SIMON FRASER UNIVERSITY
THINKING OF THE WORLD

Parameter Estimation for Dynamic Systems Models

Oksana Chkrebtii
Simon Fraser University,
SFU-UBC joint workshop
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Outline

- Introduction: dynamic systems models
- Example: modeling data by using ecological dynamics
- Parameter Estimation
  - Numerical optimization
  - Markov Chain Monte Carlo (MCMC)
- A bit about my research
  - joint with Dave Campbell (SFU), Ben Calderhead and Mark Girolami (UCL)

Dynamic Systems Models

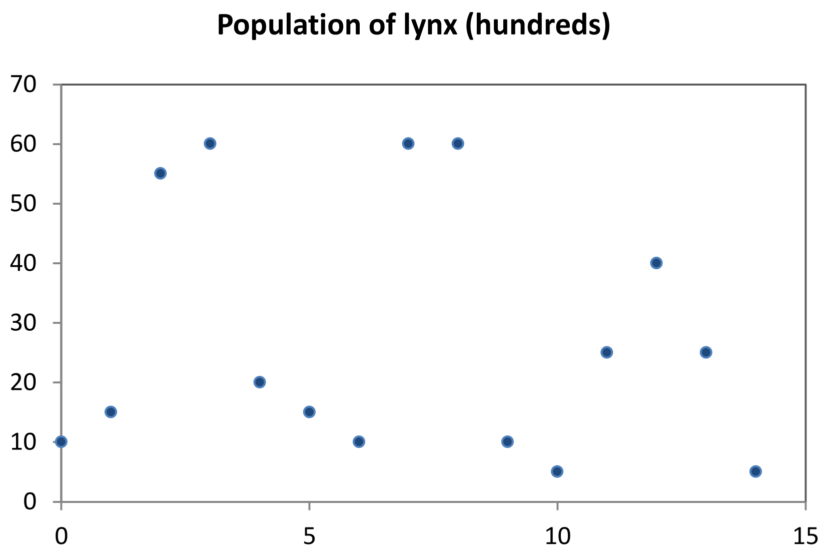
- Models that describe the behaviour of complex systems by relating variables to their derivatives with respect to space/time variables

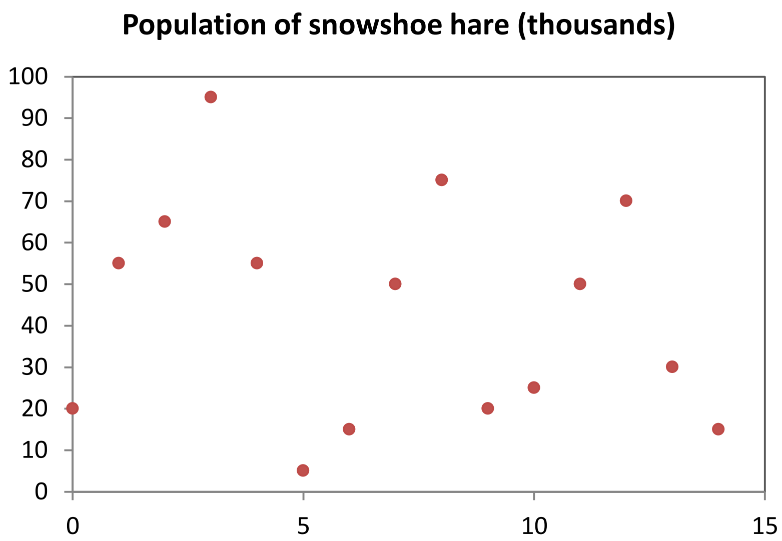
- Systems of ordinary differential equations (ODE) or partial differential equation (PDE)
  - high-dimensional, nonlinear, coupled
  - deterministic or stochastic
  - unknown parameters: some have physical interpretations

- Models that are too complex to study directly can be analyzed statistically by using computer experiments

Example with population data

- Suppose we observe two populations in a forest





- Observe a periodic pattern with some shift
- We may try fitting a periodic function to the data
- But we should try to fit a function that reflects known mechanism by which lynx and hares interact

Population dynamics

The Lotka-Volterra system with 2 states and 4 parameters

h(t) = number of hares, $l(t)$ = number of lynx

$$\frac{dh(t)}{dt} = \alpha h(t) - \beta h(t)l(t)$$

← Hares are eaten by lynx and are not limited by food supply

$$\frac{dl(t)}{dt} = \delta l(t)h(t) - \gamma l(t)$$

← Lynx feed on hare and compete with one another for food

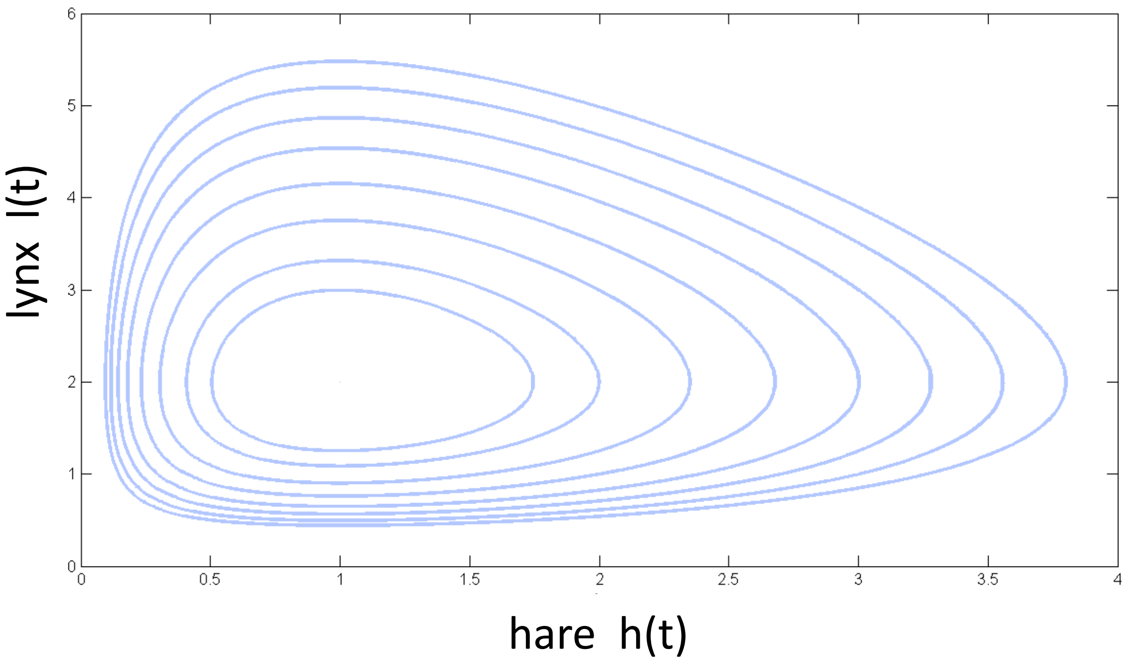
$$l(0) = l_0, \qquad h(0) = h_0$$

← Populations start out at these values

Rates of change of the populations depend on the number of predators and prey present at time t

Population dynamics

- This system has no closed form solution, so we use numerical methods instead:



Each ellipse is a solution to the system under the parameters

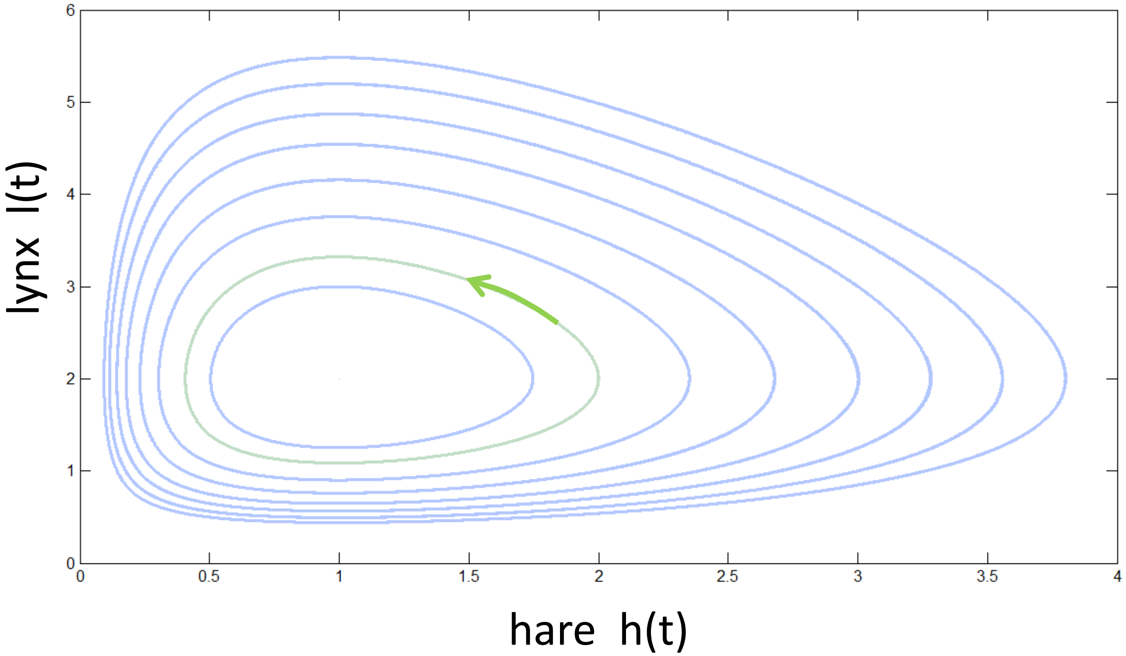
$$\alpha = 2, \qquad \beta = 1,$$
$$\gamma = 1, \qquad \delta = 1.$$

and different initial conditions

- Let's look at the solution corresponding to the initial conditions $h(0) = 1$ and $l(0) = 1$

Population dynamics

- This system has no closed form solution, so we use numerical methods instead:



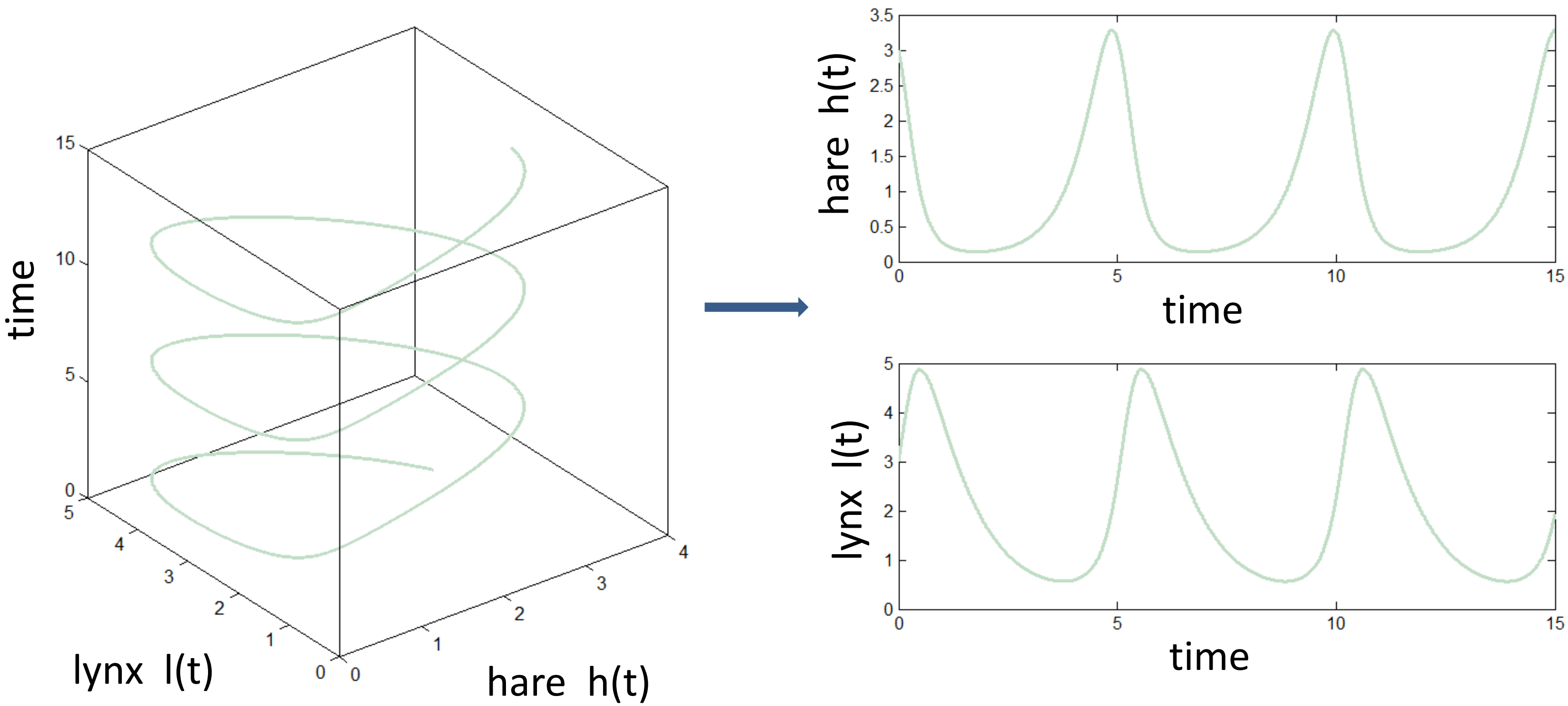
$$\frac{dh(t)}{dt} = \alpha h(t) - \beta h(t) l(t)$$

$$\frac{dl(t)}{dt} = \delta l(t) h(t) - \gamma l(t)$$

- Let's look at the solution corresponding to the initial conditions $h(0) = 1$ and $l(0) = 1$

Population dynamics

solution under parameters $(\alpha, \beta, \gamma, \delta, l_0, h_0) = (2,1,1,1,1,1)$



So we get a family of functions that depend on the system parameters, which we can fit to our data!

Parameter estimation from ODEs

- Suppose we have a complex ODE model relating states to their derivatives with respect to time
- We observe the state variables and not their derivatives
- Solution $x(t; \boldsymbol{\theta}, \boldsymbol{x_0})$ is a nonlinear function of time
- We solve the system by using a numerical ODE solver

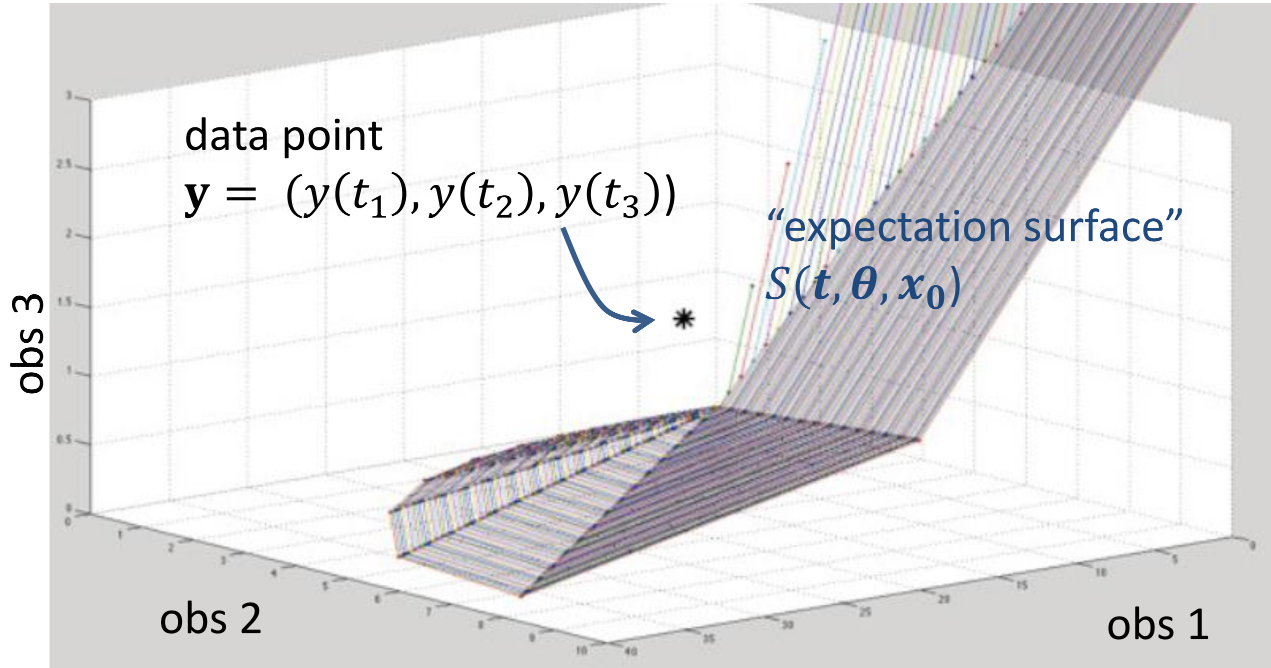
$$\boldsymbol{x}(t; \boldsymbol{\theta}, \boldsymbol{x_0}) \approx S(t\,; \boldsymbol{\theta}, \boldsymbol{x_0})$$

- Model the data as a noisy version of the solver function

$$\boldsymbol{y}(t) = S(t\,; \boldsymbol{\theta}, \boldsymbol{x_0}) + \epsilon$$

Parameter estimation from ODEs

- This is a nonlinear regression problem
- Choose parameters $\boldsymbol{\theta}$ so that $S(\boldsymbol{t}; \boldsymbol{\theta}, \boldsymbol{x_0})$ is "close" to the data $\boldsymbol{y}$



We can visualize this problem by thinking of only three observations of one state

Parameter estimation from ODEs

- Likelihood is one way to measure distance

$$L\left(y(t)\,|\theta, x_0\right) = \mathrm{N}(\,y(t)\,|\,S(t;\theta, x_0), \sigma^2)$$

- No closed form solution => no closed form L
  - Luckily: optimization and MCMC only require evaluating likelihood at a number of points

- Nonlinear Least Squares optimization methods
  - Require sensitivity equations (estimated numerically)
  - Numerical optimization works well for very simple systems, unlike the one on the next slide…

Squid Neurons

- Model for the spike potential in the giant axon of squid neurons.

V(t) = voltage,   R(t) = recovery

$$\frac{dV(t)}{dt} = \gamma\,[V(t) - R(t)^3 + R(t)]$$

← Voltage changes over time across cell membrane

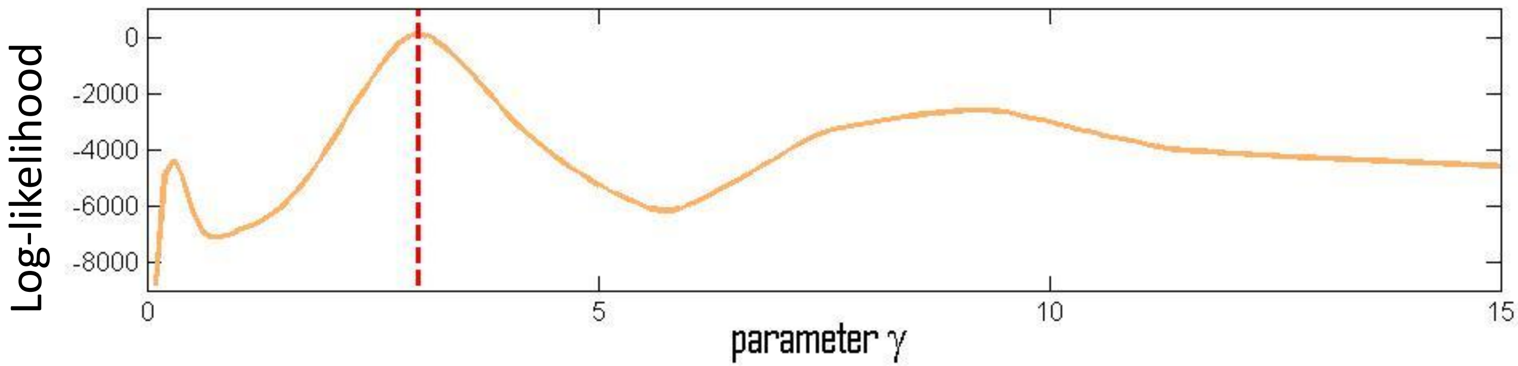
$$\frac{dR(t)}{dt} = \frac{1}{\gamma}[V(t) - \alpha + \beta R(t)]$$

← Rate of change of recovery depends on voltage at time t

$$V(t) = v_0, \qquad R(0) = r_0$$

← Initial conditions

Squid Neurons: likelihood function



David Campbell, Russell J. Steele: Smooth functional tempering for nonlinear differential equation models. Statistics and Computing 22(1): 429-443 (2012)

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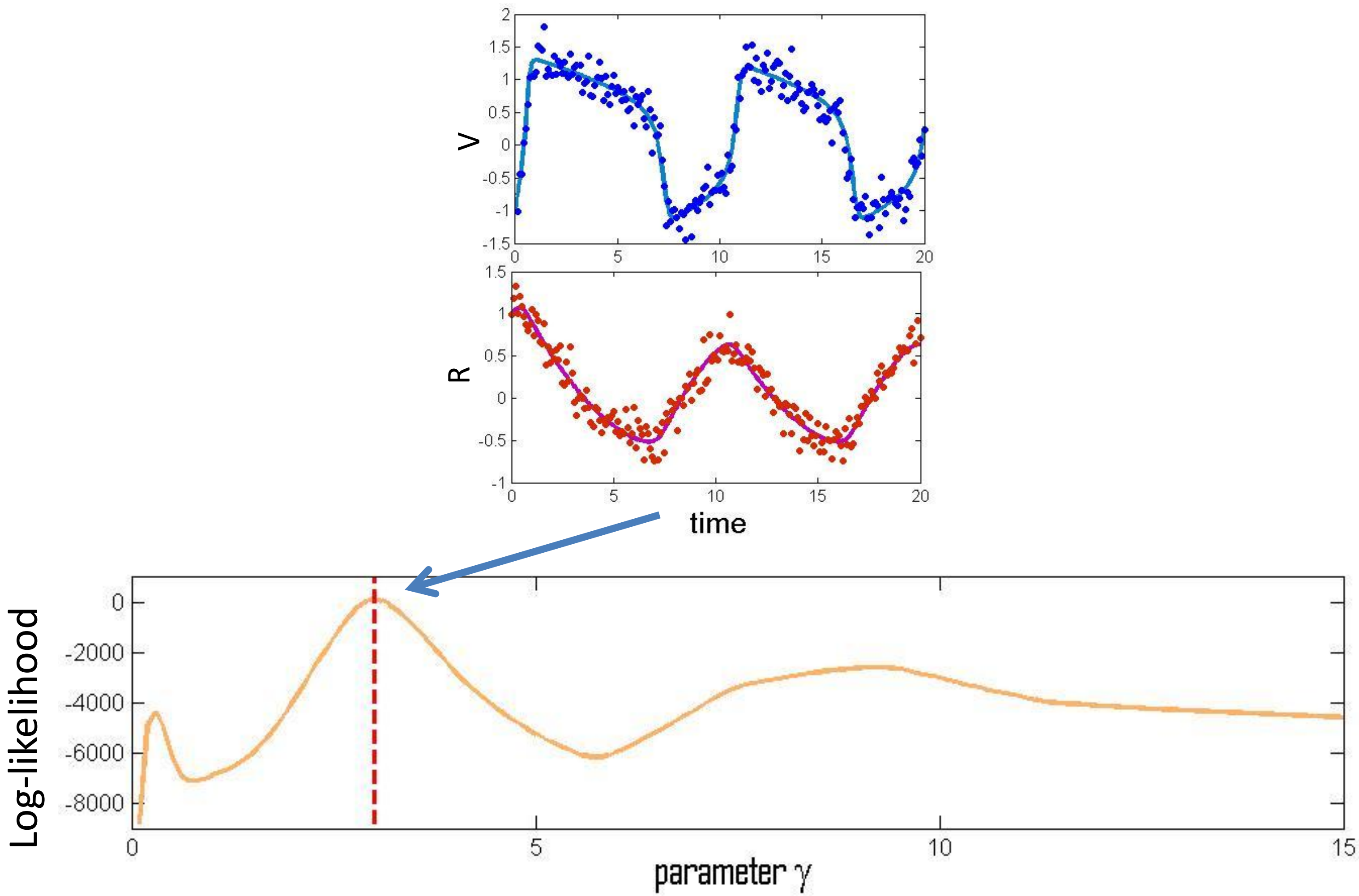

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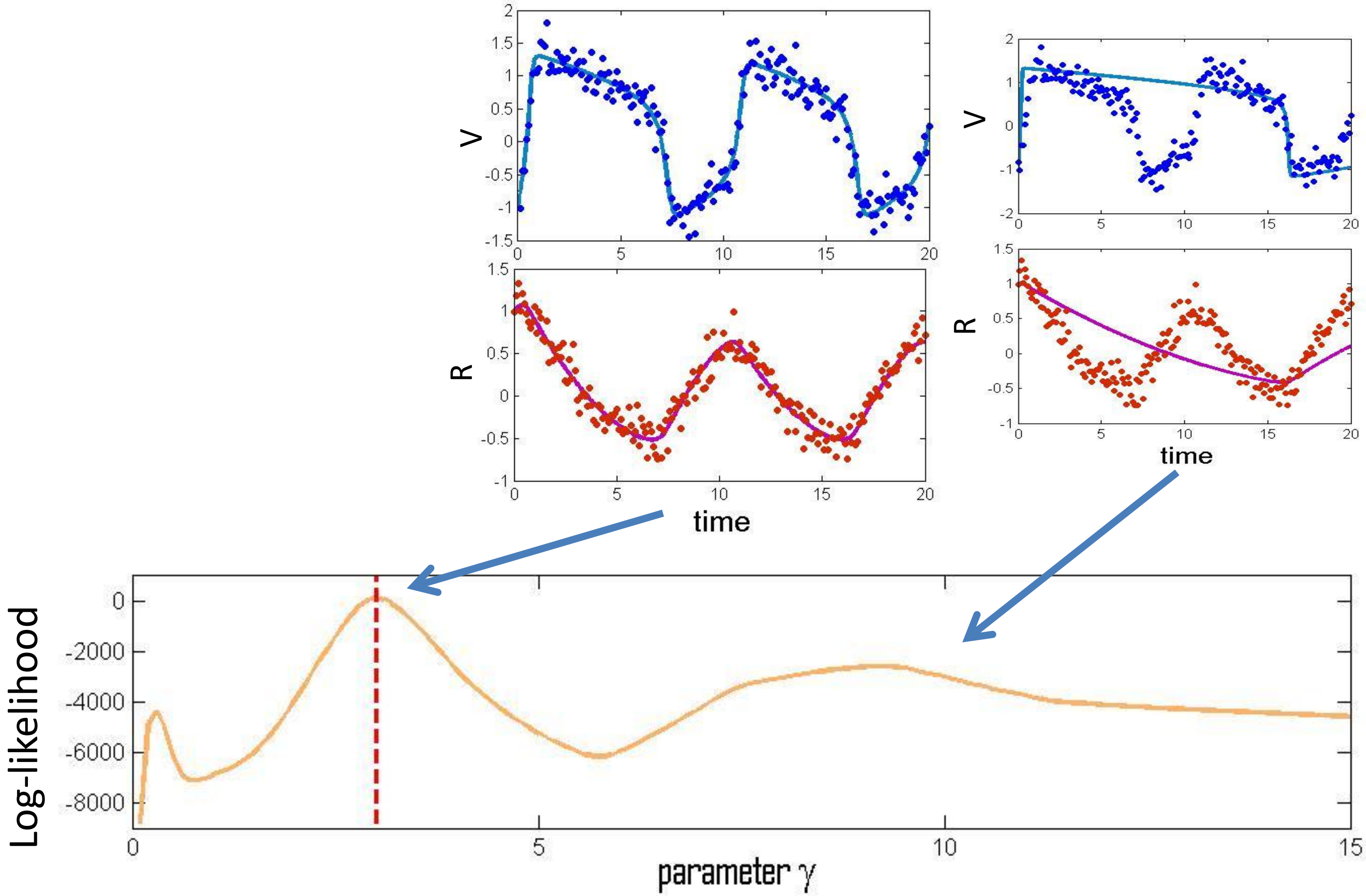

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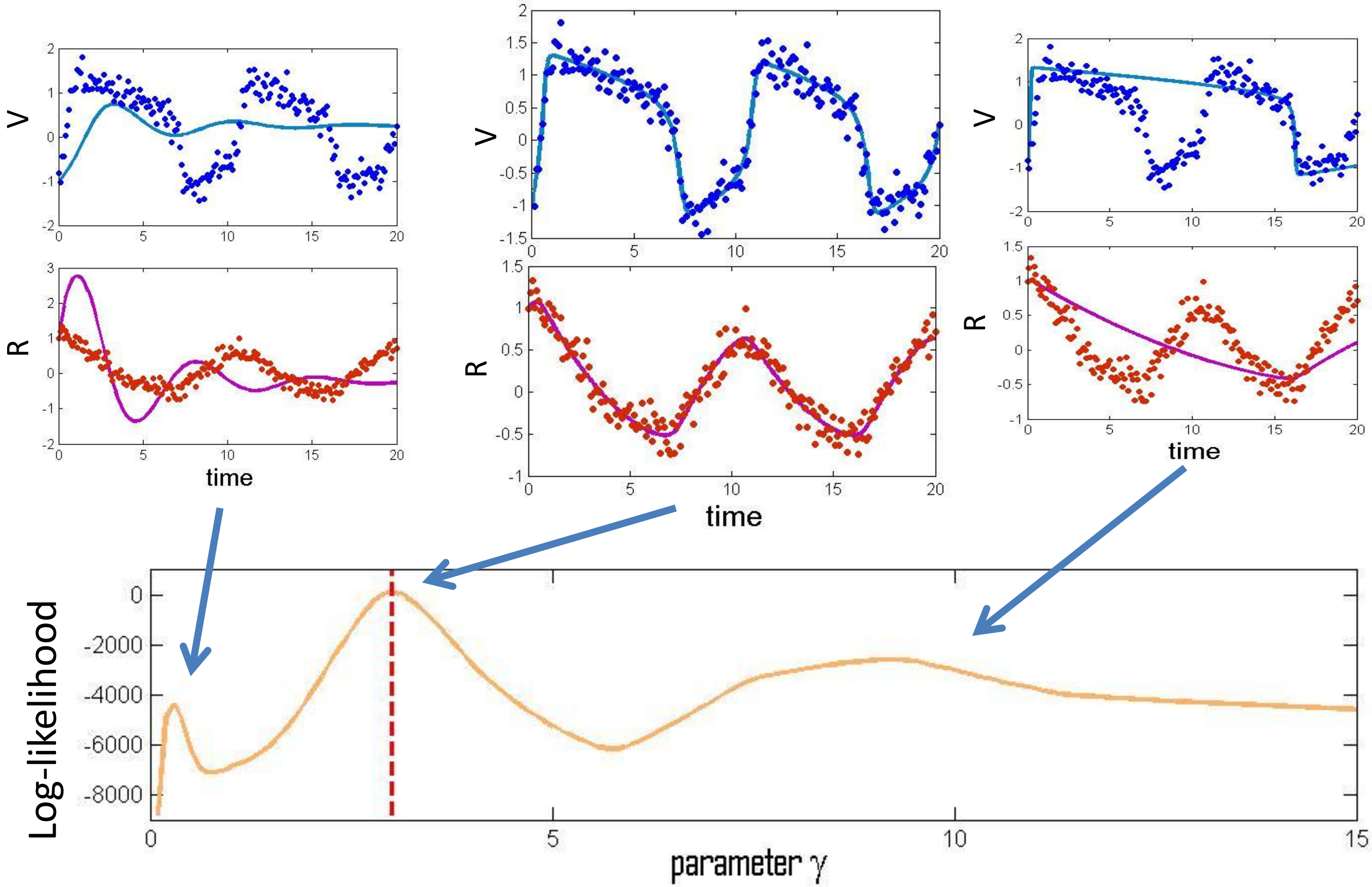

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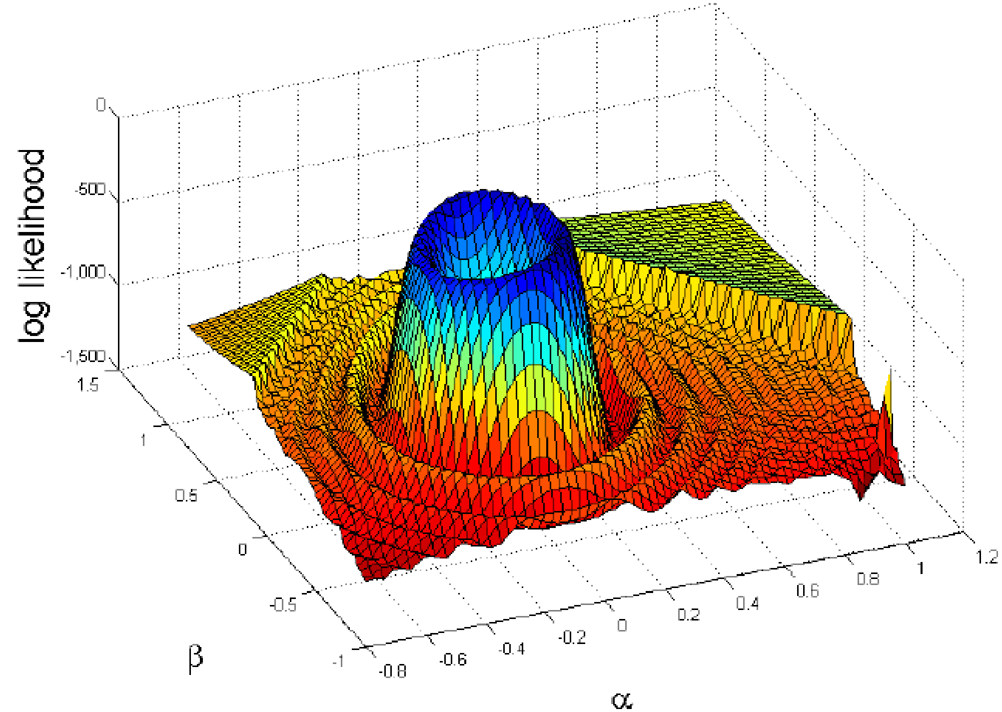


Ramsay, J. O., Hooker, G., Campbell, D. and Cao, J. (2007), Parameter estimation for differential equations: a generalized smoothing approach. Journal of the Royal Statistical Society: Series, 69: 741–796.

- Numerical optimizers may only find local optima
- Instead, we can estimate any functional of the posterior by using MCMC methods

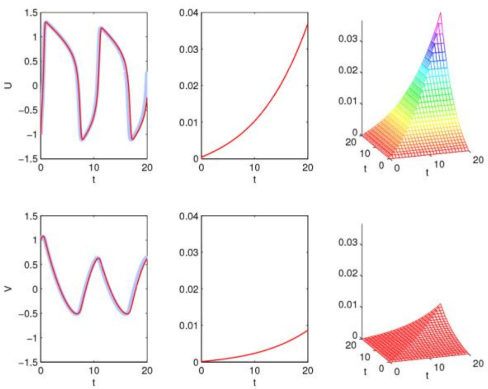
Estimation via MCMC

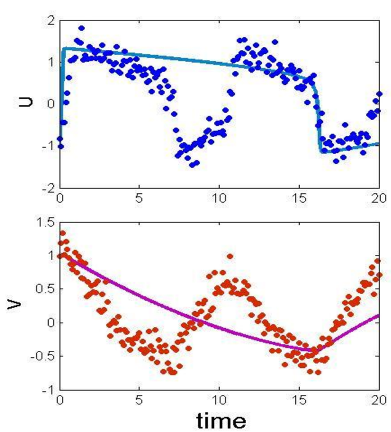
- complex posterior topology and high dimensions delay convergence
- guaranteed to get a good sample from the posterior distribution if you wait long enough
- to guarantee eventual graduation:
  - use fancy MCMC methods
    - parallel tempering, smooth functional tempering, adaptive MCMC, etc.
  - or redefine the problem:
    - estimate the DE solution nonparametrically
    - model the solution function as a stochastic process

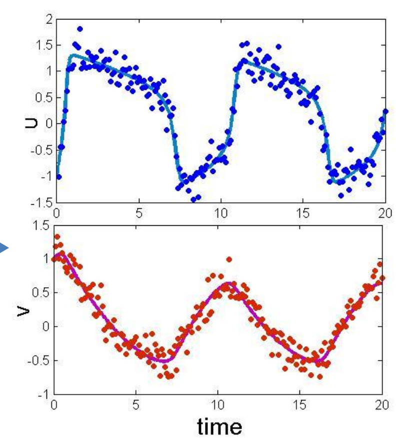
A bit about my research

Classical parameter estimation techniques ignore the error associated with solving ODEs numerically. By modeling the solution as a stochastic process we obtain an approximation to the ODE solution with associated estimation uncertainty.

We have developed a sequential ODE solver that quantifies the error in the estimation of ODE solutions in a probabilistic way. Solution uncertainty can now be incorporated into the inference process for ODE models.







Our work has very useful implications for parameter estimation.

questions?

email: ochkrebt@sfu.ca

Many thanks to:

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