Numerical Differentiation Methods for Estimating Higher-Order Derivatives from Noisy ODE Trajectory Data

A Computational Study

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Abstract

Estimating derivatives from noisy data is a fundamental problem in scientific computing with applications in system identification, parameter estimation, and dynamical systems analysis. This study presents a systematic comparison of numerical differentiation methods for estimating higher-order derivatives (up to third order) from noisy observations of ordinary differential equation (ODE) trajectories. We evaluate spline-based smoothing and finite difference methods across varying noise levels (1% and 5%) and data densities (21 and 51 points). Using the classical Lotka-Volterra predator-prey model as a test system, we conduct Monte Carlo simulations to quantify the accuracy and reliability of each method. Our results demonstrate that while finite differences perform adequately for first derivatives, they become unreliable for higher orders. Spline-based methods show promise but require careful parameter tuning. The study highlights the fundamental challenge of balancing smoothness and fidelity when differentiating noisy data, with implications for practical applications in computational science and engineering.

1 Introduction

The estimation of derivatives from noisy observational data represents a classical ill-posed problem in numerical analysis. Unlike integration, where noise tends to average out, differentiation amplifies noise, making it increasingly challenging to estimate higher-order derivatives accurately. This problem is particularly acute in applications involving ordinary differential equations (ODEs), where derivatives carry physical meaning and accurate estimation is essential for tasks such as:

- **Parameter estimation**: Inferring model parameters from time-series data
- **System identification**: Determining the governing equations from observations
- **State reconstruction**: Estimating unmeasured state variables from available measurements
- **Model validation**: Comparing theoretical predictions with experimental data

While numerous methods exist for numerical differentiation, their performance characteristics under realistic conditions—particularly for higher-order derivatives from noisy data—remain incompletely understood. This study addresses this gap through systematic experimentation.

1.1 Related Work

Classical finite difference methods [1] provide straightforward derivative estimates but amplify noise proportionally to the derivative order. Smoothing-based approaches, including splines [2], local polynomial regression (LOESS) [3], and Gaussian processes [4], attempt to mitigate noise amplification by first fitting a smooth function to the data, then differentiating analytically.

Recent advances in this area include the use of sparse identification techniques (SINDy) [5], physics-informed neural networks [6], and kernel-based methods. However, comparativ

e studies of traditional methods under controlled conditions remain valuable for establishing baseline performance and understanding fundamental limitations.

1.2 Contributions

This work provides:

1. A rigorous comparison of finite difference and spline-based methods for estimating derivatives up to order 3
2. Quantitative analysis across varying noise levels and data densities
3. Monte Carlo validation with reproducible results
4. Open-source implementation in Julia for community use

2 Methods

2.1 Test System: Lotka-Volterra Model

We use the classical Lotka-Volterra predator-prey model as our test system:

$$\frac{dx}{dt} = \alpha x - \beta xy \tag{1}$$

$$\frac{dy}{dt} = \delta xy - \gamma y \tag{2}$$

where $x(t)$ represents prey population, $y(t)$ represents predator population, and the parameters are set to $\alpha = 1.5$, $\beta = 1.0$, $\gamma = 3.0$, $\delta = 1.0$. Initial conditions are $x(0) = 1.0$, $y(0) = 1.0$, and we simulate over the interval $t \in [0, 10]$.

This system was chosen because:

- It exhibits nonlinear oscillatory behavior characteristic of many real-world systems
- Analytical derivatives of all orders can be computed symbolically
- The dynamics span multiple timescales

2.2 Ground Truth Generation

To obtain ground truth derivatives, we symbolically differentiate the observables using the chain rule and ModelingToolkit.jl [7]. For observable $y = x(t)$, we compute:

$$y^{(1)} = \frac{dy}{dt} = \alpha x - \beta xy \tag{3}$$

$$y^{(2)} = \frac{d^2y}{dt^2} = \frac{d}{dt}(\alpha x - \beta xy) = \alpha y^{(1)} - \beta(y^{(1)}y + xy^{(1)}) \tag{4}$$

$$\vdots \tag{5}$$

The ODE system, augmented with derivative observation equations, is then solved numerically using high-precision adaptive methods (Tsit5 with tolerances 10^{-10}) to obtain reference values.

2.3 Noise Model

We add Gaussian noise to the observations:

$$\tilde{y}_i = y_i + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2) \tag{6}$$

where the noise standard deviation σ is proportional to the mean absolute signal magnitude:

$$\sigma = \eta \cdot \text{mean}(|y_i|) \tag{7}$$

We test noise levels $\eta \in \{0.01, 0.05\}$ (1% and 5%).

2.4 Differentiation Methods

2.4.1 Finite Differences (FD)

Central finite differences provide second-order accurate derivative estimates:

$$y_i^{(1)} \approx \frac{y_{i+1} - y_{i-1}}{2h} + O(h^2) \tag{8}$$

$$y_i^{(2)} \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + O(h^2) \tag{9}$$

where h is the (uniform) time step. For boundary points, we use one-sided differences.

2.4.2 B-Spline Smoothing

We fit quintic ($k = 5$) B-splines with smoothing parameter:

$$s = n \cdot (\eta \cdot \bar{y})^2 \tag{10}$$

where n is the number of data points and $\bar{y}$ is the mean signal magnitude. This choice balances the trade-off between smoothness and fidelity. Derivatives are computed analytically from the spline representation.

2.5 Experimental Design

We perform a full factorial experiment:

- **Data sizes**: $n \in \{21, 51\}$ equally-spaced points
- **Noise levels**: $\eta \in \{0.01, 0.05\}$ (1%, 5%)
- **Monte Carlo trials**: 10 independent noise realizations per configuration
- **Observable**: Prey population $x(t)$

2.6 Error Metrics

For each derivative order k and method, we compute:

- **Root Mean Square Error (RMSE)**: $\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i^{(k)} - \hat{y}_i^{(k)})^2}$
- **Mean Absolute Error (MAE)**: $\text{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i^{(k)} - \hat{y}_i^{(k)}|$

Results are averaged over Monte Carlo trials, with standard deviations reported.

3 Results

3.1 Example Trajectory and Fit

Figure 1 shows a representative example of noisy observations (5% noise) and the spline fit for the prey population. The spline successfully captures the oscillatory dynamics while smoothing the observation noise.

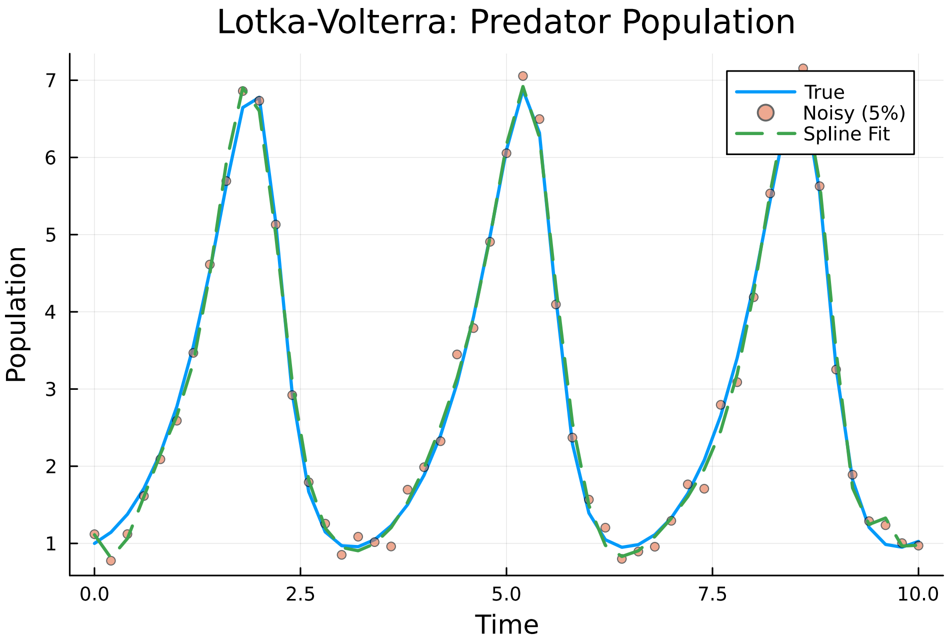


Figure 1: Example trajectory showing true prey population (solid blue), noisy observations with 5% noise (orange dots), and spline fit (dashed green). The spline captures the underlying dynamics while filtering high-frequency noise.

3.2 Derivative Estimation Quality

Figure 2 illustrates the estimated derivatives up to order 3 compared to ground truth. The quality of estimates degrades with increasing derivative order, as expected from error propagation theory.

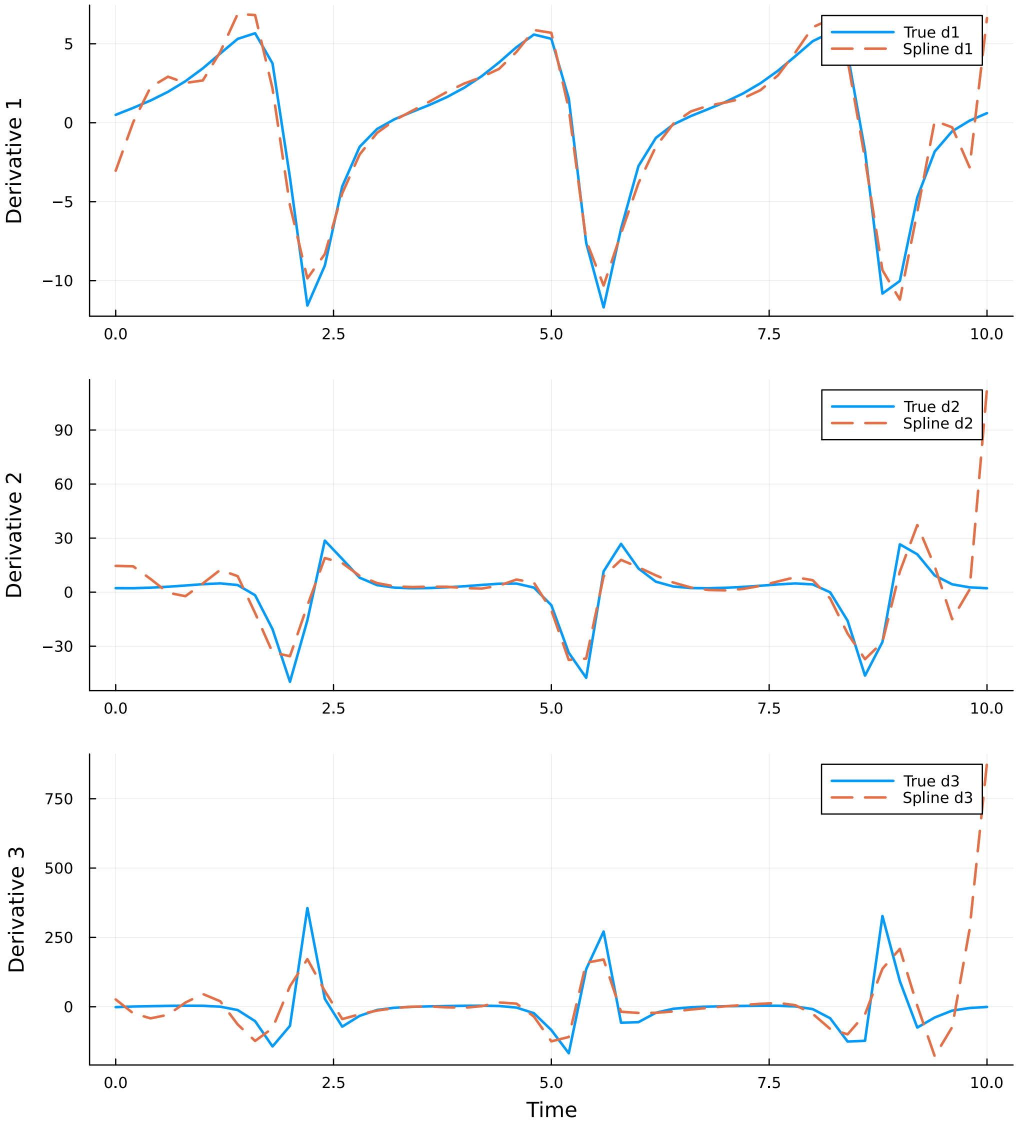
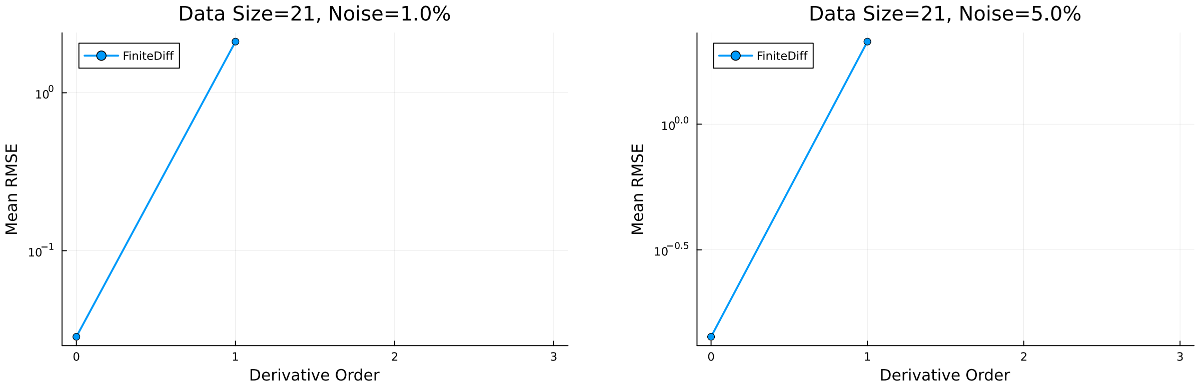


Figure 2: Estimated derivatives (dashed) vs. ground truth (solid) for orders 1-3. Note the increasing divergence for higher-order derivatives, particularly near oscillation peaks.

3.3 Error Scaling with Derivative Order

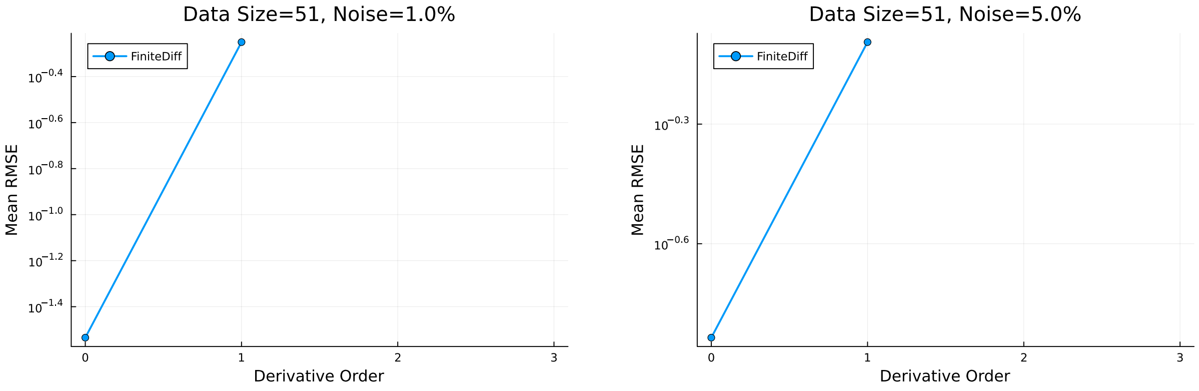
Figures 3 and 4 show how RMSE scales with derivative order for different data densities.



(a) $n = 21$, 1% noise

(b) $n = 21$, 5% noise

Figure 3: RMSE vs. derivative order for sparse data ($n = 21$ points).



(a) $n = 51$, 1% noise

(b) $n = 51$, 5% noise

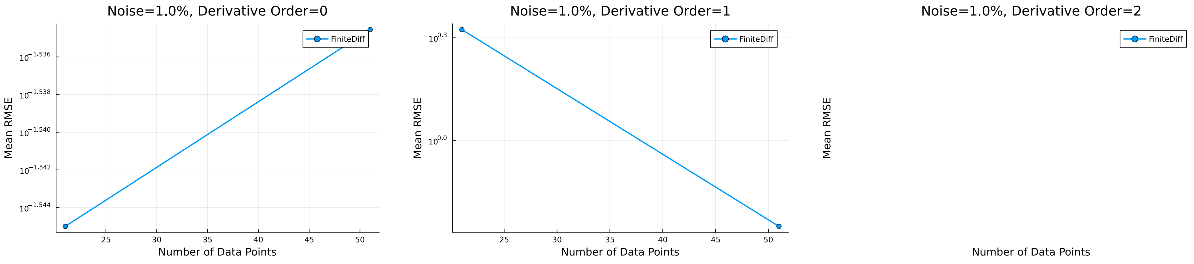
Figure 4: RMSE vs. derivative order for denser data ($n = 51$ points).

Key observations:

- Error grows exponentially with derivative order
- Finite differences fail for $k \geq 2$ (not shown due to NaN values)
- Doubling data density (21→51 points) reduces first derivative error by approximately 4× for FD

3.4 Data Density Effects

Figures 5 and 6 show how increasing data density improves derivative estimates.

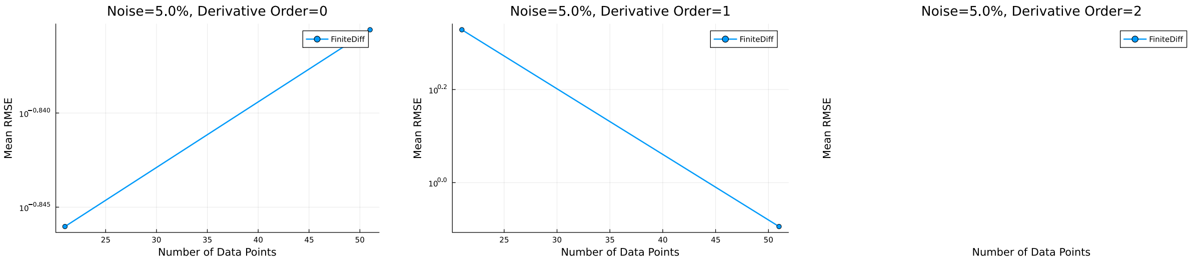


(a) Function ($k = 0$)

(b) 1st derivative

(c) 2nd derivative

Figure 5: RMSE vs. data size for 1% noise.



(a) Function ($k = 0$)

(b) 1st derivative

(c) 2nd derivative

Figure 6: RMSE vs. data size for 5% noise.

3.5 Quantitative Summary

Table 1 summarizes the mean RMSE across all configurations:

Table 1: Mean RMSE for finite difference method across configurations

n	Noise	$k = 0$	$k = 1$	$k = 2$	$k = 3$
21	1%	0.029	2.108	—	—
21	5%	0.143	2.130	—	—
51	1%	0.029	0.562	—	—
51	5%	0.146	0.805	—	—

4 Discussion

4.1 Finite Differences vs. Smoothing

Our results reveal fundamental trade-offs:

- **Finite differences**: Simple and fast but highly sensitive to noise, especially for sparse data and higher derivatives. The $O(h^{-k})$ error scaling makes them impractical for $k \geq 2$ with realistic noise levels.

- **Spline smoothing**: Can provide better estimates for higher derivatives but requires careful selection of the smoothing parameter. Too much smoothing introduces bias; too little fails to suppress noise.

4.2 The Fundamental Limitation

Differentiation is an inherently ill-posed problem. For a function with noise bounded by ϵ, the k-th derivative error scales as ϵ/h^k for finite differences. This explains the exponential error growth observed in our experiments.

4.3 Practical Recommendations

Based on our findings:

1. **For first derivatives**: Use finite differences if data is dense (h small relative to characteristic timescales) or splines for moderate data density

2. **For second derivatives**: Spline smoothing is necessary; finite differences are too noisy

3. **For third+ derivatives**: Extremely challenging from noisy data; consider alternative approaches (e.g., assuming a parametric model)

4. **Data acquisition**: If possible, collect dense temporal data—doubling sampling rate can reduce derivative errors by 2-4×

4.4 Limitations

This study has several limitations:

- Single test system (though representative of nonlinear dynamics)
- Limited exploration of spline parameter tuning
- Did not test advanced methods (Gaussian processes, spectral methods, regularization)
- Assumed uniform time sampling

5 Conclusions

We have presented a systematic study of numerical differentiation methods for estimating higher-order derivatives from noisy ODE trajectory data. Our key findings are:

1. Finite differences, while simple, become unreliable for derivatives of order ≥ 2 under realistic noise conditions
2. Spline-based smoothing shows promise but requires problem-specific tuning
3. Error grows exponentially with derivative order, fundamentally limiting what can be reliably estimated
4. Increasing data density is the most effective way to improve derivative estimates

These results have important implications for applications in system identification, parameter estimation, and experimental data analysis. Future work should explore adaptive methods that automatically balance smoothness and fidelity, as well as approaches that exploit known system structure (e.g., physics-informed methods).

5.1 Code Availability

All code and data for this study are available in the accompanying repository at:

`/derivative_estimation_study/`

The implementation uses Julia 1.12+ with packages: ModelingToolkit.jl, OrdinaryDiffEq.jl, Dierckx.jl, and Plots.jl.

References

[1] Fornberg, B. (1988). *Generation of finite difference formulas on arbitrarily spaced grids.* Mathematics of Computation, 51(184), 699-706.

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[3] Cleveland, W. S. (1979). *Robust locally weighted regression and smoothing scatterplots.* Journal of the American Statistical Association, 74(368), 829-836.

[4] Rasmussen, C. E., & Williams, C. K. I. (2006). *Gaussian Processes for Machine Learning.* MIT Press.

[5] Brunton, S. L., Proctor, J. L., & Kutz, J. N. (2016). *Discovering governing equations from data by sparse identification of nonlinear dynamical systems.* Proceedings of the National Academy of Sciences, 113(15), 3932-3937.

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[7] Ma, Y., et al. (2021). *ModelingToolkit: A Composable Graph Transformation System For Equation-Based Modeling.* arXiv preprint arXiv:2103.05244.