n-TangentProp: A Quasilinear Algorithm for Taking Derivatives of Neural Networks

Kyle R. Chickering
UC Davis

1. Motivation
2. PINNs + Neural Networks
3. Autodiff
4. TangentProp + n-TangentProp
5. Results
6. Conclusions

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Paper online, work under Dr. P. Simard in Feb. of last year

Motivation I

- The Navier-Stokes Existence & Smoothness (T. Tao in Notices)

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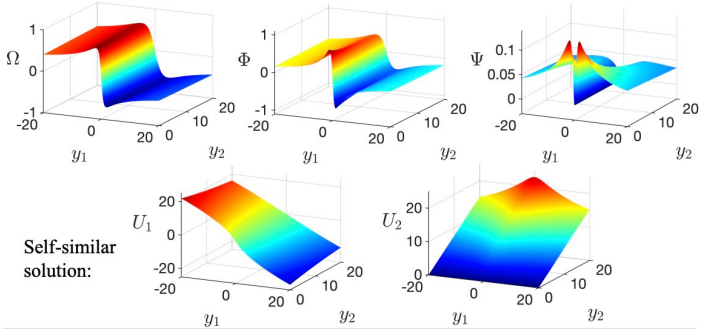

Boussinesq

$$
\begin{aligned}
\Omega + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla \Omega &= \Phi\,, \\
(2 + \partial_{y_1} U_1)\Phi + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla \Phi &= -\partial_{y_1} U_2 \Psi\,, \\
(2 + \partial_{y_2} U_2)\Psi + ((1+\lambda)\mathbf{y} + \mathbf{U}) \cdot \nabla \Psi &= -\partial_{y_2} U_1 \Phi\,, \\
\operatorname{div} \mathbf{U} &= 0\,.
\end{aligned}
\tag{3}
$$

Hard to solve numerically!

From Wang, Lai, Gómez-Serrano, Buckmaster '23

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- PINNs!

PINN's Neural Networks

Neural Networks I

- Repeated functional composition

$$u = \sigma(W^n \cdot \sigma(W^{n-1} \cdot \sigma(\cdots \sigma(W^1 \cdot x))))$$

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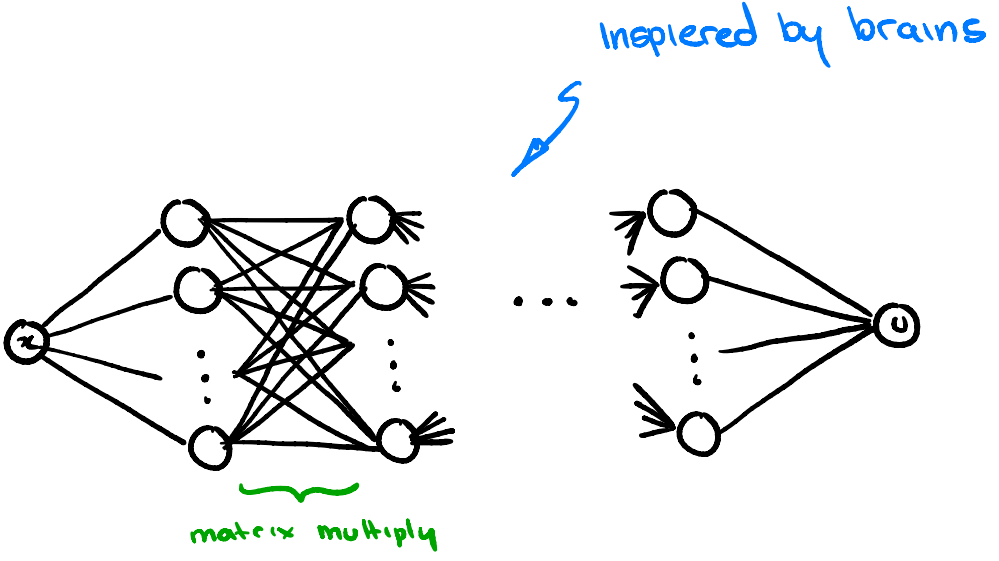

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- As width $\longrightarrow \infty$ we can approximate any continuous function on a compact domain
- Does not tell us <u>how</u> to get approximation

Neural Networks III

- Suppose I have a labled dataset $X = \{(x_i, y_i)\}_{i \in \mathcal{I}}$, & I want a function to approximate or generalize X, i.e. $f(x_i) \sim y_i \ \forall \ i \in \mathcal{I}$.

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- Loss: $$L(u_W) = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} |u_W(x_i) - y_i|^2$$
- Update params: $$W \leftarrow W - \alpha \nabla_W L(u_W)$$
- Gradient descent: $\nabla_W L(u_W) \to 0$ means critical pt.

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- NNs as functional approximator, $u_\theta \longrightarrow u$ during training!

Accuracy Gains

- Sobolev Loss

$$L_{Sob.}^{(m)}(v_\theta) = \frac{1}{N} \sum_{k=1}^{N} \sum_{j=0}^{m} a_j \left| \nabla_x^j F(a^\alpha v_\theta; x_k) \right|^2 + BC$$

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Key takeaway: More enforced derivatives gives better accuracy & training efficiency

(Maddu et al. '22)

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→ More Derivatives!

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- "Cold Water" Papers

PINN Use Cases

- Combined Forward-Inverse Problems
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  - → measurements from a fluid experiment
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- Auxillary Conditions
  - → For example: Enforcing smoothness
- If you can do it easily w/o a PINN, you probably don't need a PINN!

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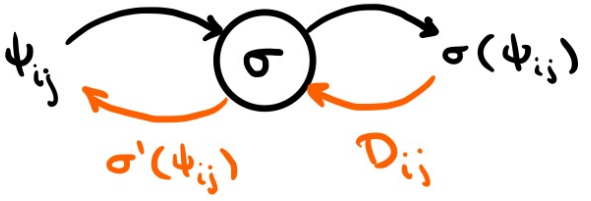

- Forward: $\sigma(\psi)$

Autodiff

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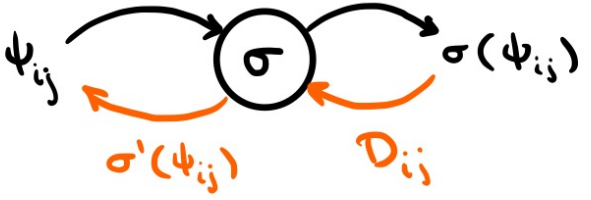

- Forward: $\sigma(\psi)$
- Backwards: $D \odot \sigma'(\psi)$

Computation Graph for NN

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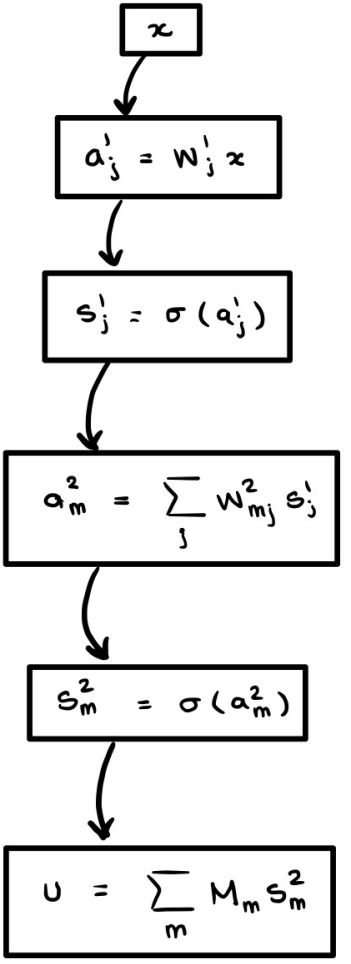
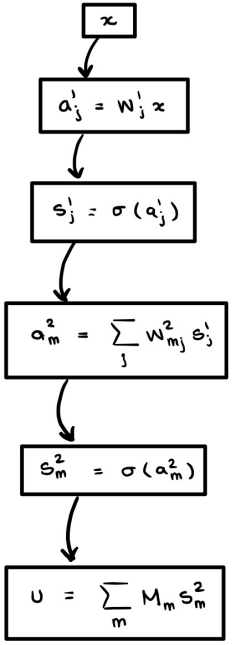


Autodiff Algorithm

- Forwards → Backwards → New Graph



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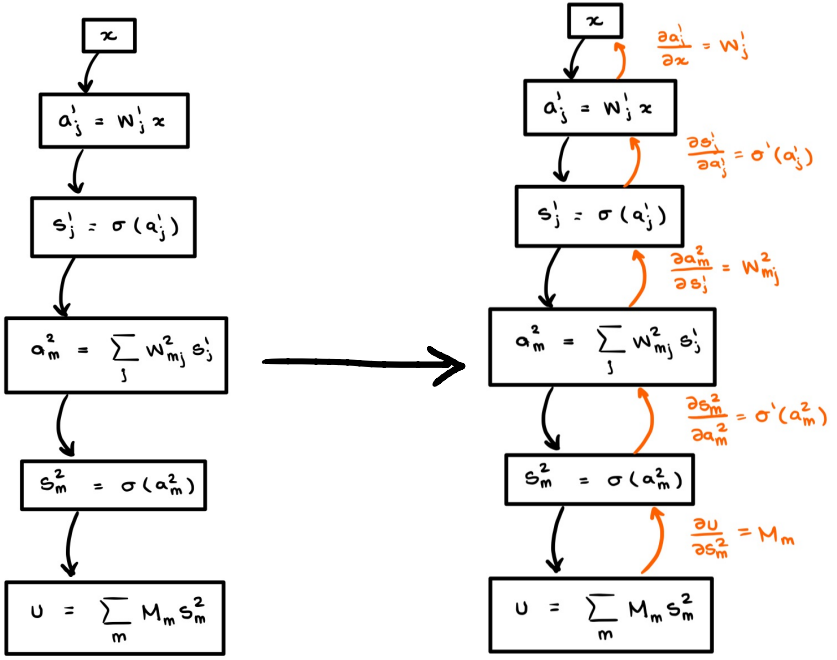

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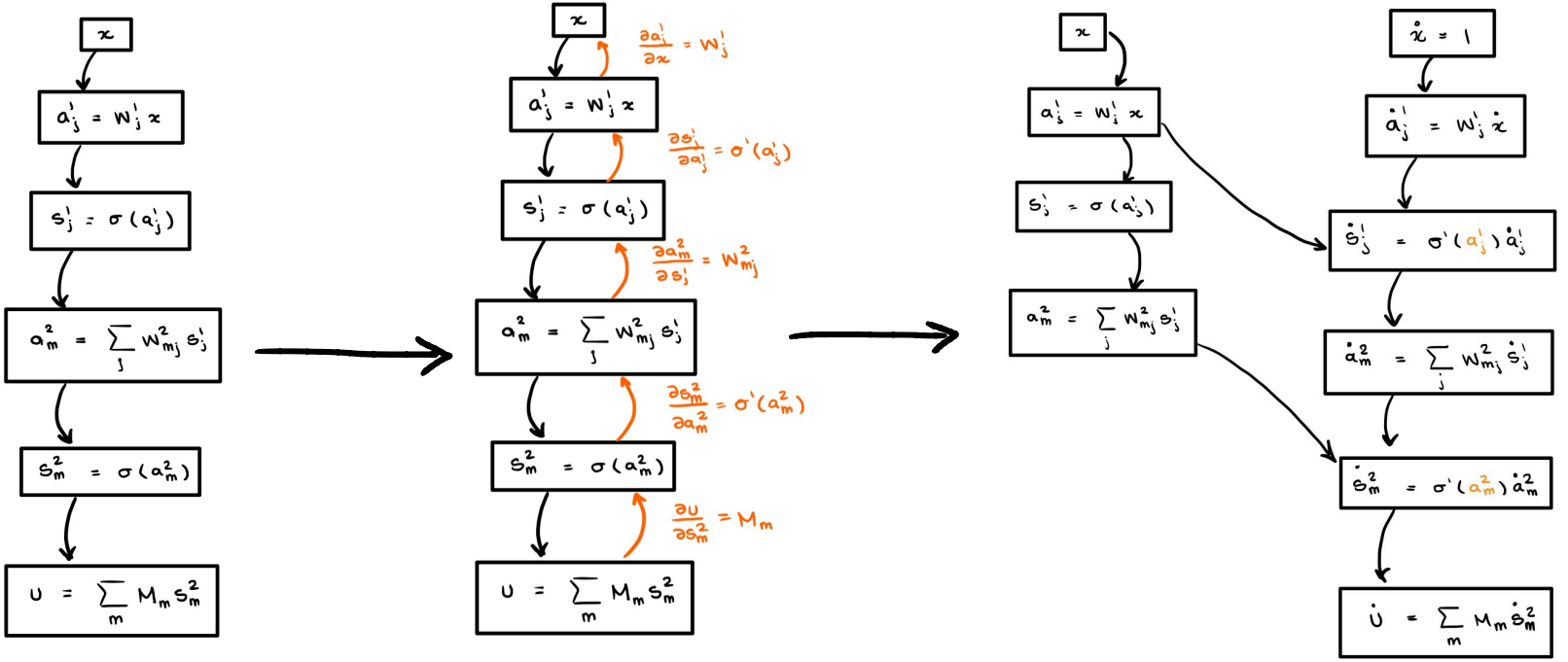

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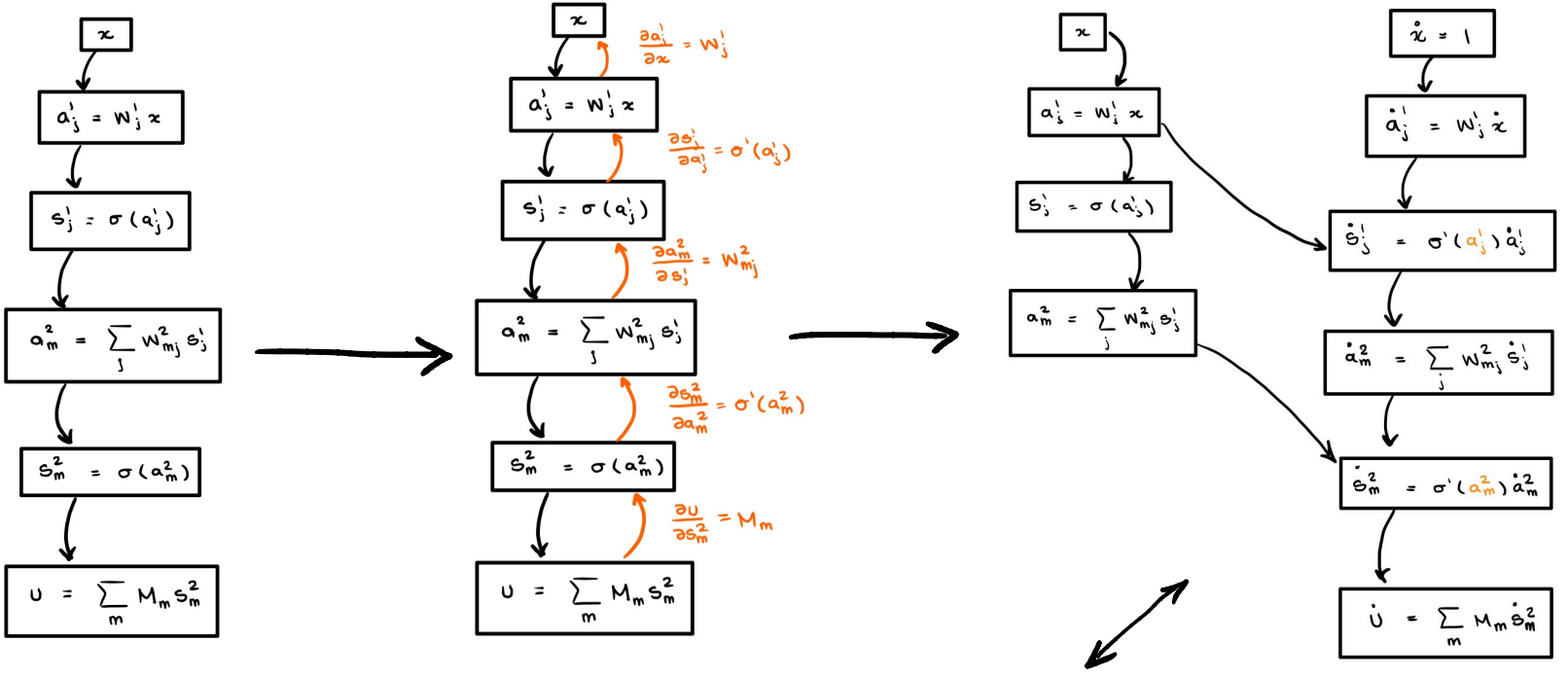
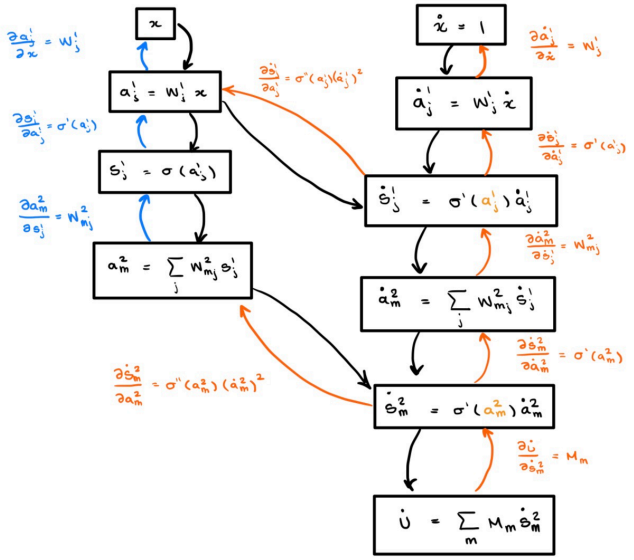


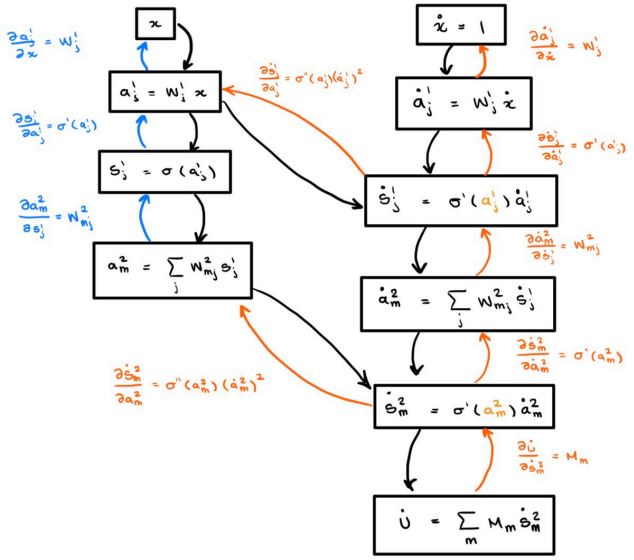
$$U' = M \cdot \sigma'(W^2 \cdot \sigma(W^1 x)) \cdot (W^2 \cdot \sigma'(W^1 x)) \cdot W^1$$

Computation is Repeated Through Chain Rule



Computation is Repeated Through Chain Rule

We already computed these!



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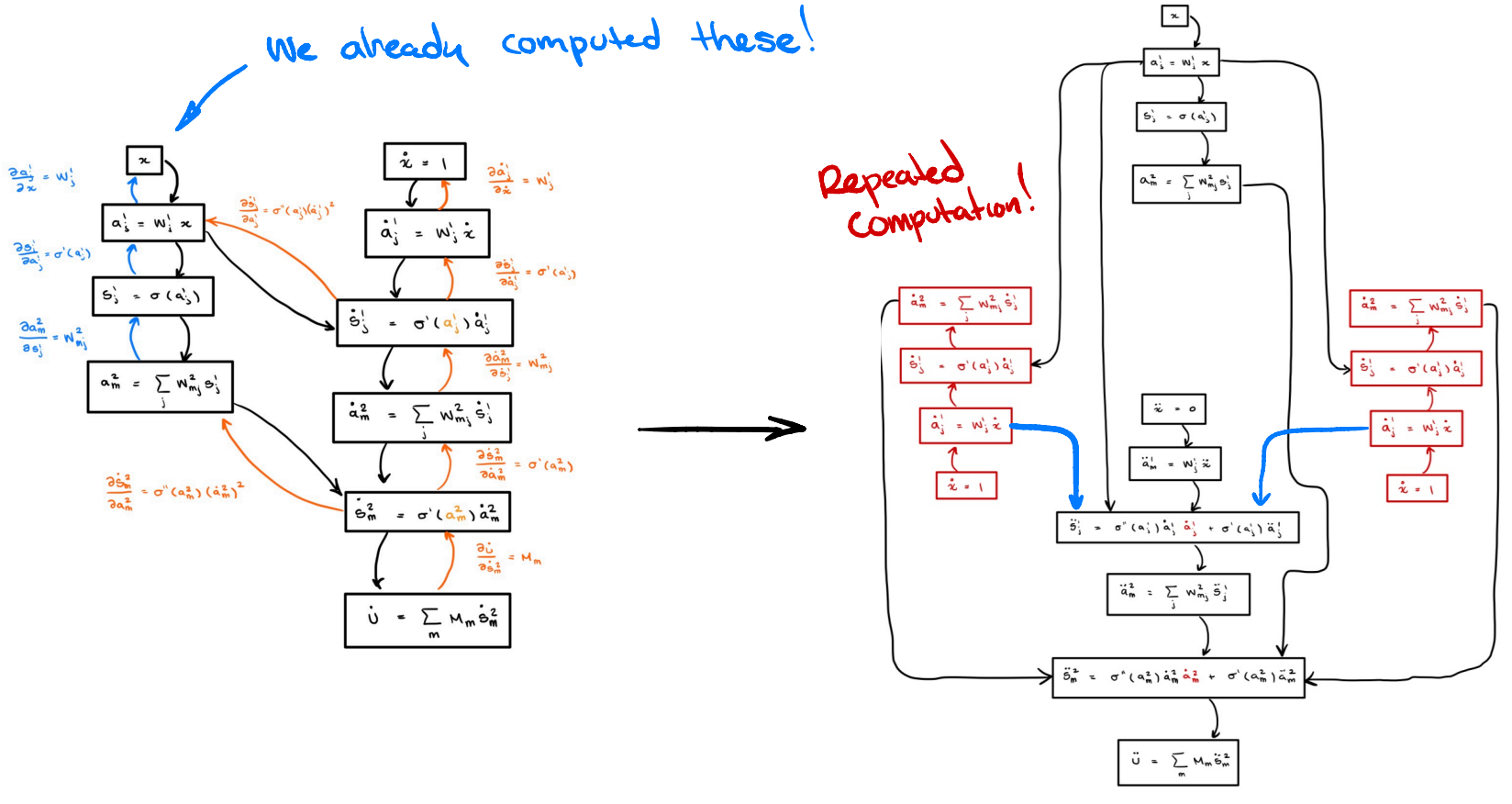
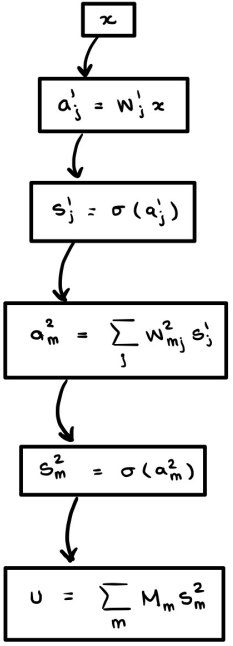


Autodiff Graph Grows Exponentially!



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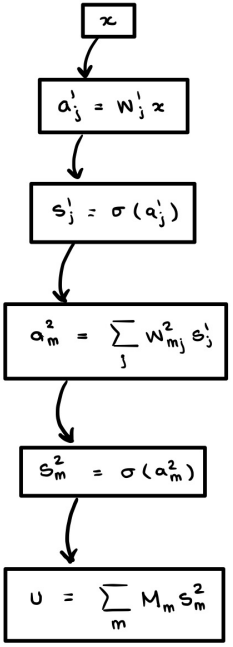

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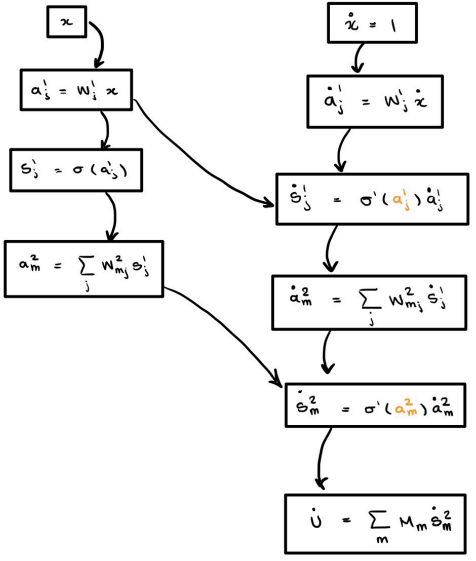

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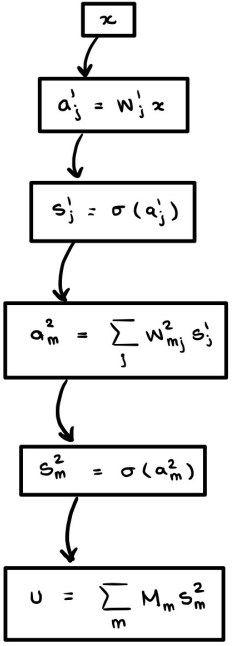

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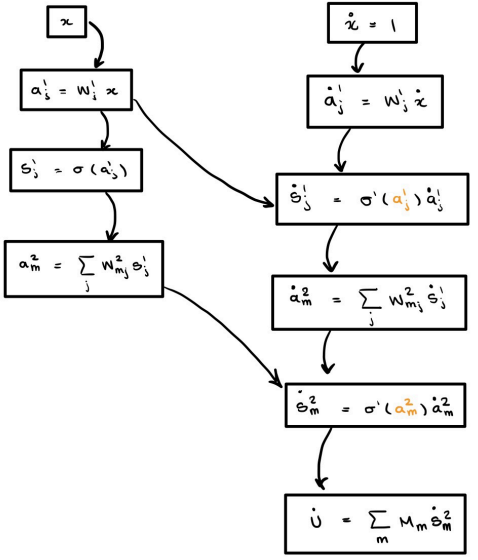

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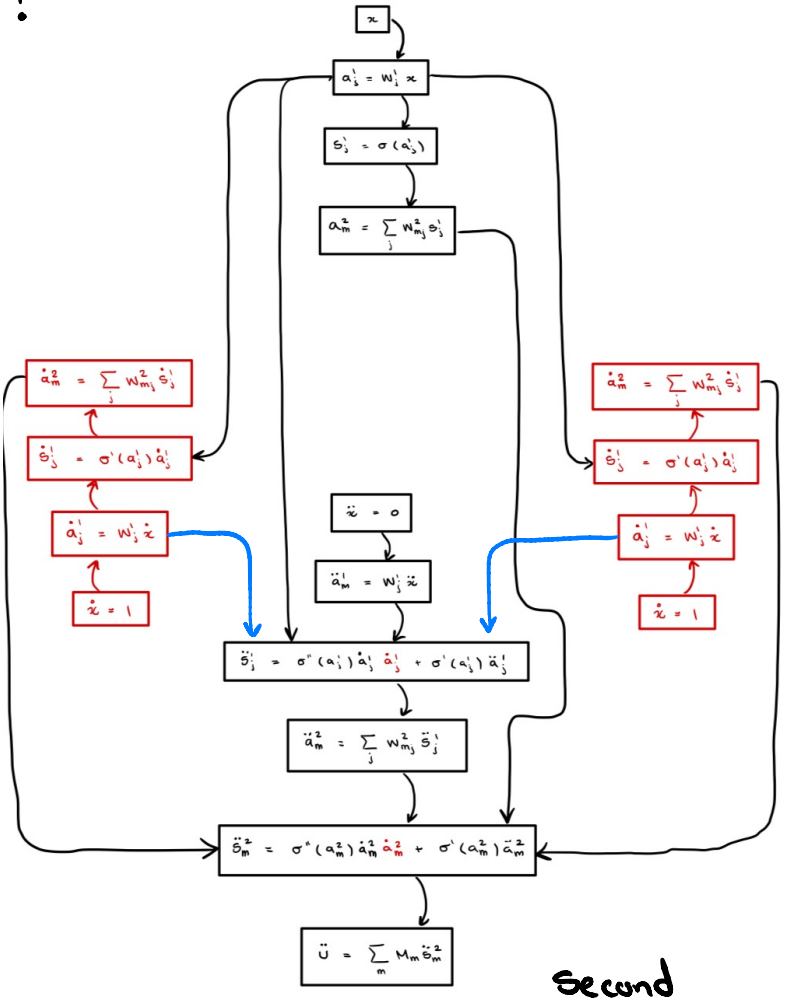
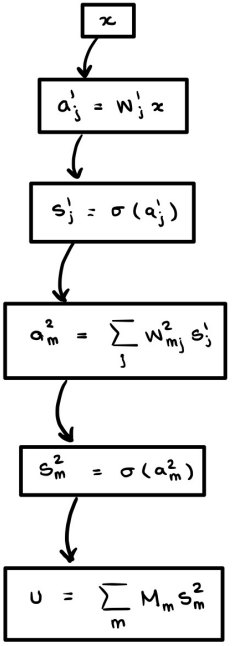
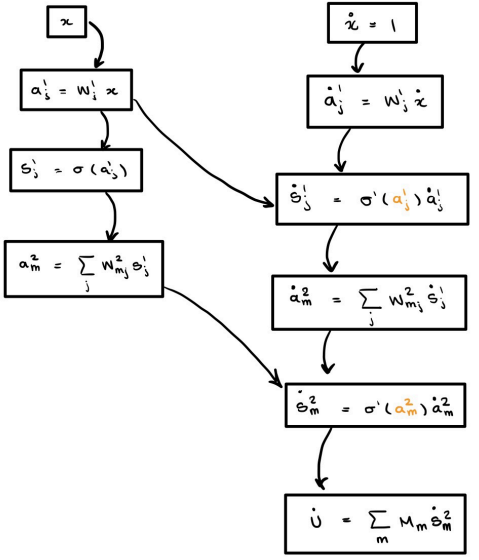


Second

Counting Nodes I





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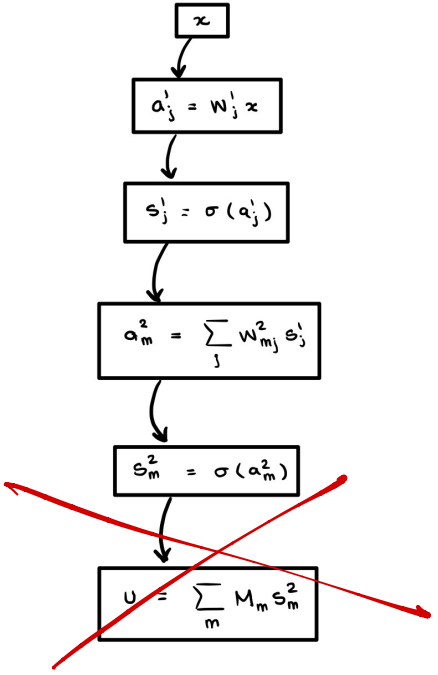

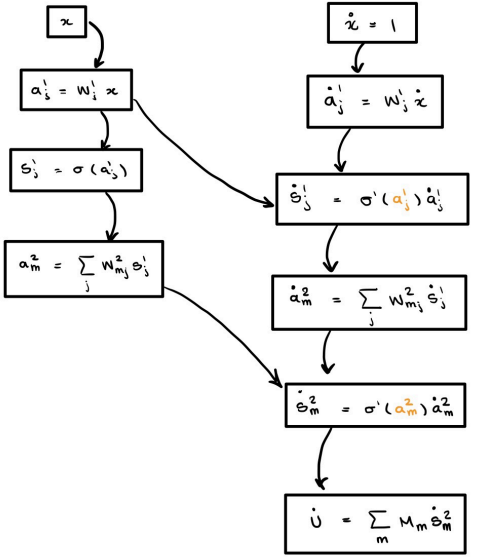

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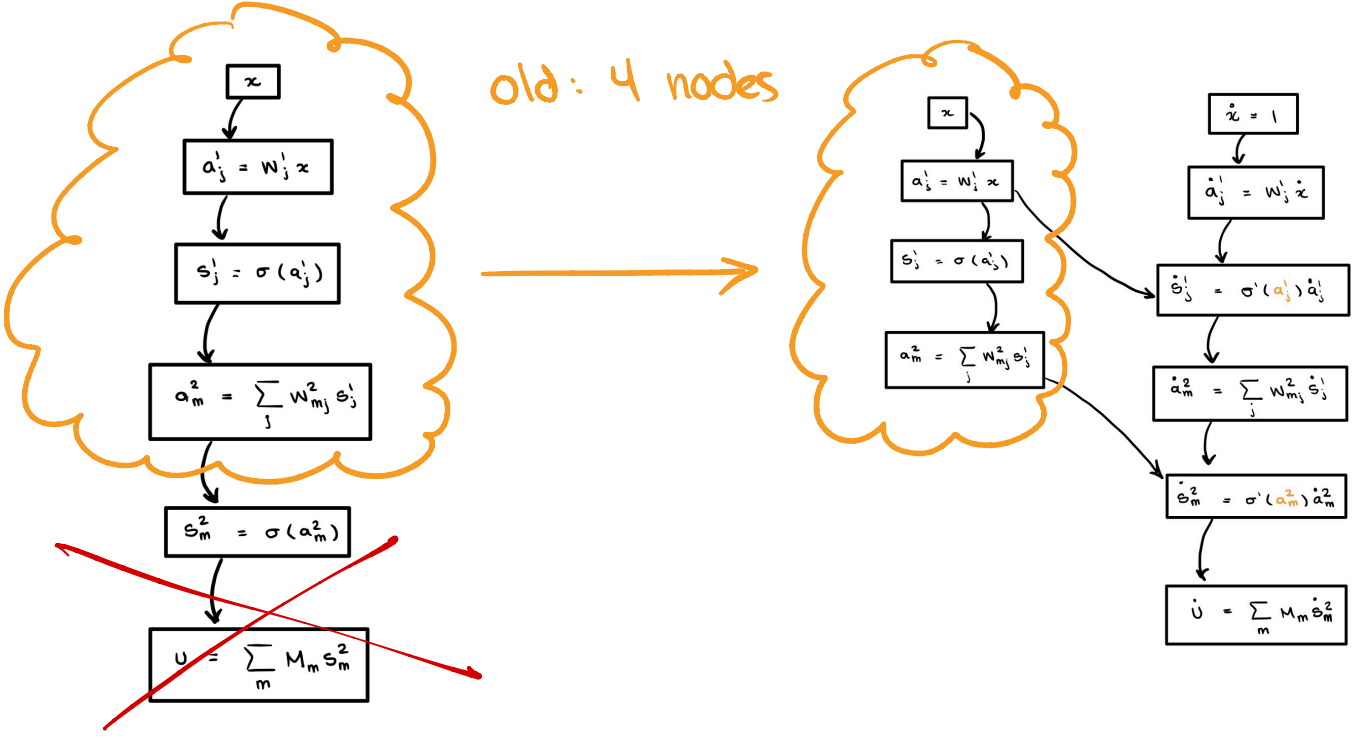

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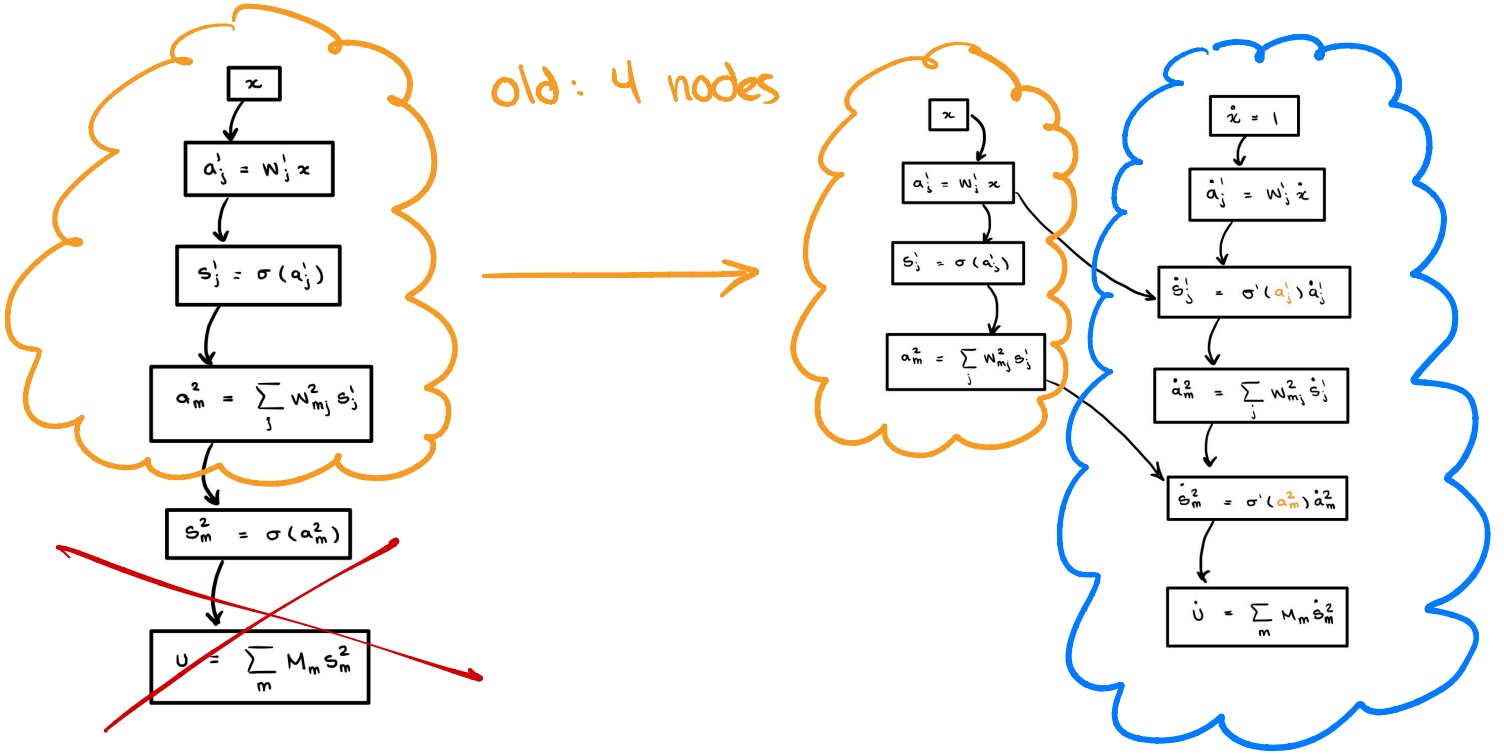
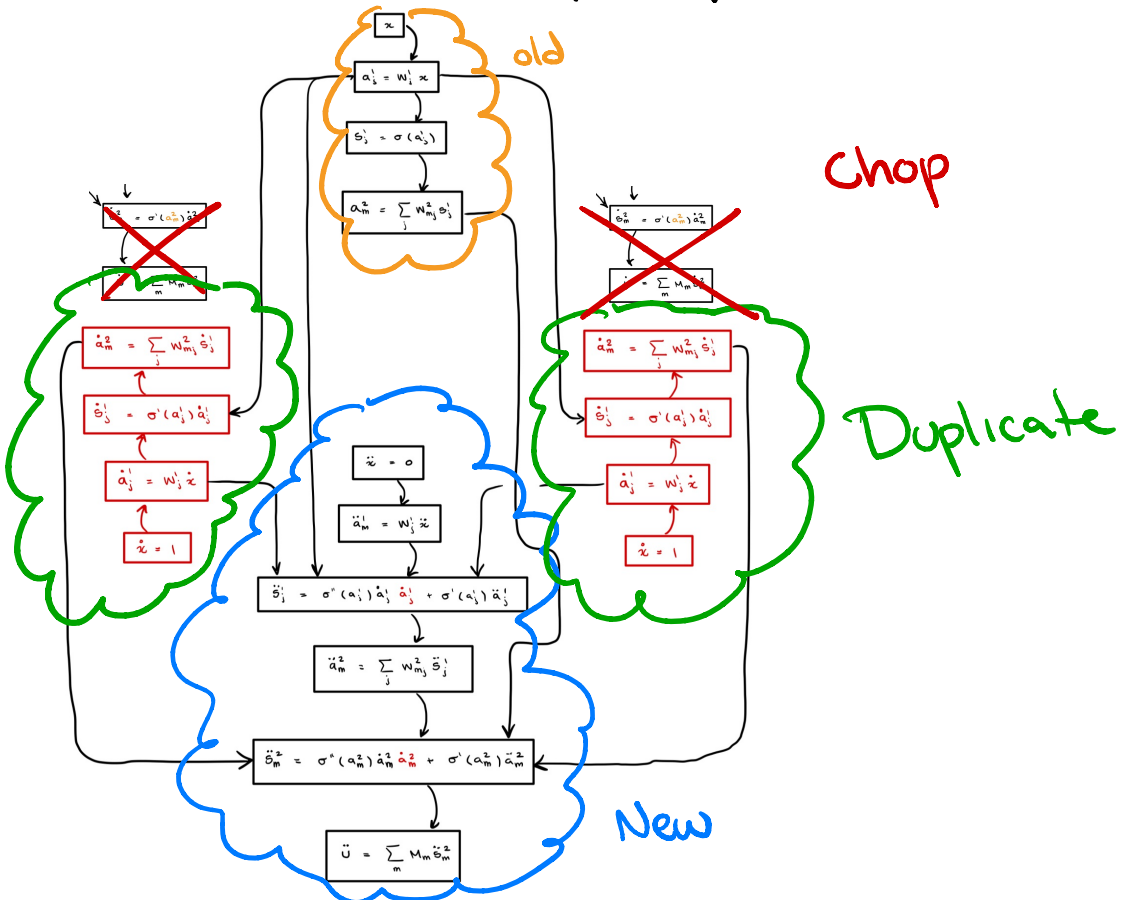
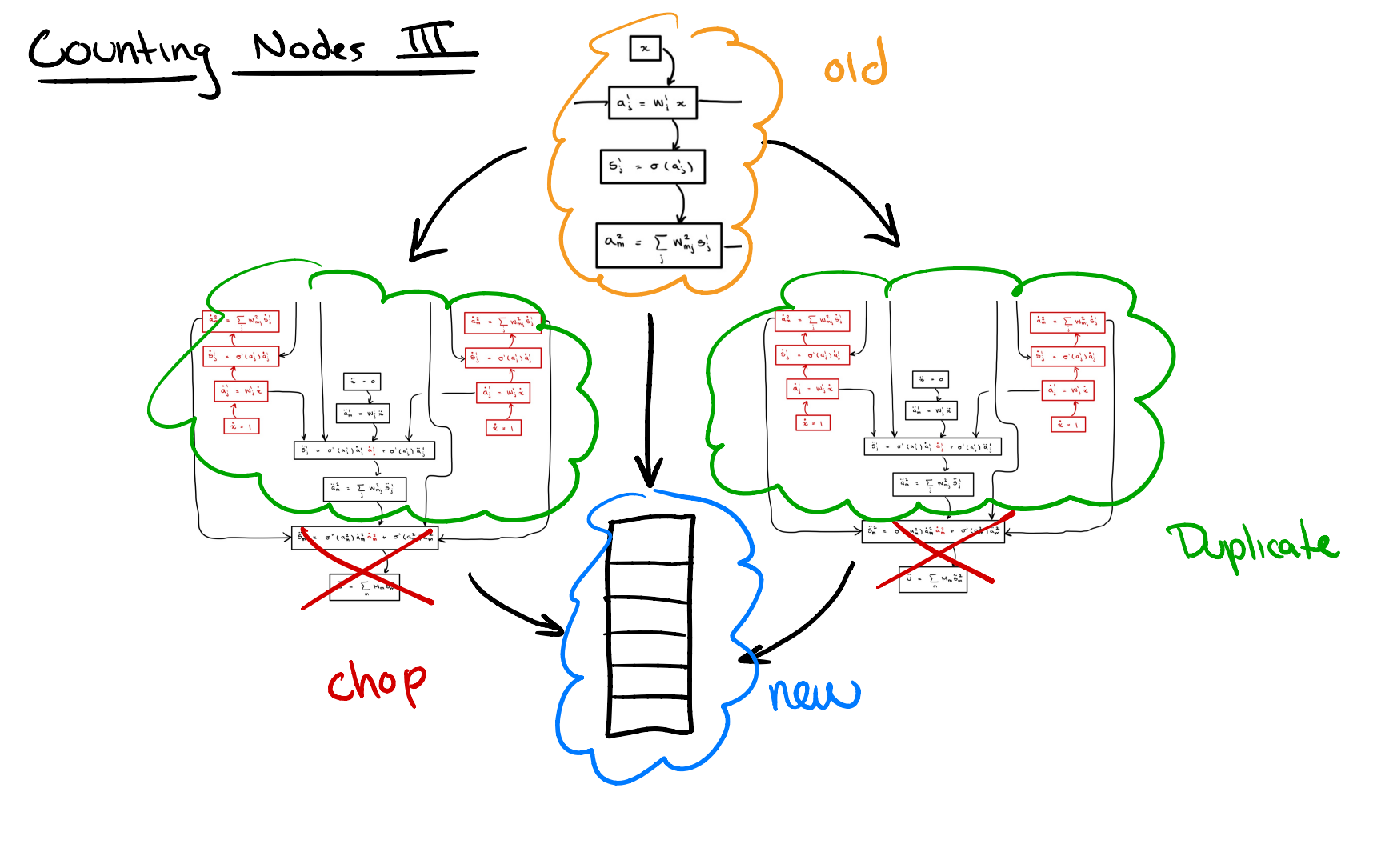


Counting Nodes II

- 6 new, 4 old, chop & duplicate the rest



Counting Nodes III



Counting Nodes III:

- # Nodes (n) = 10 + 2 × (# Nodes (n-1) - 6)
- # Nodes (0) = 6

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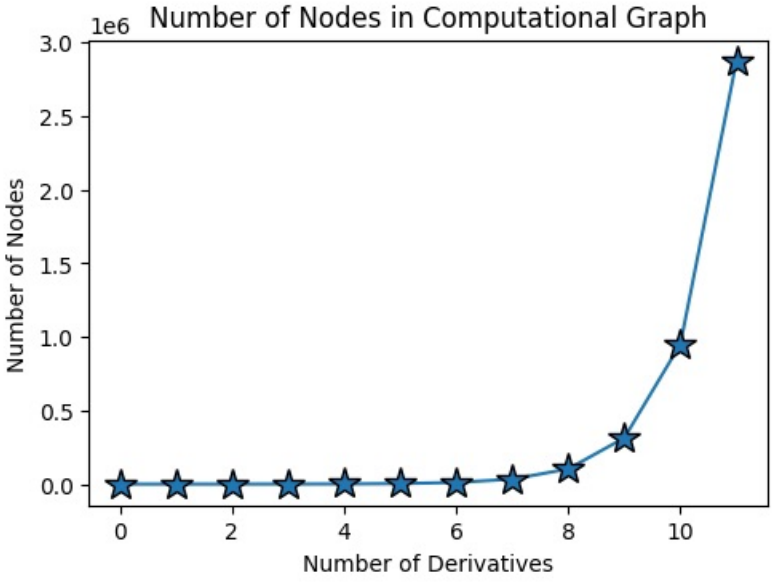
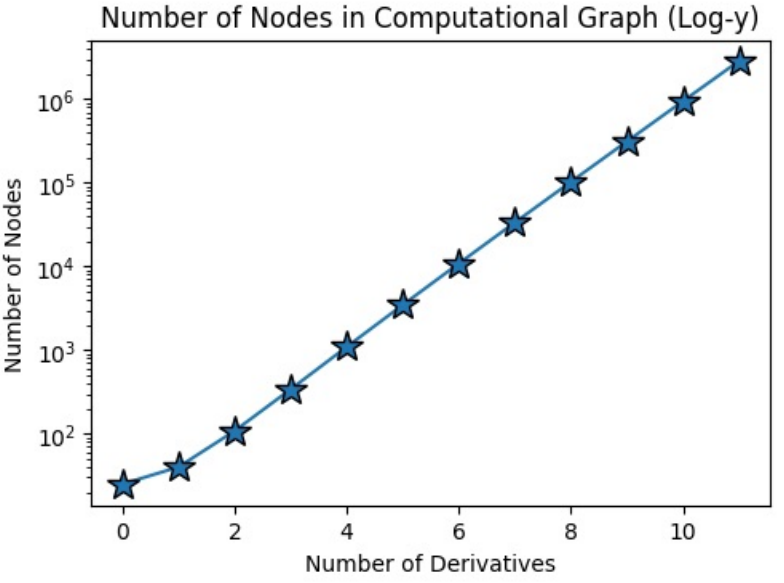
- $\#\text{Nodes}(0) = 6$
- $\Rightarrow \#\text{Nodes}(n) = 2^{n+1} - 2$
- Worse if we have to evaluate <u>all</u> derivatives up to n

$$\sum_{k=0}^{n} \#\text{Nodes}(k) = 2^{n+2} - 2$$

Counting Nodes V : Empirical





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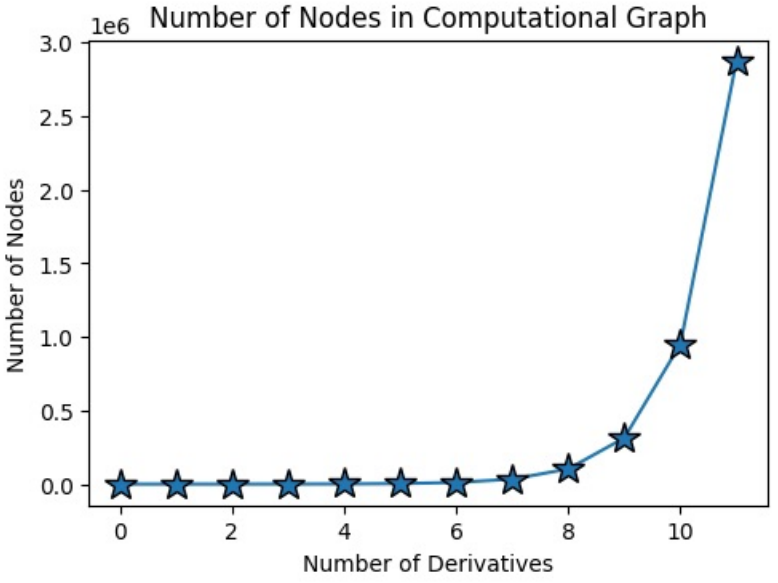

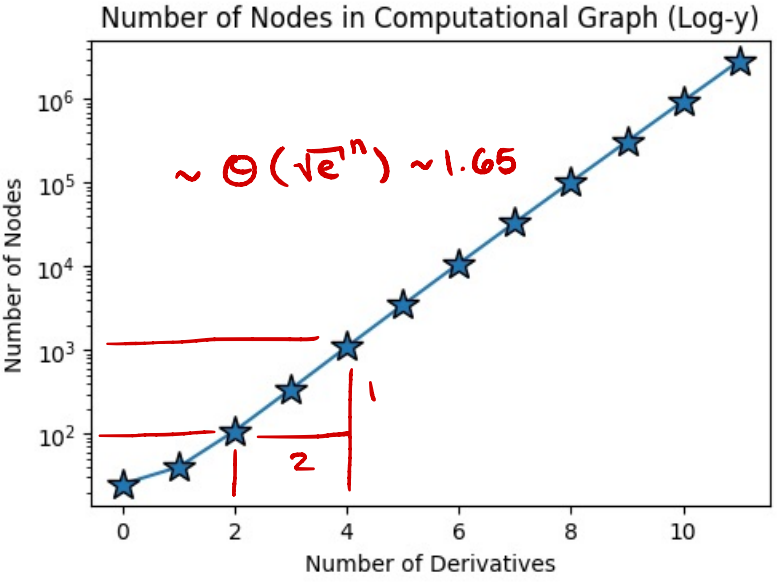

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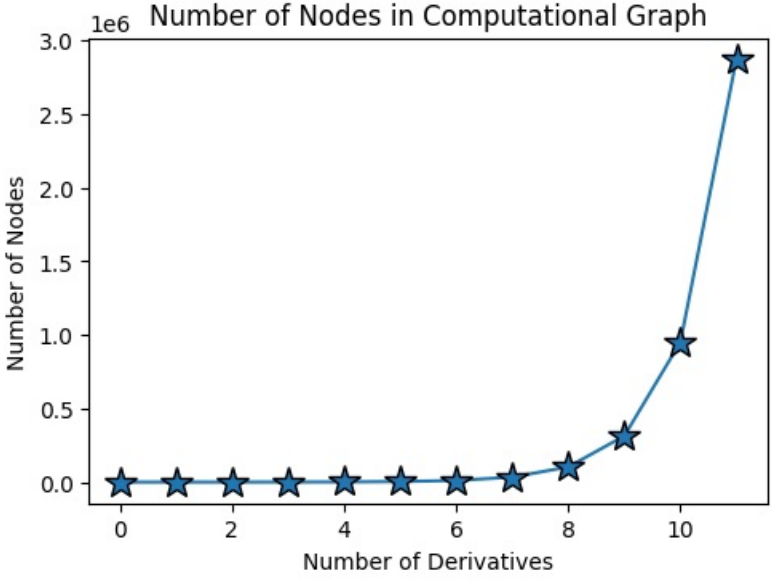
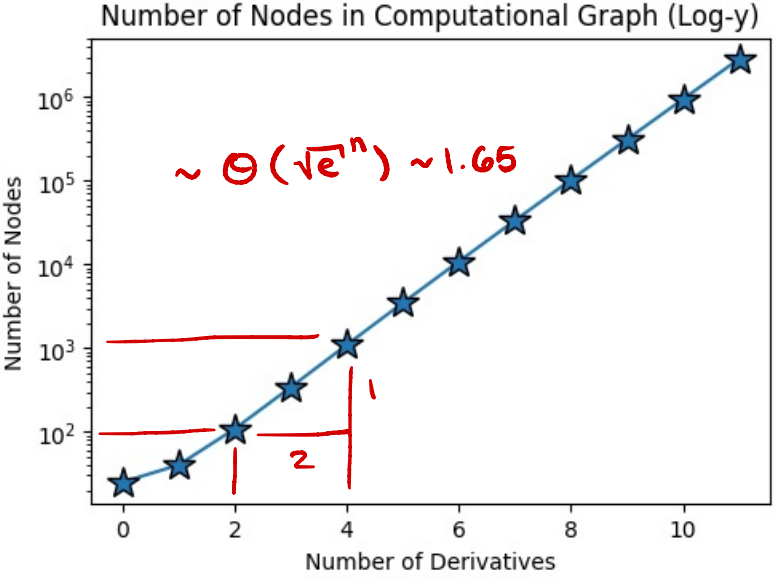
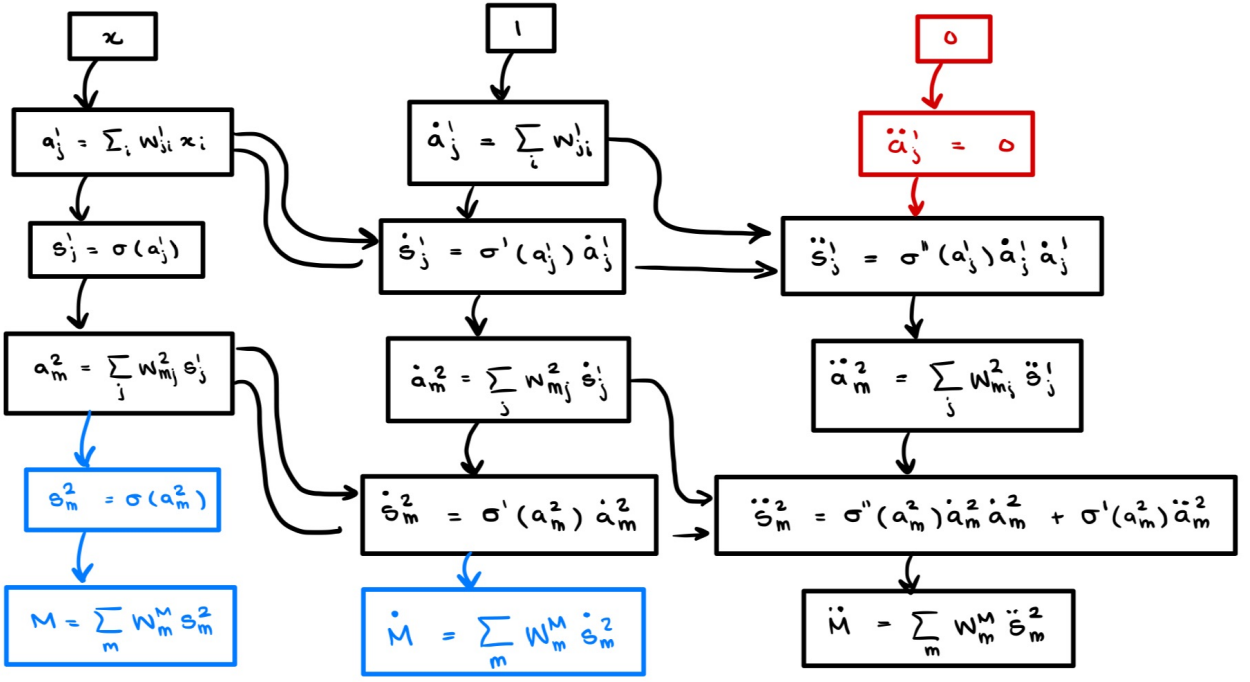




- Graph optimizations beat 2^n, but still exponential!

What Does the Minimal Graph for v^4 look like?



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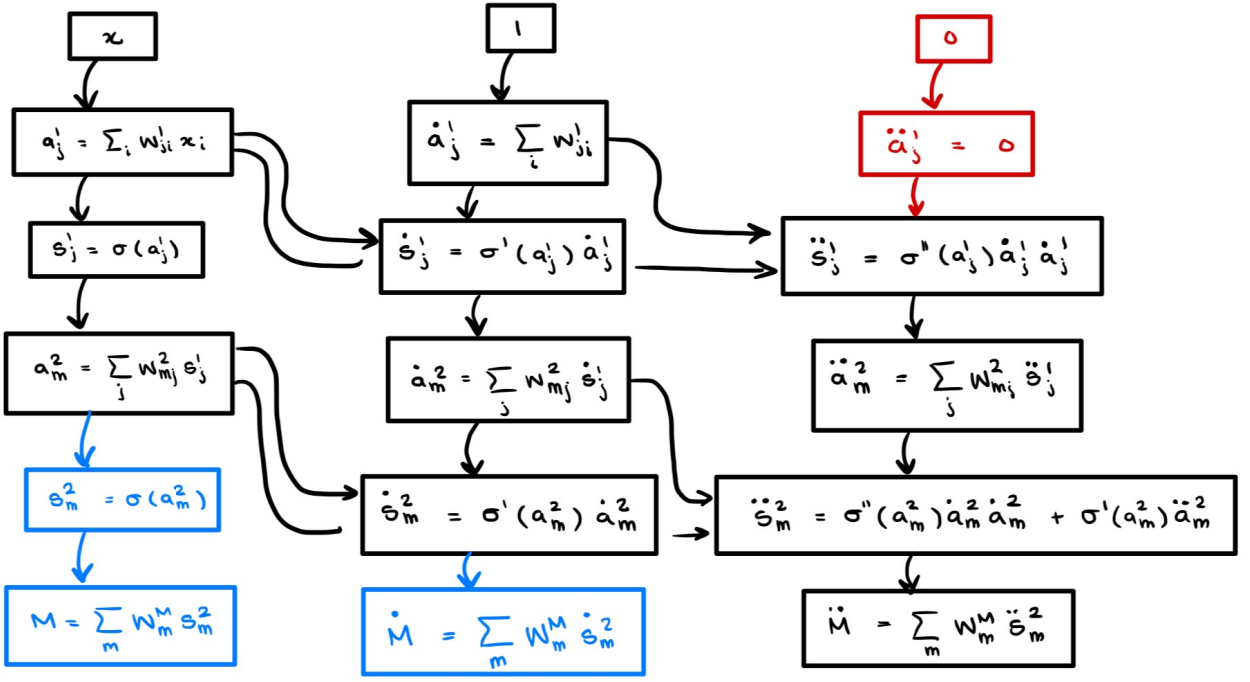

→ n-TangentProp will construct this instead!

TangentProp & n-TangentProp

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- Developed before Autodiff was in widespread use

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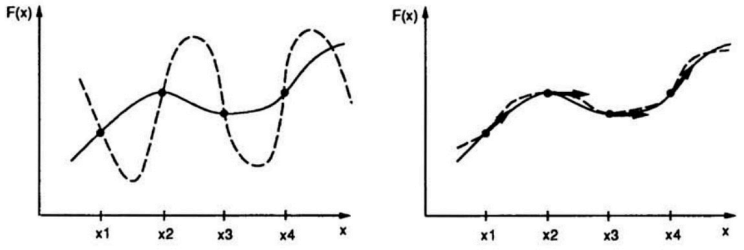
- First order constraint improves training convergence (c.f. Sobolev Loss!)



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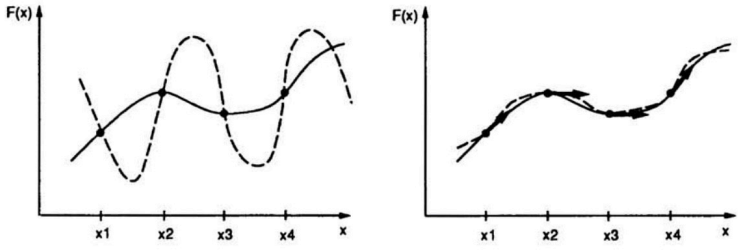

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- $a_i^l = \sum_j w_{ij}^l x_j^{l-1}$, $x_j^l = \sigma(a_j^l)$

Derivative

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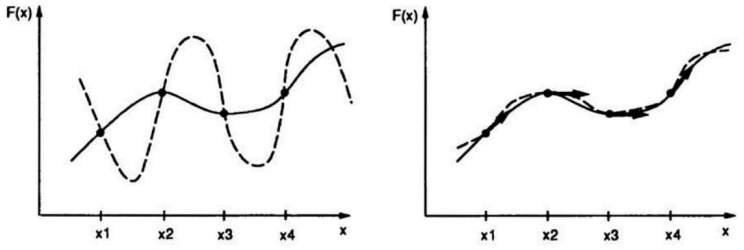

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- Both computed during forward

n-Tangent Prop I

- Leibniz formula: Product Rule

$$\frac{d^n}{dx^n}(fg) = \sum_{k=0}^{n} C^L(k,n) f^{(k)} g^{(n-k)}$$

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- Faà di Bruno formula: Chain Rule

$$\frac{d^n}{dx^n}(f \circ g) = \sum_{\bar{p} \in P(n)} C^F_{\bar{p},n} f^{(|\bar{p}|)} \circ g \prod_{j=1}^{n} \left(g^{(j)}\right)^{p_j}$$

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$$\partial^m a_i^l = \sum_j w_{ij}^l \partial^m z_j^{l-1},$$

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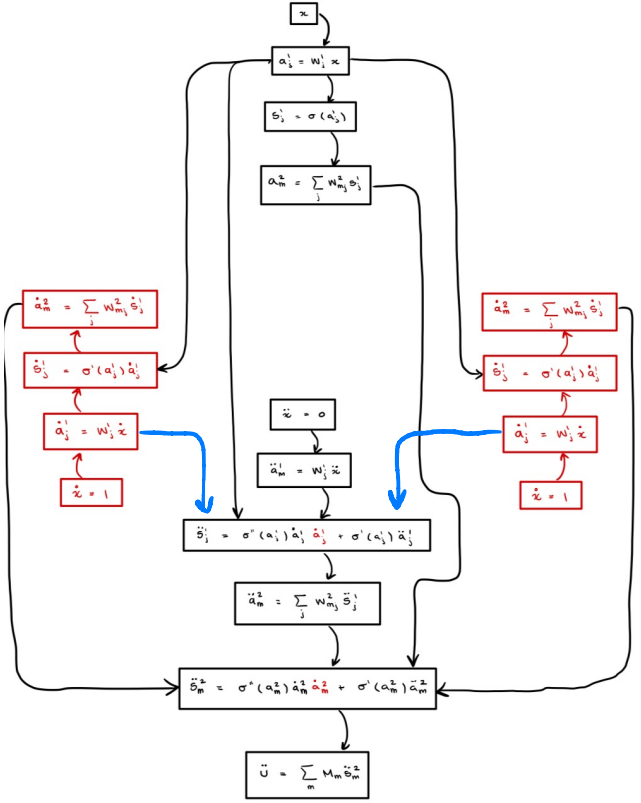
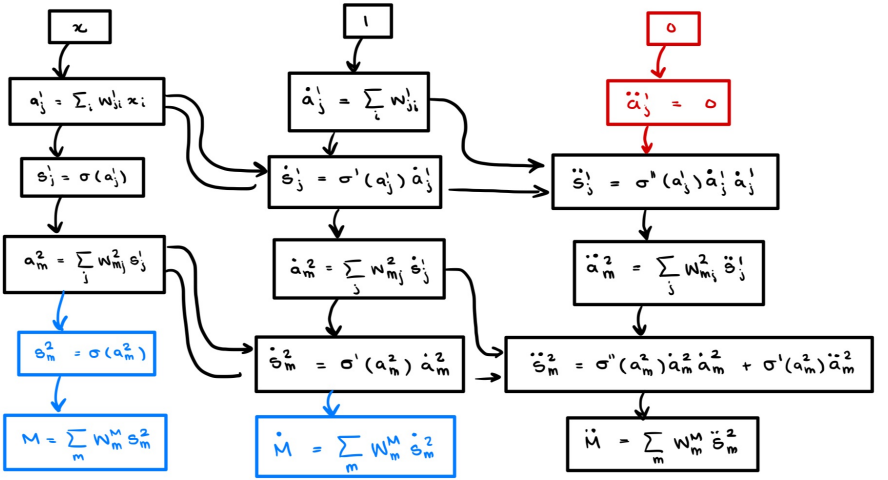
* Forces us to compute derivatives in order!

Computational Graphs



Autodiff



n-Tangent Prop

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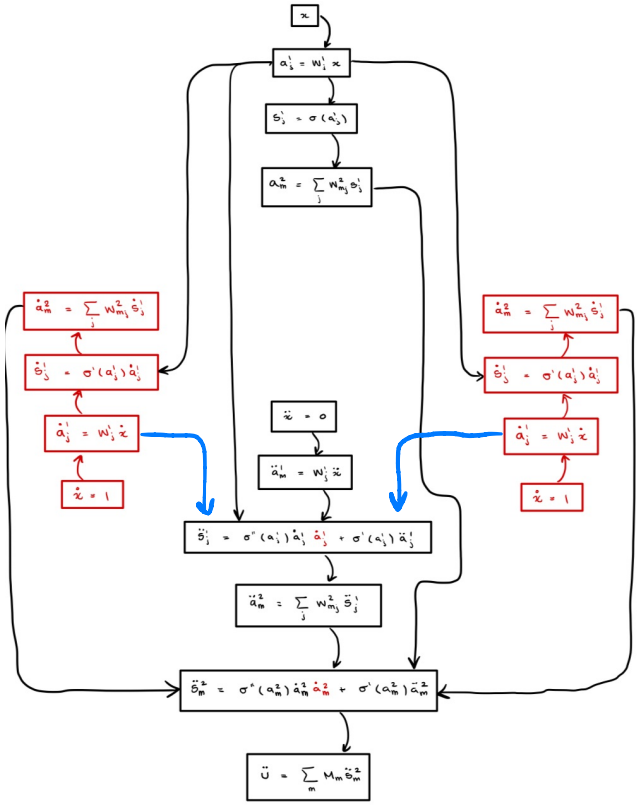

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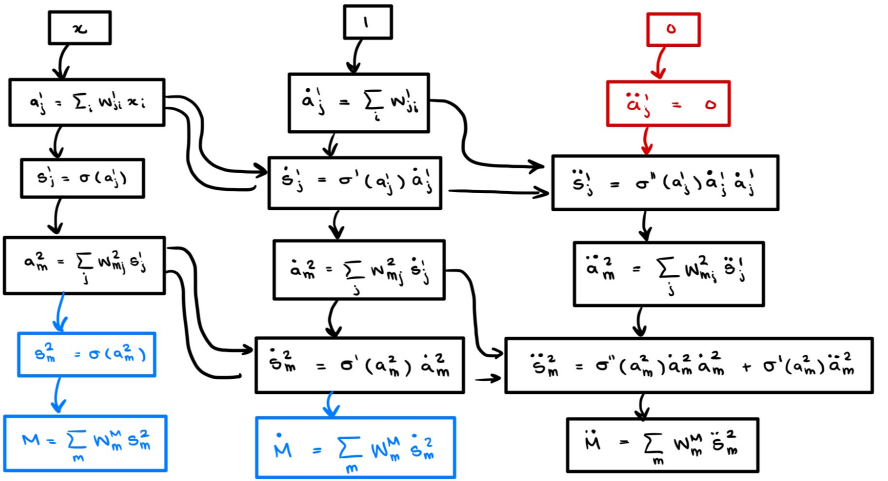

n-Tangent Prop

To compute 0, 1, 2 derivs:

AD: 18 + 10 + 6 = 34 nodes

nTP: 18 nodes

Runtime Analysis

- Linear # of nodes in computation graph

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- Assume original computation time is $\Theta(C)$, then

Ad: $\Theta(2^n C)$, exponential

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- Ignores a lot: We will do empirical analysis below

Pedantic Runtime Analysis I

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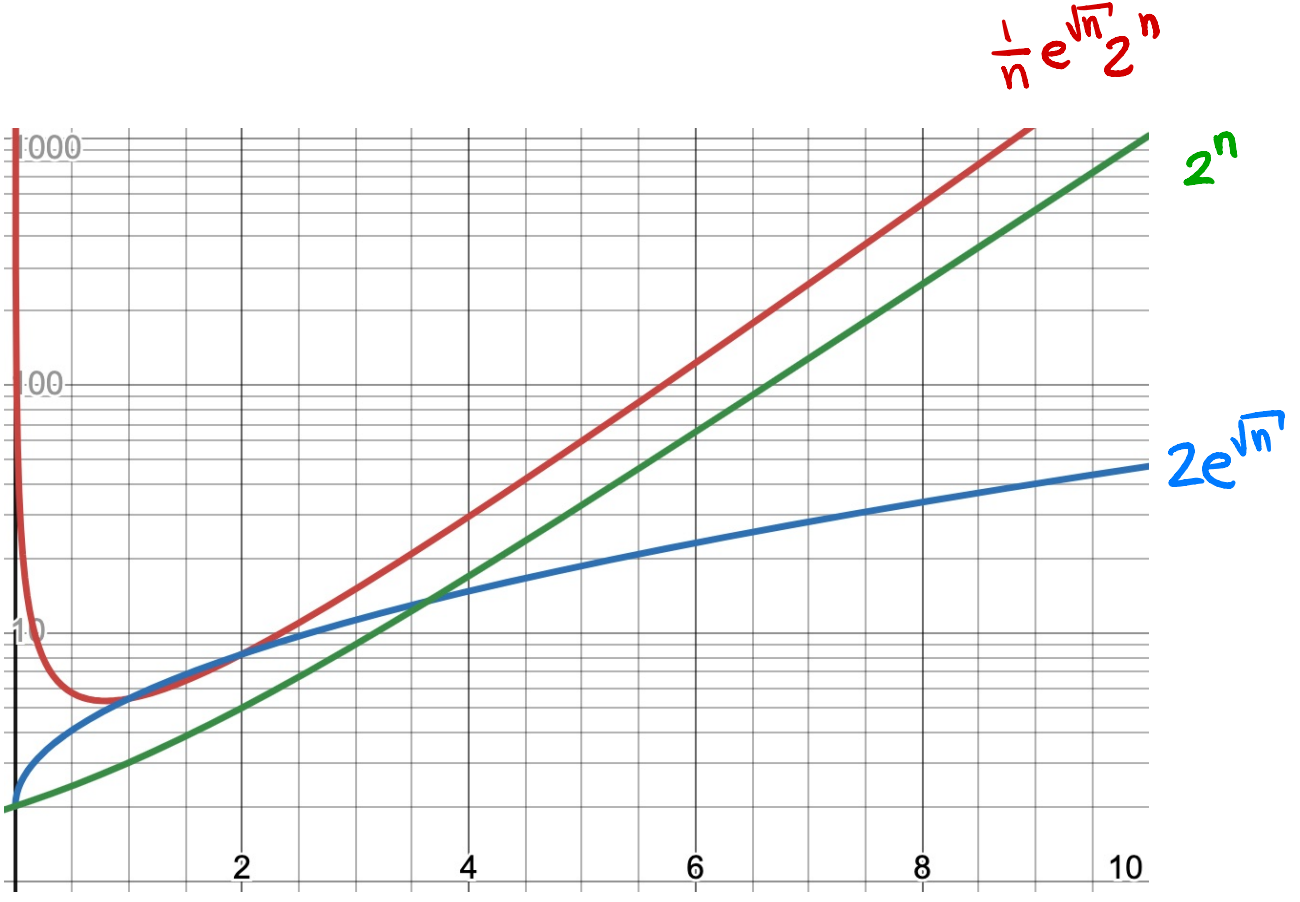
$$\text{AD} = \Theta\left(\frac{e^{\sqrt{n}}}{n} 9^n\right), \quad \text{nTP} = \Theta\left(e^{\sqrt{n}}\right)$$

Pedantic Runtime Analysis II



Results

Results: Neural Network I

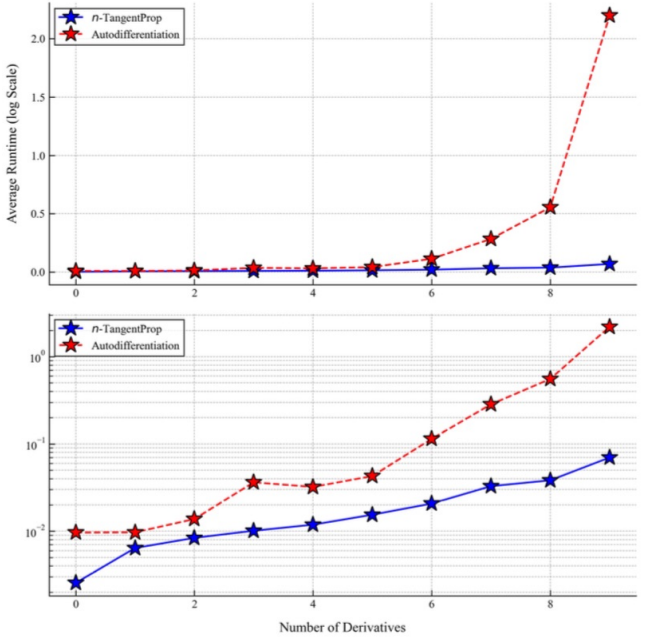


Fig. 1. Average runtime for a combined forward and backwards pass using autodifferentiation (red) and n-TangentProp (blue). The top and bottom frames show the same data, however the bottom frame is plotted with a logarithmic y-axis. Each model is run 100 times and the average for each trial is plotted. The network has 3 hidden layers of 24 neurons each, a common PINN architecture. The batch size is $2^8 = 256$ samples. The forward and backwards pass times are shown separately in Figures 2 and 3 respectively.

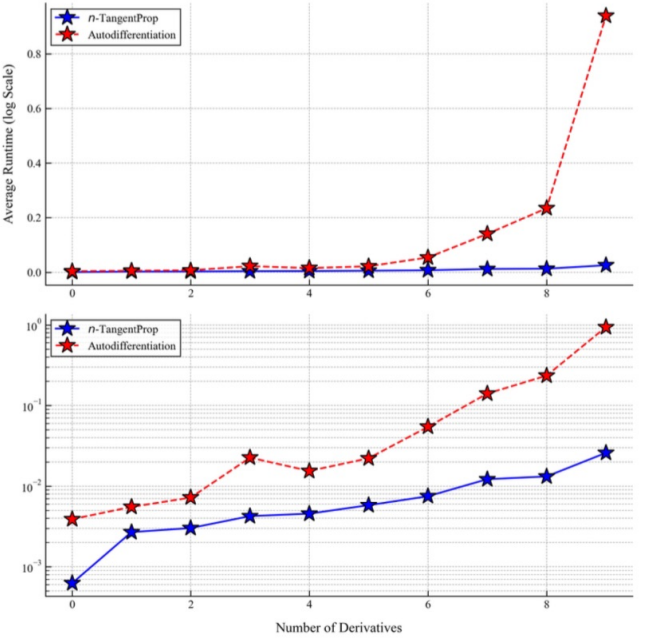
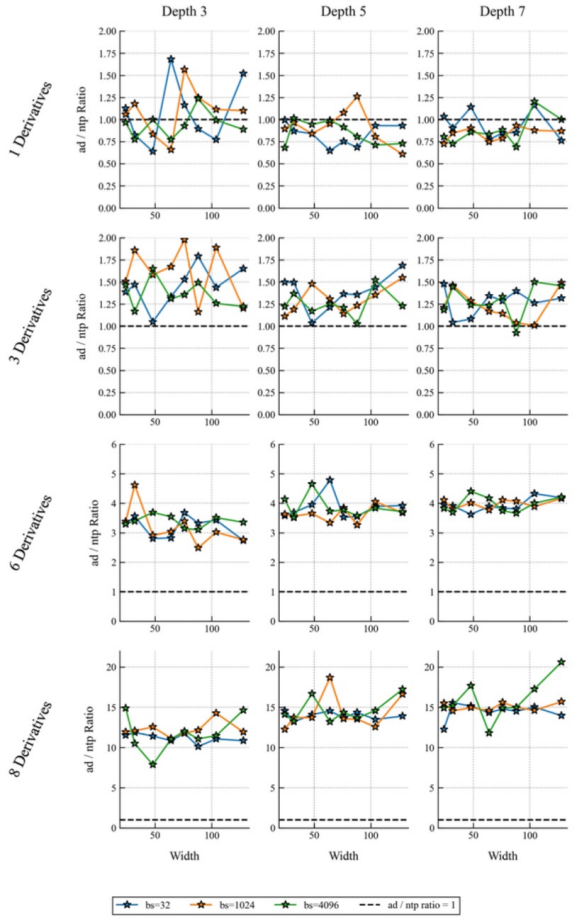


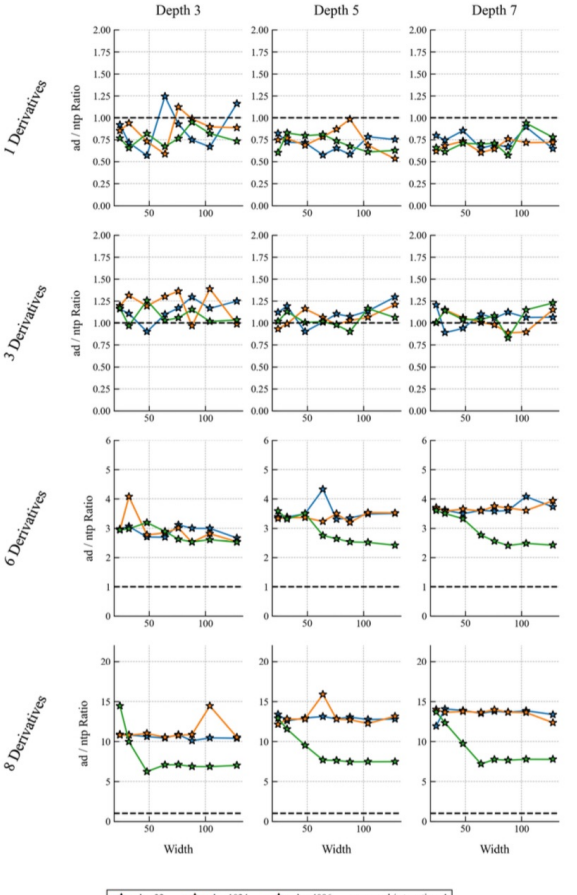
Fig. 2. Forward pass times for the model shown in Figure 1. The top and bottom frames show the same data, however the bottom frame is plotted with a logarithmic y-axis. Each model is run 100 times and the average for each trial is plotted. The network has 3 hidden layers of 24 neurons each, a common PINN architecture. The batch size is $2^8 = 256$ samples.

Results: Neural Networks II

Forward



Combined



Self-Similar Burgers I

- Burgers: $\partial_t u + u \partial_x u = 0$

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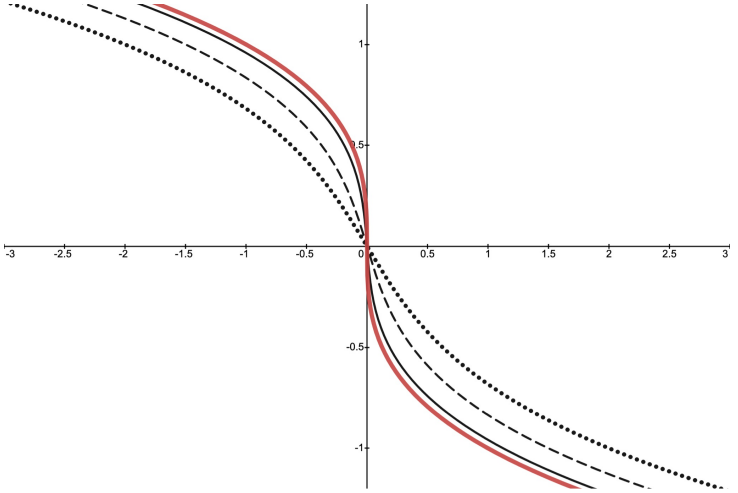

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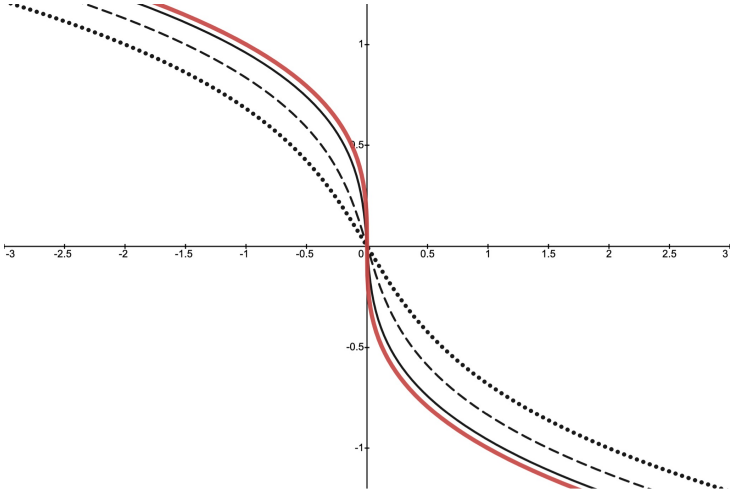

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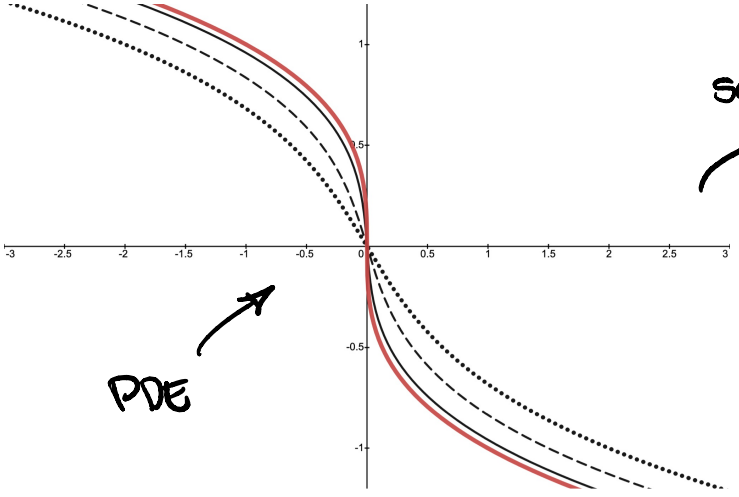
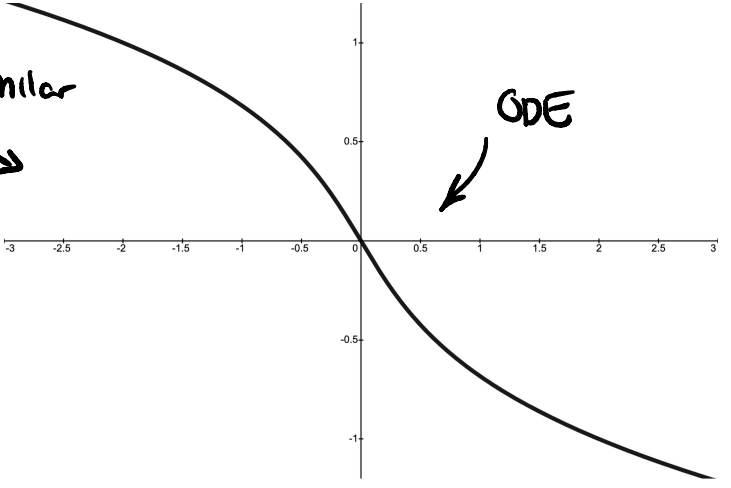


self-similar



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- PINN: Solve for W, λ <u>simultaneously</u>

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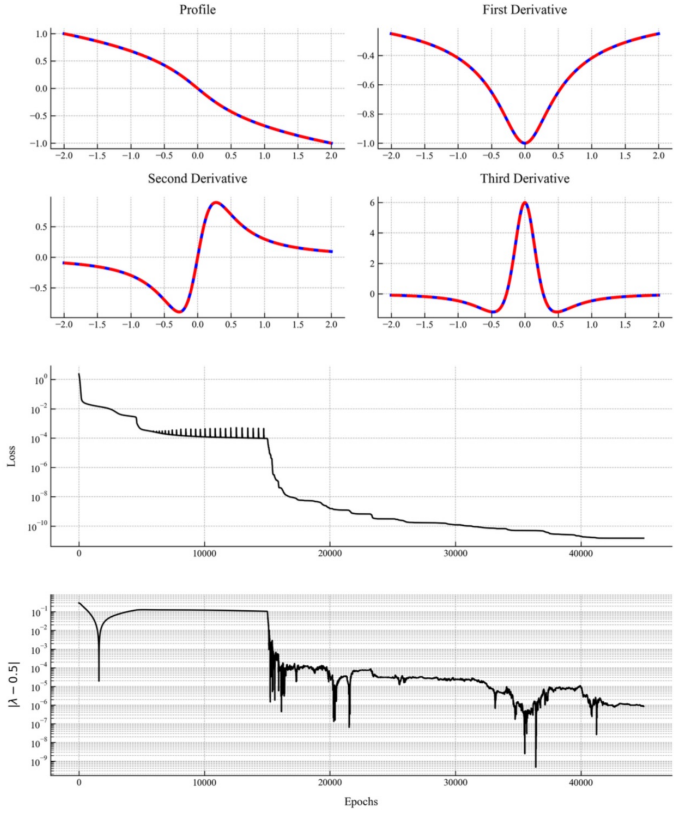

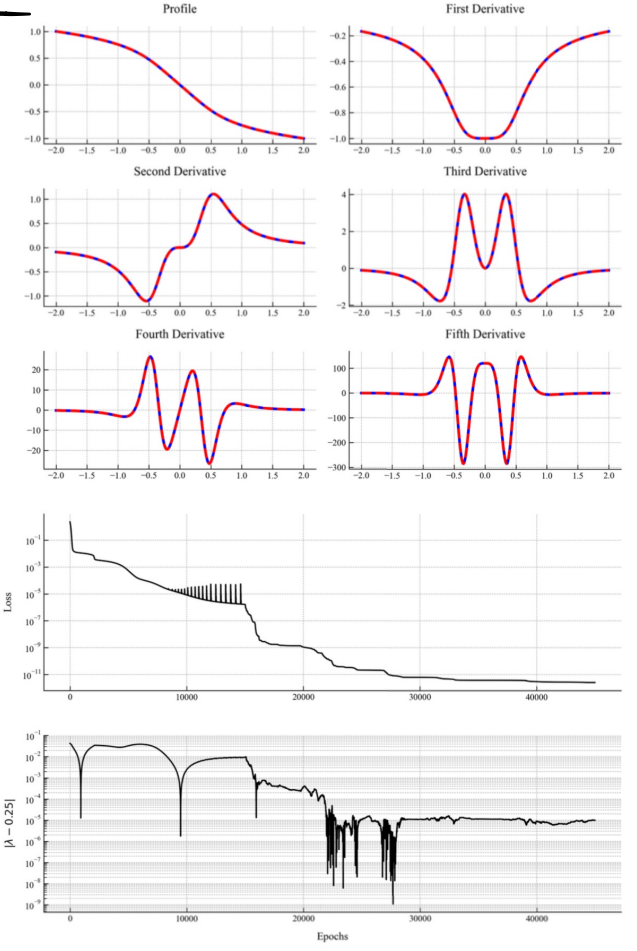

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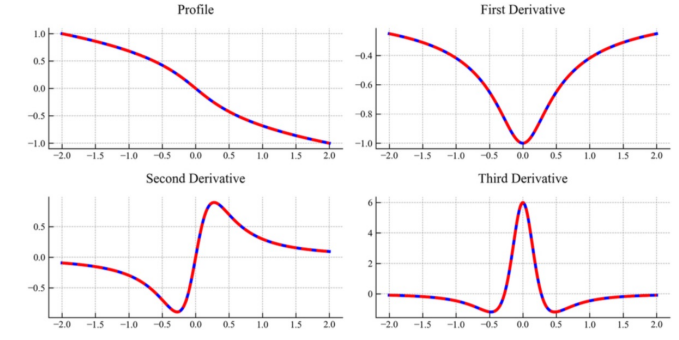
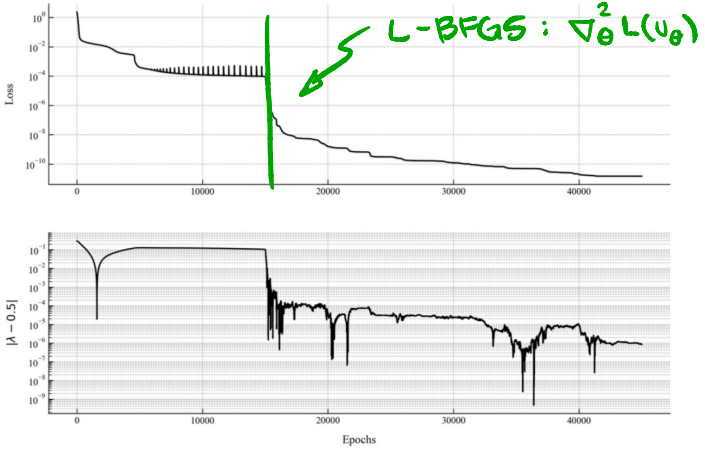
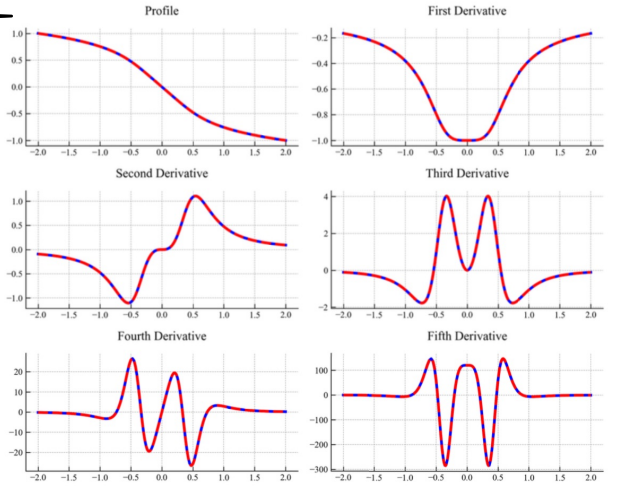
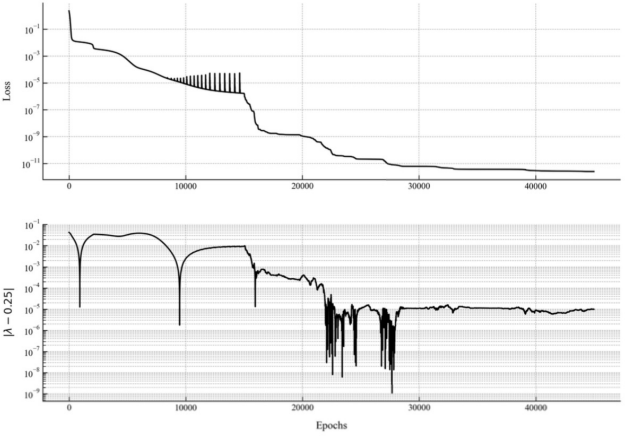
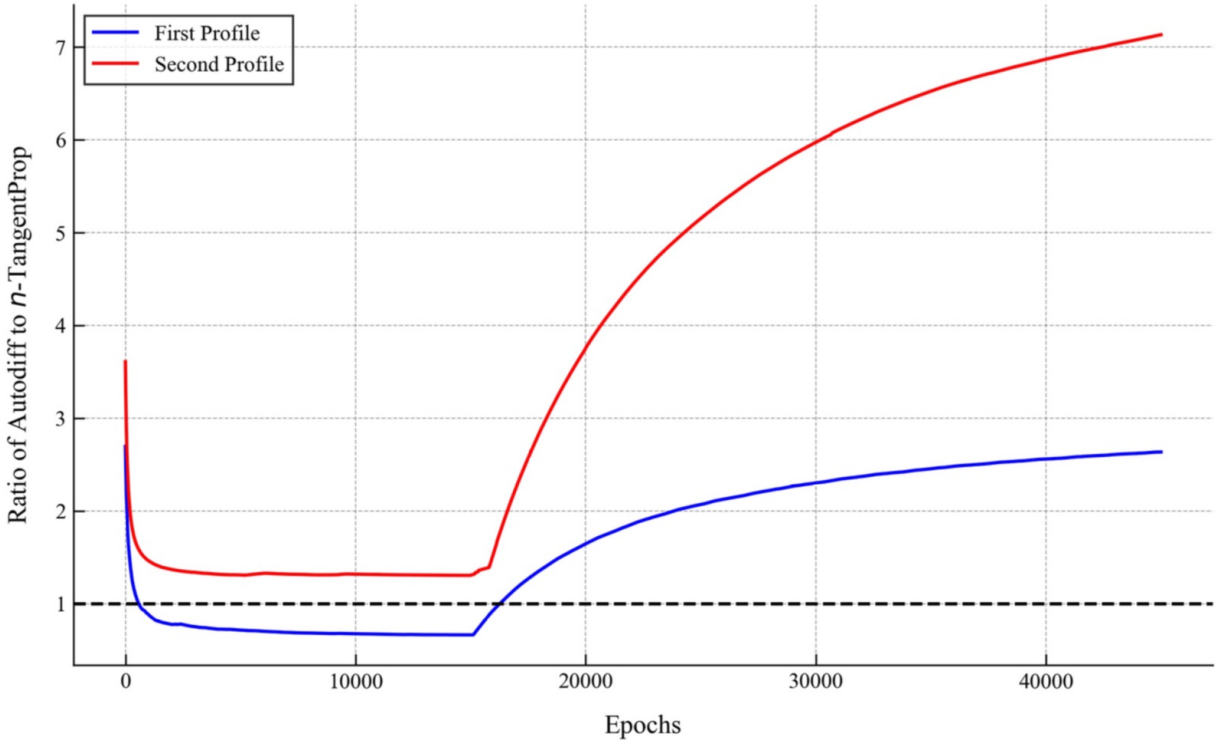








Results: Self-Similar Burgers II



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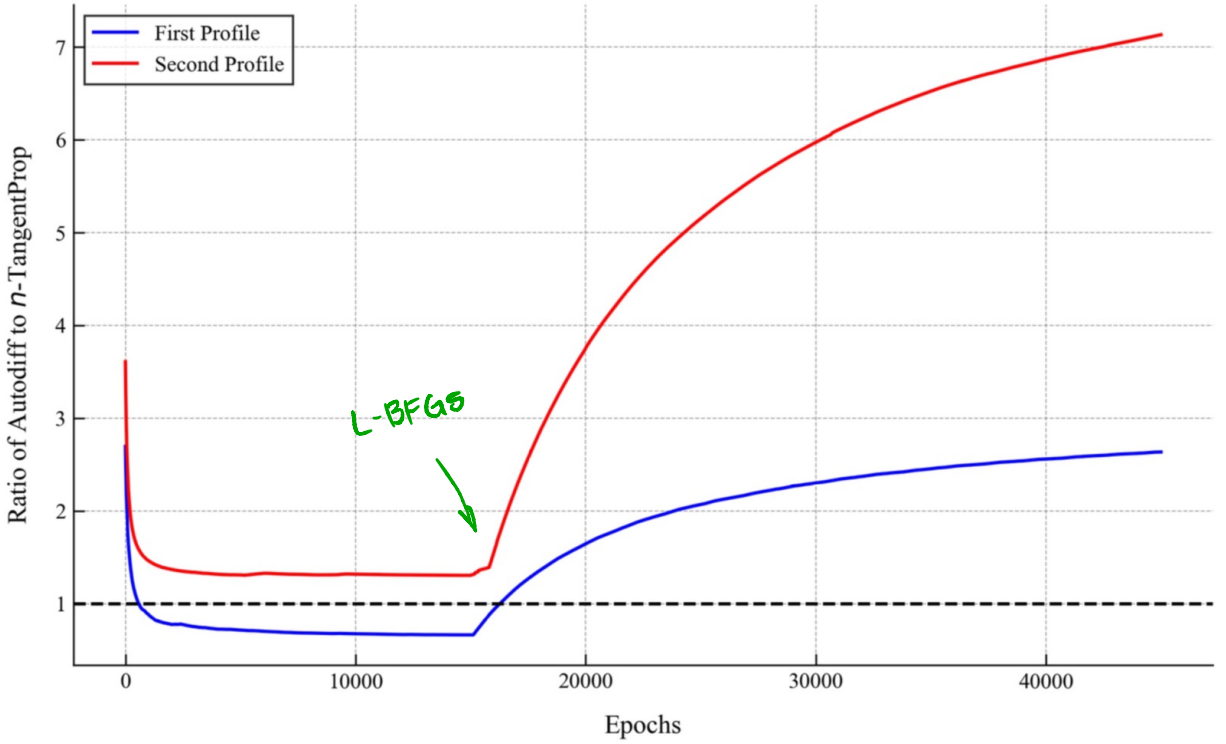
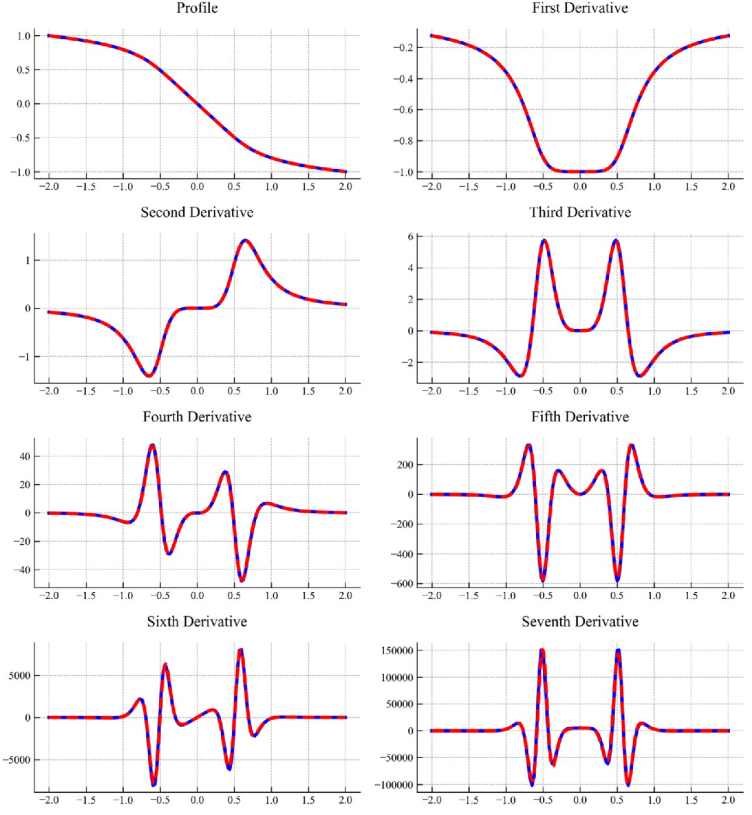
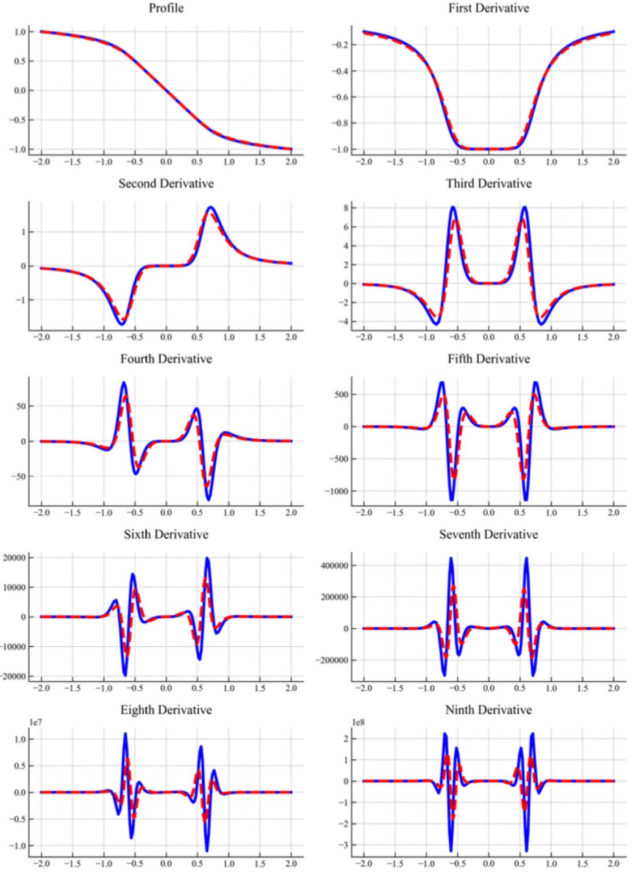


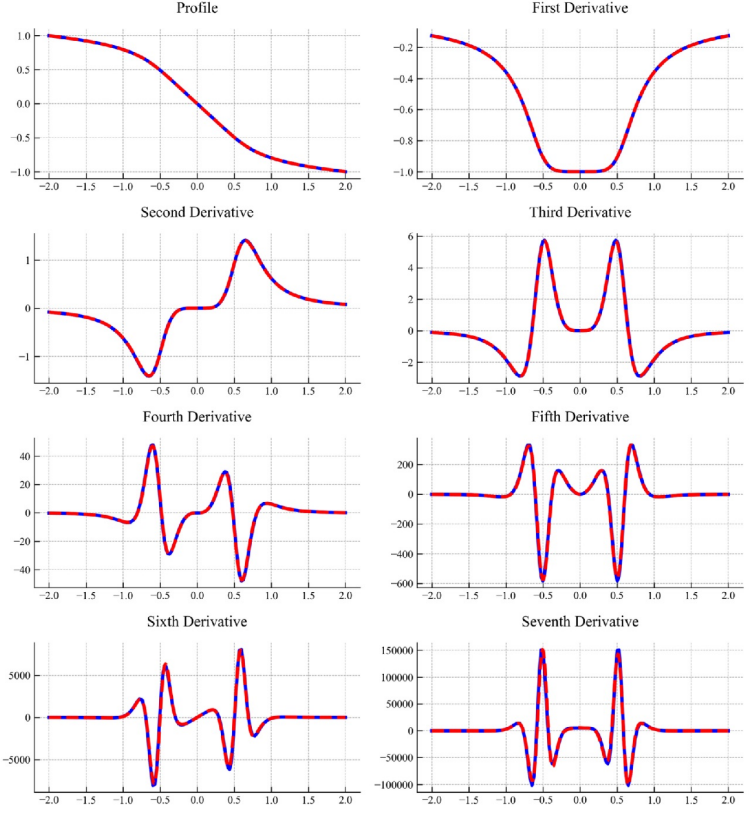
Results : Self-Similar Burgess III

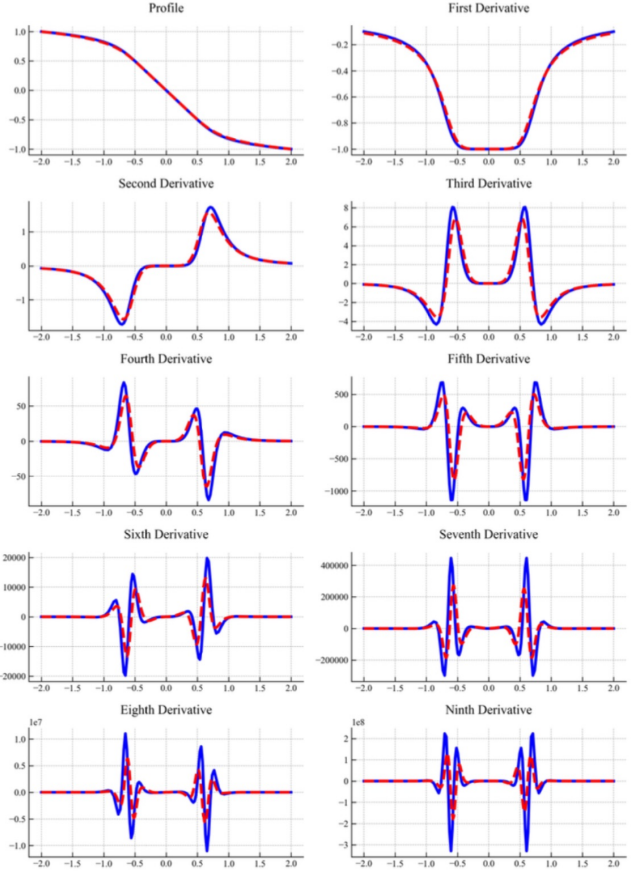




Results : Self-Similar Burgess III

26x Faster





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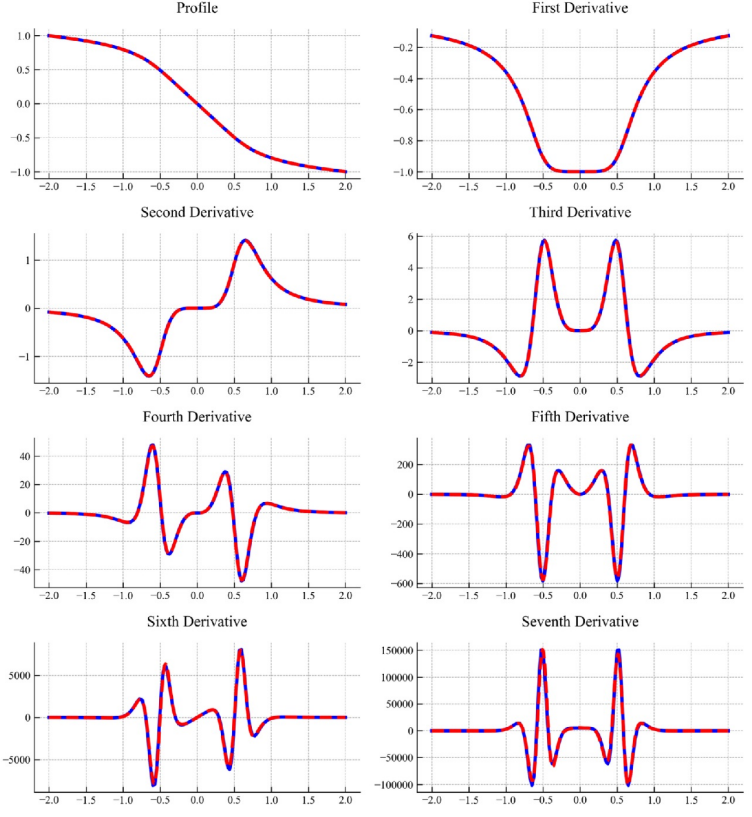
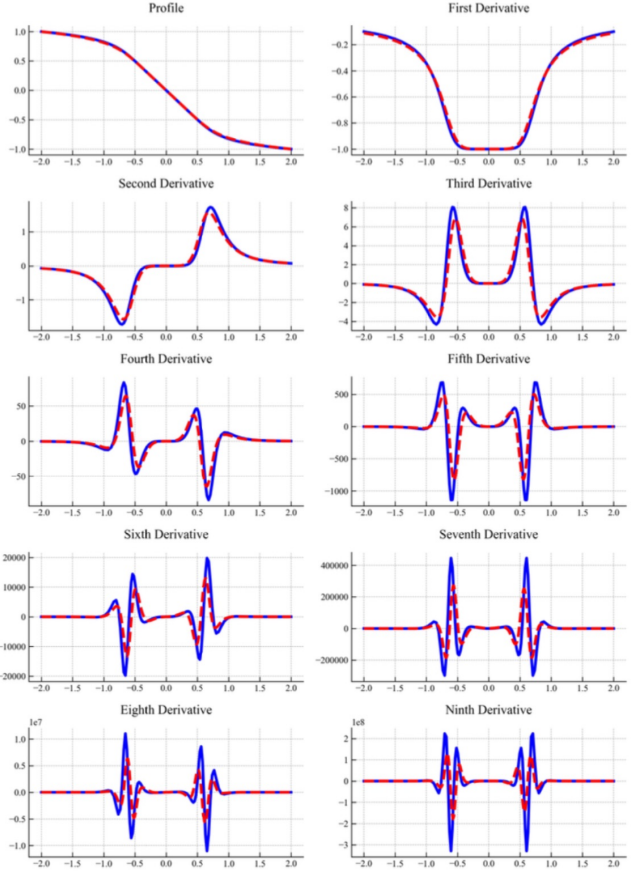


65x Faster



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- More accurate solutions, ~3x faster for simple problem, 65+ x faster on harder problem.

Thank You!