A 3-stage Parameter Estimation Procedure for ODEs and DDEs

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Problem Statement:

Given **noisy observations** of the system state and a model of the system dynamics, determine model parameters which best fit the data, in the **least squares** sense:

$$\frac{dx}{dt}(t)=f(t,x(t),p);x(0)=x_0;t\in[0,T]$$

ODE model

$$\hat{x}(t_i)=x(t_i)+N(0,\sigma)$$

observations

Gaussian Noise

$$\sum_{i=1}^{n_t}\left\|\hat{x}(t_i)-x(t_i,p)\right\|^2$$

Least Squares Objective Function

Motivation:

- If the parameter search space is large, this optimization can be **expensive**.
- Can we take advantage of the model and observations to **reduce the search space**?
- Once the search space is reduced, should a **global** or **local** optimization strategy be used?

Example: Barnes Problem

Simple Predator-Prey Model specified by:

$$\frac{dx_1}{dt}(t)=ax_1(t)-bx_1(t)x_2(t)$$

$$\frac{dx_2}{dt}(t)=bx_1(t)x_2(t)-cx_2(t)$$

- Parameters: **a = b = c = x_1(0) =1, x_2(0) = 0.3**

Stage I: Refined Initial Guess

- Apply expert knowledge
- Use the noisy observations and the model to formulate an **alternative optimization problem**, which should be **inexpensive**.

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Initial Parameter Range

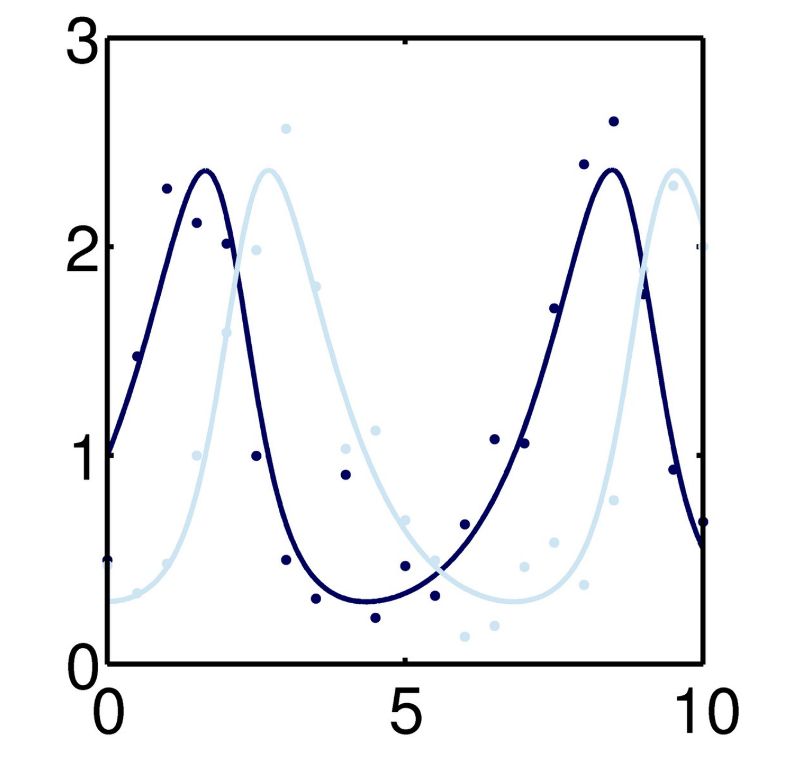
I. Refined Initial Guess

II. Global Optimization

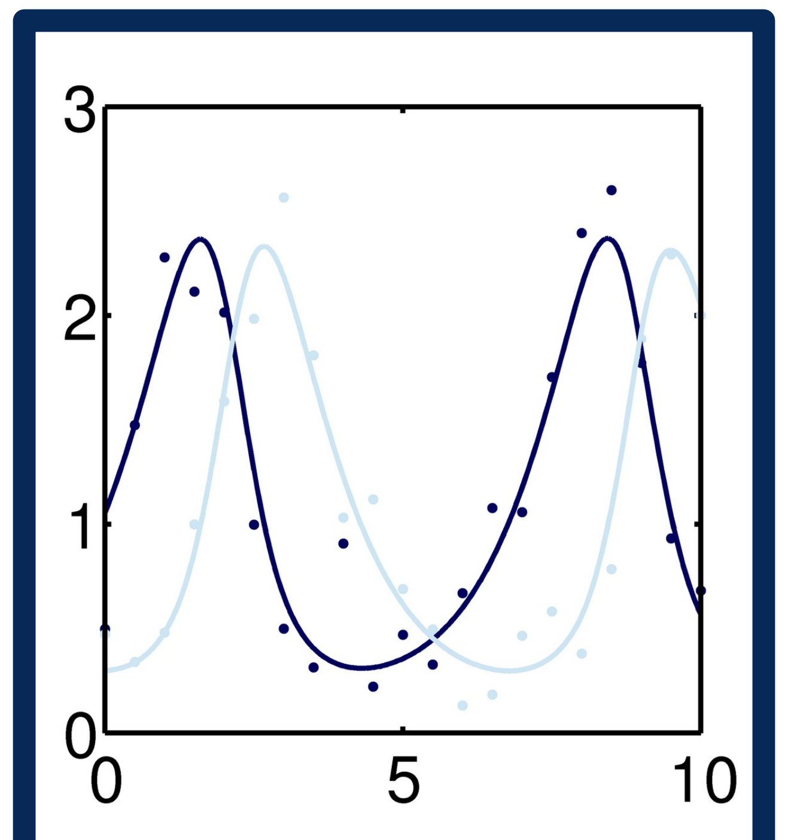
III. Local Optimization

Hybrid Optimization

Parameter Estimates



Noisy Observations (σ = 0.2)
And
Underlying True Trajectory



Best Fit Trajectory

Divided Differences:

- Differentiate the observations
- Avoid simulating the model

$$\frac{d\hat{x}}{dt}(t_i)\approx\frac{\hat{x}(t_{i+1})-\hat{x}(t_i)}{t_{i+1}-t_i}$$

$$\sum_{i=1}^{n_t-1}\left\|\frac{d\hat{x}}{dt}(t_i)-f(t_i,\hat{x}(t_i),p)\right\|^2$$

Data Driven Simulation:

$$\frac{dx}{dt}(t)=f(t,spline(\hat{x},t),p)$$

- Replace the dependence on x with dependence on the observations
- Still use the original least squares objective function, so still have to simulate the trajectory

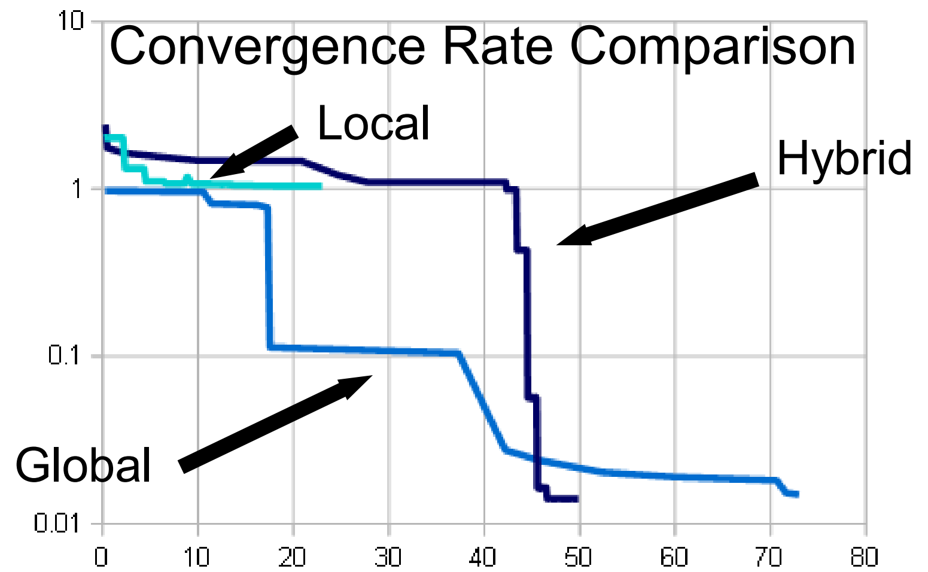
Comparison of Stage I Strategies:

Divided Differences		Data driven simulation		# of samples	Noise Level (σ)
Time (s)	Relative Error	Time (s)	Relative Error		
0.021	0.35	1.5	0.15	20	0.2
0.022	0.24	1.1	0.08		0.1
0.021	0.21	1.0	0.05	100	0.2
0.022	0.07	0.98	0.04		0.1
Inexpensive		**Expensive**		Optimizations performed in MATLAB	
Data Sensitive					

Stages II / III: Hybrid Optimization

Global	Local
• Slow, Heuristic-Based	• Fast, Gradient-Based
• Black-box Optimization	• We use a Levenberg Marquardt algorithm for least squares problems
• We use a Cross-Entropy based approach (importance sampling)	

- Model trajectories and gradients are accurately computed using a Continuous Runge-Kutta (CRK) method, implemented in the DDEM package



- How soon we switch greatly impacts performance of the hybrid

Results:

Method	Stage 1 Time (s)	Stage 2 Time (s)	Stage 3 Time (s)	Total Time (s)
Stage II Only	-	9.98	-	9.98
Stages II and III	-	5.05	0.08	5.13
All Stages	0.016	1.716	0.078	**1.81**
Multiple Shooting	-	-	-	2.47

- Addition of each stage reduces total time
- Timing of 3-stage procedure comparable to multiple shooting

Future Work:

- Application to stochastic models and larger systems
- Efficient solution of the data driven simulation Stage I optimization
- Alternative Stage I techniques for the case of partial observations

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