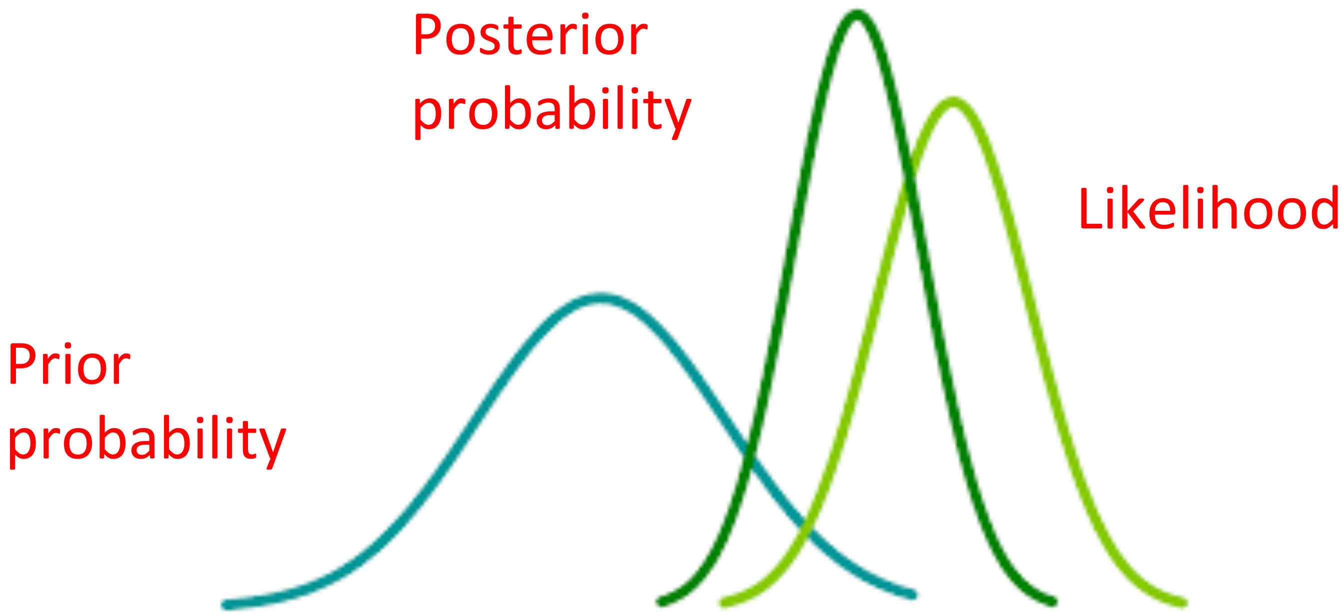
Part 4
Uncertainty quantification

Dirk Husmeier

University of Glasgow | School of Mathematics & Statistics



$$p(\theta|y) \ \propto \ p(y|\theta)p(\theta)$$

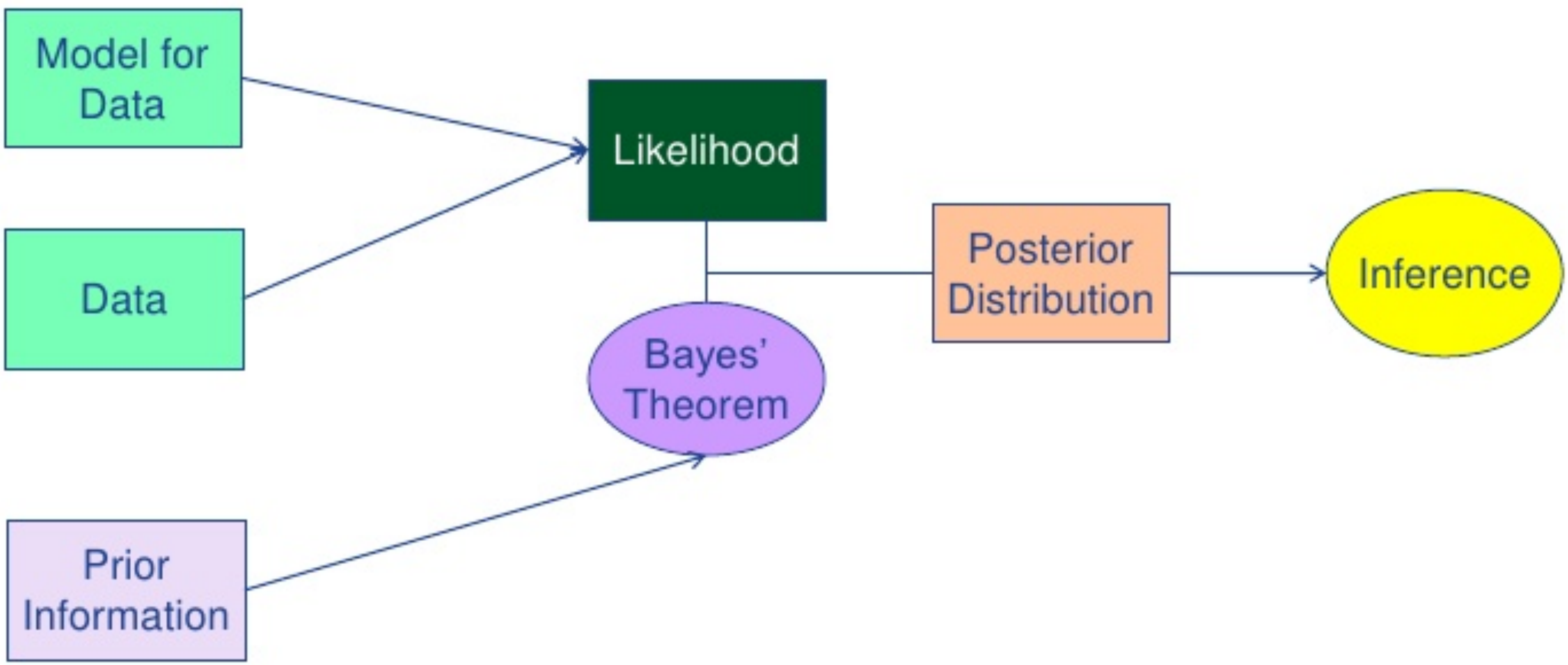
Posterior probability

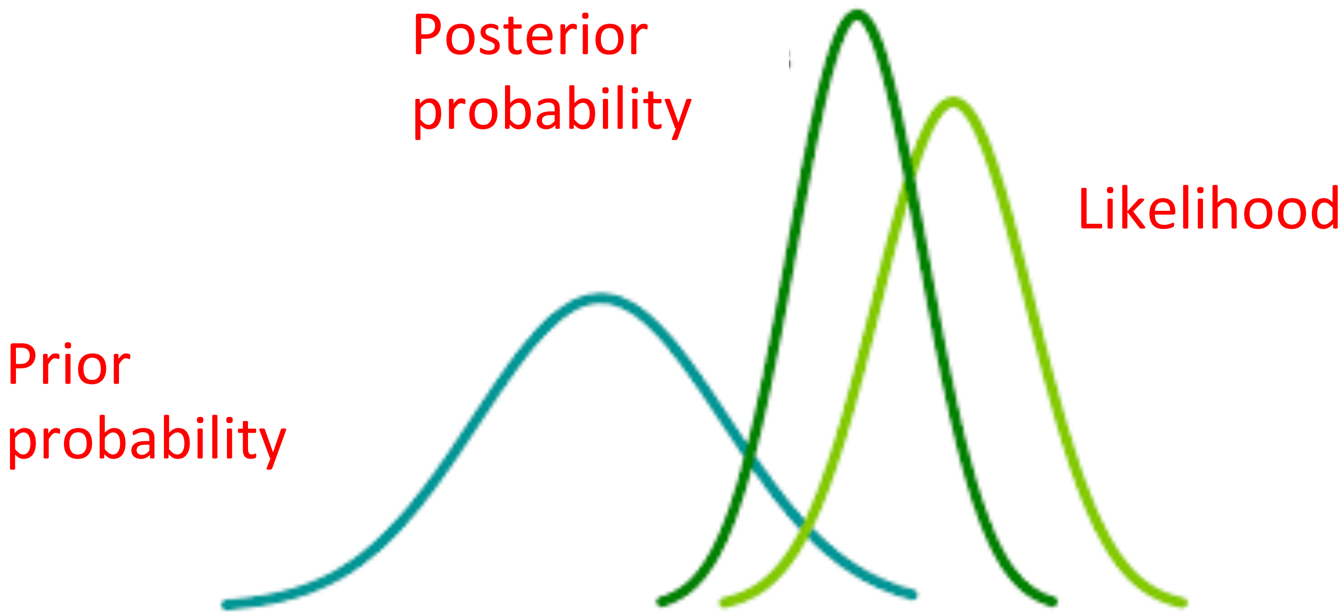
Likelihood

Prior probability

Bayes theorem

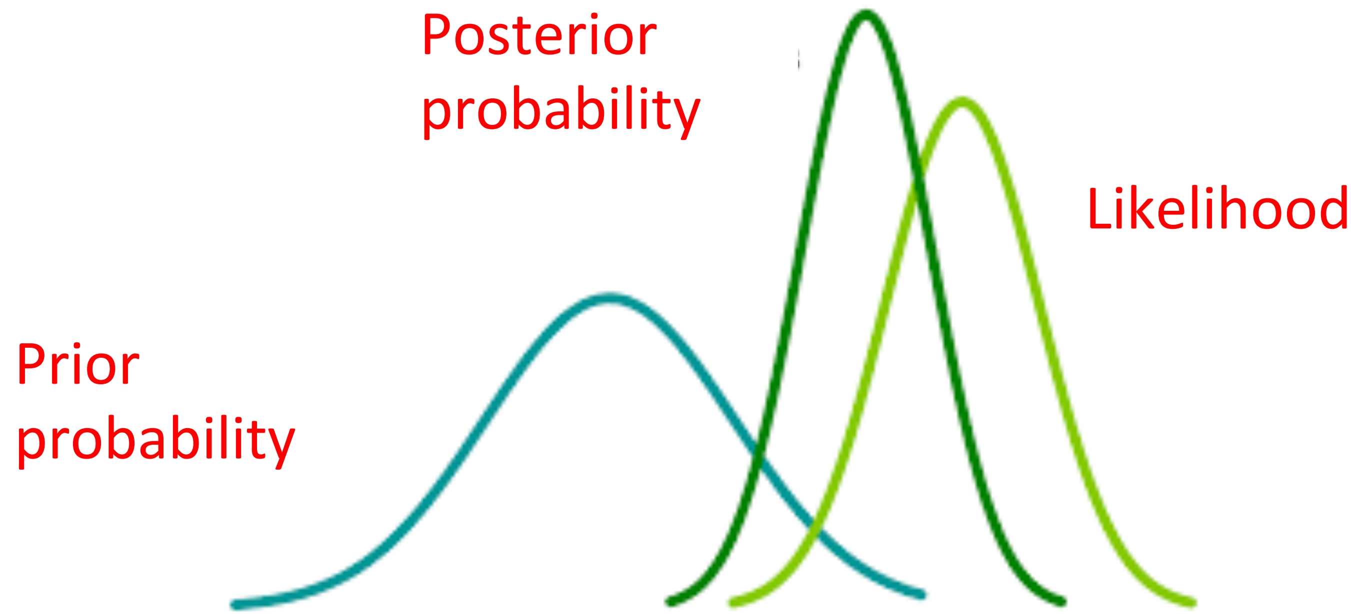
Illustration of Bayesian inference





$$p(\theta|y) \propto p(y|\theta)p(\theta) = \frac{p(y|\theta)p(\theta)}{\int p(y|\theta')p(\theta')d\theta'}$$

Usually intractable



$$p(\theta|y) \;\propto\; p(y|\theta)p(\theta) \;=\; \frac{p(y|\theta)p(\theta)}{\int p(y|\theta')p(\theta')d\theta'}$$

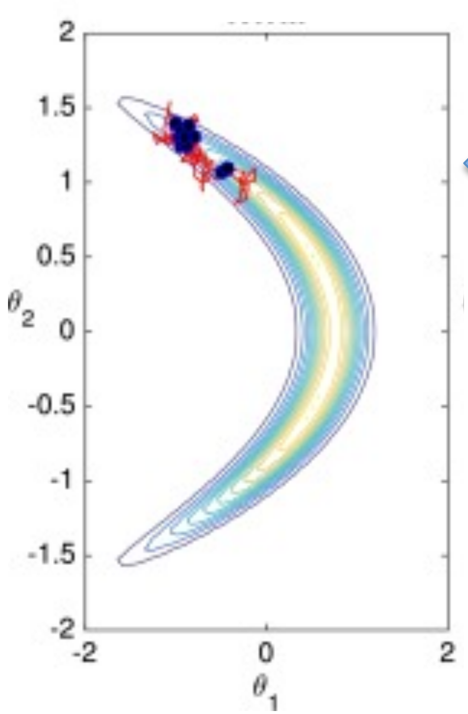
$$\theta' \sim q(\theta')$$

MCMC

Accept with probability

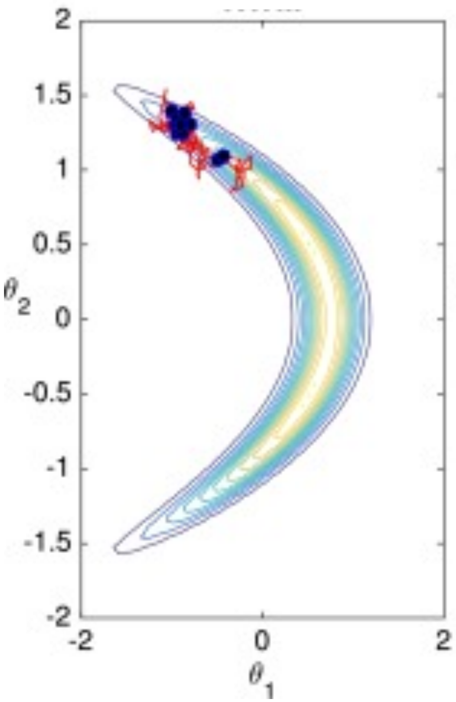
$$\min\left\{1, \frac{p(y|\theta')}{p(y|\theta)} \times \frac{p(\theta')}{p(\theta)} \times \frac{q(\theta)}{q(\theta')}\right\}$$

Example: Banana-shaped log likelihood



Standard MCMC

Example: Banana-shaped log likelihood



Standard
MCMC

Hamiltonian
Monte Carlo

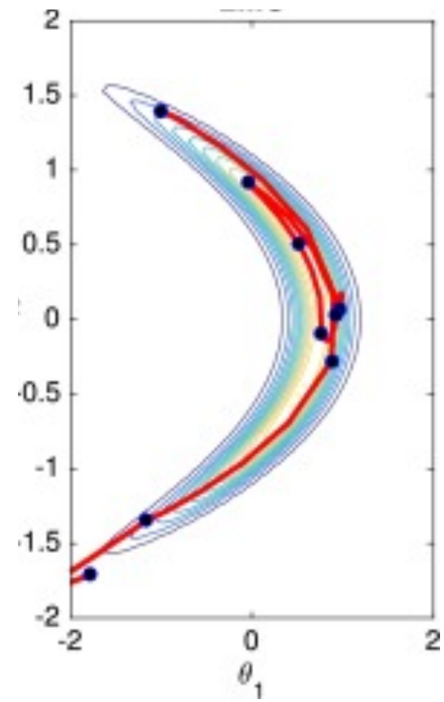


Illustration:

Hamiltonian Mechanics: The Oscillator

$$H = KE + PE = T + V$$

$$H = \frac{1}{2} m v^2 + \frac{1}{2} k x^2$$

$$= \frac{1}{2m} m^2 \dot{x}^2 + \frac{1}{2} k x^2$$

$$= \frac{1}{2m} p^2 + \frac{1}{2} k x^2$$

$$\frac{\partial H}{\partial x} = kx \qquad \frac{\partial H}{\partial p} = \frac{1}{m} p = v = \dot{x}$$

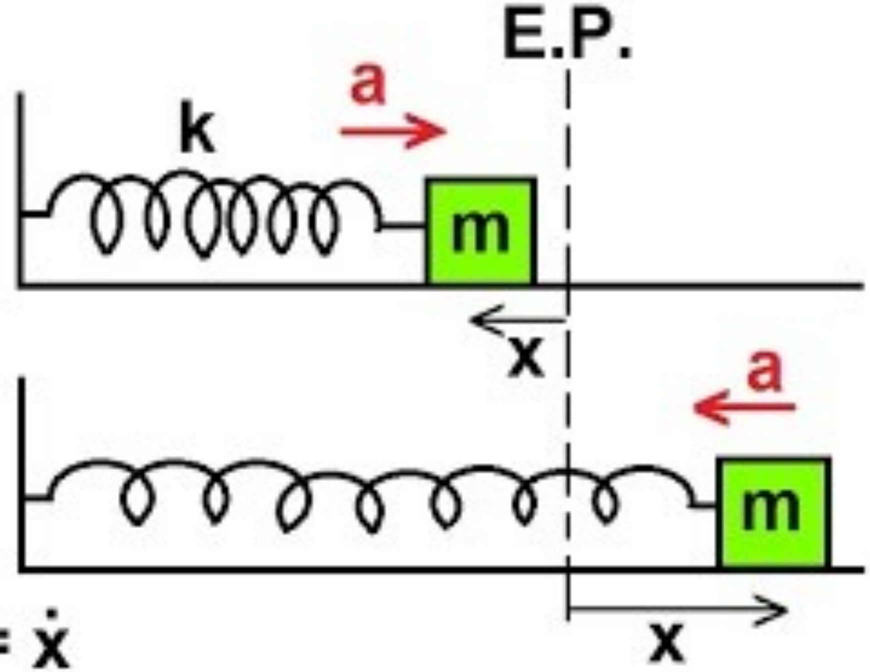


Illustration:

Hamiltonian Mechanics: The Oscillator

$$H = KE + PE = T + \boxed{V}$$

$$H = \frac{1}{2}mv^2 + \boxed{\frac{1}{2}kx^2}$$

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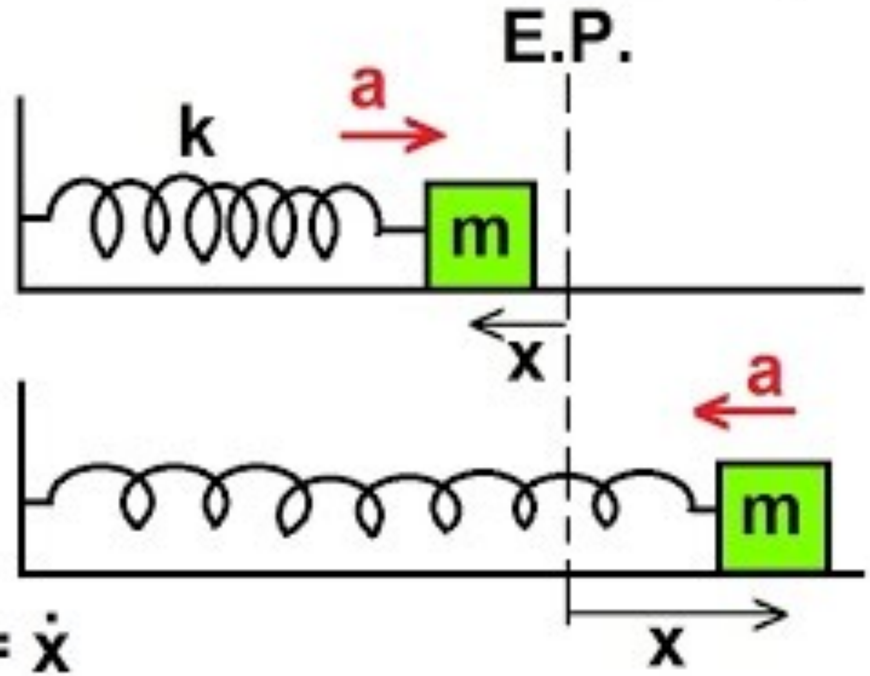

Potential energy V depending on position x.

Illustration:

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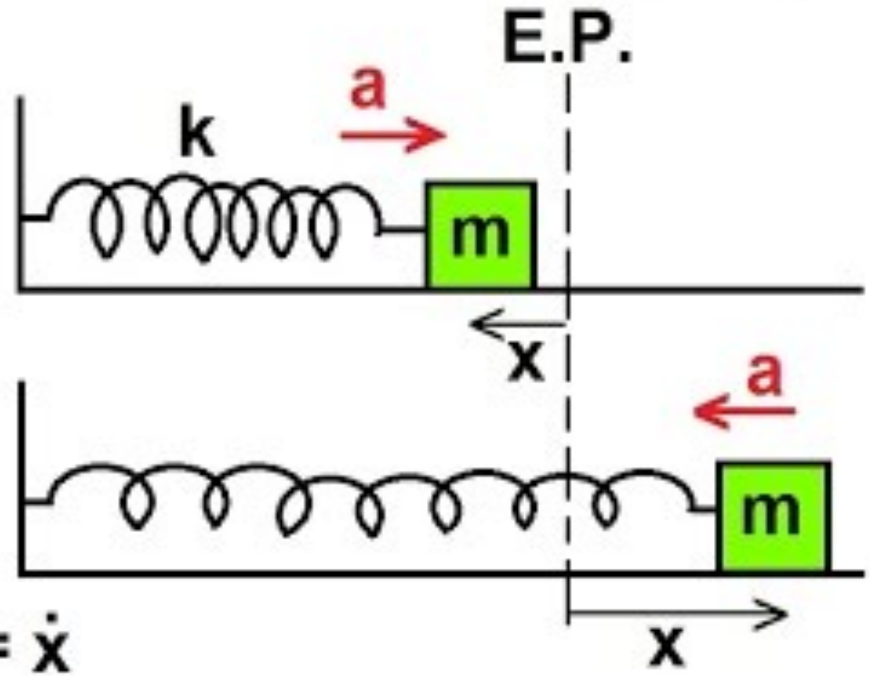

Potential energy V depending on position x.
Kinetic energy T depending on momentum p.

Illustration:

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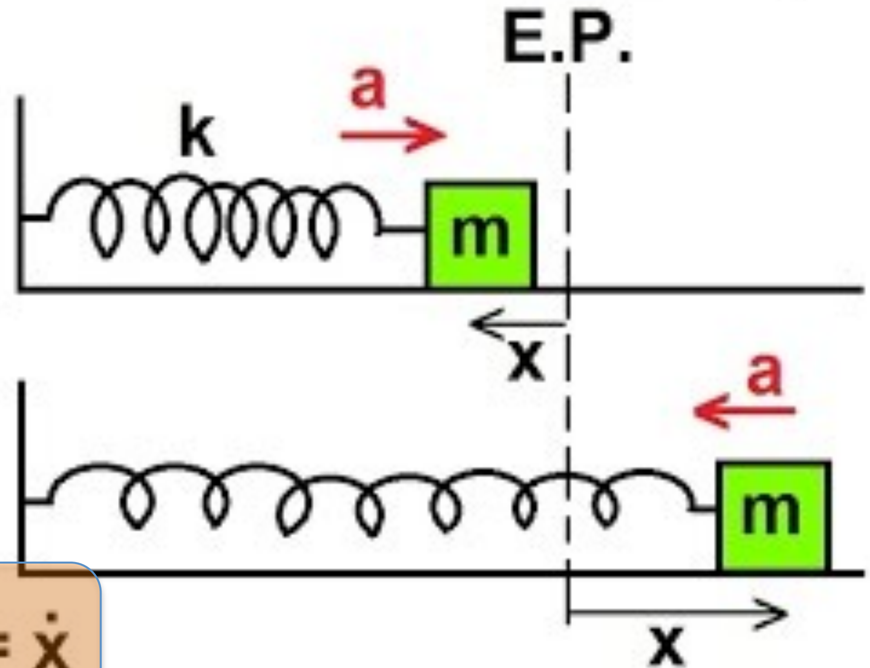

Potential energy V depending on position x.
Kinetic energy T depending on momentum p.
The Hamiltonian equations determine the dynamics of the system.

Illustration:

Hamiltonian Mechanics: The Oscillator

$$H = KE + PE = T + \boxed{V}$$

$$H = \frac{1}{2}mv^2 + \boxed{\frac{1}{2}kx^2}$$

$$= \frac{1}{2m}m^2\dot{x}^2 + \boxed{\frac{1}{2}kx^2}$$

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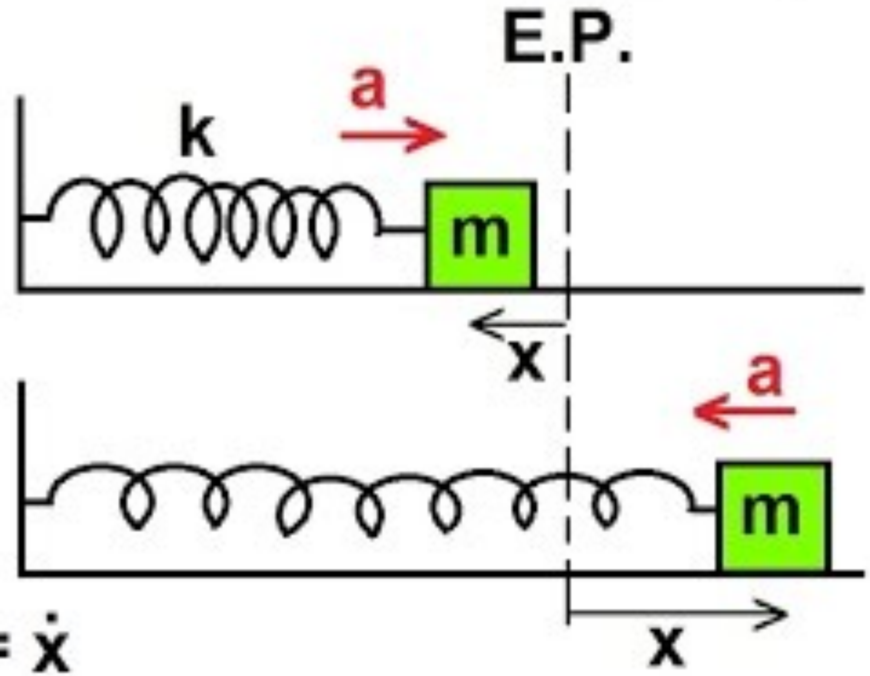
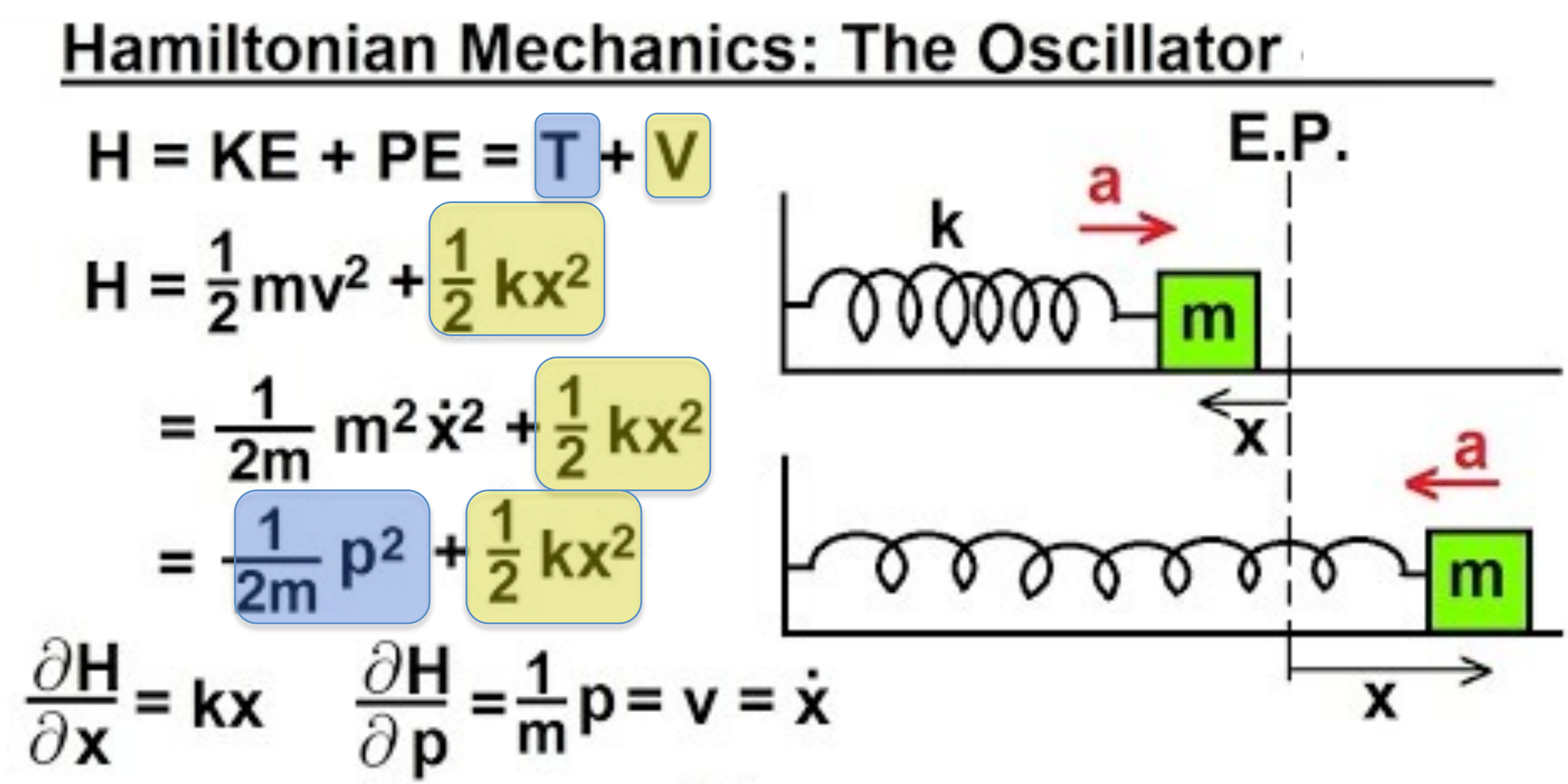


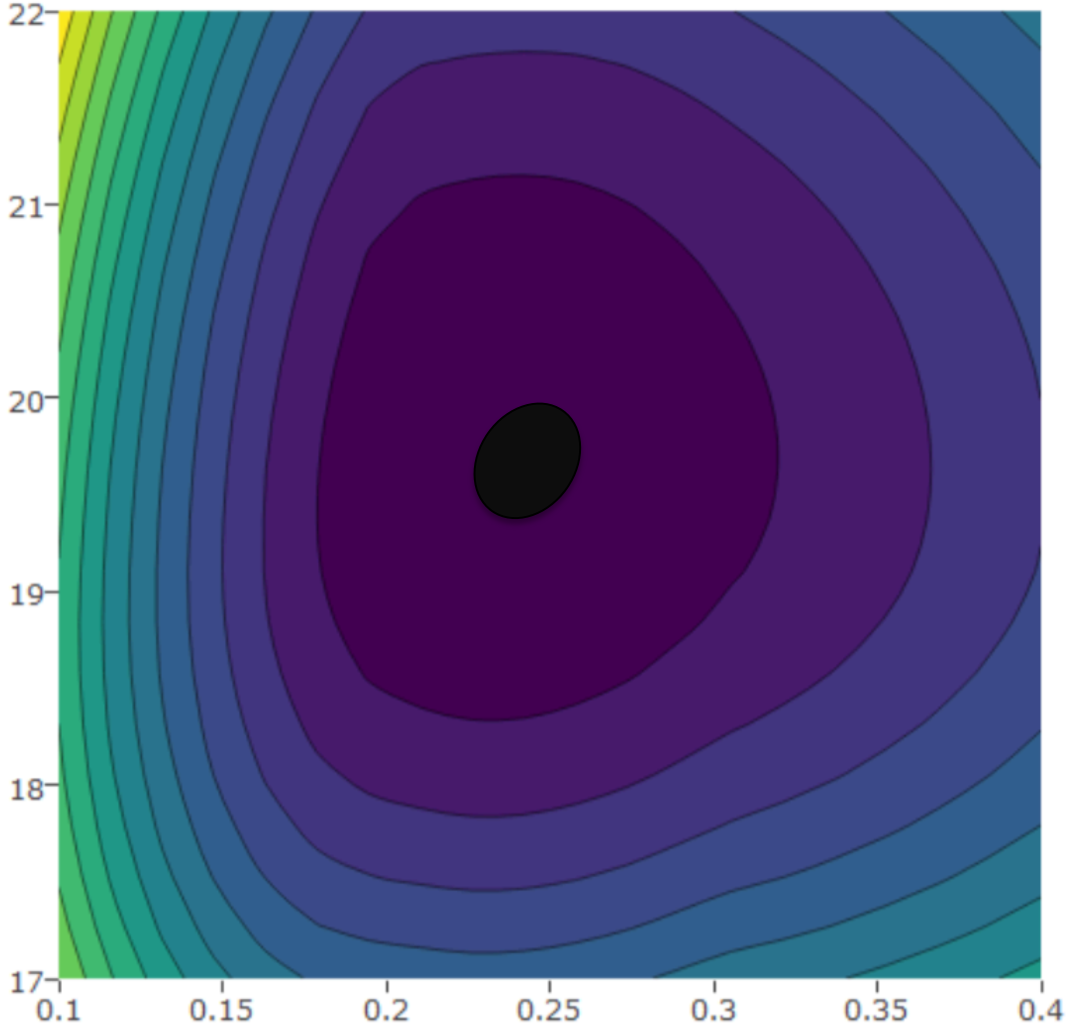
The log posterior probability corresponds to the potential energy V, the model parameters correspond to the positions x.

Illustration:

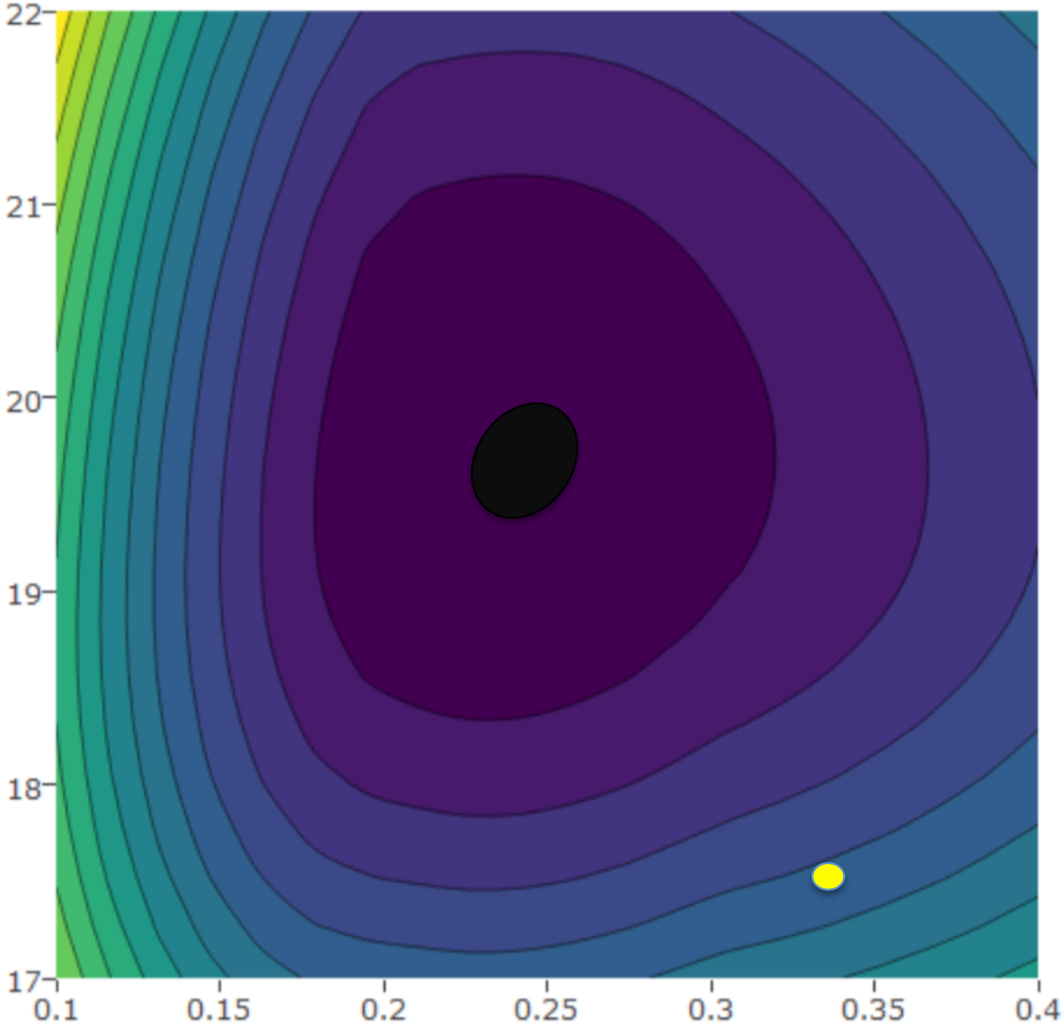


The log posterior probability corresponds to the potential energy V, the model parameters correspond to the positions x.
The momentum variables p, which determine the kinetic energy T, get discarded after the numerical integration.

Log posterior contour plot

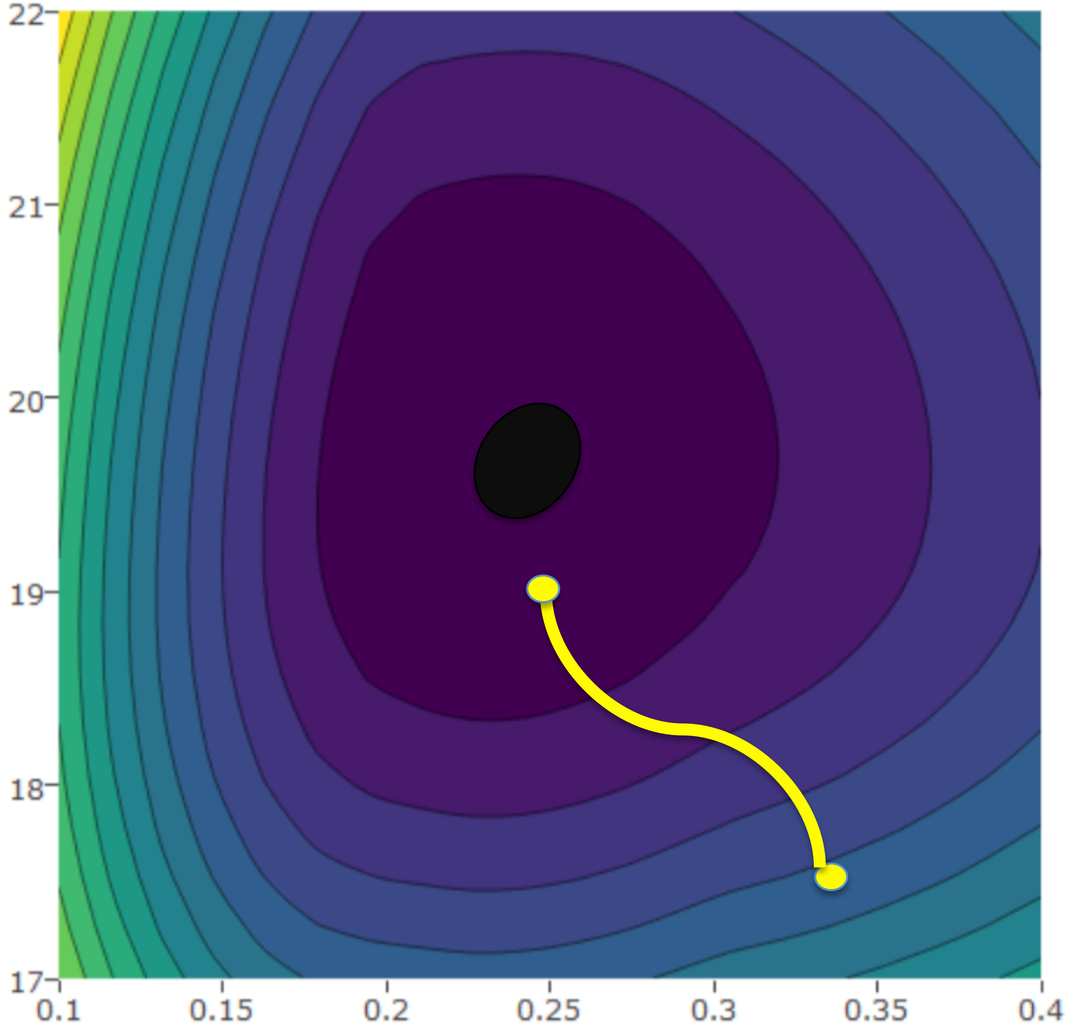


Log posterior contour plot



Starting position

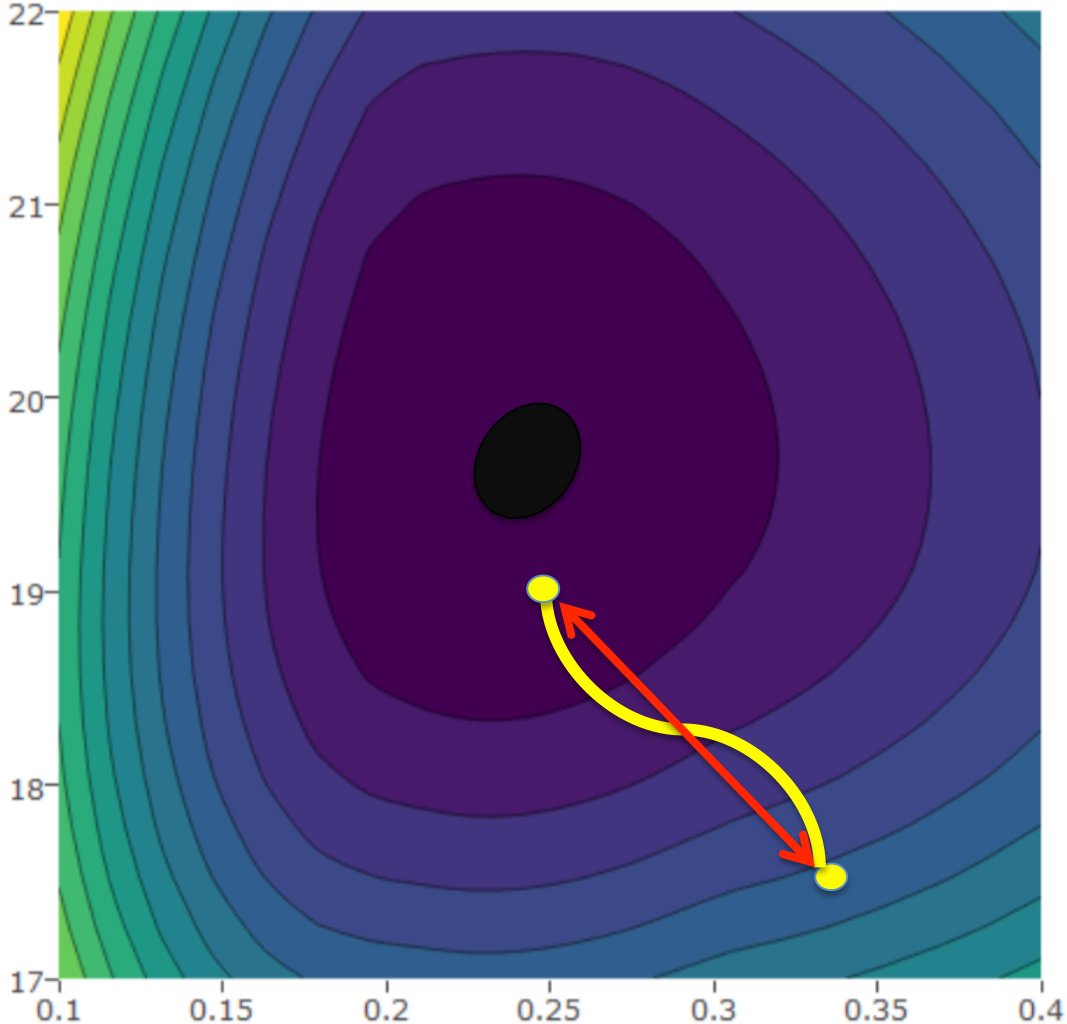
Log posterior contour plot



Starting position

Numerically integrate the Hamiltonian equations over L steps.

Log posterior contour plot

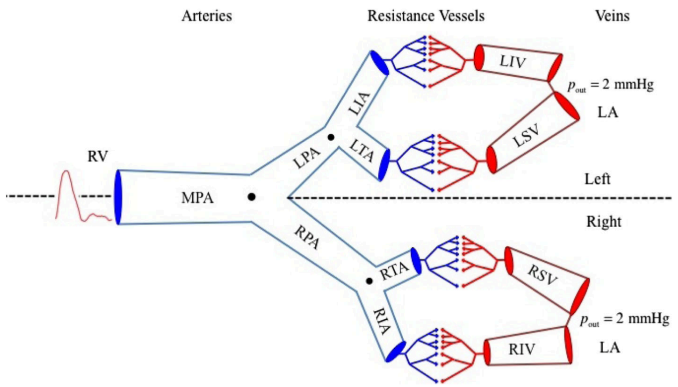


Starting position

Numerically integrate the Hamiltonian equations over L steps.

Correct for finite step-size numerical integration errors with a Metropolis-Hastings acceptance/ rejection step.

Dynamical System



$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{A}\right) + \frac{A}{\rho}\frac{\partial p}{\partial x} = -\frac{2\pi\nu r}{\delta}\frac{q}{A}$$

Closed-form solution

Experimental data

Model prediction

Posterior probability

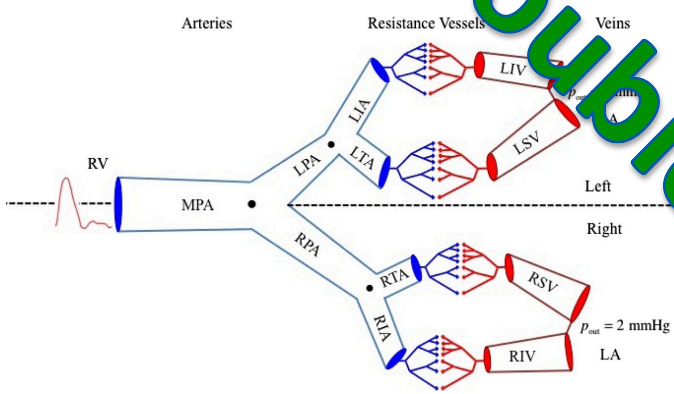
Analytically intractable

Dynamical System

Experimental data

Model prediction

Double intractable



Posterior probability

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{A}\right) + \frac{A}{\rho}\frac{\partial p}{\partial x} = -\frac{2\pi\nu r}{\delta}\frac{q}{A}$$

Analytically intractable

Analytically intractable

BAYESIAN STATISTICS 7, pp. 651–659
J. M. Bernardo, M. J. Bayarri, J. O. Berger, A. P. Dawid,
D. Heckerman, A. F. M. Smith and M. West (Eds.)

Gaussian Processes to Speed up Hybrid Monte Carlo for Expensive Bayesian Integrals

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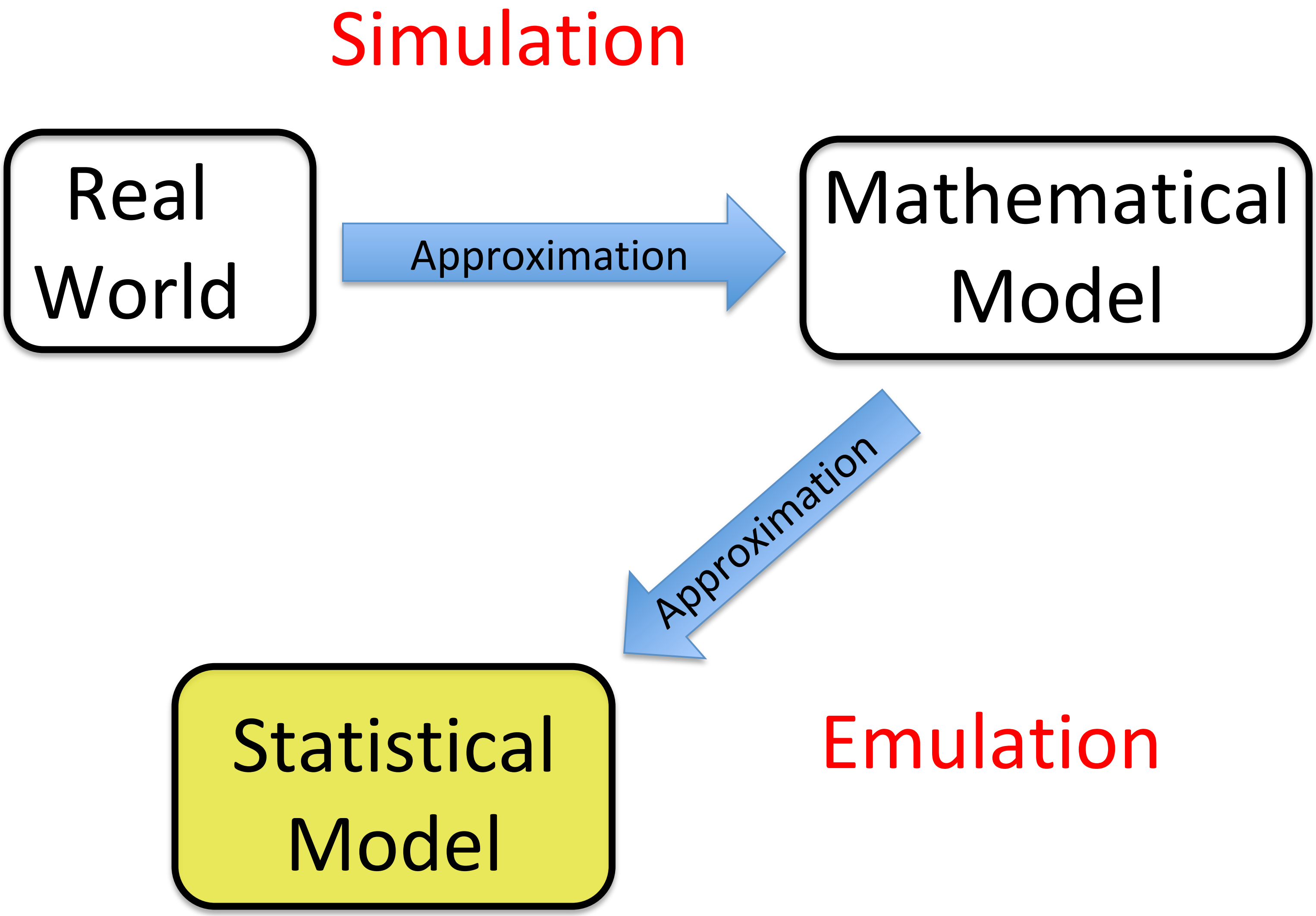
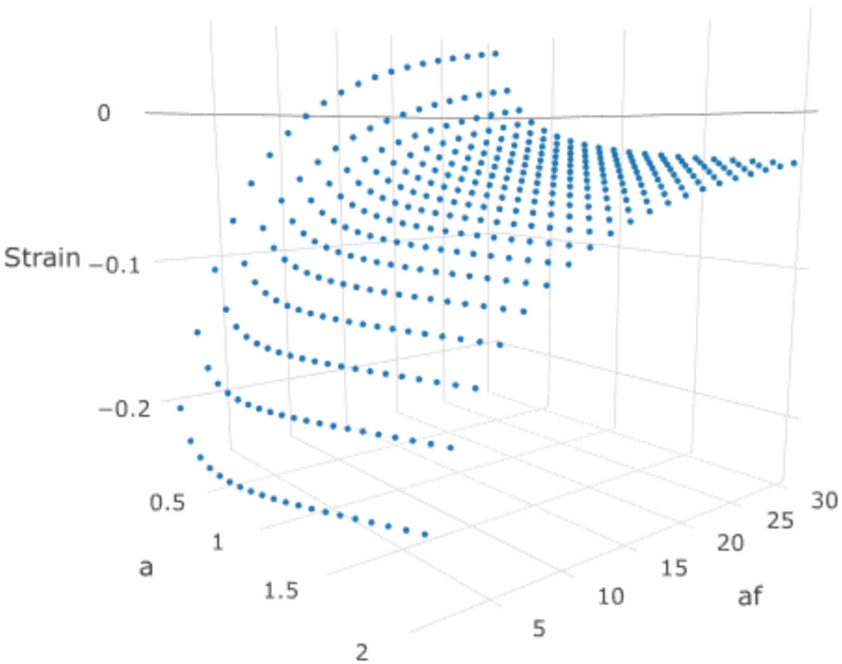
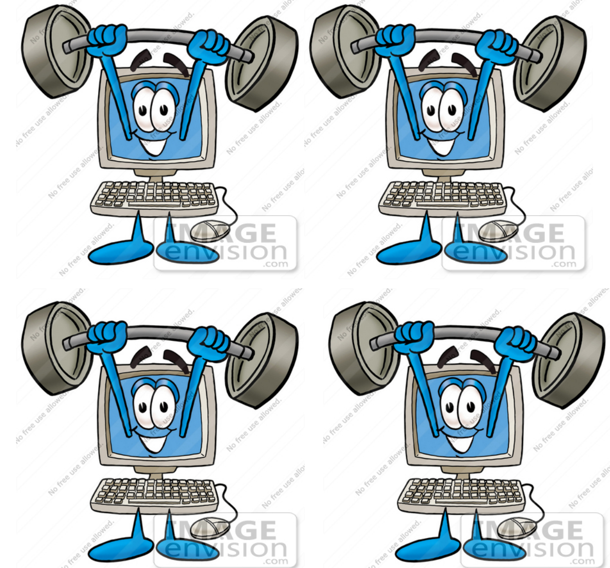
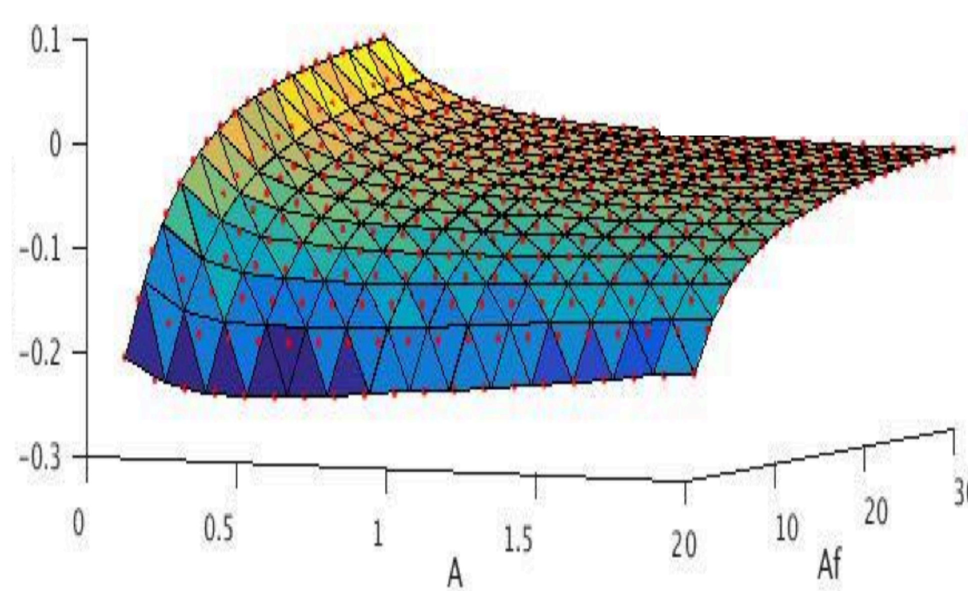

Simulation
Real World
Approximation
Mathematical Model
Approximation
Statistical Model
Emulation



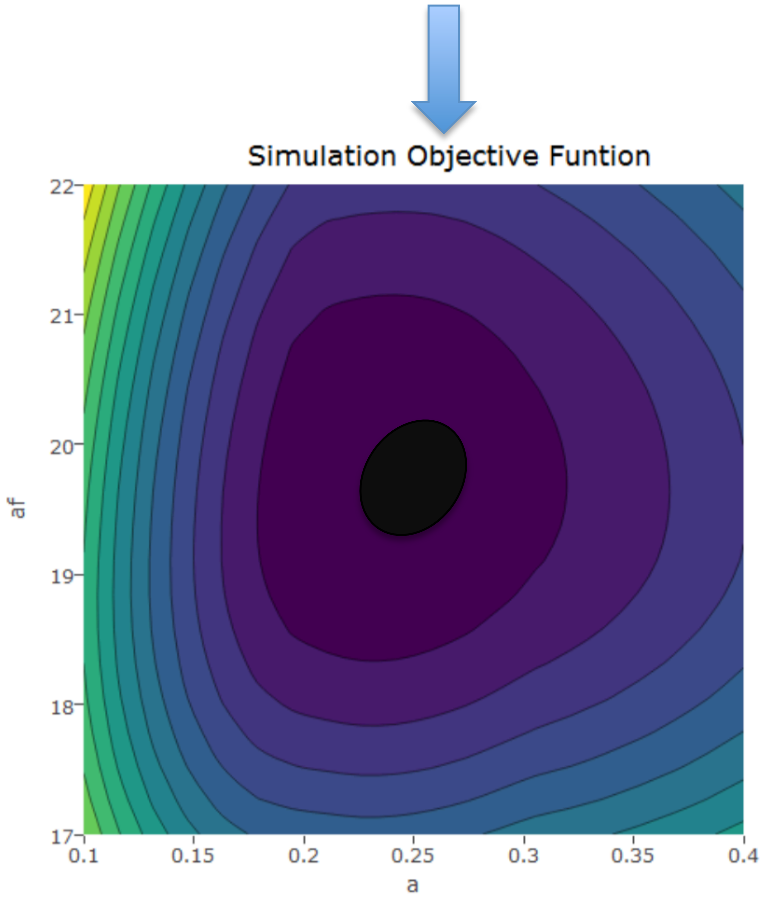
Parallel processing

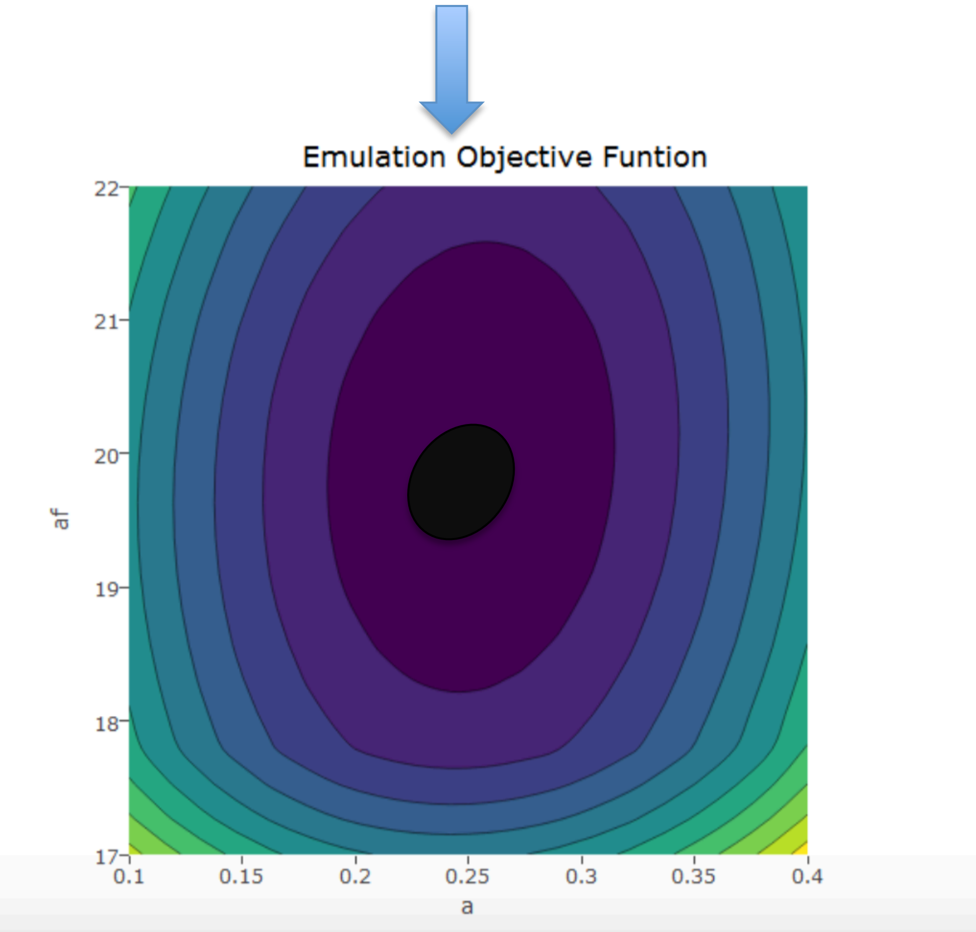


Statistical nonlinear regression

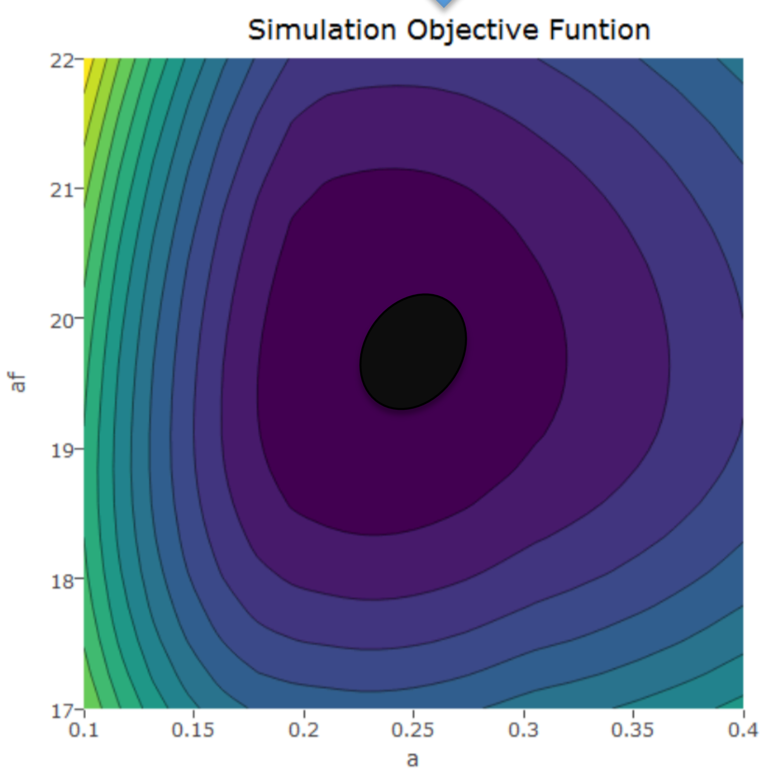


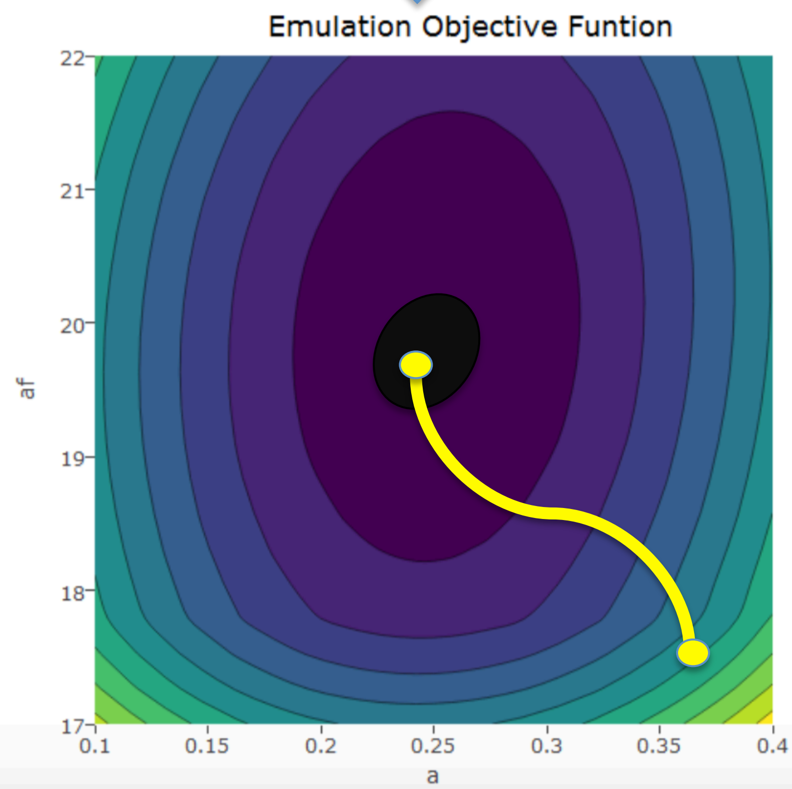
Simulation versus Emulation





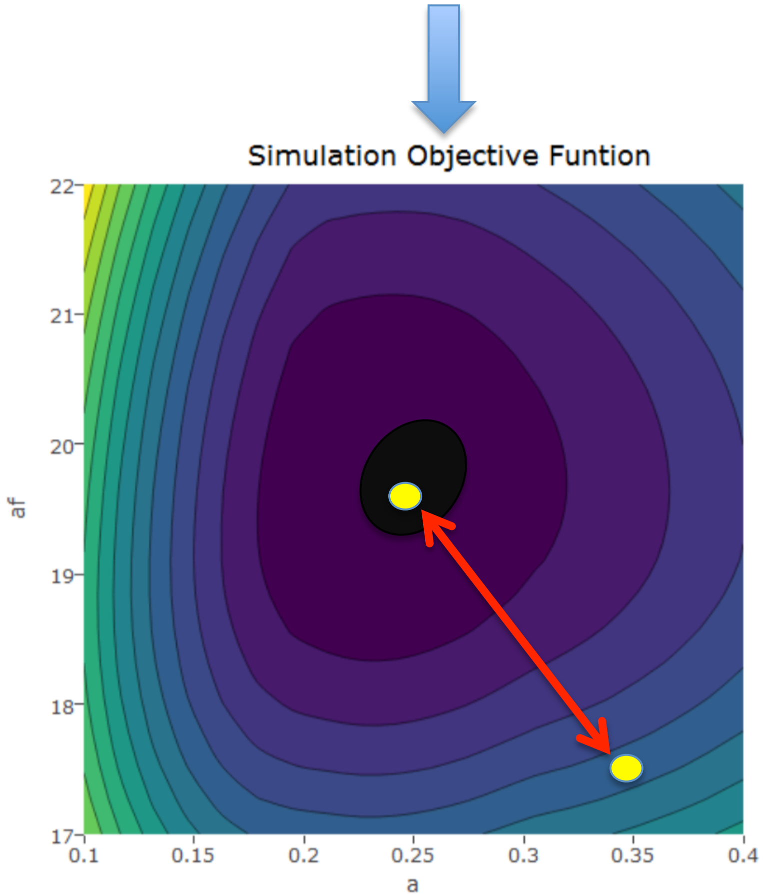
Simulation versus Emulation



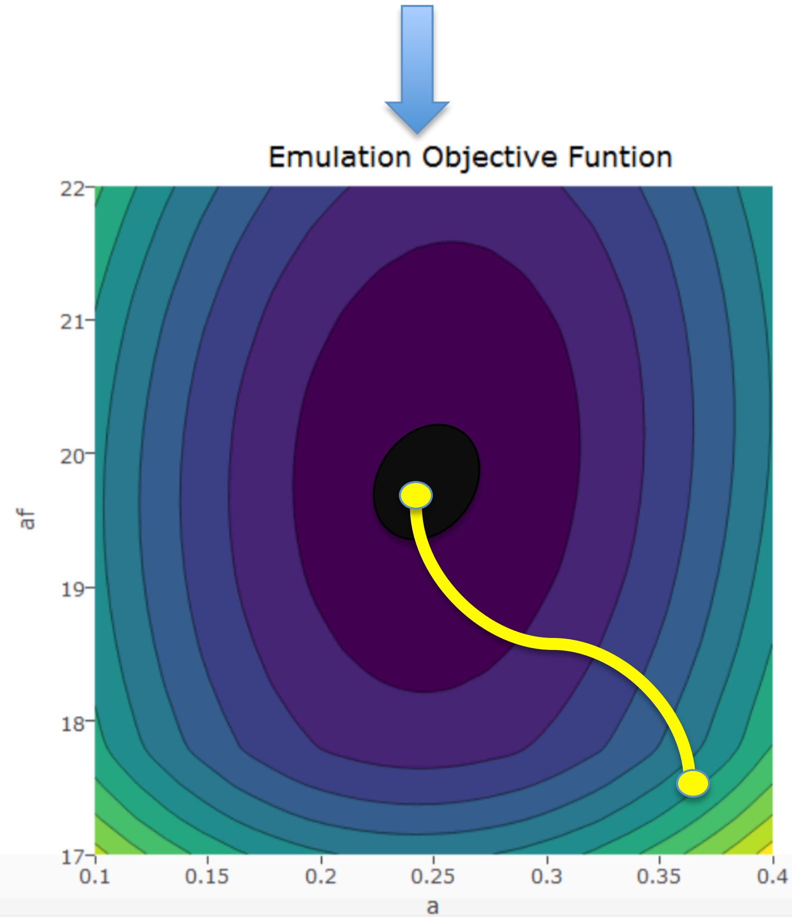


Numerical integration of the Hamiltonian equations on the emulated log posterior

Simulation versus Emulation



Metropolis-Hastings bias correction using the true log posterior probability



Numerical integration of the Hamiltonian equations on the emulated log posterior

Tuning parameters of HMC

Numerical integration step size
λ

Number of numerical integration steps
L

Tuning parameters of HMC

Numerical integration step size

λ

Too small:
Excessive computational costs

Too large:
High rejection rate

Number of numerical integration steps

L

Tuning parameters of HMC

Numerical integration step size

λ

Too small:
Excessive computational costs

Too large:
High rejection rate

Number of numerical integration steps

L

Too small:
Random walk behaviour

Too large:
Small sample size

Tuning parameters of HMC

Numerical integration step size

λ

How can we optimise these parameters ?

Number of numerical integration steps

L

Tuning parameters of HMC

Numerical integration step size

λ

How can we optimise these parameters ?

Number of numerical integration steps

L

What is our optimality criterion?

MCMC standard error

$$\text{MCMC-SE} \equiv \sqrt{\frac{\mathrm{Var}_{\pi}[f]}{\mathrm{ESS}}}.$$

Effective sample size

$$\mathrm{ESS} = \frac{N}{1 + 2\sum_{l=1}^{\infty} \rho_l}$$

Autocorrelation

$$\rho_k = c_k / c_0 \qquad c_k = \frac{1}{(N-k)} \sum_{t=1}^{N-k} (x_t - \bar{x})(x_{t+k} - \bar{x})$$

Adaptive Hamiltonian and Riemann Manifold Monte Carlo Samplers

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University of British Columbia Vancouver, Canada

Shakir Mohamed SHAKIRM@CS.UBC.CA
University of British Columbia Vancouver, Canada

Nando de Freitas NANDO@CS.UBC.CA
University of British Columbia Vancouver, Canada

ICML 2013
Proceedings of the 30th International Conference on Machine Learning

Use Bayesian optimization to optimize the ESS per computational time

We combine both ideas and use emulation twice

We combine both ideas and use emulation twice

Emulation of the log likelihood for faster HMC

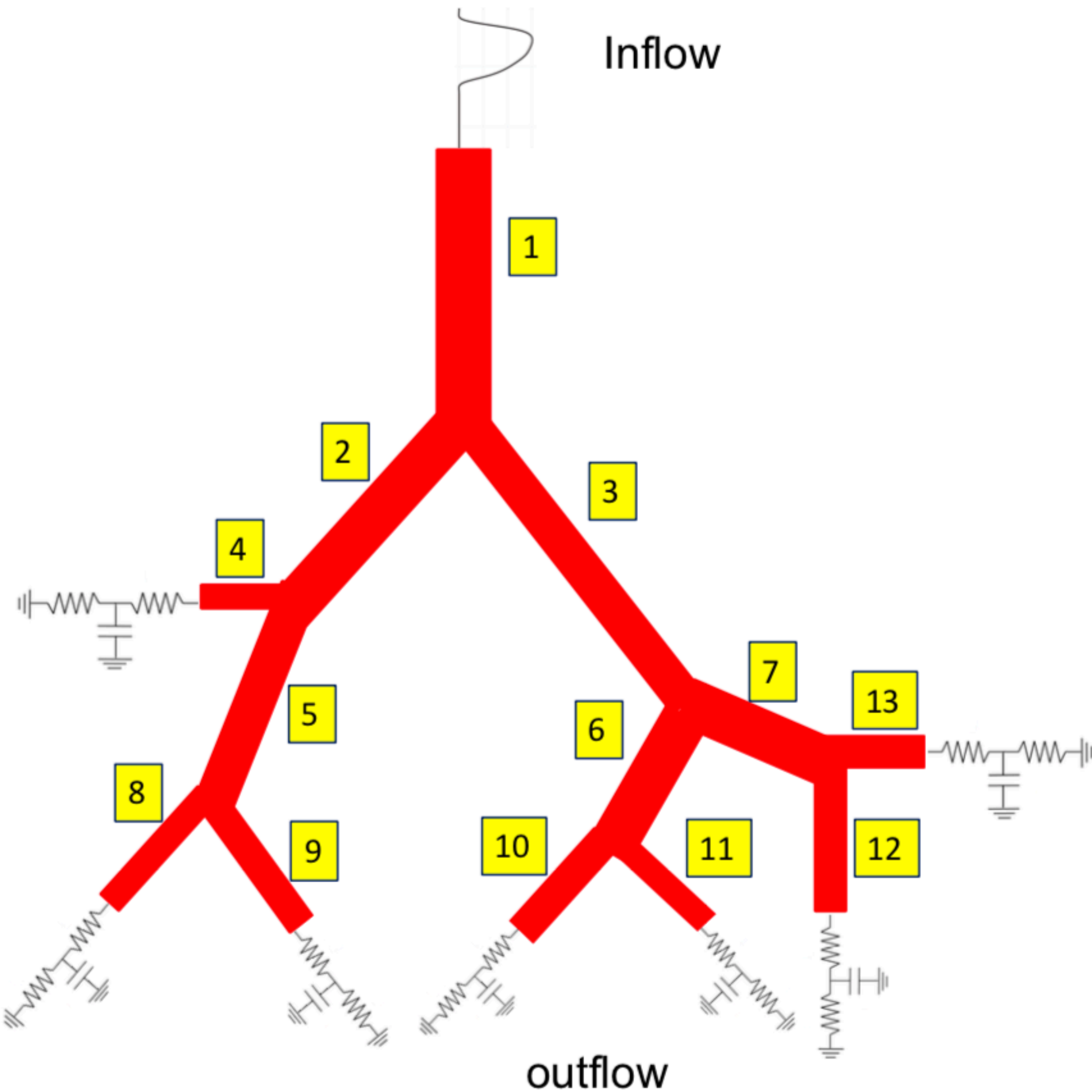
Emulation of the HMC objective function as part of Bayesian optimization

Mihaela Paun

5th International Conference on Computational and Mathematical Biomedical Engineering - CMBE2017
10–12 April 2017, United States
P. Nithiarasu, A.M. Robertson (Eds.)

SIMULATING THE EFFECTS OF HYPOXIA ON PULMONARY HEMODYNAMICS IN MICE

Muhammad U. Qureshi[1], **Mansoor A. Haider**[1], **Naomi C. Chesler**[2], **and Mette S. Olufsen**[1]
[1]Department of Mathematics, North Carolina State University, Raleigh, NC, USA
[2]Department of Biomedical Engineering, University of Wisconsin-Madison, Madison, WI, USA


Inflow
1
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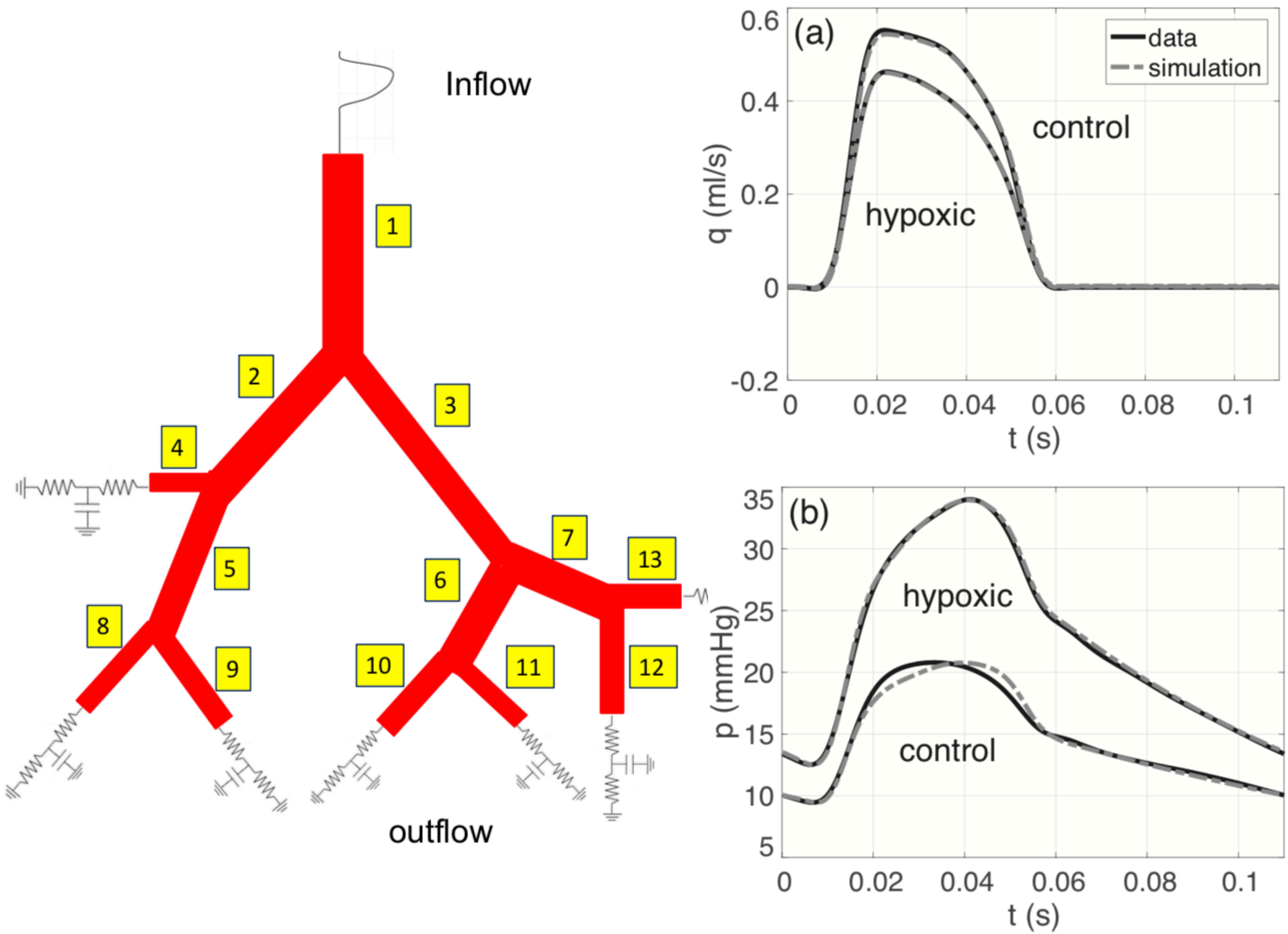
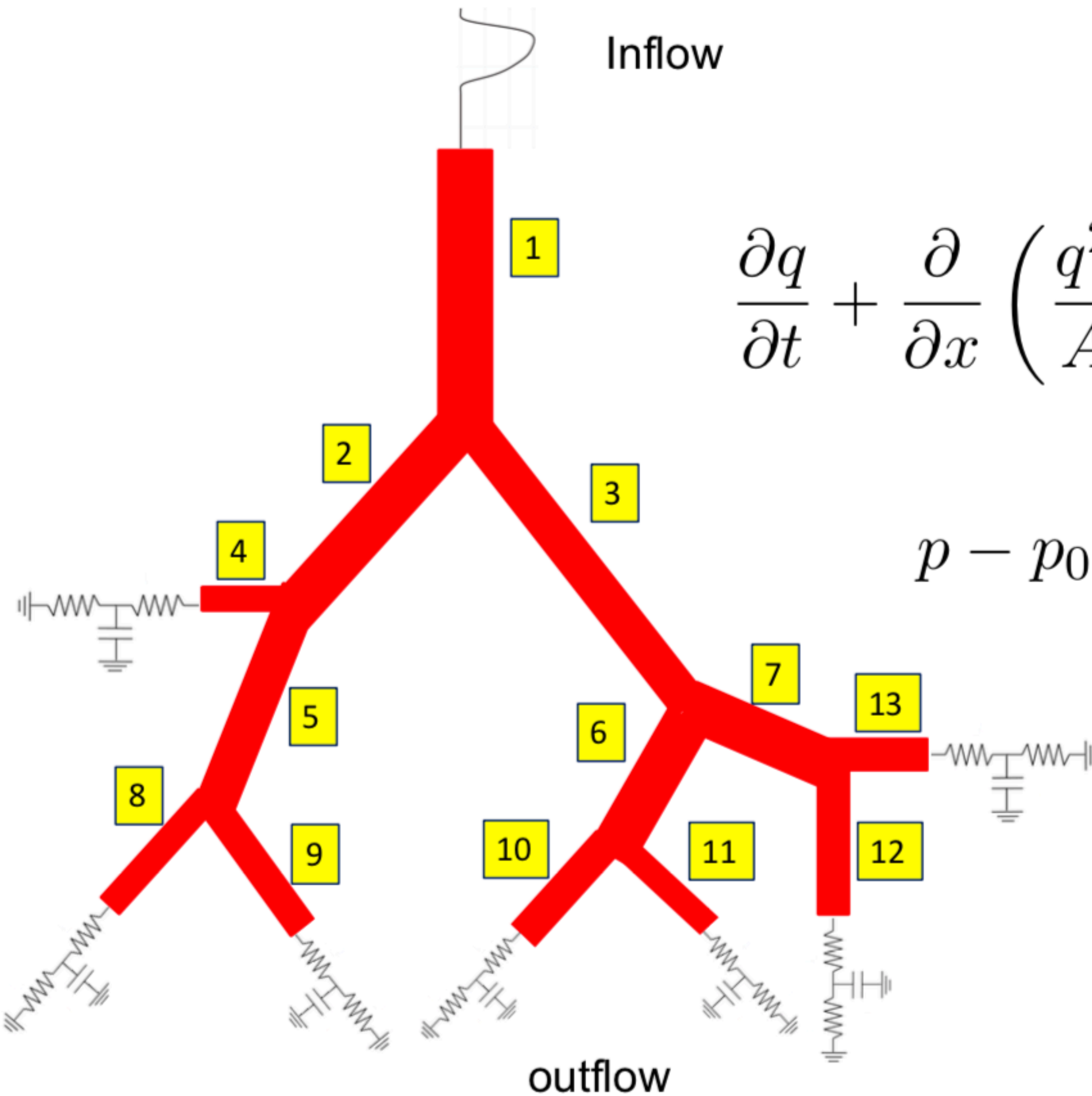
5
6
7
13
8
9
10
11
12
outflow



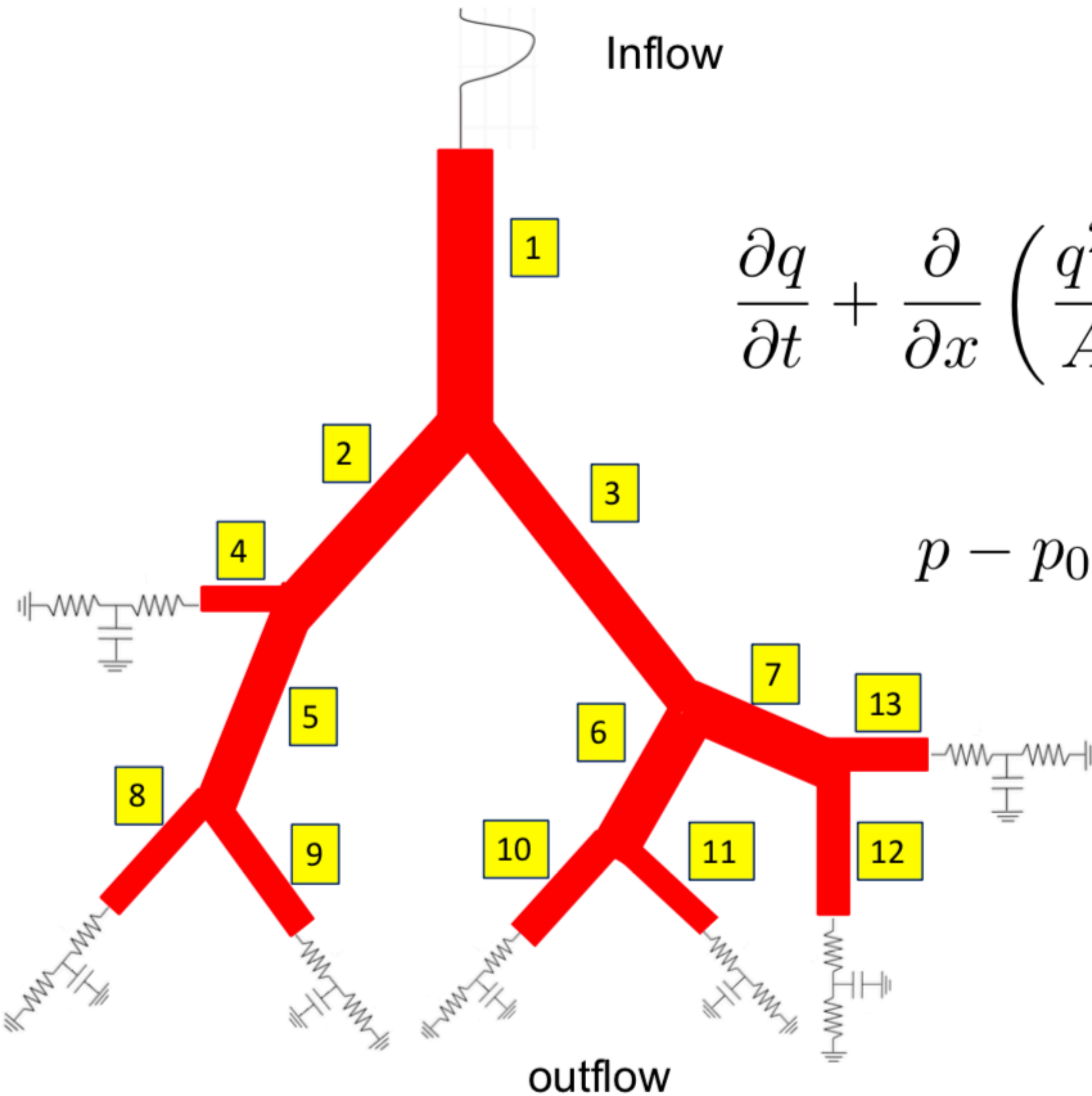
Inflow
1
2
3
4
5
6
7
8
9
10
11
12
13
outflow
(a)
data
simulation
control
hypoxic
q (ml/s)
t (s)
(b)
hypoxic
control
p (mmHg)
t (s)



$$\frac{\partial A}{\partial t} + \frac{\partial q}{\partial x} = 0$$

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{A}\right) + \frac{A}{\rho}\frac{\partial p}{\partial x} = -\frac{2\pi\nu r}{\delta}\frac{q}{A}$$

$$p - p_0 = \frac{4}{3}\,\mathrm{f}\left(1 - \sqrt{\frac{A_0}{A}}\right)$$



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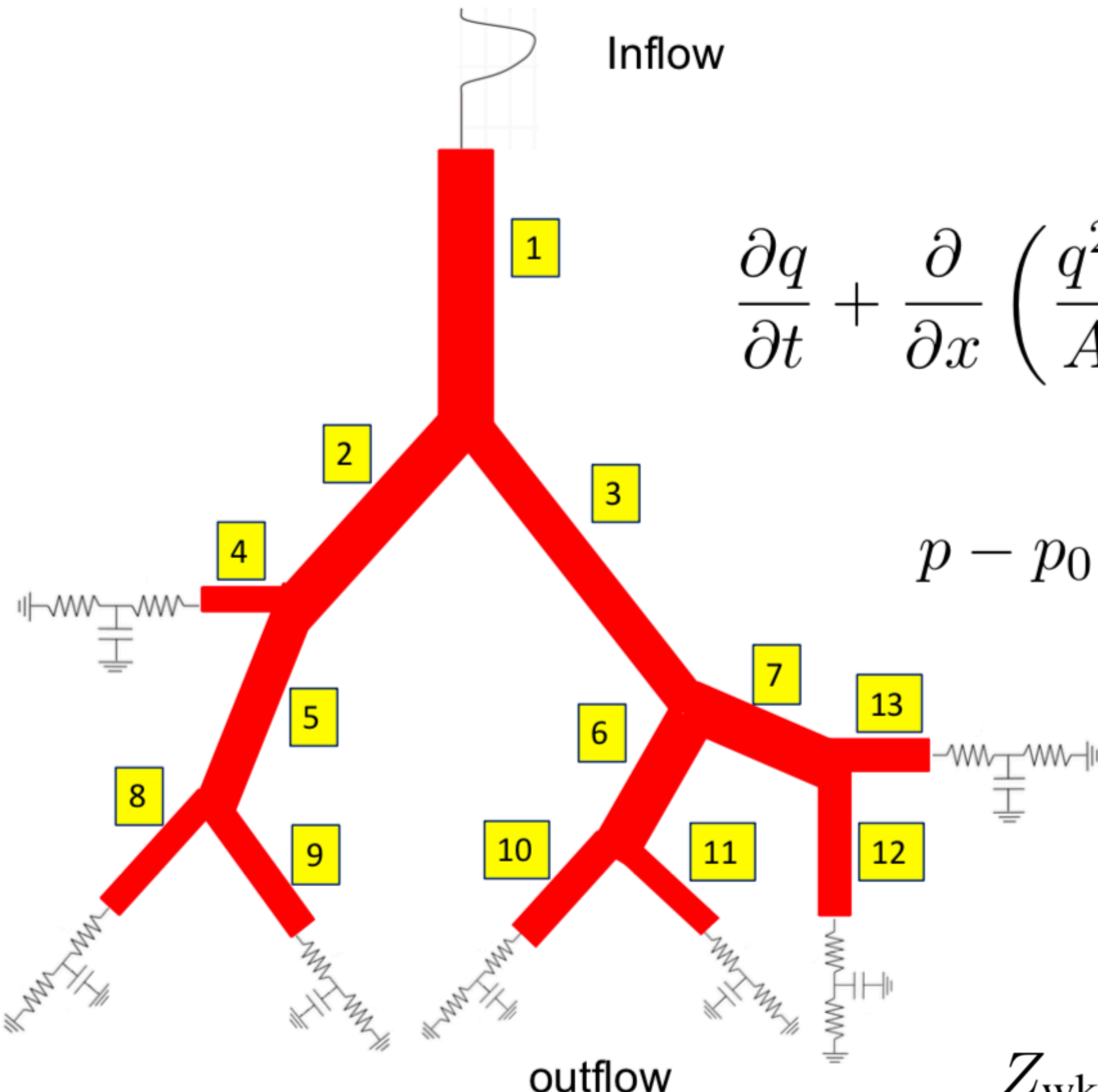
$$p - p_0 = \frac{4}{3}\boxed{f}\left(1 - \sqrt{\frac{A_0}{A}}\right)$$

Stiffness parameter



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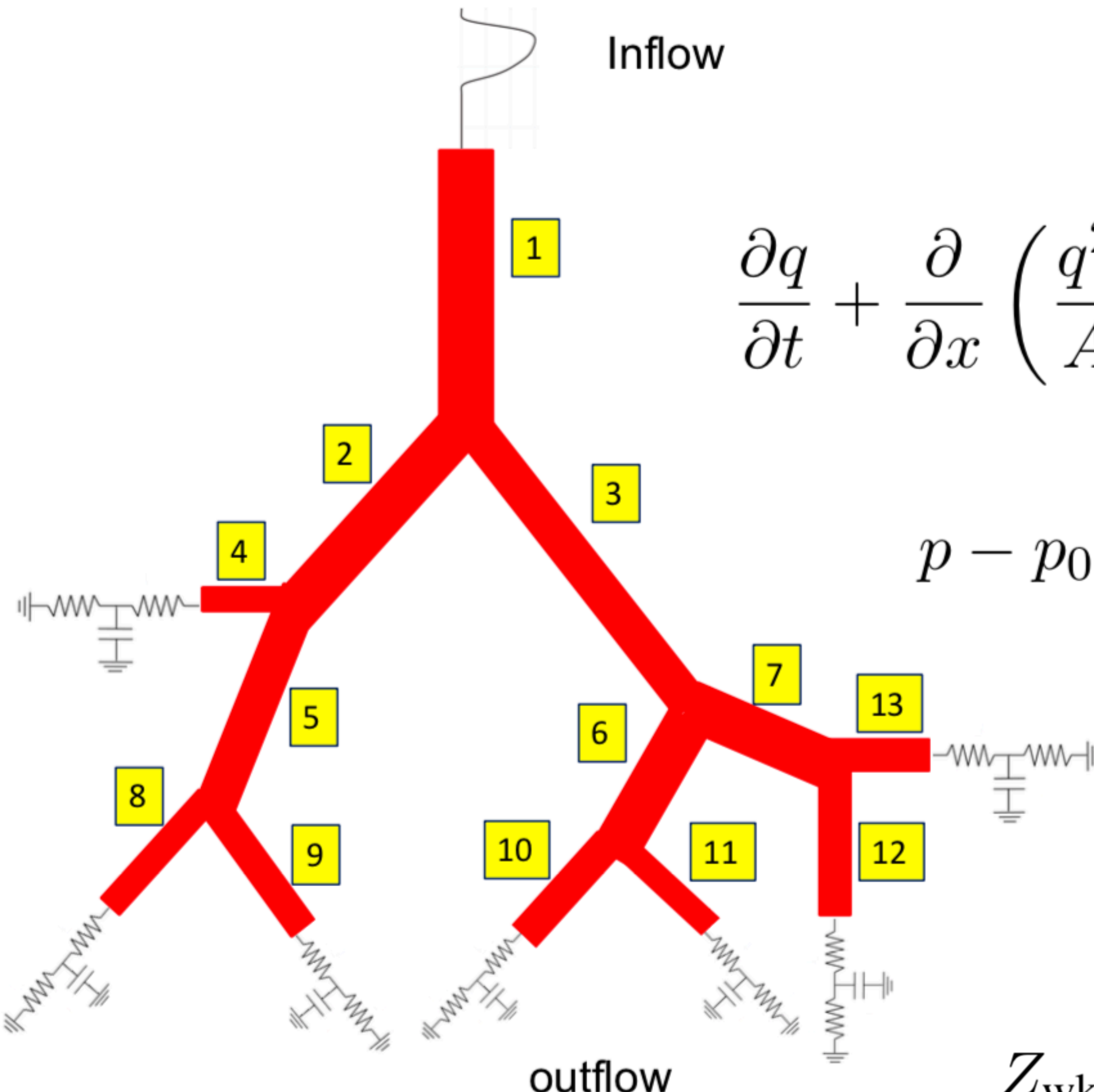
$$p - p_0 = \frac{4}{3}\,\mathrm{f}\left(1 - \sqrt{\frac{A_0}{A}}\right)$$

$$Z_{\mathrm{wk}}(\omega) = R_1 + \frac{R_2}{1 + i\omega C R_2}$$



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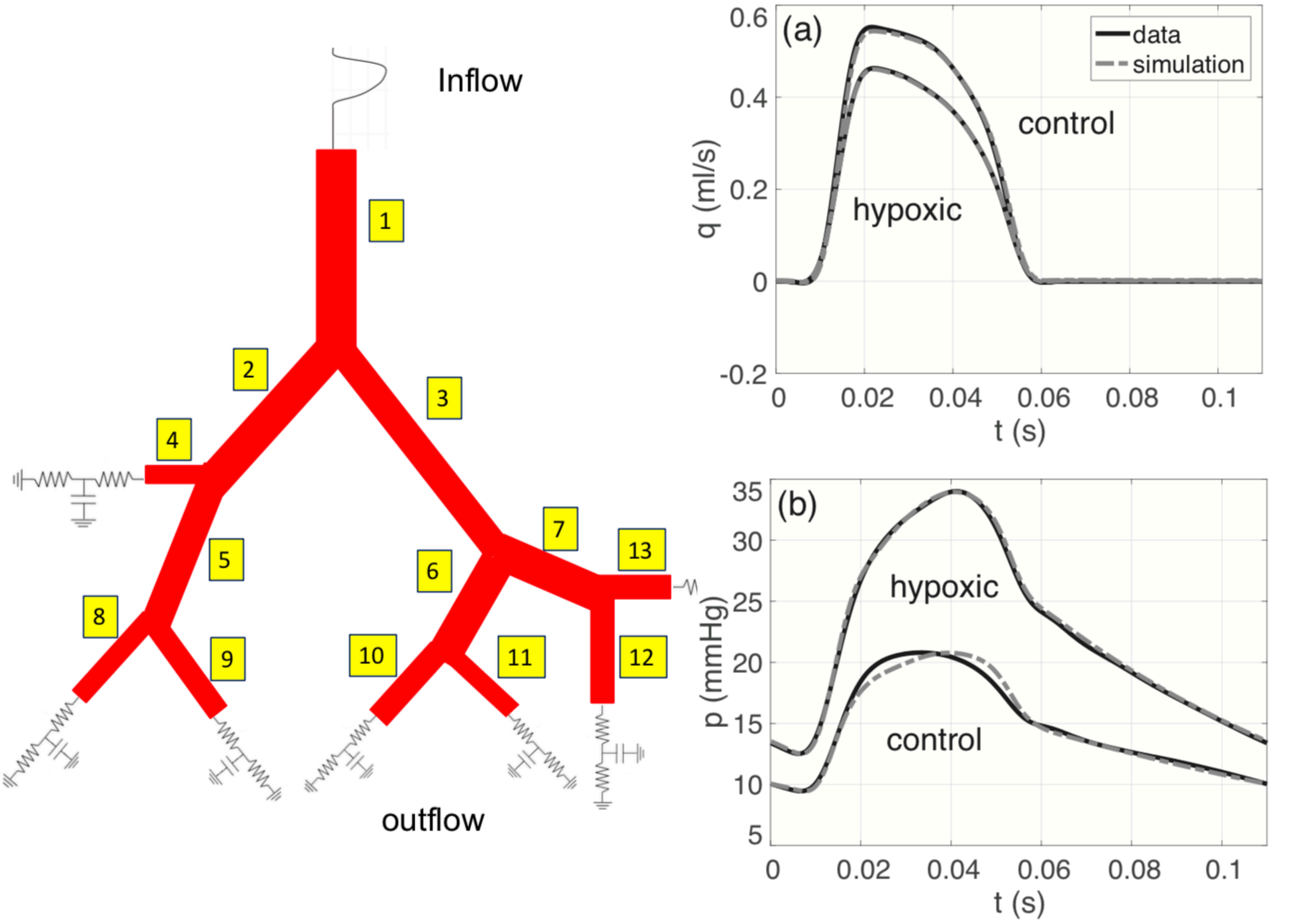
$$p-p_0=\frac{4}{3}\boxed{f}\left(1-\sqrt{\frac{A_0}{A}}\right)$$

?

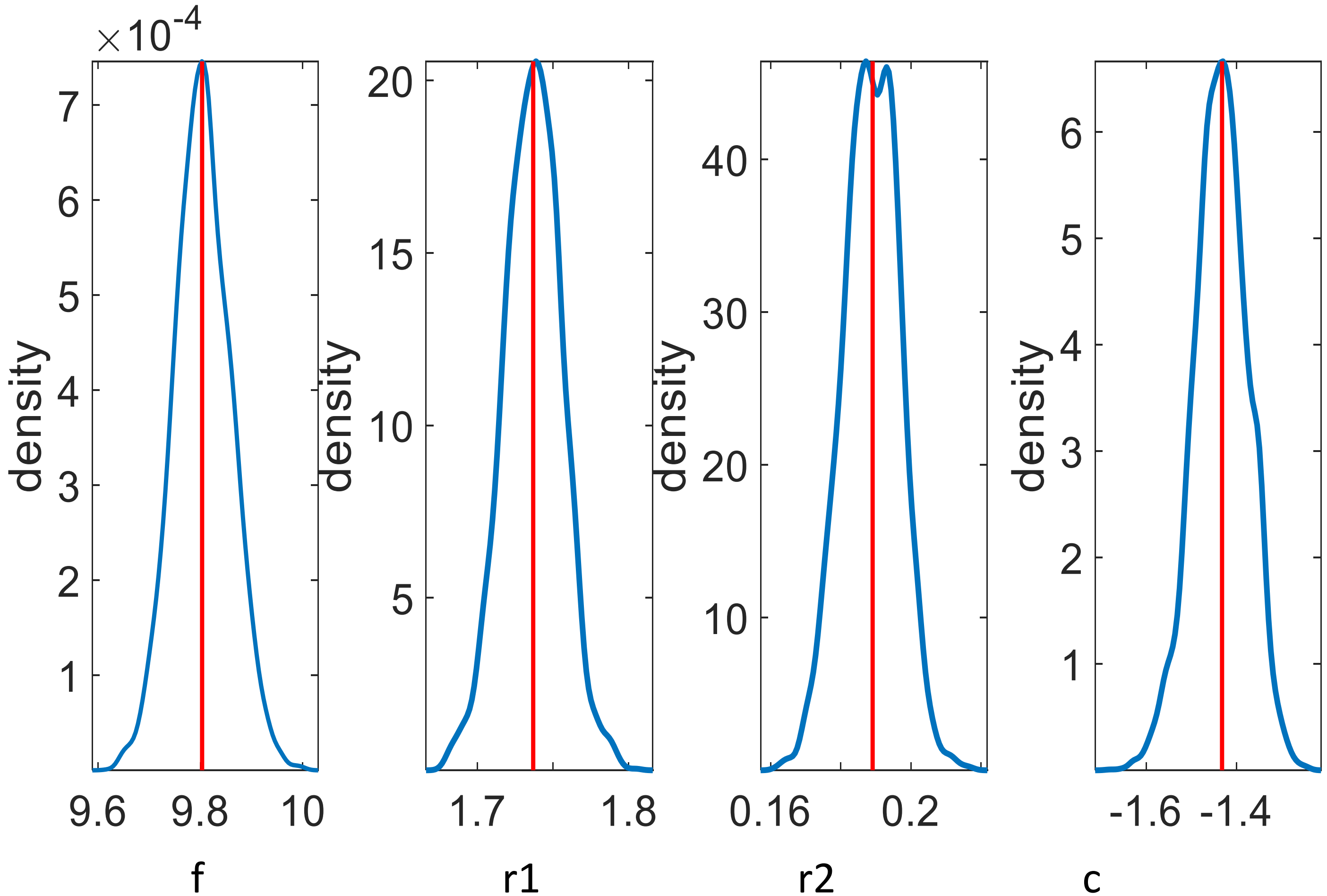
$$Z_{\mathrm{wk}}(\omega)=\boxed{R_1}+\frac{\boxed{R_2}}{1+i\omega\boxed{C}R_2}$$

Data

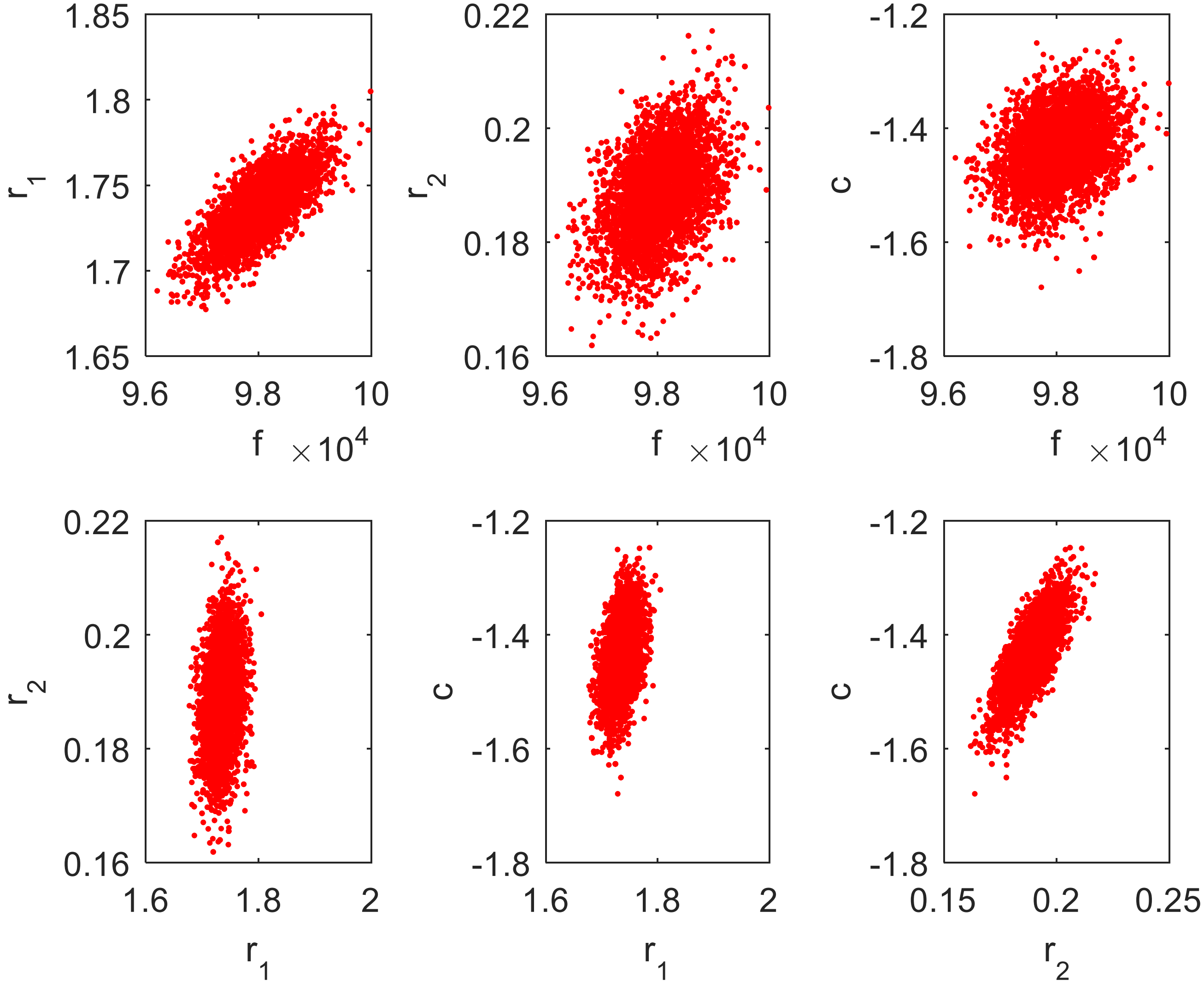


Inflow
1
2
3
4
5
6
7
8
9
10
11
12
13
outflow
(a)
data
simulation
control
hypoxic
q (ml/s)
0.6
0.4
0.2
0
-0.2
0
0.02
0.04
0.06
0.08
0.1
t (s)
(b)
hypoxic
control
p (mmHg)
35
30
25
20
15
10
5
0
0.02
0.04
0.06
0.08
0.1
t (s)

Posterior probability



Posterior correlations



Computational complexity

Target: ESS= 1500

PSRF <= 1.1

- **Standard MCMC:**

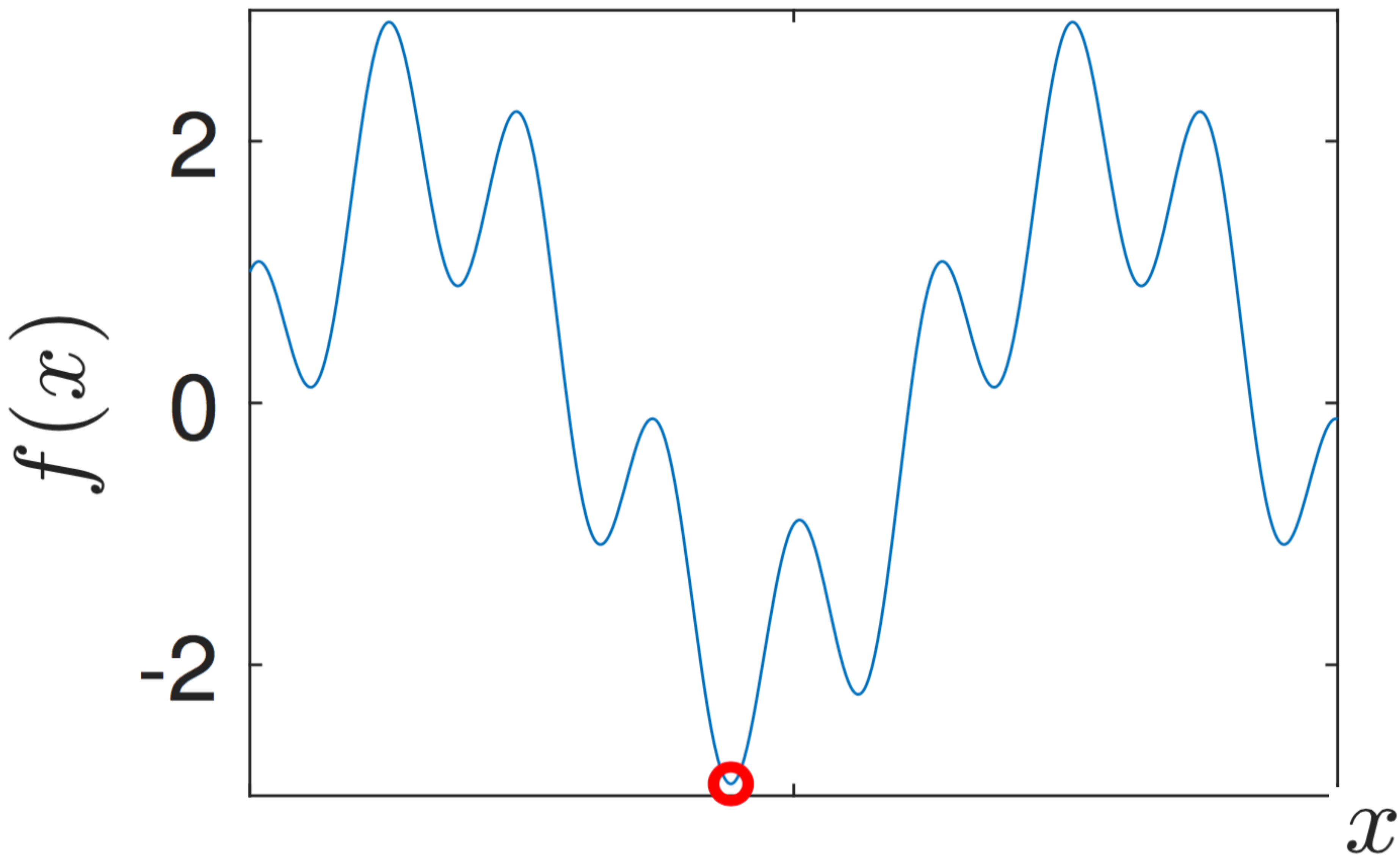
  3 weeks

- **HMC combined with emulation and BO:**

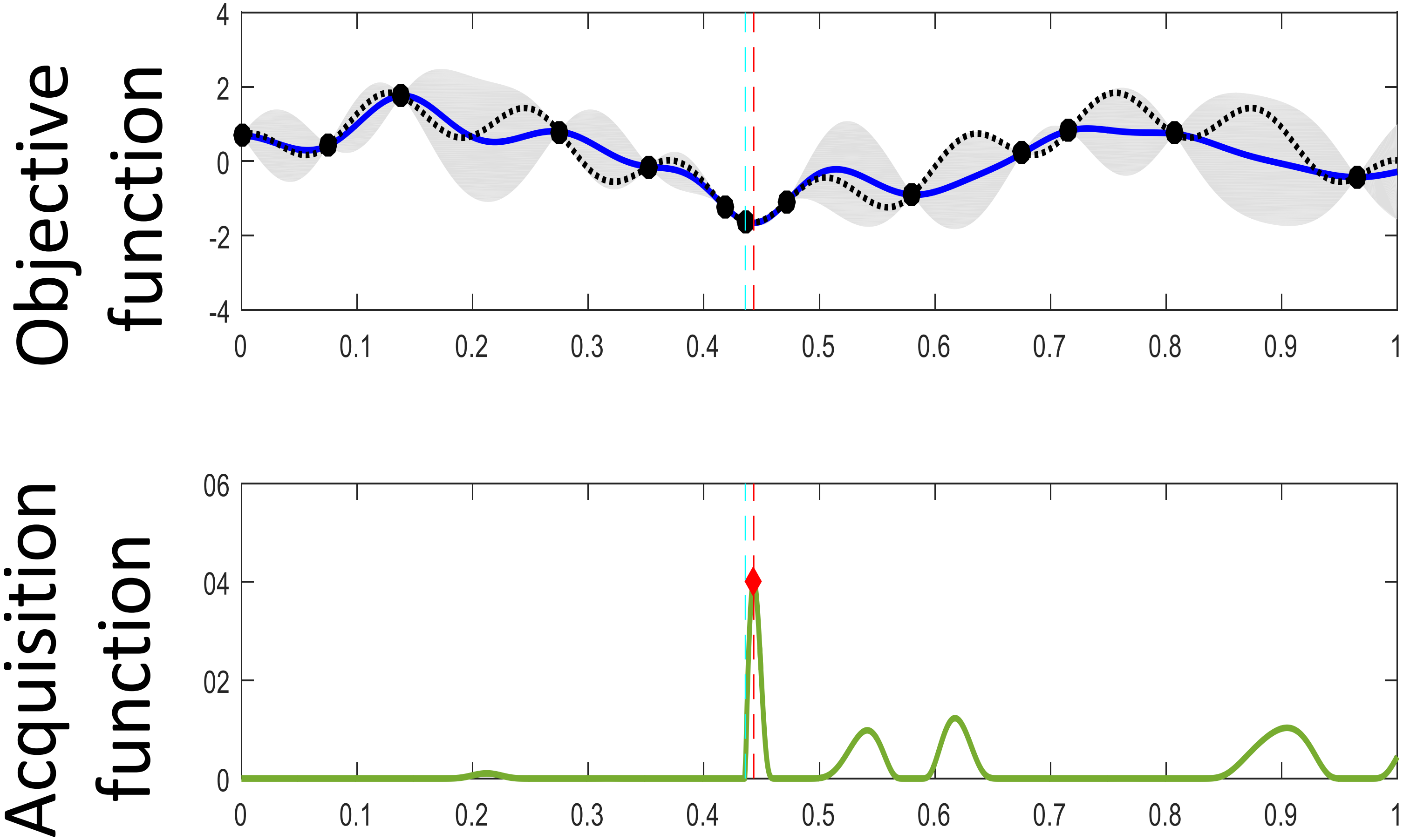
  2 days

Computer tutorial

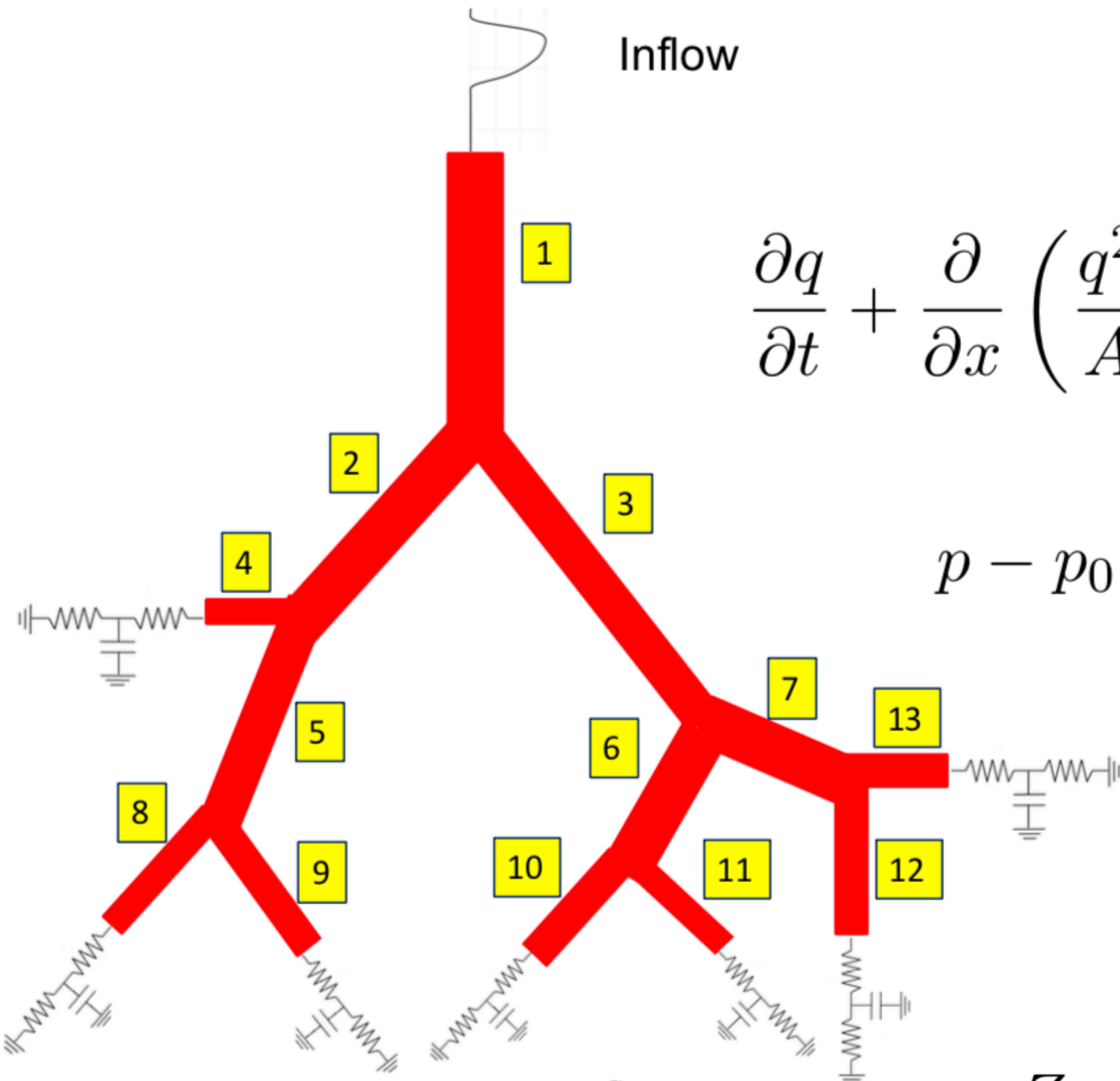
Exercise 1: Bayesian optimization



Recall ...


Objective function
Acquisition function
4
2
0
-2
-4
06
04
02
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Exercise 2: Bayesian optimization



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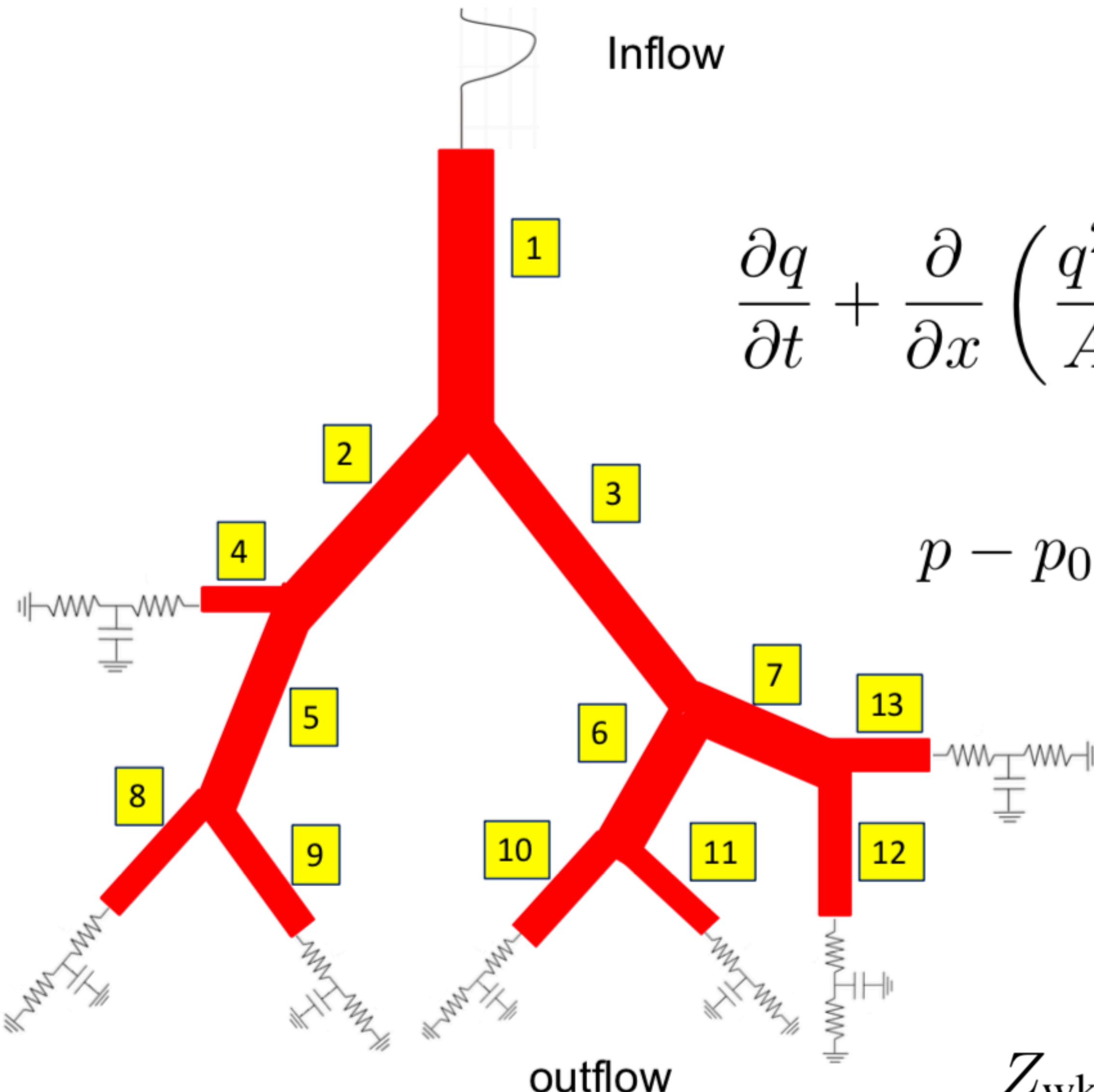
$$p - p_0 = \frac{4}{3}\boxed{f}\left(1 - \sqrt{\frac{A_0}{A}}\right)$$

?

$$Z_{\mathrm{wk}}(\omega) = \boxed{R_1} + \frac{\boxed{R_2}}{1 + i\omega\boxed{C}R_2}$$

Exercise 2: Bayesian optimization



$$\frac{\partial A}{\partial t} + \frac{\partial q}{\partial x} = 0$$

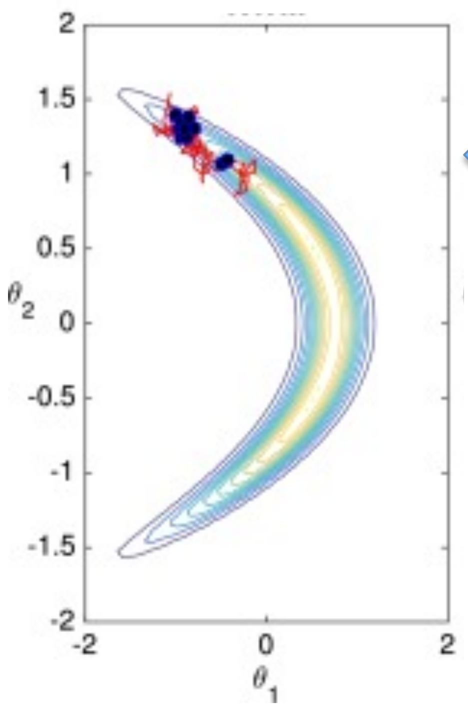
$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{A}\right) + \frac{A}{\rho}\frac{\partial p}{\partial x} = -\frac{2\pi\nu r}{\delta}\frac{q}{A}$$

$$p - p_0 = \frac{4}{3}\boxed{f}\left(1 - \sqrt{\frac{A_0}{A}}\right)$$

?

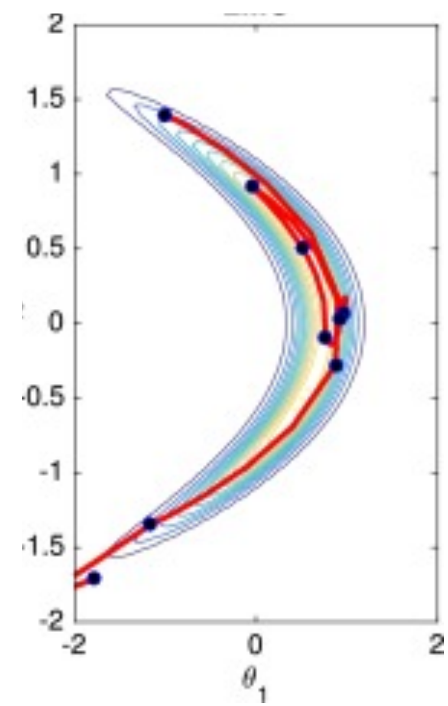
$$Z_{\mathrm{wk}}(\omega) = R_1 + \frac{R_2}{1 + i\omega C R_2}$$

Exercise 3
Hamiltonian Monte Carlo



Standard
MCMC

Hamiltonian
Monte Carlo



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Any Questions?