

## Uncertainty analysis for computer models.

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\*Thanks to EPSRC, NERC, MRc, Leverhulme, for funding. Thanks to Ian Vernon for pictures. Energy systems work with Antony Lawson, Amy Wilson, Chris Dent.

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The science in each of these applications is completely different. However, the underlying methodology for handling uncertainty is the same.

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the optimal assignment of any decision inputs,  $d$ , in the model.

## Simple 1D Exponential Growth Example

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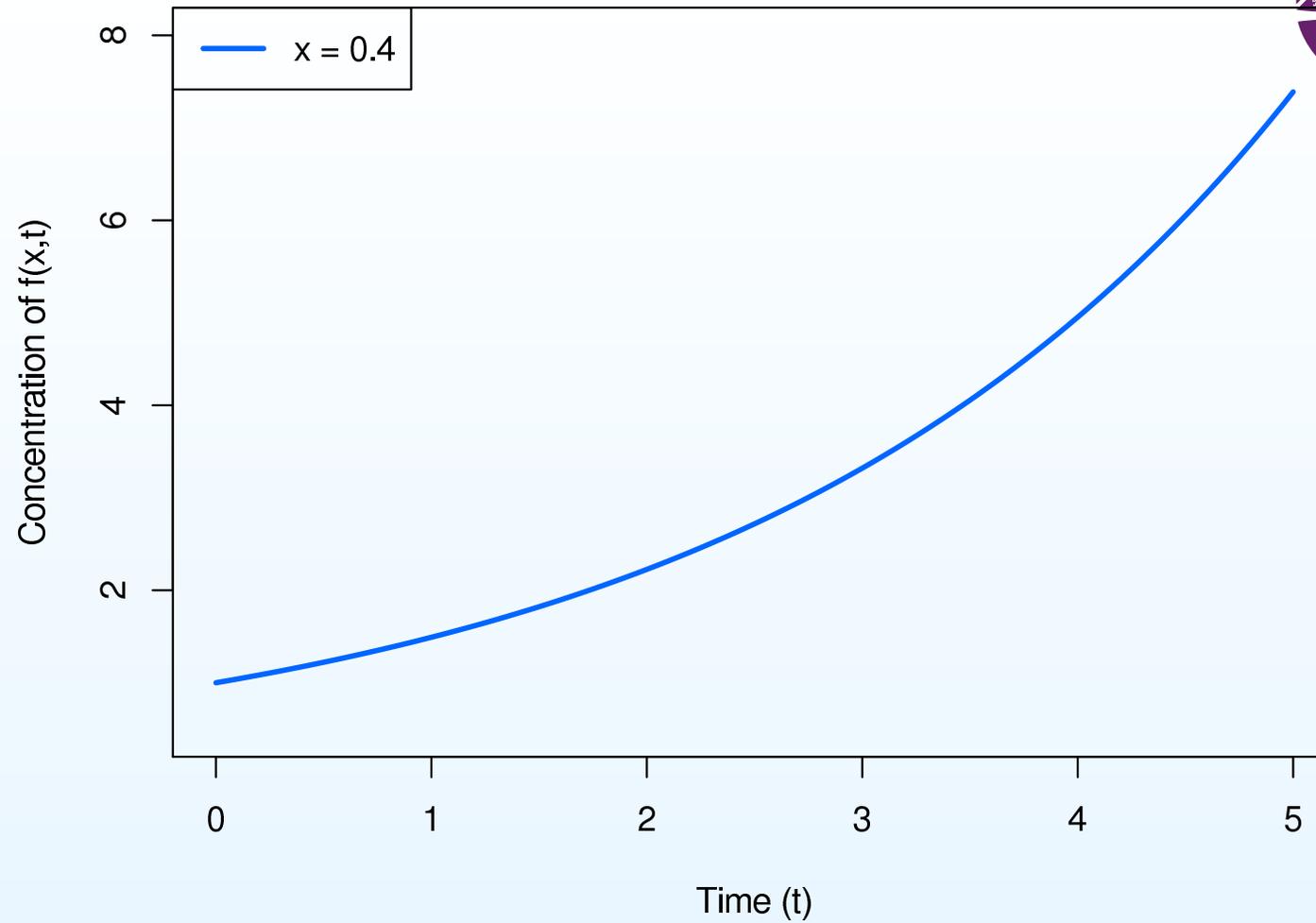
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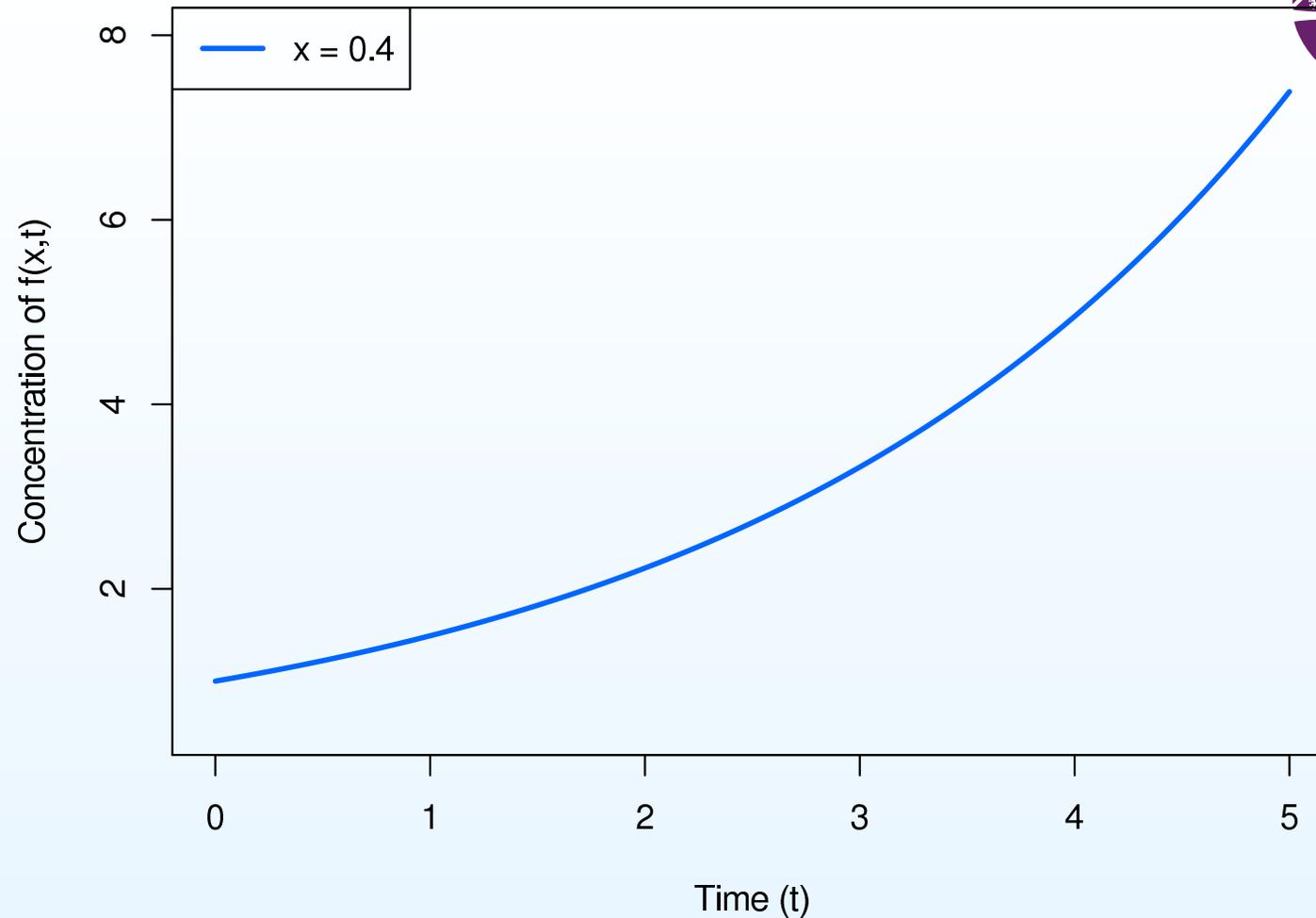
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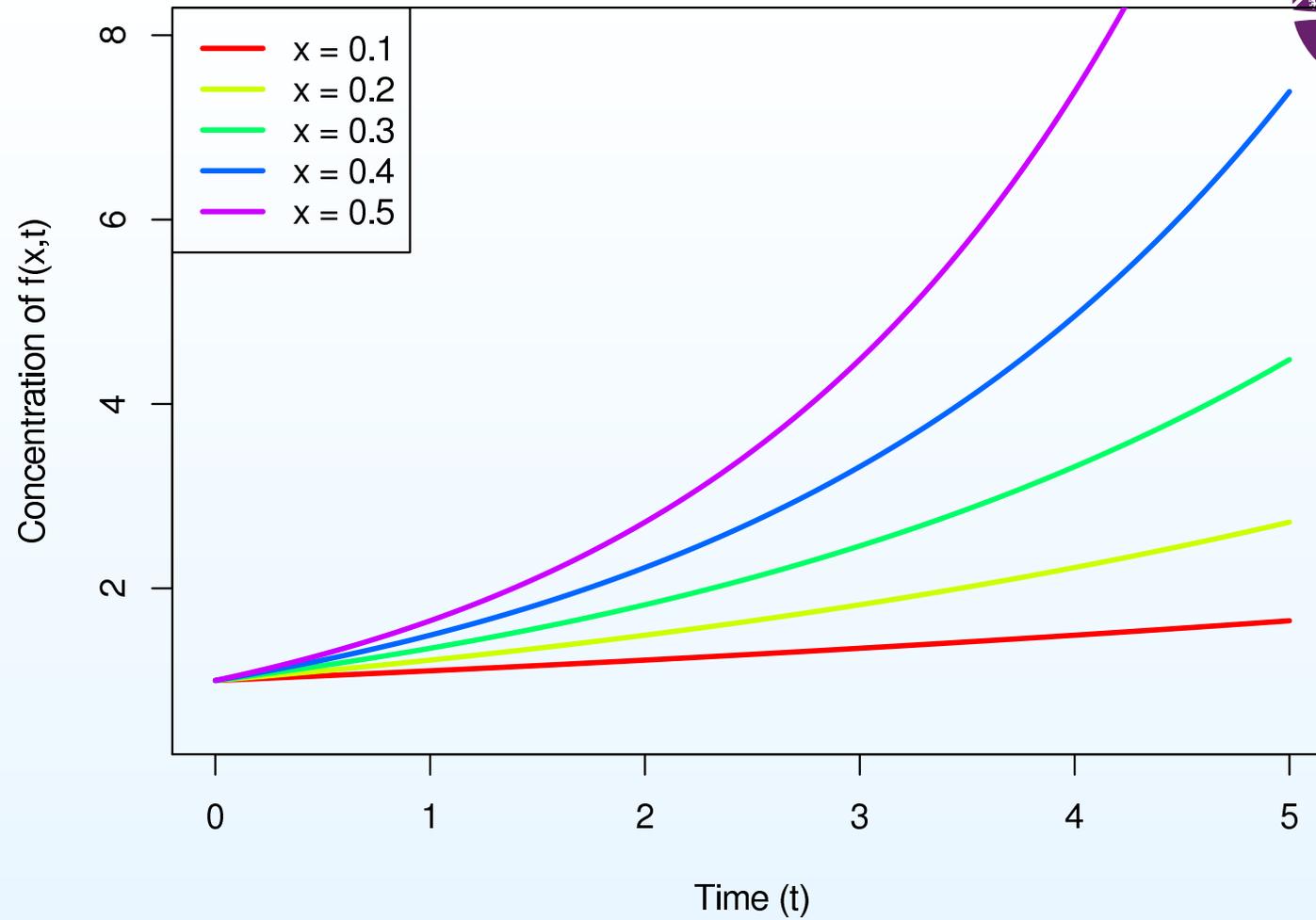
- We will temporarily assume the initial conditions are  $f_0 = f(x, t = 0) = 1$ .
- Model features an input parameter  $x$  which **we want to learn about**.
- Note that normally we would **not** have the analytic solution for  $f(x, t)$ .



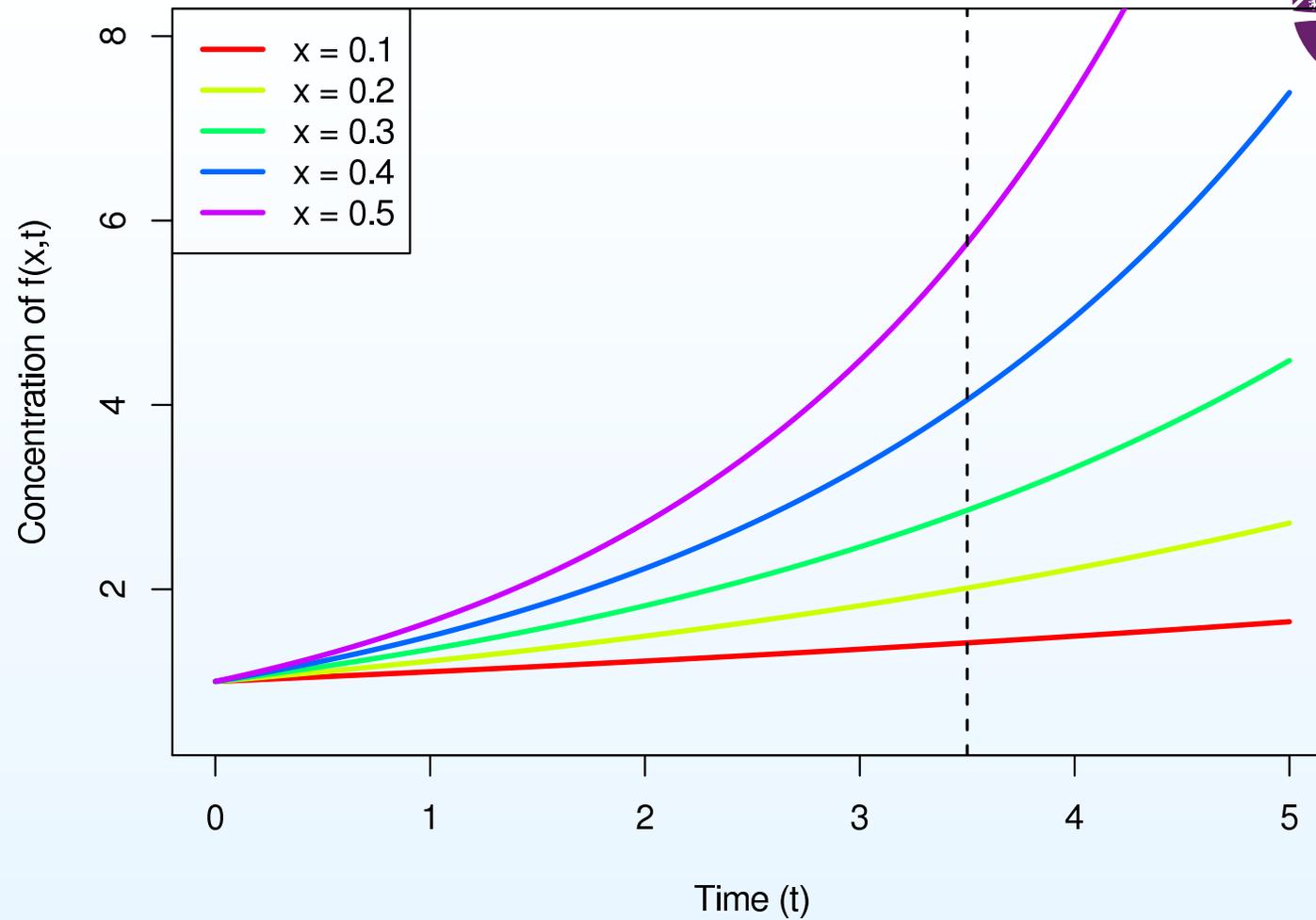
- One “model run” with the input parameter  $x = 0.4$



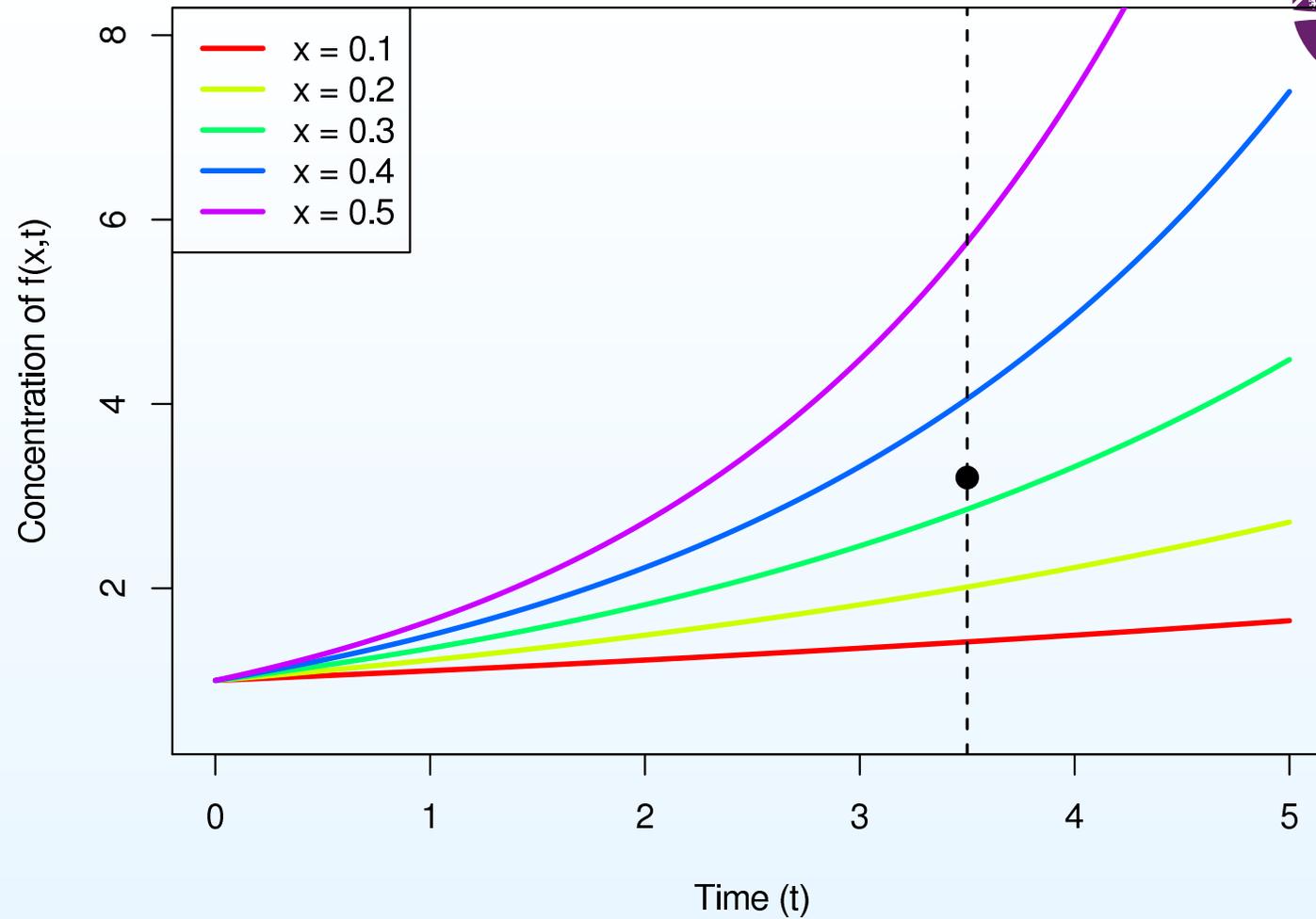
- One “model run” with the input parameter  $x = 0.4$
- If we did not know the analytic solution for  $f(x, t)$  this would be generated by numerically solving the differential equation.



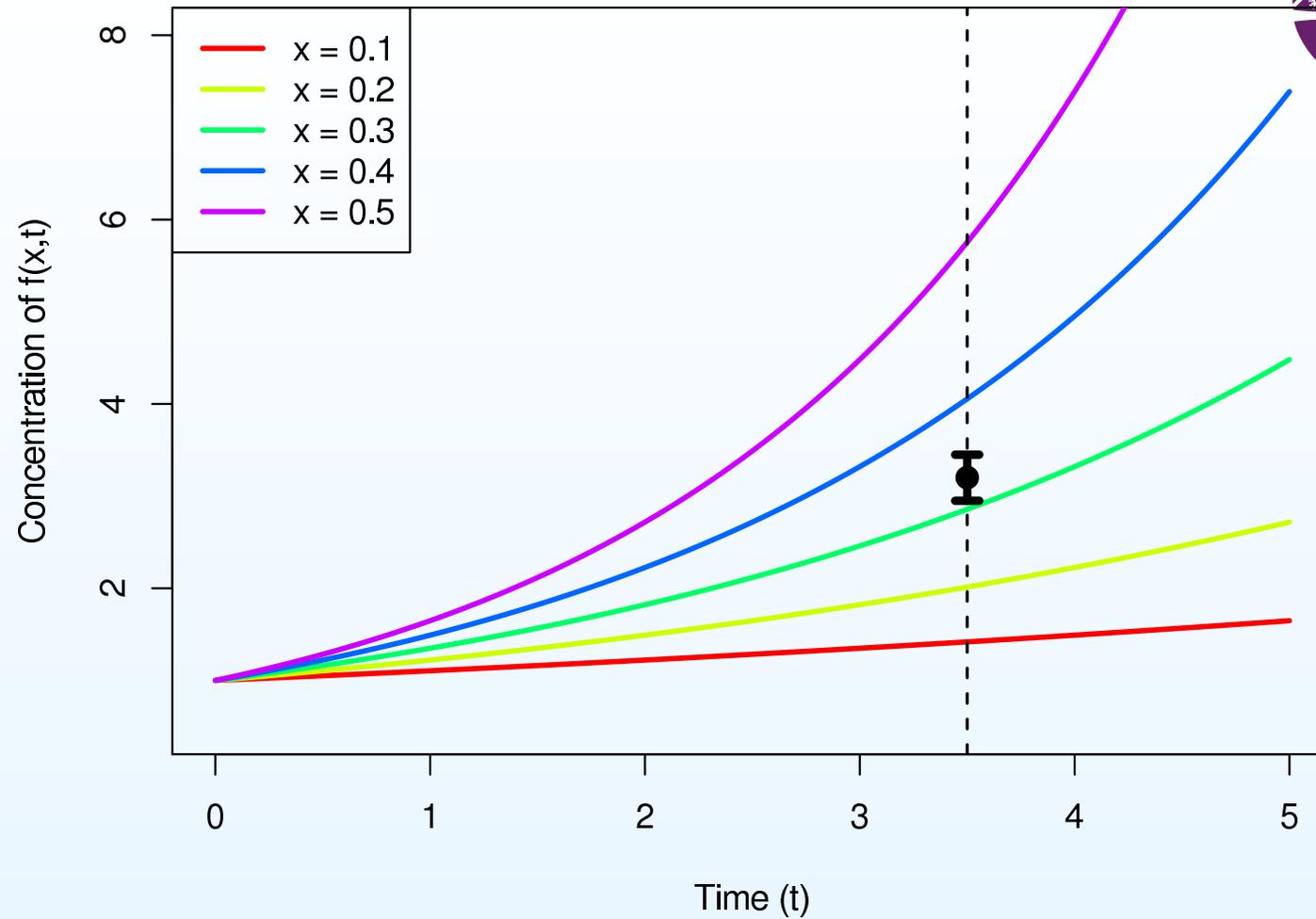
- Five model runs with the input parameter varying from  $x = 0.1$  to  $x = 0.5$



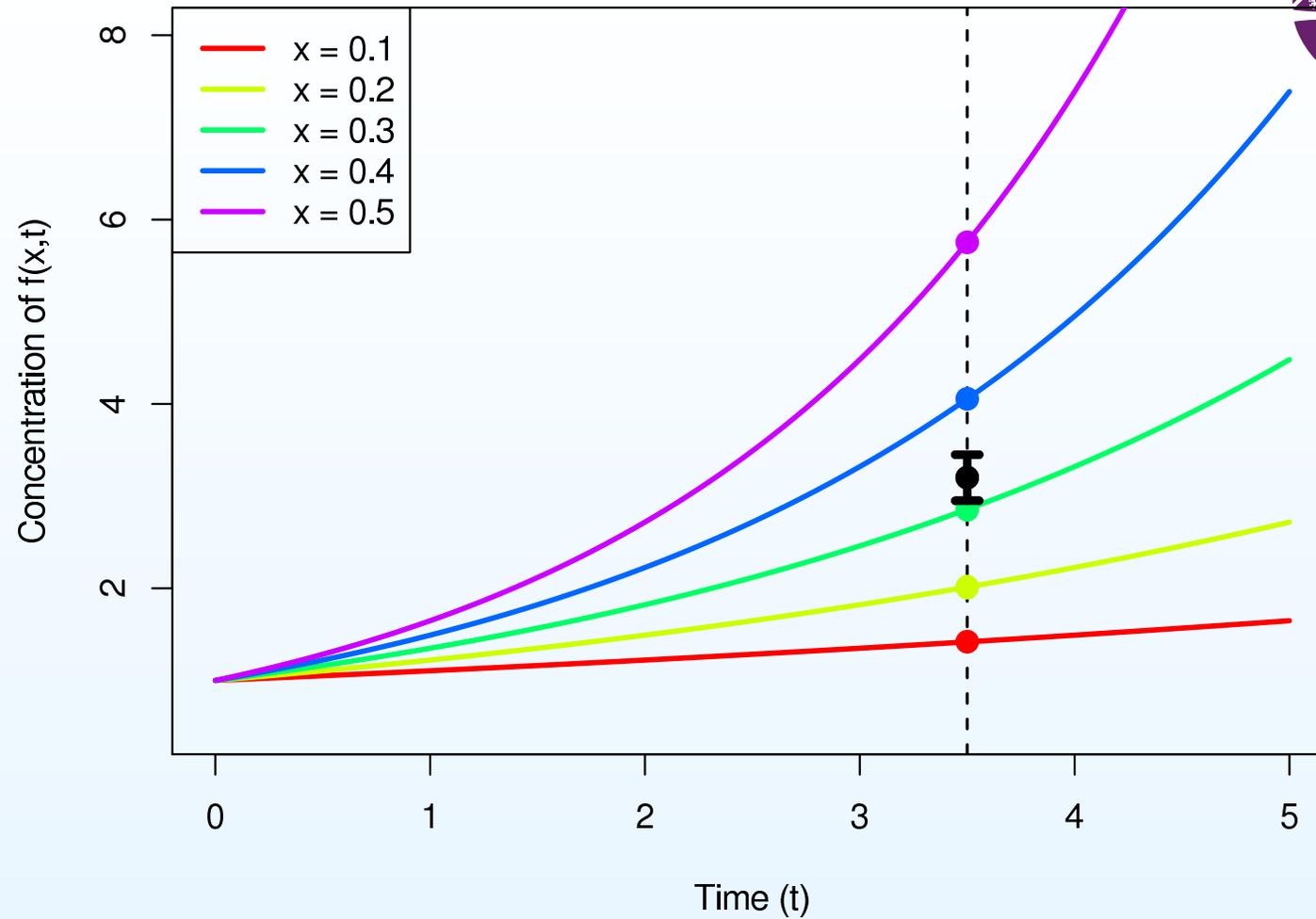
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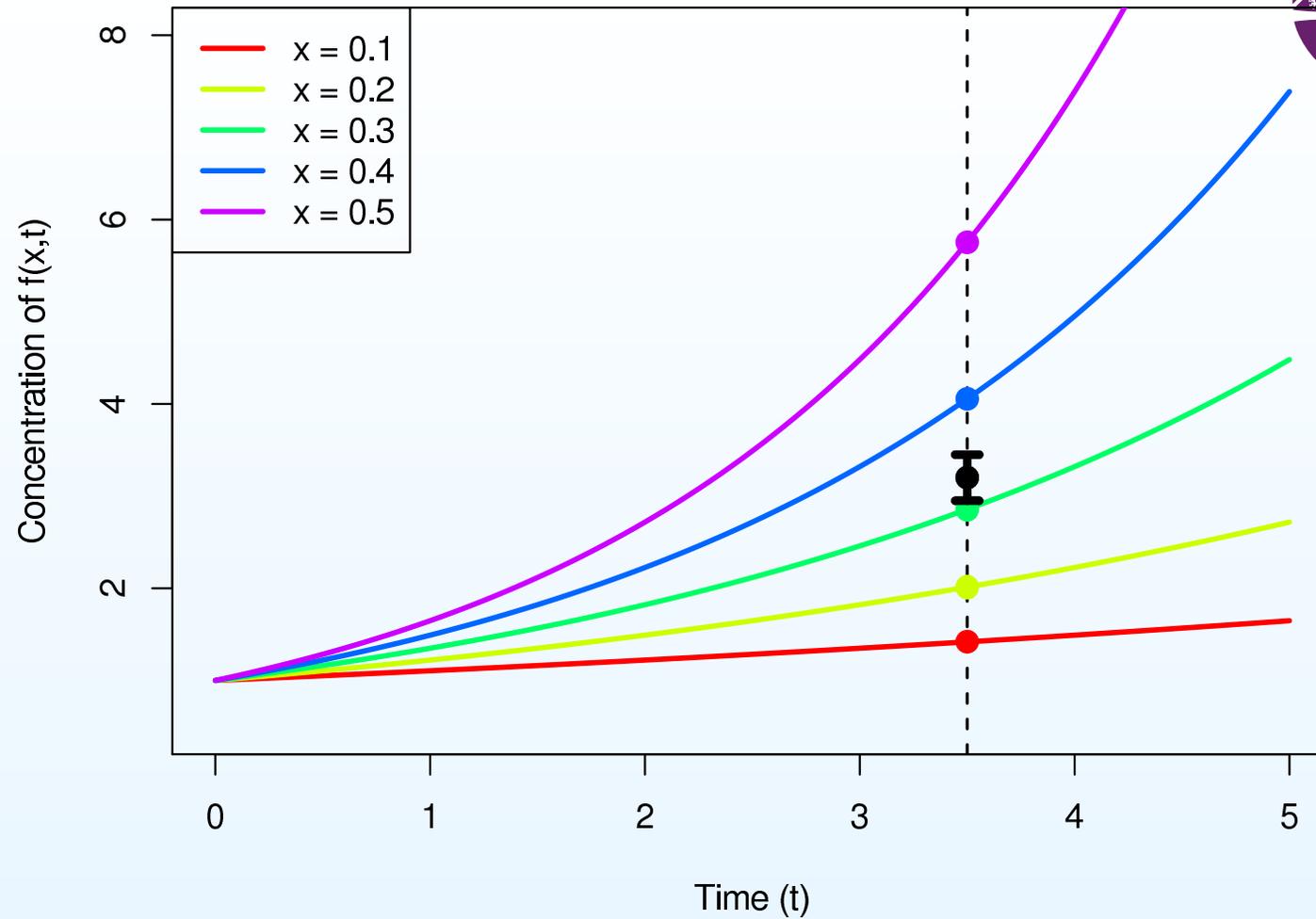
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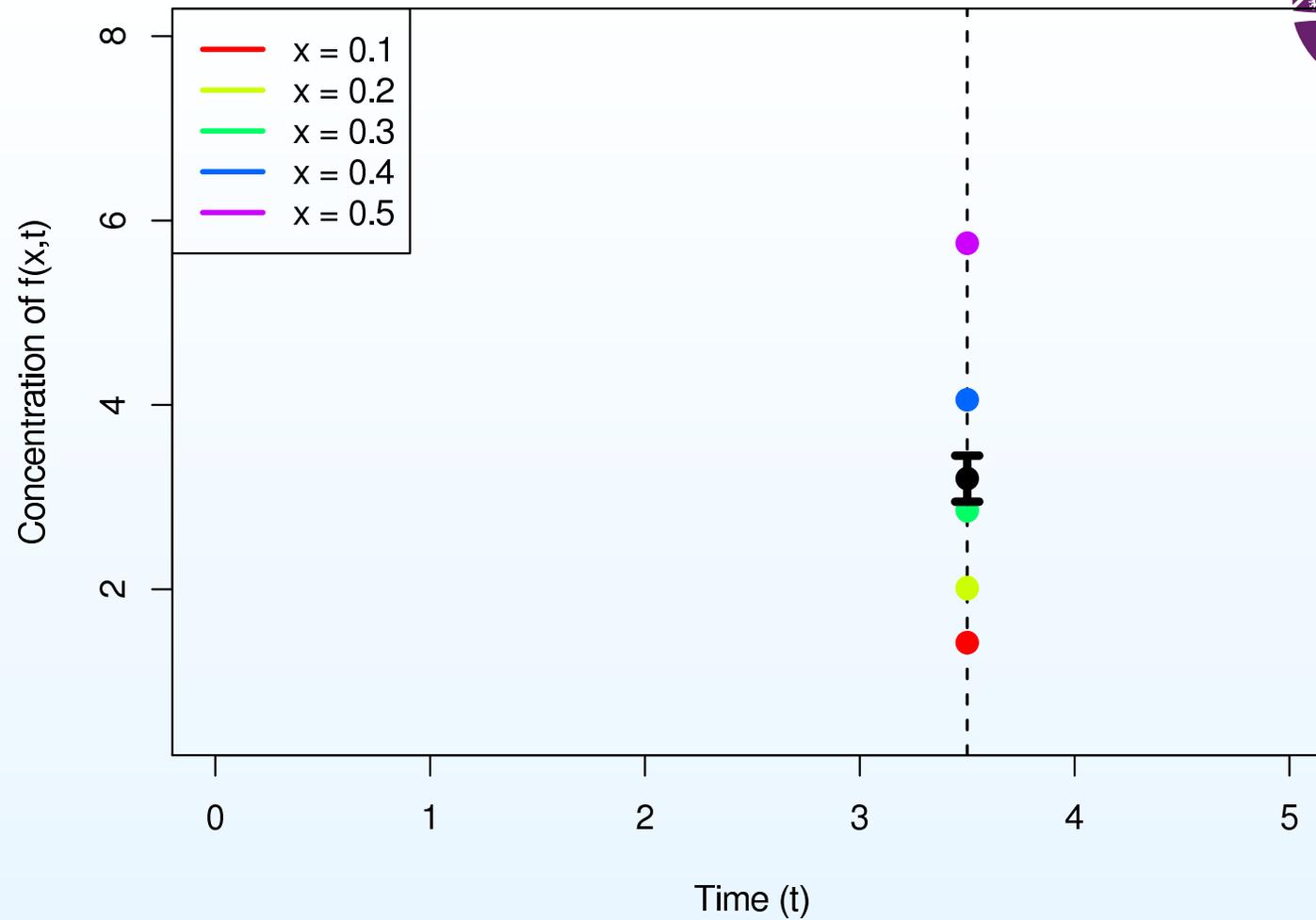
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- We are going to measure  $f(x, t)$  at  $t = 3.5$
- The measurement is **not a point** but comes with **measurement error**.



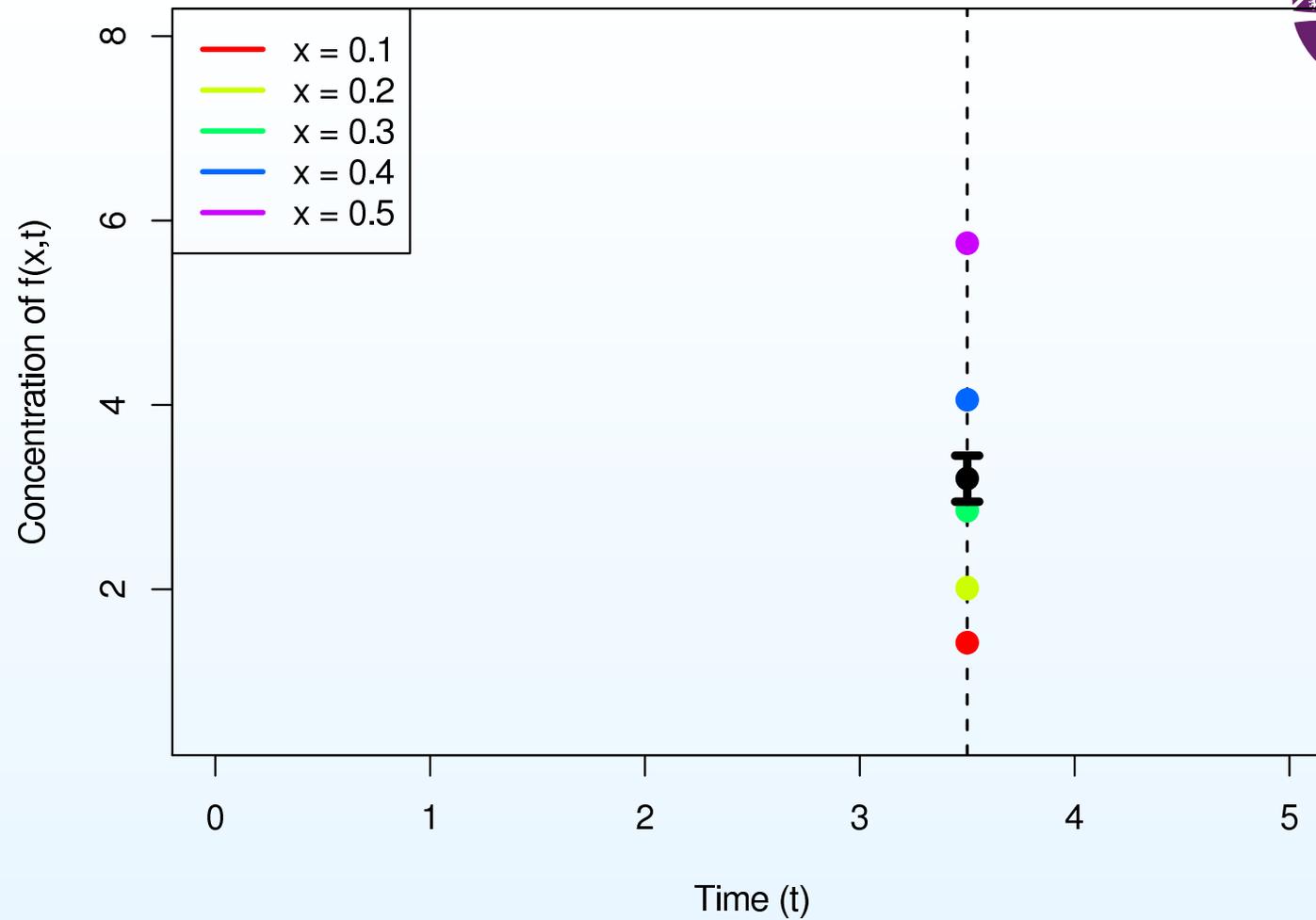
- **Question:** which values of  $x$  ensure the output  $f(x, t = 3.5)$  is consistent with the observations?



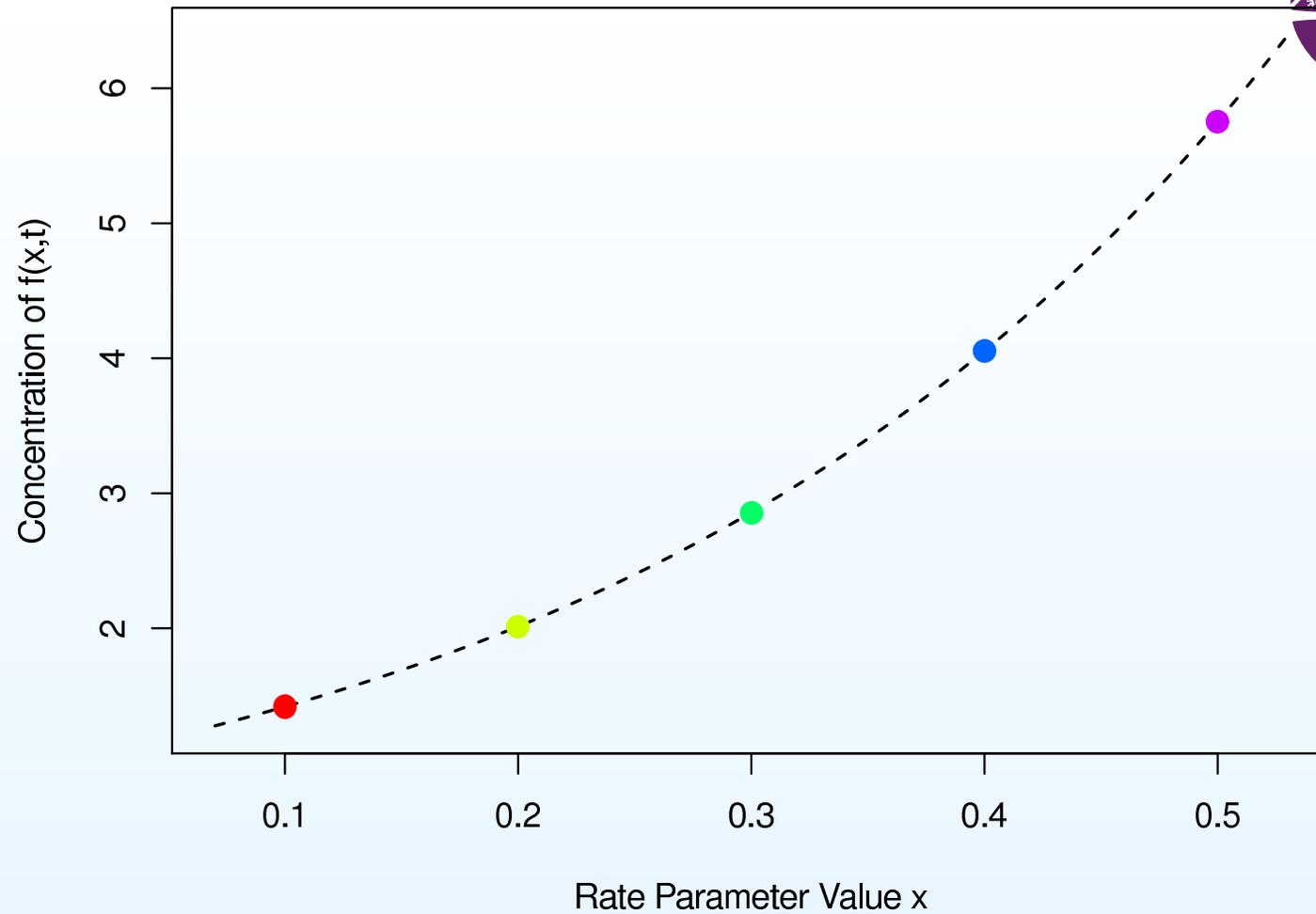
- Question: which values of  $x$  ensure the output  $f(x, t = 3.5)$  is consistent with the observations?
- It would seem that  $x$  has to be at least between 0.3 and 0.4.



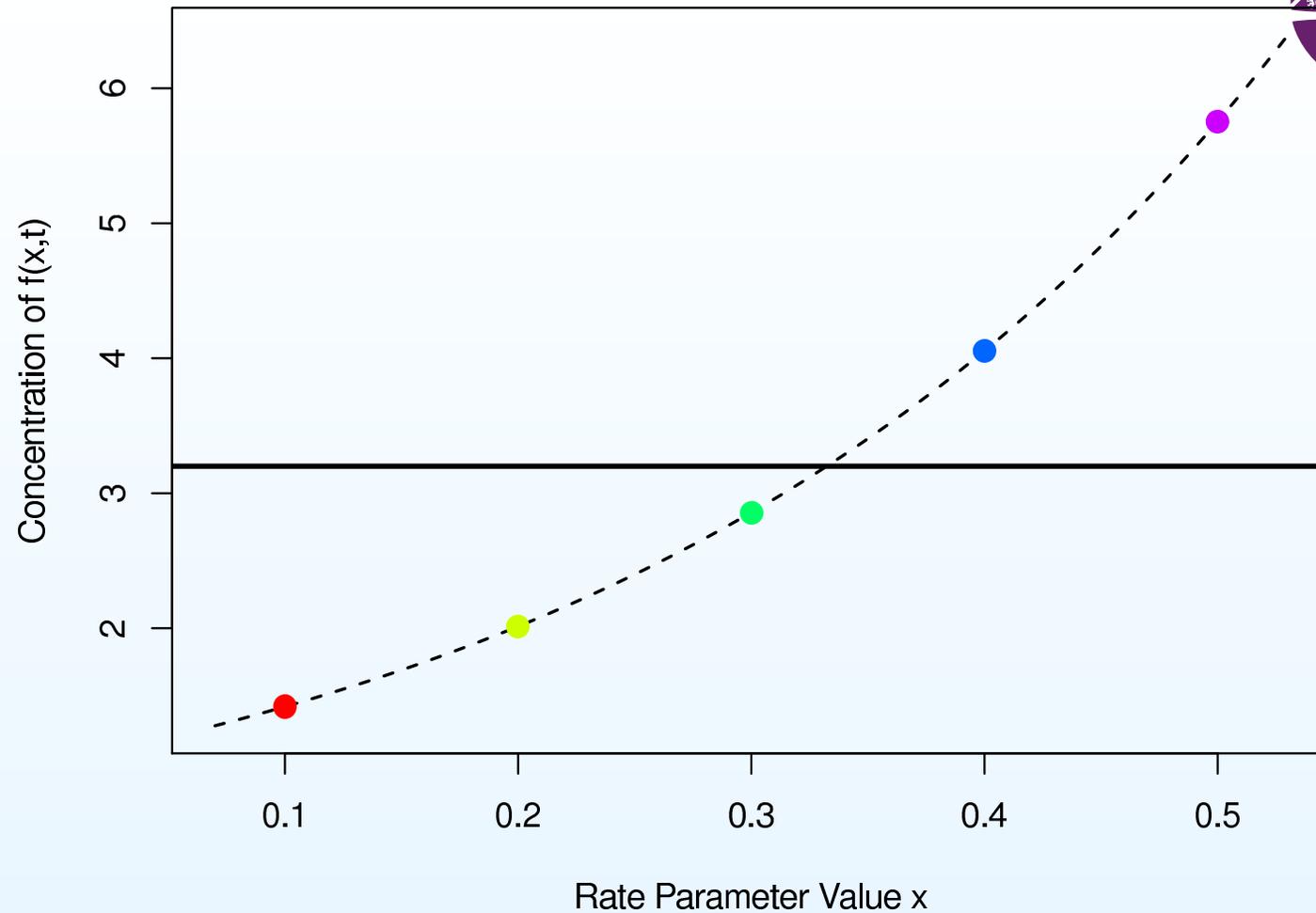
- To answer this, we can now discard other values of  $f(x, t)$  and think of  $f(x, t = 3.5)$  as a function of  $x$  only.



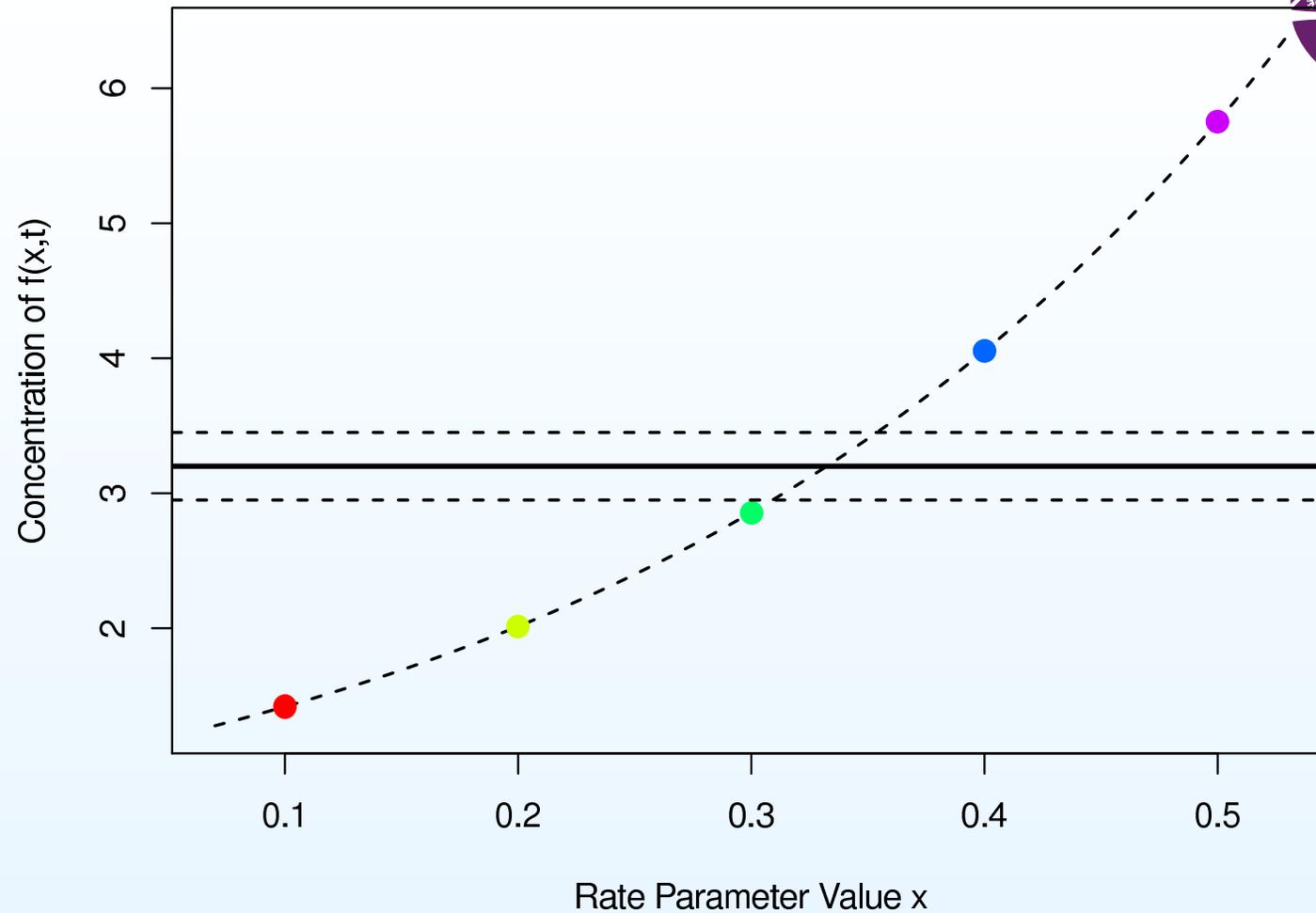
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- That is take  $f(x) \equiv f(x, t = 3.5)$



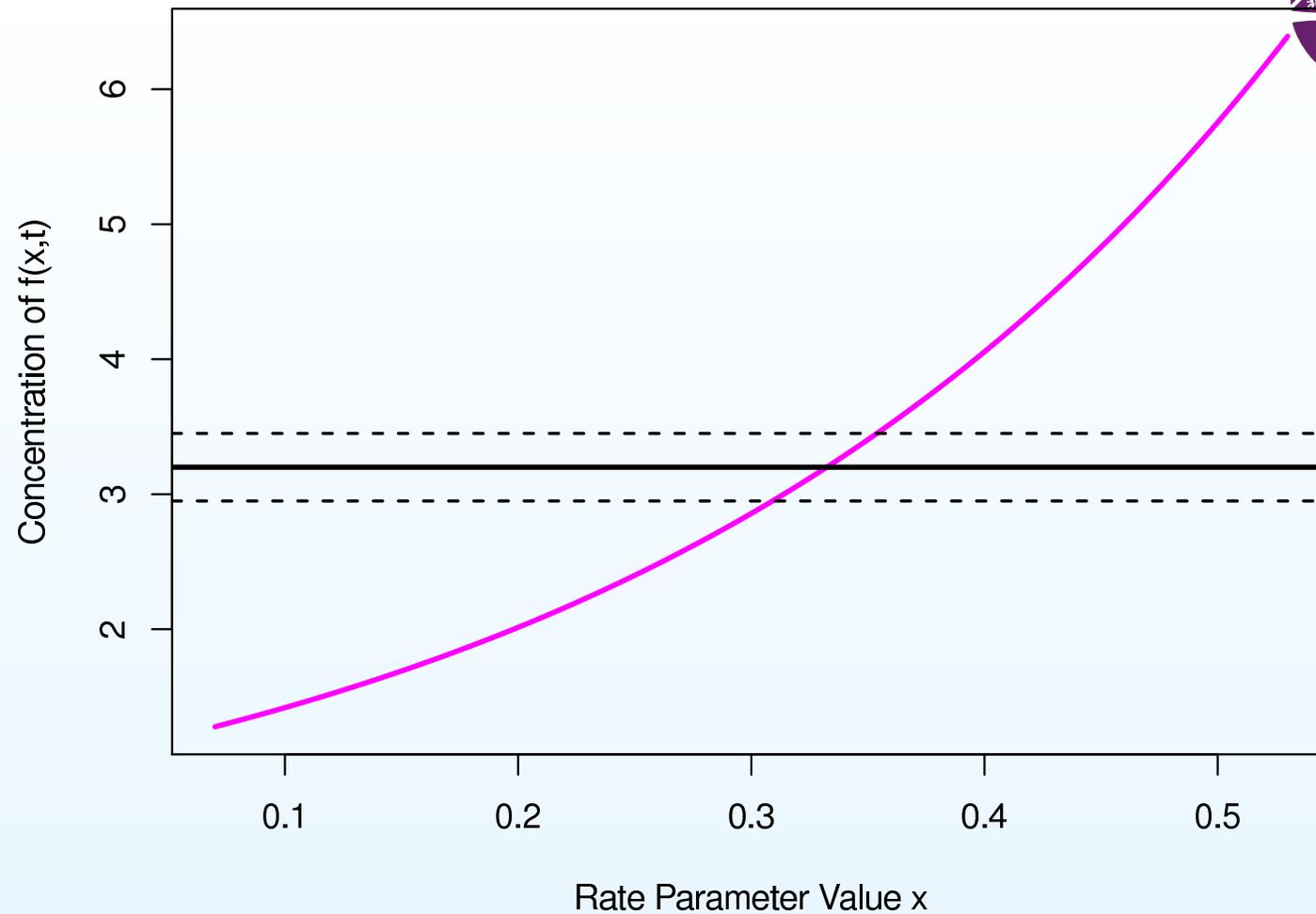
- We can now plot the concentration  $f(x)$  as a function of the input parameter  $x$ .



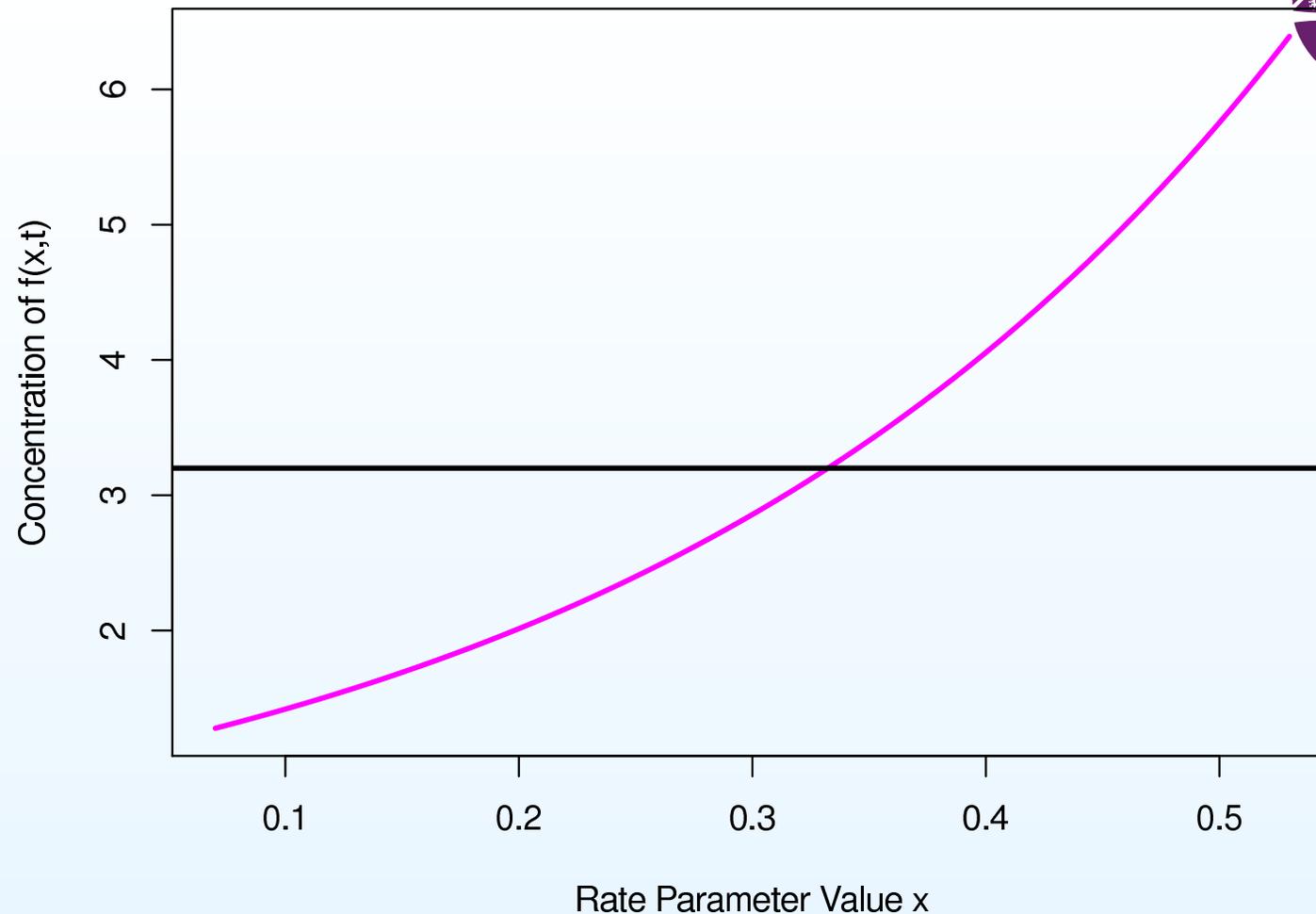
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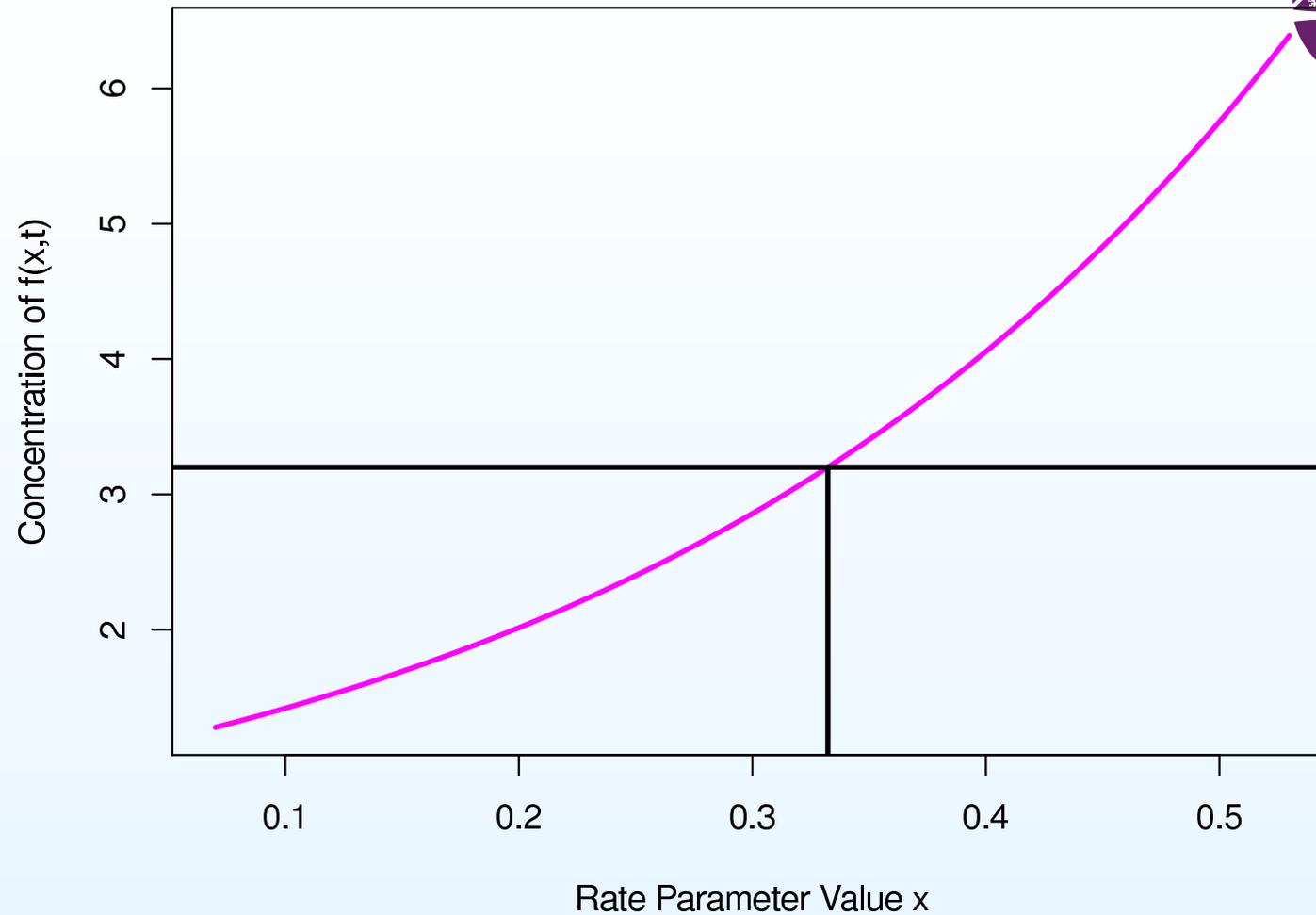
- We can now plot the concentration  $f(x)$  as a function of the input parameter  $x$ .
- Black horizontal line: the observed measurement of  $f$
- Dashed horizontal lines: the measurement errors



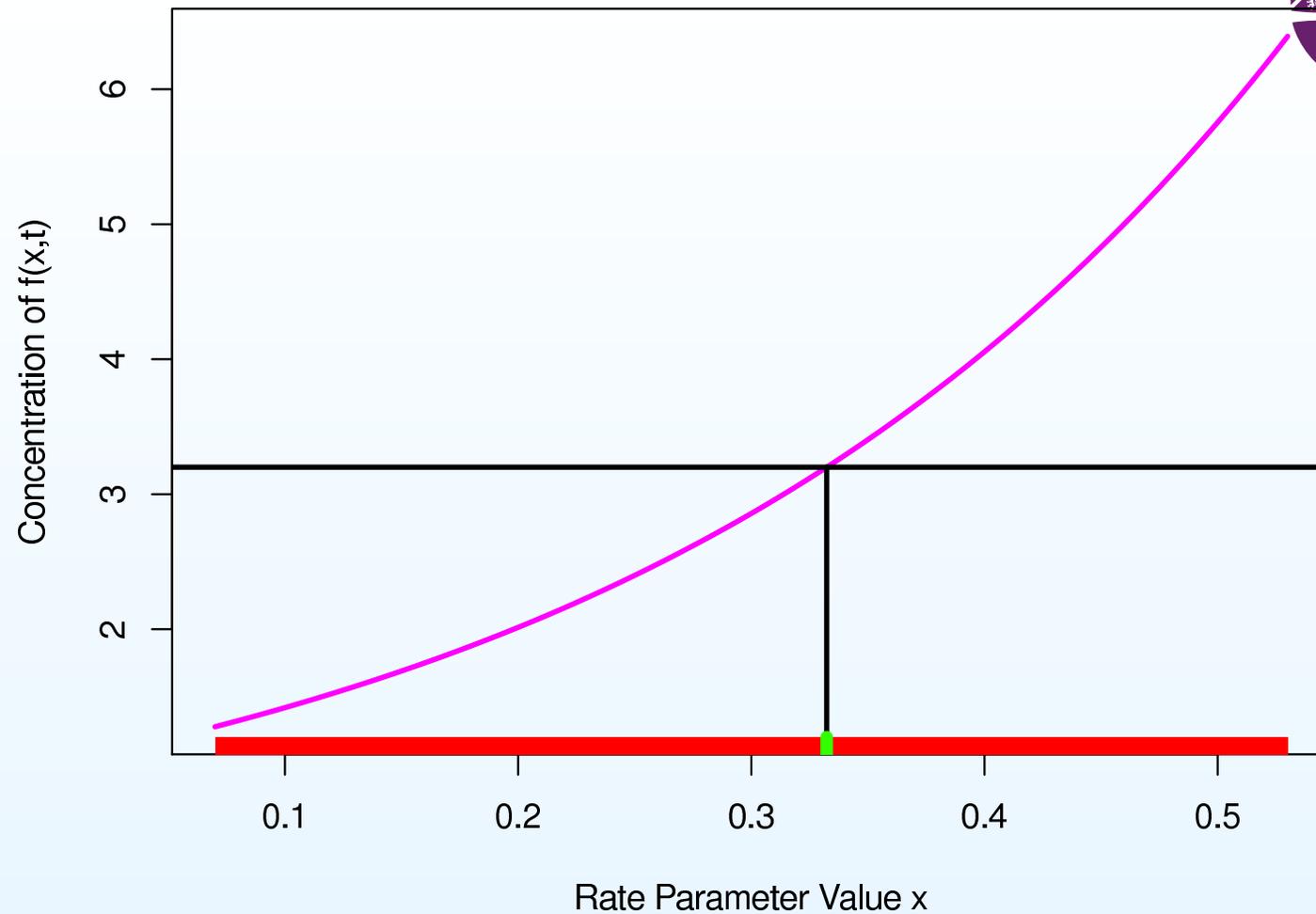
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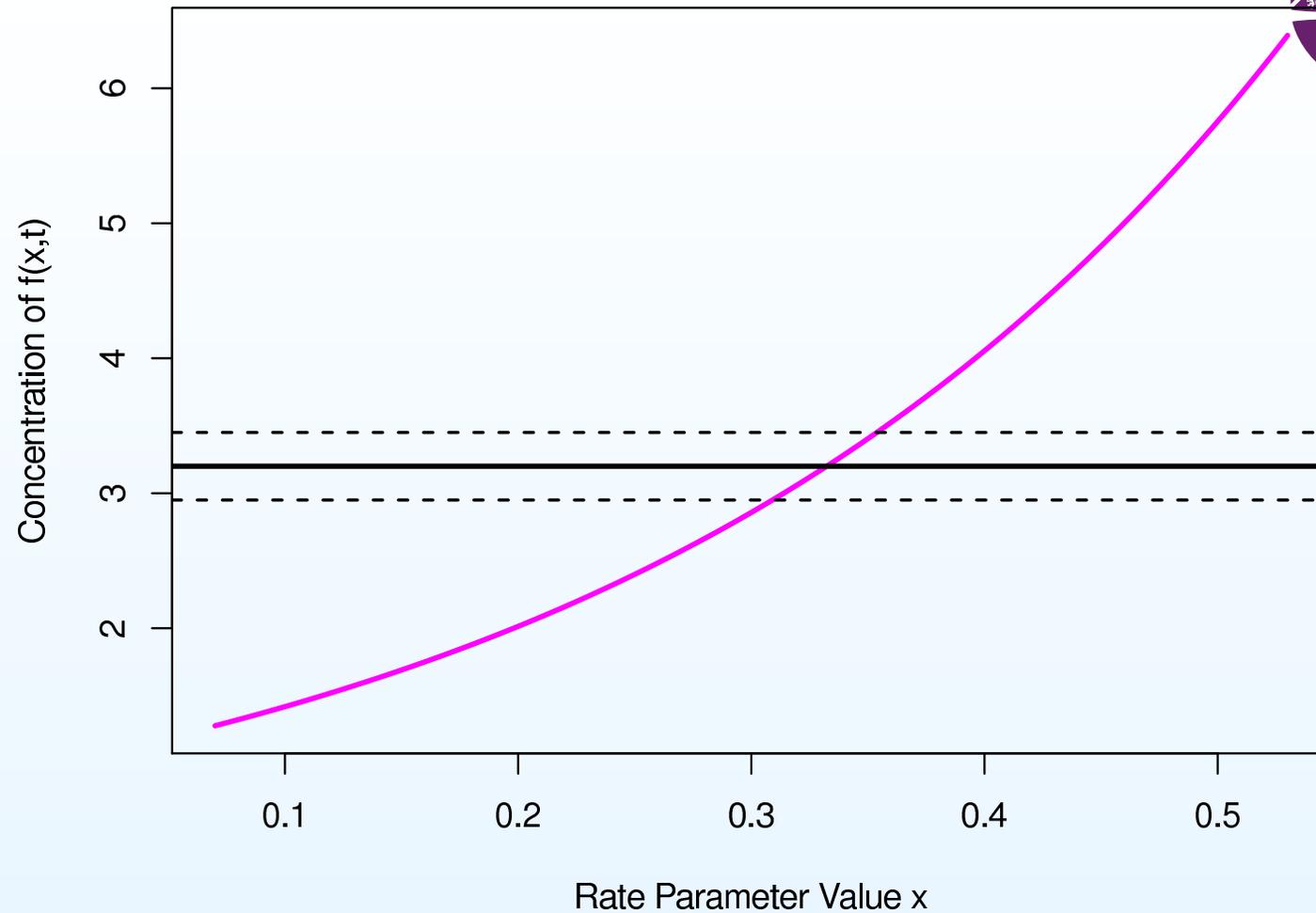
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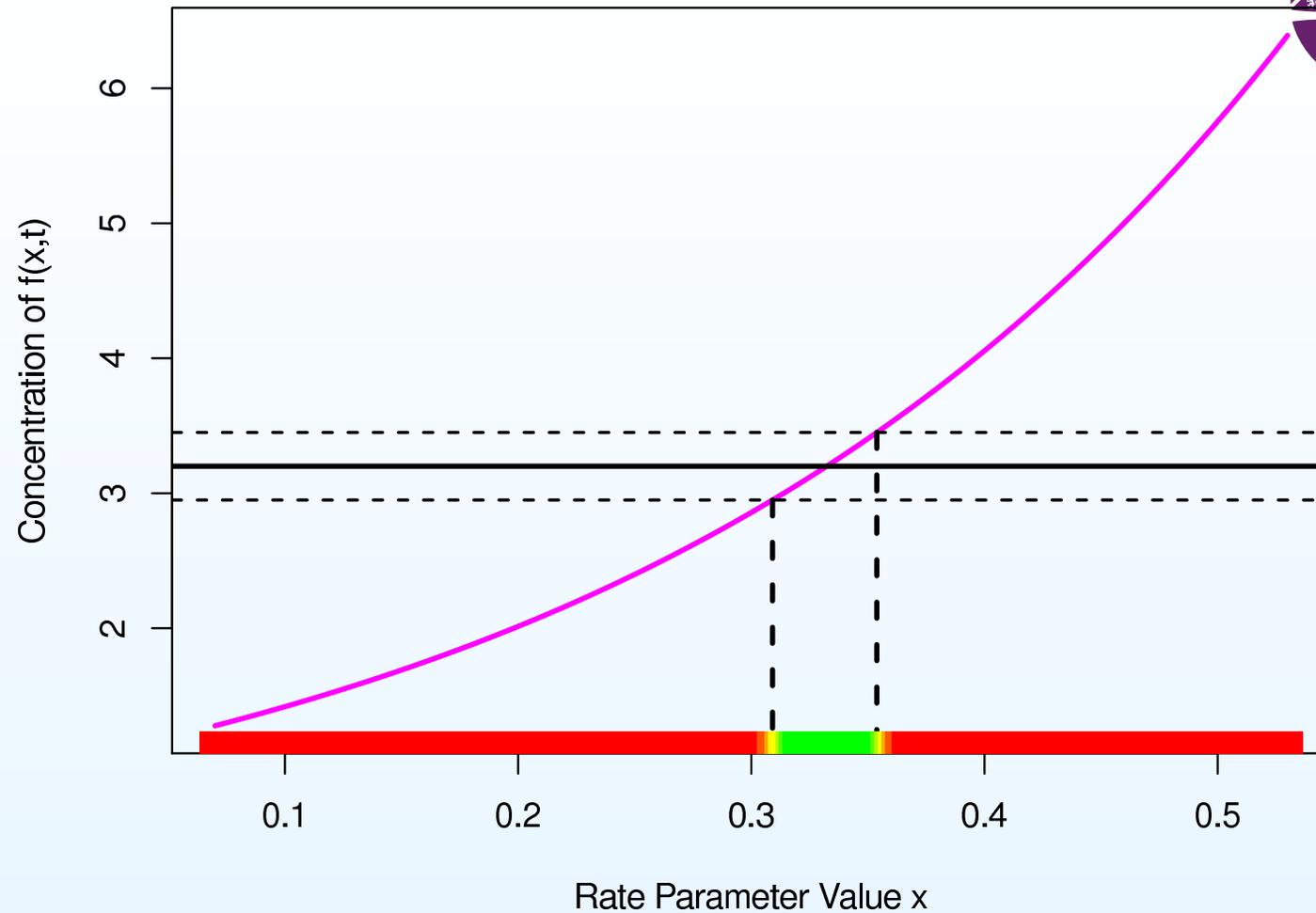
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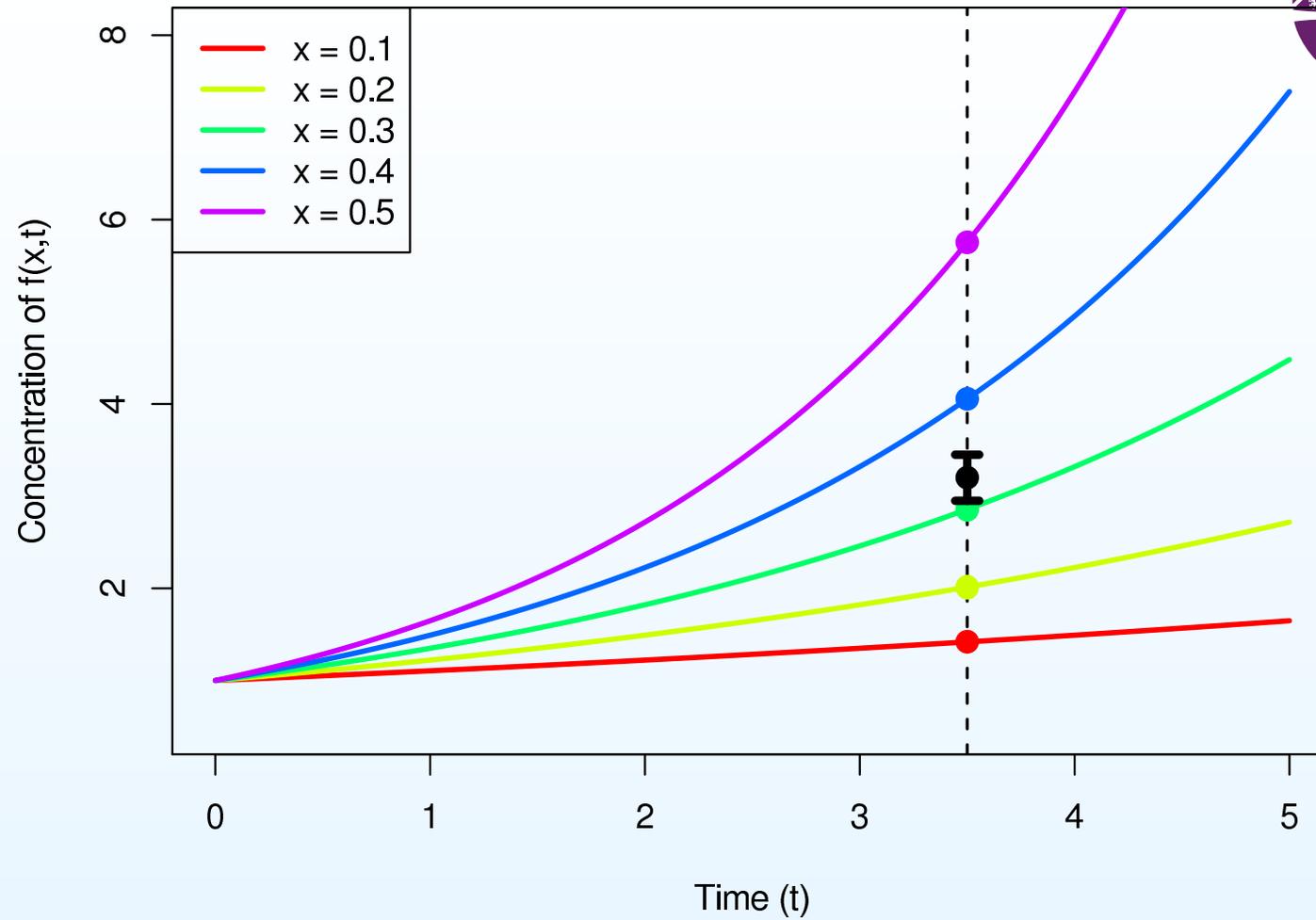
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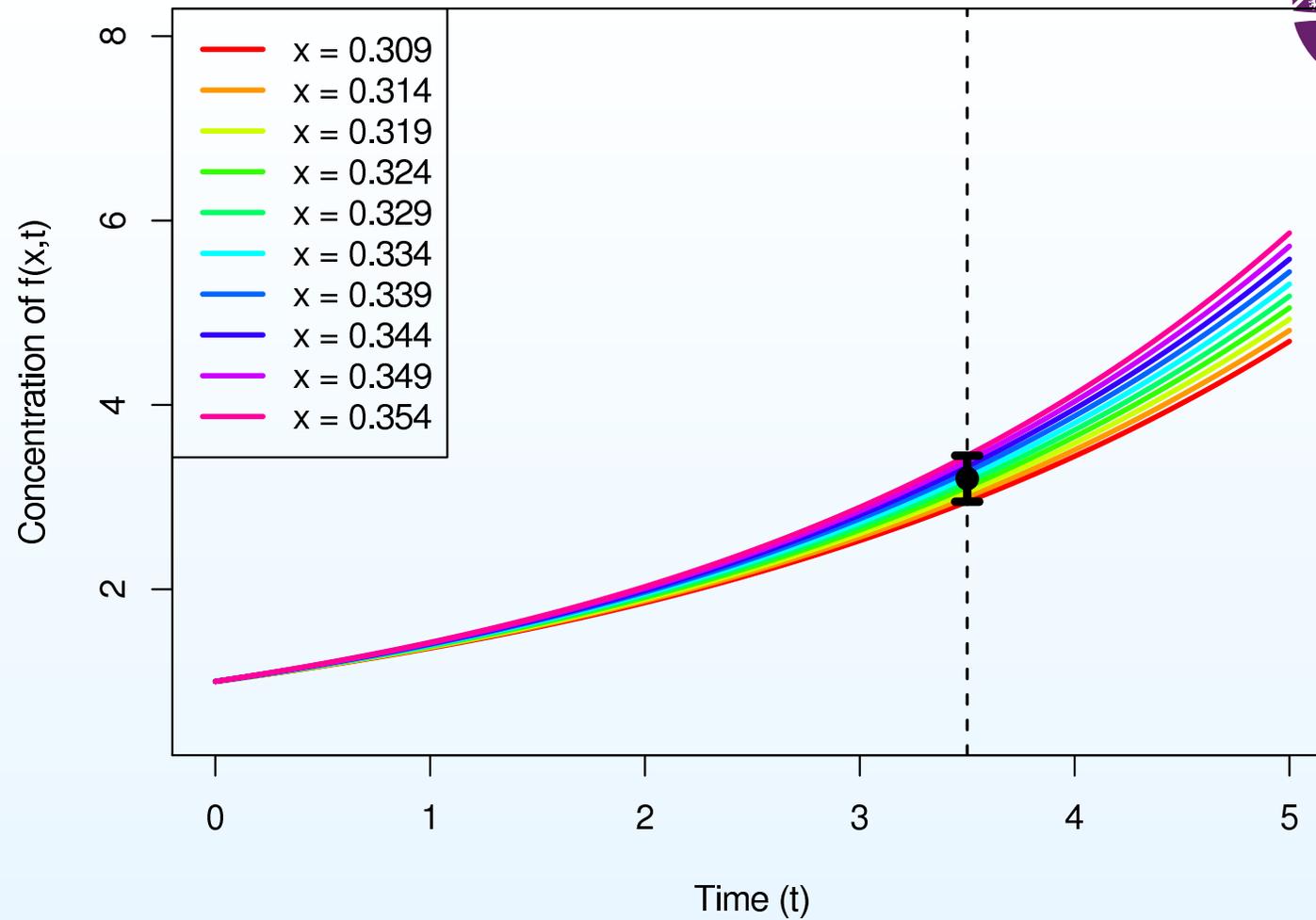
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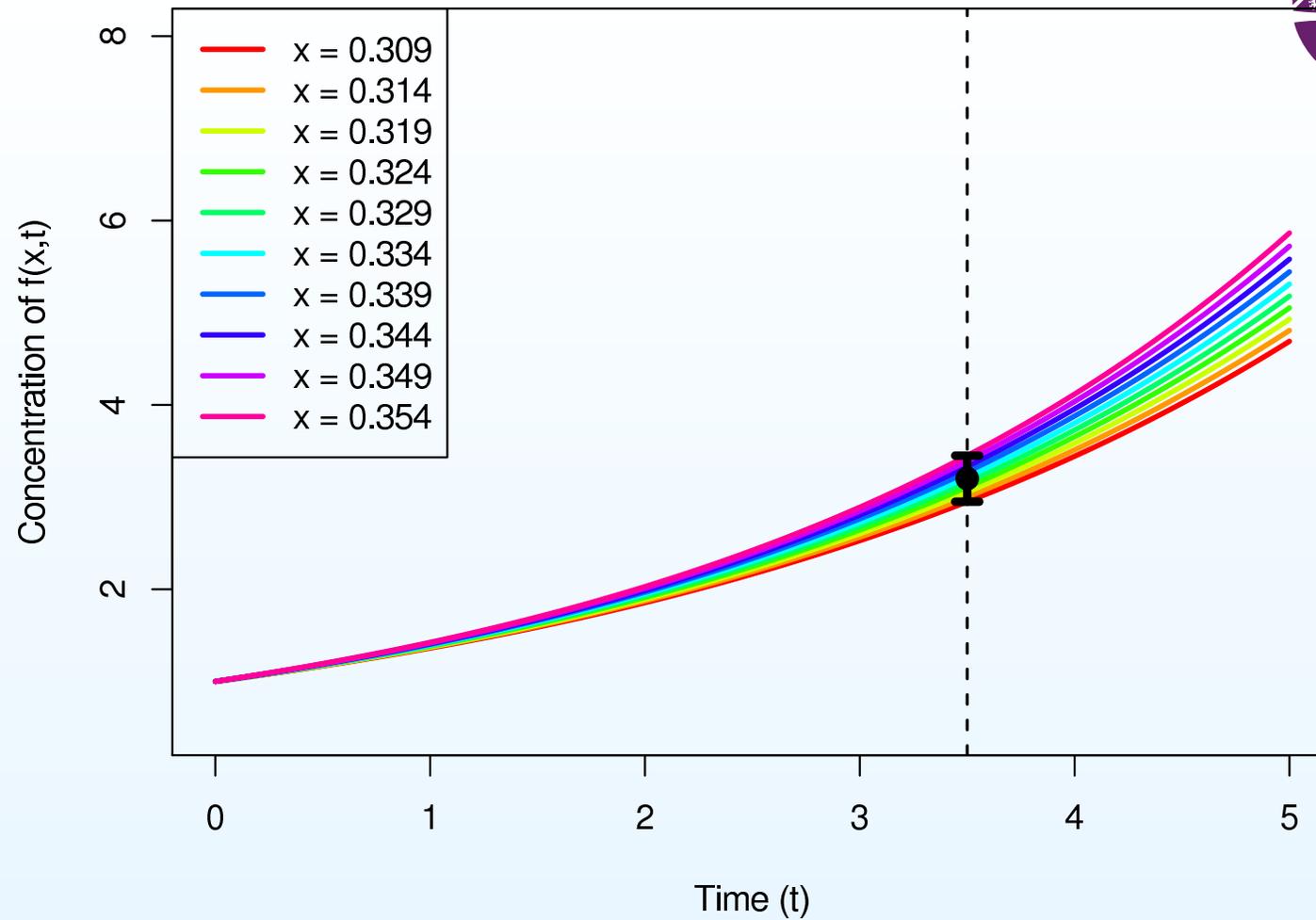
- Uncertainty in the measurement of  $f(x, t = 3.5)$  leads to uncertainty in the inferred values of  $x$ .
- Hence we see a range (green/yellow) of possible values of  $x$  consistent with the measurements, with all the implausible values of  $x$  in red.



- Constraints on  $x$  from observations impose constraints on  $f(x, t)$  in the future.



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



- This shows us the range of possible predictions of future system behaviour consistent with the model structure and the past measurements.

## Function emulation

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- (i) an approximation to the simulator and
- (ii) an assessment of the likely magnitude of the error of the approximation.

Unlike the original simulator, the emulator is fast to evaluate for any choice of inputs.

## Form of the emulator

We may represent beliefs about component  $f_i$  of  $f$ , using an emulator:

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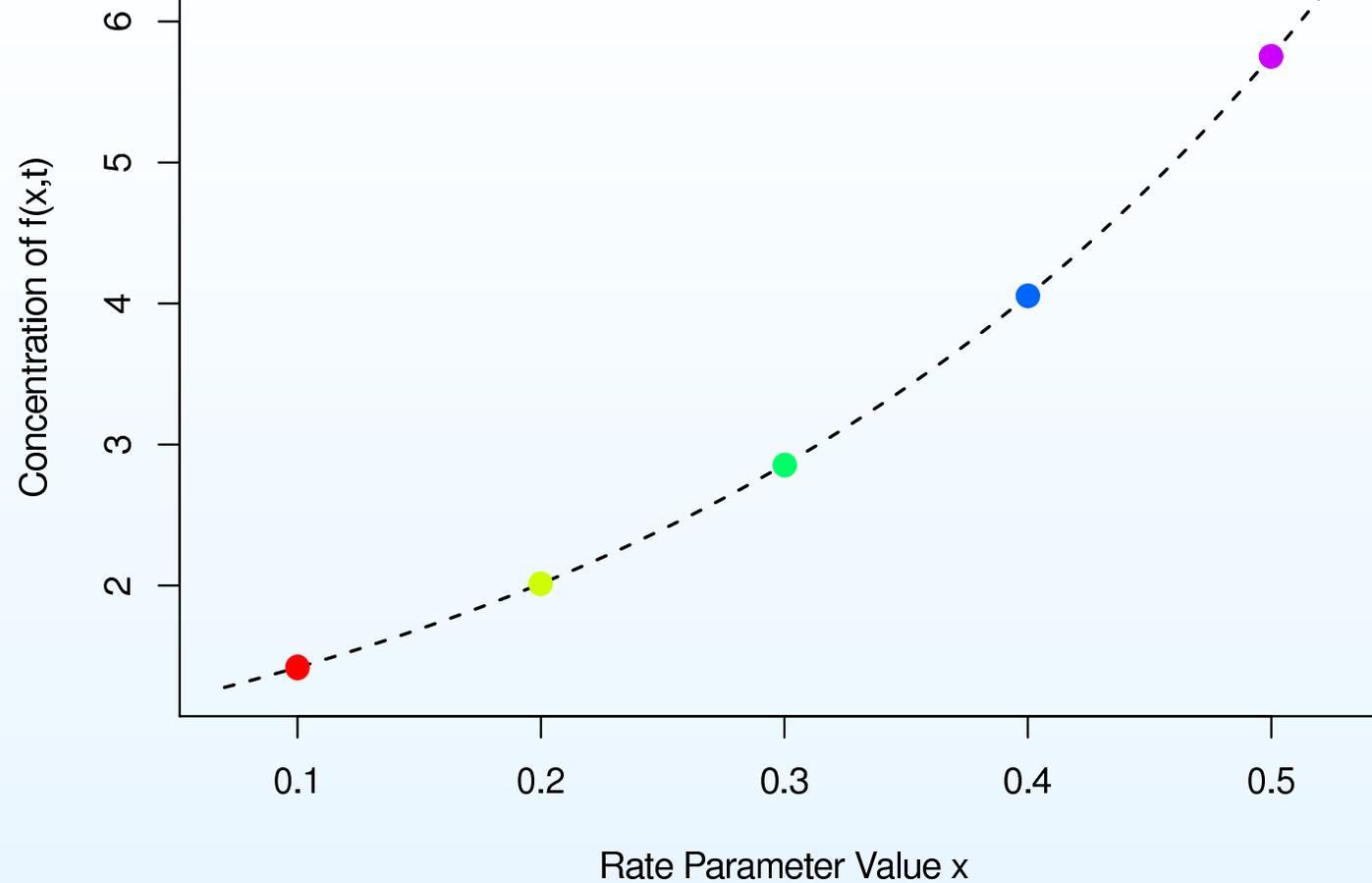
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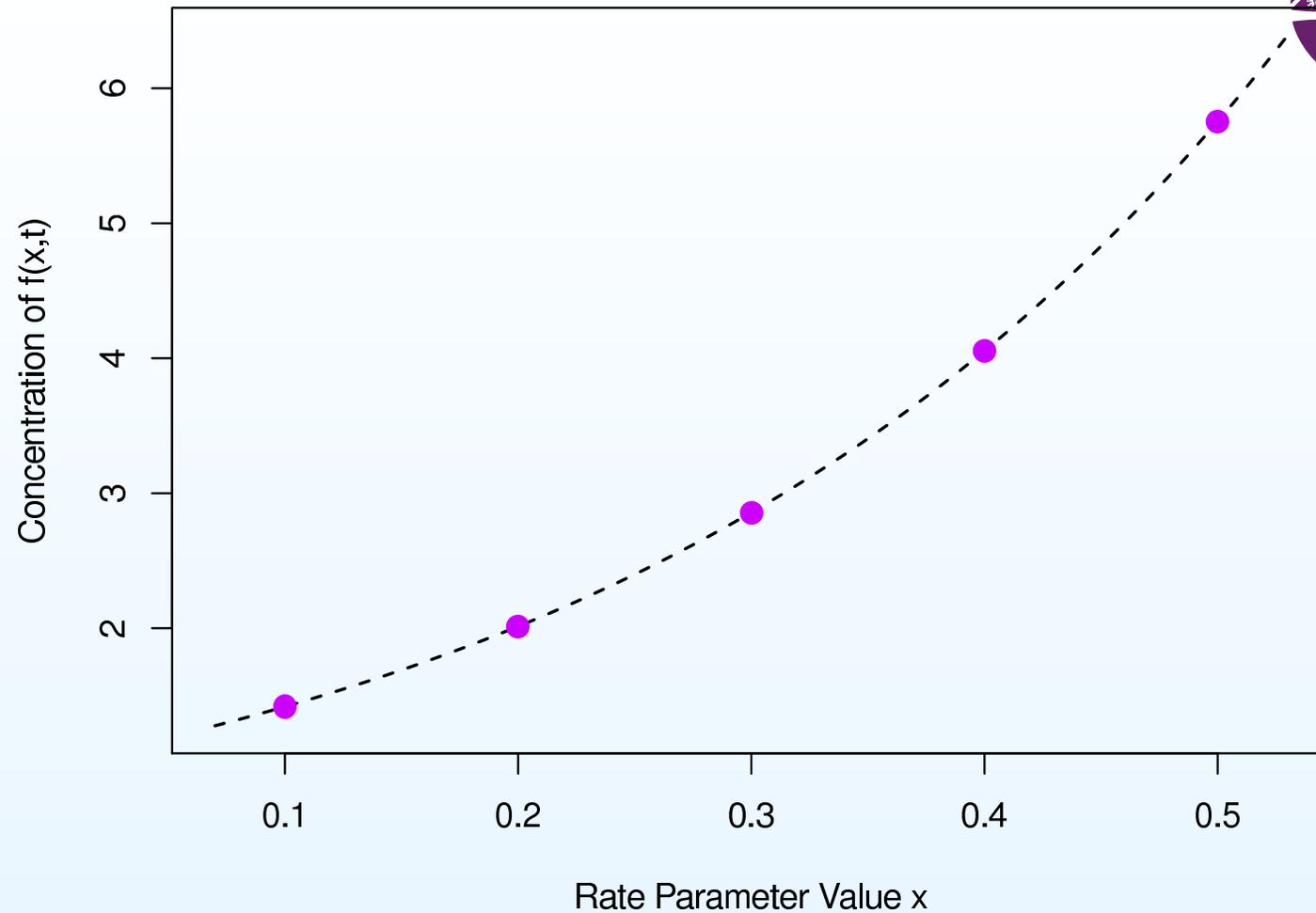
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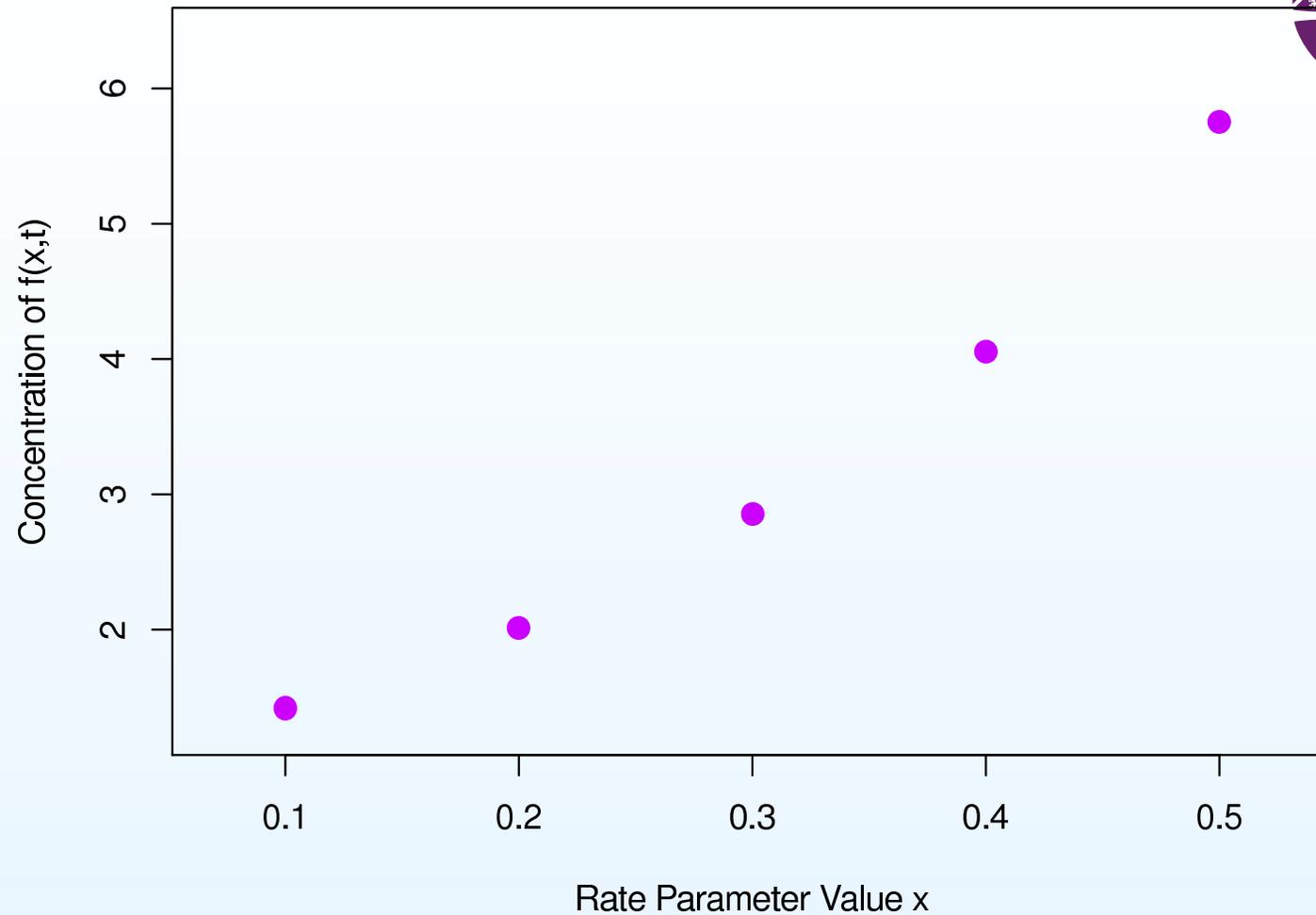
## Emulating the Model: Simple 1D Example



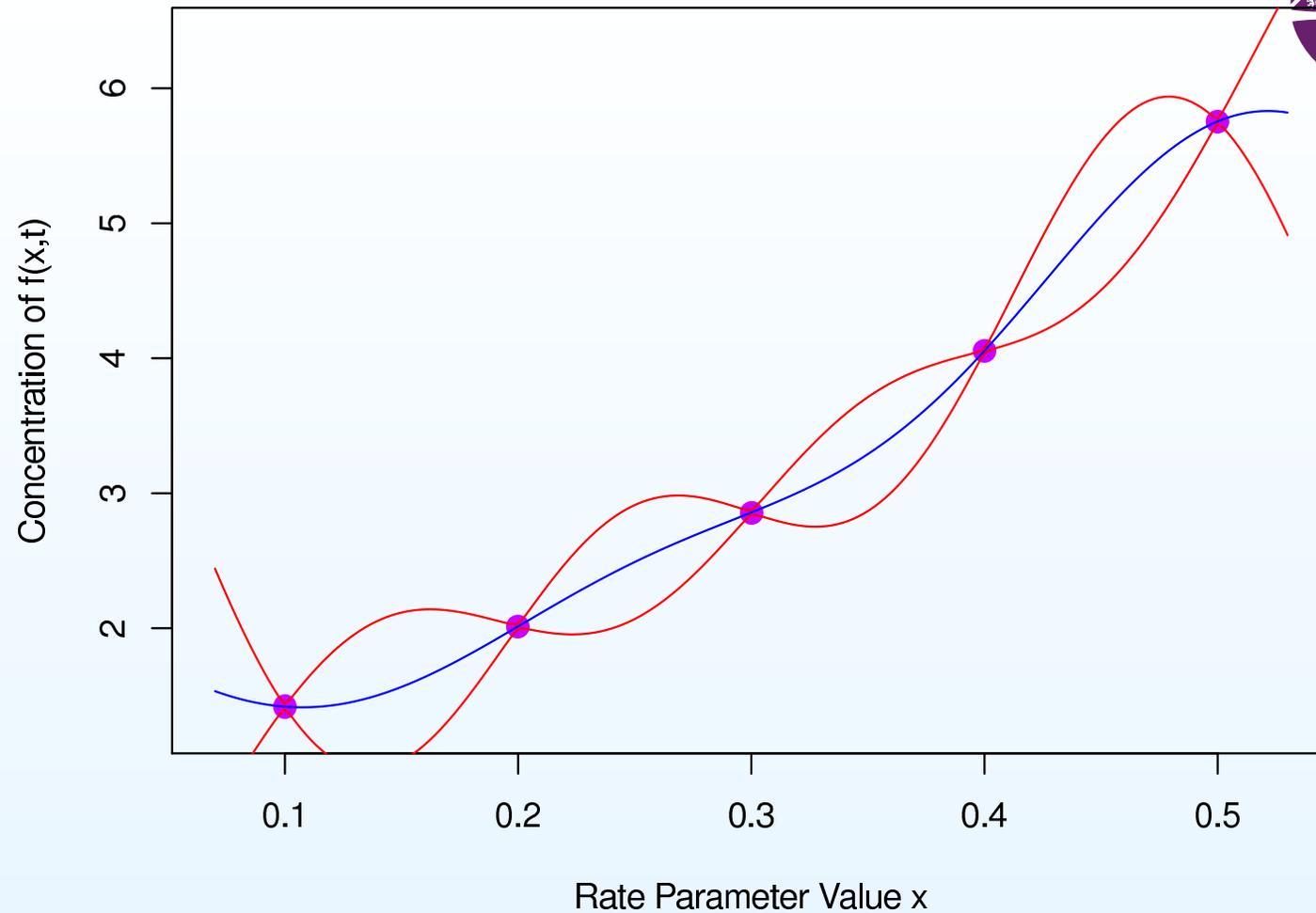
- Consider the graph of  $f(x)$ : in general we do not have the analytic solution of  $f(x)$ , here given by the dashed line.



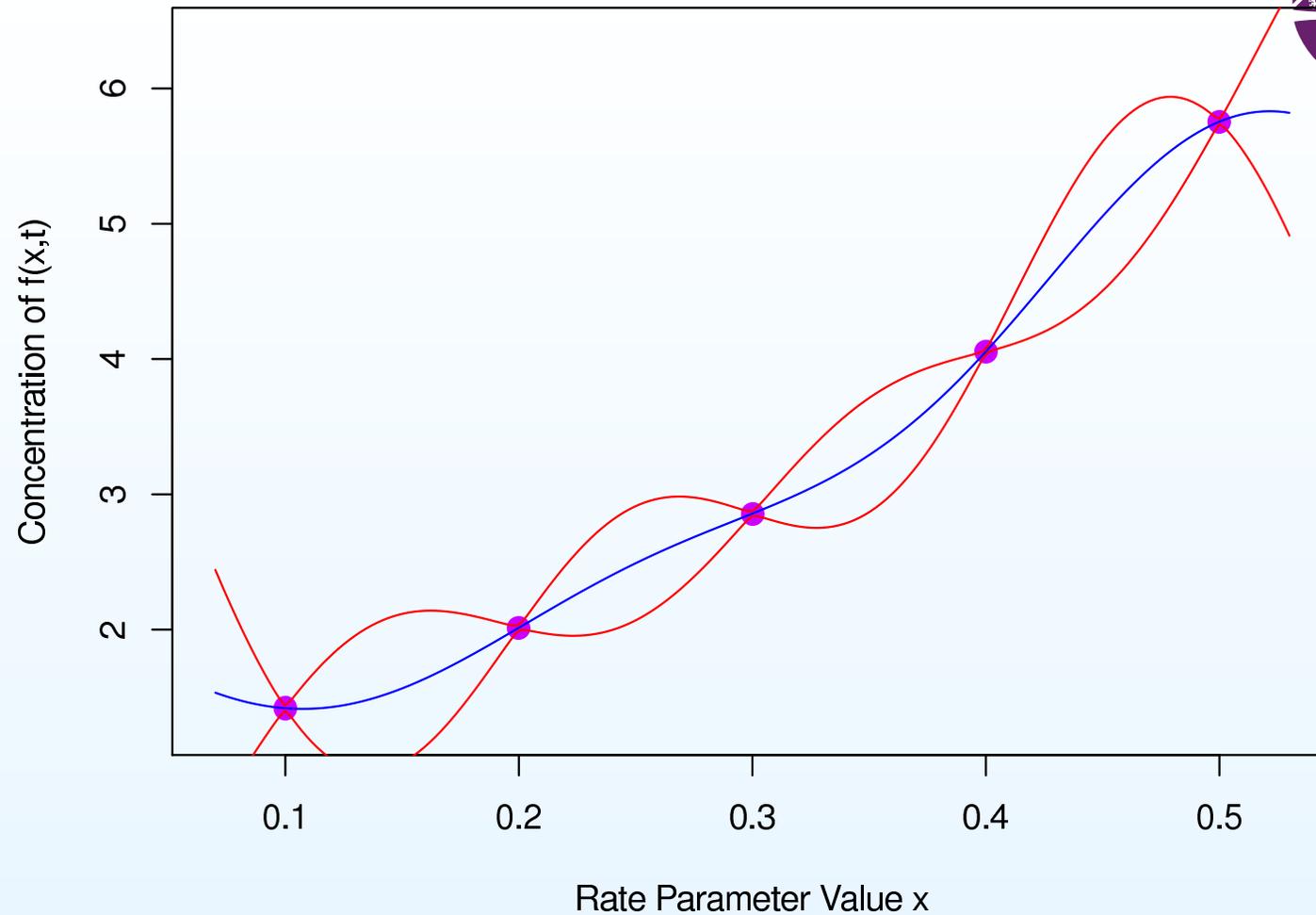
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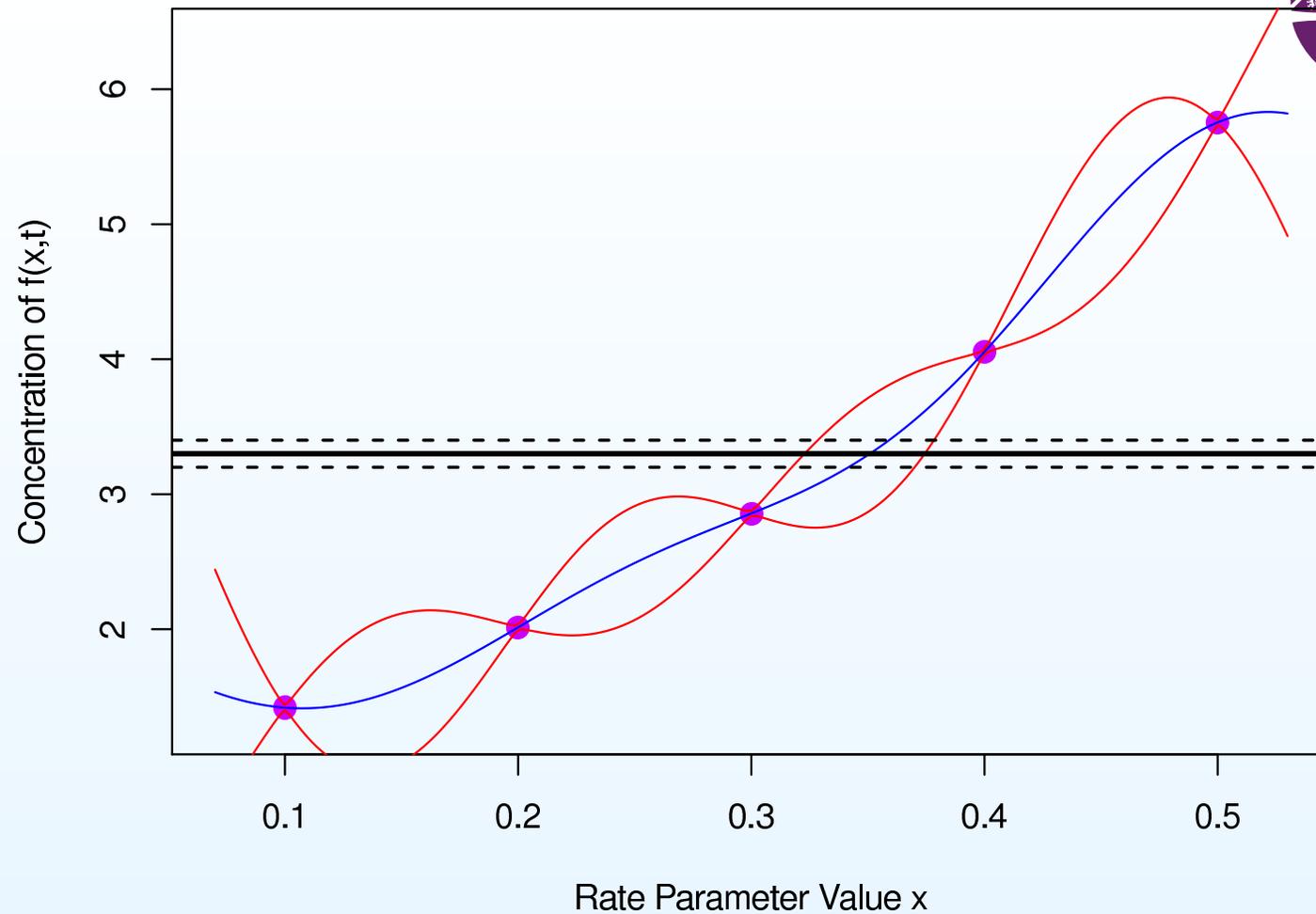
- Consider the graph of  $f(x)$ : in general we do not have the analytic solution of  $f(x)$ , here given by the dashed line.
- Instead we only have a **finite number** of runs of the model, in this case five.



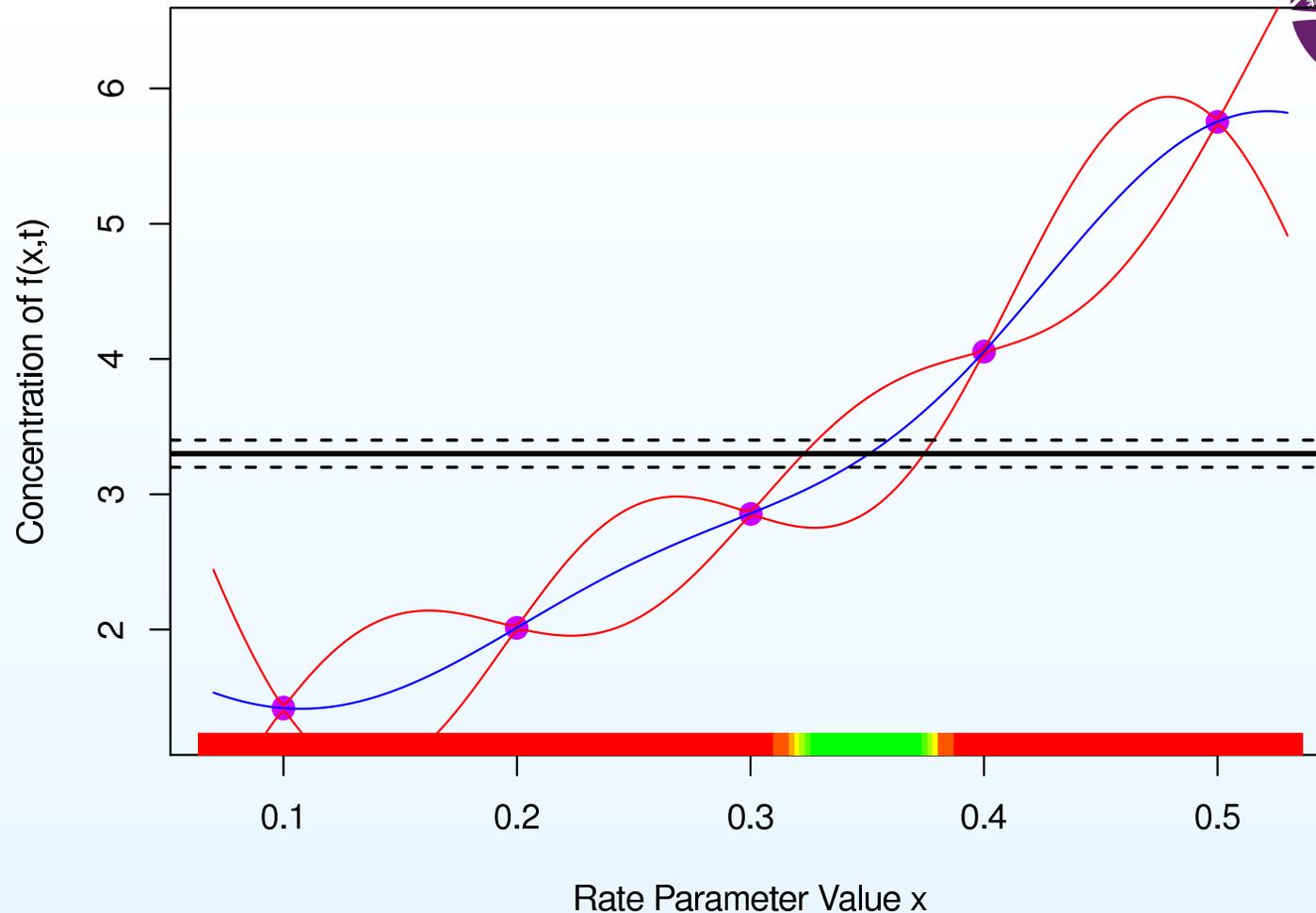
- The emulator can be used to represent our beliefs about the behaviour of the model at untested values of  $x$ , and is fast to evaluate.



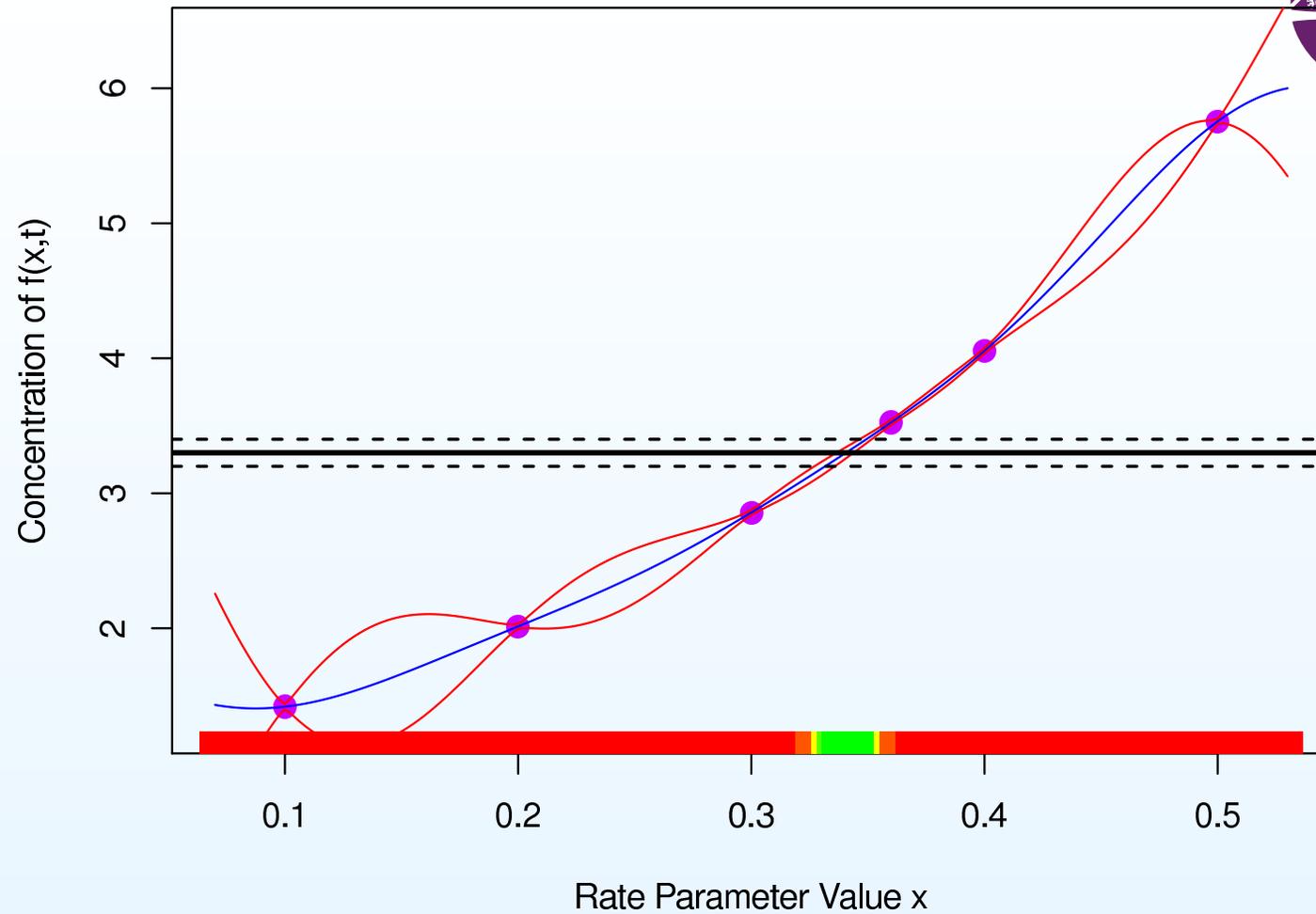
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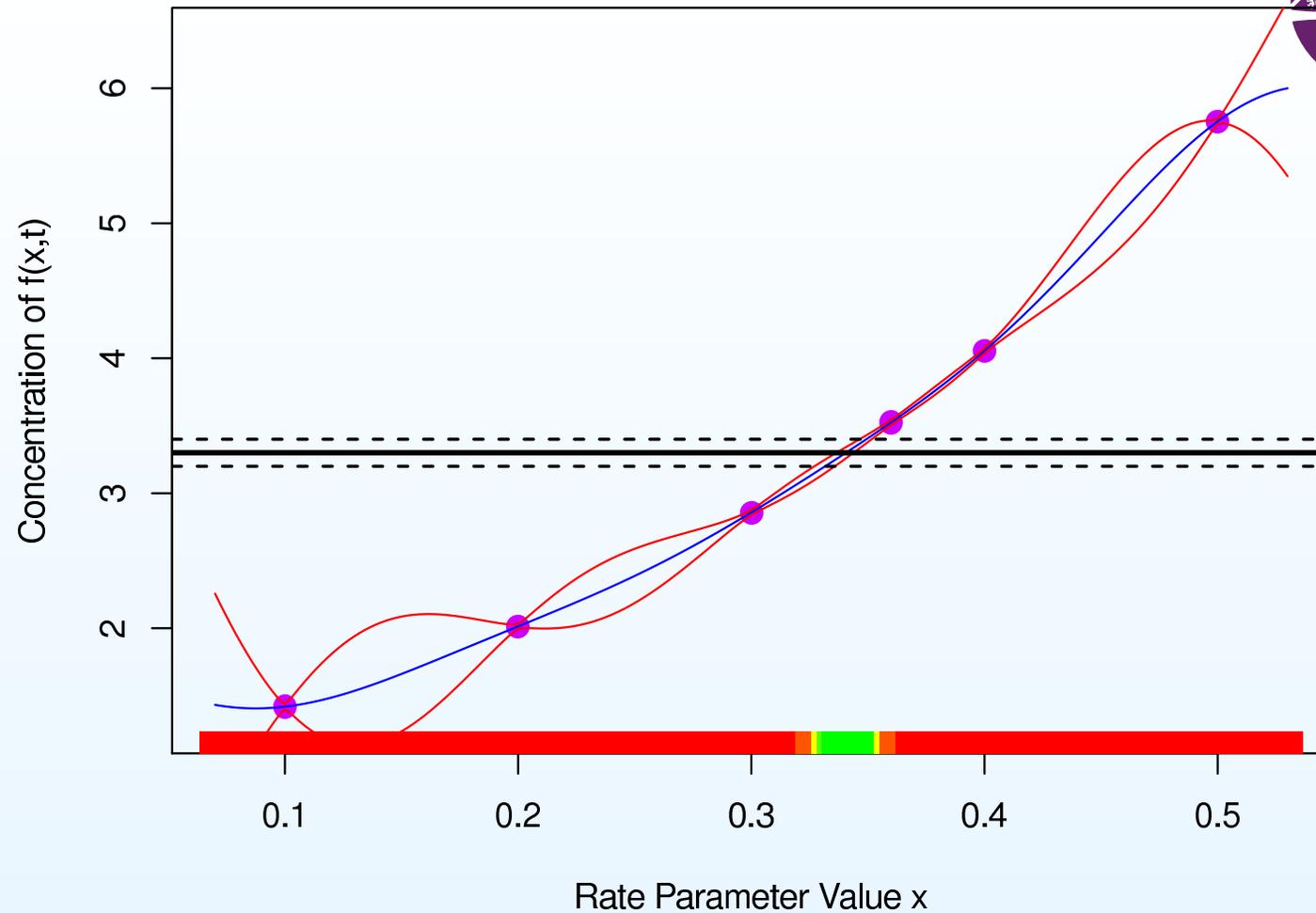
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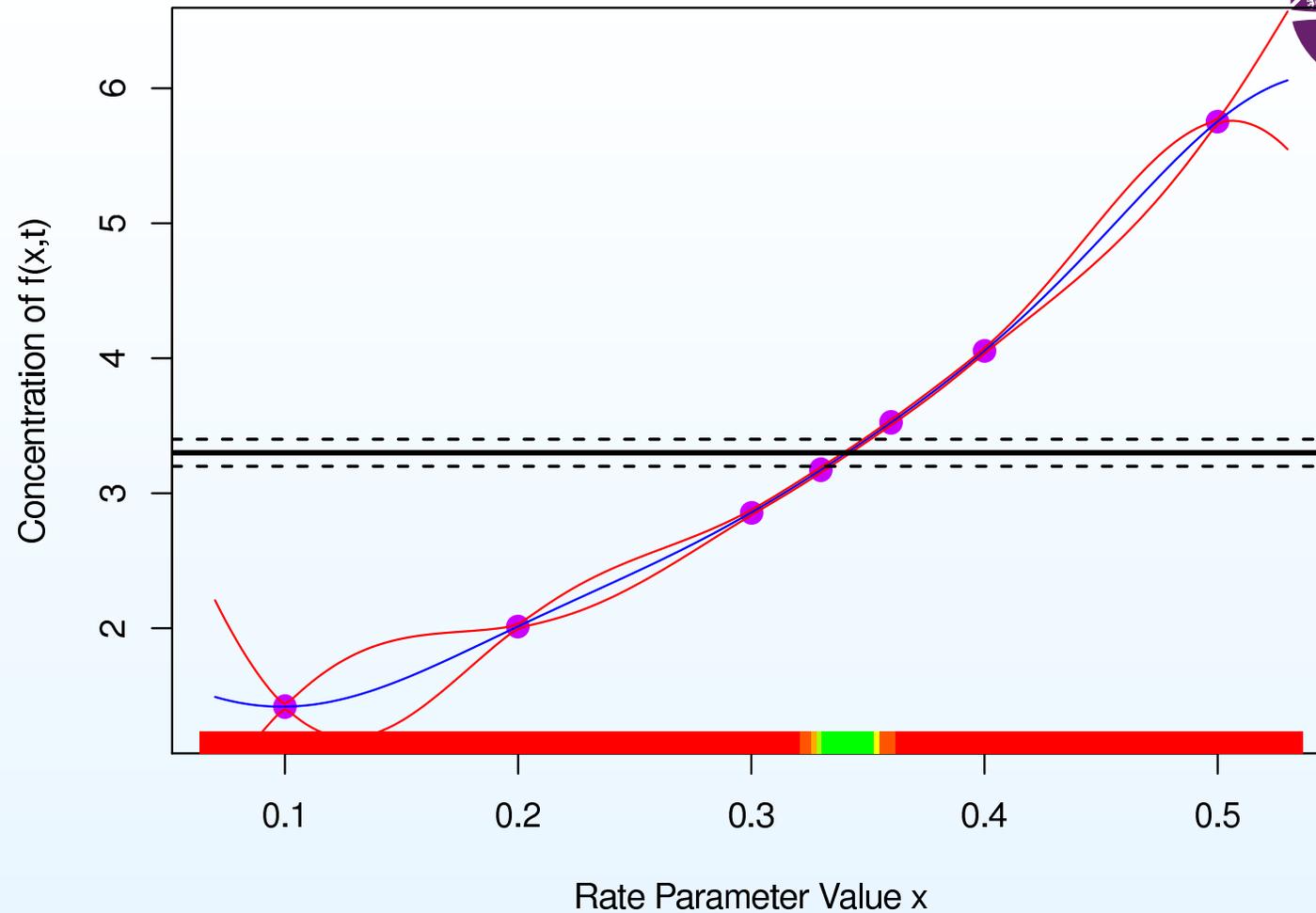
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- Note the uncertainty on  $x$  now includes uncertainty coming from the emulator.



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## Emulation methods

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Unlike the model, the emulator is fast to evaluate. Therefore construction of the emulator allows us to go beyond scenario analysis and explore the future behaviour of the model across the whole range of physically meaningful input specifications.

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Bayesian statistics provides a wide range of tools for constructing and validating such uncertainty judgements and decision choices.

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You take the test and get a positive result. Do you have the disease?

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For a detailed treatment, see

Bayes linear Statistics: Theory and Methods, 2007, (Wiley)

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## Limitations of physical models

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Neither of these approximations invalidates the modelling process. Problems only arise when we forget these simplifications and confuse the analysis of the model with the corresponding analysis for the physical system itself.

# Relating the model and the system

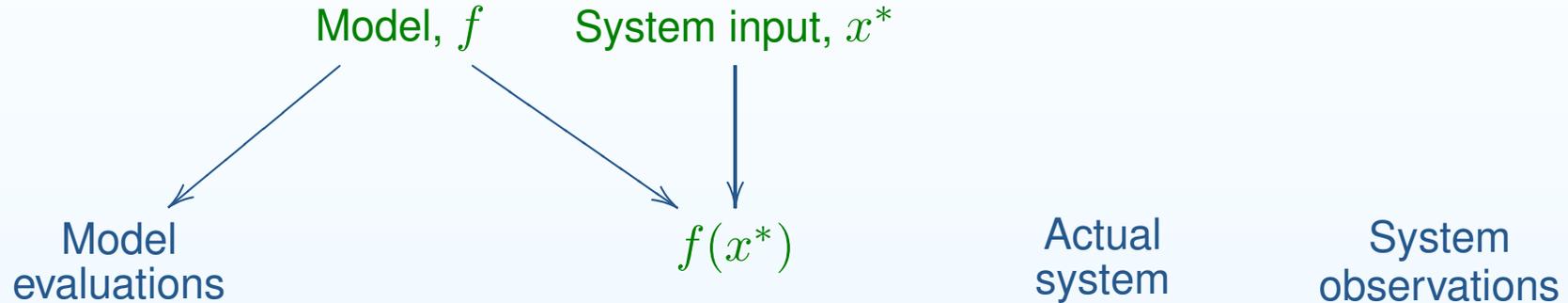
Model  
evaluations

Actual  
system

System  
observations

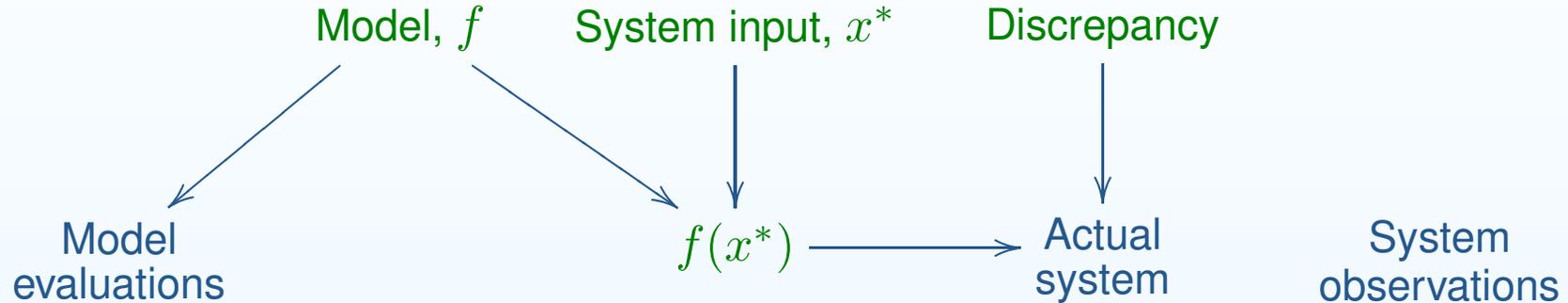
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2. We link the model evaluations to the evaluation of the model at the (unknown) system values  $x^*$  for the inputs
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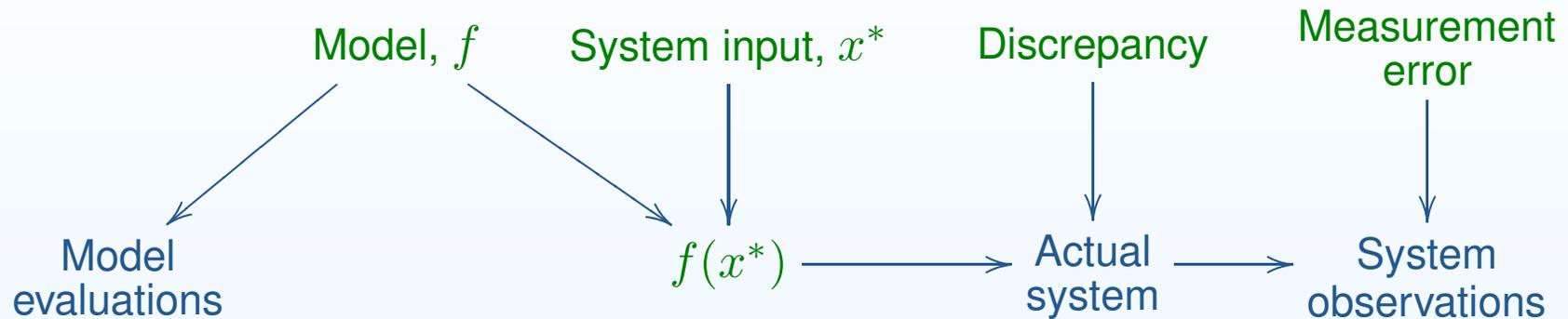
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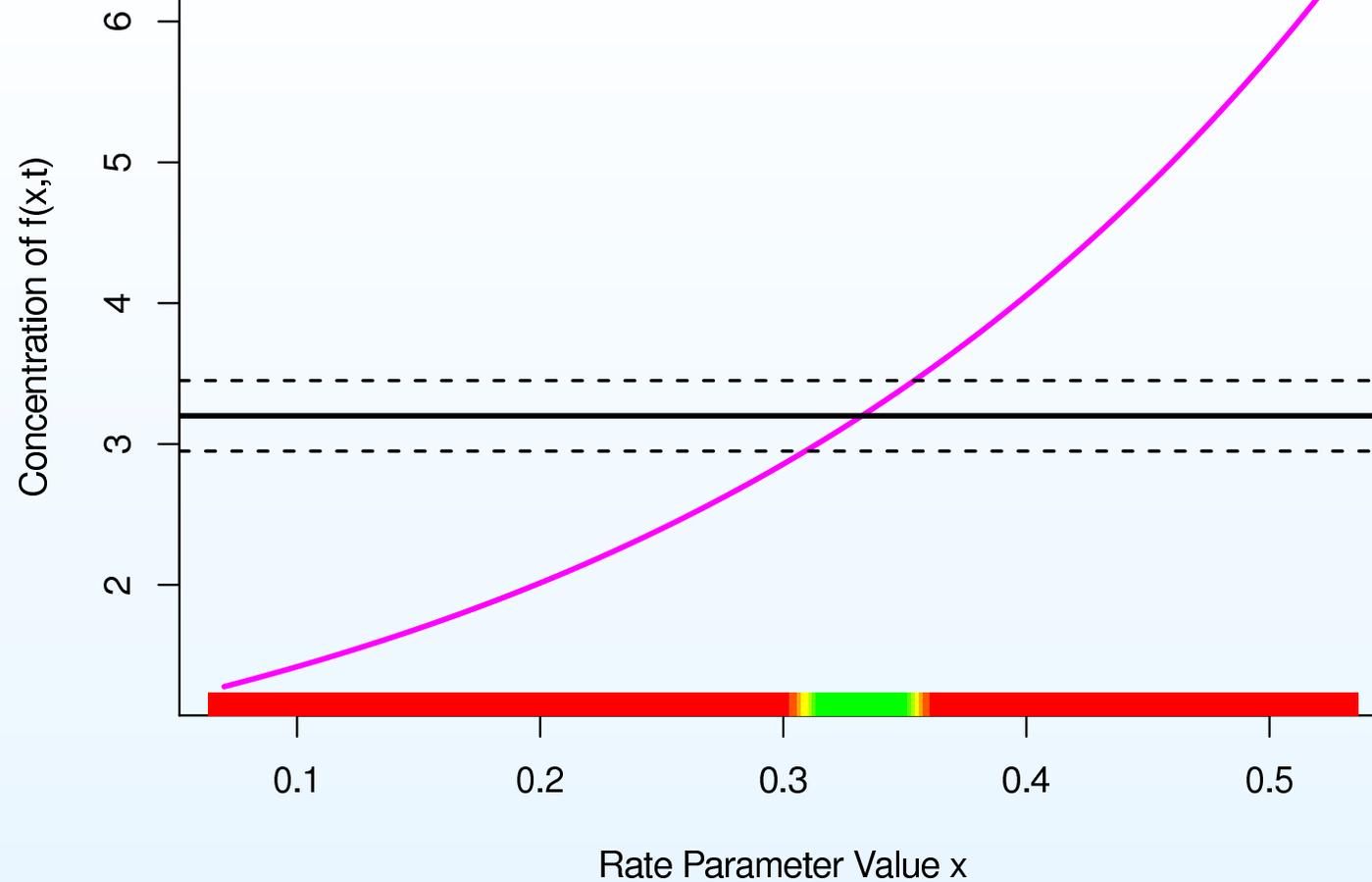
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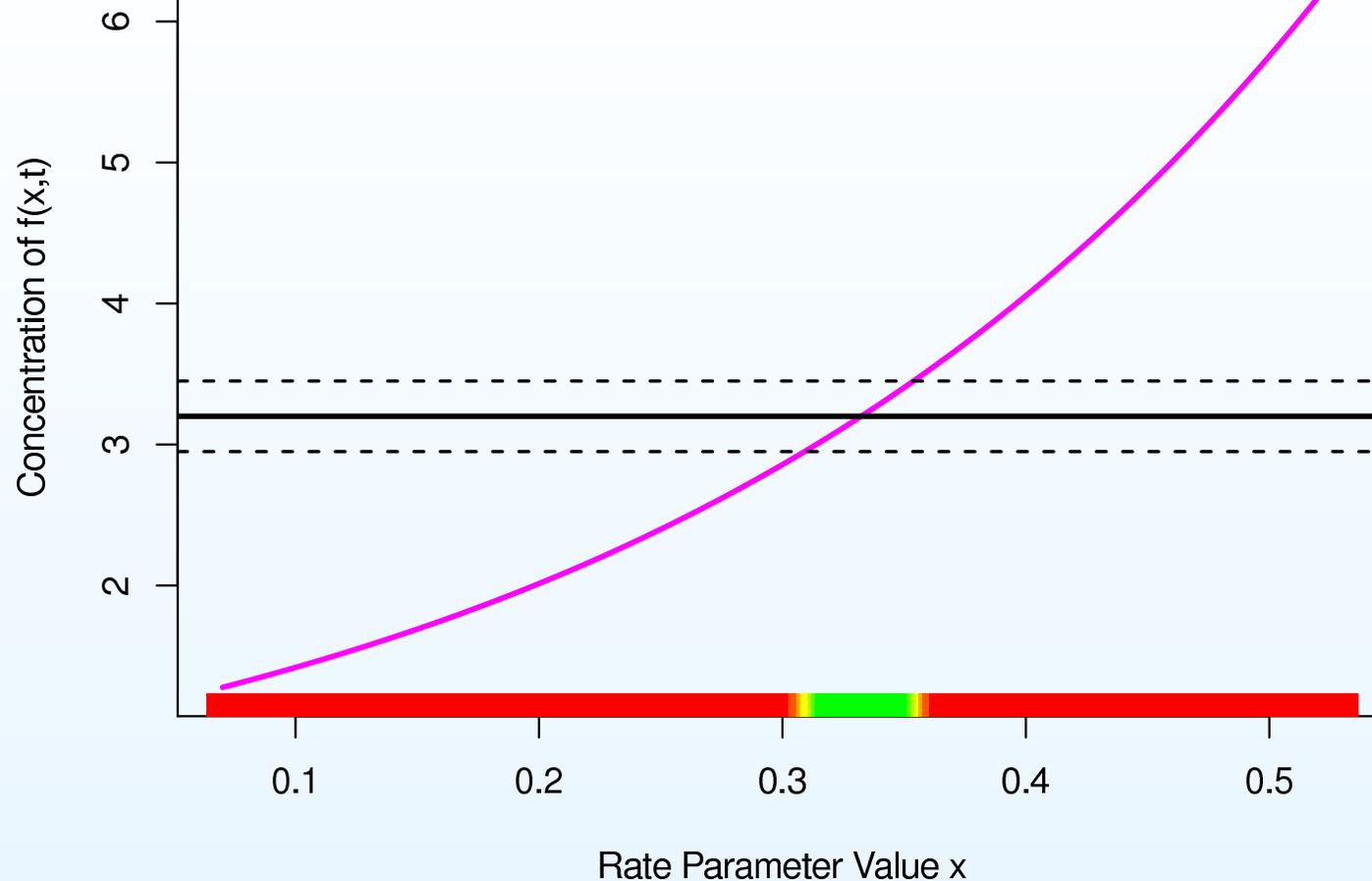
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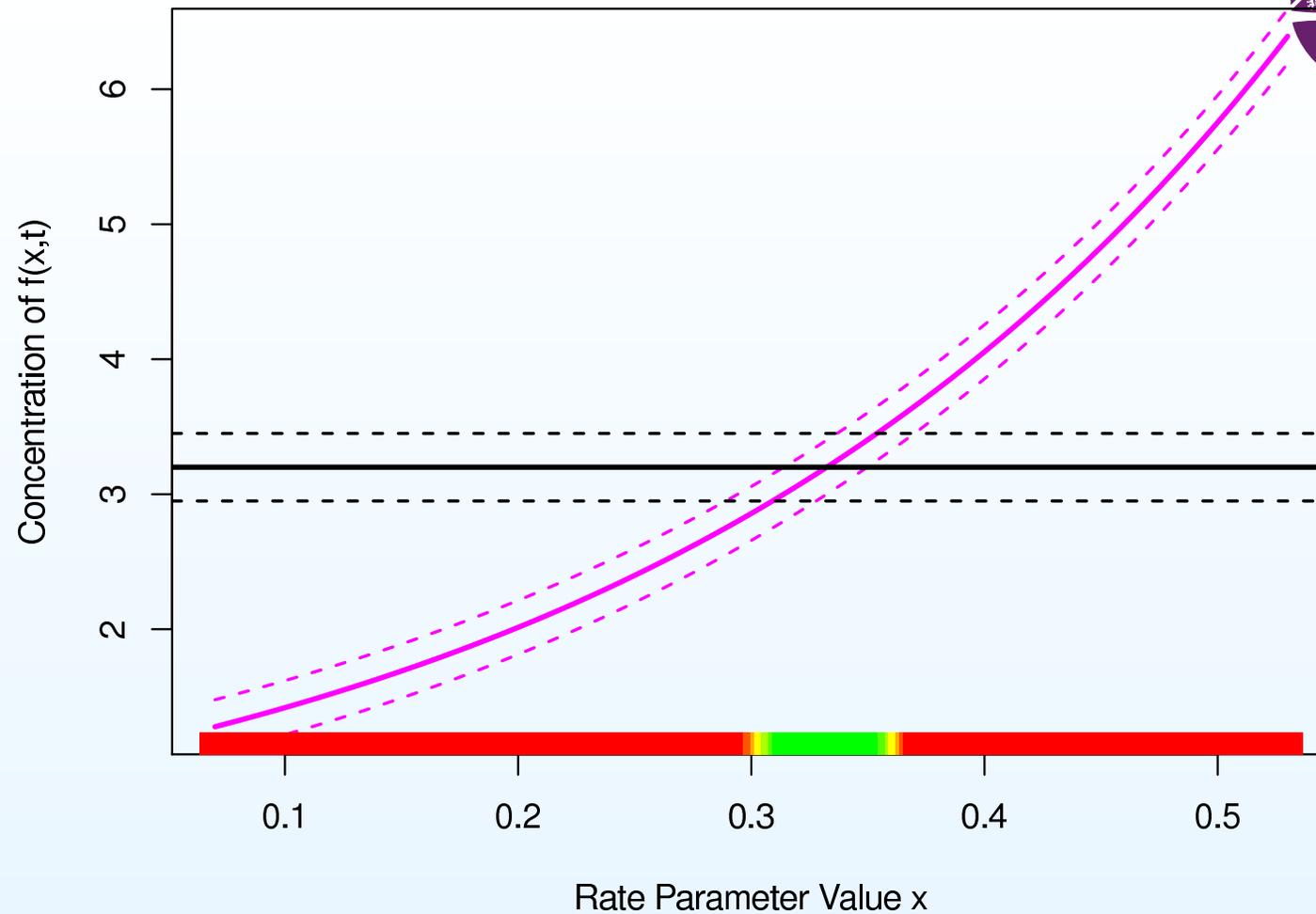


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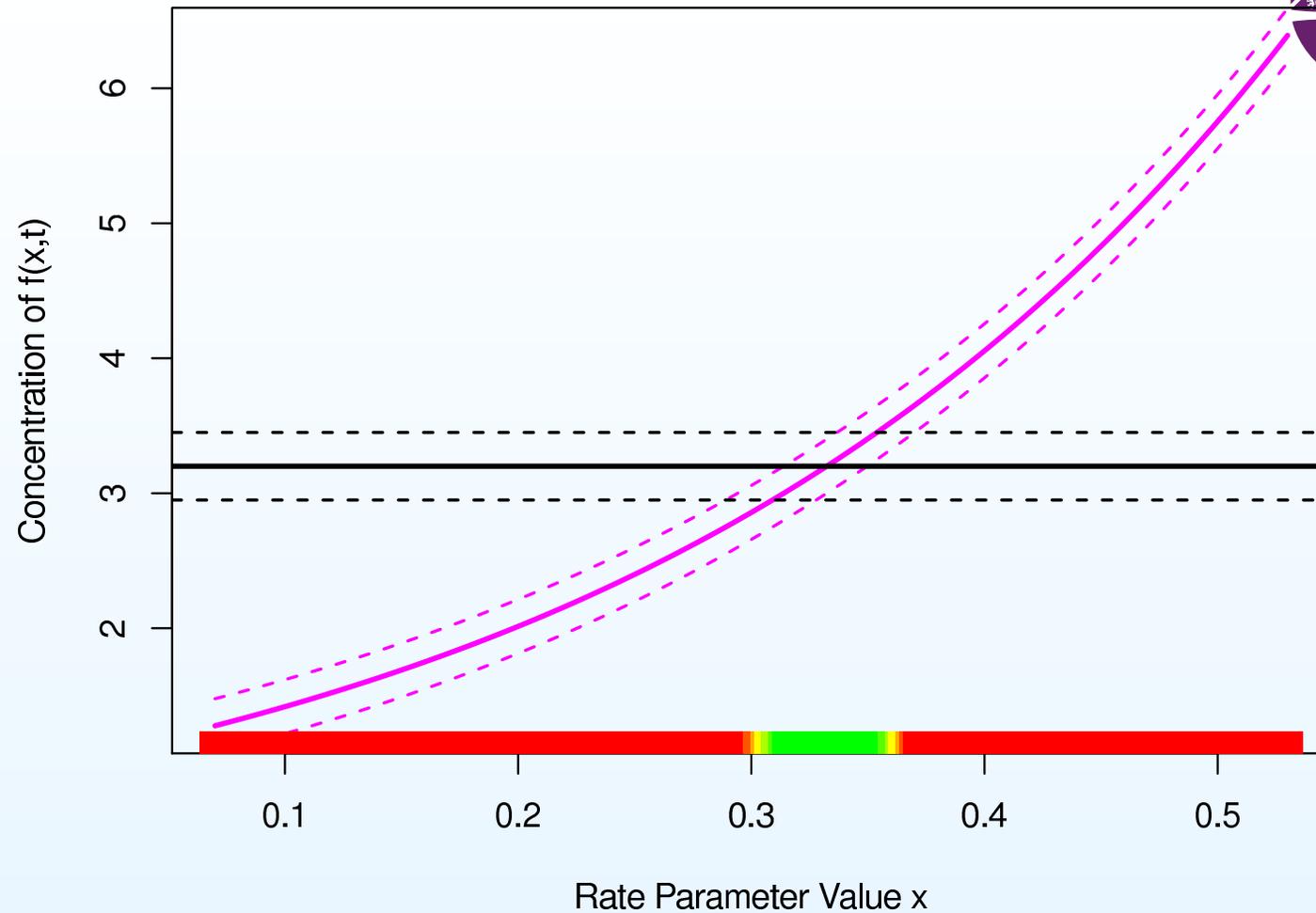
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- The notion of **model discrepancy** is related to how accurate we believe the model to be.
- This uncertainty arises from many issues e.g. is the form of the model (the differential equation) appropriate, is the model a simplified description of a more complex system, is there uncertainty in the initial conditions etc?



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We assess structural discrepancy for

(i) historical system outputs to improve our model fitting to data and

(ii) for future system outputs to improve our uncertainty statements for future system forecasts.

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## Energy systems integration



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  - (ii) making random draws  $\hat{u}$  from  $\hat{f}_2(\hat{y}, w) + \delta_2$

This approach is modular. We can emulate and assess structural discrepancy over each model separately, then combine all of the specifications to carry out the composite uncertainty analysis over any collection of subsystems of interest.

## Concluding comments

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if the simulator represents a model with many assumptions, make it easy to access and modify the code to allow simulator runs to quantify (internal) structural discrepancy.

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