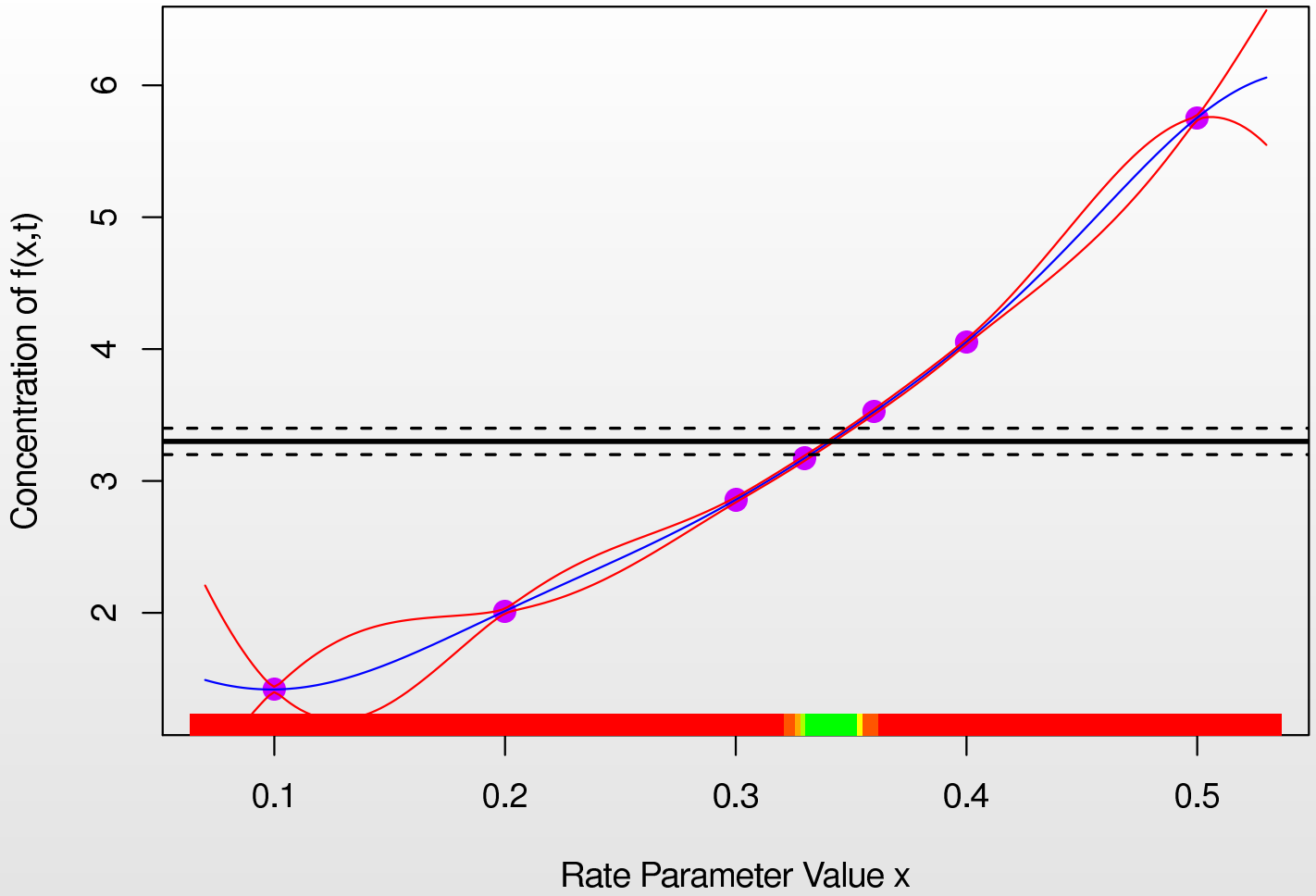

- We perform a 2nd iteration or wave of runs to improve emulator accuracy.
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- Now the emulator is more accurate than the observation, and we can identify the set of all x values of interest.

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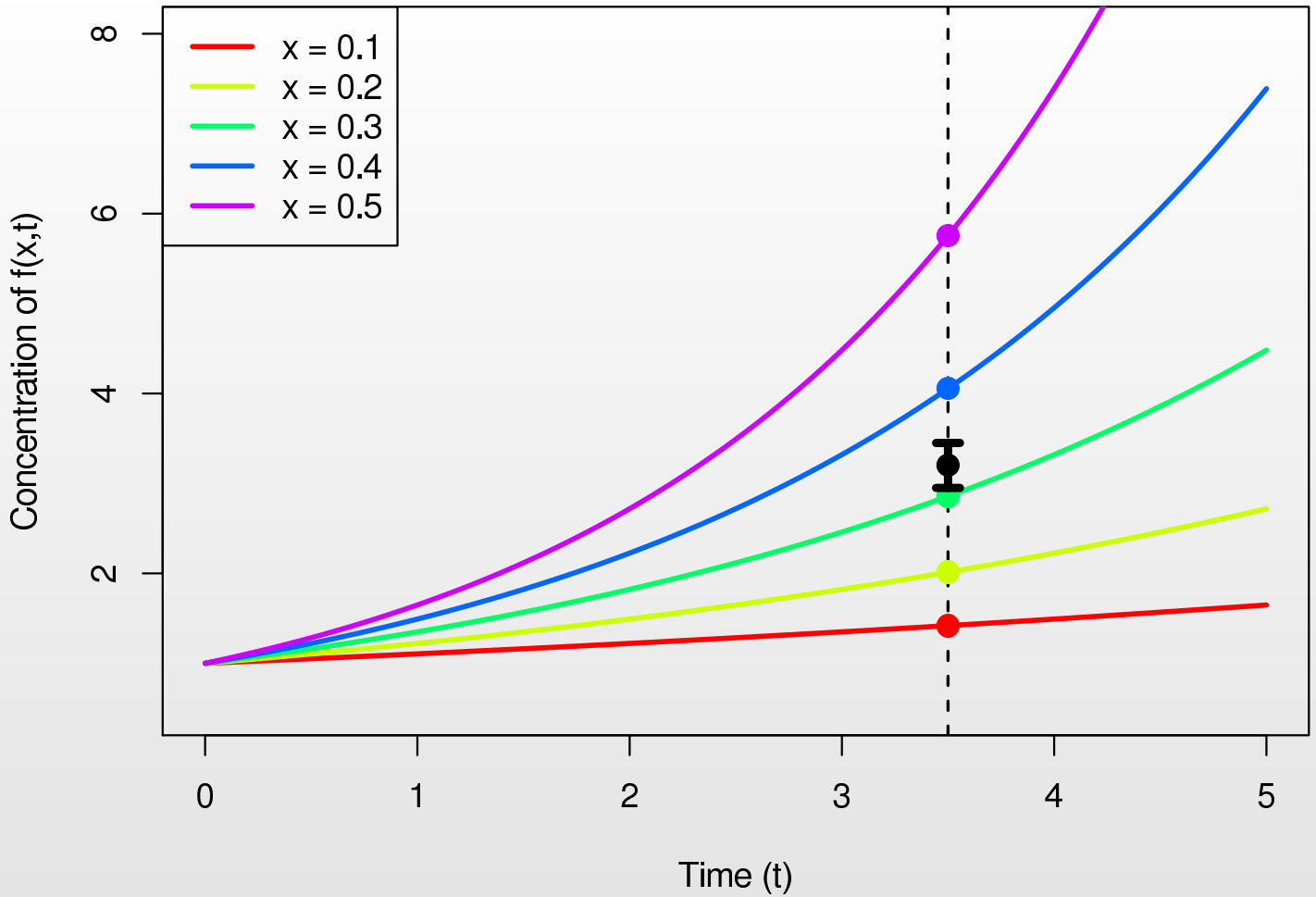
- We can use the model's predictions at $t = 2$ and $t = 5$ to determine which experiment A or B is expected to be most informative about the input parameter x, given our knowledge about $f(x, t)$ at $t = 3.5$.



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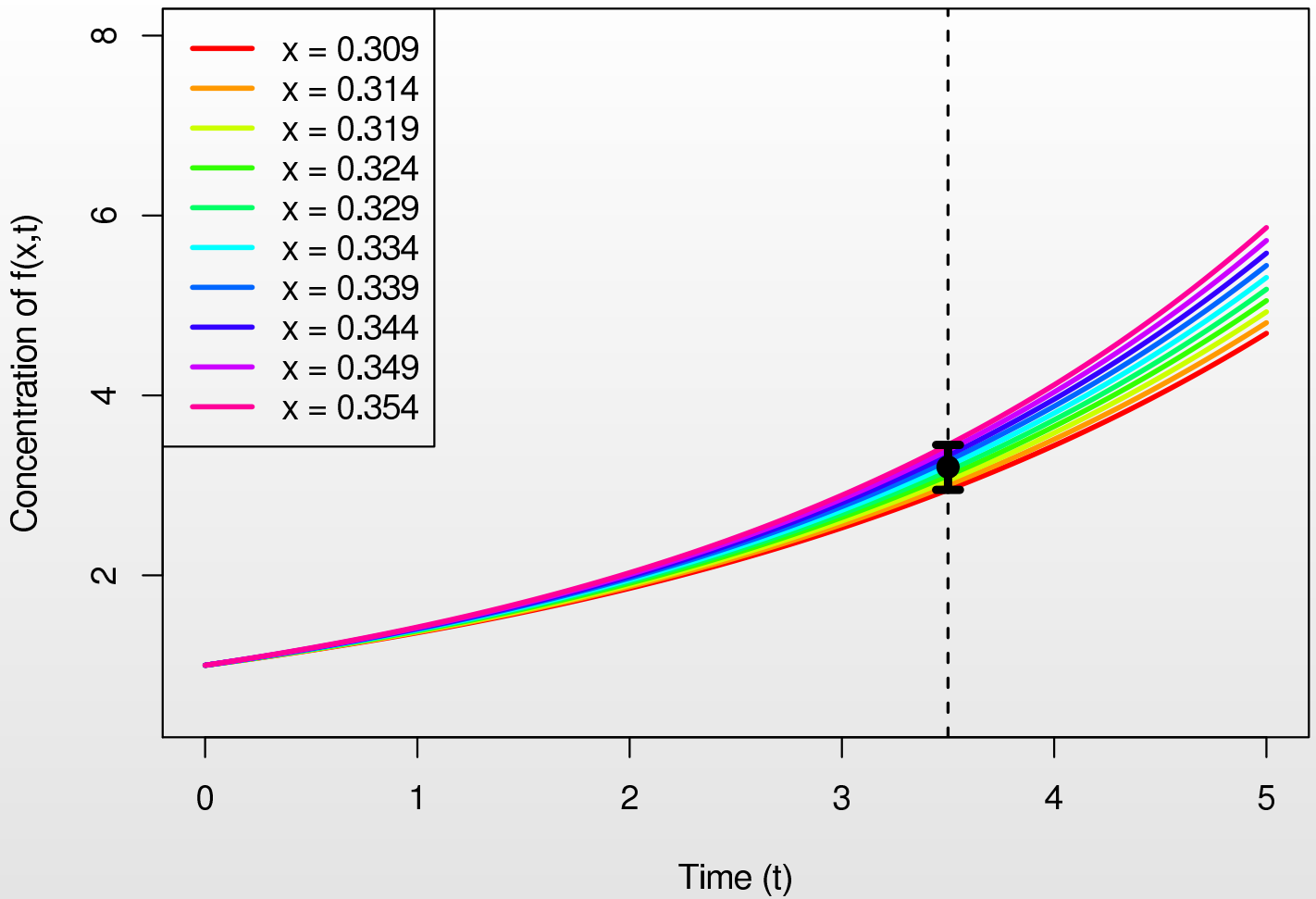

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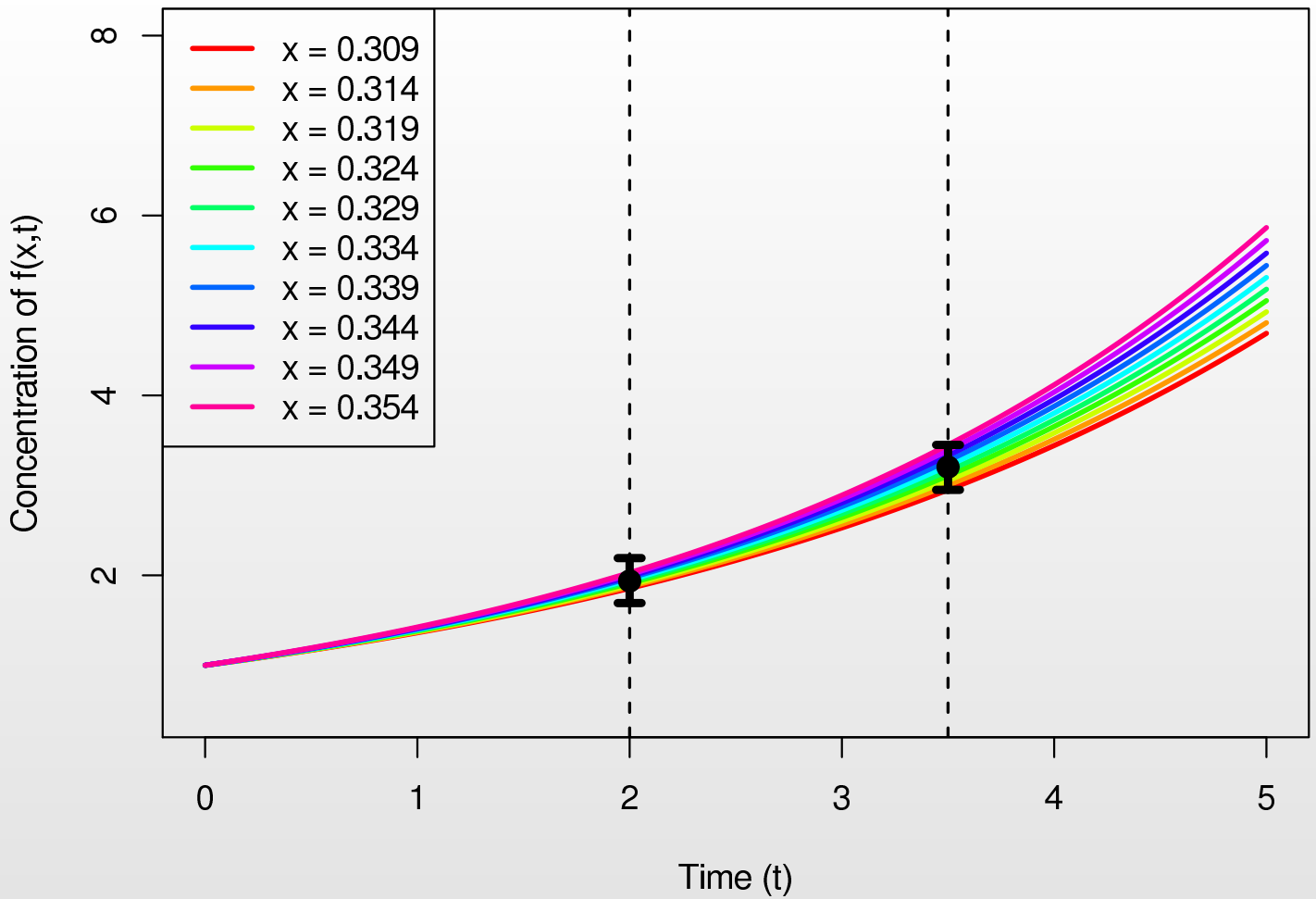

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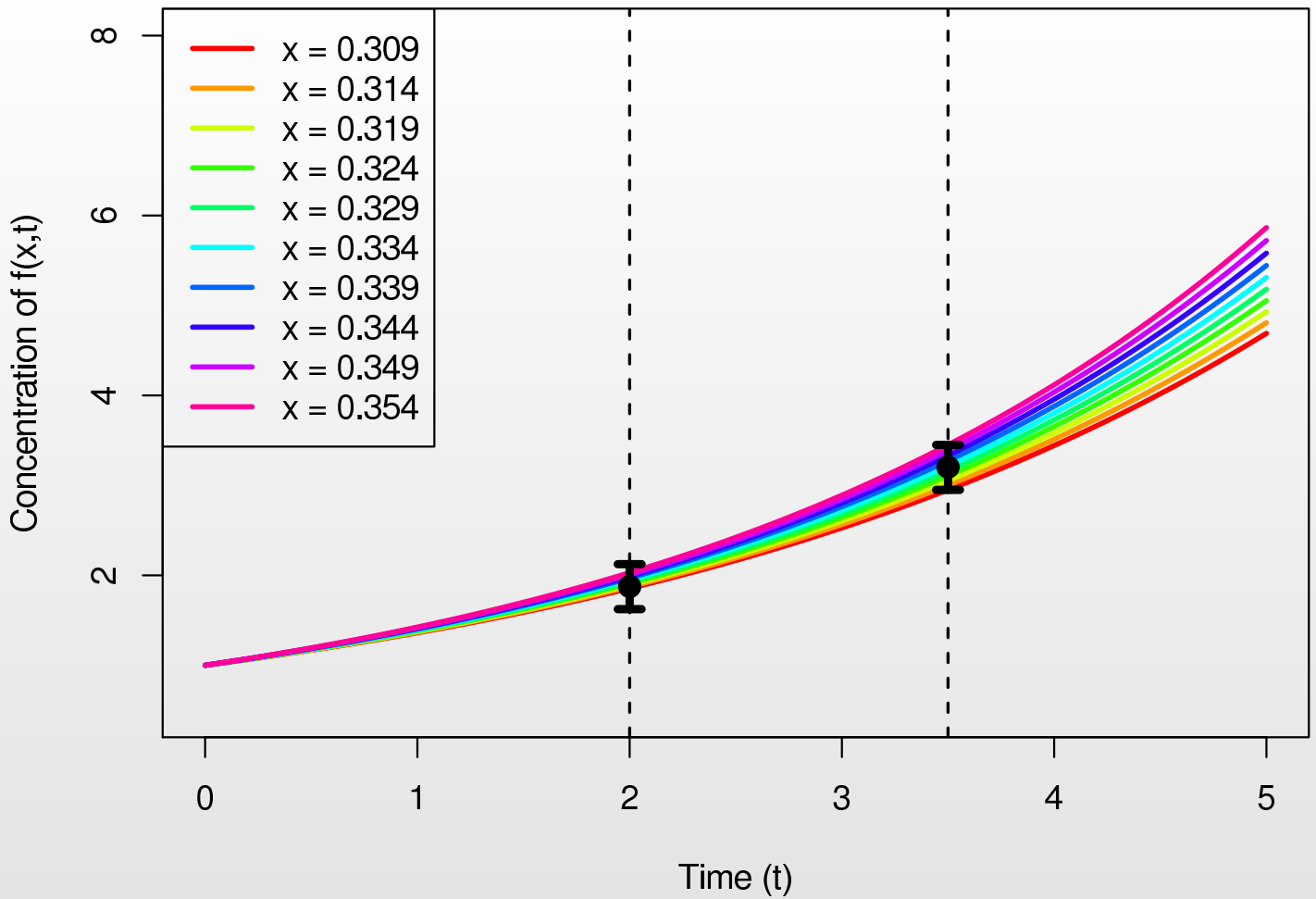

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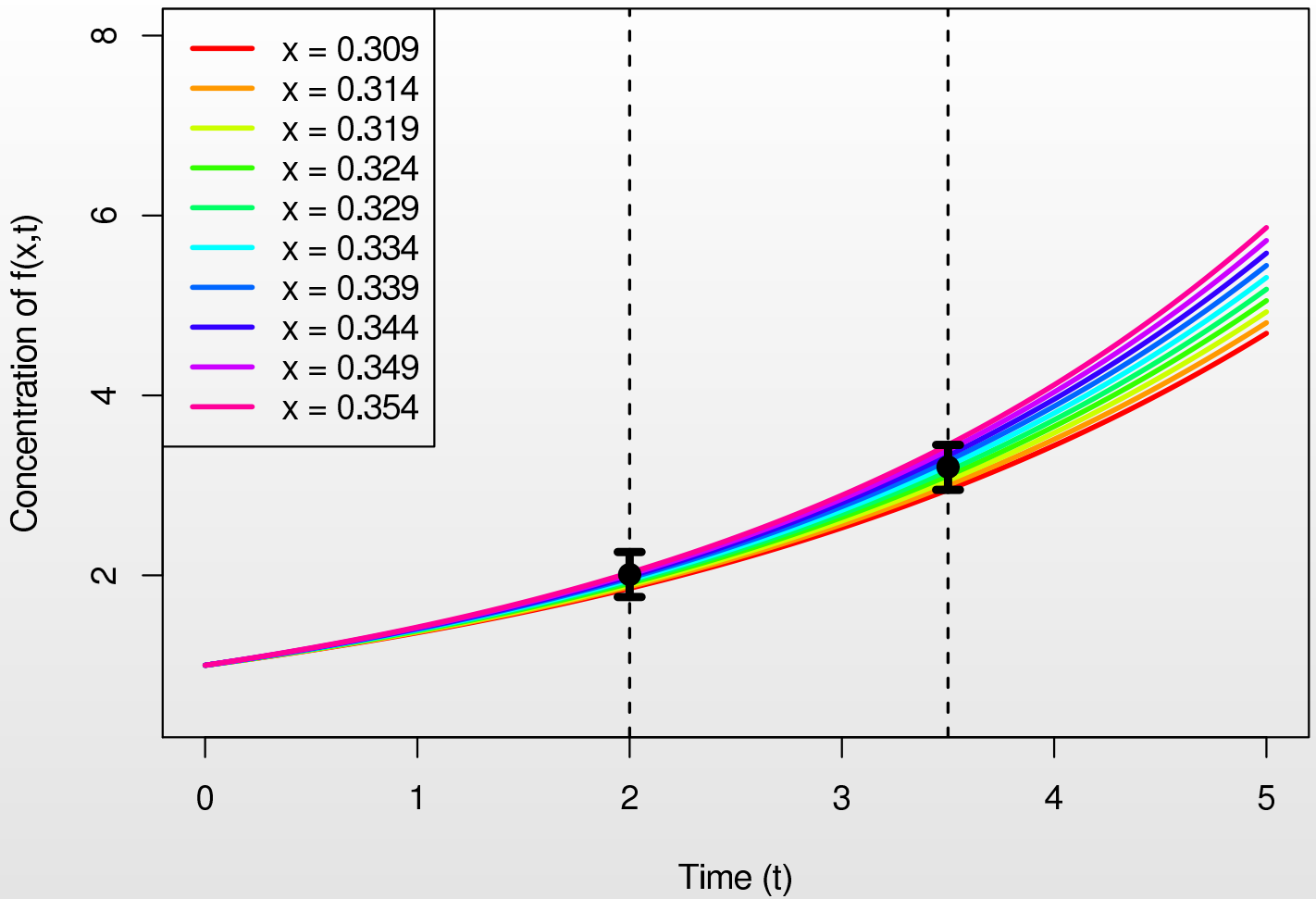
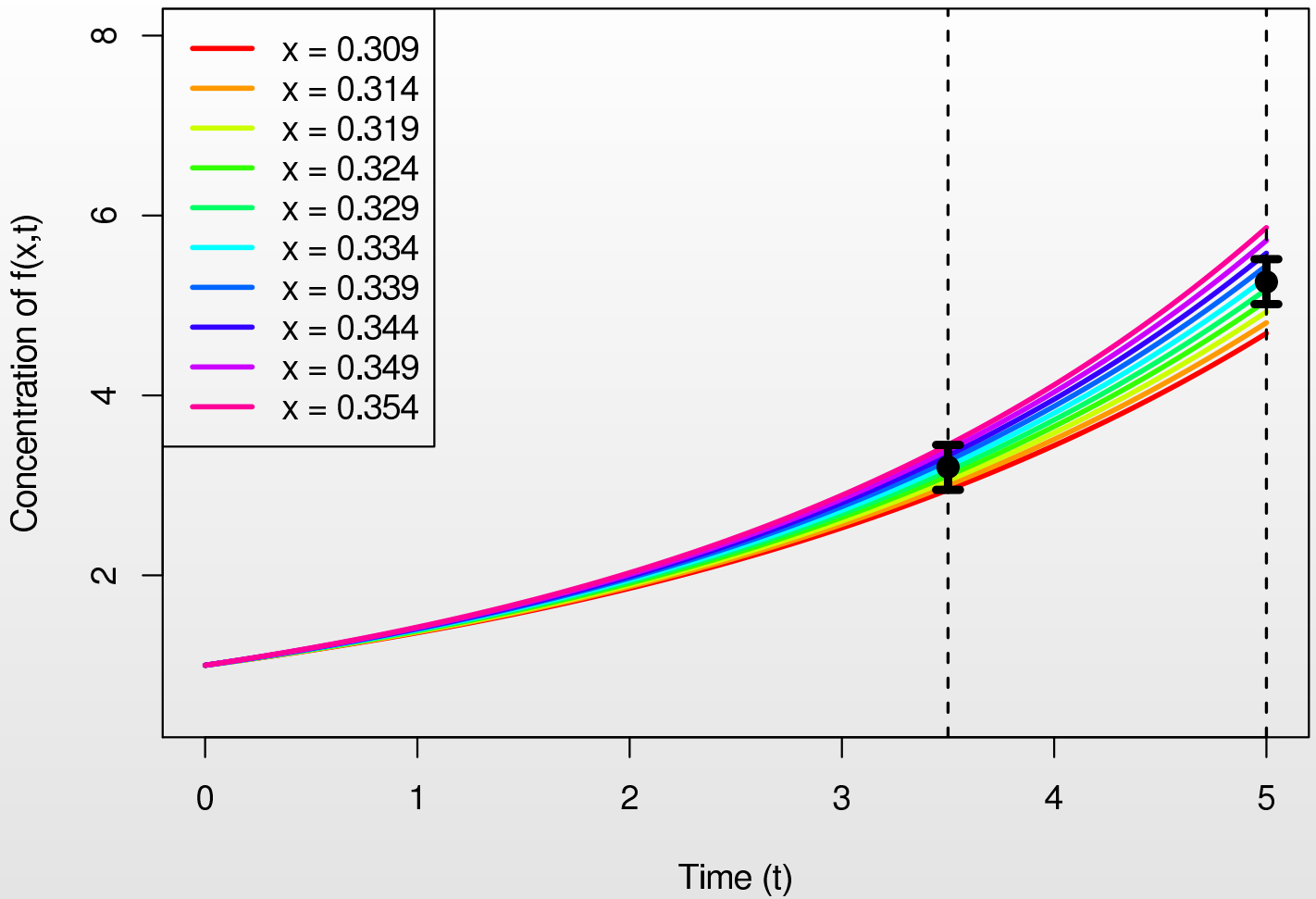


- The predictions imply that any measurement of $f(x, t = 2)$ is highly unlikely to be informative for x.
- This is due to the measurement errors swamping the signal from the model output $f(x, t = 2)$.



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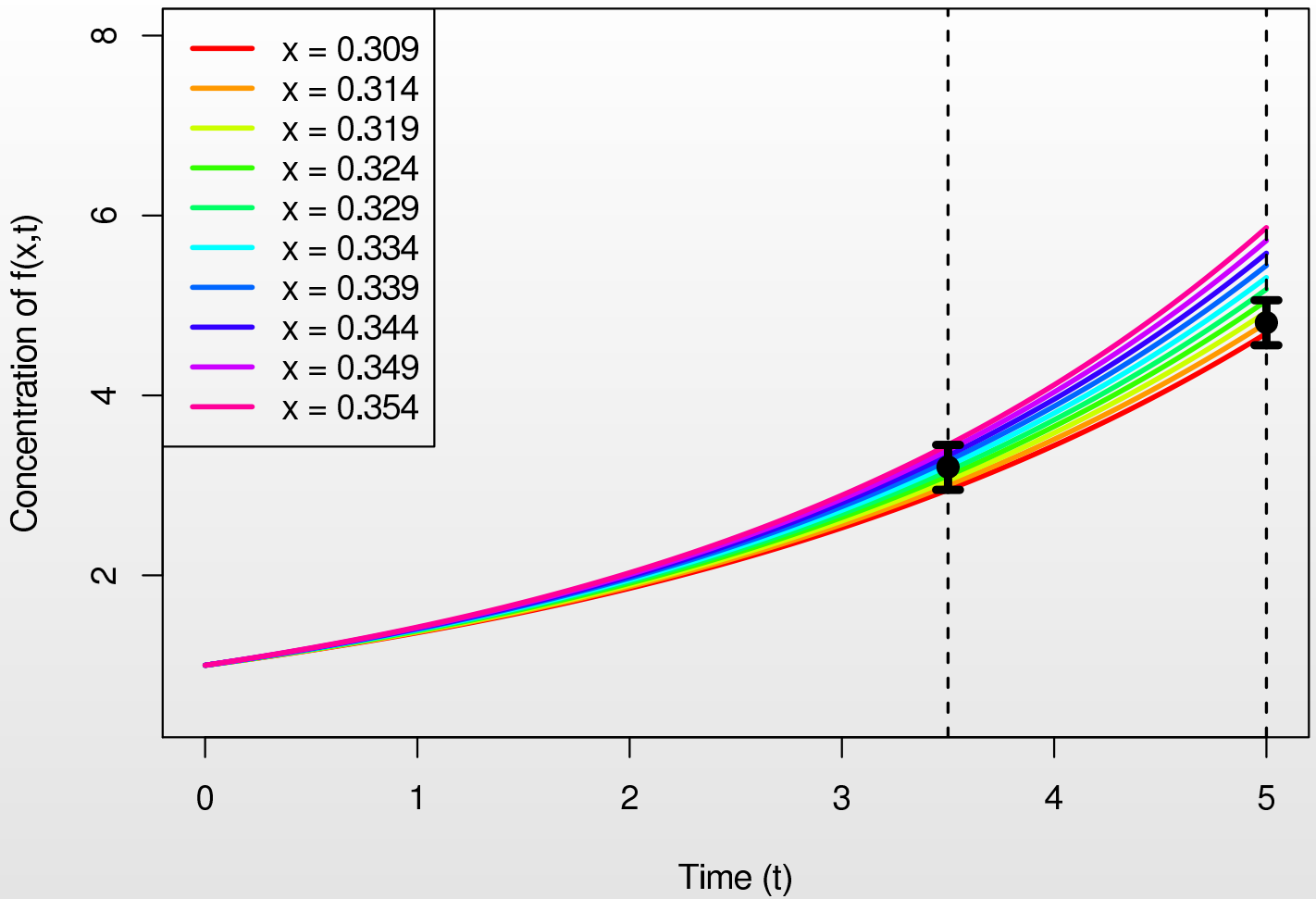

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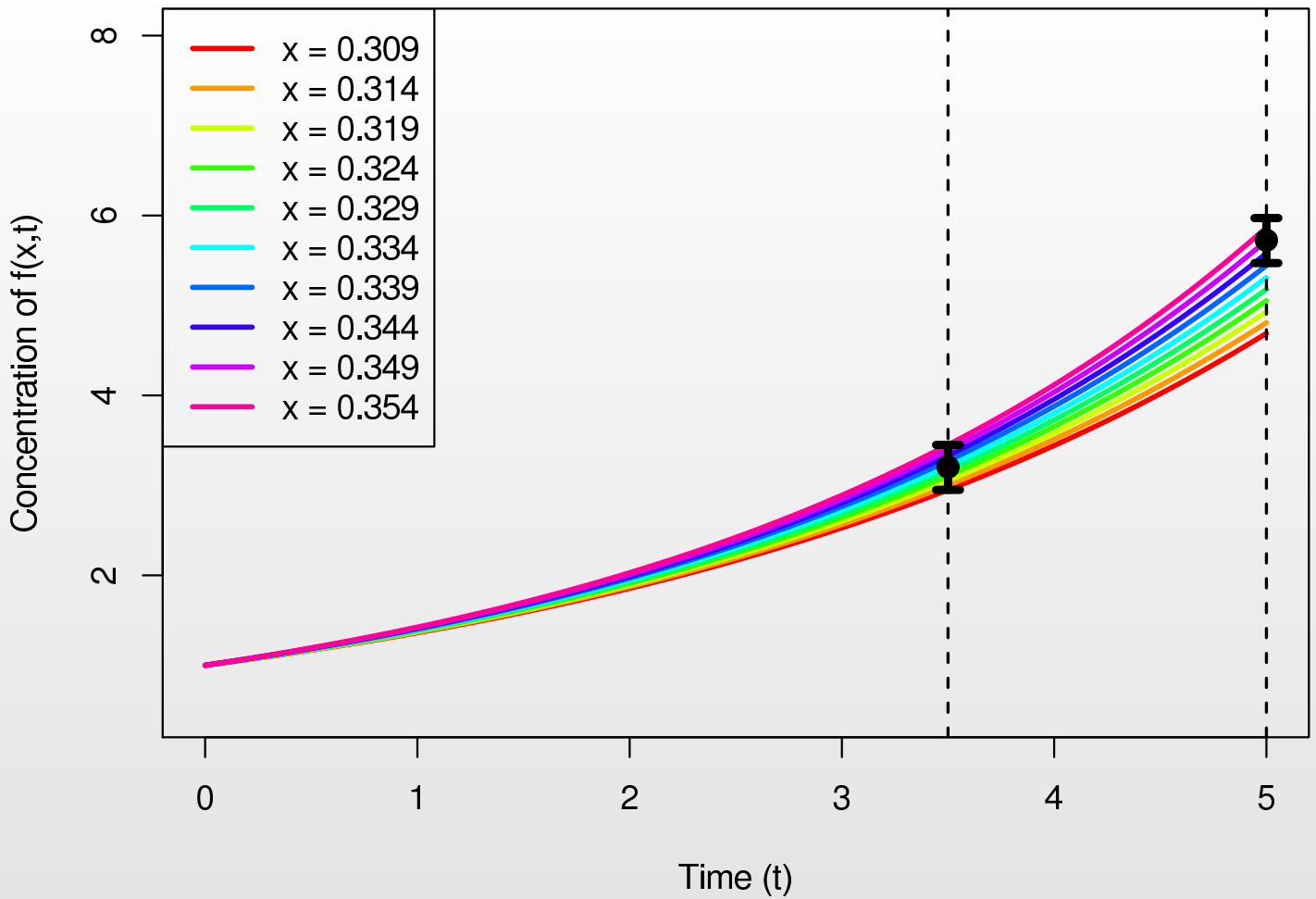
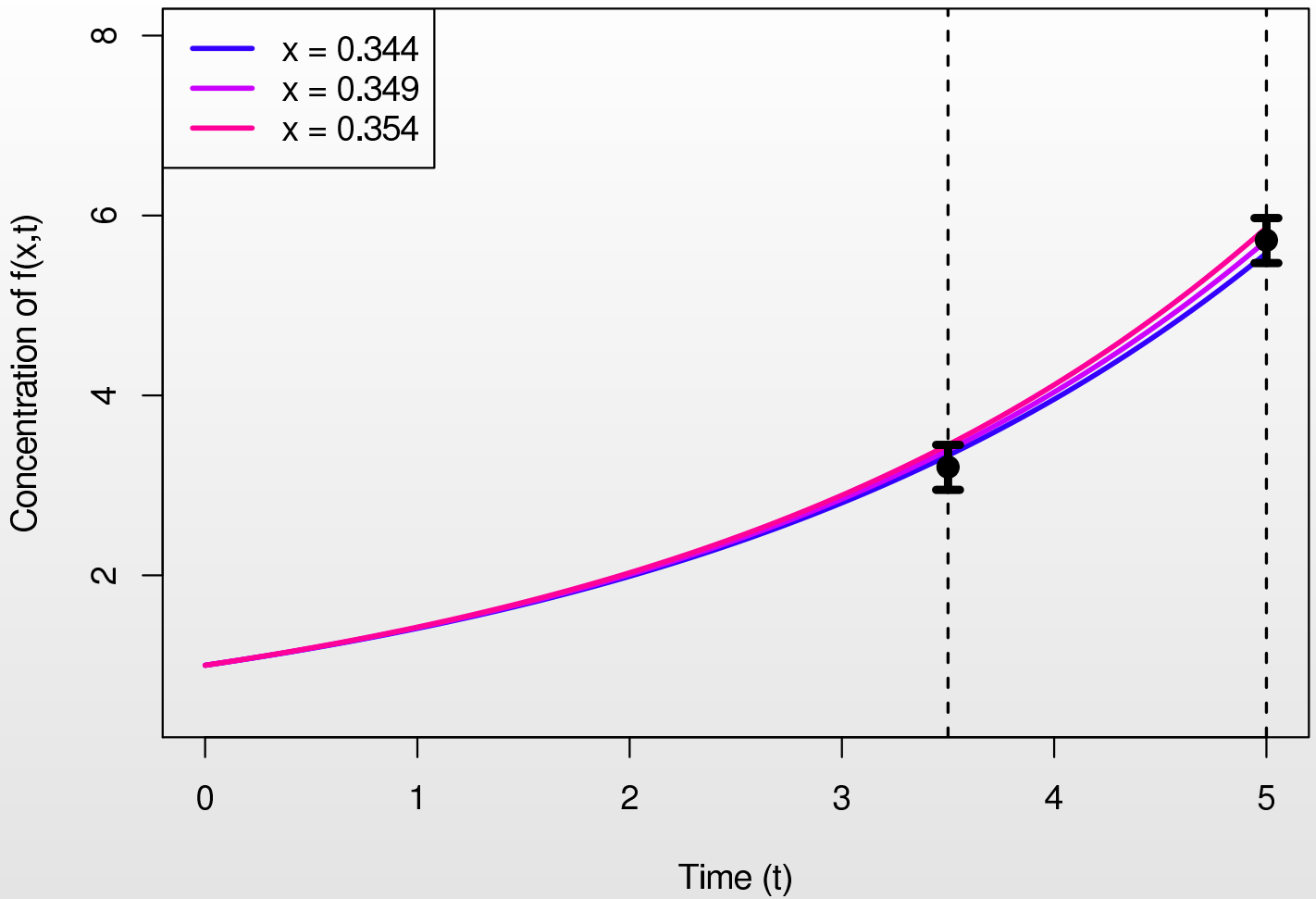
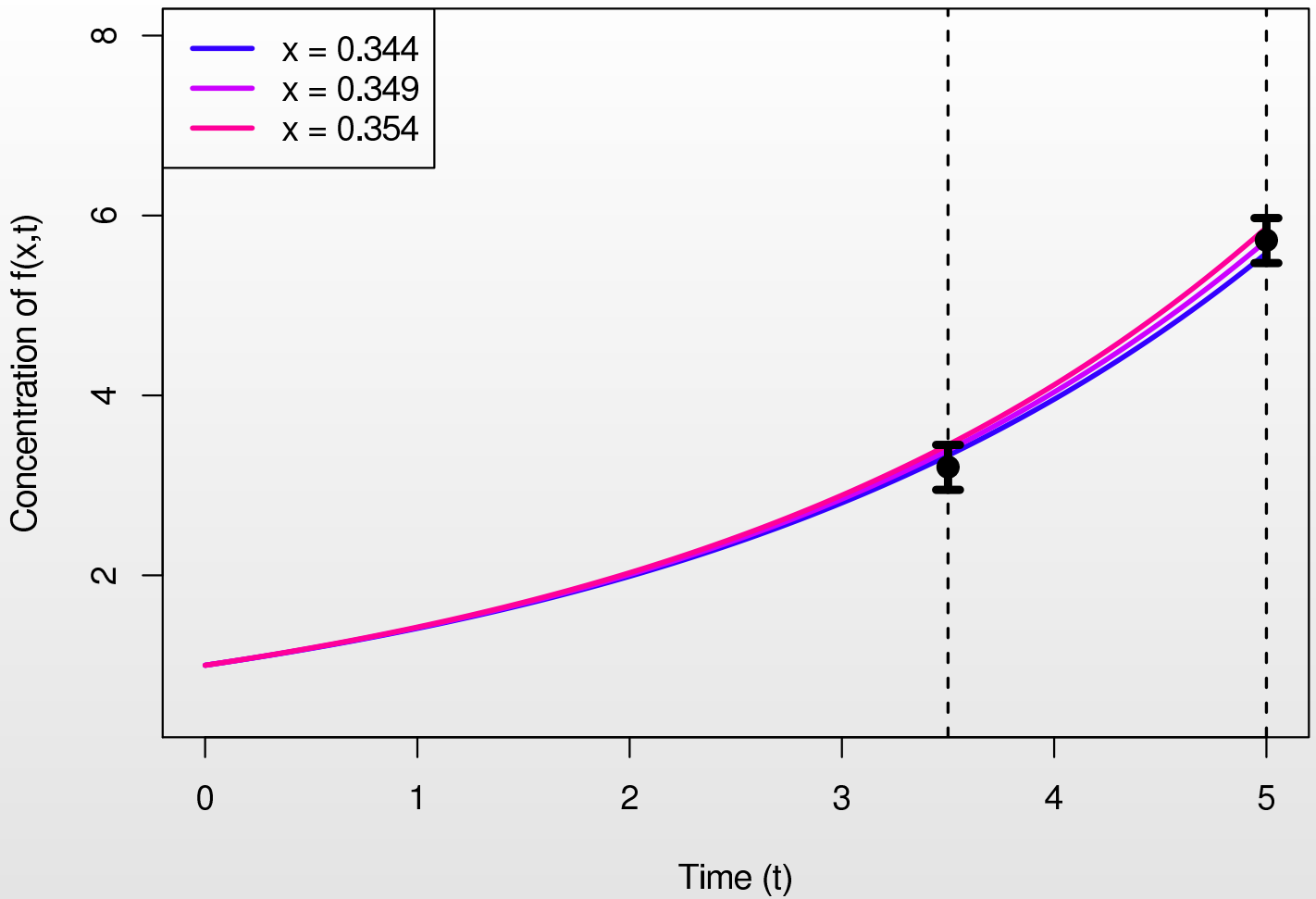


- The predictions for $f(x, t = 5)$ show a different conclusion.
- For each possible measurement of $f(x, t = 5)$ it is highly likely that we will be able to rule out several more values of x as implausible.



- For one possible measurement, we see that non-implausible values of x would lie approximately between 0.344 and 0.354, ruling out approximately 70% of the possible values of x.



- For one possible measurement, we see that non-implausible values of x would lie approximately between 0.344 and 0.354, ruling out approximately 70% of the possible values of x.
- This high expected space reduction in x implies that Experiment B, measuring $f(x,t)$ at $t = 5$, is clearly the best choice.

Simple Example: Conclusions

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- Note that although this method requires trusting the model predictions, in general we would incorporate a model discrepancy term to allow for a certain level of inaccuracy of the model.

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- Here the input x is a vector of length 32, but the output $f(x)$ is of length 96.

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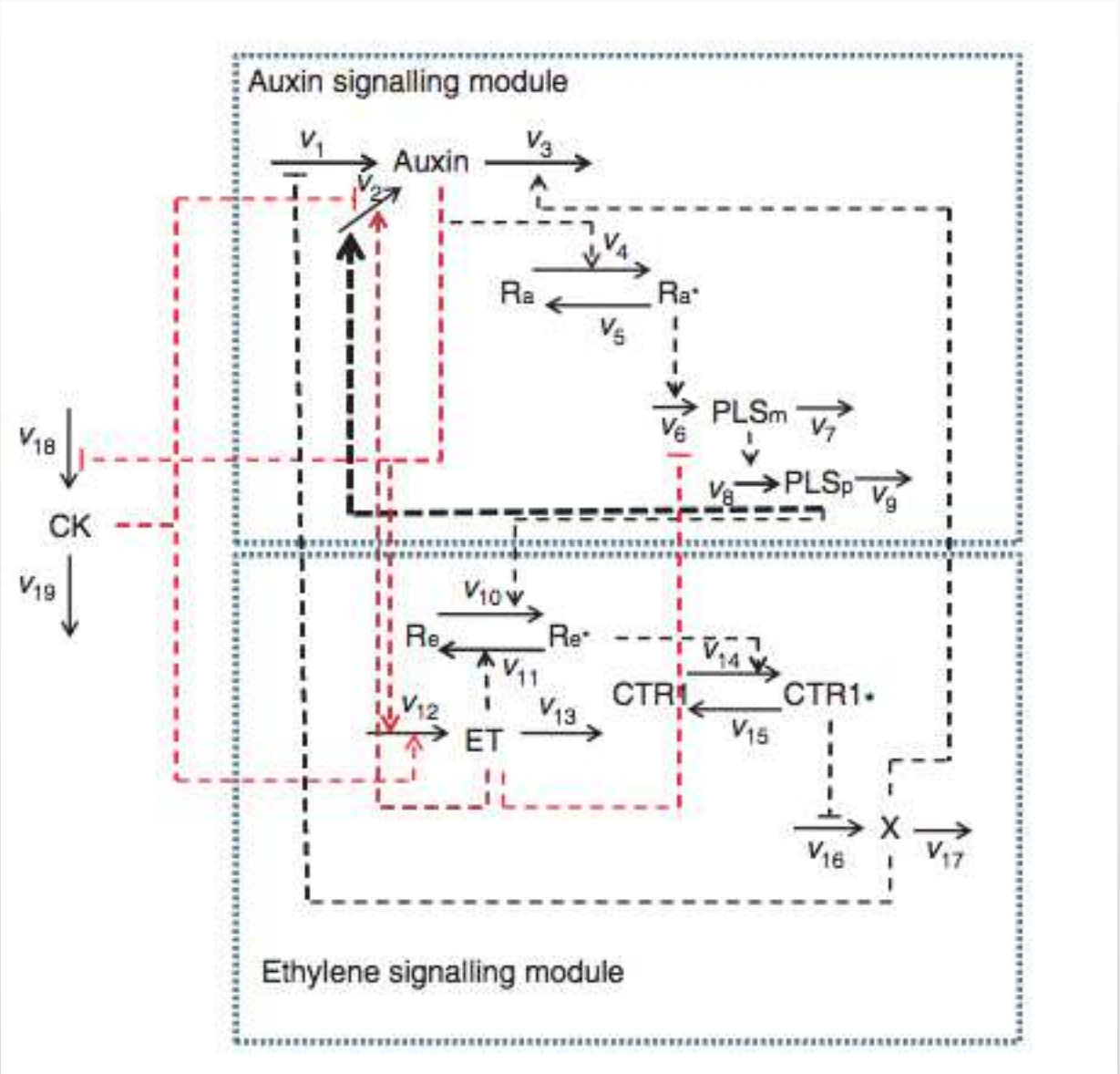
  - Use the results of the History Match to obtain model predictions for all future experiments that are consistent with current observations.
  - Choose the most efficient experiment based on an Expected Space Reduction criteria and complementary robustness considerations.
- This will result in a design for a new experiment that is expected to be highly informative about the input or rate parameters of the Arabidopsis system.

Slides describing model inputs and outputs.

Chemical Output	Initial concentration	Measurable
Auxin	0.1	Yes
X	0.1	
PLSp	0.1	Yes
Ra	0	
Ra_star	1	
CK	0.1	Yes
ET	0.1	Yes
PLSm	0.1	
Re	0	
Re_star	0.3	
CTR1	0	
CTR1_star	0.3	
IAA	0	
cytokinin	0	
ACC	0	

Reaction Network Model



32 Reaction Rates: 32 Input parameters

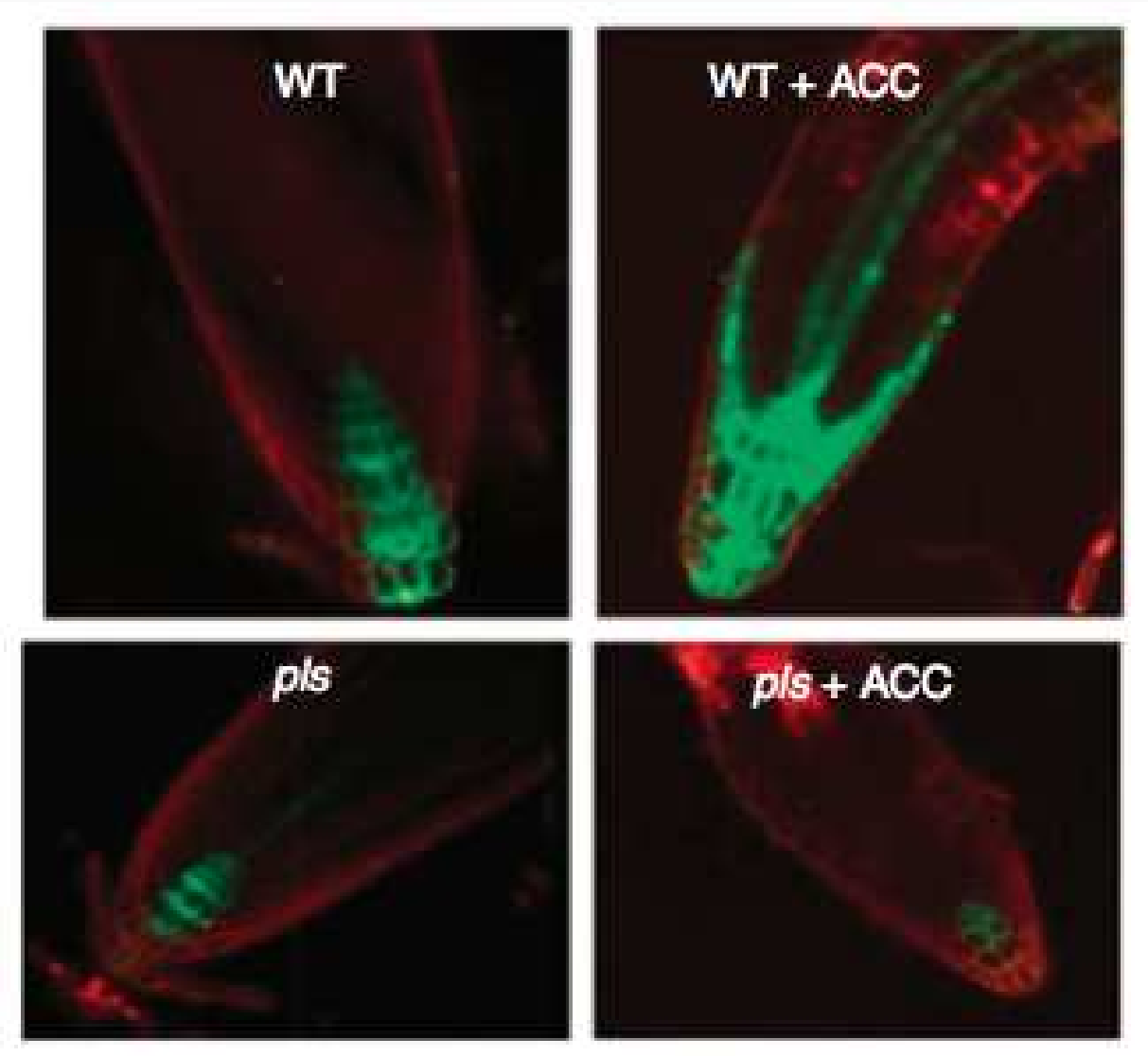
Input	min	max	Input	min	max
k1	0.001	100	k1a	0.001	100
k2	0.0002	20	k2a	0.0028	280
k2b	0.001	100	k2c	1×10^{-5}	1
k3	0.002	200	k3a	0.00045	45
k4	0.001	100	k5	0.001	100
k6	0.3	0.3	k6a	0.0002	20
k7	0.001	100	k8	0.001	100
k9	0.001	100	k10	3×10^{-7}	0.03
k10a	0.0005	50	k11	0.005	500
k12	0.0001	10	k12a	0.0001	10
k13	0.001	100	k14	0.003	300
k15	8.5×10^{-5}	8.5	k16	0.0003	30
k16a	0.001	100	k17	0.0001	10
k18	0.0001	10	k18a	0.001	100
k19	0.001	100	k1vauxin	0.001	100
k1vCK	0.001	100	k1veth	0.001	100

- So now the input $x =$ (k1, k1a, k2, k2a, . . . ,k19, k1vauxin, k1vCK, k1veth)

Arabidopsis Model

$$
\begin{aligned}
\frac{dAuxin}{dt} &= \frac{k_{1a}}{1+\frac{X}{k_1}} + k_2 + \frac{k_{2a}ET}{1+\frac{CK}{k_{2b}}}\frac{PLSp}{k_{2c}+PLSp} - \\
&\quad (k_3 + k_{3a}X)Auxin + k_{1vauxin}IAA \\
\frac{dX}{dt} &= k_{16} - k_{16a}CTR1_{star} - k_{17}X \\
\frac{dPLSp}{dt} &= k_8 PLSm - k_9 PLSp \\
\frac{dRa}{dt} &= -k_4 AuxinRa + k_5 Ra_{star} \\
\frac{dRa_{star}}{dt} &= k_4 AuxinRa - k_5 Ra_{star} \\
\frac{dCK}{dt} &= \frac{k_{18a}}{1+\frac{Auxin}{k_{18}}} - k_{19}CK + k_{1vCK}cytokinin \\
\frac{dET}{dt} &= k_{12} + k_{12a}AuxinCK - k_{13}ET + k_{1veth}ACC \\
\frac{dPLSm}{dt} &= \frac{k_6 Ra_{star}}{1+\frac{ET}{k_{6a}}} - k_7 PLSm \\
\frac{dRe}{dt} &= k_{11}Re_{star}ET - (k_{10} + k_{10a}PLSp)Re \\
\frac{dRe_{star}}{dt} &= -k_{11}Re_{star}ET + (k_{10} + k_{10a}PLSp)Re \\
\frac{dCTR1}{dt} &= -k_{14}Re_{star}CTR1 + k_{15}CTR1_{star} \\
\frac{dCTR1_{star}}{dt} &= k_{14}Re_{star}CTR1 - k_{15}CTR1_{star} \\
\frac{dIAA}{dt} &= 0, \quad \frac{dcytokinin}{dt} = 0, \quad \frac{dACC}{dt} = 0
\end{aligned}
$$

Measurements of root hormone level.



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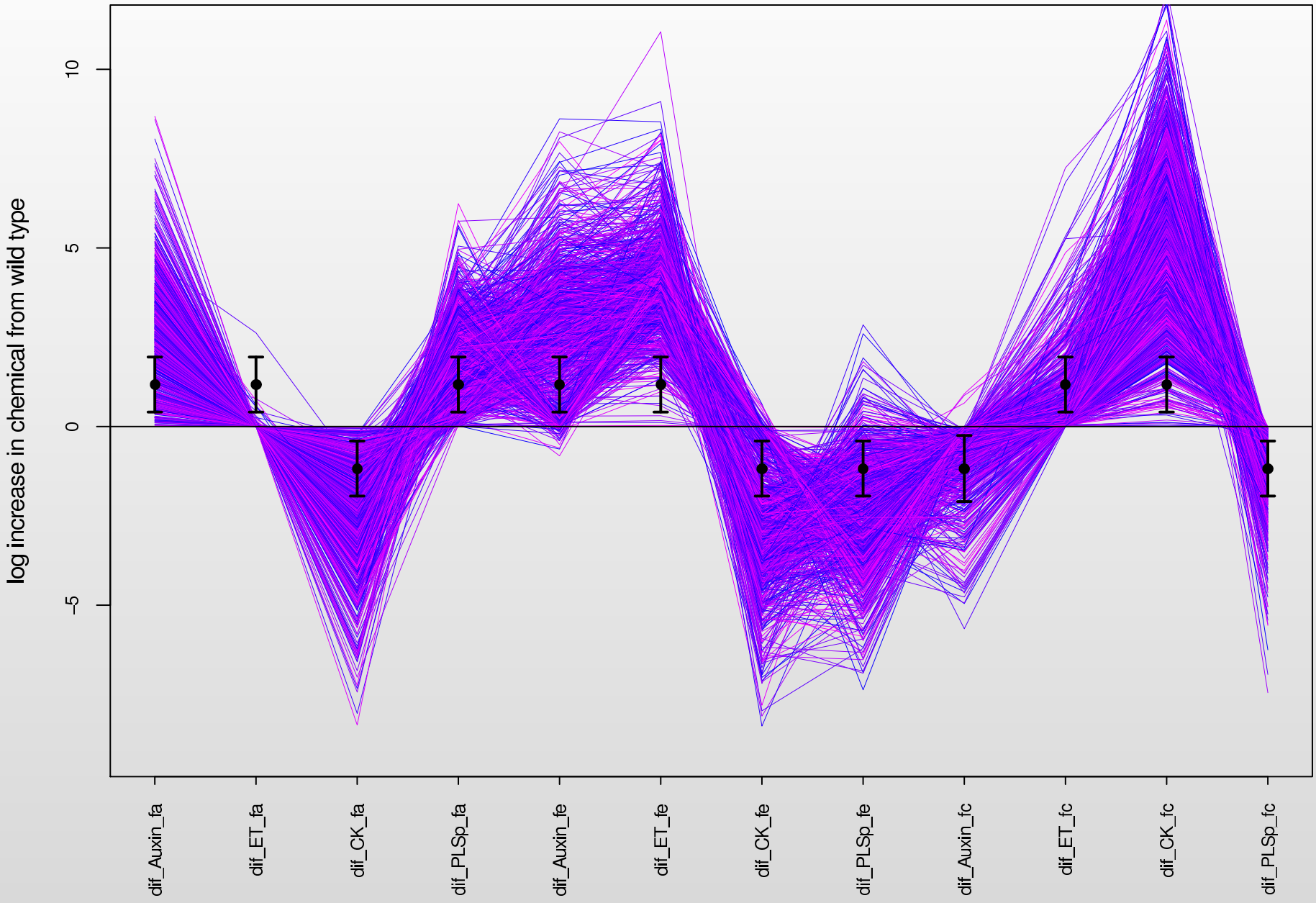
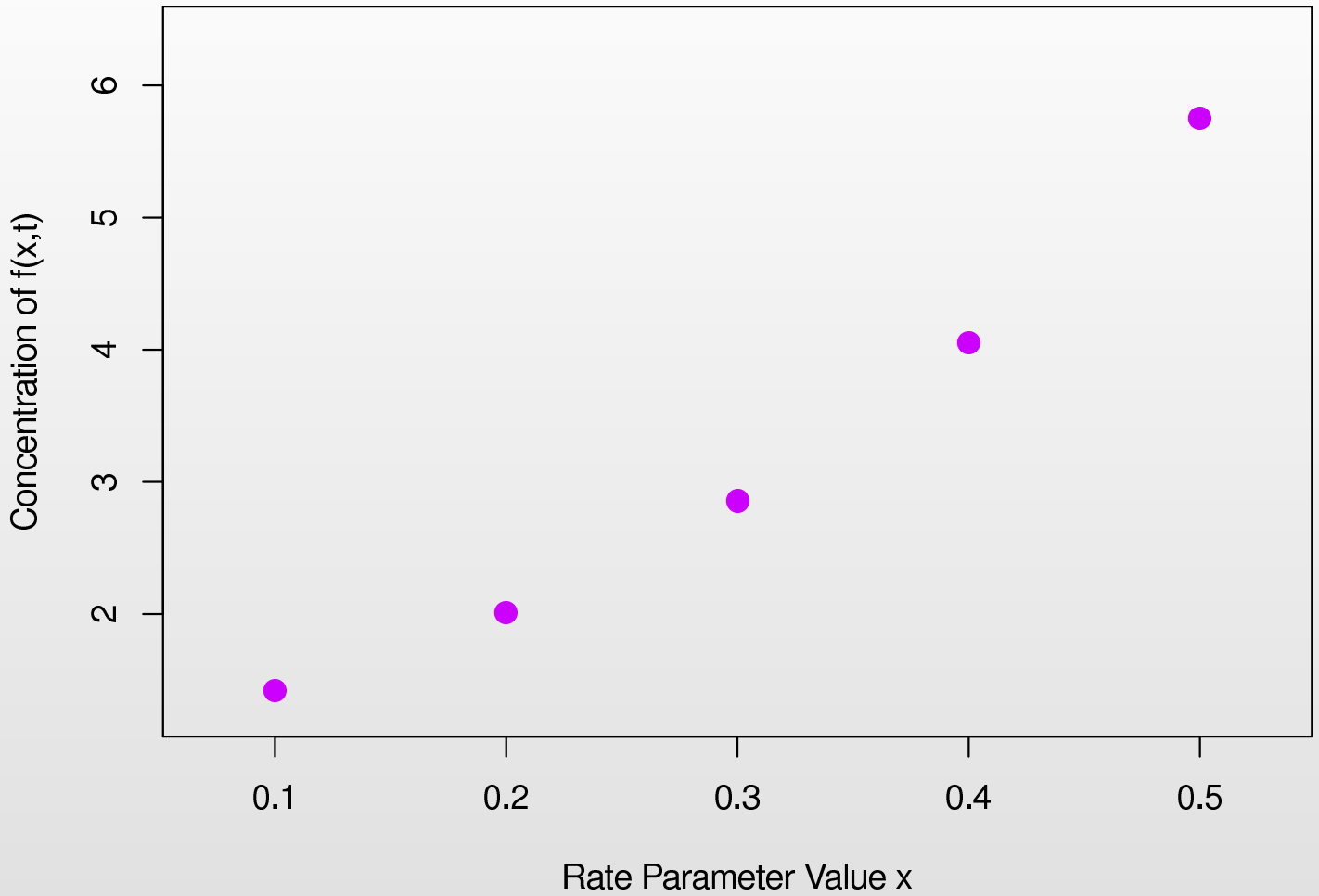
3 What design of future experiment will reduce this set $\mathcal{X}(z)$, and hence resolve uncertainty about the rate parameters?

Observed Trends plus 2000 runs of the model



Emulation: 1D example



- Consider the graph of $f(x)$: in general we do not have the analytic solution of $f(x)$, here given by the dashed line.
- Instead we only have a finite number of runs of the model, in this case five.

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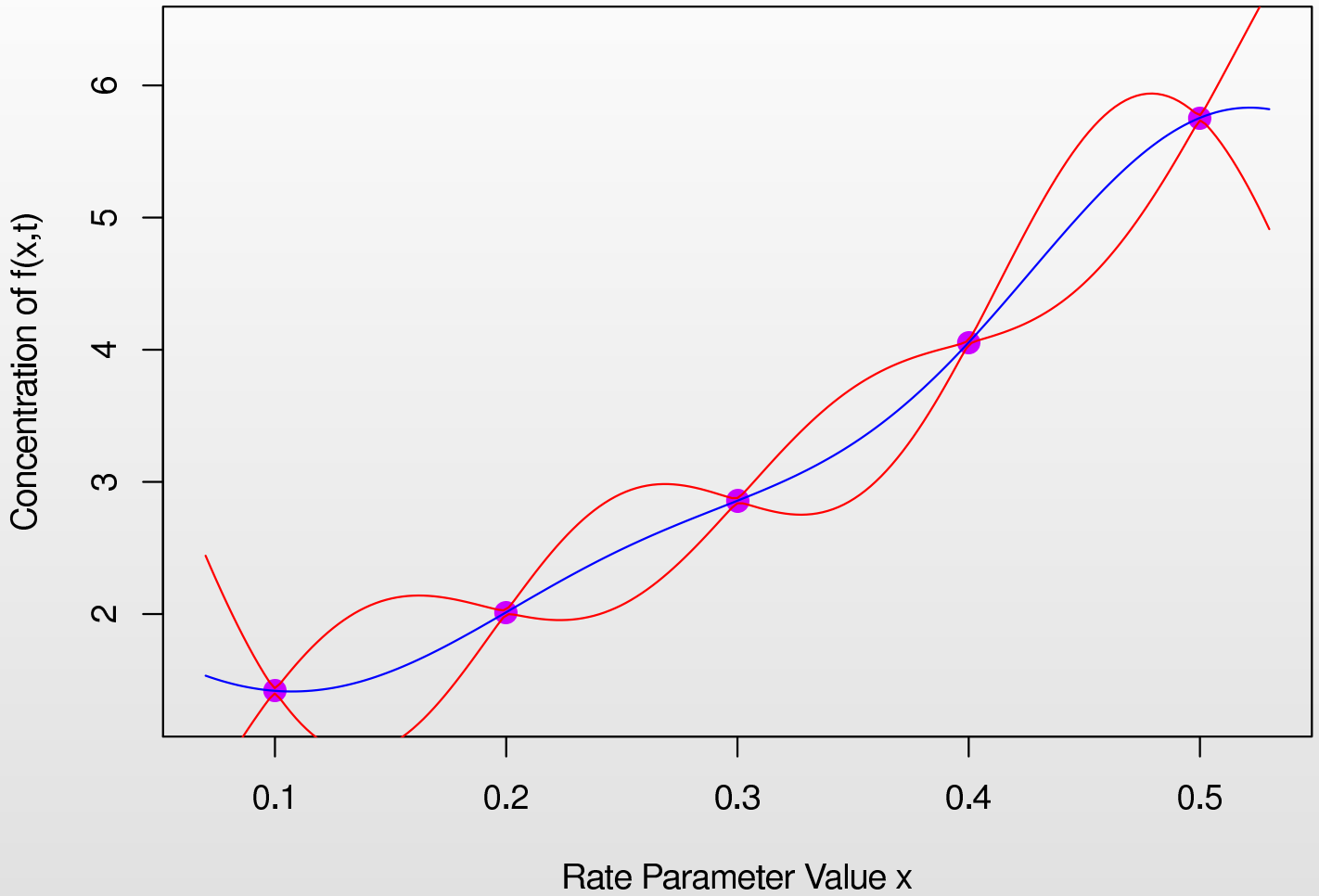

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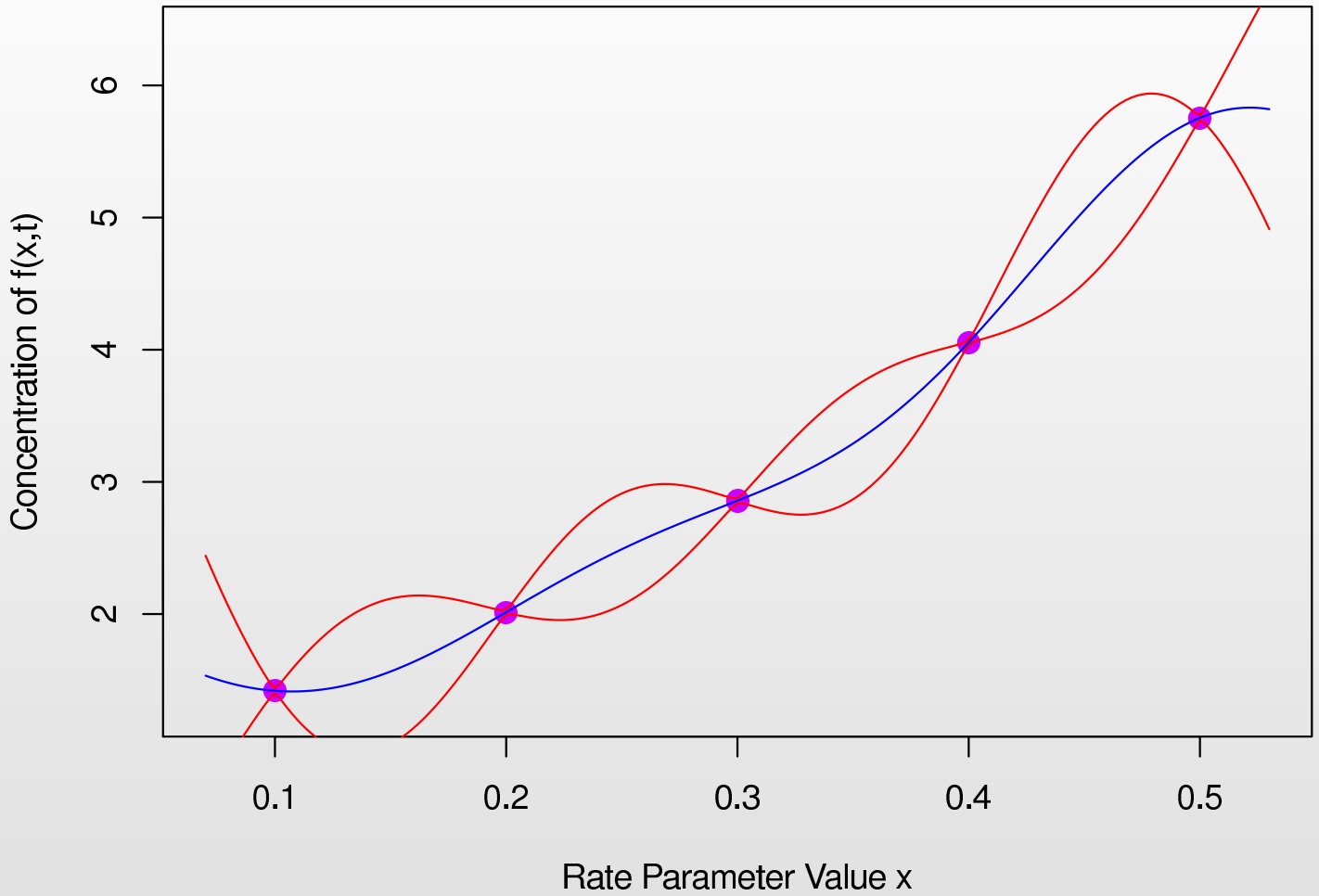

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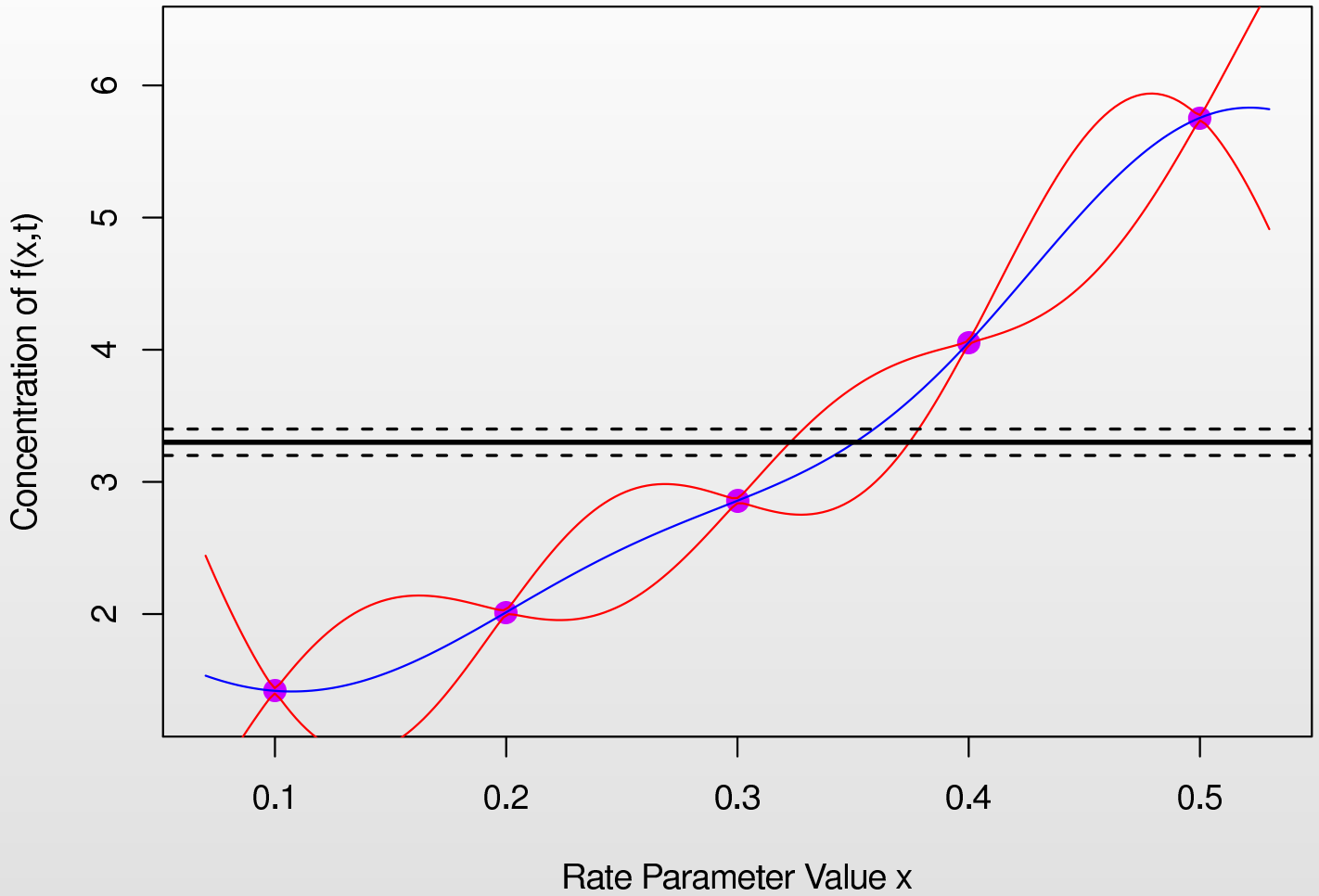
Implausibility Measures: 1D example



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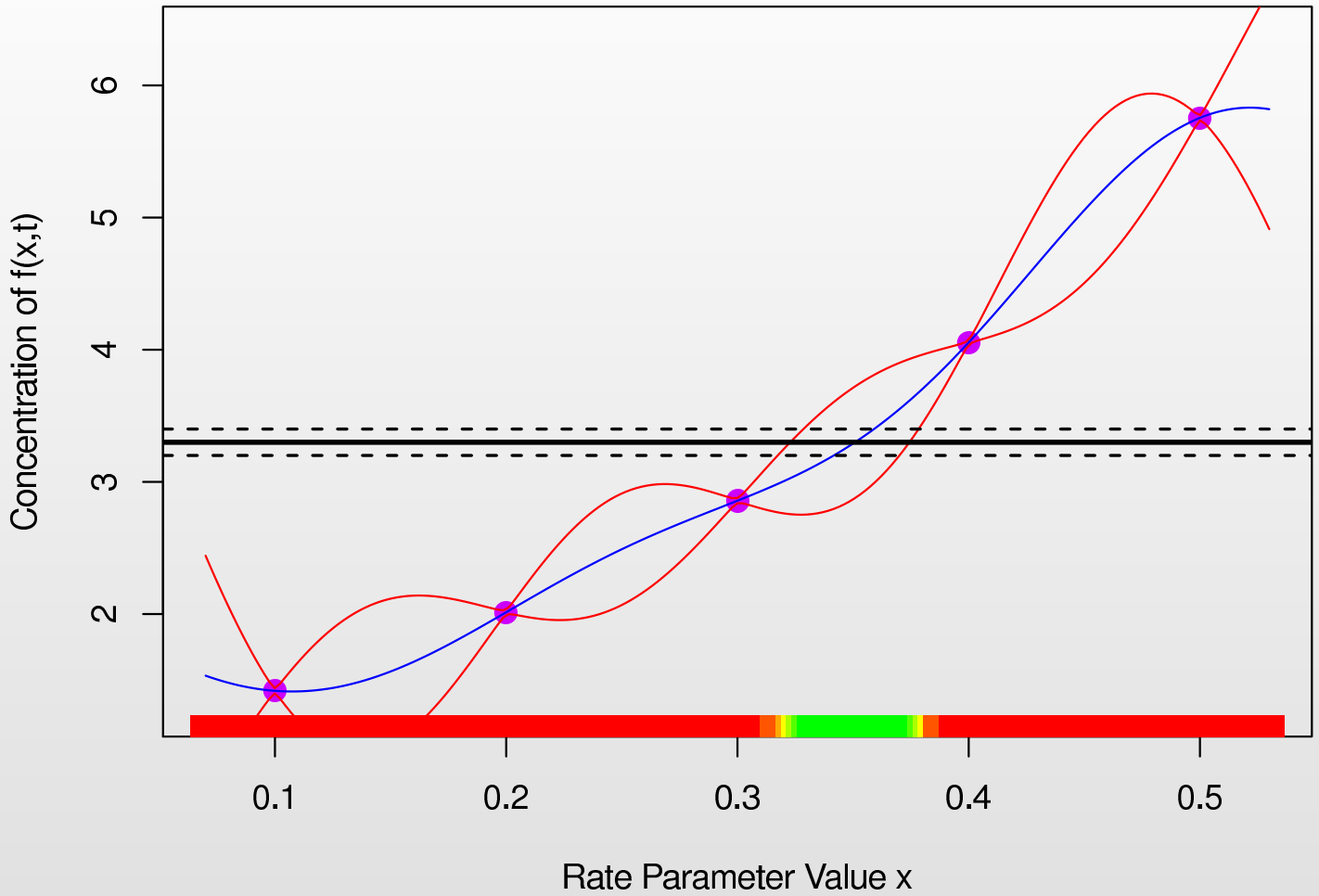

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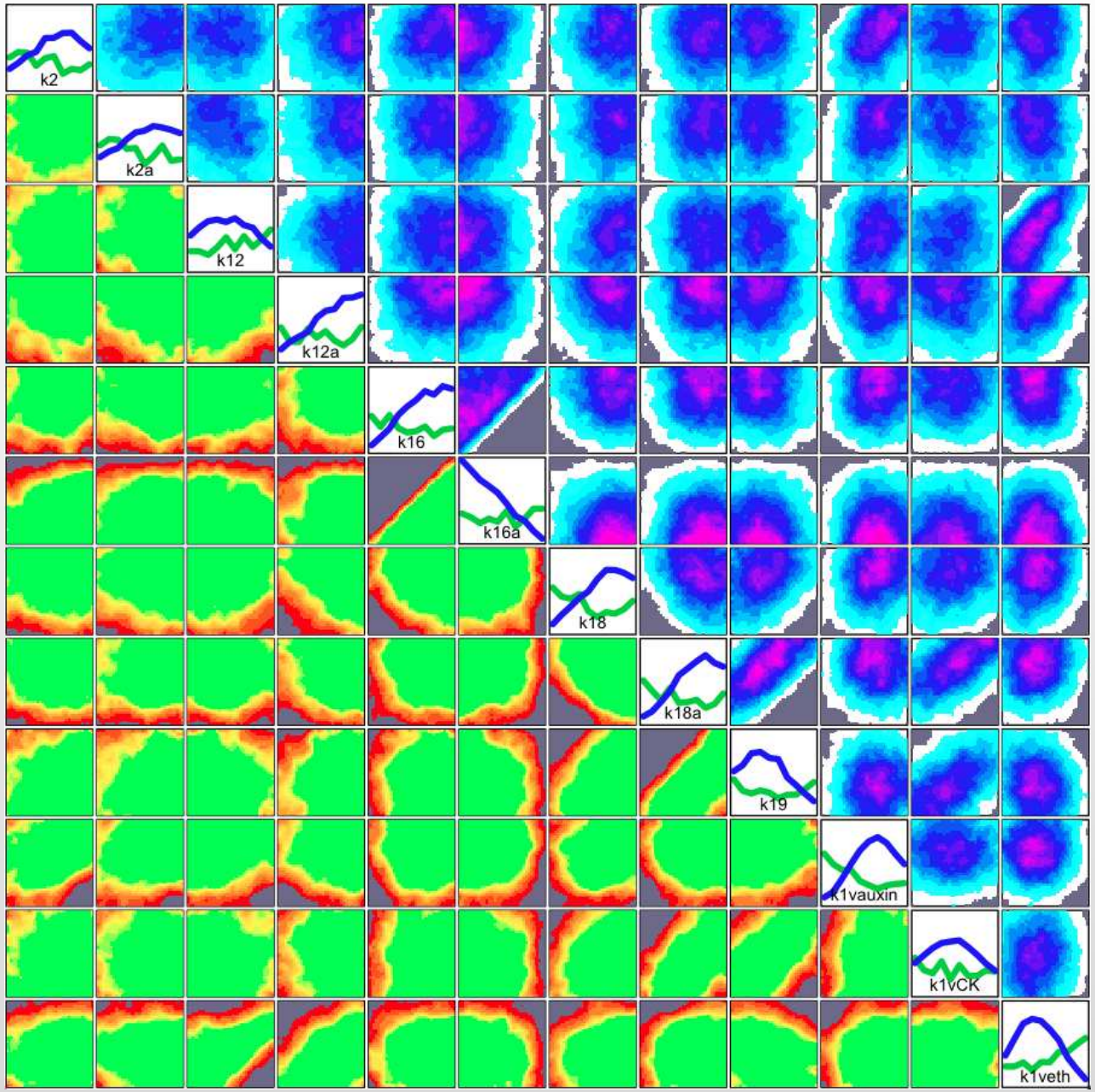
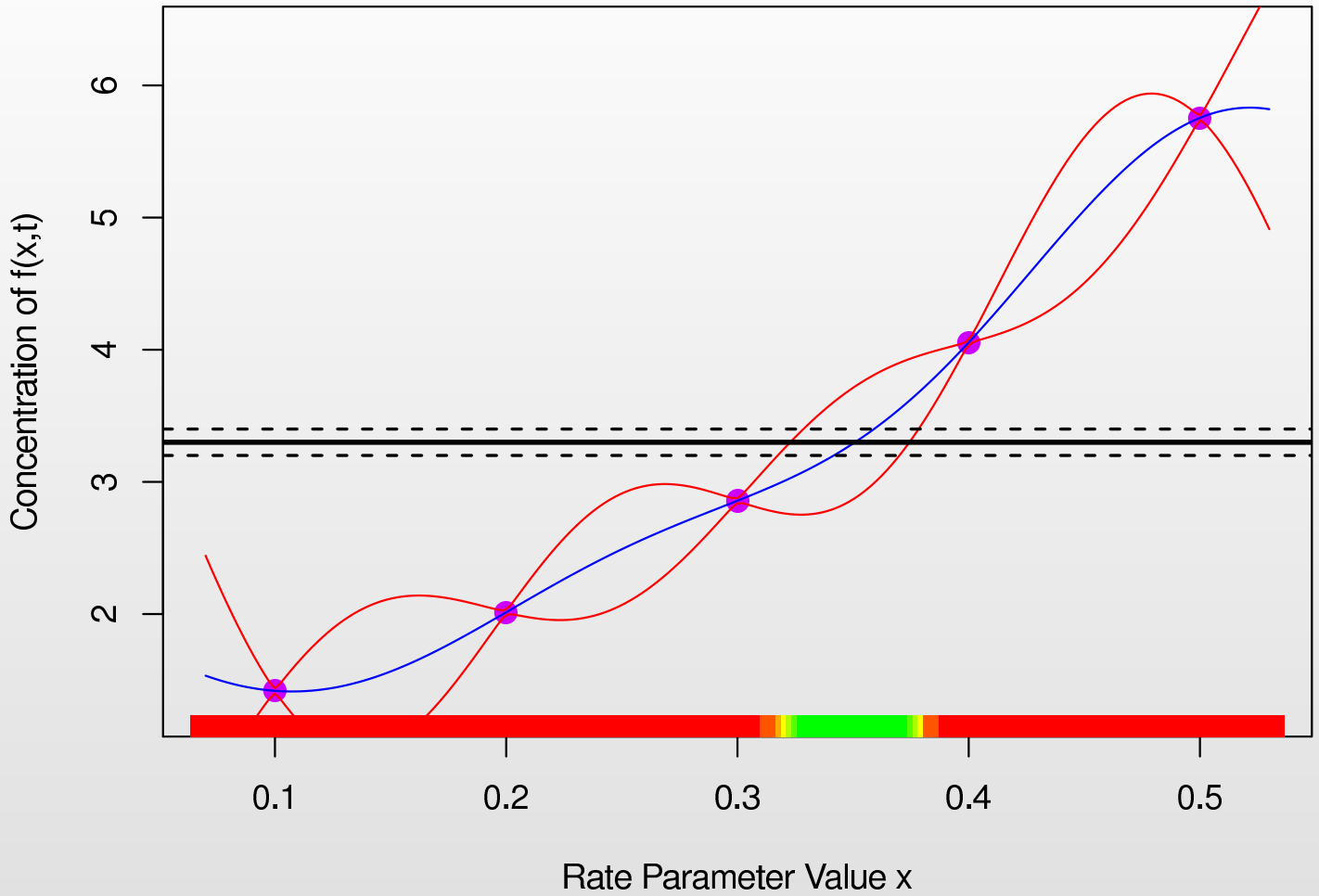
Implausibility Measures: Arabidopsis Model

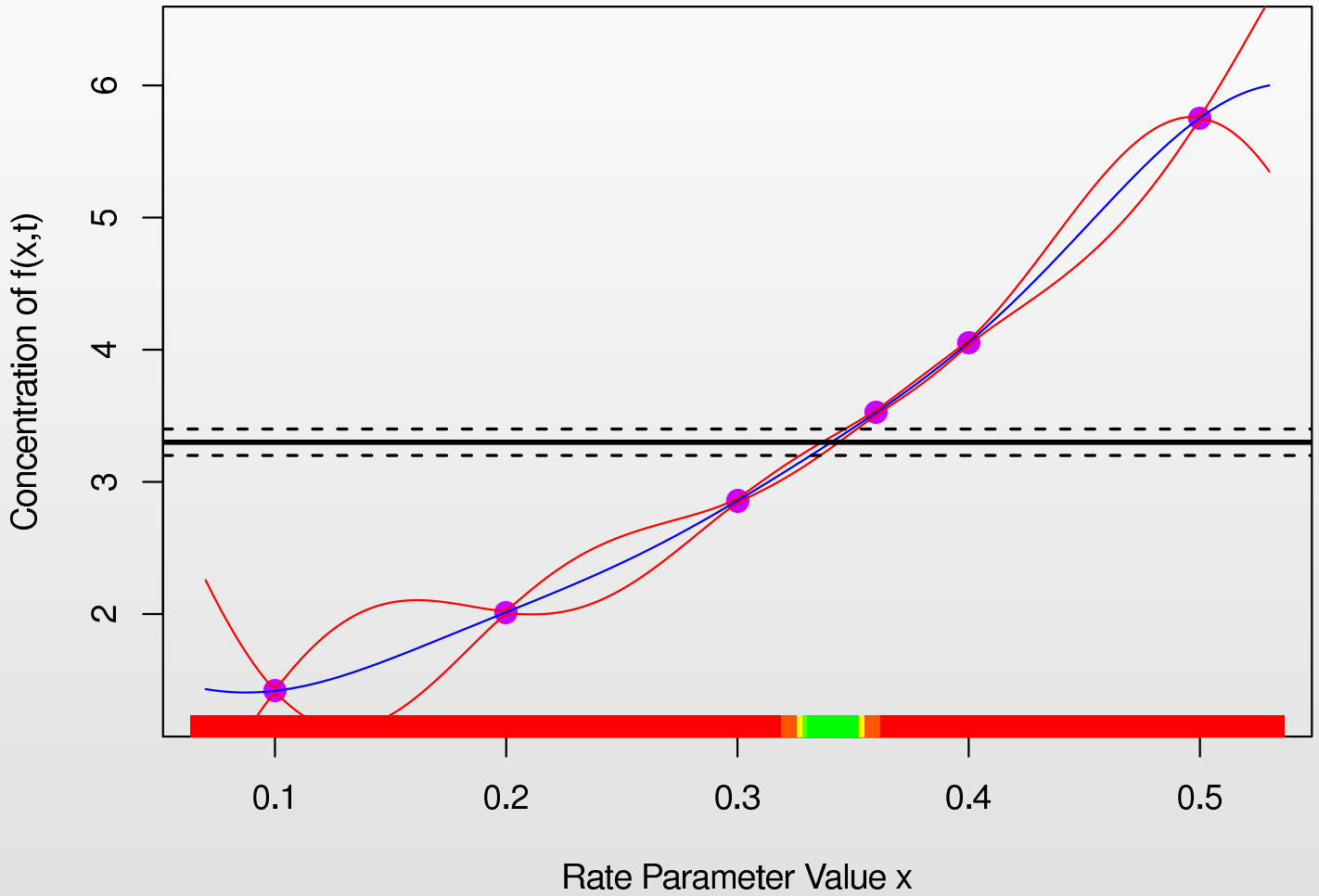


Iterative Input Space Reduction: 1D example



- Comparing the emulator to the observed measurement we again identify the set of x values currently consistent with this data (the observed errors here have been reduced for clarity).
- Note: uncertainty on x now includes uncertainty coming from the emulator.

Iterative Input Space Reduction: 1D example



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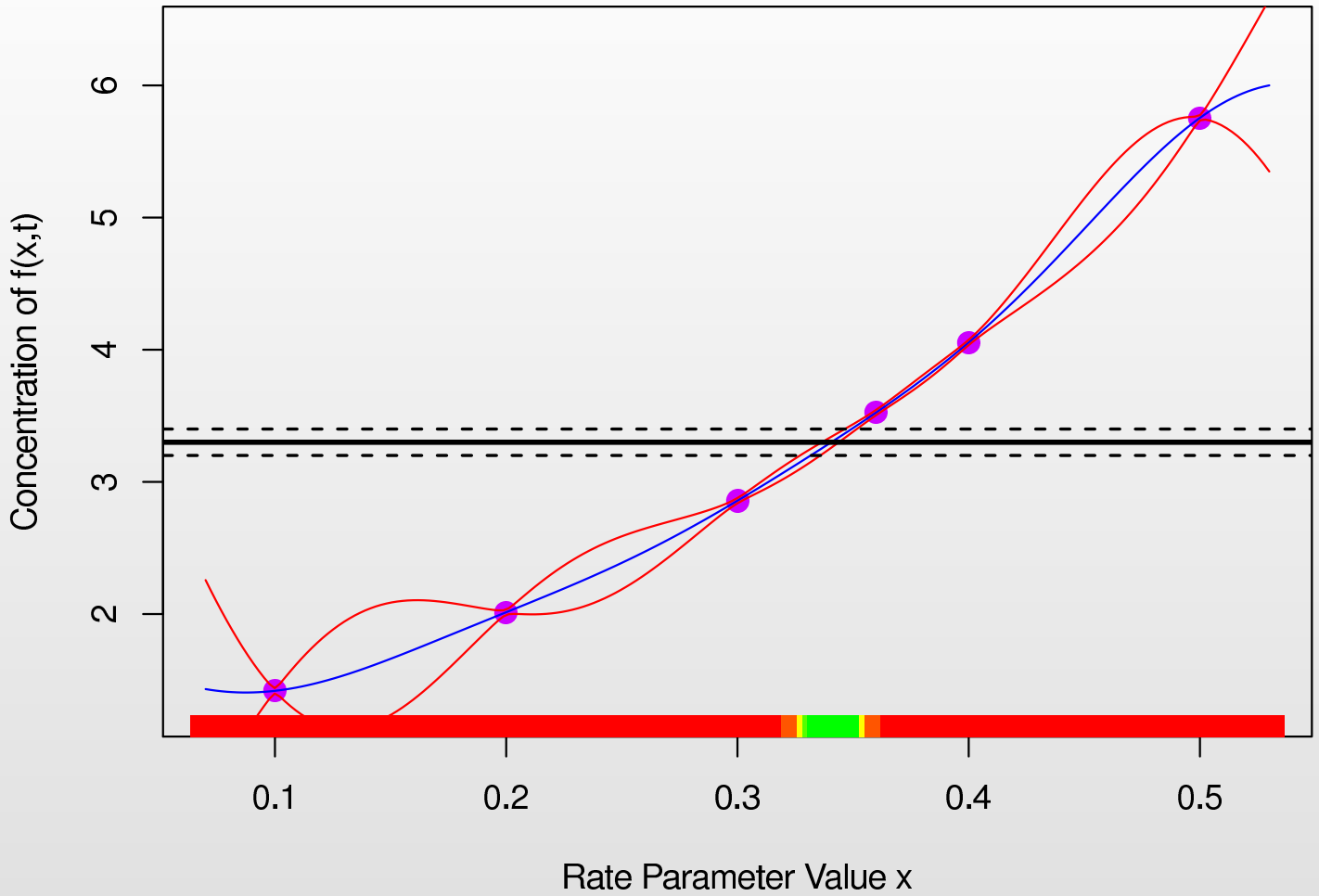

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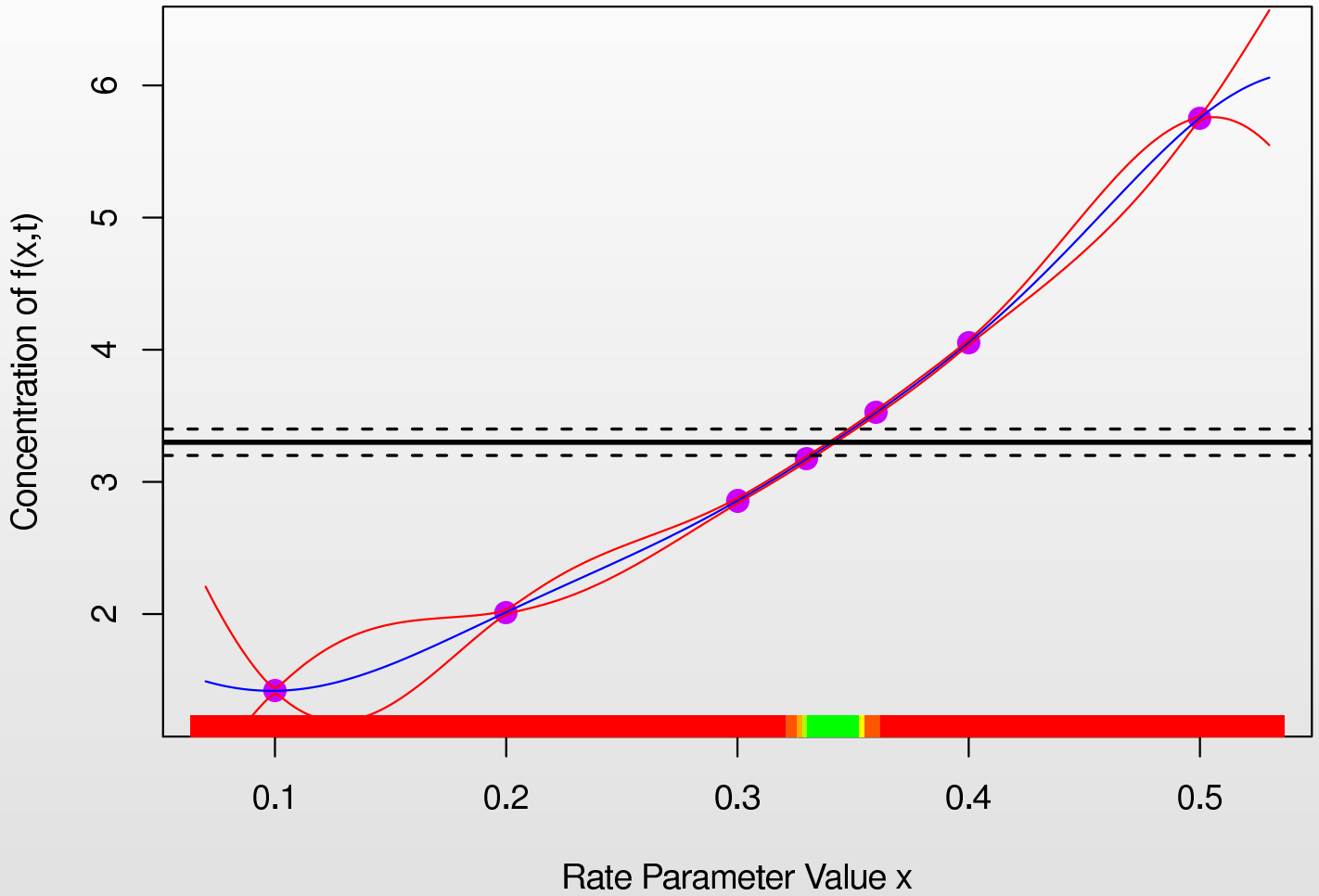
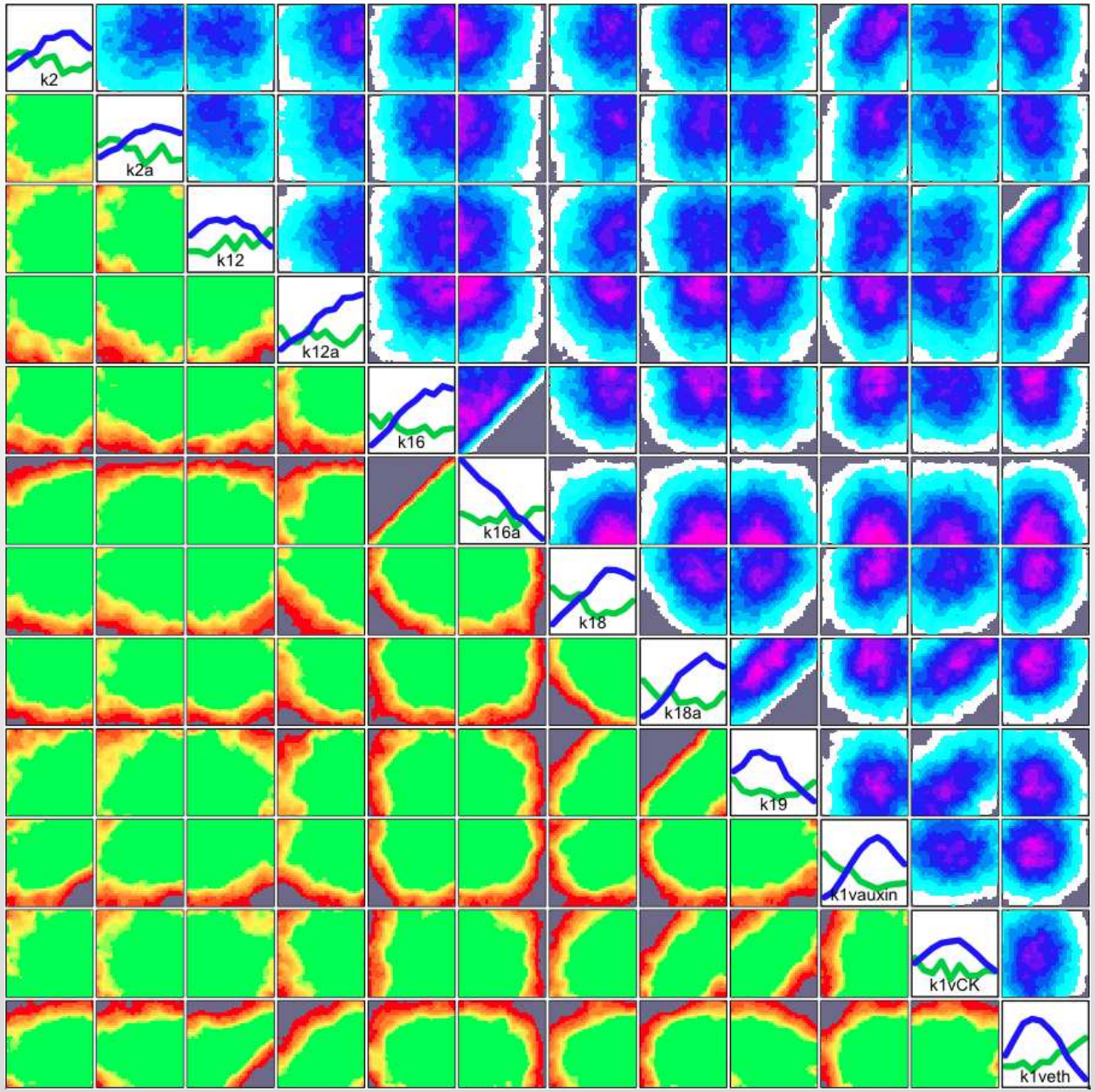
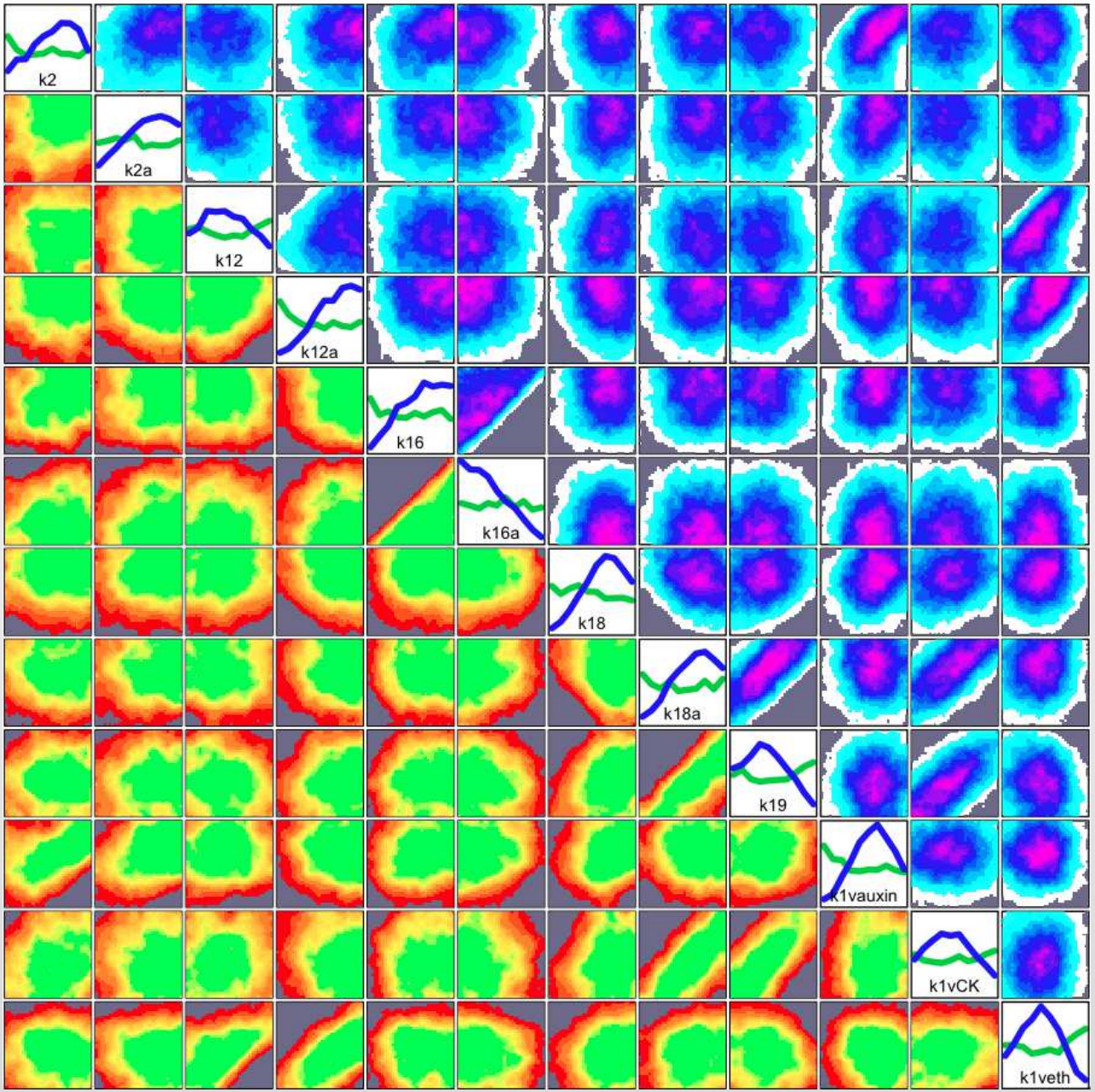


- We perform a 2nd iteration or wave of runs to improve emulator accuracy.
- The runs are located only at non-implausible (green/yellow) points.
- Now the emulator is more accurate than the observations, and we can identify the set of all x values of interest.

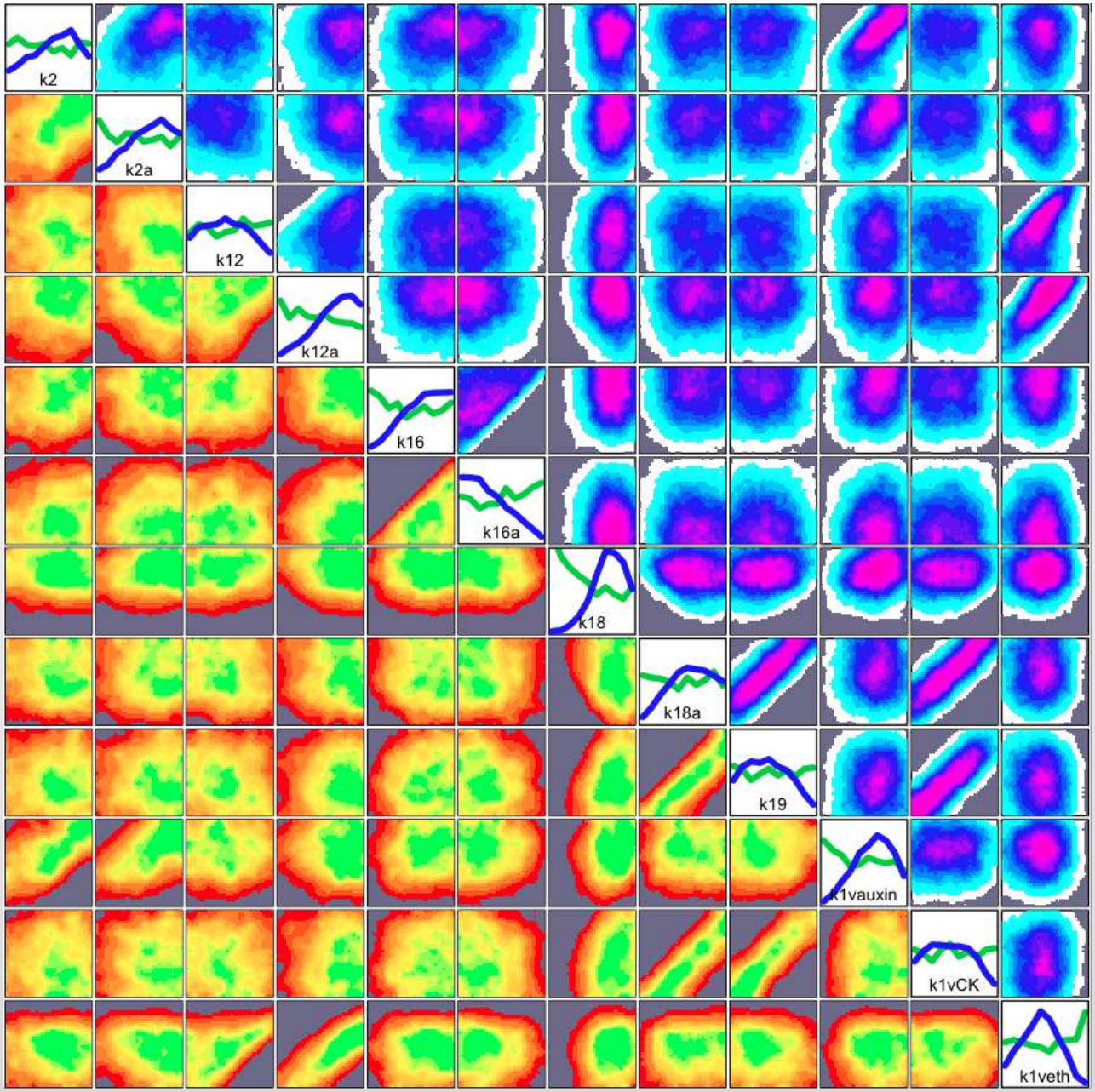
Iterative Input Space Reduction: Arabidopsis Model Wave 1



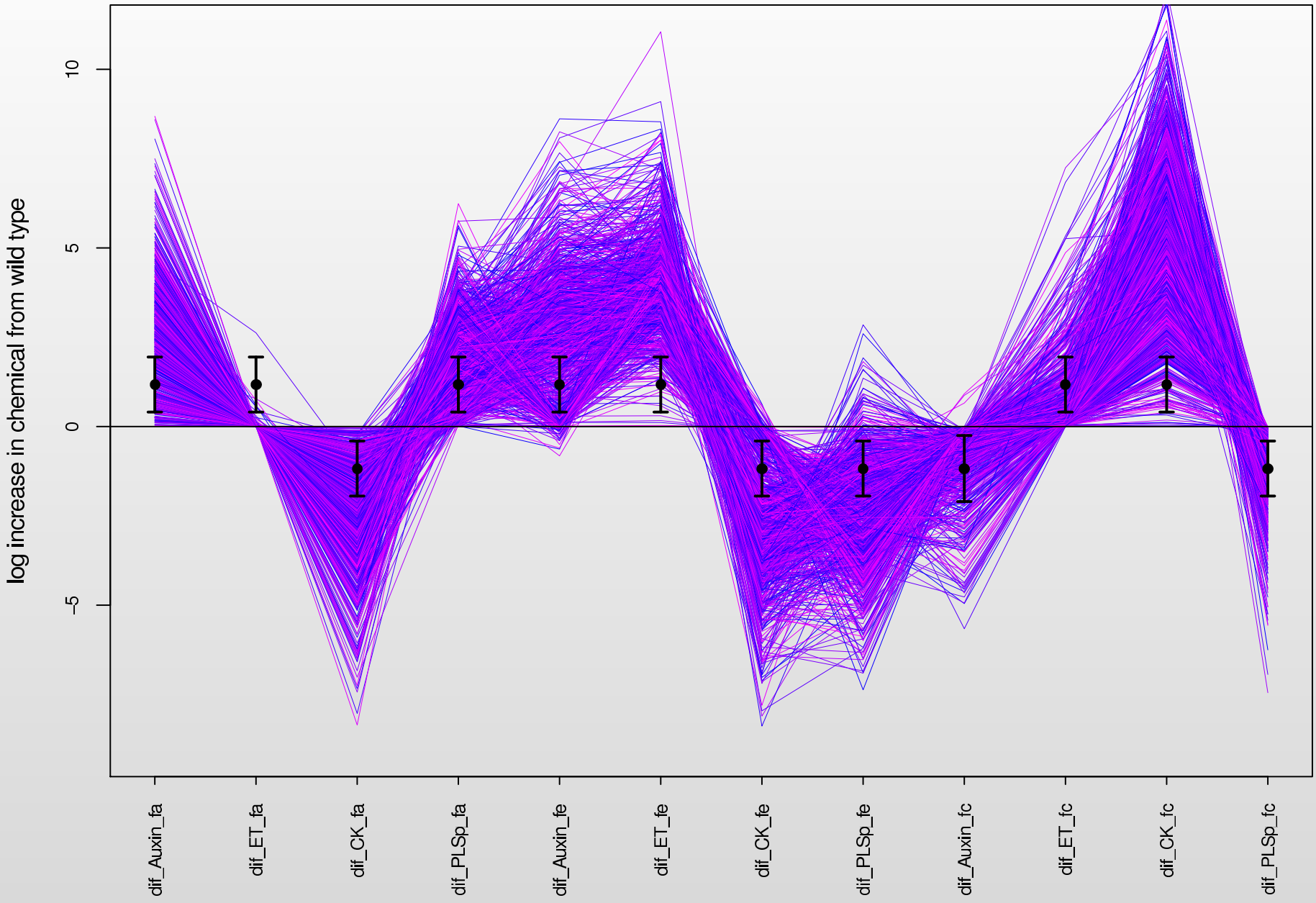
Iterative Input Space Reduction: Arabidopsis Model Wave 2



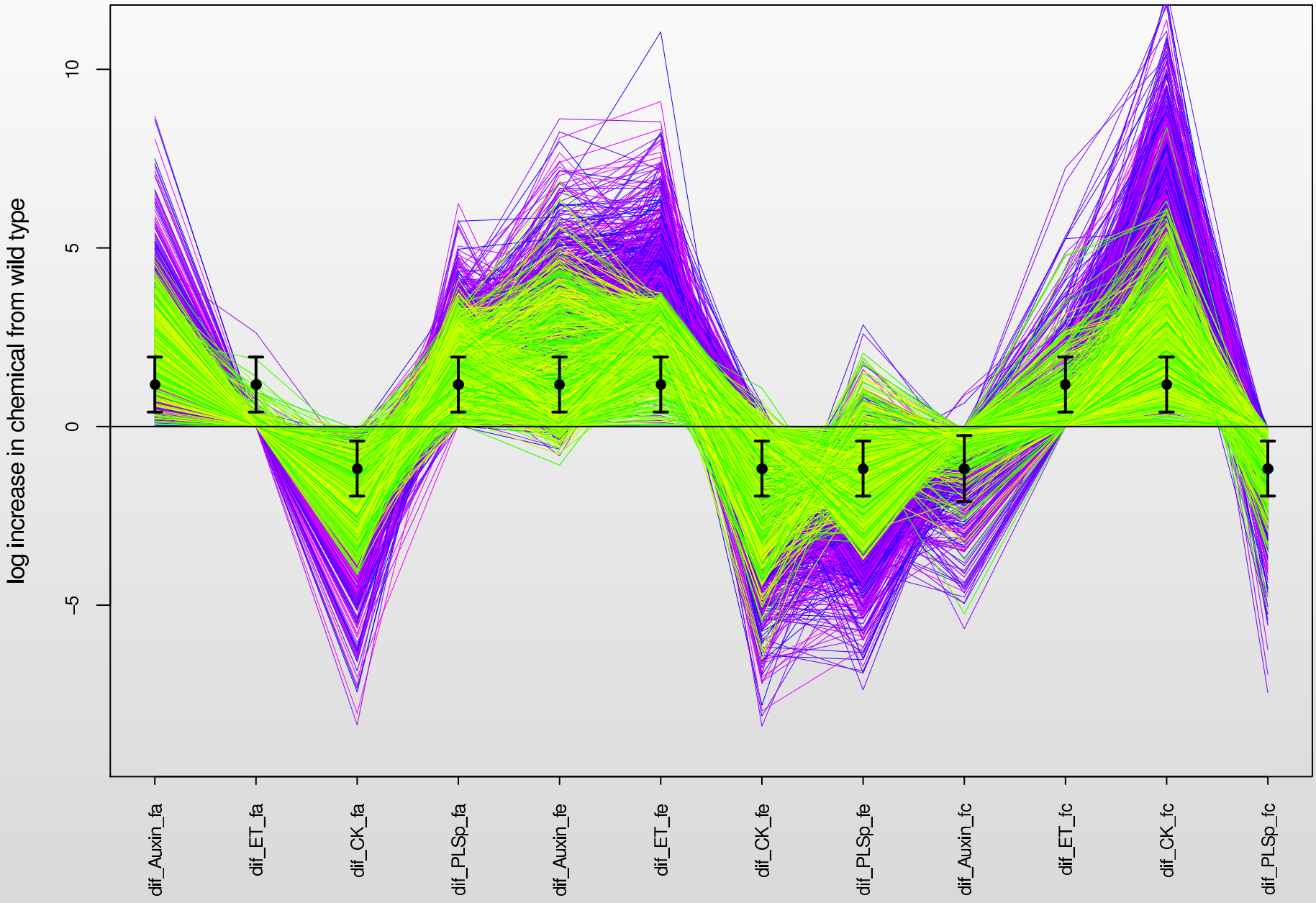
Iterative Input Space Reduction: Arabidopsis Model Wave 3



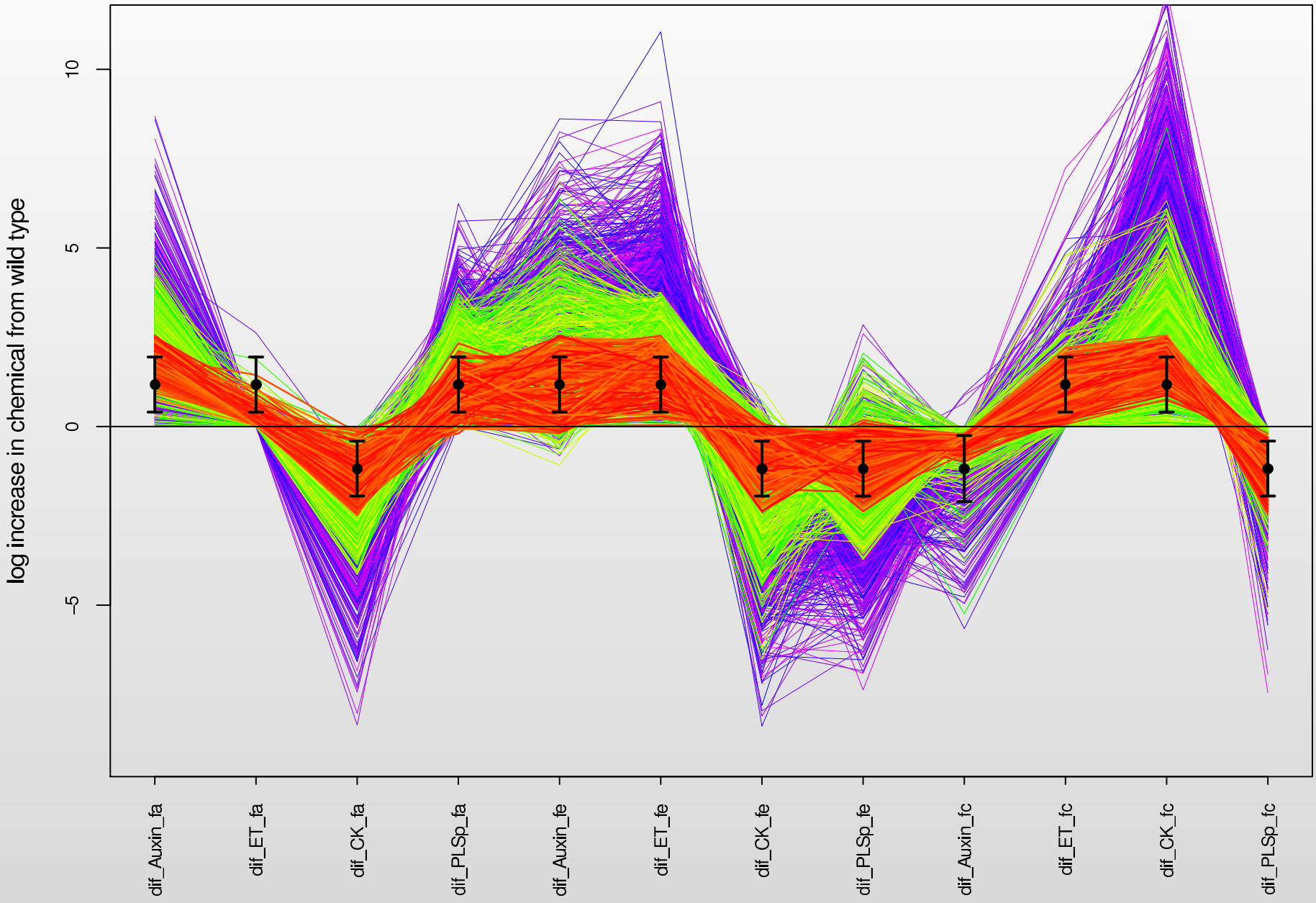
Iterative Strategy for Arabidopsis Model: Wave 1



Iterative Strategy for Arabidopsis Model: Waves 1 and 2



Iterative Strategy for Arabidopsis Model: Wave 1, 2 and 3



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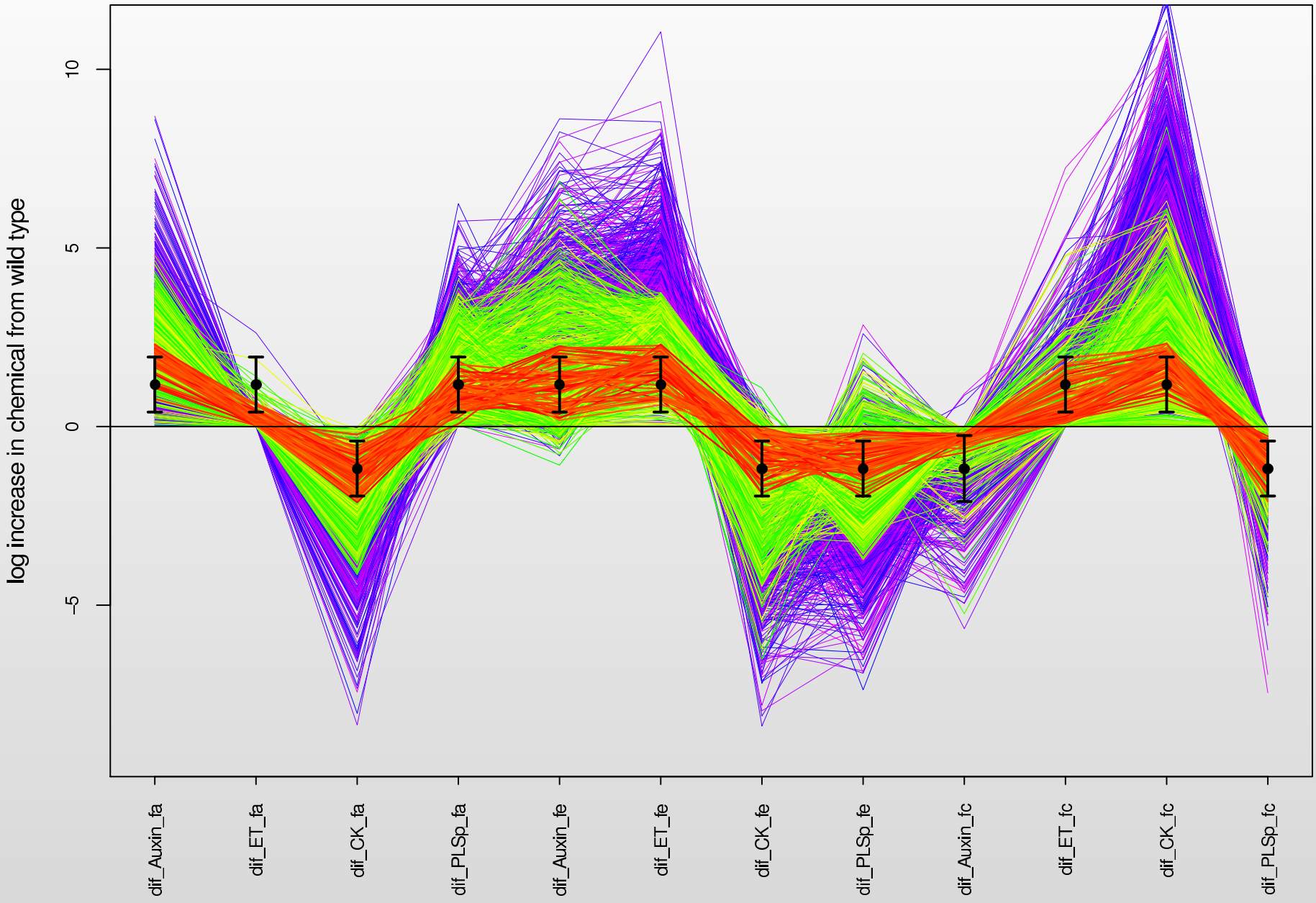
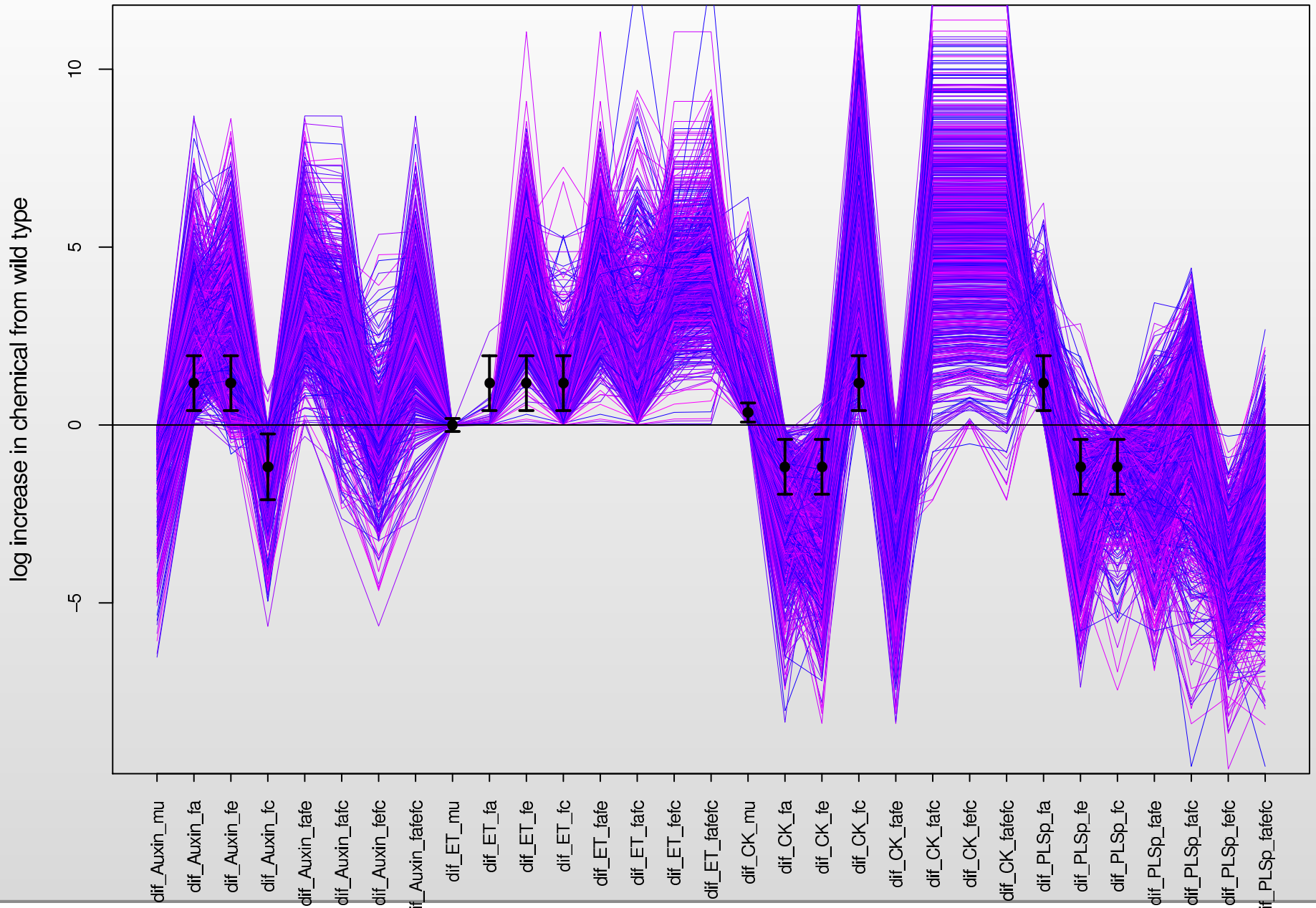
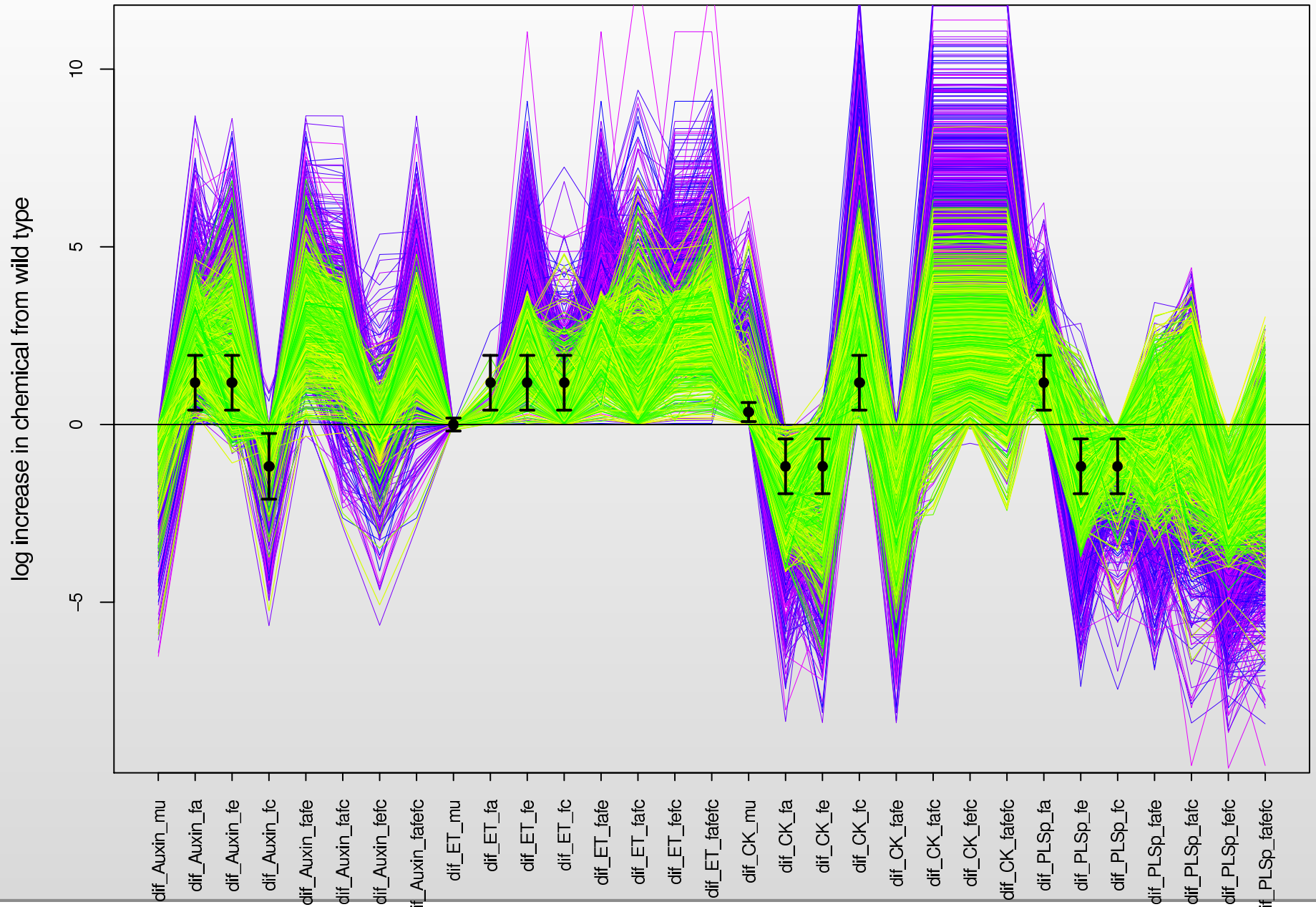


Iterative Strategy for Arabidopsis Model: Wave 1



Iterative Strategy for Arabidopsis Model: Waves 1 and 2



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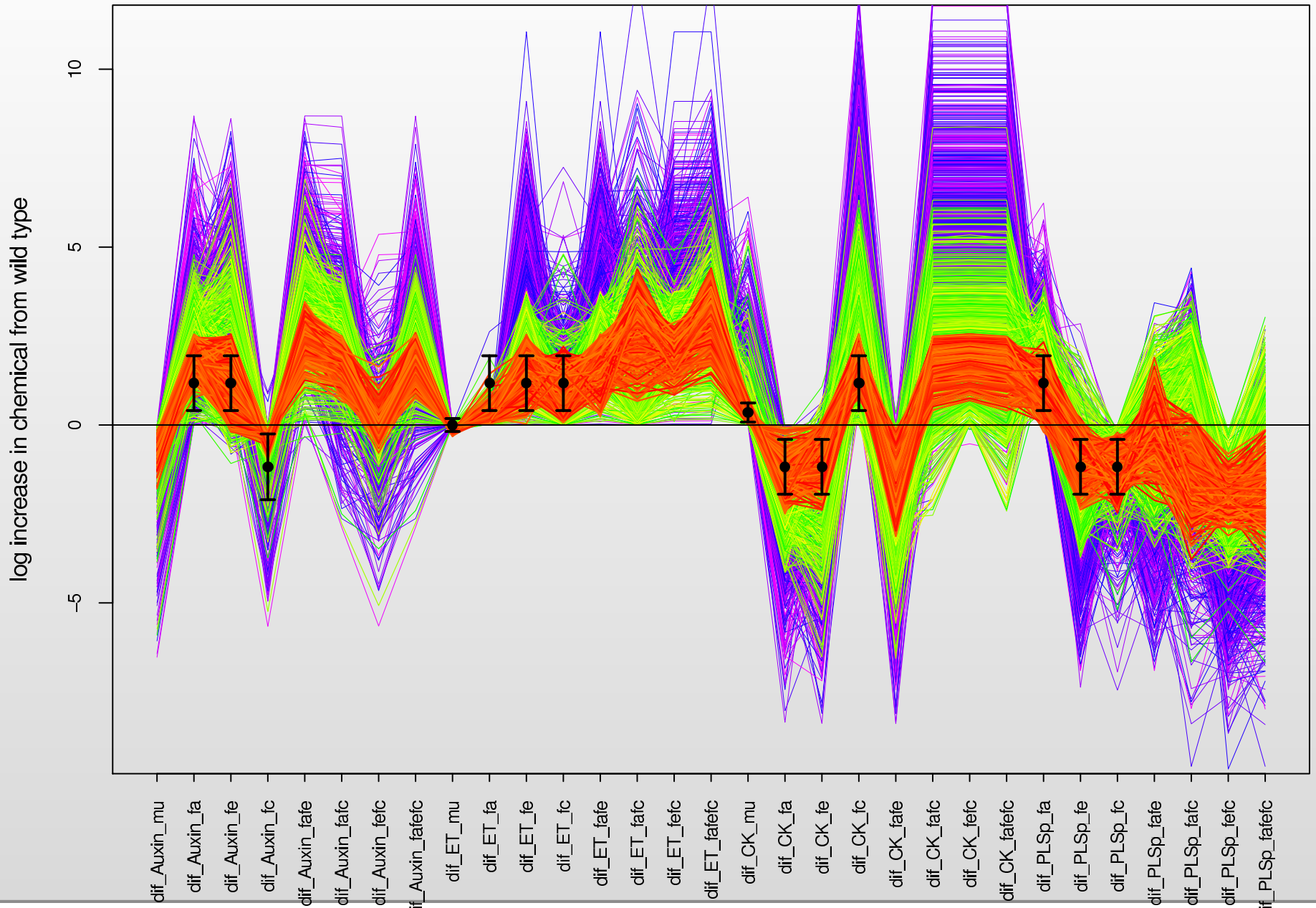

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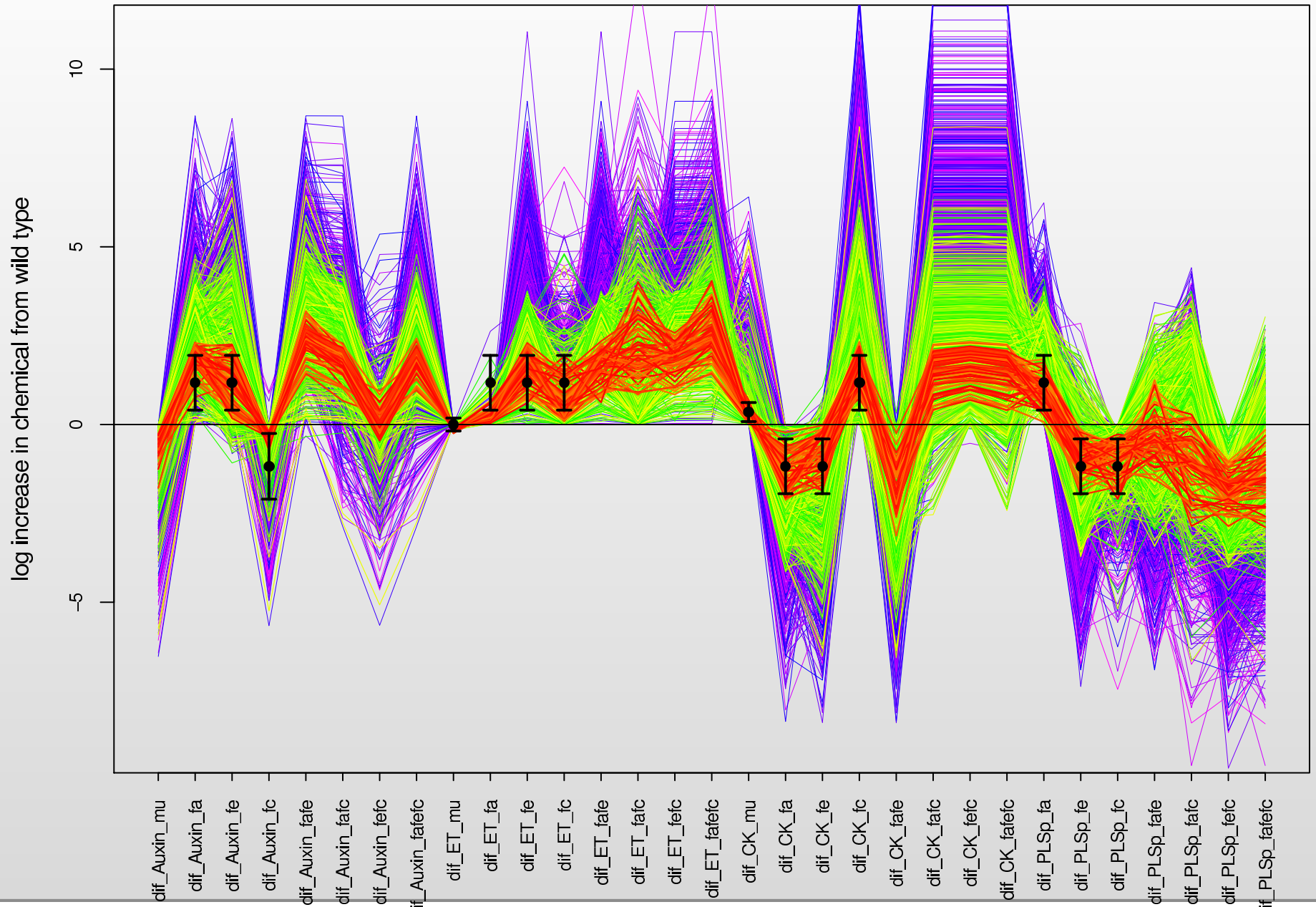

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- We hence expect to learn most efficiently about the rate parameters x from this design of 4 experiments.

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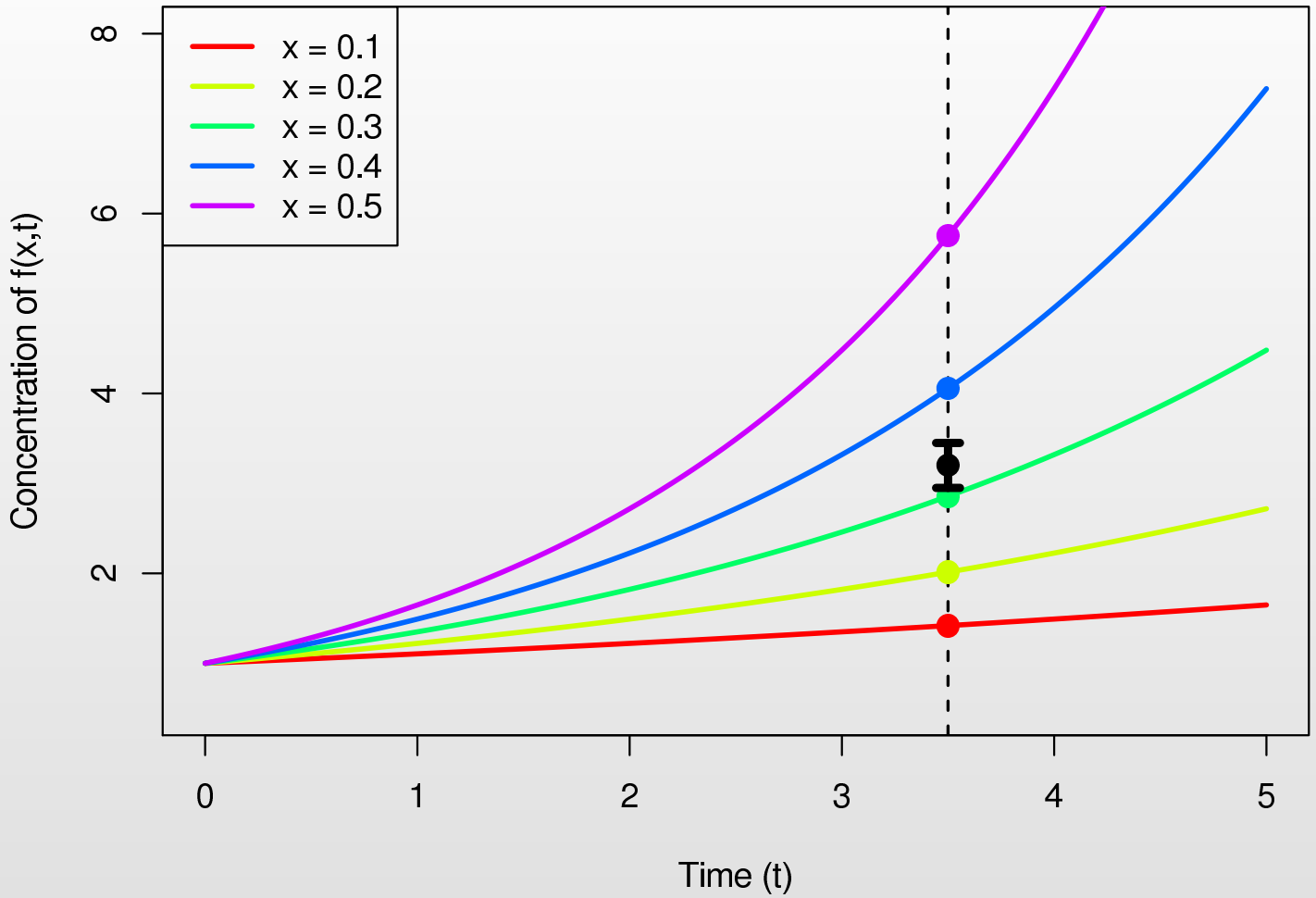

- Using the emulator we can choose several values of x consistent with the measurement of $f(x,t)$ at $t = 3.5$, and perform corresponding runs of the model.

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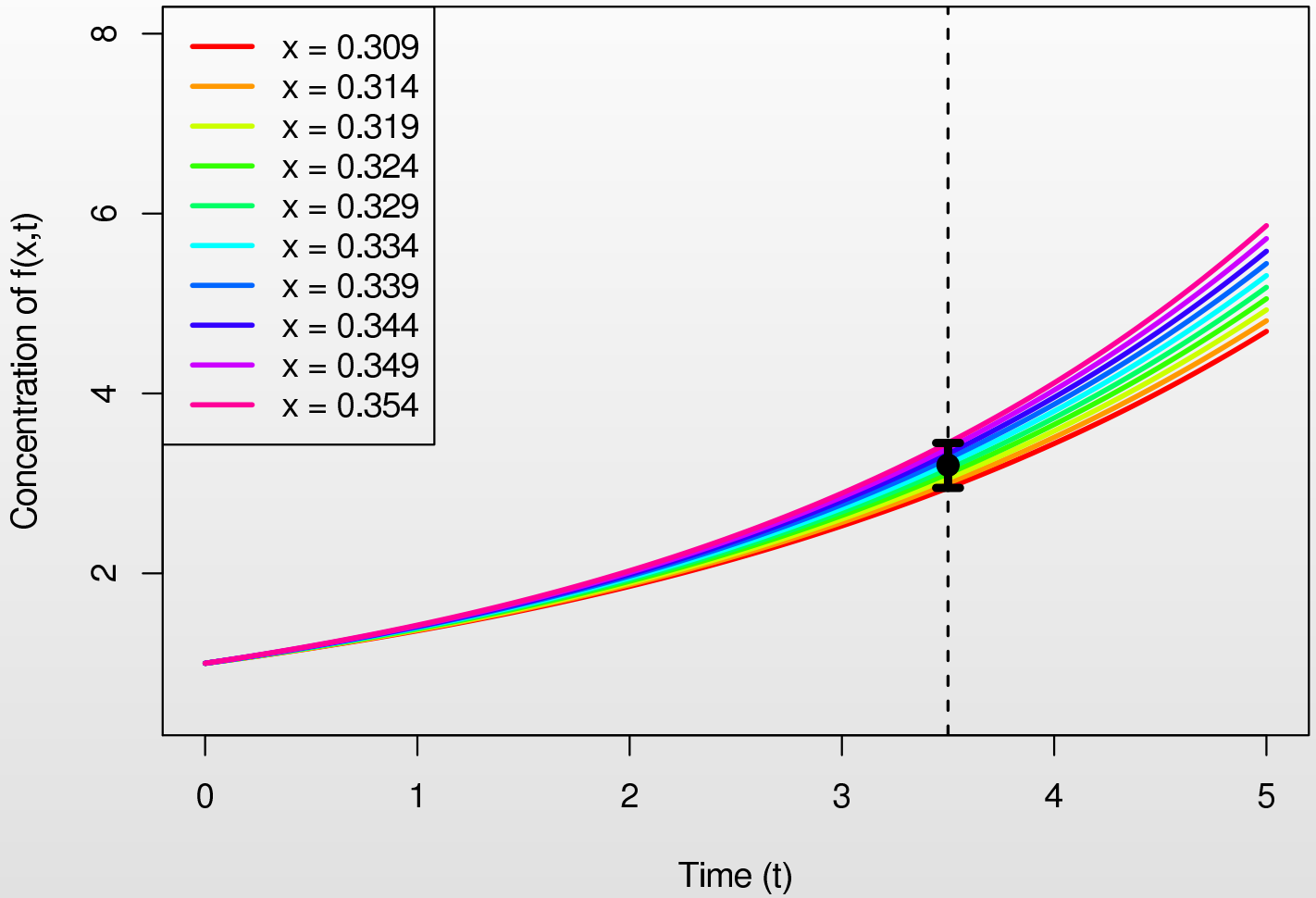

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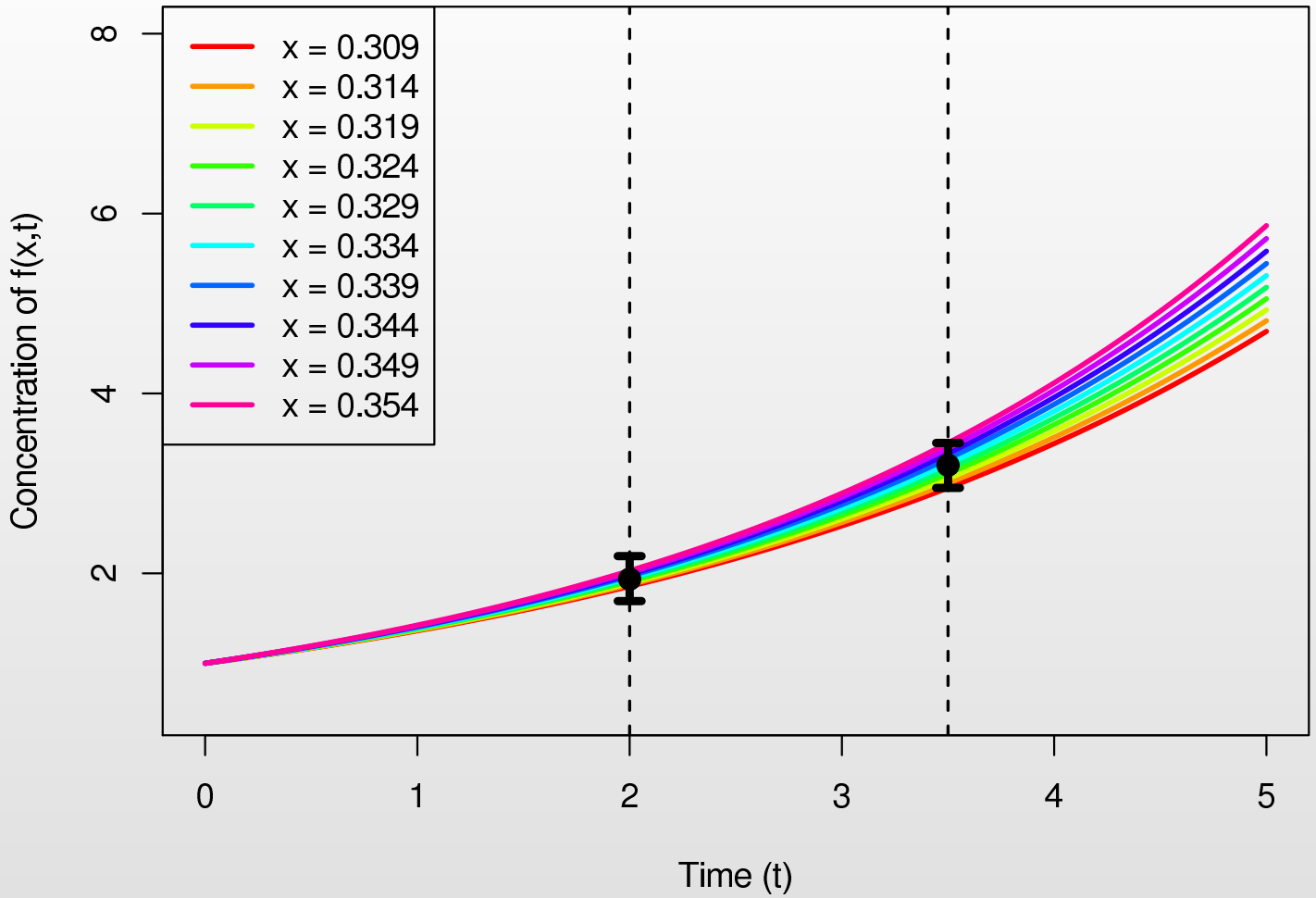

- Using the emulator we can choose several values of x consistent with the measurement of $f(x,t)$ at $t = 3.5$, and perform corresponding runs of the model.
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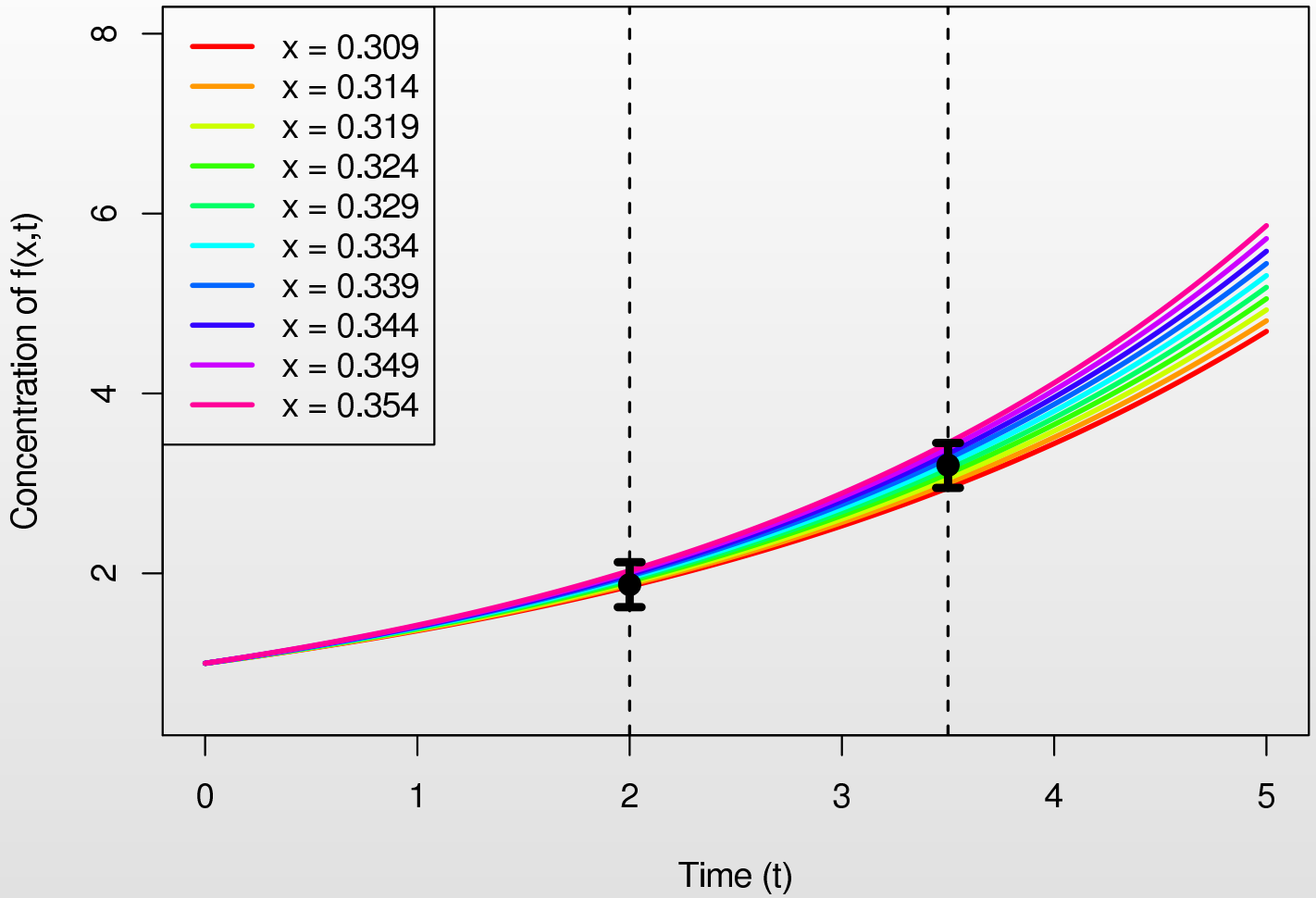

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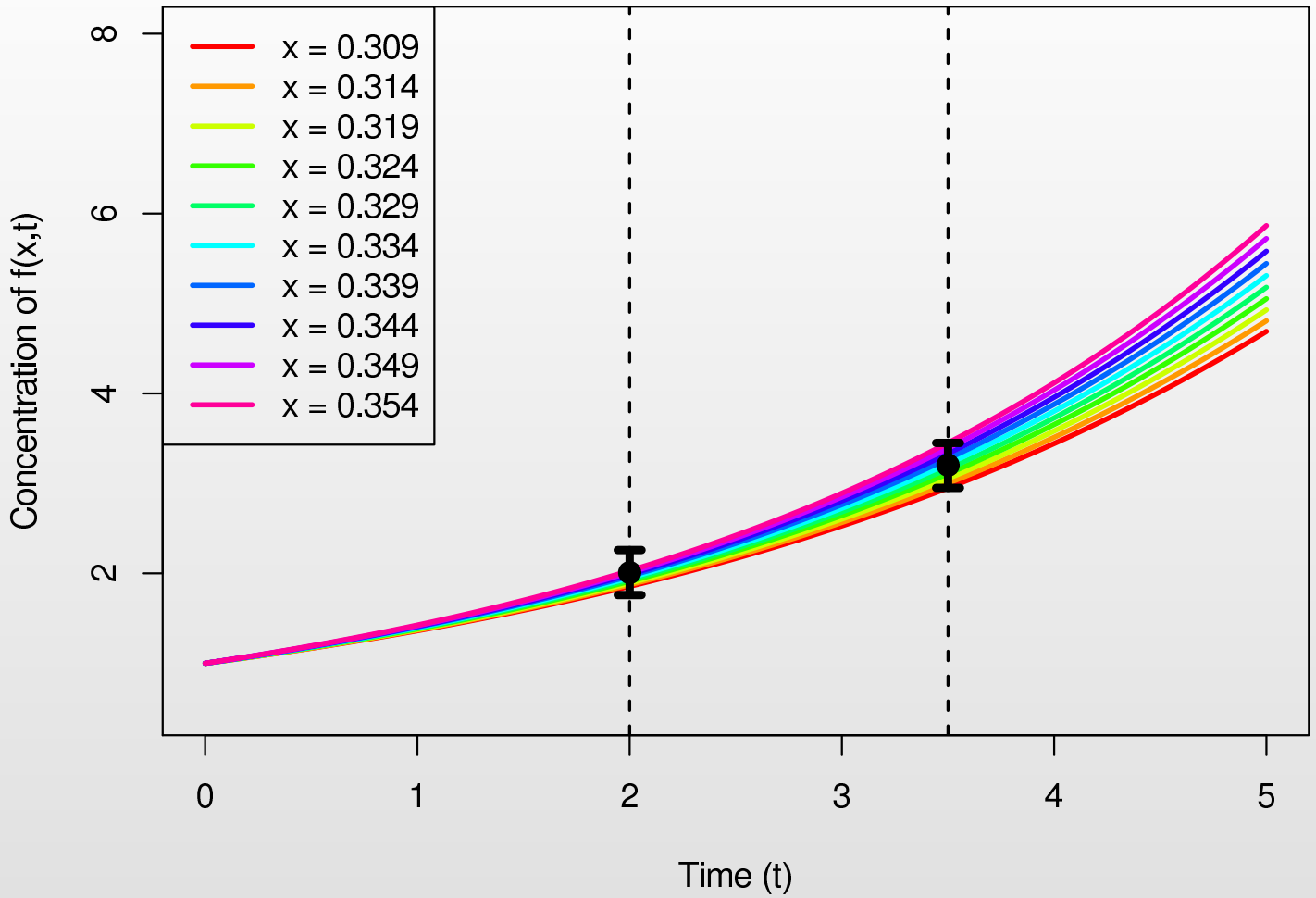

- The predictions imply that any measurement of $Y(t = 2)$ is highly unlikely to be informative for x.
- This is due to the measurement errors swamping the signal from the model output $Y(t = 2)$.

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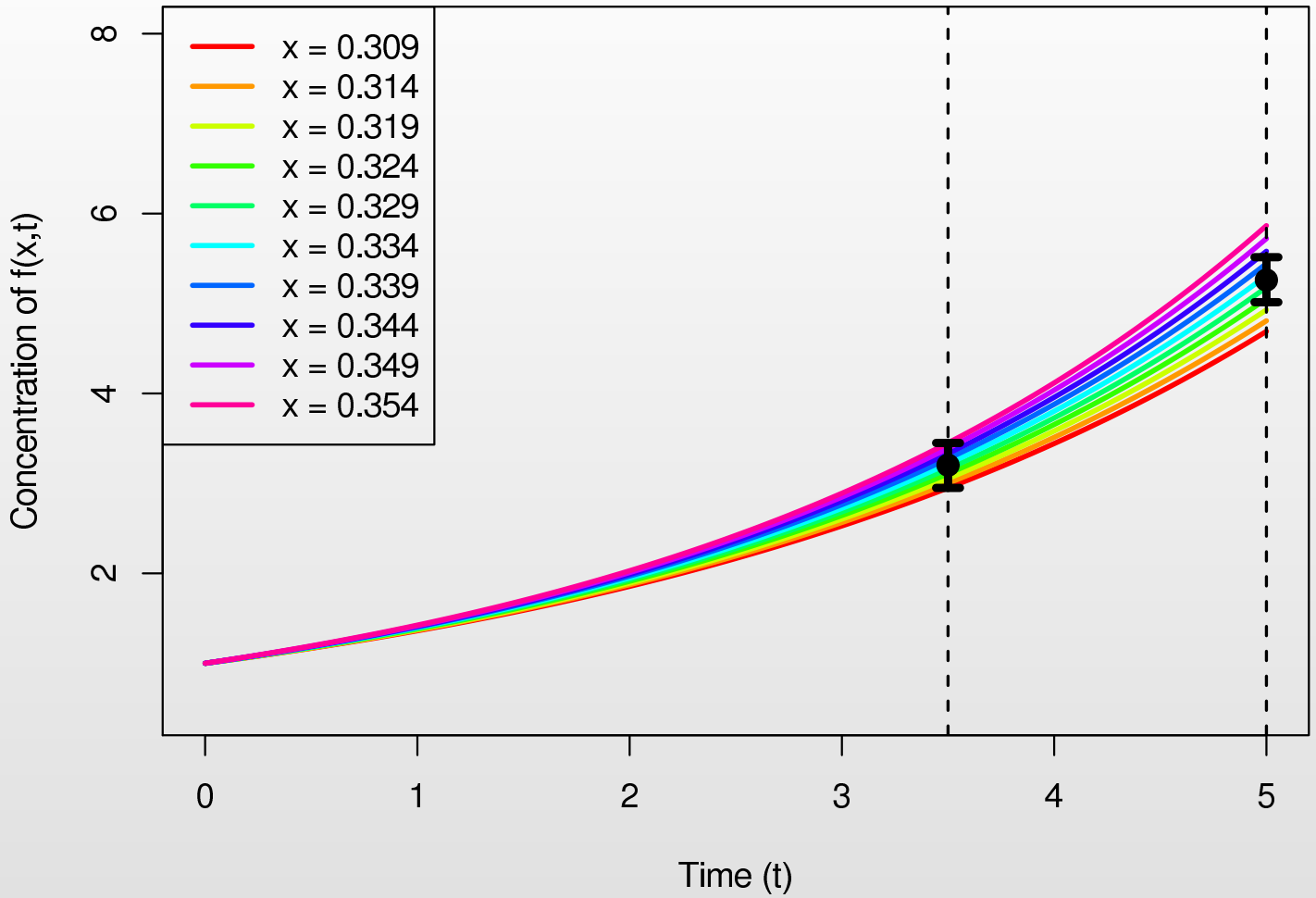

- The predictions for $Y(t = 5)$ show a different conclusion.

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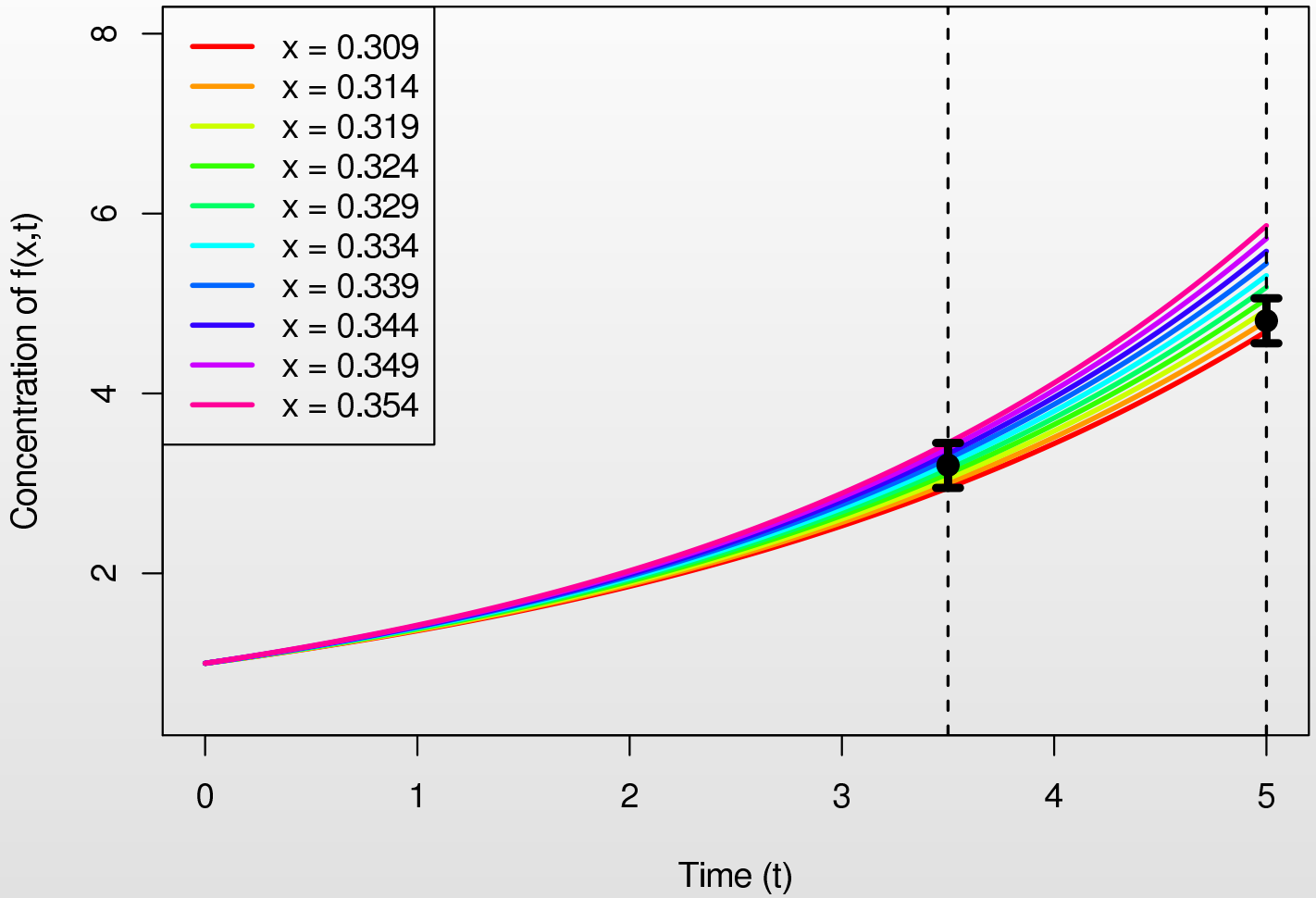

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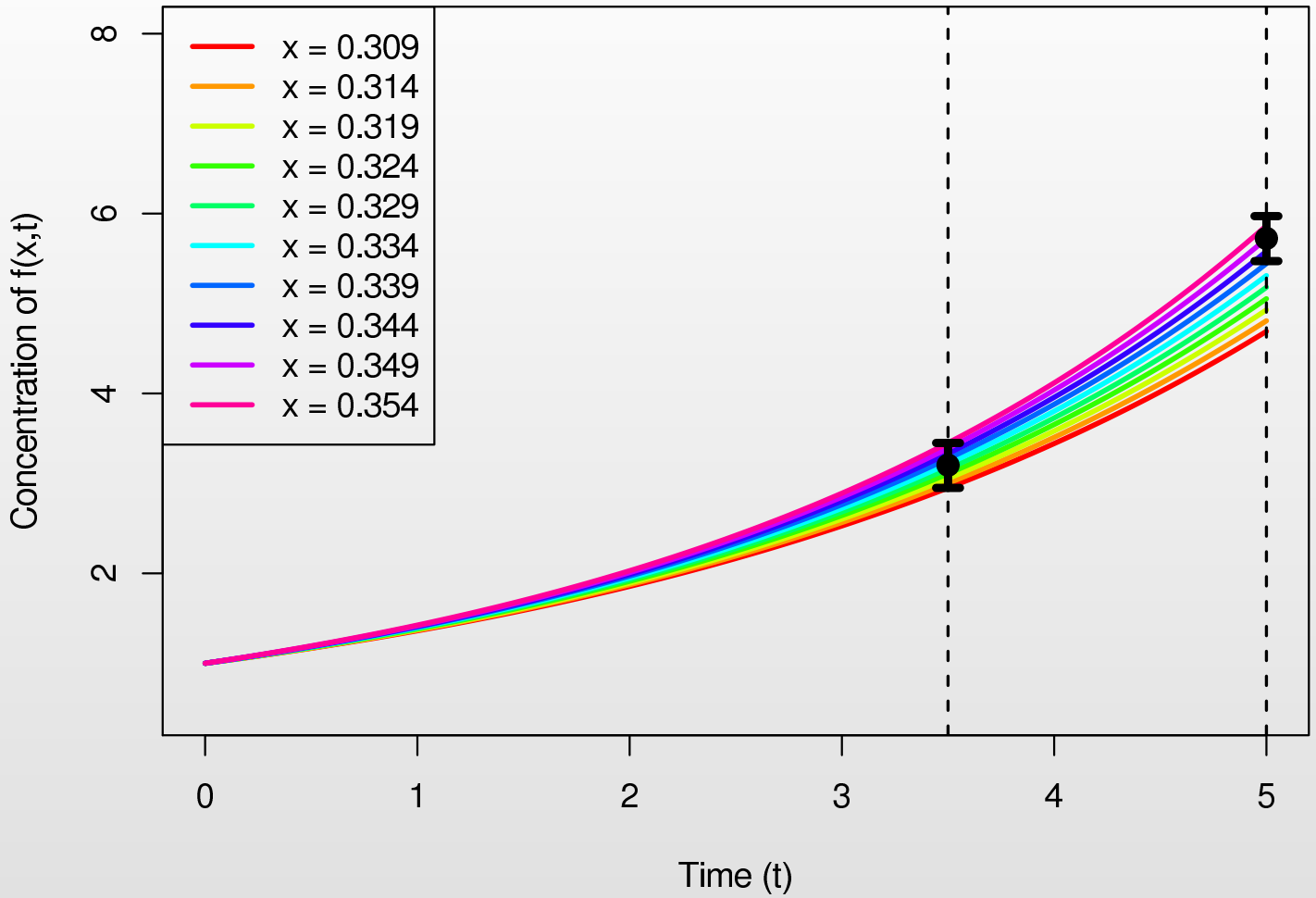
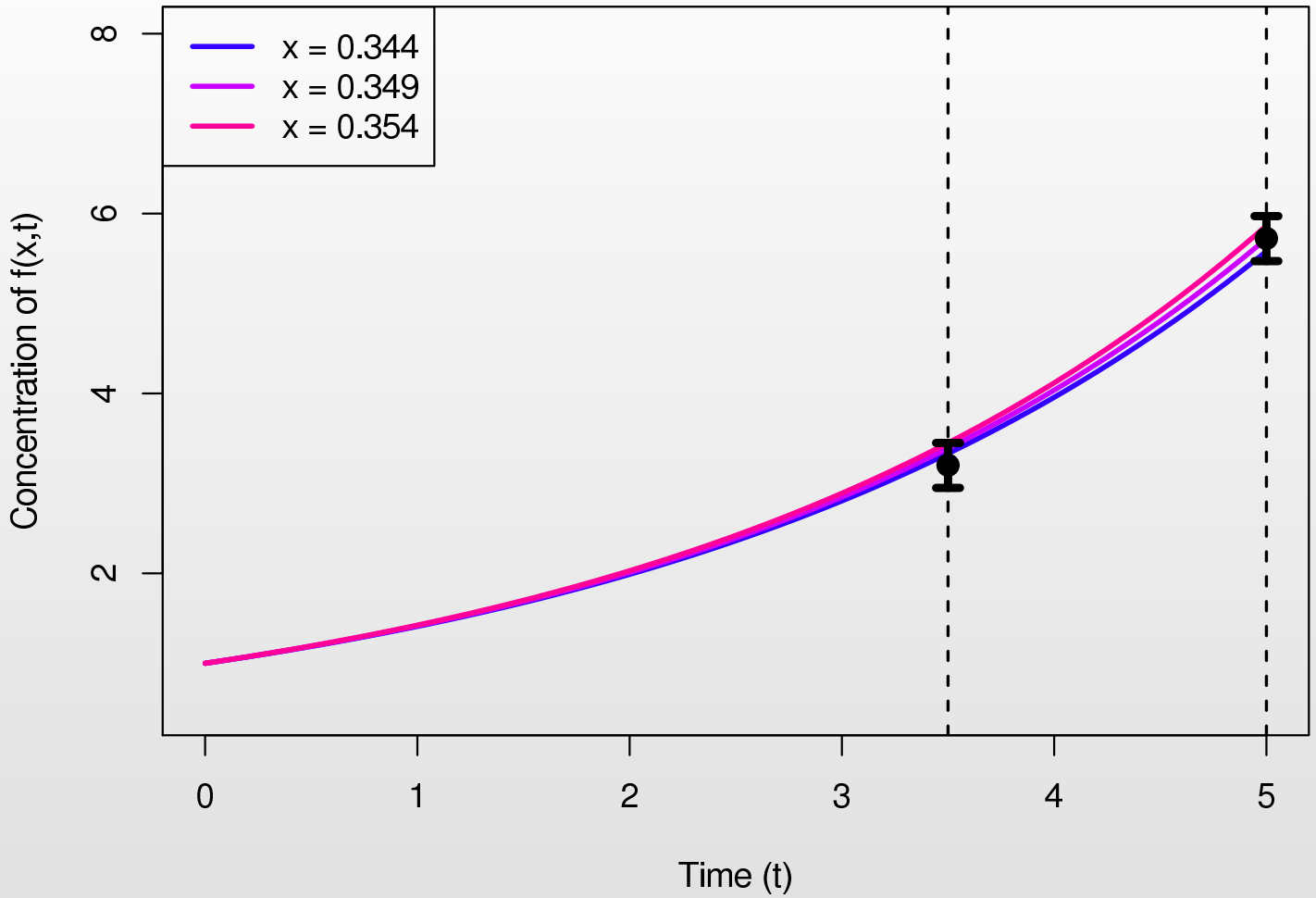


- The predictions for $Y(t = 5)$ show a different conclusion.
- For each possible measurement of $Y(t = 5)$ it is highly likely that we will be able to rule out several more values of x as implausible.

Designing new experiment: 1D example



- For one possible measurement, see that non-implausible values of x would lie between 0.344 and 0.354, ruling out 70% of the possible values of x.

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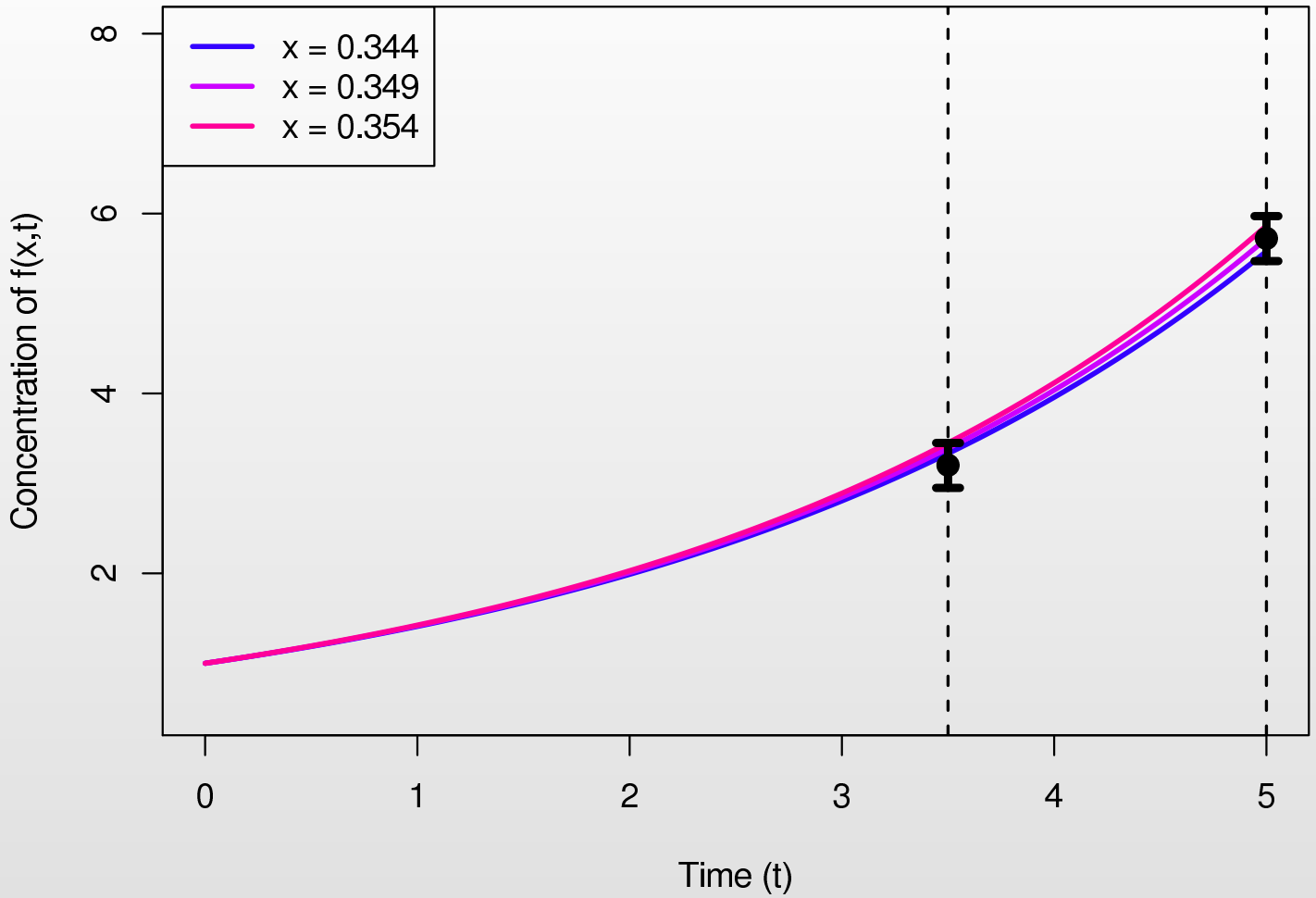
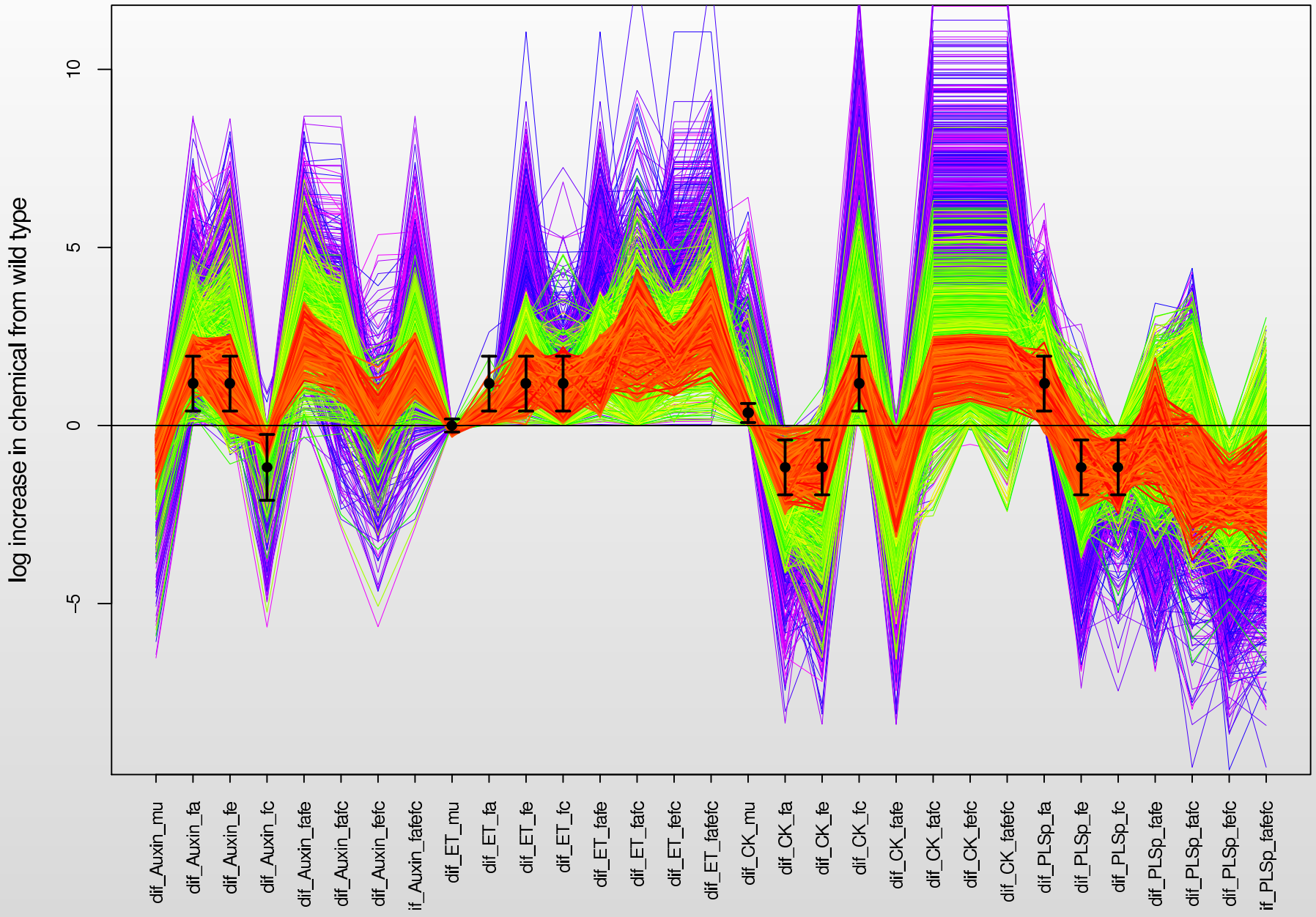
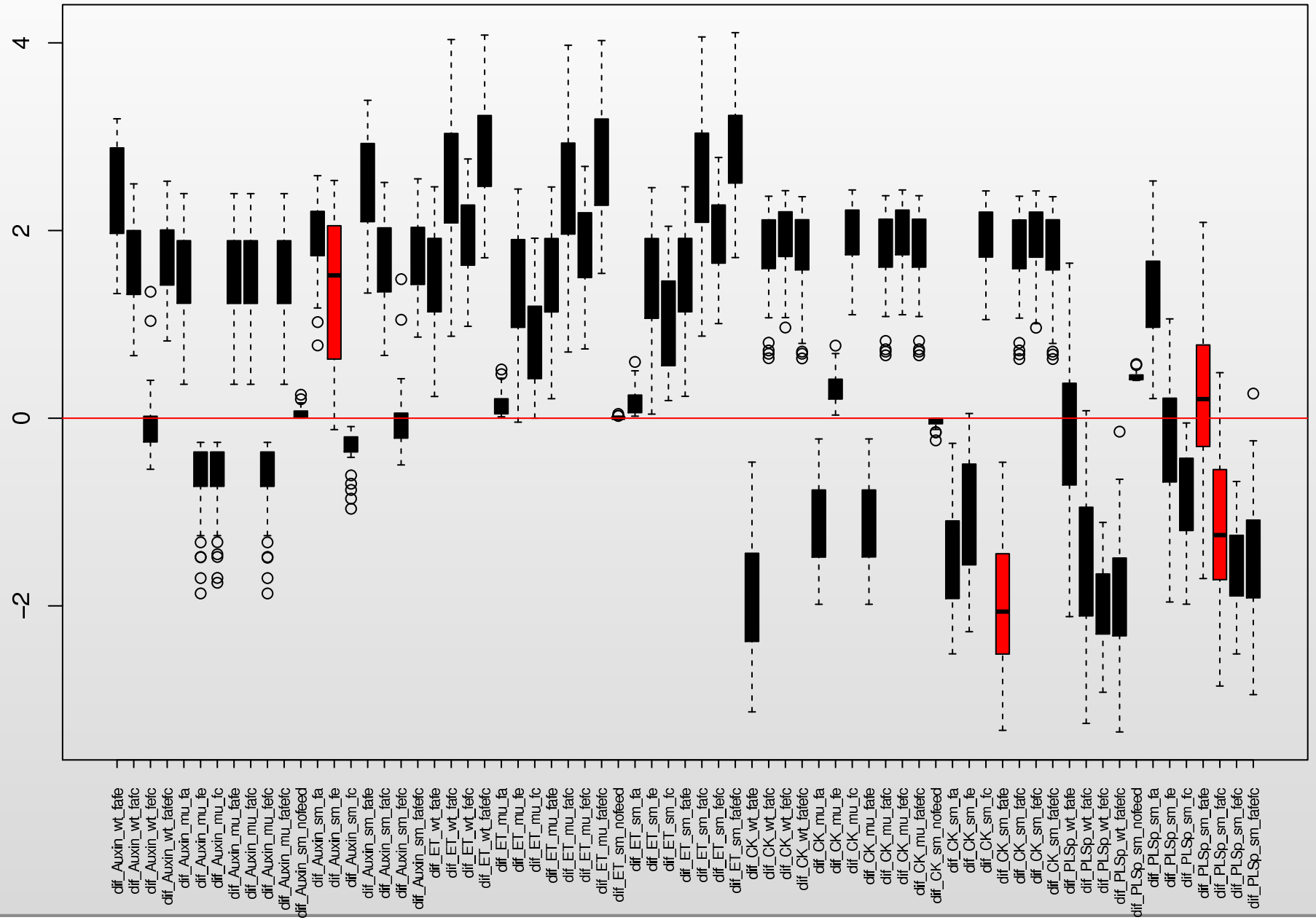


- For one possible measurement, see that non-implausible values of x would lie between 0.344 and 0.354, ruling out 70% of the possible values of x.
- This high expected space reduction in x implies that Experiment B, measuring $f(x,t)$ at $t = 5$, is clearly the best choice.

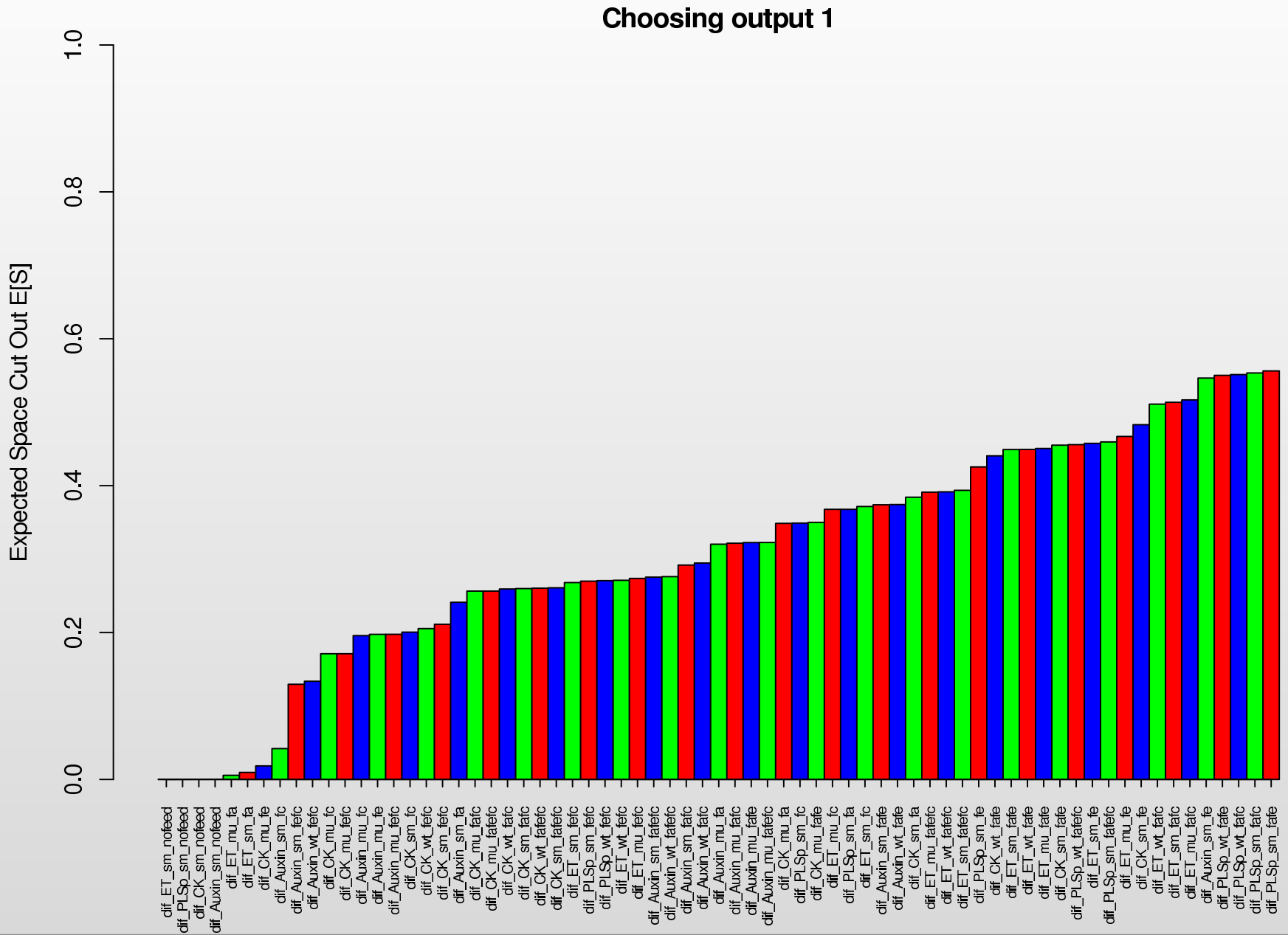
History Matching Plots Plus New Outputs



Predictions for New Outputs



Space Cut Out Criteria for New Outputs



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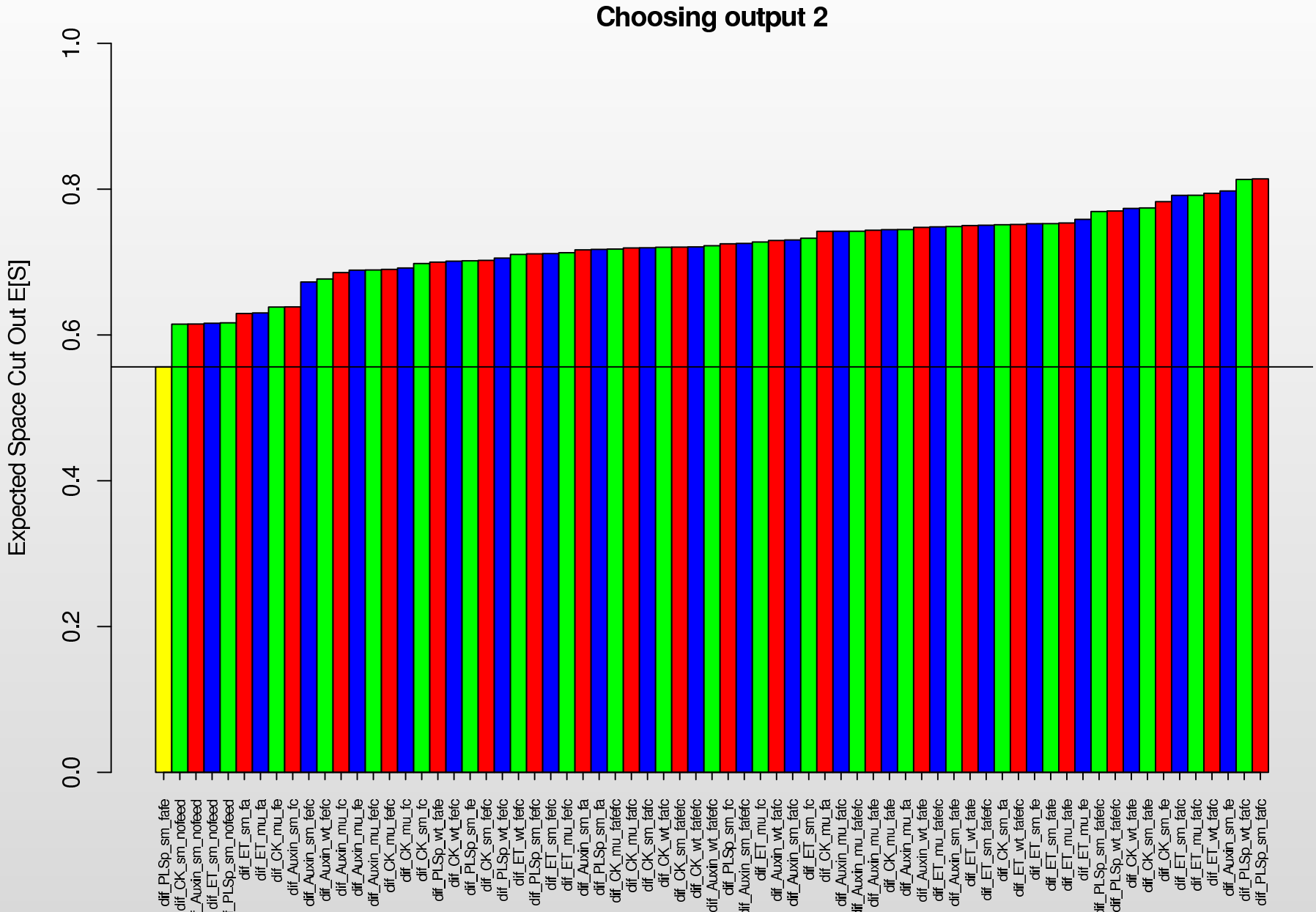

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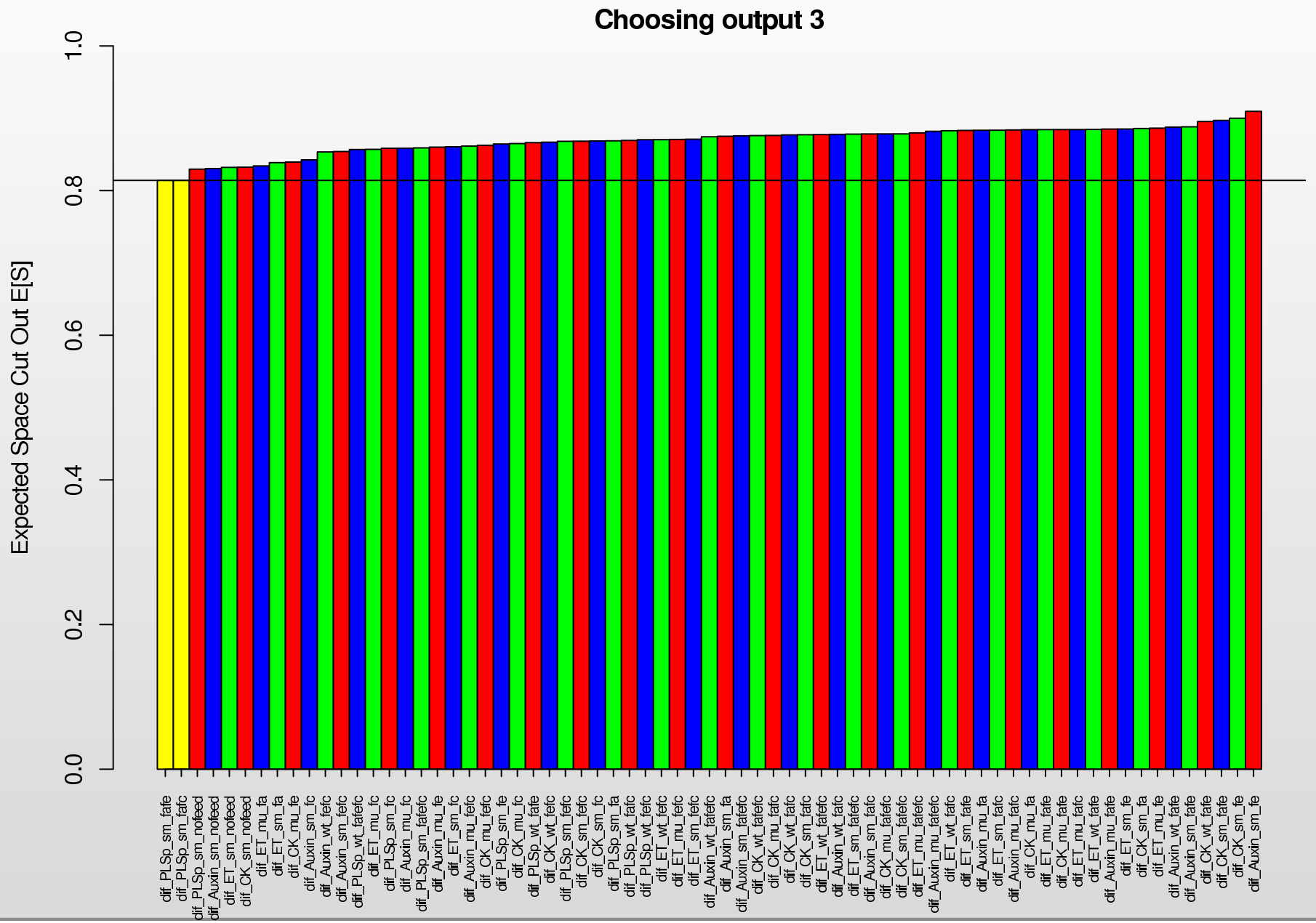

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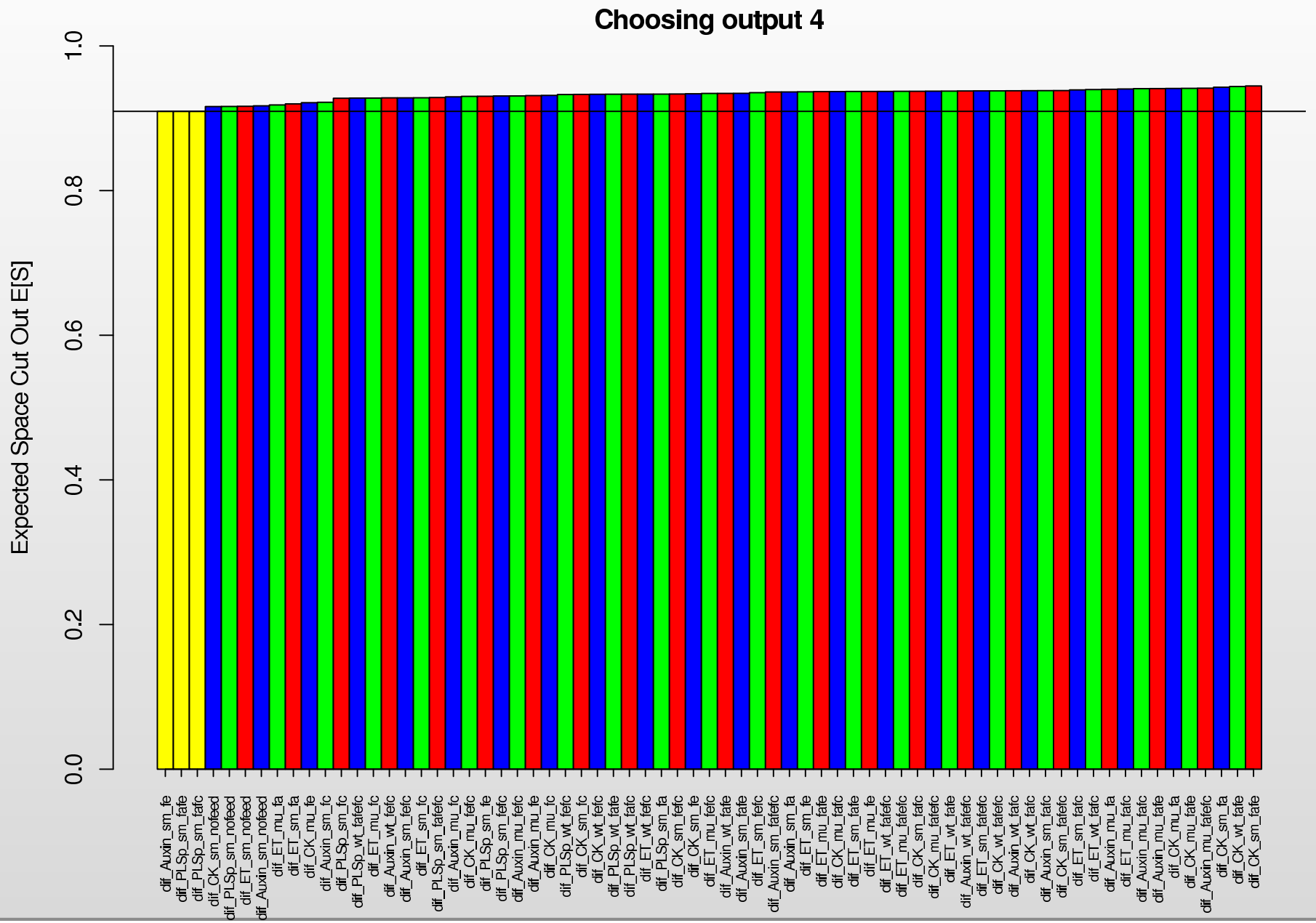

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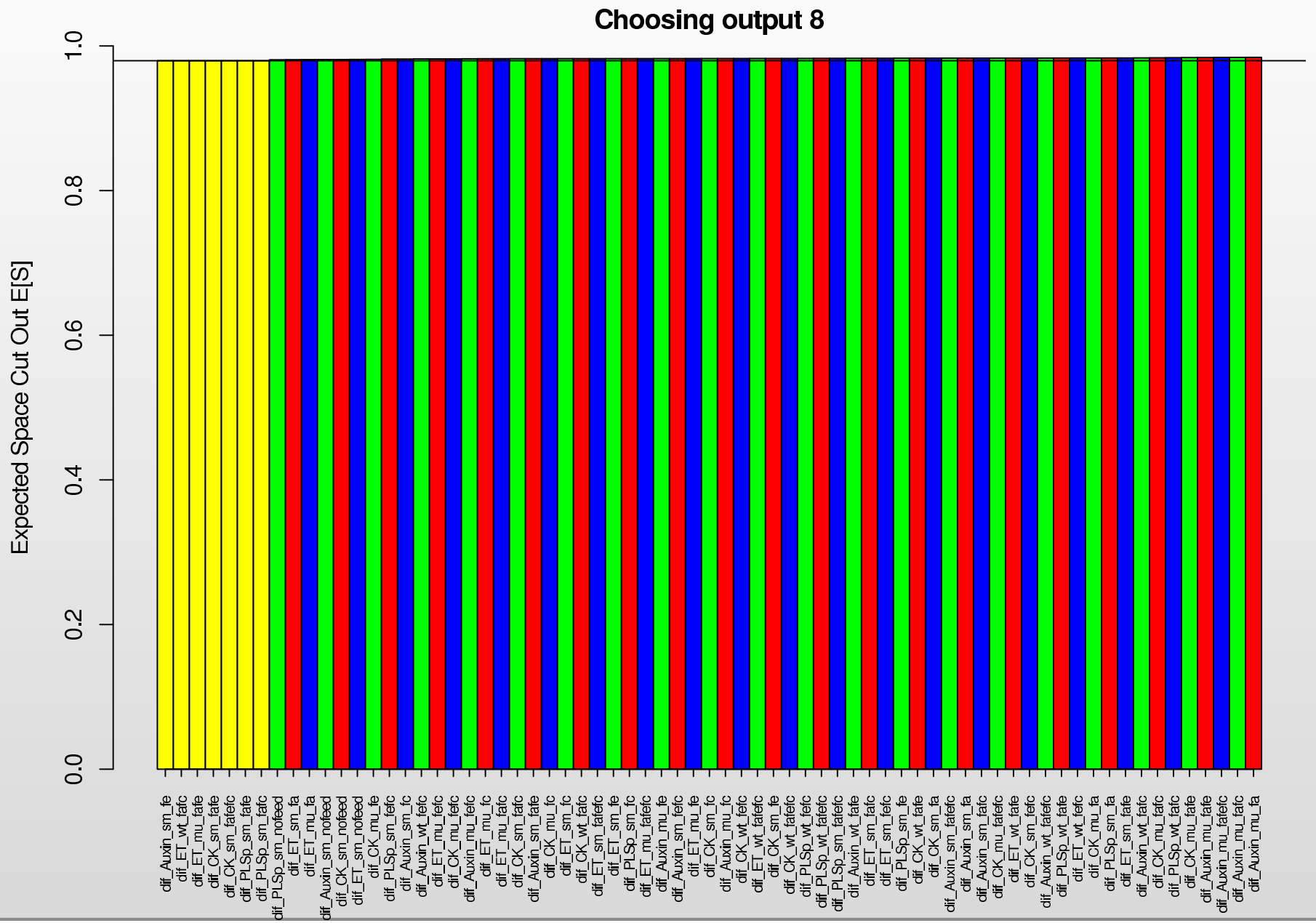

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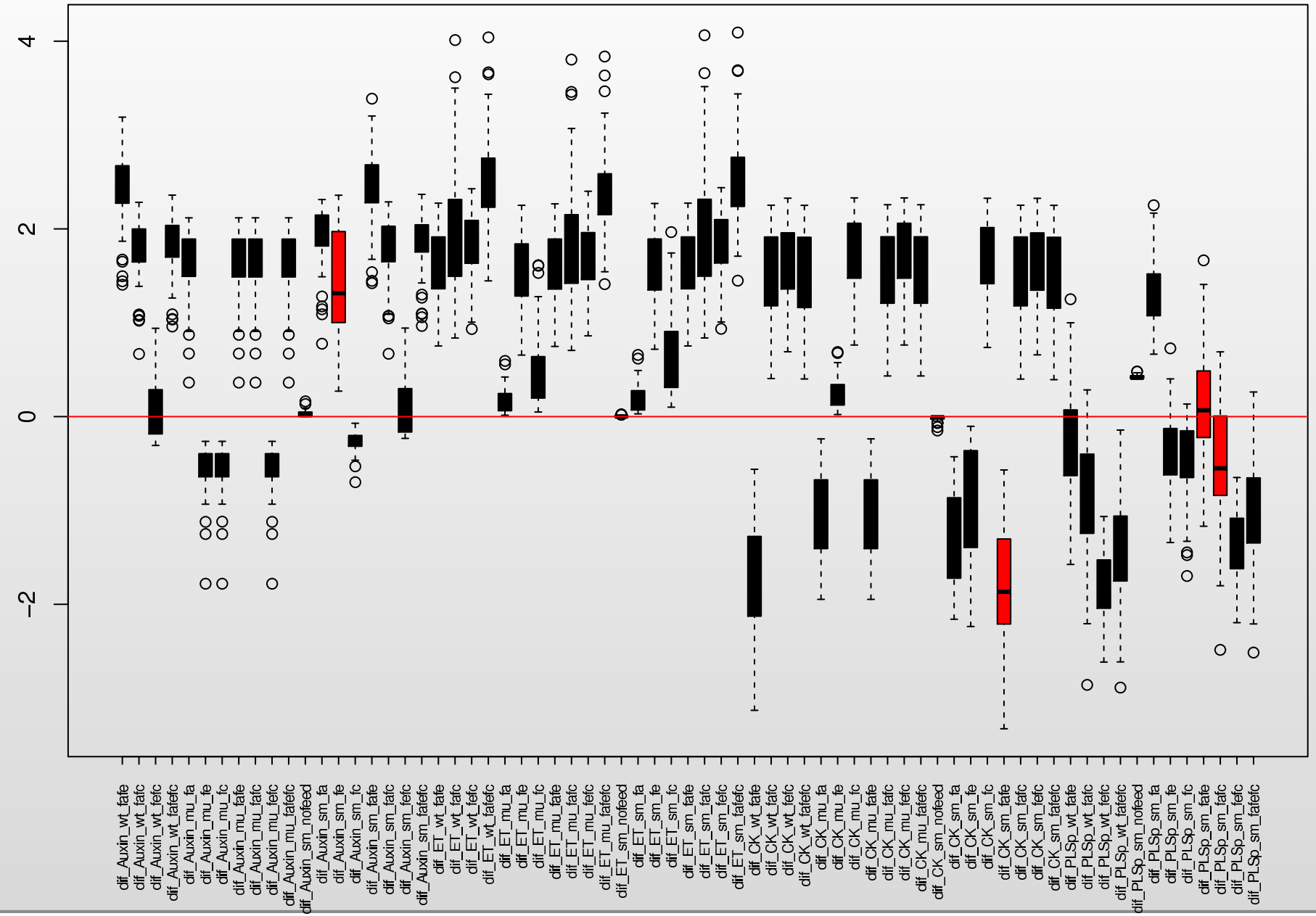

Space Cut Out Criteria

- Consider the implausibility measure for a future measurement z_i :

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

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- For given z_i, the fraction of space cutout S_i due to output i is:

$$S_i(z_i) = \frac{1}{V_{\mathcal{X}}} \int_{x \in \mathcal{X}} \mathrm{I}_i(x, z_i) dx$$

Space Cut Out Criteria

- Given the best input x^*, and distributional assumptions for z_i we have that:

$$z_i|x^* \quad \sim \quad N(\mu_i(x^*), \sigma_i^2(x^*) + \mathrm{Var}(\epsilon_i) + \mathrm{Var}(e_i))$$

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$$\mathrm{E}(S_i|x^*) = \frac{1}{V_{\mathcal{X}}} \int_{z_i} \int_{x \in \mathcal{X}} \mathrm{I}_i(x, z_i) \pi(z_i|x^*) dx dz_i$$

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- and the expected space cut out S_i for new output i is

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- If we want to identify our Utility U_i with the space cutout S_i, we will then choose the experiment to measure output i to maximise $\mathrm{E}(S_i)$.

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- and the expected space cut out S_i for new output i is

$$\mathrm{E}(S_i) = \frac{1}{V_{\mathcal{X}}^2} \int_{x^* \in \mathcal{X}} \int_{z_i} \int_{x \in \mathcal{X}} \mathrm{I}_i(x, z_i) \pi(z_i|x^*) dx dz_i dx^*$$

- If we want to identify our Utility U_i with the space cutout S_i, we will then choose the experiment to measure output i to maximise $\mathrm{E}(S_i)$.
- In fact we want to choose 4 outputs i, j, k, l such that the analogous expected space cut out $\mathrm{E}(S_{i,j,k,l})$ is maximised.

Approximate Space Cut Out Criteria

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- Should really do this using emulators, but for this calculation the runs may be sufficient.
- This is because the runs would inform the most important parts of the integrals.
- Again, we are interested in the analogous multivariate quantity $\mathrm{E}(S_{i,j,k,l})$

Experimental Design Results: 4 new experiments chosen

- Selected outputs by stepping up to 8 outputs, then back down to 4: robust.

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plant	chemical measured	feeding regime	expected space cut
PSLox	PLSp	auxin + ethylene	56%
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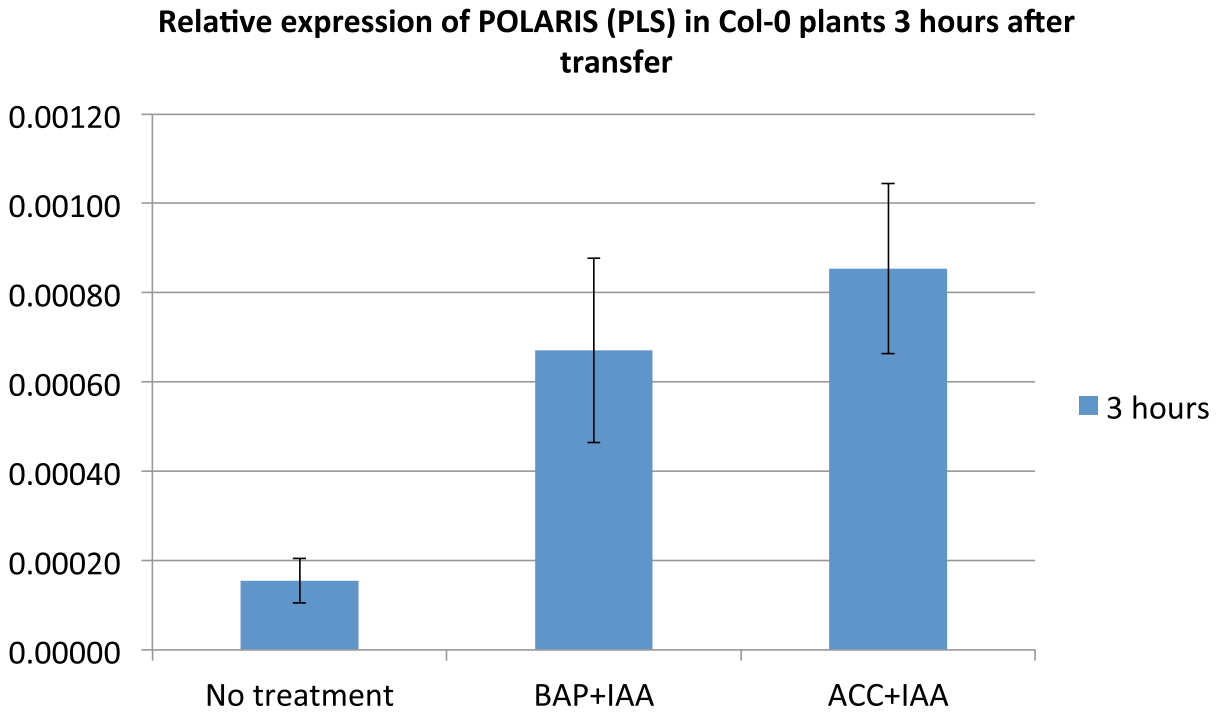
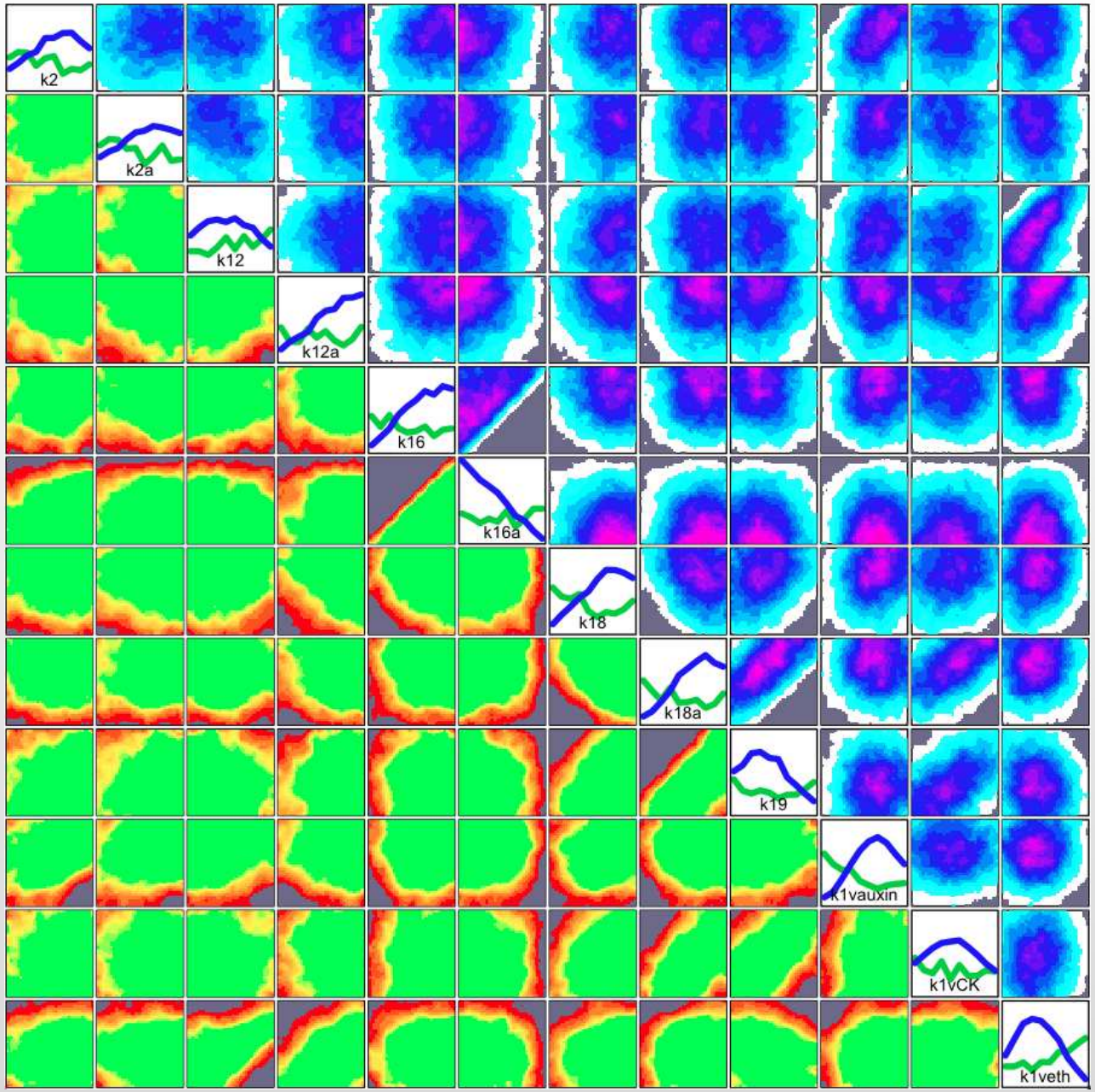
- First two experiments completed.

Results for First Two New Experiments

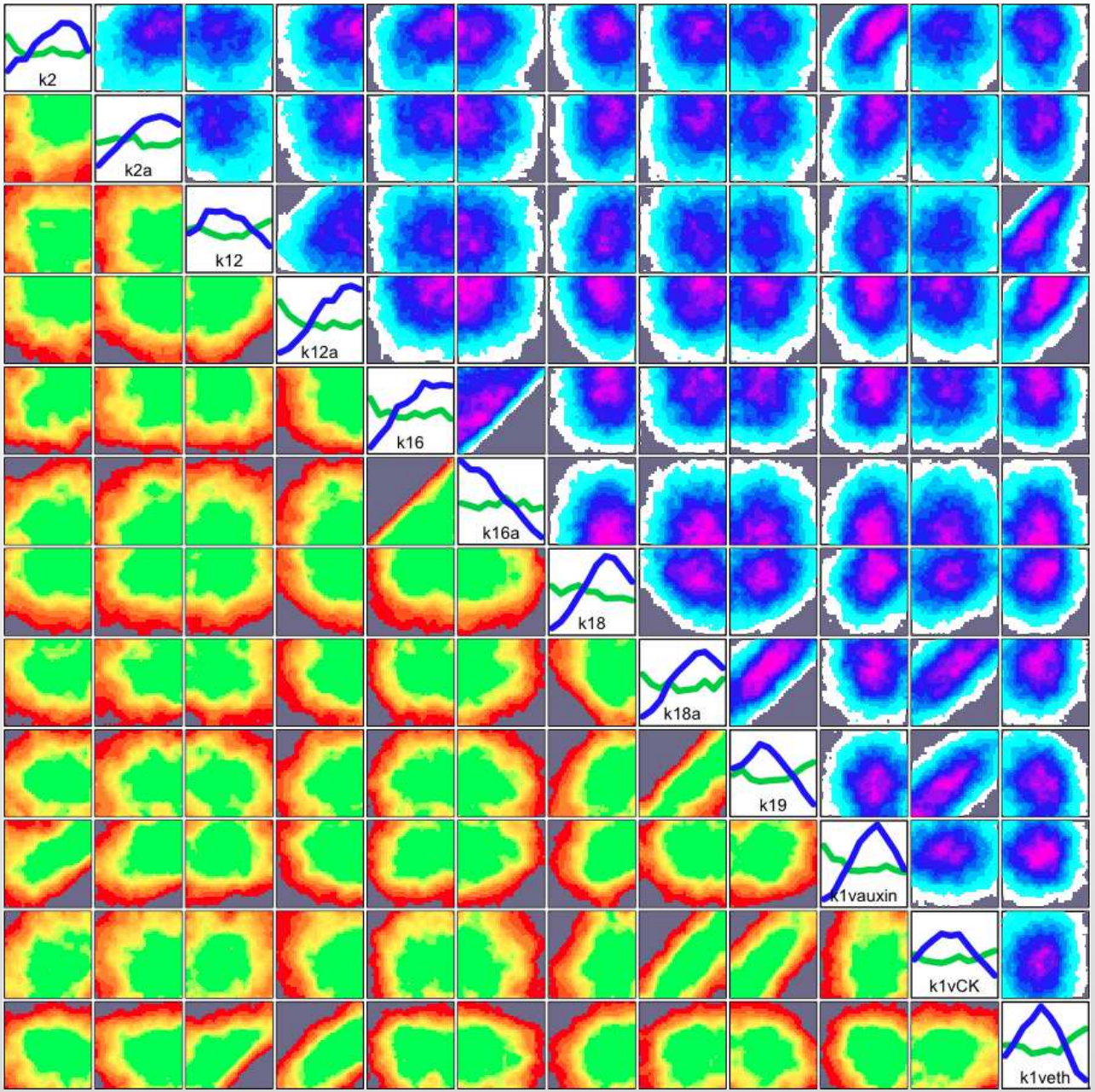


Seven day old Columbia wildtype plants were transferred to media containing either cytokinin and auxin (BAP + IAA), an ethylene precursor and auxin (ACC + IAA) or no hormone treatment. After three hours, the relative abundance (expression) of the POLARIS mRNA was measured with qPCR. Three separate biological replicates were used and error bars represent the standard error of the mean.

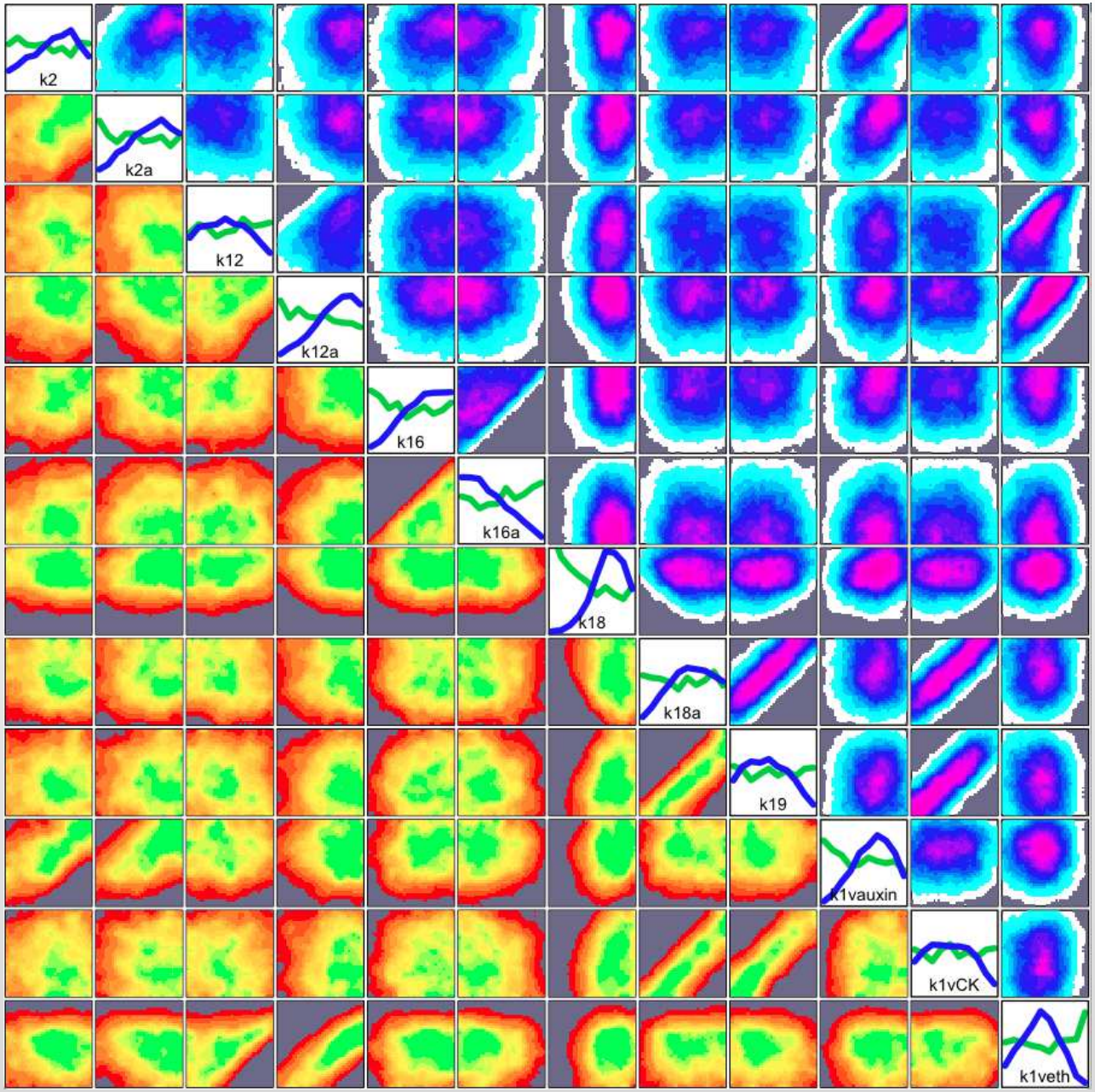
Iterative Input Space Reduction: Arabidopsis Model Wave 1



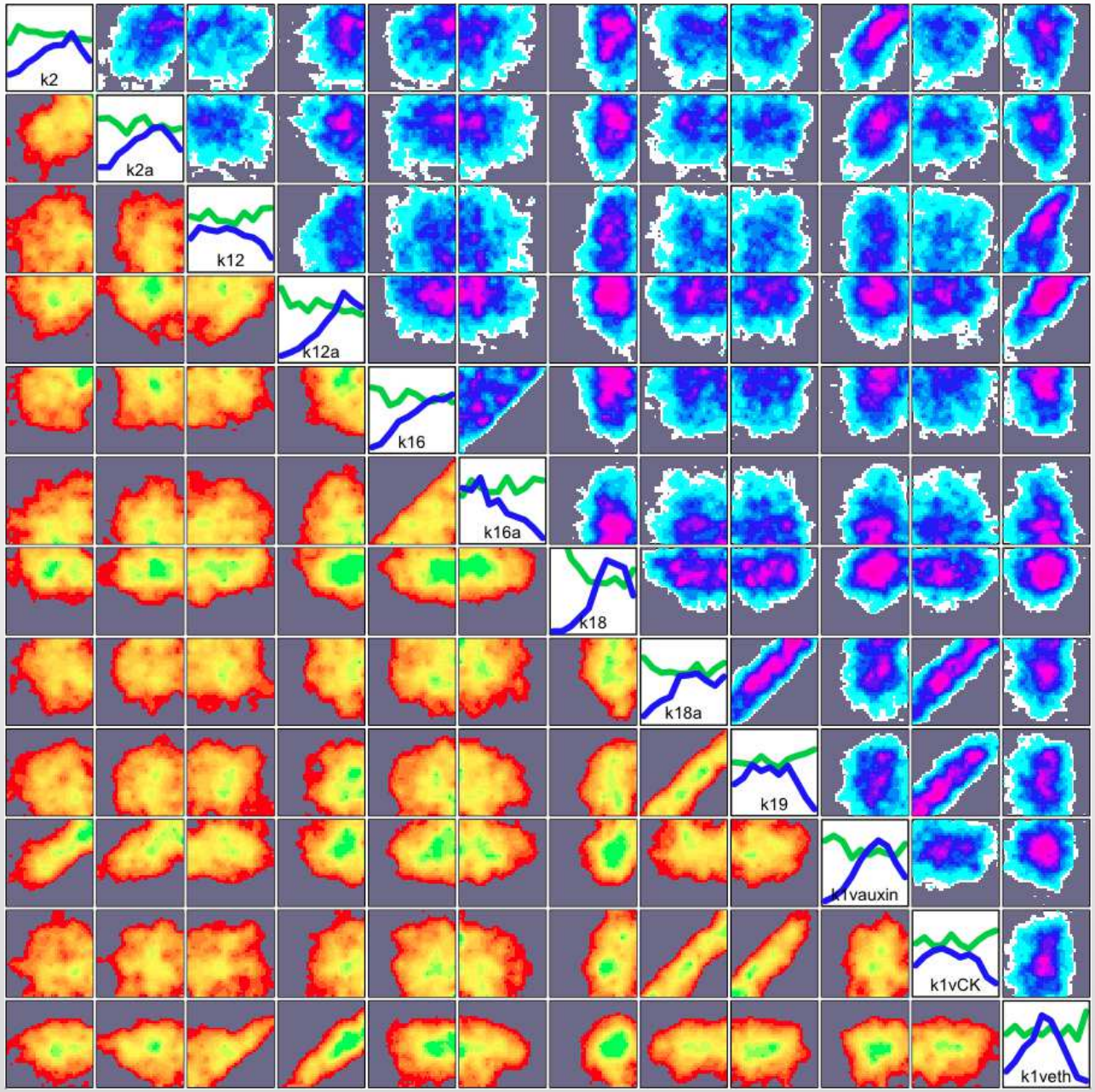
Iterative Input Space Reduction: Arabidopsis Model Wave 2



Iterative Input Space Reduction: Arabidopsis Model Wave 3



Arabidopsis Model with 2 New Results



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- We can also design experiments to challenge the model, i.e. to validate it if necessary.

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- The correct treatment of uncertainty is vital: without this, any analysis will be problematic and untrustworthy.
- The emulation methods we describe can be used to exhaustively explore model features (helpful when developing models).
- Due to the need to synthesis many sources of uncertainty within one coherent calculation, a Bayesian approach is ideal.

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Developments in Emulation

- Much work in the emulation of deterministic models (much to be done too!). Some decent papers are (see Managing Uncertainty in Complex Models website http://www.mucm.ac.uk):

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For the Arabidopsis model used in this talk see (further papers in preparation:

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