

PyDelt: Advanced Numerical Function Approximation and Differentiation for Dynamical Systems

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Abstract—Numerical differentiation from noisy data represents one of the fundamental challenges in computational science—a challenge that has grown increasingly critical as we seek to understand complex systems ranging from classical physics to modern epidemiological networks. This paper presents PyDelt, a comprehensive software library that transforms the poorly conditioned problem of numerical differentiation into a tractable computational task through advanced interpolation methods, multivariate calculus operations, and noise-resistant algorithms. We trace the development of PyDelt from its theoretical foundations to its practical implementation, demonstrating how it addresses long-standing challenges in derivative estimation. Through rigorous evaluation on both traditional test functions and real-world complex adaptive systems (CAS) applications—including epidemiological monitoring, financial contagion analysis, ecological stability assessment, and control optimization—we show that PyDelt achieves superior performance: GLLA and GOLD methods reduce errors by 40% for clean data, while LOWESS/LOESS methods show only 2× error increase with 5% noise (vs. 9-10× for finite differences). This combination of theoretical rigor and practical effectiveness makes PyDelt suitable for both classical dynamics and the inherently noisy, high-dimensional data characteristic of modern complex systems.

Index Terms—numerical differentiation, dynamical systems, complex adaptive systems, interpolation, noise robustness, multivariate calculus, network dynamics, stability analysis

1 INTRODUCTION

1.1 Motivation: The Ubiquitous Challenge of Numerical Differentiation

The ability to compute derivatives from empirical data lies at the heart of scientific discovery and engineering innovation. From Newton’s laws of motion to modern machine learning, derivatives provide the mathematical language for describing change, optimization, and dynamics. Yet despite centuries of mathematical development, a fundamental challenge persists: given noisy data points (x_i, y_i) where $y_i = f(x_i) + \epsilon_i$, how can we accurately and reliably estimate derivatives $f'(x)$, $\nabla f(\mathbf{x})$, or $\mathbf{J}_f(\mathbf{x})$?

This question is not merely academic—it arises daily in laboratories, hospitals, financial institutions, and research centers worldwide. Whether analyzing experimental measurements in physics, sensor data in engineering, financial time series, or epidemiological observations, scientists and engineers face the same core problem: extracting reliable

derivative information from noisy, discrete observations of continuous phenomena.

This challenge is particularly acute in two complementary domains:

1.1.1 Traditional Dynamical Systems

In classical physics and engineering, we often know the analytical form of governing equations but need numerical derivatives for:

- **Experimental Validation:** Comparing theoretical predictions with noisy measurements
- **Parameter Estimation:** Fitting models to observed trajectories
- **Control Design:** Computing feedback gains from system responses
- **Sensitivity Analysis:** Understanding how perturbations affect system behavior

1.1.2 Complex Adaptive Systems

In emerging CAS applications—epidemiological networks, financial markets, ecological systems, social dynamics—the governing equations are often unknown and must be inferred from data:

- **Early Warning Signals:** Detecting approaching tipping points via gradient changes
- **Influence Networks:** Identifying interaction strengths through Jacobian analysis
- **Stability Assessment:** Evaluating system resilience via Hessian eigenvalues
- **Adaptive Control:** Steering systems toward desired states using gradient-based methods

Both domains share a common mathematical challenge: extracting reliable derivative information from noisy, potentially high-dimensional observations where $\mathbf{y}_i = \mathbf{f}(\mathbf{x}_i) + \epsilon_i$.

1.2 The Poorly Conditioned Nature of Numerical Differentiation

The fundamental difficulty stems from the poorly conditioned nature of differentiation. For a linear operator L mapping functions to their derivatives, the condition number κ can be expressed as:

$$\kappa(L) = \sup_{f \neq 0} \frac{\|Lf\|}{\|f\|} \cdot \sup_{g \neq 0} \frac{\|L^{-1}g\|}{\|g\|} \quad (1)$$

where $\|\cdot\|$ denotes a suitable function norm, \sup represents the supremum (least upper bound), and L^{-1} is the inverse operator (integration). For differentiation operators, this condition number is unbounded, explaining why small noise in data can lead to arbitrarily large errors in derivative estimates. This affects both traditional and CAS applications, though the challenges manifest differently:

Traditional Systems: Known equations, moderate noise, need for high accuracy

Complex Adaptive Systems: Unknown dynamics, high noise, high dimensionality, critical transitions

As noted by van Breugel et al. [6], “Even with noise of moderate amplitude, a naïve application of finite differences produces derivative estimates that are far too noisy to be useful.”

Existing methods for addressing this challenge include:

- 1) **Simple Divided Differences:** Methods like forward, backward, and central differences that approximate derivatives using nearby points. For a function $f(x)$ sampled at points x_i , these methods compute derivatives as:

$$\text{Forward difference: } f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \quad (2)$$

$$\text{Backward difference: } f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \quad (3)$$

$$\text{Central difference: } f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} \quad (4)$$

While computationally efficient, these methods amplify noise significantly [7]. For data with noise variance σ^2 , the variance of the derivative estimate using central differences is approximately $\frac{2\sigma^2}{(\Delta x)^2}$, demonstrating how noise is amplified by a factor inversely proportional to the square of the step size.

- 2) **Smoothing Followed by Differentiation:** Applying filters (e.g., Butterworth, Gaussian) to smooth data before differentiation. For a Gaussian filter with standard deviation σ_g , the smoothed function \tilde{f} is given by the convolution:

$$\tilde{f}(x) = (f * g)(x) = \int_{-\infty}^{\infty} f(t) \cdot g(x - t) dt \quad (5)$$

where $g(x) = \frac{1}{\sigma_g \sqrt{2\pi}} e^{-\frac{x^2}{2\sigma_g^2}}$ is the Gaussian kernel, σ_g controls the smoothing bandwidth, and $*$ denotes the convolution operator. This approach often attenuates important features along with noise [8].

- 3) **Polynomial Fitting:** Fitting polynomials locally (e.g., Savitzky-Golay filters) or globally to data before differentiation. For a local polynomial of degree

d fit to a window of $2w + 1$ points centered at x_i , the model is:

$$\hat{f}(x) = \sum_{j=0}^d a_j (x - x_i)^j \quad (6)$$

where a_j are polynomial coefficients, w is the window half-width, and the coefficients are determined by minimizing $\sum_{k=-w}^w (f(x_{i+k}) - \hat{f}(x_{i+k}))^2$. The derivative is then $\hat{f}'(x) = \sum_{j=1}^d j \cdot a_j (x - x_i)^{j-1}$. These methods struggle with the appropriate selection of window size w and polynomial order d [1].

- 4) **Spline Interpolation:** Using various spline functions to interpolate data before differentiation. A cubic spline $S(x)$ consists of piecewise cubic polynomials with continuous first and second derivatives:

$$S(x) = \begin{cases} S_1(x) & x_1 \leq x < x_2 \\ S_2(x) & x_2 \leq x < x_3 \\ \vdots & \vdots \\ S_{n-1}(x) & x_{n-1} \leq x \leq x_n \end{cases} \quad (7)$$

where each $S_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$ is a cubic polynomial on interval $[x_i, x_{i+1}]$, and a_i, b_i, c_i, d_i are coefficients determined by continuity constraints. While more robust than simple differences, traditional spline methods still require careful parameter tuning [3].

- 5) **Regularization Approaches:** Methods like Total Variation Regularization that formulate differentiation as an optimization problem with smoothness constraints. These approaches minimize functionals of the form:

$$J[f] = \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda \int |f''(x)|^p dx \quad (8)$$

where $J[f]$ is the objective functional, $\lambda > 0$ is the regularization parameter controlling the trade-off between data fidelity (first term) and smoothness (second term), and p determines the type of regularization ($p = 2$ for Tikhonov, $p = 1$ for total variation). These approaches often involve complex parameter selection [9].

All these methods face a fundamental trade-off between faithfulness to the data and smoothness of the derivative estimate. This trade-off can be formalized through the bias-variance decomposition of the mean squared error (MSE):

$$\text{MSE}[\hat{f}'] = \text{Bias}[\hat{f}']^2 + \text{Var}[\hat{f}'] \quad (9)$$

where $\text{Bias}[\hat{f}']$ represents the systematic error (deviation from the true derivative) and $\text{Var}[\hat{f}']$ represents the variance (sensitivity to noise). As smoothing increases, bias typically increases (the estimate deviates more from the true derivative) while variance decreases (the estimate becomes less sensitive to noise). As highlighted in mathematical literature, this trade-off creates a poorly conditioned problem where no single parameter choice minimizes both noise sensitivity and bias [10].

1.3 The PyDelt Solution: From Theory to Practice

PyDelt was developed to bridge the gap between theoretical understanding and practical application of numerical differentiation. Rather than offering a single "best" method, PyDelt provides a unified framework that recognizes a fundamental truth: different problems require different solutions. The library's development philosophy centers on three key principles:

1. Theoretical Rigor: Every method in PyDelt is grounded in solid mathematical foundations, with clear error bounds and complexity analyses.

2. Practical Flexibility: A universal API allows seamless switching between methods, enabling users to find the optimal approach for their specific problem.

3. Comprehensive Coverage: From univariate derivatives to tensor calculus, from deterministic to stochastic systems, PyDelt provides the tools needed for modern scientific computing.

The library implements a comprehensive suite of methods, each designed to excel in specific scenarios:

- **Spline interpolation:** Enhanced with adaptive smoothing parameters. The smoothing spline $S(x)$ minimizes:

$$E[S] = \sum_{i=1}^n (y_i - S(x_i))^2 + \lambda \int_{x_1}^{x_n} |S''(t)|^2 dt \quad (10)$$

where $E[S]$ is the energy functional, y_i are observed data values, $S(x_i)$ are spline values at data points, $\lambda \geq 0$ is the smoothing parameter (automatically selected using generalized cross-validation), and the integral penalizes curvature.

- **Local Linear Approximation (LLA):** Robust sliding-window approach for noisy data. For each point x_i , LLA fits a local model:

$$f(x) \approx a_i + b_i(x - x_i) \quad (11)$$

where a_i is the local intercept and b_i is the local slope, determined using weighted least squares within a window of size w . The derivative estimate is then $f'(x_i) = b_i$.

- **Generalized Local Linear Approximation (GLLA):** Higher-order local approximations using an embedding dimension m and derivative order n . GLLA fits local models of the form:

$$f(x) \approx \sum_{j=0}^m a_{i,j} (x - x_i)^j \quad (12)$$

where m is the polynomial degree (embedding dimension), $a_{i,j}$ are local polynomial coefficients, and derivatives are computed as $f^{(n)}(x_i) = n! \cdot a_{i,n}$ where $n!$ is the factorial.

- **Generalized Orthogonal Local Derivative (GOLD):** Orthogonalization-based approach for improved numerical stability. GOLD uses Hermite polynomials $H_j(x)$ for the local basis:

$$f(x) \approx \sum_{j=0}^m c_{i,j} H_j \left(\frac{x - x_i}{h} \right) \quad (13)$$

where H_j are Hermite polynomials of order j , $c_{i,j}$ are expansion coefficients, $h > 0$ is a scale parameter, and the orthogonality of Hermite polynomials improves numerical stability.

- **Locally Weighted Scatterplot Smoothing (LOWESS):** Non-parametric methods resistant to outliers. LOWESS assigns weights to points based on their distance from the evaluation point:

$$w_j(x) = W \left(\frac{|x_j - x|}{d(x)} \right) \quad (14)$$

where $w_j(x)$ is the weight for point x_j when evaluating at x , W is a weight function (typically tri-cubic), $d(x)$ is the distance to the q -th nearest neighbor of x , with $q = \lfloor f \cdot n \rfloor$ where $f \in (0, 1]$ is the smoothing parameter (fraction of points used) and $\lfloor \cdot \rfloor$ is the floor function.

- **Local Regression (LOESS):** Adaptive local polynomial fitting with robust weight functions that reduce the influence of outliers:

$$\hat{f}(x) = \arg \min_{g \in \mathcal{P}_d} \sum_{i=1}^n w_i(x) \rho(y_i - g(x_i)) \quad (15)$$

where $\hat{f}(x)$ is the estimated function value, $\arg \min$ denotes the minimizing argument, \mathcal{P}_d is the space of polynomials of degree d , $w_i(x)$ are distance-based weights, and ρ is a robust loss function (e.g., bisquare).

- **Functional Data Analysis (FDA):** Sophisticated smoothing with optimal parameter selection using basis function expansions:

$$f(x) \approx \sum_{k=1}^K c_k \phi_k(x) \quad (16)$$

where K is the number of basis functions, $\phi_k(x)$ are basis functions (typically B-splines), and coefficients c_k are determined by penalized least squares.

- **Neural network-based methods:** Deep learning with automatic differentiation for complex patterns. A neural network model $f_\theta(x)$ is trained to minimize:

$$L(\theta) = \sum_{i=1}^n (f_\theta(x_i) - y_i)^2 + \lambda R(\theta) \quad (17)$$

where $L(\theta)$ is the loss function, θ represents network parameters (weights and biases), $f_\theta(x_i)$ is the network output at x_i , $\lambda \geq 0$ is the regularization strength, and $R(\theta)$ is a regularization term (e.g., L_2 norm). Derivatives are then computed using automatic differentiation: $f'_\theta(x) = \frac{\partial f_\theta(x)}{\partial x}$.

1.4 Development Journey: Building a Unified Framework

The development of PyDelt was motivated by a simple observation: while numerous numerical differentiation methods exist in the literature, practitioners often struggle to select and implement the right approach for their specific problem. Existing tools either provide limited method

choices, lack theoretical guidance, or fail to handle the diverse requirements of modern applications.

PyDelt's development addressed these gaps through systematic innovation:

- 1) **Method Integration:** We implemented and optimized eight distinct interpolation approaches, from classical splines to modern neural networks, each with carefully tuned parameters and error handling.
- 2) **Universal Interface:** The `.fit().differentiate()` API pattern provides consistency across all methods, enabling fair comparison and easy method switching.
- 3) **Multivariate Extensions:** We extended univariate methods to handle gradients, Jacobians, Hessians, and Laplacians, enabling applications in high-dimensional spaces.
- 4) **Advanced Features:** Tensor calculus operations and stochastic derivatives were added to support specialized applications in continuum mechanics and financial mathematics.
- 5) **Rigorous Validation:** Comprehensive testing against analytical solutions and comparison with established libraries ensures reliability.

The result is a library that achieves what seemed contradictory: superior accuracy (40% error reduction vs. traditional methods), exceptional noise robustness (2× vs. 9-10× error increase), comprehensive functionality (univariate to tensor calculus), and computational efficiency (millisecond-scale evaluation times).

PyDelt builds upon the multi-objective optimization framework of van Breugel et al. [6], extending it with new methods, multivariate support, and a production-ready implementation suitable for both classical dynamical systems and emerging complex adaptive systems applications.

2 METHODOLOGY: FROM CONCEPT TO IMPLEMENTATION

2.1 Mathematical Foundations: The Core Innovation

2.1.1 Interpolation-Based Differentiation Framework

The central insight driving PyDelt's design is deceptively simple yet profoundly powerful: transform the poorly conditioned problem of numerical differentiation into a well-conditioned interpolation problem. This paradigm shift can be understood through a two-step process:

- 1) **Reconstruction:** Given noisy data points (x_i, y_i) where $y_i = f(x_i) + \epsilon_i$, construct an interpolant \hat{f} that approximates the underlying function f while filtering noise.
- 2) **Differentiation:** Analytically differentiate the smooth interpolant to obtain the derivative estimate: $\hat{f}'(x) = \frac{d\hat{f}(x)}{dx}$.

This approach fundamentally reframes the problem: instead of directly differentiating noisy data (which amplifies noise catastrophically), we first reconstruct a smooth representation of the underlying function, then differentiate that smooth representation analytically. The quality of the

derivative estimate depends critically on how well the interpolant balances two competing objectives: fidelity to the observed data and smoothness of the resulting function.

This interpolation-first philosophy distinguishes PyDelt from traditional finite difference methods and forms the theoretical foundation for all methods in the library.

2.2 Validation Strategy: Bridging Theory and Practice

To demonstrate PyDelt's effectiveness across diverse applications, we designed a comprehensive validation strategy that spans from idealized test cases to realistic complex systems. This dual approach ensures both theoretical soundness and practical utility:

2.2.1 Traditional Test Functions

Standard benchmark functions for validating numerical accuracy:

- **Sine function:** $f(x) = \sin(x)$ with analytical derivatives $f'(x) = \cos(x)$, $f''(x) = -\sin(x)$
- **Exponential function:** $f(x) = e^x$ with analytical derivatives $f^{(n)}(x) = e^x$ for all orders n
- **Polynomial function:** $f(x) = x^3 - 2x^2 + 3x - 1$ with analytical derivatives $f'(x) = 3x^2 - 4x + 3$, $f''(x) = 6x - 4$
- **Multivariate scalar function:** $f(x, y) = \sin(x) + \cos(y)$ with gradient $\nabla f(x, y) = [\cos(x), -\sin(y)]$
- **Multivariate vector function:** $f(x, y) = [\sin(x) \cos(y), x^2 + y^2]$ with Jacobian $J_f(x, y) = \begin{bmatrix} \cos(x) \cos(y) & -\sin(x) \sin(y) \\ 2x & 2y \end{bmatrix}$

2.2.2 Real-World Applications: Complex Adaptive Systems

Beyond traditional validation, PyDelt's true value emerges in modern complex adaptive systems where derivatives reveal hidden structure in noisy, high-dimensional data. We demonstrate PyDelt's capabilities across four critical application domains:

2.2.3 Epidemiological Network Monitoring

For disease spread dynamics, we observe infection counts $I(\mathbf{x}, t)$ as functions of spatial location \mathbf{x} and time t . PyDelt computes:

- **Spatial Gradient:** $\nabla_{\mathbf{x}} I$ reveals spread direction and velocity
- **Laplacian:** $\nabla^2 I$ measures diffusion rate and identifies outbreak centers
- **Temporal Derivative:** $\frac{\partial I}{\partial t}$ tracks acceleration of spread

2.2.4 Financial Contagion Analysis

For systemic risk in financial networks, asset returns $\mathbf{r}(t)$ and portfolio values $V(\mathbf{r})$ require:

- **Jacobian Matrix:** $\mathbf{J}_{ij} = \frac{\partial r_i}{\partial r_j}$ constructs the contagion network
- **Gradient:** ∇V identifies portfolio sensitivities for risk management
- **Hessian Eigenvalues:** Detect instabilities and approaching market crashes

2.2.5 Ecological Stability Assessment

For predator-prey and ecosystem dynamics with populations $\mathbf{N}(t)$:

- **Jacobian at Equilibrium:** $\mathbf{J}(\mathbf{N}^*)$ determines stability via eigenvalue analysis
- **Gradient Flow:** $\nabla F(\mathbf{N})$ reveals attractors and repellors
- **Bifurcation Detection:** Hessian singularities signal regime shifts

2.3 Mathematical Framework for CAS

2.3.1 Unknown Function Approximation

Unlike traditional applications where analytical forms are known, CAS require inferring dynamics purely from data. Given noisy observations $(\mathbf{x}_i, \mathbf{y}_i)$ where $\mathbf{y}_i = \mathbf{f}(\mathbf{x}_i) + \epsilon_i$:

- 1) **Function Reconstruction:** Construct interpolant $\hat{\mathbf{f}}$ that approximates unknown dynamics \mathbf{f}
- 2) **Derivative Extraction:** Compute $\nabla \hat{\mathbf{f}}, \mathbf{J}_{\hat{\mathbf{f}}}, \mathbf{H}_{\hat{\mathbf{f}}}$ analytically or numerically
- 3) **Uncertainty Quantification:** Assess confidence in derivatives based on data density and noise levels

This approach is essential for CAS where governing equations are unknown and must be learned from observations.

2.3.2 Universal Differentiation Interface

PyDelt implements a consistent mathematical framework across all interpolation methods through its universal differentiation interface. For any interpolator I fitted to data (x_i, y_i) , the derivative of order n at point x is computed as:

$$D^n[I](x) = \frac{d^n I(x)}{dx^n} \quad (18)$$

where $D^n[I]$ denotes the n -th order derivative operator applied to interpolator I , and $n \in \mathbb{N}$ is the derivative order. This operation is implemented through the `differentiate(order=n)` method, which returns a callable function that can be evaluated at arbitrary points. For multivariate functions, partial derivatives with respect to specific input dimensions can be computed using a mask parameter:

$$D_{\mathbf{m}}^n[I](\mathbf{x}) = \frac{\partial^n I(\mathbf{x})}{\partial x_{m_1} \partial x_{m_2} \cdots \partial x_{m_n}} \quad (19)$$

where $\mathbf{m} = [m_1, m_2, \dots, m_n]$ specifies the input dimensions for differentiation, and $\mathbf{x} \in \mathbb{R}^d$ is the evaluation point in d -dimensional space.

2.4 CAS-Inspired Test Cases

We evaluated PyDelt's performance on functions representative of CAS dynamics:

2.4.1 Epidemic Spread Model

Spatial SIR dynamics: $I(x, y, t) = I_0 e^{-\frac{(x-vt)^2 + y^2}{2\sigma^2}}$ modeling disease diffusion with:

- Gradient ∇I for spread direction
- Laplacian $\nabla^2 I$ for diffusion rate
- Temporal derivative $\frac{\partial I}{\partial t}$ for acceleration

2.4.2 Financial Contagion Network

Asset correlation dynamics: $\mathbf{r}(t) = \mathbf{A}(t)\mathbf{r}(t-1) + \boldsymbol{\eta}(t)$ with time-varying influence matrix $\mathbf{A}(t)$:

- Jacobian $\mathbf{J} = \frac{\partial \mathbf{r}_t}{\partial \mathbf{r}_{t-1}}$ reveals contagion pathways
- Eigenvalues of \mathbf{J} determine stability

2.4.3 Ecosystem Dynamics

Lotka-Volterra with spatial variation: $\frac{dN}{dt} = f(N, P, x, y)$ for prey N and predator P :

- Jacobian at equilibrium for stability analysis
- Hessian for bifurcation detection
- Gradient for optimal harvesting control

2.4.4 Social Network Opinion Dynamics

Opinion evolution: $\mathbf{o}(t+1) = \mathbf{W}\mathbf{o}(t) + \boldsymbol{\xi}(t)$ with influence weights \mathbf{W} :

- Gradient flow toward consensus states
- Jacobian for influence network construction

These CAS-inspired test cases include realistic noise levels (5-20%), irregular sampling, and high dimensionality characteristic of real-world complex systems.

2.5 Evaluation Metrics

We assessed the performance using a comprehensive set of metrics designed to evaluate different aspects of numerical differentiation quality:

- 1) **Accuracy:** We quantified accuracy using both point-wise and aggregate error metrics:

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |\hat{f}'(x_i) - f'(x_i)| \quad (20)$$

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (\hat{f}'(x_i) - f'(x_i))^2} \quad (21)$$

$$\text{Max Error} = \max_{i=1, \dots, n} |\hat{f}'(x_i) - f'(x_i)| \quad (22)$$

where $\hat{f}'(x_i)$ is the estimated derivative and $f'(x_i)$ is the true analytical derivative.

- 2) **Noise Robustness:** We evaluated robustness by adding Gaussian noise with standard deviation $\sigma = \alpha \cdot \sigma_f$, where σ_f is the standard deviation of the function values and $\alpha \in \{0.01, 0.05, 0.1\}$ represents noise levels of 1%, 5%, and 10%. The robustness ratio is defined as:

$$R(\alpha) = \frac{\text{MAE}_{\text{with noise } \alpha}}{\text{MAE}_{\text{without noise}}} \quad (23)$$

where $R(\alpha)$ is the error amplification factor at noise level α , and MAE denotes mean absolute error. Lower values of $R(\alpha)$ indicate better noise robustness.

- 3) **Computational Efficiency:** We measured both fitting time T_{fit} and evaluation time T_{eval} separately, as well as the total computation time $T_{\text{total}} = T_{\text{fit}} + T_{\text{eval}}$.

For real-time applications, T_{eval} is often more critical, while for batch processing, T_{total} is the relevant metric.

- 4) **Dimensionality Handling:** For multivariate functions, we evaluated gradient accuracy using the Euclidean norm error:

$$E_{\nabla f}(\mathbf{x}) = \|\hat{\nabla} f(\mathbf{x}) - \nabla f(\mathbf{x})\|_2 \quad (24)$$

where $E_{\nabla f}$ is the gradient error, $\hat{\nabla} f$ is the estimated gradient, ∇f is the true gradient, and $\|\cdot\|_2$ denotes the Euclidean (L2) norm. We also evaluated Jacobian accuracy using the Frobenius norm error:

$$E_{J_f}(\mathbf{x}) = \|\hat{J}_f(\mathbf{x}) - J_f(\mathbf{x})\|_F = \sqrt{\sum_{i,j} |\hat{J}_{ij}(\mathbf{x}) - J_{ij}(\mathbf{x})|^2} \quad (25)$$

where E_{J_f} is the Jacobian error, \hat{J}_f is the estimated Jacobian matrix, J_f is the true Jacobian, $\|\cdot\|_F$ denotes the Frobenius norm, and the sum is over all matrix elements i, j .

We also assessed the ability to compute higher-order derivatives by comparing the Hessian matrices using a similar Frobenius norm metric.

These metrics provide a comprehensive evaluation framework that captures the multiple dimensions of performance relevant to numerical differentiation methods.

3 RESULTS: VALIDATING THE APPROACH

3.1 Univariate Performance: Accuracy Meets Robustness

Our comprehensive evaluation reveals that PyDelt's methods achieve a remarkable combination of accuracy and noise robustness that surpasses traditional approaches. These results validate the interpolation-based framework and demonstrate the practical value of method diversity.

3.1.1 Error Analysis for First-Order Derivatives

PyDelt's GLLA and GOLD interpolators consistently achieve 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. This superior performance can be attributed to their mathematical formulation, which balances local adaptivity with global smoothness constraints.

For the GLLA method, the error behavior can be characterized by the following bound: For a function $f \in C^{m+1}[a, b]$ with bounded $(m+1)$ -th derivative, the error in the first derivative estimate is:

$$|f'(x) - \hat{f}'(x)| \leq C \cdot h^m + K \cdot \frac{\sigma}{\sqrt{n}} \quad (26)$$

where $f'(x)$ is the true derivative, $\hat{f}'(x)$ is the estimated derivative, $C^{m+1}[a, b]$ denotes the space of $(m+1)$ -times continuously differentiable functions on interval $[a, b]$, $h > 0$ is the effective window size, $m \geq 1$ is the embedding dimension (polynomial degree), $\sigma \geq 0$ is the noise standard deviation, n is the number of points in the local window, and $C, K > 0$ are constants depending on the function's

smoothness properties. This bound illustrates the trade-off between approximation error (first term) and noise amplification (second term).

The GOLD method, which uses orthogonalization techniques based on Hermite polynomials, shows particularly good stability for higher-order derivatives. Its error behavior benefits from the orthogonality properties of the basis functions, which reduce numerical instabilities in the coefficient estimation process.

For second-order derivatives, PyDelt's Spline and FDA interpolators show slightly better performance than GLLA in some test cases. This can be explained by their global optimization approach, which enforces continuity constraints across the entire domain rather than just locally.

3.1.2 Noise Robustness Analysis

LOWESS and LOESS interpolators demonstrate exceptional robustness to noise, with the smallest increase in error when noise is added. This robustness stems from their robust weighting schemes, which can be mathematically expressed as:

$$\hat{f}(x) = \arg \min_{g \in \mathcal{P}_d} \sum_{i=1}^n w_i(x) \rho \left(\frac{y_i - g(x_i)}{s} \right) \quad (27)$$

where $\hat{f}(x)$ is the estimated function value at x , $\arg \min$ denotes the minimizing argument, \mathcal{P}_d is the space of polynomials of degree d , $w_i(x)$ are distance-based weights, ρ is a robust loss function (typically bisquare: $\rho(u) = (1 - u^2)^2$ for $|u| < 1$ and 0 otherwise), $s > 0$ is a scale parameter estimated from the data, and y_i are observed values. This formulation effectively downweights outliers, making the derivative estimates more stable in the presence of noise.

Neural network methods show the best overall noise robustness, though at a higher computational cost. Their robustness can be attributed to the regularization techniques employed during training, which implicitly enforce smoothness constraints. For a neural network model $f_\theta(x)$ trained with L_2 regularization, the optimization problem becomes:

$$\min_{\theta} \sum_{i=1}^n (f_\theta(x_i) - y_i)^2 + \lambda \|\theta\|_2^2 \quad (28)$$

where \min_{θ} denotes minimization over network parameters θ , the first term is the data fidelity (mean squared error), $\lambda \geq 0$ is the regularization strength, and $\|\theta\|_2^2 = \sum_j \theta_j^2$ is the squared L2 norm of parameters. This regularization effectively constrains the complexity of the learned function, leading to smoother derivatives even when the training data contains noise.

3.1.3 Theoretical Error Decomposition

To better understand the performance differences between methods, we can decompose the mean squared error (MSE) of the derivative estimates into bias and variance components:

$$\text{MSE}[\hat{f}'] = \text{Bias}[\hat{f}']^2 + \text{Var}[\hat{f}'] \quad (29)$$

where $\text{MSE}[\hat{f}'] = \mathbb{E}[(\hat{f}' - f')^2]$ is the expected squared error, $\text{Bias}[\hat{f}'] = \mathbb{E}[\hat{f}'] - f'$ is the systematic error, $\text{Var}[\hat{f}'] =$

TABLE 1: 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 GOLD	0.0033	0.0030	0.0022	0.0028
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 2: Error Increase Factor with 5% Noise (First Derivatives)

Method	Sine	Exponential	Polynomial	Average
PyDelt GLLA	2.7×	2.9×	3.1×	2.9×
PyDelt GOLD	2.5×	2.7×	2.9×	2.7×
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×

$\mathbb{E}[(\hat{f}' - \mathbb{E}[\hat{f}'])^2]$ is the variance, and $\mathbb{E}[\cdot]$ denotes expectation. For methods with high smoothing (e.g., LOWESS with large span parameter), the bias term dominates as the estimate systematically deviates from the true derivative. For methods with minimal smoothing (e.g., finite differences), the variance term dominates due to noise amplification. PyDelt’s methods, particularly GLLA and GOLD, achieve a favorable balance between these components, explaining their superior overall performance.

3.2 Multivariate Performance: Scaling to High Dimensions

The true test of any numerical differentiation framework lies in its ability to handle multivariate functions—the domain where most real-world applications reside. PyDelt’s multivariate capabilities demonstrate that the interpolation-based approach scales effectively to high-dimensional problems.

3.2.1 Gradient Computation: Dimension-by-Dimension Excellence

PyDelt’s multivariate derivatives show significantly better accuracy than NumDiffTools, especially with noisy data. This improvement can be attributed to PyDelt’s approach of fitting separate univariate interpolators for each input dimension, which allows for adaptive smoothing based on the specific characteristics of each partial derivative.

For a scalar function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, PyDelt computes the gradient $\nabla f(\mathbf{x})$ by fitting n separate univariate interpolators I_j to the data projected along each input dimension j . The gradient is then constructed as:

$$\nabla f(\mathbf{x}) = \left[\frac{\partial f}{\partial x_1}(\mathbf{x}), \frac{\partial f}{\partial x_2}(\mathbf{x}), \dots, \frac{\partial f}{\partial x_n}(\mathbf{x}) \right]^T \quad (30)$$

where $\nabla f(\mathbf{x}) \in \mathbb{R}^n$ is the gradient vector, $\frac{\partial f}{\partial x_j}$ denotes the partial derivative with respect to the j -th input dimension, and $[\cdot]^T$ denotes the transpose operation.

where each partial derivative $\frac{\partial f}{\partial x_j}(\mathbf{x})$ is computed using the corresponding univariate interpolator I_j .

The LOESS and LOWESS variants demonstrate the best noise robustness for gradient computation. This can be understood through the lens of influence functions from robust statistics. For a point \mathbf{x} and a perturbation δ in the data, the influence function $IF(\mathbf{x}, \delta)$ measures the effect of this perturbation on the gradient estimate. For LOESS and LOWESS methods with robust weighting, this influence function is bounded:

$$\|IF(\mathbf{x}, \delta)\|_2 \leq M \quad (31)$$

where $IF(\mathbf{x}, \delta)$ is the influence function measuring sensitivity to data perturbations, δ represents a data perturbation (e.g., outlier), $M > 0$ is a finite constant, and $\|\cdot\|_2$ denotes the Euclidean norm. This bound holds for some constant M , regardless of the magnitude of δ . This bounded influence property ensures that outliers or noise in the data have limited effect on the gradient estimates.

3.2.2 Jacobian and Higher-Order Tensor Derivatives

For vector-valued functions $\mathbf{f} : \mathbb{R}^n \rightarrow \mathbb{R}^m$, PyDelt computes the Jacobian matrix $\mathbf{J}_f(\mathbf{x})$ by fitting $m \times n$ separate univariate interpolators, one for each output-input dimension pair. The Jacobian is constructed as:

$$\mathbf{J}_f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1}(\mathbf{x}) & \frac{\partial f_1}{\partial x_2}(\mathbf{x}) & \cdots & \frac{\partial f_1}{\partial x_n}(\mathbf{x}) \\ \frac{\partial f_2}{\partial x_1}(\mathbf{x}) & \frac{\partial f_2}{\partial x_2}(\mathbf{x}) & \cdots & \frac{\partial f_2}{\partial x_n}(\mathbf{x}) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(\mathbf{x}) & \frac{\partial f_m}{\partial x_2}(\mathbf{x}) & \cdots & \frac{\partial f_m}{\partial x_n}(\mathbf{x}) \end{bmatrix} \quad (32)$$

where $\mathbf{J}_f(\mathbf{x}) \in \mathbb{R}^{m \times n}$ is the Jacobian matrix, f_i denotes the i -th output component of \mathbf{f} , and $\frac{\partial f_i}{\partial x_j}$ is the partial derivative of the i -th output with respect to the j -th input.

PyDelt’s Jacobian computation shows good accuracy compared to analytical solutions, with GLLA and LOESS methods providing the best balance of accuracy and noise robustness. The error in the Jacobian estimate can be bounded as:

$$\|\mathbf{J}_f(\mathbf{x}) - \hat{\mathbf{J}}_f(\mathbf{x})\|_F \leq \sqrt{\sum_{i=1}^m \sum_{j=1}^n \left| \frac{\partial f_i}{\partial x_j}(\mathbf{x}) - \frac{\partial \hat{f}_i}{\partial x_j}(\mathbf{x}) \right|^2} \quad (33)$$

where $\mathbf{J}_f(\mathbf{x})$ is the true Jacobian, $\hat{\mathbf{J}}_f(\mathbf{x})$ is the estimated Jacobian, $\|\cdot\|_F$ denotes the Frobenius norm, and the error in each partial derivative $\frac{\partial \hat{f}_i}{\partial x_j}$ is bounded by the corresponding univariate error bound.

3.2.3 Mixed Partial Derivatives and Limitations

A notable limitation of PyDelt’s traditional interpolation approach for multivariate functions is the approximation of mixed partial derivatives as zero. For a scalar function $f(\mathbf{x})$, the mixed partial derivative $\frac{\partial^2 f}{\partial x_i \partial x_j}$ for $i \neq j$ is

TABLE 3: 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 GOLD	0.0158	0.0492	0.0998
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

approximated as zero because each dimension is treated independently.

This limitation is addressed in PyDelt’s neural network-based approach, which uses automatic differentiation to compute exact mixed partials. For a neural network model $f_\theta(\mathbf{x})$, the mixed partial derivative is computed as:

$$\frac{\partial^2 f_\theta(\mathbf{x})}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i} \left(\frac{\partial f_\theta(\mathbf{x})}{\partial x_j} \right) \quad (34)$$

where $\frac{\partial^2 f_\theta}{\partial x_i \partial x_j}$ is the mixed second-order partial derivative with respect to inputs x_i and x_j (where $i \neq j$), and the computation is performed using the chain rule of automatic differentiation.

This exact computation of mixed partials makes neural network methods particularly valuable for applications where cross-dimensional interactions are important, such as in fluid dynamics or elasticity theory.

3.3 Computational Efficiency

3.3.1 Algorithmic Complexity Analysis

The computational efficiency of numerical differentiation methods can be characterized by their algorithmic complexity in both the fitting and evaluation phases. Let n be the number of data points and d be the dimensionality of the input space.

For traditional interpolation methods in PyDelt, the time complexity can be analyzed as follows:

- **Spline Interpolation:** The fitting phase involves solving a tridiagonal system of equations, which has complexity $O(n)$. Evaluation at a single point has complexity $O(\log n)$ due to binary search for the appropriate interval, followed by constant-time polynomial evaluation.
- **LLA/GLLA Methods:** These methods use local windows of fixed size w , resulting in fitting complexity $O(n \cdot w^2)$ for solving n local least squares problems. Evaluation has complexity $O(w^2)$ per point, as it requires solving a local least squares problem.
- **LOWESS/LOESS:** These methods require sorting the data points by distance for each evaluation point, resulting in fitting complexity $O(n^2 \log n)$ in the worst case. However, PyDelt implements spatial indexing structures that reduce this to approximately $O(n \log n)$ in practice. Evaluation complexity is $O(k \cdot d)$ per point, where k is the number of nearest neighbors used.

TABLE 4: Average Computation Time (milliseconds)

Method	Fit Time	Evaluation Time	Total Time
PyDelt GLLA	1.24	0.31	1.55
PyDelt GOLD	1.31	0.33	1.64
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 TensorFlow	2743.21	1.87	2745.08
PyDelt NN PyTorch	2156.43	1.52	2157.95
JAX	N/A	0.89	0.89

For multivariate functions with d input dimensions, the complexity scales linearly with d for gradient computation and quadratically for Hessian computation, as separate univariate interpolators are fitted for each dimension or dimension pair.

3.3.2 Performance Benchmarks

Our empirical measurements confirm these theoretical complexity analyses. The traditional interpolation methods in PyDelt show competitive performance with SciPy and finite difference methods, with total computation times within the same order of magnitude for moderate-sized datasets.

Neural network methods have significantly higher training (fit) times but reasonable evaluation times once trained. The training complexity is $O(n \cdot e \cdot h)$, where e is the number of training epochs and h is the size of the hidden layers. However, the evaluation complexity is only $O(h)$, independent of the original dataset size.

3.3.3 Memory Complexity

Memory requirements also differ significantly between methods:

- **Finite Difference Methods:** Require $O(n)$ memory to store the original data points.
- **Spline Interpolation:** Requires $O(n)$ memory to store spline coefficients.
- **LLA/GLLA Methods:** Require $O(n \cdot w)$ memory to store local coefficients for each point.
- **Neural Network Methods:** Require $O(h^2)$ memory to store network weights, independent of the dataset size once training is complete.

This memory complexity analysis is particularly relevant for large datasets or high-dimensional problems, where memory constraints may influence method selection.

4 PRACTICAL GUIDANCE: CHOOSING THE RIGHT TOOL

4.1 Method Selection: A Decision Framework

One of PyDelt’s key innovations is recognizing that no single method is optimal for all problems. Instead, we provide a principled framework for method selection based on problem characteristics and performance requirements.

The selection of an appropriate numerical differentiation method can be formalized as a multi-objective optimization problem that balances accuracy, robustness, and computational efficiency. Let $\mathcal{A}(f, M)$ represent the accuracy of method M for function f , $\mathcal{R}(f, M, \sigma)$ represent the robustness to noise of level σ , and $\mathcal{C}(f, M, n)$ represent the computational cost for n data points.

The optimal method M^* can be expressed as:

$$M^* = \arg \max_{M \in \mathcal{M}} [w_A \cdot \mathcal{A}(f, M) + w_R \cdot \mathcal{R}(f, M, \sigma) - w_C \cdot \mathcal{C}(f, M, n)] \quad (35)$$

where M^* is the optimal method, $\arg \max$ denotes the maximizing argument, \mathcal{M} is the set of available methods, $\mathcal{A}(f, M) \in [0, 1]$ is a normalized accuracy metric, $\mathcal{R}(f, M, \sigma) \in [0, 1]$ is a normalized robustness metric, $\mathcal{C}(f, M, n) \geq 0$ is the computational cost, and $w_A, w_R, w_C \geq 0$ are weights (with $w_A + w_R + w_C = 1$) reflecting the relative importance of each criterion for the specific application.

Based on our comprehensive analysis and this theoretical framework, we recommend:

- 1) **For general-purpose differentiation:** Use PyDelt GLLA, which achieves the best balance of accuracy ($\mathcal{A} \approx 0.997$), robustness ($\mathcal{R} \approx 0.35$ at 5% noise), and computational efficiency ($\mathcal{C} \approx 1.55$ ms).
- 2) **For noisy data:** Use PyDelt LOWESS/LOESS, which maximize robustness ($\mathcal{R} \approx 0.5$ at 5% noise) through their robust weighting schemes that effectively downweight outliers. The theoretical foundation for this robustness lies in their bounded influence functions.
- 3) **For high-dimensional data (3D):** Use PyDelt MultivariateDerivatives with GLLA, which scales efficiently with dimensionality due to its $O(d)$ complexity for gradient computation, compared to $O(d^2)$ for finite difference methods.
- 4) **For performance-critical applications:** Use PyDelt LLA, which minimizes computational cost ($\mathcal{C} \approx 1.13$ ms) while maintaining reasonable accuracy ($\mathcal{A} \approx 0.996$) through its simplified local linear model.
- 5) **For numerically challenging functions:** Use PyDelt GOLD, which provides enhanced numerical stability through orthogonalization, reducing condition number issues in the local basis representation.
- 6) **For exact mixed partial derivatives:** Use PyDelt Neural Network, which computes exact mixed partials through automatic differentiation, avoiding the zero-approximation limitation of traditional methods.
- 7) **For higher-order derivatives (2):** Use PyDelt Spline/FDA/GOLD, which maintain analytical continuity in higher derivatives through their global optimization approach or orthogonal basis functions.

4.2 Parameter Tuning Guidelines: Mathematical Insights

The performance of each method depends critically on its parameters. We provide theoretical insights for optimal parameter selection:

- **PyDelt GLLA:** The embedding dimension m and derivative order n determine the local polynomial approximation. The approximation error scales as $O(h^{m+1-n})$ for the n -th derivative, where h is the effective window size. For optimal performance:

$$m_{\text{optimal}} = \arg \min_m \left[C_1 h^{m+1-n} + C_2 \frac{\sigma}{\sqrt{n}} \binom{m}{n} \right] \quad (36)$$

where m_{optimal} is the optimal embedding dimension, $\arg \min_m$ denotes minimization over m , $C_1, C_2 > 0$ are constants depending on the function, $h > 0$ is the effective window size, $\sigma \geq 0$ is the noise level, n is the number of local points, and $\binom{m}{n}$ is the binomial coefficient. This typically yields $m = 3$ to 5 for first derivatives and $m = 4$ to 6 for second derivatives, depending on noise level σ .

- **PyDelt GOLD:** The window size w and normalization method affect both accuracy and stability. The optimal window size balances bias and variance:

$$w_{\text{optimal}} \approx \left(\frac{C_3 \sigma^2}{C_4 |f^{(m+1)}|^2} \right)^{\frac{1}{2m+1}} \quad (37)$$

where w_{optimal} is the optimal window size (number of points), $C_3, C_4 > 0$ are method-specific constants, σ^2 is the noise variance, $f^{(m+1)}$ is the $(m+1)$ -th derivative of the function (measuring smoothness), and m is the polynomial degree. This typically yields $w = 3$ to 7 points.

- **PyDelt LOESS/LOWESS:** The span parameter α (or `frac`) controls the proportion of points used in local fitting. The optimal value minimizes the asymptotic mean squared error:

$$\alpha_{\text{optimal}} \approx \left(\frac{C_5 \sigma^2}{n \cdot C_6 |f^{(p+1)}|^2} \right)^{\frac{1}{2p+1}} \quad (38)$$

where $\alpha_{\text{optimal}} \in (0, 1]$ is the optimal span parameter (fraction of points used), $C_5, C_6 > 0$ are constants, σ^2 is the noise variance, n is the total number of data points, $f^{(p+1)}$ is the $(p+1)$ -th derivative (measuring curvature), and $p \geq 1$ is the degree of the local polynomial. For noisy data, this typically yields $\alpha = 0.2$ to 0.5 .

- **PyDelt Spline:** The smoothing parameter s in smoothing splines controls the trade-off between fidelity to data and smoothness of the derivative. The optimal value from generalized cross-validation is:

$$s_{\text{optimal}} = \frac{n \cdot \sigma^2}{\text{trace}(I - A(s))^2} \quad (39)$$

where $s_{\text{optimal}} \geq 0$ is the optimal smoothing parameter, n is the number of data points, σ^2 is the noise variance, $\text{trace}(\cdot)$ denotes the matrix trace, I is the identity matrix, and $A(s) \in \mathbb{R}^{n \times n}$ is the influence (hat) matrix of the spline that maps observed values to fitted values. PyDelt implements automatic selection of this parameter using generalized cross-validation.

- **PyDelt Neural Network:** The network architecture and regularization parameter λ affect both accuracy and generalization. For derivative estimation, deeper networks (more layers) generally perform better than wider networks (more neurons per layer) due to their ability to capture higher-order derivatives more effectively.

5 BEYOND BASIC DERIVATIVES: ADVANCED CAPABILITIES

PyDelt's development extended beyond traditional numerical differentiation to address specialized needs in modern scientific computing. These advanced features demonstrate the library's versatility and comprehensive approach to derivative estimation.

5.1 Tensor Calculus: From Vectors to Continuum Mechanics

PyDelt provides comprehensive tensor calculus operations through the `TensorDerivatives` class for continuum mechanics, fluid dynamics, and physics applications. All operations are **fully implemented and production-ready**:

- 1) **Divergence:** For a vector field $\mathbf{F} : \mathbb{R}^n \rightarrow \mathbb{R}^n$, the divergence measures expansion or contraction:

$$\nabla \cdot \mathbf{F} = \sum_{i=1}^n \frac{\partial F_i}{\partial x_i} \quad (40)$$

where $\nabla \cdot \mathbf{F}$ is the divergence (a scalar field), $\mathbf{F} = [F_1, F_2, \dots, F_n]^T$ is the vector field, F_i is the i -th component of \mathbf{F} , and $\frac{\partial F_i}{\partial x_i}$ is the partial derivative of the i -th component with respect to the i -th coordinate.

Implementation: `TensorDerivatives.divergence()`

- 2) **Curl:** For 3D vector fields $\mathbf{F} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$, the curl measures rotation or vorticity:

$$\nabla \times \mathbf{F} = \begin{bmatrix} \frac{\partial F_3}{\partial x_2} - \frac{\partial F_2}{\partial x_3} \\ \frac{\partial F_1}{\partial x_3} - \frac{\partial F_3}{\partial x_1} \\ \frac{\partial F_2}{\partial x_1} - \frac{\partial F_1}{\partial x_2} \end{bmatrix} \quad (41)$$

where $\nabla \times \mathbf{F}$ is the curl (a vector field), $\mathbf{F} = [F_1, F_2, F_3]^T$ is the 3D vector field with components (F_1, F_2, F_3) corresponding to coordinates (x_1, x_2, x_3) . For 2D fields, scalar curl: $\nabla \times \mathbf{F} = \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}$ where F_x, F_y are the x and y components.

Implementation: `TensorDerivatives.curl()`

- 3) **Strain and Stress Tensors:** For displacement fields \mathbf{u} , the strain tensor is:

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (42)$$

where ϵ_{ij} is the (i, j) component of the strain tensor, $\mathbf{u} = [u_1, u_2, \dots, u_n]^T$ is the displacement field, and the symmetrization ensures $\epsilon_{ij} = \epsilon_{ji}$. The stress tensor (linear elasticity) is:

$$\sigma_{ij} = \lambda \delta_{ij} \epsilon_{kk} + 2\mu \epsilon_{ij} \quad (43)$$

where σ_{ij} is the (i, j) component of the stress tensor, λ, μ are Lamé parameters (material properties), δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ if $i = j$, else 0), and $\epsilon_{kk} = \sum_k \epsilon_{kk}$ is the trace of the strain tensor (Einstein summation convention).

Implementation: `TensorDerivatives.strain_tensor()`, `TensorDerivatives.stress_tensor()`

- 4) **Directional Derivatives:** Derivative along a specific direction \mathbf{v} :

$$D_{\mathbf{v}} f = \nabla f \cdot \mathbf{v} \quad (44)$$

where $D_{\mathbf{v}} f$ is the directional derivative of scalar function f in direction \mathbf{v} , ∇f is the gradient vector, $\mathbf{v} \in \mathbb{R}^n$ is the direction vector (typically normalized: $\|\mathbf{v}\|_2 = 1$), and \cdot denotes the dot product.

Implementation: `TensorDerivatives.directional_derivative()`

5.2 Stochastic Derivatives: Uncertainty in Motion

PyDelt supports stochastic derivatives for probabilistic modeling and uncertainty quantification in financial applications and stochastic processes:

- 1) **Itô vs. Stratonovich Calculus:** For stochastic differential equations (SDEs), derivatives transform differently:

Itô: $dY_t = f(X_t) dX_t \implies \frac{dY}{dX} = f'(X_t)$

Stratonovich: $dY_t = f(X_t) \circ dX_t \implies \frac{dY}{dX} = f'(X_t) + \frac{1}{2} f''(X_t) \sigma^2$

where Y_t and X_t are stochastic processes, dY_t and dX_t are stochastic differentials, $f'(X_t)$ is the derivative of transformation function f , \circ denotes the Stratonovich product, $f''(X_t)$ is the second derivative, and σ^2 is the diffusion coefficient (variance rate).

Implementation: `set_stochastic_link(method='ito')` or `method='stratonovich'`

- 2) **Stochastic Link Functions:** Transform derivatives through probability distributions with automatic correction terms. Supported distributions:

- **Normal:** Symmetric, unbounded (interest rates, errors)
- **Lognormal:** Positive, right-skewed (stock prices, volumes)
- **Gamma:** Positive, flexible shape (waiting times, rates)
- **Beta:** Bounded $[0,1]$ (proportions, ratios)
- **Exponential:** Memoryless (survival times)
- **Poisson:** Discrete, non-negative (count processes)

Implementation: `interpolator.set_stochastic_link(...)`

Applications: Option Greeks, risk analysis, volatility modeling, Brownian motion, population dynamics

5.3 Mixed Partial Derivatives with Neural Networks

While traditional interpolation methods approximate mixed partial derivatives as zero, PyDelt's neural network implementation computes exact mixed partials through automatic differentiation:

$$\frac{\partial^2 f_\theta(\mathbf{x})}{\partial x_i \partial x_j} = \frac{\partial}{\partial x_i} \left(\frac{\partial f_\theta(\mathbf{x})}{\partial x_j} \right) \quad (45)$$

where the mixed partial derivative is computed exactly using the chain rule of automatic differentiation, with $i \neq j$ denoting different input dimensions.

Implementation: `NeuralNetworkMultivariateDerivatives` with PyTorch/TensorFlow

5.4 Applicability to Known vs. Unknown Functions

PyDelt’s methods are applicable to both analytical functions and empirical data:

- 1) **Known Functions** (analytical form available):
 - *Use Case:* When $f(x) = \sin(x)$ or other explicit formulas are known but numerical derivatives are needed
 - *Why Numerical:* Automatic differentiation, avoiding symbolic complexity, validating analytical derivatives
 - *Best Methods:* Neural networks with autodiff (exact), splines (high accuracy), LLA/GLLA (robust)
- 2) **Unknown Functions** (only discrete data available):
 - *Use Case:* Experimental measurements, sensor data, financial time series, physical observations
 - *Challenge:* Reconstruct smooth function from noisy, sparse, or irregularly sampled data
 - *Best Methods:* LOWESS/LOESS (robust to noise), FDA (functional data), splines (smooth data), neural networks (complex patterns)

Universal Approach: All methods work seamlessly for both cases through the unified `.fit(input_data, output_data).differentiate(order)` interface.

5.5 Future Research Directions

Several areas warrant continued research:

- 1) **Optimal Regularization:** Adaptive methods that estimate function properties from data for automatic parameter tuning
- 2) **Non-uniform Sampling:** Specialized methods for highly non-uniform sampling with data gaps or clusters
- 3) **Boundary Effects:** Enhanced boundary treatment methods for improved edge accuracy
- 4) **Uncertainty Quantification:** Tighter error bounds under different noise models for reliable confidence intervals
- 5) **GPU Acceleration:** Parallel processing for multivariate derivatives to achieve near-linear speedup

6 CONCLUSION: IMPACT AND FUTURE DIRECTIONS

6.1 What We’ve Achieved: Theoretical and Practical Contributions

This paper has presented a comprehensive mathematical analysis of PyDelt’s numerical differentiation methods, demonstrating their theoretical foundations and empirical performance. Our analysis has yielded several important theoretical insights:

- 1) **Error Decomposition:** We have shown that the mean squared error of derivative estimates can be decomposed into bias and variance components, with different methods optimizing different aspects of this trade-off. The GLLA and GOLD methods achieve a favorable balance, explaining their superior overall performance.
- 2) **Robustness Mechanisms:** We have demonstrated that the exceptional noise robustness of LOWESS and LOESS methods stems from their bounded influence functions, which limit the effect of outliers on the derivative estimates.
- 3) **Complexity Analysis:** Our algorithmic complexity analysis reveals that PyDelt’s methods achieve competitive computational efficiency, with time complexity ranging from $O(n)$ for spline methods to $O(n \log n)$ for LOWESS/LOESS with spatial indexing.
- 4) **Parameter Optimization:** We have derived theoretical expressions for optimal parameter selection based on the bias-variance trade-off, providing a principled approach to method tuning.

6.2 From Software to Science: PyDelt’s Impact

PyDelt represents more than a software library—it embodies a comprehensive solution to the long-standing challenge of numerical differentiation from noisy data. The journey from initial concept to production-ready implementation has yielded a tool that serves both theoretical researchers and practical engineers. **All methods described in this paper are fully implemented, rigorously tested, and production-ready.**

The key strengths of PyDelt include:

- **Superior Accuracy:** PyDelt’s GLLA and GOLD interpolators achieve 40% lower error than SciPy’s spline methods and 85% lower error than finite difference methods for clean data.
- **Exceptional Noise Robustness:** LOWESS and LOESS interpolators show only a $2\times$ increase in error with 5% noise, compared to $9\text{--}10\times$ for finite difference methods.
- **Comprehensive Multivariate Support:** Full implementation of gradient, Jacobian, Hessian, and Laplacian operations with consistent API and superior accuracy.
- **Advanced Tensor Operations:** Divergence, curl, strain/stress tensors, and directional derivatives for continuum mechanics and fluid dynamics.

- **Stochastic Calculus:** Itô/Stratonovich corrections with six probability distributions for financial and probabilistic applications.
- **Universal API:** The consistent `.fit().differentiate()` pattern across all methods facilitates method comparison and selection.
- **Theoretical Foundations:** Each method is grounded in solid mathematical principles, with clear error bounds and complexity analyses.

6.3 Looking Forward: The Road Ahead

The development of PyDelt represents a significant milestone, but the journey continues. The field of numerical differentiation evolves alongside the problems it seeks to solve, and several promising directions emerge:

- 1) **Adaptive Intelligence:** Future versions will incorporate machine learning to automatically select methods and parameters based on data characteristics, reducing the burden on users.
- 2) **Uncertainty Quantification:** Enhanced error bounds and confidence intervals will provide users with reliable measures of derivative accuracy.
- 3) **Distributed Computing:** GPU acceleration and parallel processing will enable real-time derivative computation for massive datasets.
- 4) **Domain-Specific Extensions:** Specialized modules for specific fields (bioinformatics, climate science, robotics) will provide tailored solutions.

PyDelt's modular architecture and comprehensive feature set position it to incorporate these advances seamlessly. Our vision is clear: to provide the scientific community with the most powerful, flexible, and user-friendly numerical differentiation tools available, enabling discoveries that would otherwise remain hidden in noisy data.

The story of PyDelt is ultimately a story about transforming mathematical theory into practical tools that empower scientists and engineers to extract knowledge from data. As complex systems grow more prevalent and data more abundant, the need for robust derivative estimation will only increase. PyDelt stands ready to meet this challenge, serving as a bridge between the mathematical elegance of calculus and the messy reality of empirical observation.

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SOFTWARE AVAILABILITY AND CITATION

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Citation

If you use PyDelt in your research, please cite:

BibTeX:

```
@software{pydelt2025,
  title = {PyDelt: Advanced Numerical Function
    Interpolation and Differentiation},
  author = {Lee, Michael},
  year = {2025},
  url = {https://github.com/MikeHLee/pydelt},
  version = {0.6.1}
}
```

IEEE Style: M. Lee, "PyDelt: Advanced Numerical Function Interpolation and Differentiation," version 0.6.1, 2025. [Online]. Available: <https://github.com/MikeHLee/pydelt>

Key Features to Cite

- Universal differentiation interface across multiple interpolation methods
- Multivariate calculus operations (gradient, Jacobian, Hessian, Laplacian)
- Tensor calculus for continuum mechanics and fluid dynamics
- Stochastic derivatives with Itô/Stratonovich corrections
- Neural network integration with automatic differentiation