PyDelt: Comprehensive Analysis of Advanced Numerical Differentiation Methods

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***Abstract*—This paper presents a comprehensive analysis of numerical differentiation methods implemented in PyDelt compared to other popular libraries. We evaluate the performance of various interpolation-based, finite difference, and neural network-based methods across univariate and multivariate functions, with varying levels of noise. Our results demonstrate that PyDelt's methods offer superior accuracy and noise robustness compared to traditional approaches, while maintaining competitive computational efficiency. We provide specific recommendations for method selection based on application requirements and highlight areas for future development.**

***Index Terms*—numerical differentiation, interpolation, noise robustness, multivariate calculus, neural networks, automatic differentiation**

I. Introduction

Numerical differentiation is a fundamental operation in scientific computing, with applications ranging from signal processing and time series analysis to physics simulations and optimization algorithms. The accuracy and robustness of derivative estimates are critical in many applications, particularly when dealing with noisy data or complex functions.

PyDelt is a Python library that provides a comprehensive suite of numerical differentiation methods based on advanced interpolation techniques, including:

- Spline interpolation
- Local Linear Approximation (LLA)
- Generalized Local Linear Approximation (GLLA)
- Locally Weighted Scatterplot Smoothing (LOWESS)
- Local Regression (LOESS)
- Functional Data Analysis (FDA)
- Neural network-based methods with automatic differentiation

This paper evaluates these methods against popular alternatives from libraries such as SciPy, NumDiffTools, FinDiff, and JAX, across a range of test functions and noise conditions.

II. Methodology

A. Test Functions

We evaluated the performance of differentiation methods on the following test functions:

1) **Sine function**: $f(x) = \sin(x)$
   - First derivative: $f'(x) = \cos(x)$
   - Second derivative: $f''(x) = -\sin(x)$
2) **Exponential function**: $f(x) = e^x$
   - First derivative: $f'(x) = e^x$
   - Second derivative: $f''(x) = e^x$
3) **Polynomial function**: $f(x) = x^3 - 2x^2 + 3x - 1$
   - First derivative: $f'(x) = 3x^2 - 4x + 3$
   - Second derivative: $f''(x) = 6x - 4$
4) **Multivariate scalar function**: $f(x, y) = \sin(x) + \cos(y)$
   - Gradient: $\nabla f(x, y) = [\cos(x), -\sin(y)]$
5) **Multivariate vector function**: $f(x, y) = [\sin(x)\cos(y), x^2 + y^2]$
   - Jacobian matrix: $J_f(x, y) = \begin{bmatrix} \cos(x)\cos(y) & -\sin(x)\sin(y) \\ 2x & 2y \end{bmatrix}$

B. Evaluation Metrics

We assessed the performance of each method using the following metrics:

1) **Accuracy**: Mean absolute error (MAE) and root mean square error (RMSE) between the numerical and analytical derivatives.
2) **Noise Robustness**: Performance degradation when adding Gaussian noise with standard deviation proportional to the signal's standard deviation.
3) **Computational Efficiency**: Execution time for fitting and evaluating derivatives.
4) **Dimensionality Handling**: Ability to handle multivariate functions and compute higher-order derivatives.

C. Compared Methods

1) PyDelt Methods:

- SplineInterpolator
- LlaInterpolator
- GllaInterpolator
- LowessInterpolator
- LoessInterpolator
- FdaInterpolator
- Neural network derivatives (TensorFlow and PyTorch)
- MultivariateDerivatives

2) External Libraries:

- SciPy (UnivariateSpline, CubicSpline)
- NumDiffTools
- FinDiff
- JAX automatic differentiation

TABLE I
MEAN ABSOLUTE ERROR FOR FIRST-ORDER DERIVATIVES (NO NOISE)

Method	Sine	Exponential	Polynomial	Average
PyDelt GLLA	0.0031	0.0028	0.0019	0.0026
PyDelt LLA	0.0045	0.0042	0.0037	0.0041
PyDelt Spline	0.0089	0.0076	0.0053	0.0073
PyDelt LOESS	0.0124	0.0118	0.0097	0.0113
PyDelt LOWESS	0.0131	0.0122	0.0102	0.0118
PyDelt FDA	0.0091	0.0079	0.0058	0.0076
SciPy Spline	0.0092	0.0081	0.0061	0.0078
NumDiffTools	0.0183	0.0175	0.0142	0.0167
FinDiff	0.0187	0.0179	0.0145	0.0170
JAX	0.0001	0.0001	0.0001	0.0001

TABLE II
MEAN ABSOLUTE ERROR FOR SECOND-ORDER DERIVATIVES (NO NOISE)

Method	Sine	Exponential	Polynomial	Average
PyDelt GLLA	0.0187	0.0172	0.0103	0.0154
PyDelt LLA	0.0213	0.0198	0.0121	0.0177
PyDelt Spline	0.0156	0.0143	0.0087	0.0129
PyDelt LOESS	0.0289	0.0276	0.0198	0.0254
PyDelt LOWESS	0.0297	0.0283	0.0207	0.0262
PyDelt FDA	0.0159	0.0147	0.0091	0.0132
SciPy Spline	0.0162	0.0151	0.0094	0.0136
NumDiffTools	0.0412	0.0397	0.0312	0.0374
FinDiff	0.0423	0.0408	0.0327	0.0386
JAX	0.0001	0.0001	0.0001	0.0001

III. Results and Discussion

A. Univariate Differentiation Performance

1) First-Order Derivatives: Table I shows the mean absolute error (MAE) for first-order derivatives across different test functions with no added noise.

The PyDelt GLLA interpolator consistently achieves the highest accuracy among traditional numerical methods, with an average MAE approximately 40% lower than SciPy's spline methods and 85% lower than finite difference methods.

2) Second-Order Derivatives: For second-order derivatives, PyDelt's Spline and FDA interpolators show slightly better performance than GLLA, likely due to their analytical computation of higher-order derivatives.

3) Noise Robustness: To evaluate noise robustness, we added Gaussian noise with standard deviation equal to 5% of the signal's standard deviation and computed the relative increase in error.

LOWESS and LOESS interpolators demonstrate exceptional robustness to noise, with the smallest increase in error. Neural network methods show the best overall noise robustness, though at a higher computational cost.

B. Multivariate Differentiation Performance

1) Gradient Computation: PyDelt's multivariate derivatives show significantly better accuracy than NumDiffTools, especially with noisy data. The LOESS and LOWESS variants demonstrate the best noise robustness for gradient computation.

TABLE III
ERROR INCREASE FACTOR WITH 5% NOISE (FIRST DERIVATIVES)

Method	Sine	Exponential	Polynomial	Average
PyDelt GLLA	2.7×	2.9×	3.1×	2.9×
PyDelt LLA	2.9×	3.2×	3.4×	3.2×
PyDelt Spline	4.8×	5.2×	5.7×	5.2×
PyDelt LOESS	1.9×	2.1×	2.3×	2.1×
PyDelt LOWESS	1.8×	2.0×	2.2×	2.0×
PyDelt FDA	4.5×	4.9×	5.3×	4.9×
SciPy Spline	5.1×	5.6×	6.2×	5.6×
NumDiffTools	8.7×	9.3×	10.1×	9.4×
FinDiff	8.9×	9.6×	10.4×	9.6×
PyDelt NN	1.5×	1.7×	1.9×	1.7×

TABLE IV
MEAN EUCLIDEAN ERROR FOR GRADIENT COMPUTATION

Method	No Noise	5% Noise	10% Noise
PyDelt MV Spline	0.0143	0.0731	0.1482
PyDelt MV LLA	0.0167	0.0512	0.1037
PyDelt MV GLLA	0.0152	0.0487	0.0993
PyDelt MV LOWESS	0.0218	0.0437	0.0876
PyDelt MV LOESS	0.0212	0.0428	0.0862
PyDelt MV FDA	0.0147	0.0724	0.1471
NumDiffTools MV	0.0376	0.3517	0.7128
JAX MV	0.0001	N/A	N/A

TABLE V
FROBENIUS NORM ERROR FOR JACOBIAN COMPUTATION

Method	No Noise	5% Noise
PyDelt MV Spline	0.0187	0.0953
PyDelt MV LLA	0.0213	0.0687
PyDelt MV GLLA	0.0196	0.0631
PyDelt MV LOWESS	0.0278	0.0567
PyDelt MV LOESS	0.0271	0.0554
PyDelt MV FDA	0.0192	0.0941
JAX MV	0.0001	N/A

TABLE VI
AVERAGE COMPUTATION TIME (MILLISECONDS)

Method	Fit Time	Evaluation Time	Total Time
PyDelt GLLA	1.24	0.31	1.55
PyDelt LLA	0.87	0.26	1.13
PyDelt Spline	0.93	0.18	1.11
PyDelt LOESS	3.76	0.42	4.18
PyDelt LOWESS	2.83	0.39	3.22
PyDelt FDA	1.02	0.21	1.23
SciPy Spline	0.78	0.15	0.93
NumDiffTools	N/A	0.67	0.67
FinDiff	N/A	0.53	0.53
PyDelt NN TF	2743.21	1.87	2745.08
PyDelt NN PT	2156.43	1.52	2157.95
JAX	N/A	0.89	0.89

2) Jacobian Computation: For vector-valued functions, we evaluated the Frobenius norm of the error in the Jacobian matrix:

C. Computational Efficiency

The traditional interpolation methods in PyDelt show competitive performance with SciPy and finite difference methods. Neural network methods have significantly higher training (fit) times but reasonable evaluation times once trained.

D. Feature Comparison

PyDelt offers the most comprehensive feature set, with particular strengths in noise robustness, multivariate derivatives, and its universal API that allows seamless switching between methods.

IV. Recommendations

A. Method Selection Guidelines

Based on our comprehensive analysis, we provide the following recommendations for method selection:

B. Parameter Tuning Guidelines

For optimal performance, we recommend the following parameter settings:

PyDelt GLLA:

- Low noise: `embedding=3, n=2`
- Medium noise: `embedding=4, n=2`
- High noise: `embedding=5, n=3`

PyDelt LOESS/LOWESS:

- Low noise: `frac=0.2` (LOESS) / default (LOWESS)
- Medium noise: `frac=0.3` (LOESS) / default (LOWESS)
- High noise: `frac=0.5` (LOESS) / default (LOWESS)

PyDelt Spline:

- Low noise: `smoothing=0.01`
- Medium noise: `smoothing=0.1`
- High noise: `smoothing=0.5`

PyDelt Neural Network:

- Low noise: `hidden_layers=[32, 16], epochs=200`
- Medium noise: `hidden_layers=[64, 32], epochs=500`
- High noise: `hidden_layers=[128, 64, 32], epochs=1000`

V. Areas for Continued Development

Despite the strong performance of PyDelt's methods, several areas warrant further development:

A. Mixed Partial Derivatives

The current implementation of PyDelt's multivariate derivatives approximates mixed partial derivatives as zero for traditional interpolation methods. This limitation arises from the separable nature of the interpolation approach. Future work should focus on:

1) **Enhanced Mixed Partials**: Developing specialized interpolation schemes that can accurately capture mixed partial derivatives.
2) **Hybrid Approaches**: Combining traditional interpolation with neural network methods to balance accuracy and computational efficiency.
3) **Tensor Product Interpolation**: Implementing true multivariate interpolation using tensor product bases.

B. Performance Optimization

While PyDelt's methods are competitive in terms of computational efficiency, several optimizations could further improve performance:

1) **GPU Acceleration**: Implementing GPU support for traditional interpolation methods to handle large datasets.
2) **Parallel Processing**: Adding multi-core support for fitting multiple interpolators simultaneously.
3) **Just-in-Time Compilation**: Integrating Numba or JAX for accelerated numerical computations.
4) **Adaptive Method Selection**: Developing an intelligent system to automatically select the optimal differentiation method based on data characteristics.

C. Higher-Order Tensor Derivatives

Extending PyDelt to support higher-order tensor derivatives would benefit applications in continuum mechanics, fluid dynamics, and quantum physics:

1) **Tensor Calculus Operations**: Implementing divergence, curl, and other tensor operations.
2) **Coordinate System Support**: Adding support for different coordinate systems (spherical, cylindrical).
3) **Differential Operators**: Implementing Laplacian, Hessian, and other differential operators for tensor fields.

D. Uncertainty Quantification

Incorporating uncertainty estimates in derivative calculations would provide valuable information for scientific applications:

1) **Confidence Intervals**: Computing confidence intervals for derivative estimates.
2) **Bayesian Methods**: Implementing Bayesian approaches to derivative estimation.
3) **Ensemble Methods**: Combining multiple differentiation methods to improve robustness and quantify uncertainty.

E. Integration with Differential Equation Solvers

Tighter integration with differential equation solvers would enhance PyDelt's utility in scientific computing:

1) **ODE/PDE Solvers**: Developing specialized solvers that leverage PyDelt's accurate derivatives.
2) **Variational Methods**: Implementing variational approaches for solving differential equations.
3) **Physics-Informed Neural Networks**: Integrating with physics-informed neural networks for solving complex PDEs.

TABLE VII
FEATURE COMPARISON OF DIFFERENTIATION METHODS

Feature	PyDelt Interpolators	PyDelt Neural Network	SciPy	NumDiffTools	FinDiff	JAX
Univariate Derivatives	✓✓✓	✓✓✓	✓✓	✓✓	✓✓	✓✓✓
Multivariate Derivatives	✓✓✓	✓✓✓	✓	✓✓	✓✓	✓✓✓
Higher-Order Derivatives	✓✓(up to 3rd)	✓✓✓(unlimited)	✓✓(up to 3rd)	✓✓	✓✓	✓✓✓
Mixed Partial Derivatives	✓(approximated)	✓✓✓(exact)	✓	✓✓	✓✓	✓✓✓
Noise Robustness	✓✓✓	✓✓✓	✓	✓	✓	N/A
Arbitrary Evaluation Points	✓✓✓	✓✓✓	✓✓✓	✓	✓	✓✓✓
GPU Acceleration	×	✓✓✓	×	×	×	✓✓✓
Memory Efficiency	✓✓	✓	✓✓	✓✓✓	✓✓✓	✓
Requires Analytical Function	×	×	×	×	×	✓
Universal API	✓✓✓	✓✓✓	✓	✓✓	✓✓	✓✓

Legend: ✓✓✓Excellent, ✓✓Good, ✓Basic, × Not supported

TABLE VIII
METHOD SELECTION GUIDELINES

Scenario	Recommended Method	Alternative
General-purpose	PyDelt GLLA	PyDelt Spline
Noisy data	PyDelt LOWESS/LOESS	PyDelt Neural Network
High-dimensional data (¿3D)	PyDelt MV with GLLA	Neural Network
Performance-critical	PyDelt LLA	FinDiff
Exact mixed partials	PyDelt Neural Network	JAX (if analytical)
Higher-order derivatives (¿2)	PyDelt Spline/FDA	PyDelt Neural Network
Real-time applications	PyDelt LLA (pre-fit)	FinDiff
Extremely noisy data	PyDelt Neural Network	PyDelt LOWESS

VI. CONCLUSION

Our comprehensive analysis demonstrates that PyDelt provides state-of-the-art numerical differentiation methods that outperform traditional approaches in terms of accuracy, noise robustness, and flexibility. The library's universal differentiation interface allows seamless switching between methods, enabling users to select the most appropriate approach for their specific application.

The key strengths of PyDelt include:

1) **Superior Accuracy**: PyDelt's GLLA interpolator consistently achieves the highest accuracy among traditional numerical methods.
2) **Exceptional Noise Robustness**: LOWESS, LOESS, and neural network methods demonstrate remarkable resilience to noise.
3) **Comprehensive Feature Set**: Support for univariate and multivariate functions, higher-order derivatives, and arbitrary evaluation points.
4) **Universal API**: Consistent interface across all methods, facilitating method comparison and selection.

By addressing the identified areas for continued development, PyDelt can further solidify its position as the leading library for numerical differentiation in Python, serving a wide range of scientific and engineering applications.

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