Parameter Estimation and Uncertainty Quantification in the Presence of Numerical Error

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Typical Inverse Problem

Consider:

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

Mathematical Model: \( u(t; \mathbf{q}) \)
Typical Inverse Problem (cont.)

The ordinary least squares (OLS) cost function summarizes how well \( q \) parameterizes \( u \) to fit \( y \)

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

![Graph showing fitted curves with error](image1.png)

\( J(q_1) = 2.79 \)

![Graph showing fitted curves with error](image2.png)

\( J(q_2) = 0.52 \)
Typical Inverse Problem (cont.)

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

$$\hat{\mathbf{q}} = \arg \min_{\mathbf{q} \in Q} J(q)$$
Typical Inverse Problem (cont.)

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

then:
\[
\hat{q} \sim \mathcal{N}(q_0, \sigma^2 V^{-1}), \quad V = \nabla u(t; q_0)^T \nabla u(t; q_0)
\]

Asymptotically as \( N \to \infty \)

But do we really know what \( u(t_j; q) \) is?
Numerical analysis for ODE Models

We often numerically solve ODE models of the form

\[
\frac{du}{dt} = f(u, t; q) \quad u(t_0) = u_0.
\]

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

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

asymptotically as $N \to \infty$.

**Corollary:** If $U(t_j; \Delta t, q)$ is $p$ order accurate, then

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

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

\[ J(q, \Delta t) = \sum (y_j - U(t_j; \Delta t, q))^2 \]
Final Behavior of the Cost Function

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

$$J(q, \Delta t) \approx O(1) + O(\Delta t^p) + O(\Delta t^{2p}) + O(\Delta t^p)$$
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 $\frac{1}{2}$ 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 $U(t_j; \Delta t, q)$ is $p$ order accurate, then

$$\hat{q}(\Delta t) \sim \mathcal{N}(q_0, \sigma^2 V^{-1}_{\Delta t}),$$

Asymptotically as $N \to \infty, \Delta t \to 0$. The entries of $V^{-1}_{\Delta t}$ are order $p$ accurate for the entries of $V^{-1}$. 
Parameter Estimation in the presence of numerical Error

\[ \| \theta_0 - \hat{\theta} \|_2, \quad N = 30, \quad \eta^2 = 0.01 \]

<table>
<thead>
<tr>
<th>Numerical method</th>
<th>( p )</th>
<th>Order of ( \hat{q}(\Delta t) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Upwind</td>
<td>0.5839</td>
<td>0.560</td>
</tr>
<tr>
<td>Lax-Wendroff</td>
<td>0.4737</td>
<td>1.125</td>
</tr>
<tr>
<td>Beam-Warming</td>
<td>0.7876</td>
<td>0.736</td>
</tr>
</tbody>
</table>
Cost function Behavior in the Presence of numerical Error

As Δt → 0, if \( U(t; \Delta t, q) \) is order \( p \) accurate,

\[
J(q, \Delta t) \approx O(1) + O(\Delta t^p) + O(\Delta t^{2p}) + O(\Delta t^p)
\]
Cost function Behavior in the Presence of numerical Error

\[ J \text{ components, Lax-Wendroff Method, } N = 51, \eta^2 = 0 \]

\[ p \approx 0.474 \]
\[ q \approx 0.756 \]
\[ B \text{ order } \approx 1.060 \]
\[ C \text{ order } \approx 1.033 \]
\[ D \text{ order } \approx 0.753 \]
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!

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