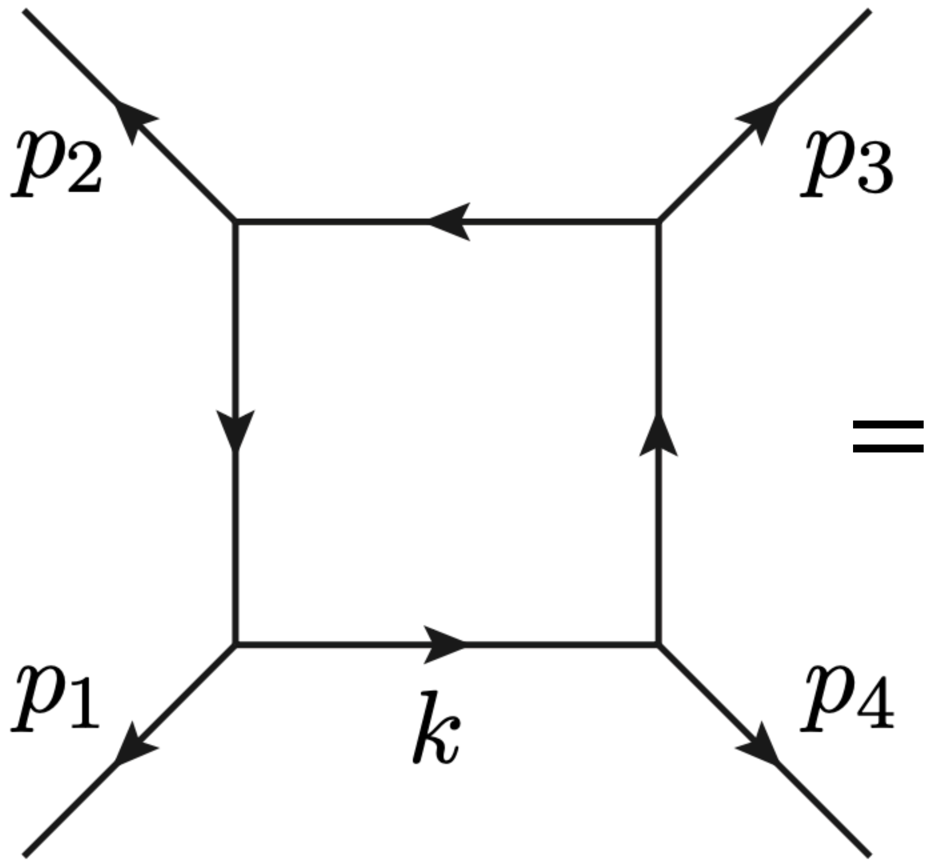
Learning Feynman integrals from differential equations with neural networks

Simone Zoia

Francesco Calisto, Ryan Moodie, SZ (arXiv:2312.02067)

Milan Christmas Meeting, 20th Dec 2023

We need to evaluate Feynman integrals



$$= \int \frac{\mathrm{d}^D k}{\mathrm{i}\pi^{D/2}} \frac{1}{k^2 \, (k+p_1)^2 \, (k+p_1+p_2)^2 \, (k+p_1+p_2+p_3)^2}$$

Essential ingredients of perturbative computations → particle phenomenology

Also: gravitational waves, cosmology, statistical mechanics, mathematics…

Many techniques developed over many years, yet they remain a bottleneck

Integrating by differentiating

[Barucchi, Ponzano ’73; Kotikov ’91; Bern, Dixon, Kosower ‘94; Gehrmann, Remiddi 2000; Henn 2013]

View Feynman integrals as solutions to PDEs

$$\frac{\partial}{\partial s_{12}} \vec{\mathrm{F}}(s;\epsilon) = A_{s_{12}}(s;\epsilon) \cdot \vec{\mathrm{F}}(s;\epsilon)$$

Most powerful tool for analytic computation of Feynman integrals

Neat connection with study of special functions

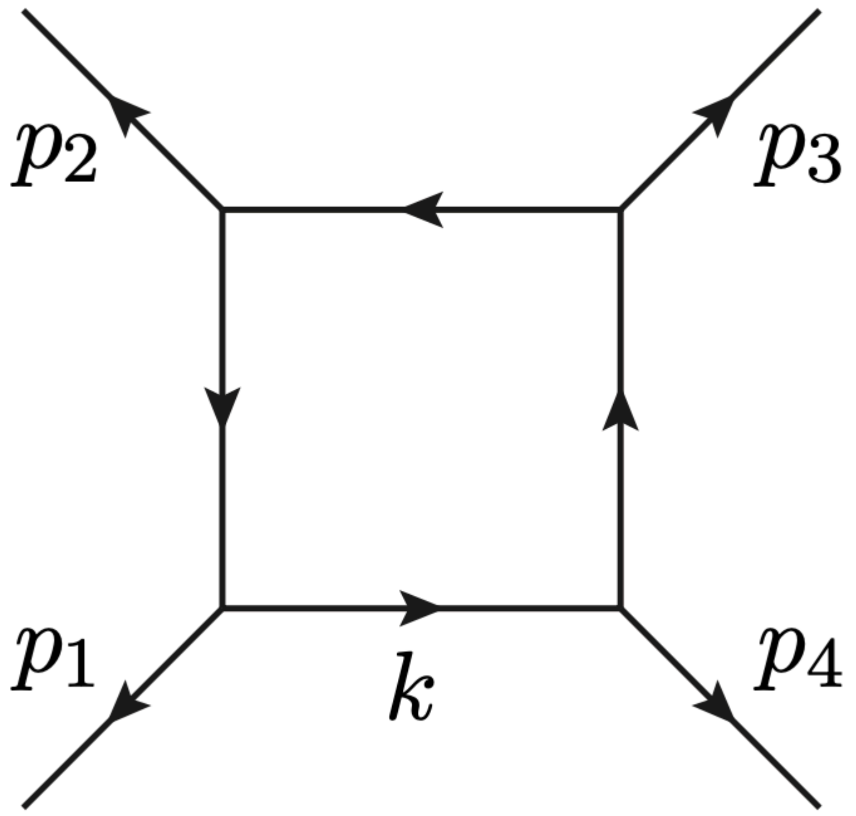
Growing interest for numerical solution

Method of differential equations

$$\frac{\partial}{\partial s_{12}} \overrightarrow{\mathrm{F}}(s;\epsilon) = A_{s_{12}}(s;\epsilon) \cdot \overrightarrow{\mathrm{F}}(s;\epsilon)$$

Integral families and master integrals

Scalar Feynman integrals with the same propagator structure = **integral family**



$$\mathrm{I}_{\vec{a}}(s,t;\epsilon) = \int \frac{\mathrm{d}^D k}{\mathrm{i}\pi^{D/2}} \frac{1}{D_1^{a_1} \ldots D_4^{a_4}}$$

$$\left\{ \mathrm{I}_{\vec{a}}(s,t;\epsilon) \,|\, \forall\, \vec{a} \in \mathbb{Z}^4 \right\}$$

$$D_1 = k^2$$
$$D_2 = (k + p_1)^2$$
$$D_3 = (k + p_1 + p_2)^2$$
$$D_4 = (k - p_4)^2$$

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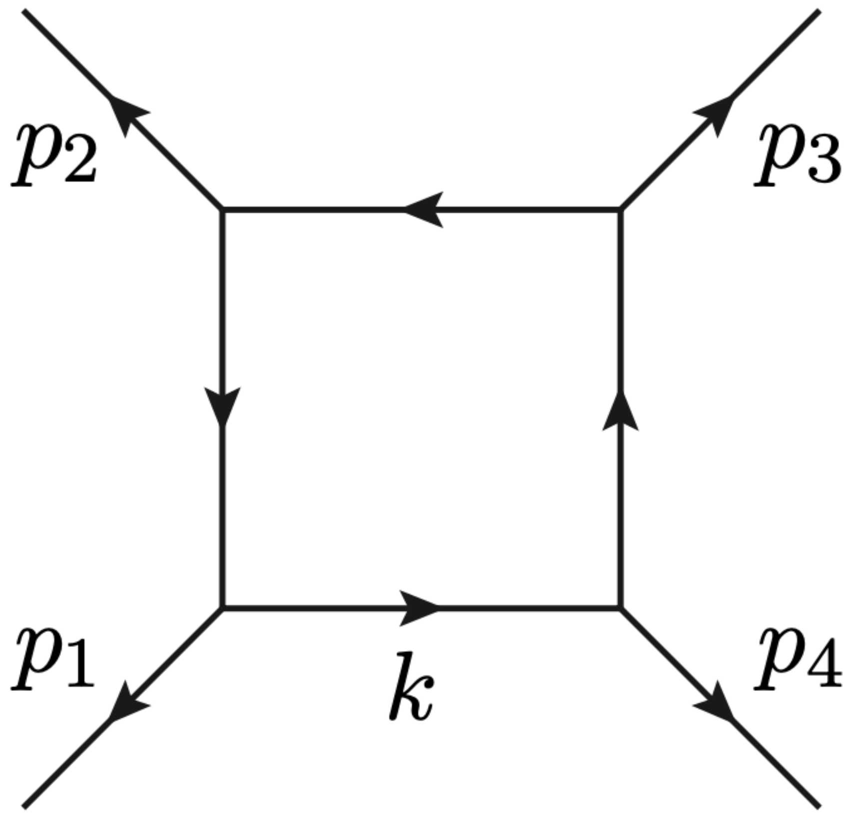

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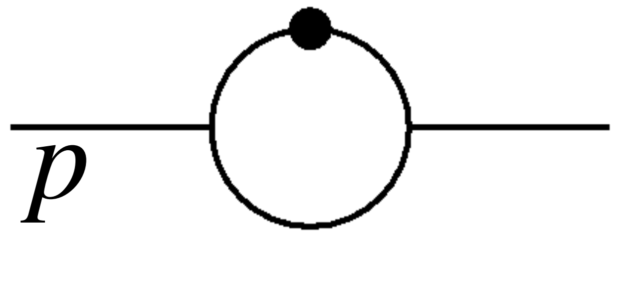
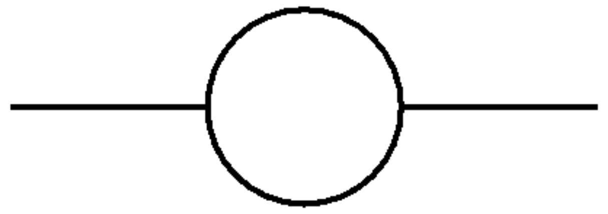
Identities among the $\mathrm{I}_{\vec{a}}$'s



$$= \frac{3-D}{p^2} \times$$



e.g. Integration-By-Parts relations

[Chetyrkin, Tkachov '81; Laporta 2000]

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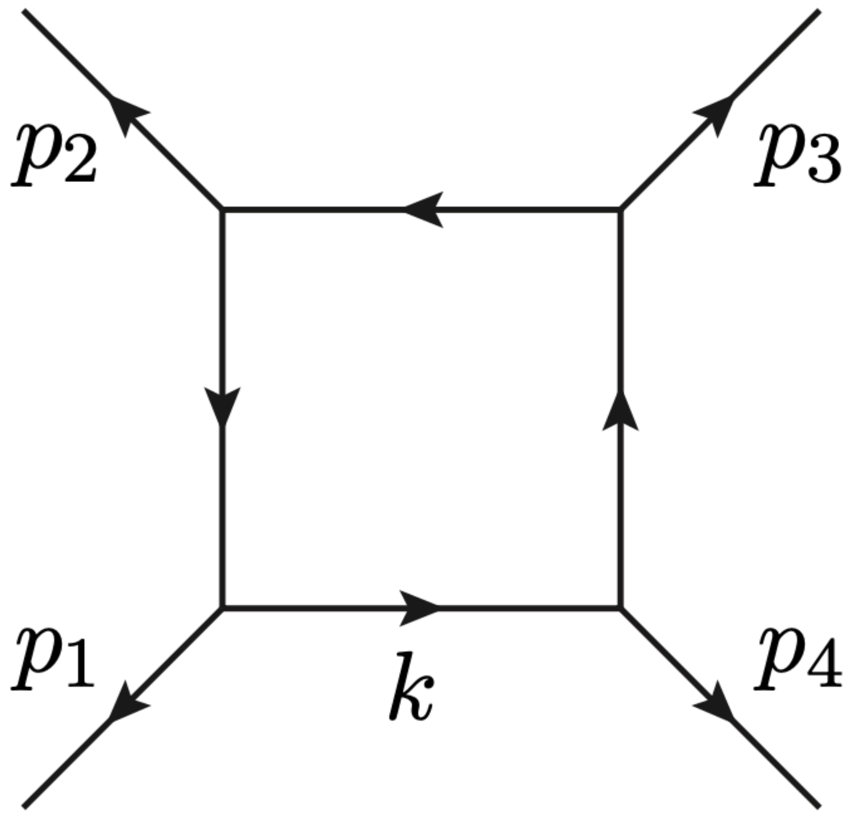

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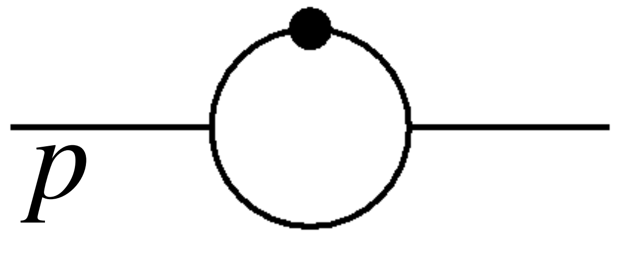
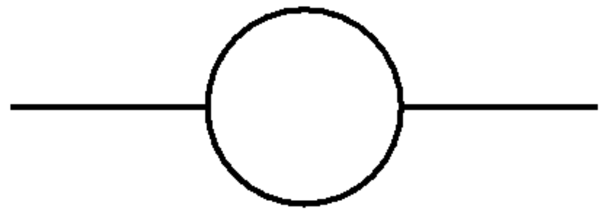


$= \frac{3-D}{p^2} \times$


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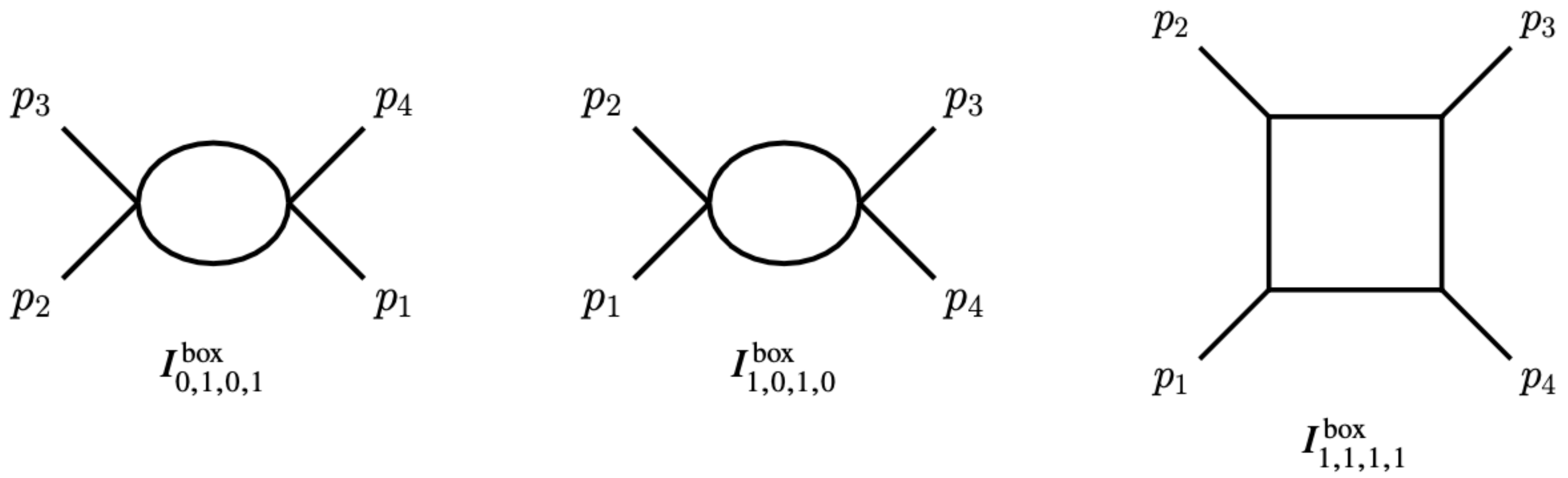
$\Rightarrow$

Finite-dimensional basis:
master integrals $\overrightarrow{\mathrm{F}}(s,t;\epsilon)$



Integrating by differentiating

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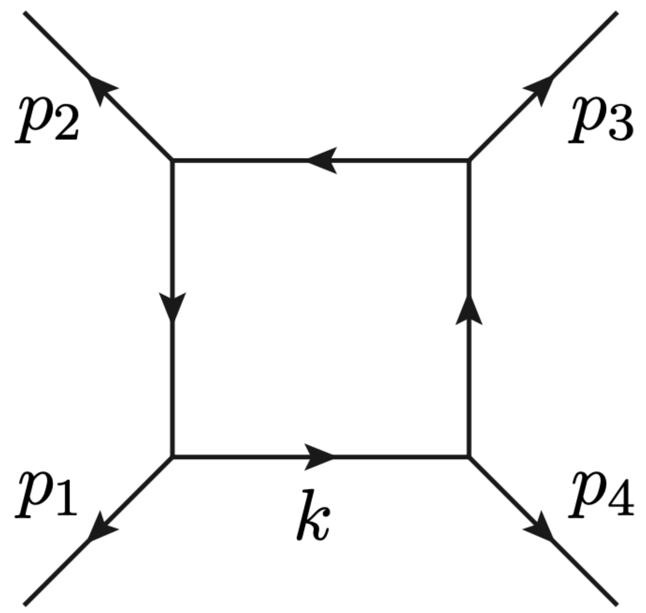
$$\frac{\partial}{\partial s_{12}} \vec{\mathrm{F}}(s;\epsilon) = \sum_{\vec{a}} c_{\vec{a}}\, \mathrm{I}_{\vec{a}}$$

$$= A_{s_{12}}(s;\epsilon) \cdot \vec{\mathrm{F}}\,(s;\epsilon)$$

IBP reduction

$$\frac{\partial}{\partial s}\vec{F}(s,t;\epsilon) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{\epsilon}{s} & 0 \\ \frac{2(2\epsilon-1)}{st(s+t)} & \frac{2(1-2\epsilon)}{s^2(s+t)} & -\frac{s+t+\epsilon t}{s(s+t)} \end{pmatrix} \cdot \vec{F}(s,t;\epsilon)$$



$\Rightarrow$ System of 1st order linear PDEs for the MIs $\vec{\mathrm{F}}$

How do we solve it? $$\vec{\mathrm{F}}(s;\epsilon) = \sum_{w \geq w_{\min}} \epsilon^w\, \vec{\mathrm{F}}^{(w)}(s)$$

Analytic solution not always feasible

Choose MIs such that DEs take **canonical form** *[Henn 2013]* ← No general algorithm!

Best understood cases: solution in terms of multiple polylogarithms 🥳

More complicated classes of functions do appear (e.g. elliptic MPLs)

→ Mathematical technology much less mature 😵‍💫

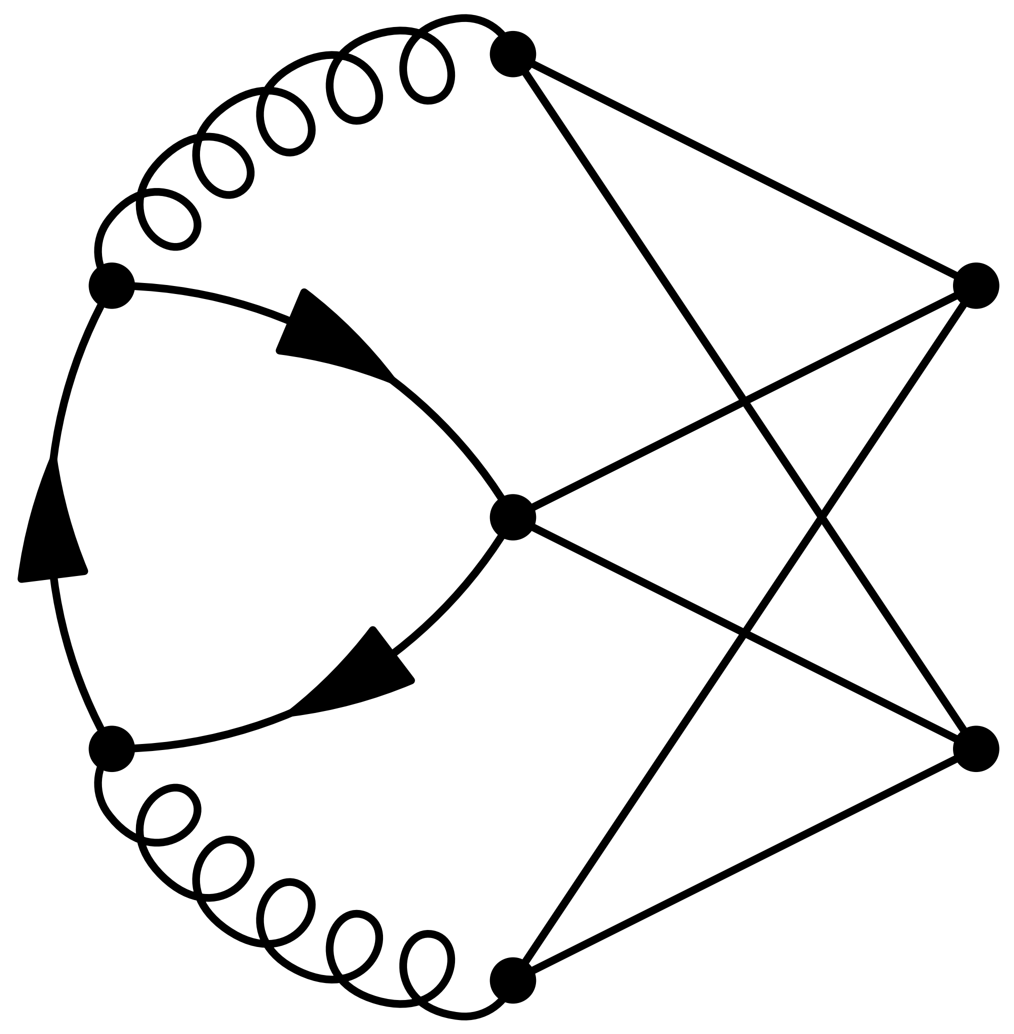
Growing interest for semi-numerical solution based on series expansions *[Moriello 2019]* → G. Fontana's talk

DiffExp *[Hidding 2020]*, SeaSyde *[Armadillo et al. 2022]*, AMFlow *[Ma, Liu 2022]*

😄 Very flexible (canonical form not required)

🙁 Long evaluation times

Physics-informed deep learning



Neural networks are universal function approximators

[Hornik, Stinchcombe, White '89]

Typical problem: approximate function $f(x)$ from large dataset of values $f(x_i)$

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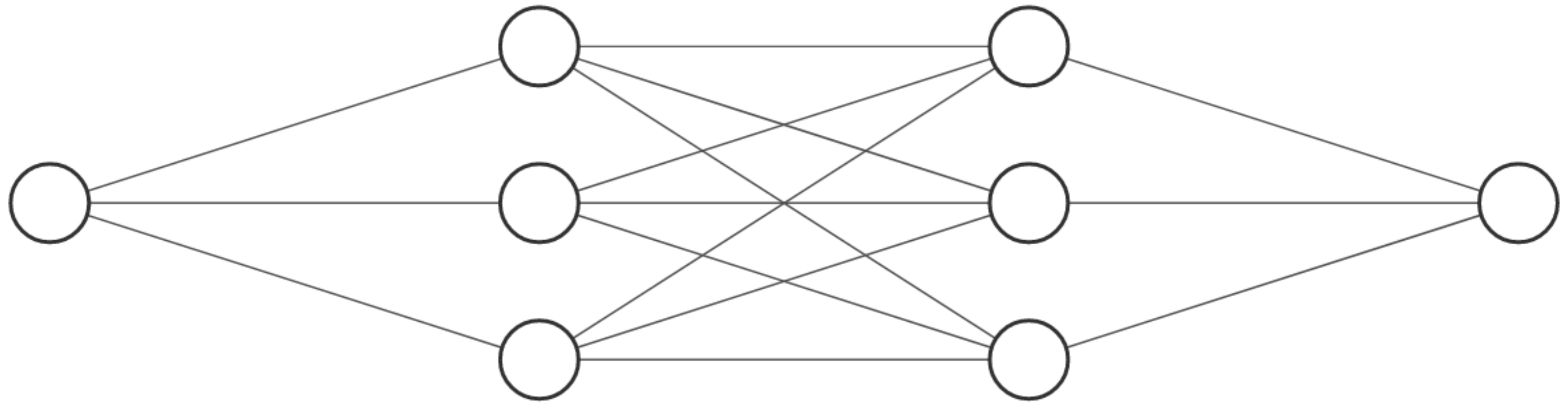

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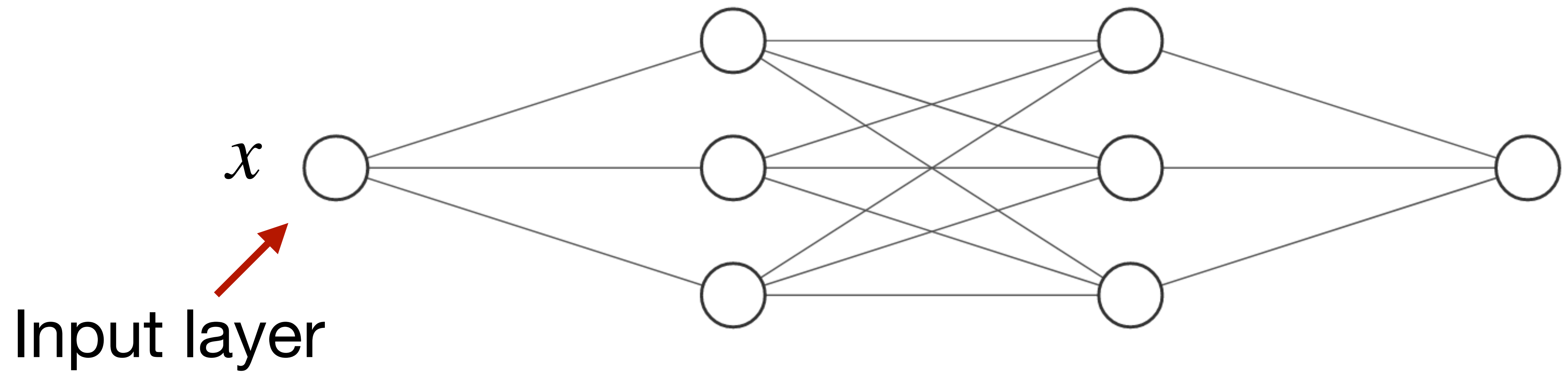

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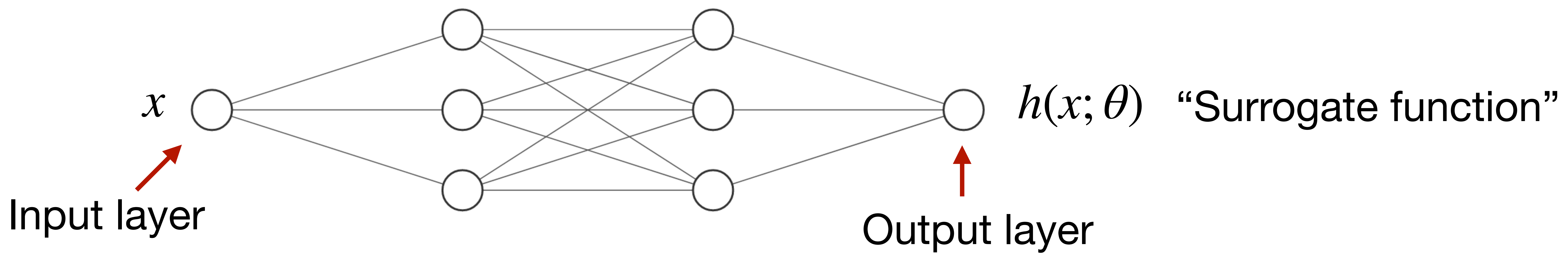

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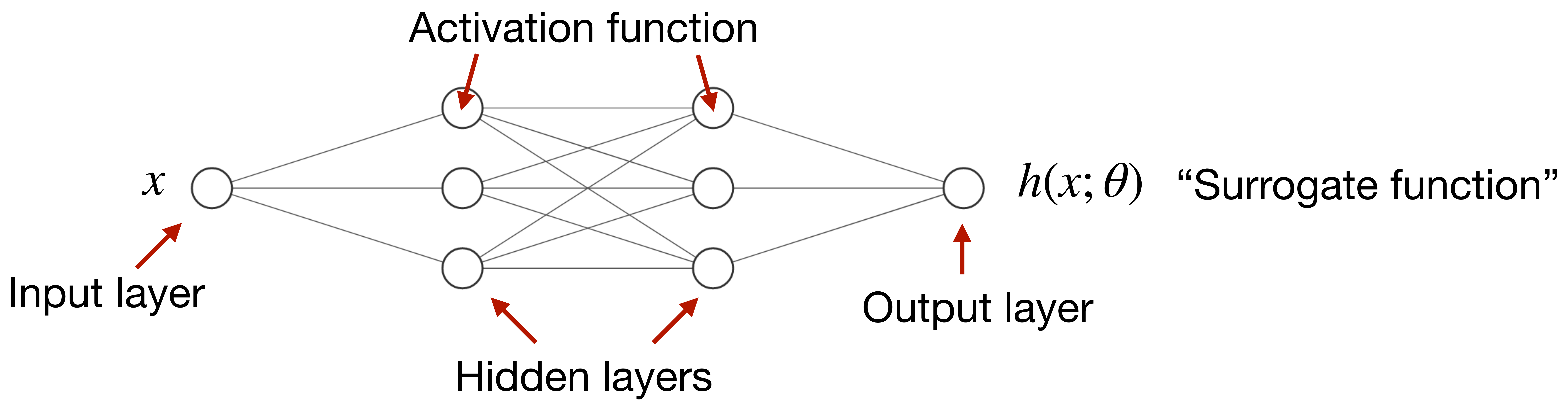

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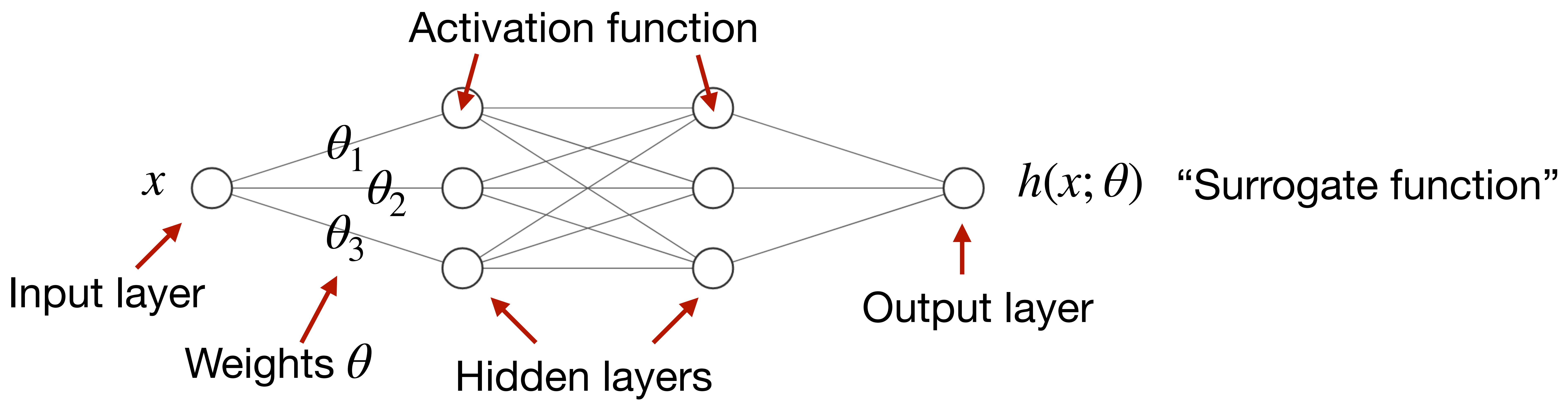

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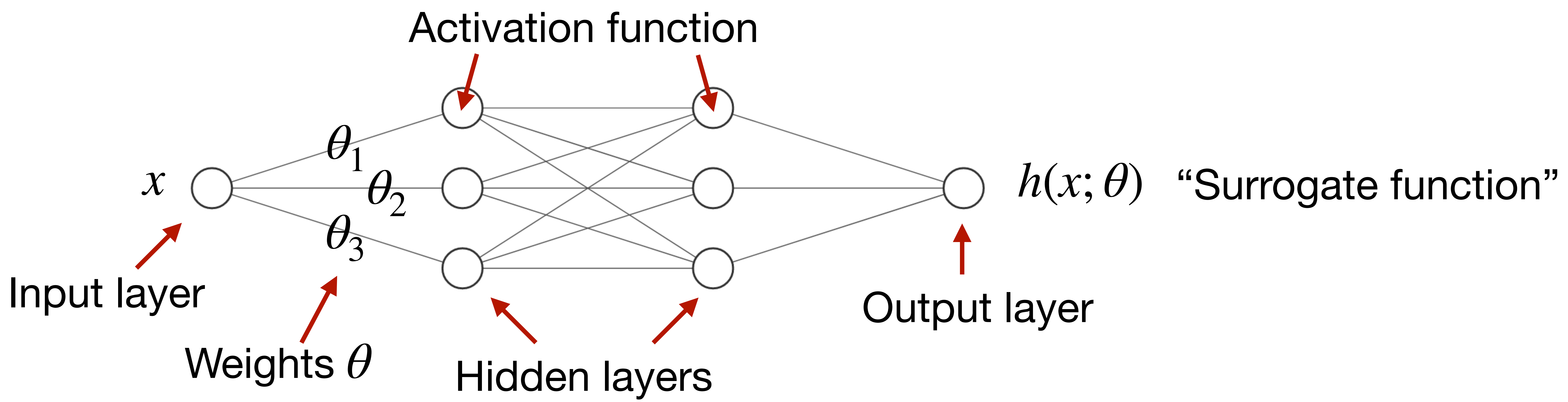

Optimisation problem: find weights θ such that a **loss function** is minimised

$$L(\mathrm{D};\theta) = \frac{1}{N}\sum_{i=1}^{N}\left[f(x_i) - h(x_i;\theta)\right]^2$$

We don’t have a large dataset…

What we have:

- Small dataset of values (at least 1), obtained numerically in other ways

  E.g. AMFlow *[Liu, Ma 2022]* → Expensive evaluation, but very flexible

- Differential equations: $$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = A(x)\,f(x)$$

Physics-informed deep learning

[Raissi, Perdikaris, Karniadakis 2017]

💡 Idea: include the DEs in the loss function

$$L(\mathrm{D};\theta) = \overline{\sum_i} \left[h(x_i;\theta) - f(x_i)\right]^2 + \overline{\sum_j} \left[\left.\frac{\mathrm{d}h(x;\theta)}{\mathrm{d}x}\right|_{x=x_j} - A(x_j)\, h(x_j;\theta)\right]^2$$

Small “boundary” dataset

Infinite dimensional “DE” dataset

Derivatives of the NN computed with automatic differentiation *[Griewank, Walther 2008]*

Input: few boundary values + the analytic DEs

The canonical form of the DEs is not needed

We make mild assumptions to simplify the problem:

$$\frac{\partial}{\partial v_i}\overrightarrow{F}(\vec{v};\epsilon) = A_{v_i}(\vec{v};\epsilon)\cdot\overrightarrow{F}(\vec{v};\epsilon) \quad \forall\, i = 1,\ldots,n_v$$

$\vec{v}$: kinematic variables

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$\vec{v}$: kinematic variables

1. The matrices $A_{v_i}(\vec{v};\epsilon)$ are rational functions $\Rightarrow$ Separate Re/Im parts, only deal with real numbers

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$\vec{v}$: kinematic variables

1. The matrices $A_{v_i}(\vec{v};\epsilon)$ are rational functions $\Rightarrow$ Separate Re/Im parts, only deal with real numbers

2. The matrices $A_{v_i}(\vec{v};\epsilon)$ are finite at $\epsilon = 0$,

$$A_{v_i}(\vec{v};\epsilon) = \sum_{k=0}^{k_{\max}} \epsilon^k A_{v_i}^{(k)}(\vec{v})$$

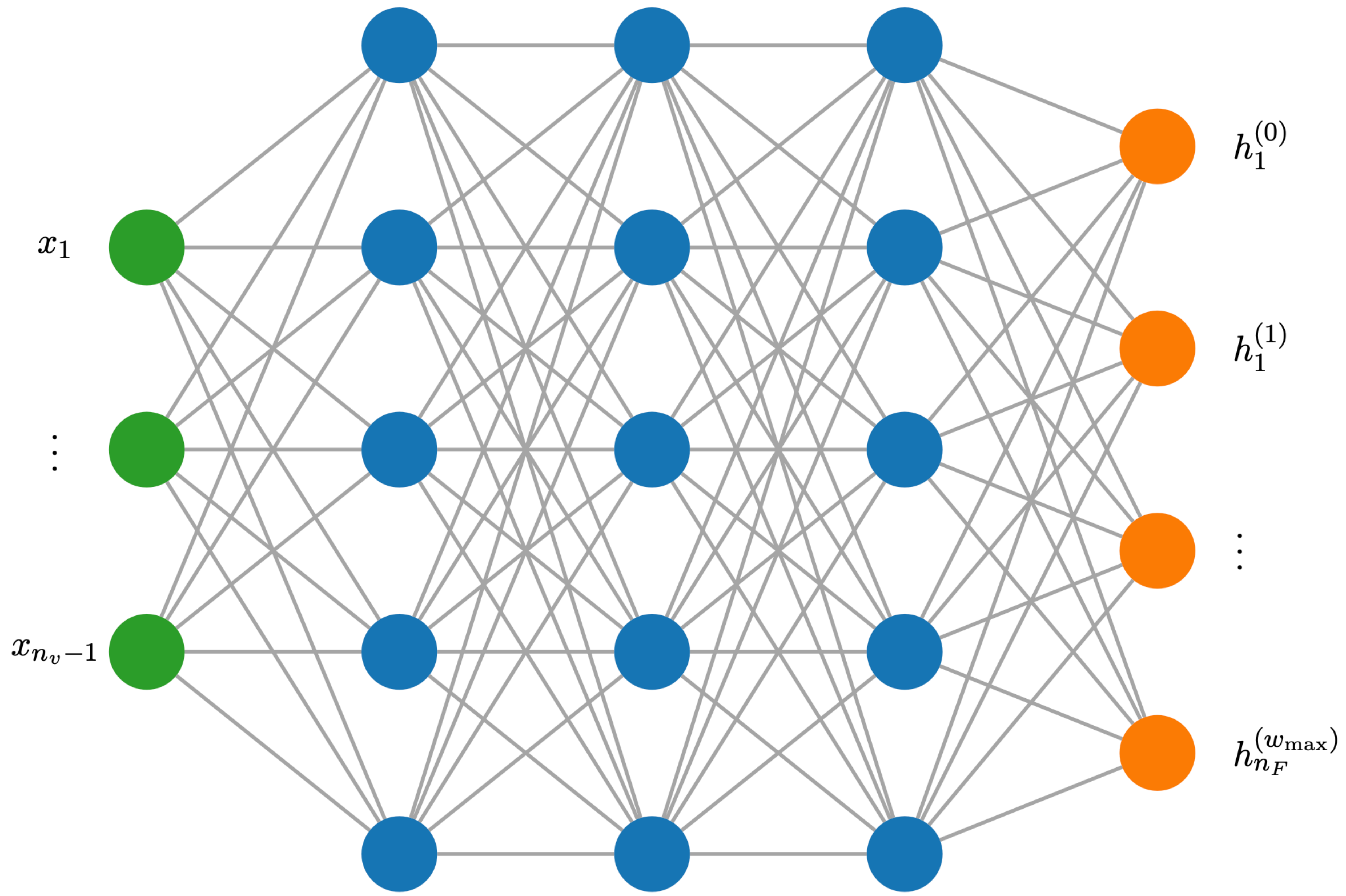
$\Rightarrow$ Simplifies the ϵ expansion of the solution

$$\overrightarrow{F}(\vec{v};\epsilon) = \epsilon^{w*} \sum_{w=0}^{w_{\max}} \epsilon^w \overrightarrow{F}^{(w)}(\vec{v})$$

Architecture

PyTorch

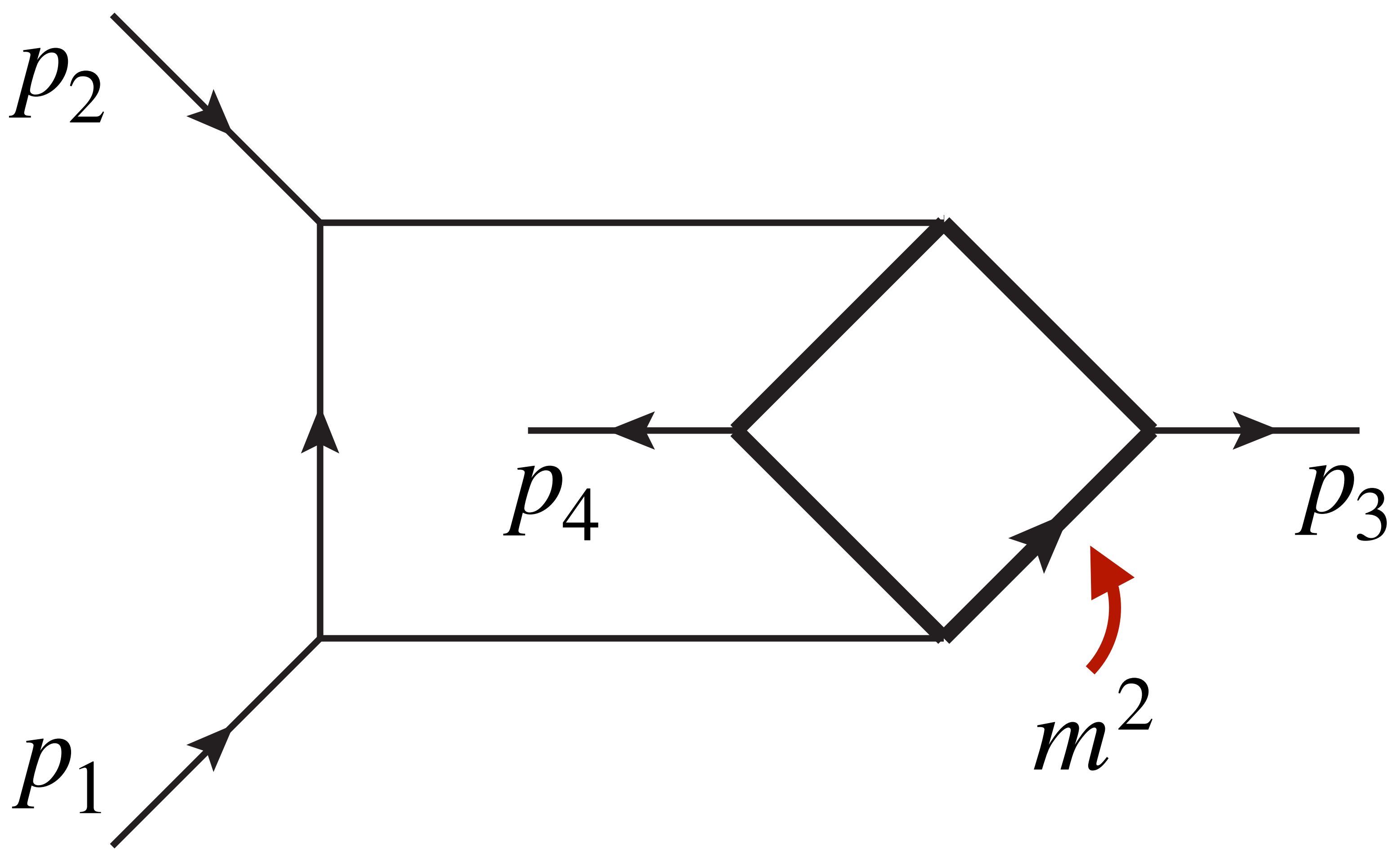
Dimensionless kinematic variables



Re or Im part of $\vec{F}^{(w)}$ up to a certain order in ϵ

In the examples we considered: 3/4 hidden layers, 32—256 nodes per layer

Heavy crossed box



3 kinematic variables, 36 MIs

$$\vec{v} = \left\{ s = (p_1 + p_2)^2 \,,\, t = (p_1 - p_3)^2 \,,\, m^2 \right\}$$

Canonical DEs / analytic solution unavailable

Subsectors involve elliptic functions

[von Manteuffel, Tancredi 2017]

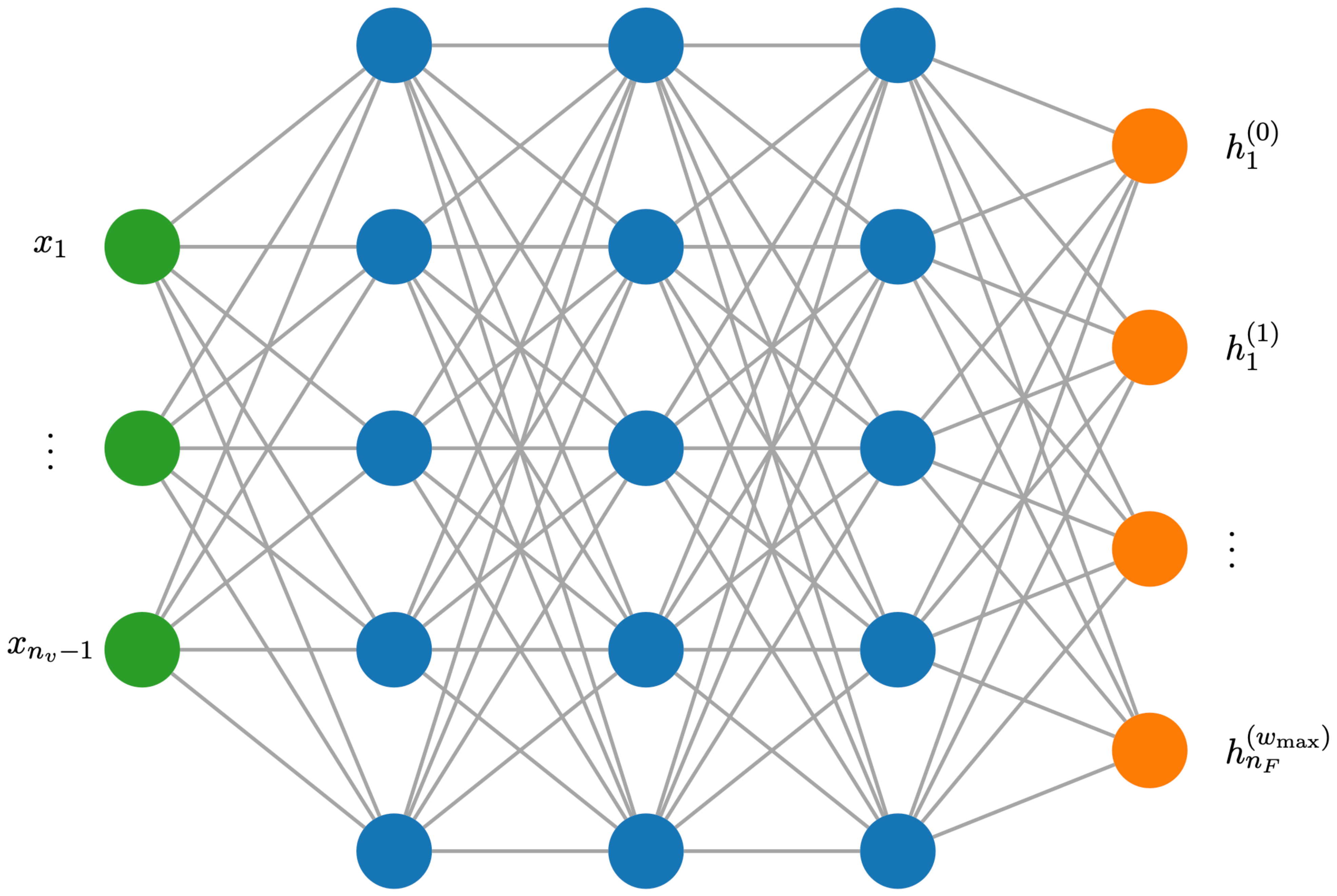
Full computation only recently, using generalised power series expansions (DiffExp)

[Becchetti, Bonciani, Cieri, Coro, Ripani 2023] *[Hidding 2020]*

MIs stripped of square roots → $A_{v_i}(\vec{v};\epsilon) = \sum_{k=0}^{2} \epsilon^k A_{v_i}^{(k)}(\vec{v})$

Heavy crossed box: architecture

2 input variables
(fix $m^2 = 1$)



3 hidden layers, 256 neurons each

MIs (Re or Im)

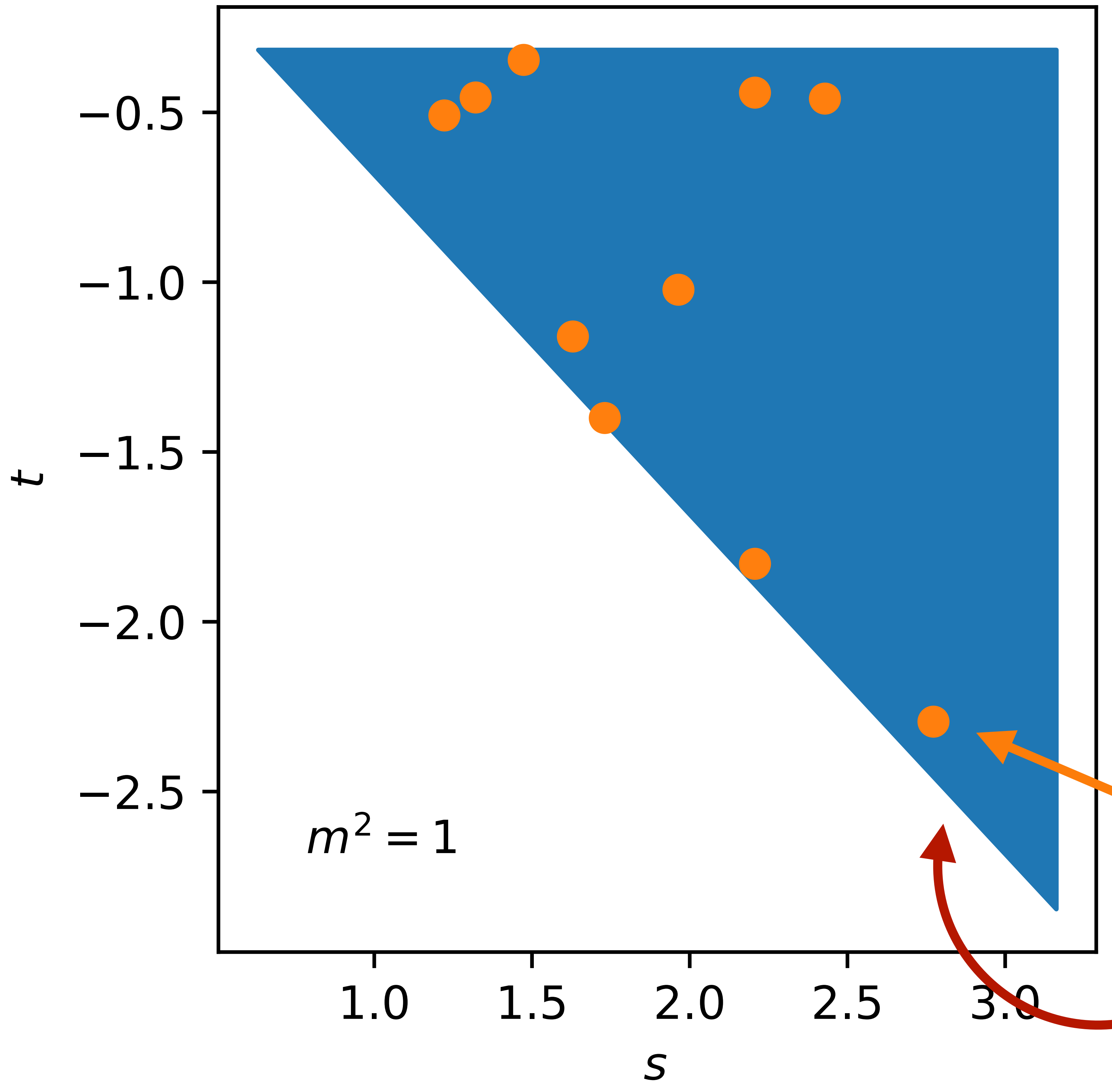
36 x 5 = 180 outputs

ϵ orders

$$\vec{F}(\vec{v};\epsilon) = \frac{1}{\epsilon^4}\sum_{w=0}^{4} \epsilon^w \vec{F}^{(w)}(\vec{v})$$

Heavy crossed box: kinematic region

s channel: $s > -t > 0 \wedge m^2 > 0$ → Never leave the chosen domain of analyticity domain, so analytic continuation is not required



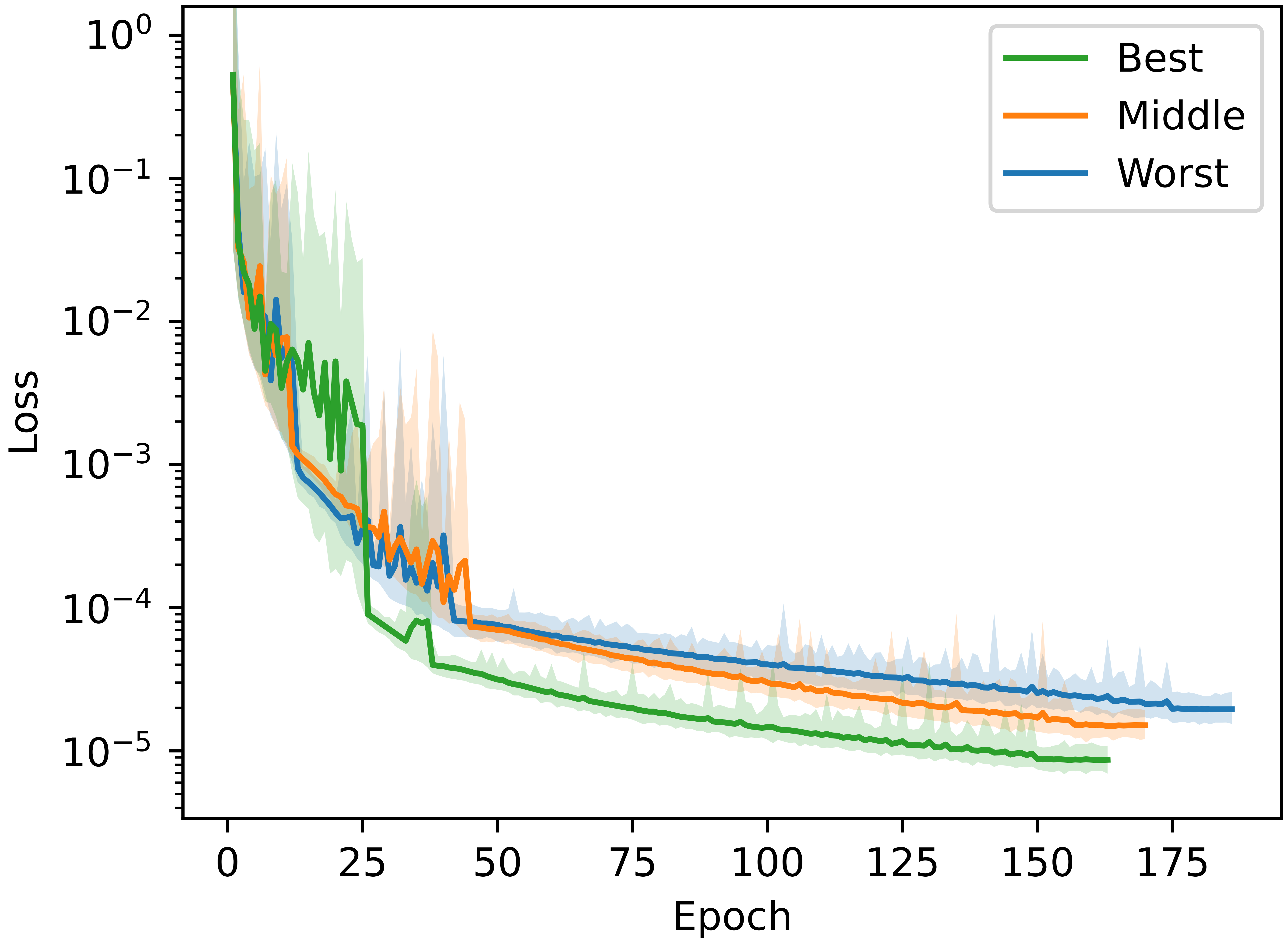
We choose $s < \sqrt{10}$

Singularities of the solution

Cut near boundaries:
$10\,\%$ of largest value ($\sqrt{10}$)

Boundary values at 10 random points, obtained with AMFlow *[Liu, Ma 2022]*

Heavy crossed box: training



Ensemble of 10 NNs

Iterations: 7.9×10^4

Time to train 1 NN: 75 min
(on a good laptop, GPU)

Use training metric for validation, as inputs for DE loss function are dynamically random sampled

Heavy crossed box: model performance

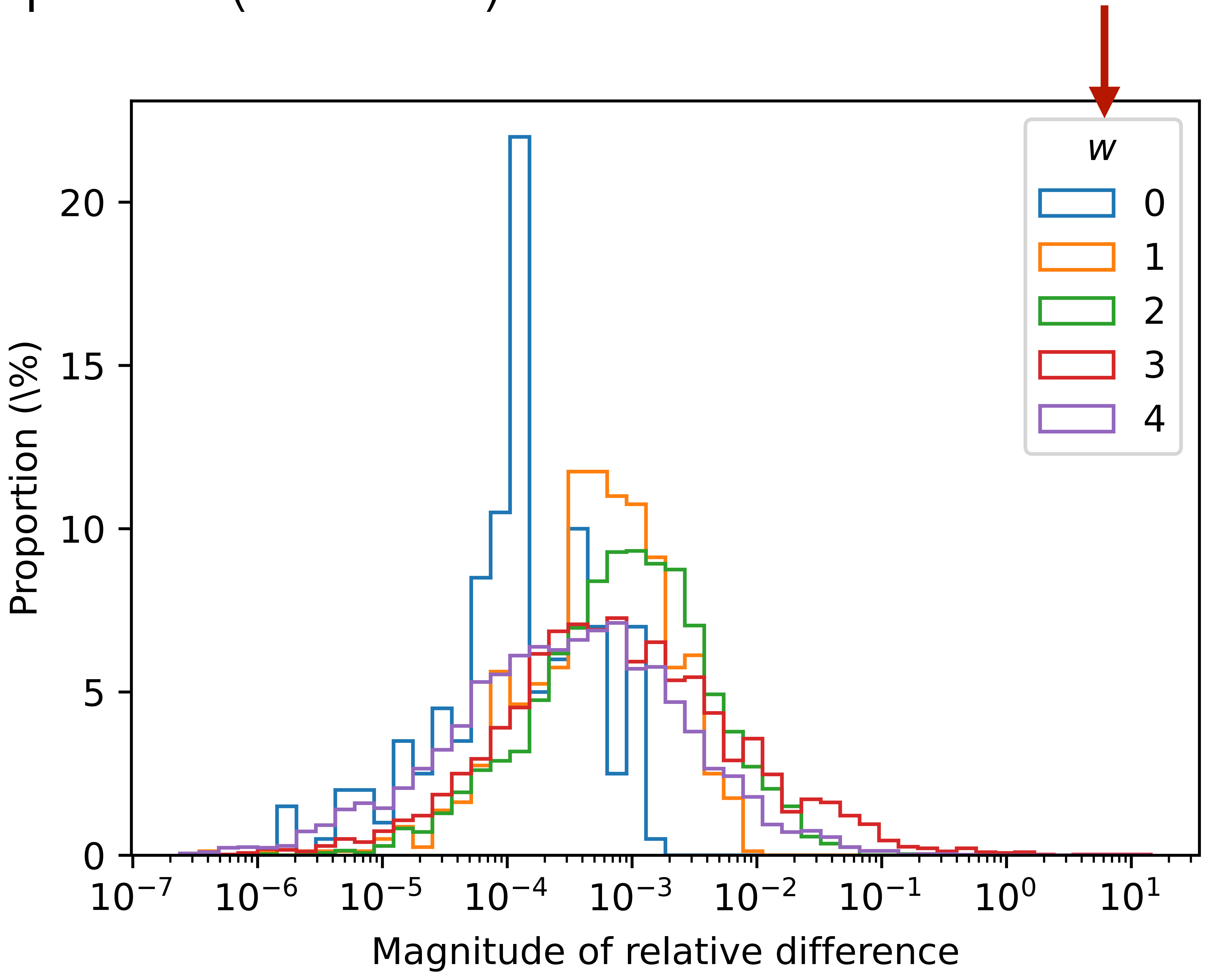
Comparison against testing dataset of 100 points (AMFlow)

ϵ orders

Mean absolute difference: 1.6×10^{-3}

Mean magnitude of rel. diff.: 7.3×10^{-3}

Evaluation time $\sim 1 - 10\ \mu s$

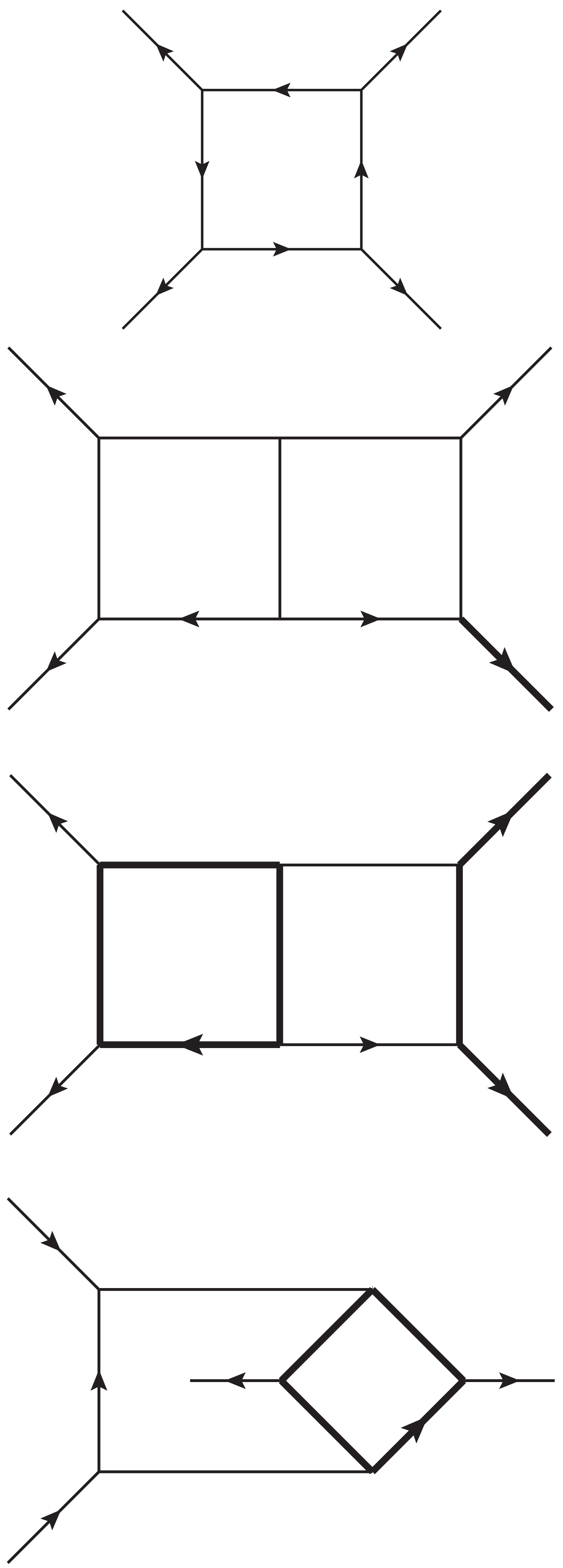


General comments

Flatness of the performance with respect to

- Analytic complexity (ϵ orders, MI) within the same family
- Across different families

Instantaneous evaluation times 🥳



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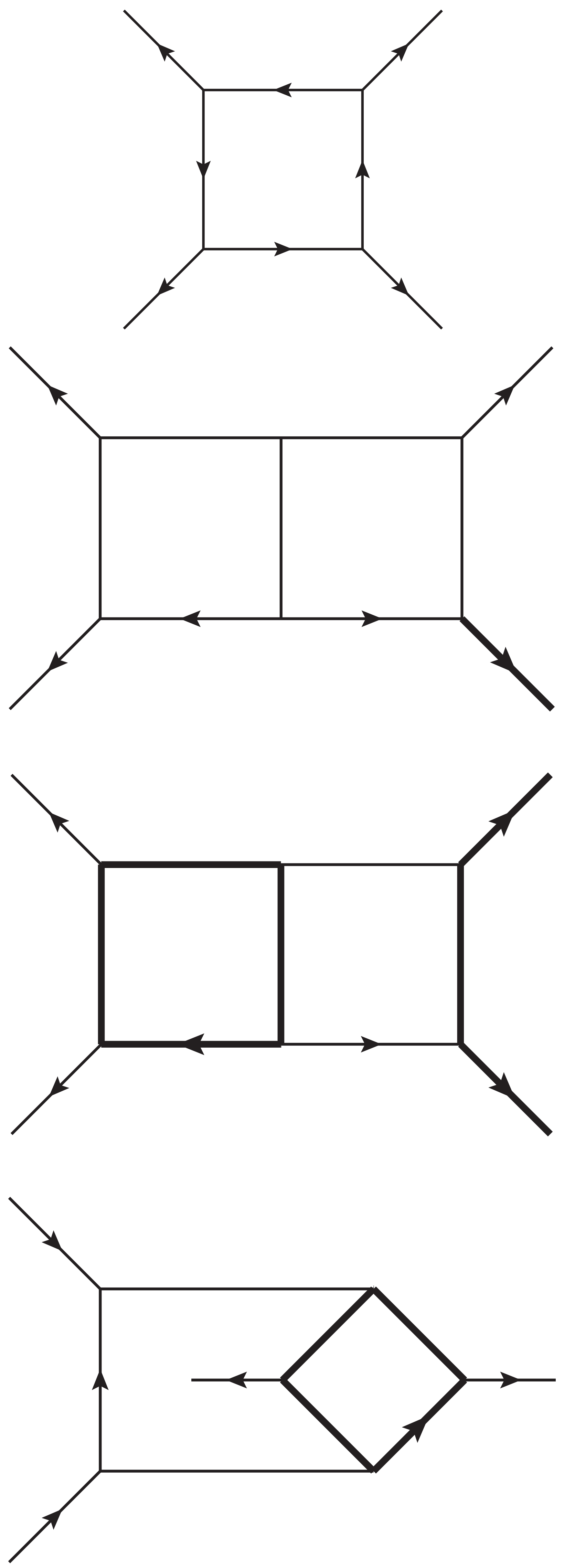
We can estimate it (ensemble uncertainty, differential error…), but unclear how to increase it arbitrarily



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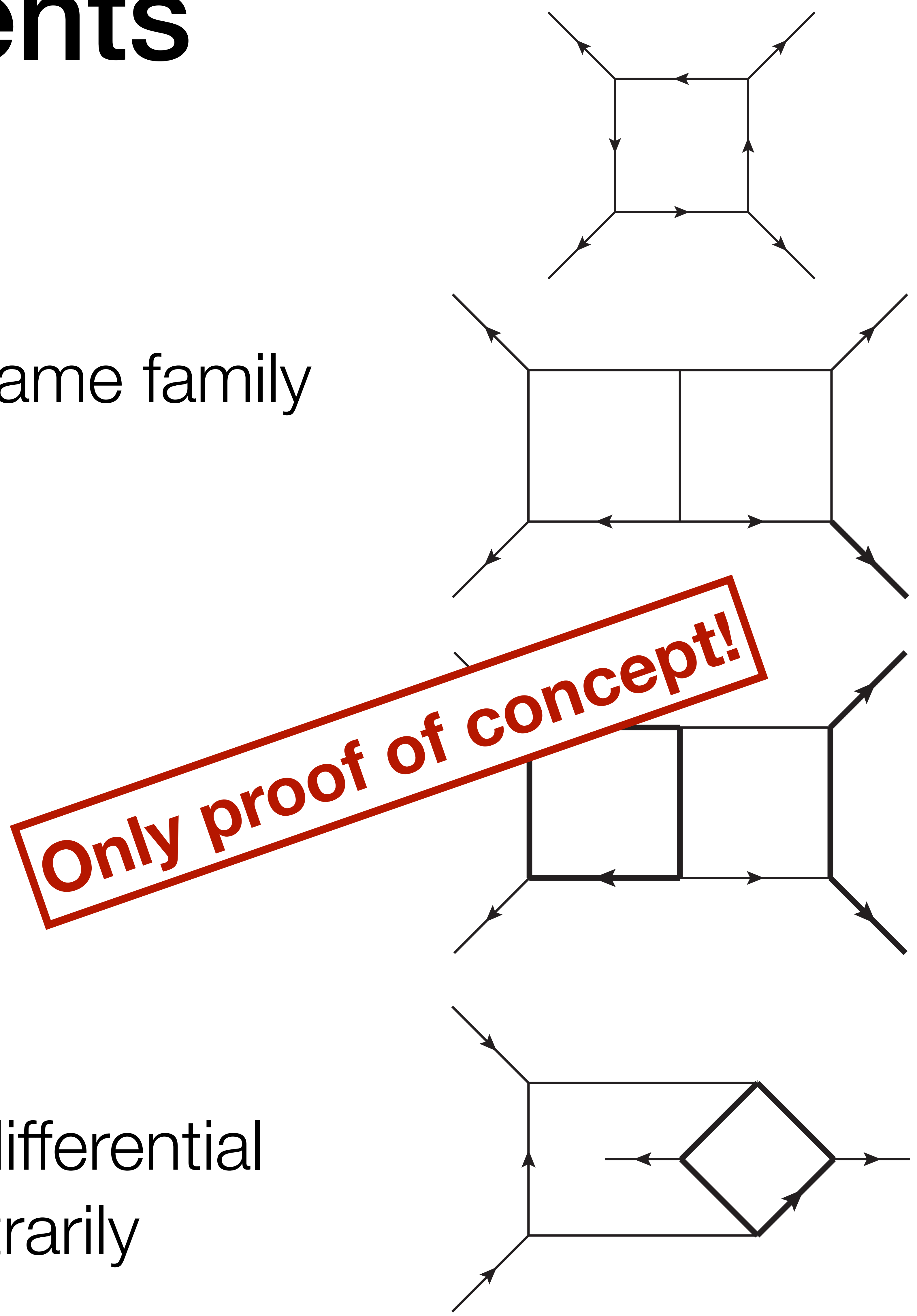

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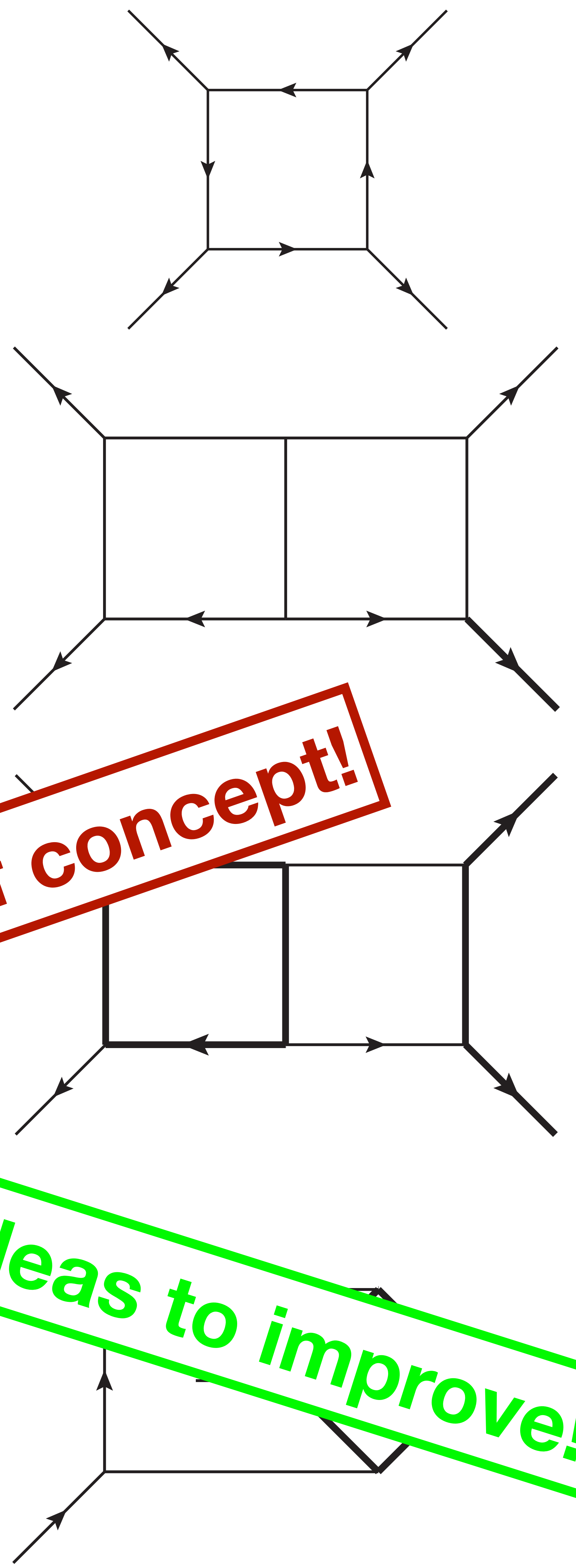

Only proof of concept!

Many ideas to improve!

Conclusion

New method to evaluate numerically Feynman integrals satisfying generic DEs using physics informed deep learning

Proof-of-concept implementation can reach 1% accuracy in cutting-edge 2-loop examples

Much room for improvement!

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Thank you!

Solution made simple by the canonical form

[Henn 2013]

Choose MIs such that the DEs take the **canonical form**

$$\mathrm{d}\overrightarrow{\mathrm{F}}(s;\epsilon) = \epsilon \; \mathrm{d}\tilde{A}\,(s) \cdot \overrightarrow{\mathrm{F}}\,(s;\epsilon)$$

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In the best understood cases (= most of the integrals computed so far):

$$\tilde{A}\,(s) = \sum_i a_i \log W_i\,(s)$$

Constant matrices

Letters: algebraic functions of kinematics
e.g. $\{s, t, s+t\}$ for the box

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Best-case scenario! 🥳

Proof-of-concept implementation

PyTorch

GELU activation function (nonzero and continuous 2nd-order derivatives)

Train with stochastic gradient descent (Adam optimiser)

Mini-batch training: iterations organised into epochs composed of small batches, taking a dynamic random sample of the inputs for each batch

- No need for regularisation to avoid overfitting
- Validation can be done on the training dataset

Loss function

$$L_{\mathrm{DE}}(\mathrm{D}_{\mathrm{DE}}, \theta) =$$

$$\overline{\sum_{\vec{x}^{(i)} \in \mathrm{D}_{\mathrm{DE}}}} \overline{\sum_{j=1}^{n_F}} \overline{\sum_{l=1}^{n_v - 1}} \overline{\sum_{w=0}^{w_{\max}}} \left[\partial_{x_l} h_j^{(w)}\left(\vec{x}^{(i)}; \theta\right) - \sum_{k=0}^{\min(w, k_{\max})} \sum_{r=1}^{n_F} A_{x_l, jr}^{(k)}\left(\vec{x}^{(i)}\right) h_r^{(w-k)}\left(\vec{x}^{(i)}; \theta\right) \right]^2$$

$$L_{\mathrm{b}}(\mathrm{D}_{\mathrm{b}}, \theta) = \overline{\sum_{\vec{x}^{(i)} \in \mathrm{D}_{\mathrm{b}}}} \overline{\sum_{j=1}^{n_F}} \overline{\sum_{w=0}^{w_{\max}}} \left[h_j^{(w)}\left(\vec{x}^{(i)}; \theta\right) - g_j^{(w)}\left(\vec{x}^{(i)}\right) \right]^2$$

Integral family	box	one-mass double box	heavy crossed box	top double box
Inputs	1	2	2	2
Hidden layers	3×32	3×256	3×256	4×128
Outputs	15	90	180	99
Learning rate	10^{-2}	10^{-3}	10^{-3}	10^{-3}
Batch size	64	256	256	256
Boundary points	2	6	10	20
c_{n_v}	$s = 10$	$s_{12} = 2.5$	$m^2 = 1$	$m_\mathrm{t}^2 = 1$
Scale bound	—	—	$s \leq \sqrt{10}$	$s_{12} \leq 5$
Physical cut (%)	10	10	10	10
Spurious cut (%)	0	0	0	1

Summary of hyperparameters

Integral family	Final loss	Iterations	Time (minutes)
box	2.7×10^{-7}	2.5×10^{5}	16
one-mass double box	3.4×10^{-4}	1.1×10^{5}	53
heavy crossed box	1.4×10^{-5}	7.9×10^{4}	75
top double box	7.1×10^{-4}	5.2×10^{4}	32

Training statistics

Integral family	MEU	MDE	MAD	MMRD	MLR	Size
box	2.8×10^{-5}	3.6×10^{-4}	2.9×10^{-5}	2.2×10^{-5}	3.9×10^{-7}	10^{5}
one-mass DB	8.1×10^{-4}	1.1×10^{-2}	2.0×10^{-3}	1.1×10^{-2}	-2.8×10^{-4}	10^{5}
heavy CB	2.8×10^{-4}	2.8×10^{-3}	1.6×10^{-3}	7.3×10^{-3}	-4.5×10^{-4}	10^{2}
top DB	1.9×10^{-4}	1.7×10^{-3}	9.0×10^{-4}	3.9×10^{-3}	1.8×10^{-4}	10^{2}

Uncertainty and testing errors