Parameter Estimation and Uncertainty Quantification in the Presence of Numerical Error

John Nardini

NCSU Tutorial Workshop on Parameter Estimation for Biological Models

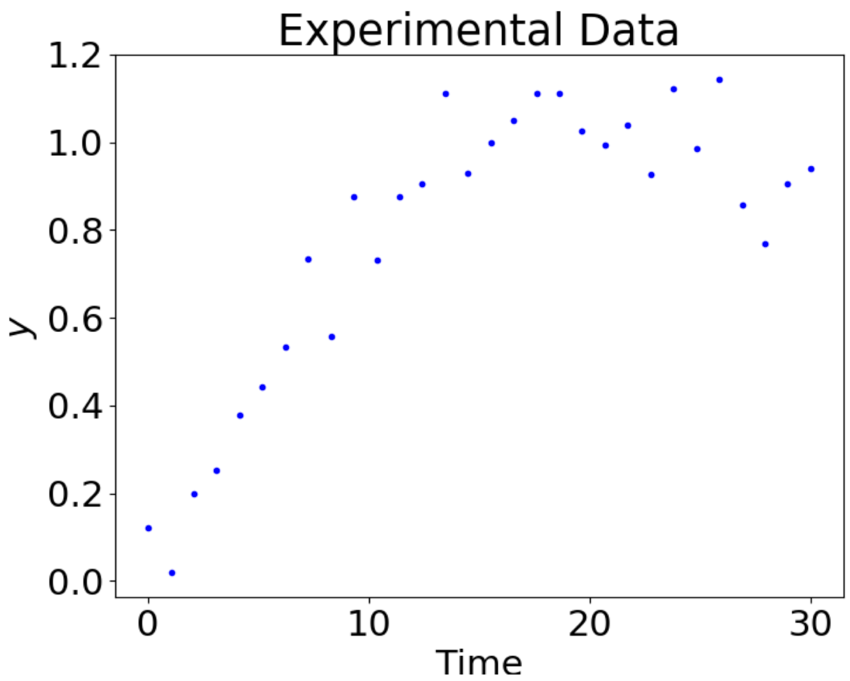
July 29, 2019

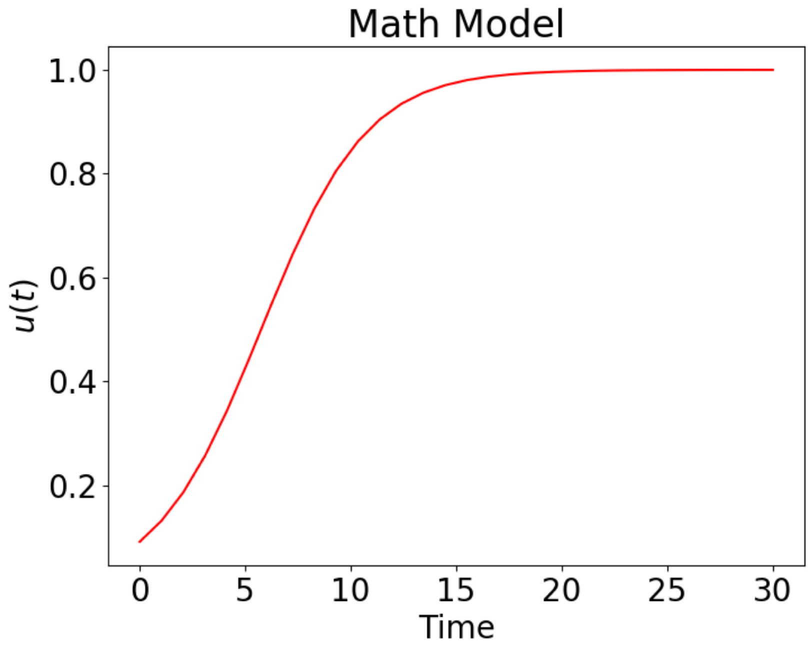
Typical Inverse Problem

Consider:

Experimental data, $\boldsymbol{y} = \{y(t_j)\}_{j=1}^{N}$, and

Mathematical Model: $u(t; \boldsymbol{q})$

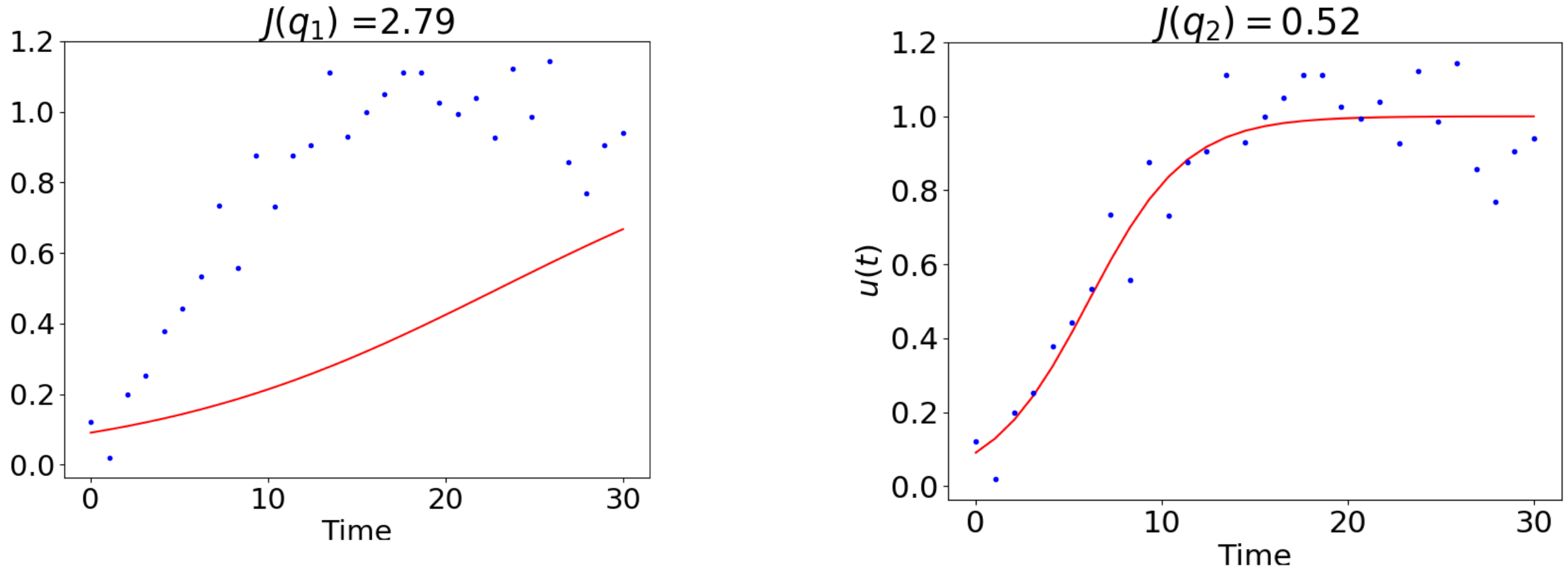




Typical Inverse Problem (cont.)

The ordinary least squares (OLS) cost function Summarizes how well $\boldsymbol{q}$ parameterizes u to fit $\boldsymbol{y}$

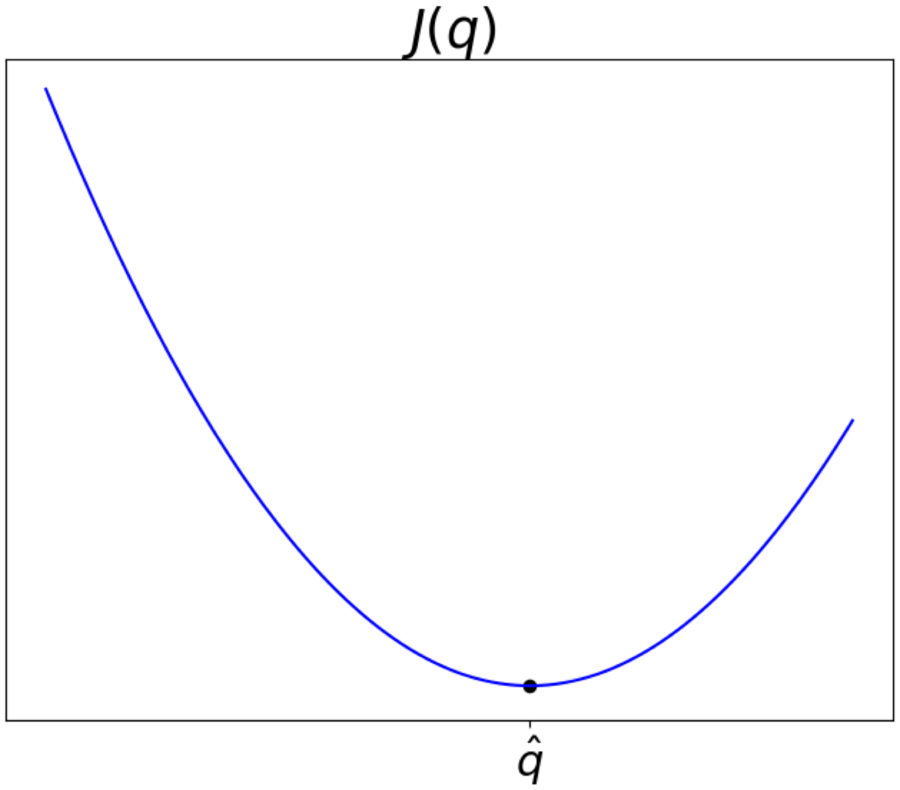
$$J(\boldsymbol{q}) = \sum_{i=1}^{N} \left(y_j - u(t_j; \boldsymbol{q})\right)^2$$



Typical Inverse Problem (cont.)

So we often parameterize $u(t;\boldsymbol{q})$ by:

$$\hat{\boldsymbol{q}} = \arg\min_{\boldsymbol{q} \in \boldsymbol{Q}} J(q)$$



Typical Inverse Problem (cont.)

Theorem:

If $y_j = u(t_j; \boldsymbol{q_0}) + \varepsilon_j$ and $\varepsilon_j \sim \mathcal{N}(0, \sigma^2), j = 1, \dots, N$

then:

$$\widehat{\boldsymbol{q}} \sim \mathcal{N}(\boldsymbol{q_0}, \sigma^2 V^{-1}), \qquad V = \nabla u(t; \boldsymbol{q_0})^T \nabla u(t; \boldsymbol{q_0})$$

Asymptotically as $N \to \infty$

But do we really know what $u(t_j; \boldsymbol{q}\,)$ is?

Numerical analysis for ODE Models

We often numerically solve ODE models of the form

$$\frac{du}{dt} = f(u, t; q) \qquad u(t_0) = u_0.$$

We call a numerical solution, $U(t; \Delta t, q)$, "*order p accurate*" if

$$\|u(t; q) - U(t; \Delta t, q)\|_1 \approx C\Delta t^p$$

Example: For MATLAB's ode45 function, $p = 4$

Revisiting the Inverse Problem Theory

Theorem:
If $y_j = u\left(t_j; \boldsymbol{q_0}\right) + \varepsilon_j$ and $\varepsilon_j \sim \mathcal{N}(0, \sigma^2), j = 1, \ldots, N$, then

$$\widehat{\boldsymbol{q}} \sim \mathcal{N}(\boldsymbol{q_0}, \sigma^2 V^{-1}), \qquad V = \nabla u(t; \boldsymbol{q_0})^T \nabla u(t; \boldsymbol{q_0})$$

asymptotically as $N \to \infty$.

Corollary: If $\mathrm{U}\left(t_j; \Delta t, \boldsymbol{q}\ \right)$ is *p order accurate*, then

$$\widehat{\boldsymbol{q}}(\Delta t) \sim \mathcal{N}\left(\boldsymbol{q_0}, \sigma^2 V_{\Delta t}^{-1}\right),$$

Asymptotically as $N \to \infty, \Delta t \to 0$. The entries of $V_{\Delta t}^{-1}$ are *order p accurate* for the entries of V^{-1}.

Behavior of the Cost Function

$$J(\boldsymbol{q}, \Delta t) = \sum \left(y_j - U\left(t_j; \Delta t, \boldsymbol{q}\right)\right)^{\mathbf{2}}$$

Final Behavior of the Cost Function

As $\Delta t \to 0$, if $U(t; \Delta t, \boldsymbol{q})$ is order p accurate,

$$J(\boldsymbol{q}, \Delta t) \approx \mathcal{O}(1) + \mathcal{O}(\Delta t^p) + \mathcal{O}(\Delta t^{2p}) + \mathcal{O}(\Delta t^p)$$

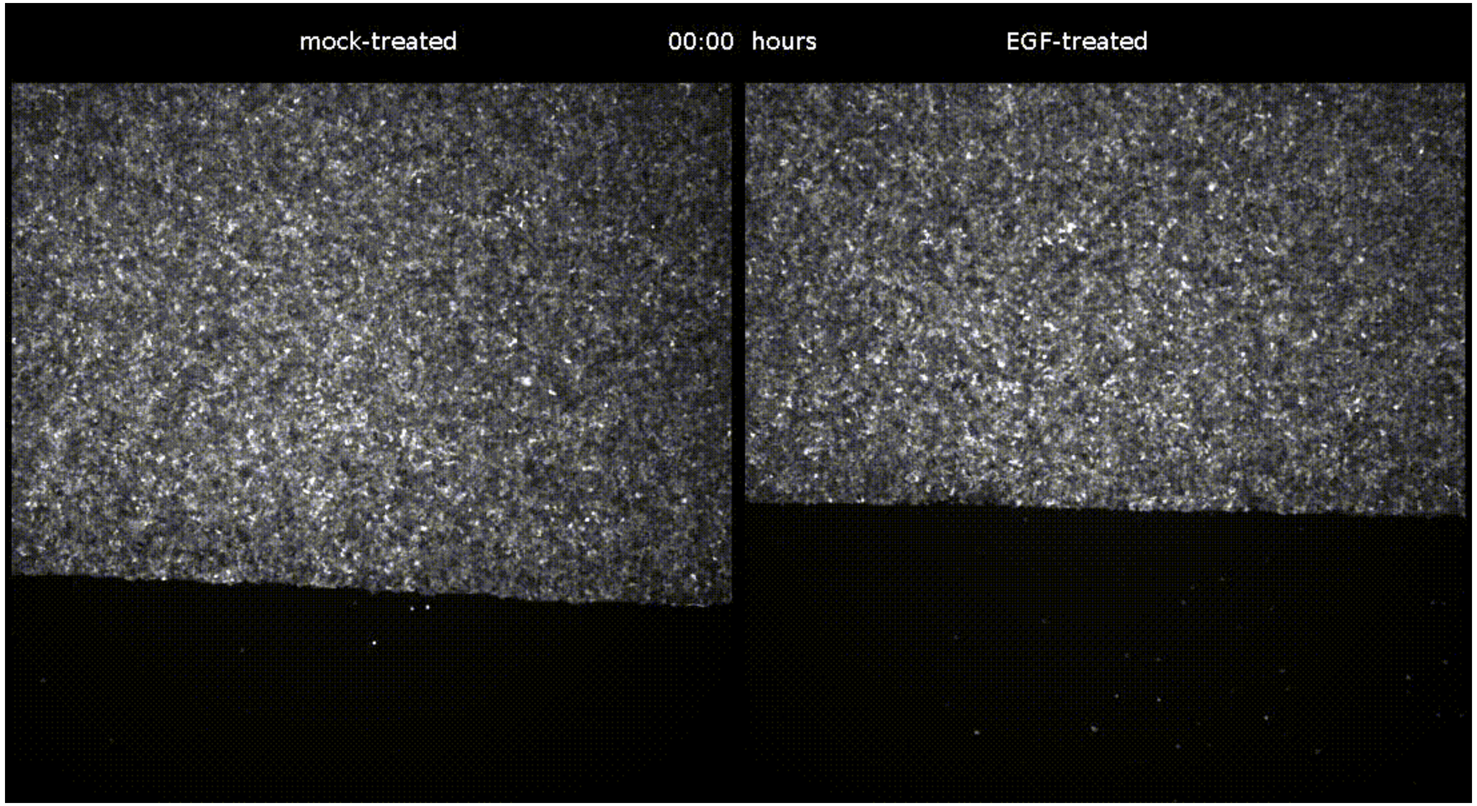
Data Noise	Inference	Numerical Error	Inference + Numerical Error

Do I really care?

Usually …. No. But there are some cases where numerical error matters!

Example: Advection Equations

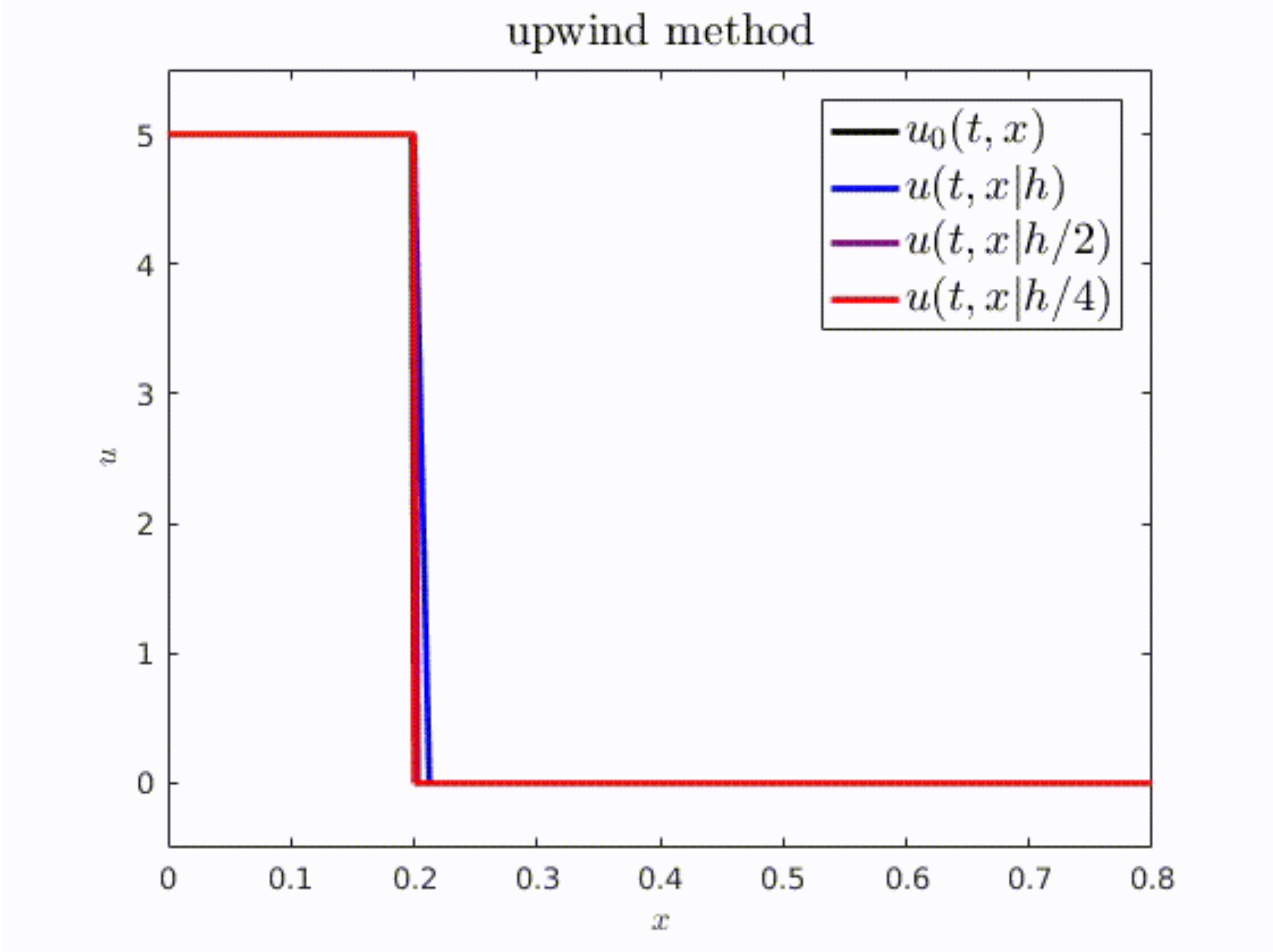
$$u_t + \nabla \cdot (vu) = 0$$
$$v = v(x)$$



Numerical Simulations for Advection Equations

The Upwind Method is order ½ accurate when $u(t, x; q)$ is discontinuous

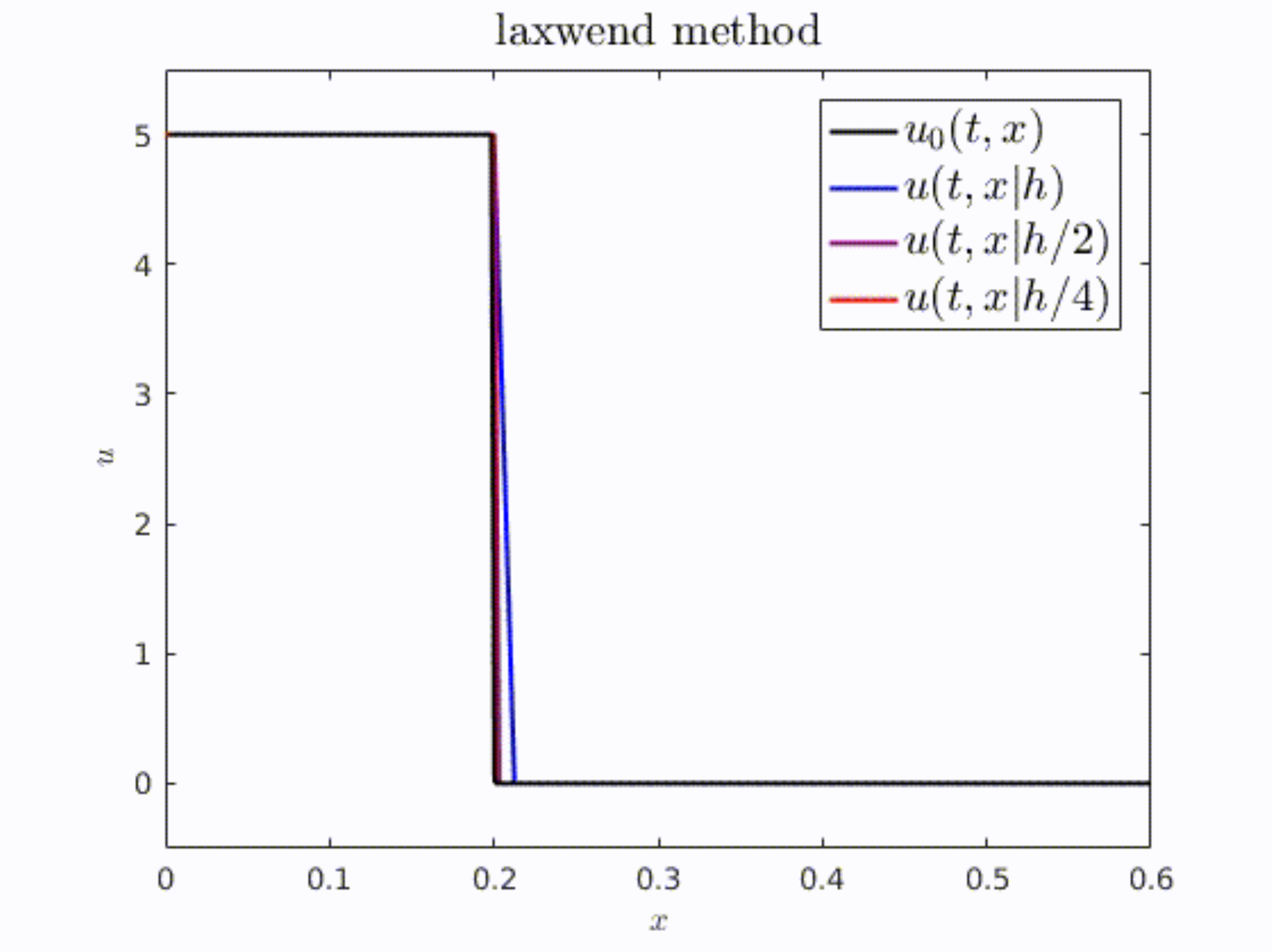
It adds numerical diffusion



Numerical Simulations for Advection Equations

The Lax-Wendroff Method is order 2/3 accurate when $u(t, x; q)$ is discontinuous

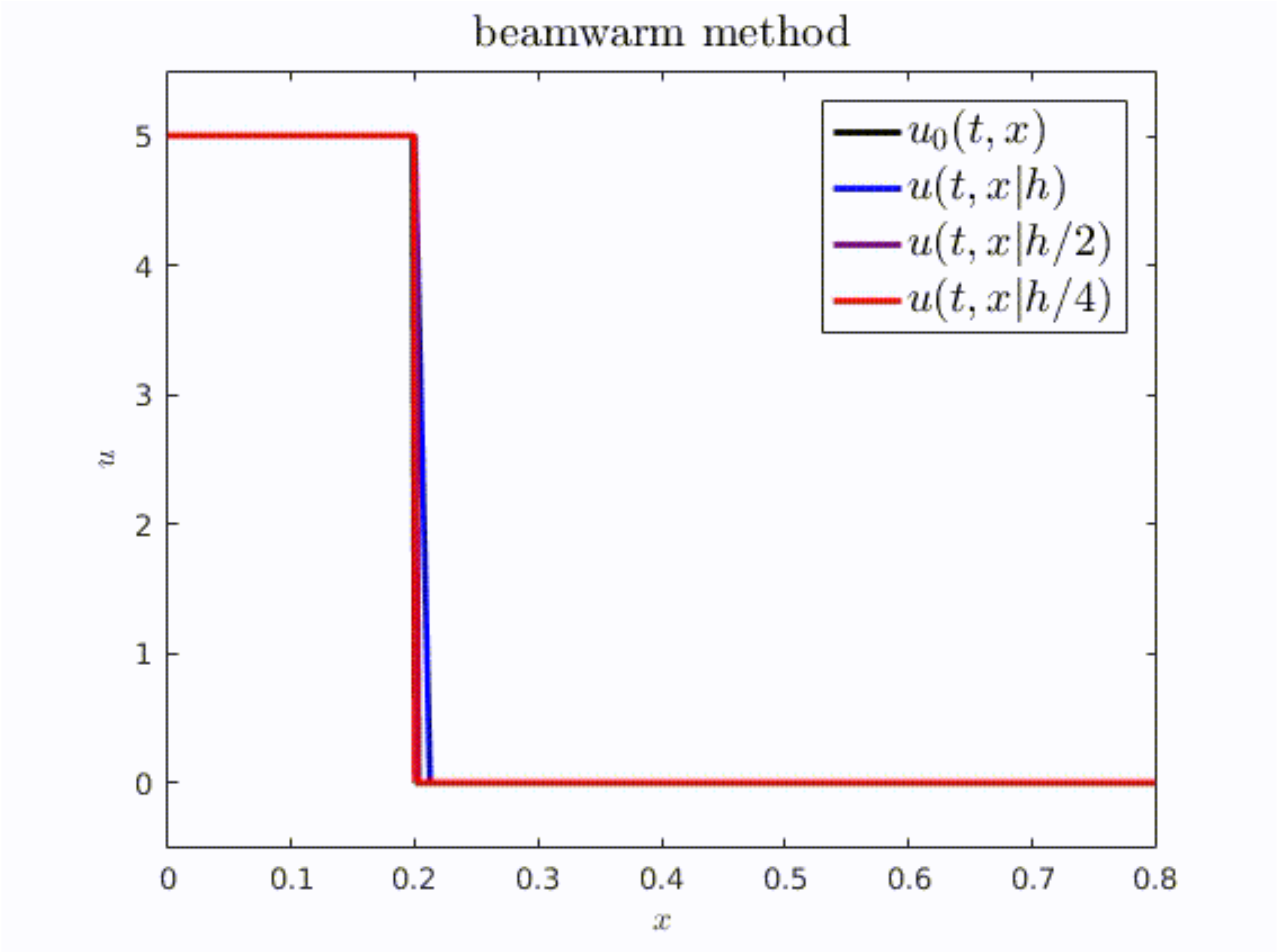
It adds numerical dispersion



Numerical Simulations for Advection Equations

The Beam-Warming Method is order 2/3 accurate when $u(t, x; q)$ is discontinuous

It adds numerical dispersion



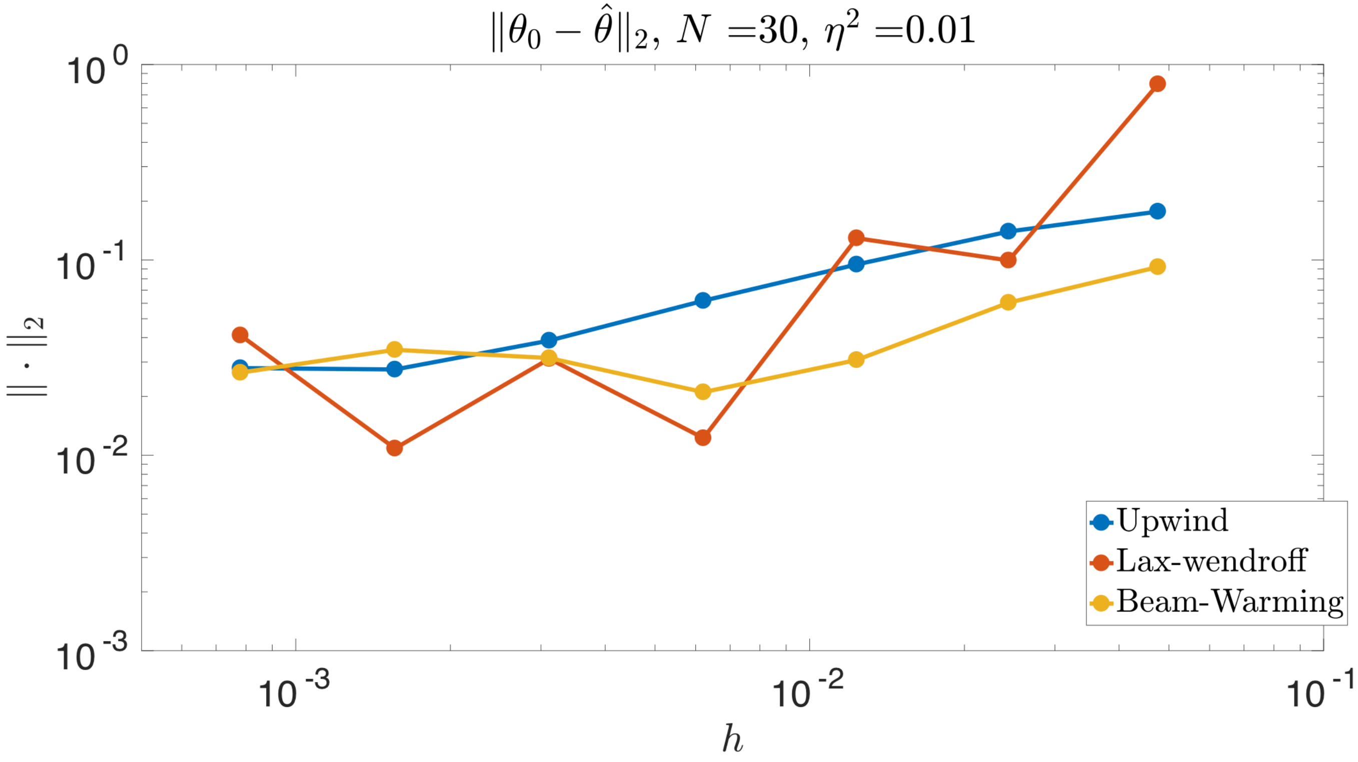
Parameter Estimation in the presence of numerical Error

Recall: If $\mathrm{U}\left(t_j;\Delta t,\boldsymbol{q}\ \right)$ is *p order accurate*, then

$$\widehat{\boldsymbol{q}}(\Delta t)\sim\mathcal{N}\left(\boldsymbol{q_0},\sigma^2 V_{\Delta t}^{-1}\right),$$

Asymptotically as $N\rightarrow\infty,\Delta t\rightarrow 0$. The entries of $V_{\Delta t}^{-1}$ are *order p accurate* for the entries of V^{-1}.

Parameter Estimation in the presence of numerical Error



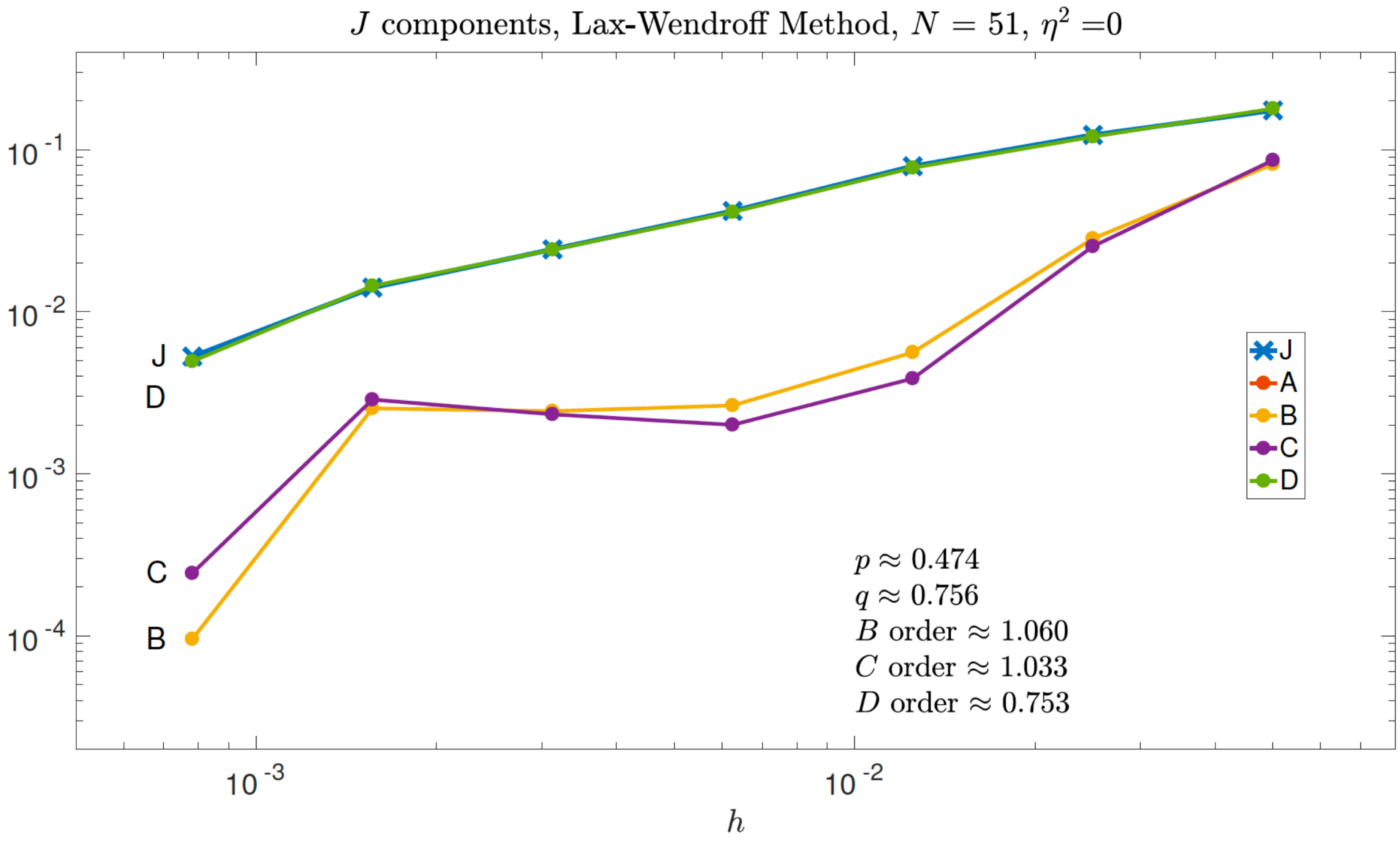
Numerical method	**p**	Order of $\hat{q}(\Delta t)$
Upwind	0.5839	0.560
Lax-Wendroff	0.4737	1.125
Beam-Warming	0.7876	0.736

Cost function Behavior in the Presence of numerical Error

As $\Delta t \rightarrow 0$, if $U(t; \Delta t, \boldsymbol{q})$ is order p accurate,

$$J(\boldsymbol{q}, \Delta t) \approx \mathcal{O}(1) + \quad \mathcal{O}(\Delta t^{p}) + \quad \mathcal{O}(\Delta t^{2p}) + \mathcal{O}(\Delta t^{p})$$

Cost function Behavior in the Presence of numerical Error



Conclusions

- Numerical Error can also impact inverse problems
- Theory regarding the behavior of the OLS estimator and cost function in the presence of numerical error
- Relevant to hyperbolic advection equations

Thank you!

Contact:
jtnardin@ncsu.edu
Johnnardini.wordpress.ncsu.edu
@jnard98

Thanks to Dr. David M. Bortz

The Joint NSF/NIH Mathematical Biology Initiative Program via grant NIGMS-R01GM126559

Nardini, J.T. and Bortz, D.M., The influence of numerical error on parameter estimation and uncertainty quantification for advective PDE models. *Inverse Problems* 35(6) p.65003 2019.