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Peer Review

Review of: "A Quasilinear Algorithm for Computing Higher-Order Derivatives of Deep Feed-Forward Neural Networks"

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This paper presents n-TANGENTPROP, a novel algorithm for computing higher-order derivatives of deep feed-forward neural networks for applications in PINNs. It addresses the exponential runtime issue of auto-differentiation in high-order derivative computations in PINNs. The proposed method leverages an extension of the TANGENTPROP formalism, aiming for significant efficiency improvements in PINN training. The authors provide both theoretical analysis and empirical validation, demonstrating the method's superior scaling properties. Specifically, the n-TANGENTPROP computes derivatives in quasilinear, instead of exponential time.

Strengths

- **Theoretical Soundness**: The derivation of n-TANGENTPROP is well-grounded in Faà di Bruno's formula and combinatorial properties of partition functions.
- **Empirical Validation**: The paper includes an experiment showing that n-TANGENTPROP outperforms auto-differentiation in training efficiency for high-order derivatives.
- **Impact on PINNs**: The method has clear practical implications, particularly for solving differential equations where multiple derivatives and higher-order derivatives are required, making PINNs more computationally viable.

Areas for Improvement

- **Discussion of PINN Benefits**: The introduction focuses on the limitations of PINNs but does not adequately highlight their advantages, such as grid-invariance, seamless data assimilation, and improved inverse problem-solving.

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- **Ordering of Figures**: Some figures are referenced out of order, which could affect readability. Ensuring a logical sequence would enhance clarity.
- **Code Optimization**: While the algorithm is shown theoretically to outperform auto-differentiation, the author acknowledges that the current implementation could be further optimized (e.g., leveraging C++ or GPU-specific optimizations). The lack of full vectorization limits its applicability and broad adoption.
- **Comparison with Alternative Methods**: The paper effectively benchmarks against auto-differentiation but does not compare n-TANGENTPROP with alternative methods such as numerical differentiation approaches or other recent advancements in efficient PINN training.
- **Test Cases**: The paper could benefit from additional test cases!

Overall Assessment

The paper presents a compelling improvement in computational efficiency for higher-order derivatives in deep neural networks. The work is **theoretically solid, well-motivated, and empirically validated**. However, further optimizations and broader comparative analysis would strengthen the impact of the proposed method.

Declarations

Potential competing interests: No potential competing interests to declare.