Learning to integrate

DANIEL MAÎTRE
IPPP, DURHAM UNIVERSITY

Based on arXiv:2211.02834 with Roi Santos-Mateos

Introduction

- Consider parametric integrals of the form

$$I(s_1, ..., s_m) = \int_0^1 dx_1 \cdots \int_0^1 dx_k \; f(s_1, ..., s_m; x_1, ..., x_k)$$

- x_i are auxiliary variables and s_i are the parameters
- Example: sector decomposition of loop integrals

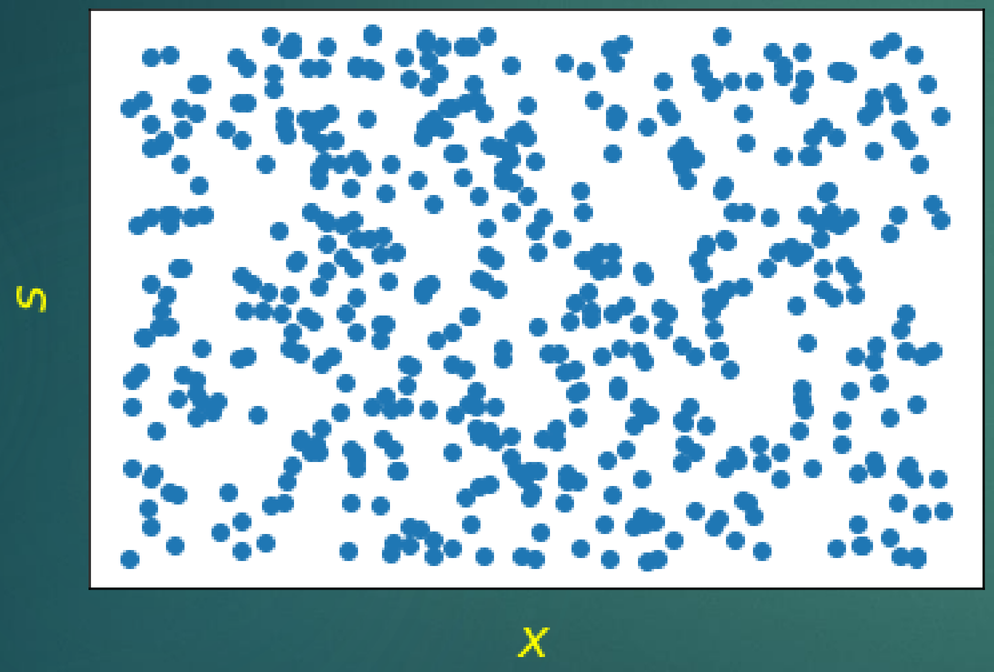
Typical solution

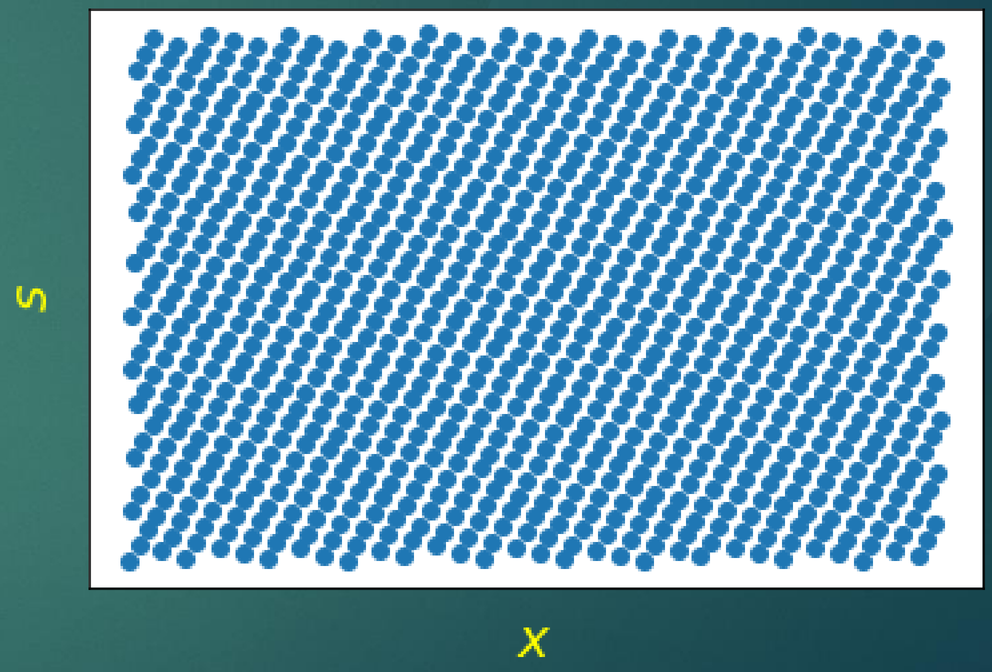
- Monte Carlo integration for each values of the parameters

- Each run is independent

Alternative

- Sample the x-s space more uniformly





- Can leverage information on the integrand between separate evaluations

Primitive function

- Suppose we had a function with

$$\frac{d^k F(s_1, ..., s_m; x_1, ..., x_k)}{dx_1 \ldots dx_k} = f(s_1, ..., s_m; x_1, ..., x_k)$$

- We can evaluate the integral as

$$I(s_1, ..., s_m) = \sum_{x_1, ..., x_k = 0,1} (-1)^{k - \sum x_i} F(s_1, ..., s_m; x_1, ..., x_k)$$

NN approximation

- We introduce a neural network approximation for the the primitive function

$$\mathcal{N}(s_1, ..., s_m; x_1, ..., x_k)$$

- Train it such that its derivative matches the integrand function

$$L = \text{MSE}\left(f(s_1, ..., s_m; x_1, ..., x_k), \frac{d\mathcal{N}(s_1, ..., s_m; x_1, ..., x_k)}{dx_1 ... dx_k}\right)$$

NN

- Standard network with *L* hidden layers

$$a_i^{(l)} = \phi\left(z_i^{(l)}\right) , \quad z_i^{(l)} = \sum_j w_{ij}^{(l)} a_j^{(l-1)} + b_i^l .$$

- Inputs

$$a_i^{(0)} = x_i \text{ for } i \leq k , \quad a_i^{(0)} = s_{i-k} \text{ for } i > k .$$

- output

$$y = \sum_j w_j^{(L+1)} a_j^{(L)} + b^{(L)}$$

Derivatives in the loss function

- The derivative in the loss function contains all the derivatives of the activation function up to degree k

$$\frac{d^p z_i^{(l)}}{dx_1 dx_2 \dots dx_p} = \sum_j w_{ij}^{(l)} \frac{d^p a_i^{(l-1)}}{dx_1 dx_2 \dots dx_p}$$

$$\begin{aligned}
\frac{d^3 a_i^{(l)}}{dx_1 dx_2 dx_3} &= \phi^{(3)}(z_i^{(l)}) \frac{dz_i^{(l)}}{dx_1} \frac{dz_i^{(l)}}{dx_2} \frac{dz_i^{(l)}}{dx_3} \\
&+\phi''(z_i^{(l)}) \left[\frac{d^2 z_i^{(l)}}{dx_1 dx_3} \frac{dz_i^{(l)}}{dx_2} + \frac{dz_i^{(l)}}{dx_1} \frac{d^2 z_i^{(l)}}{dx_2 dx_3} + \frac{d^2 z_i^{(l)}}{dx_1 dx_2} \frac{dz_i^{(l)}}{dx_3} \right] \\
&+\phi'(z_i^{(l)}) \frac{d^3 z_i^{(l)}}{dx_1 dx_2 dx_3}
\end{aligned}$$

Example 1

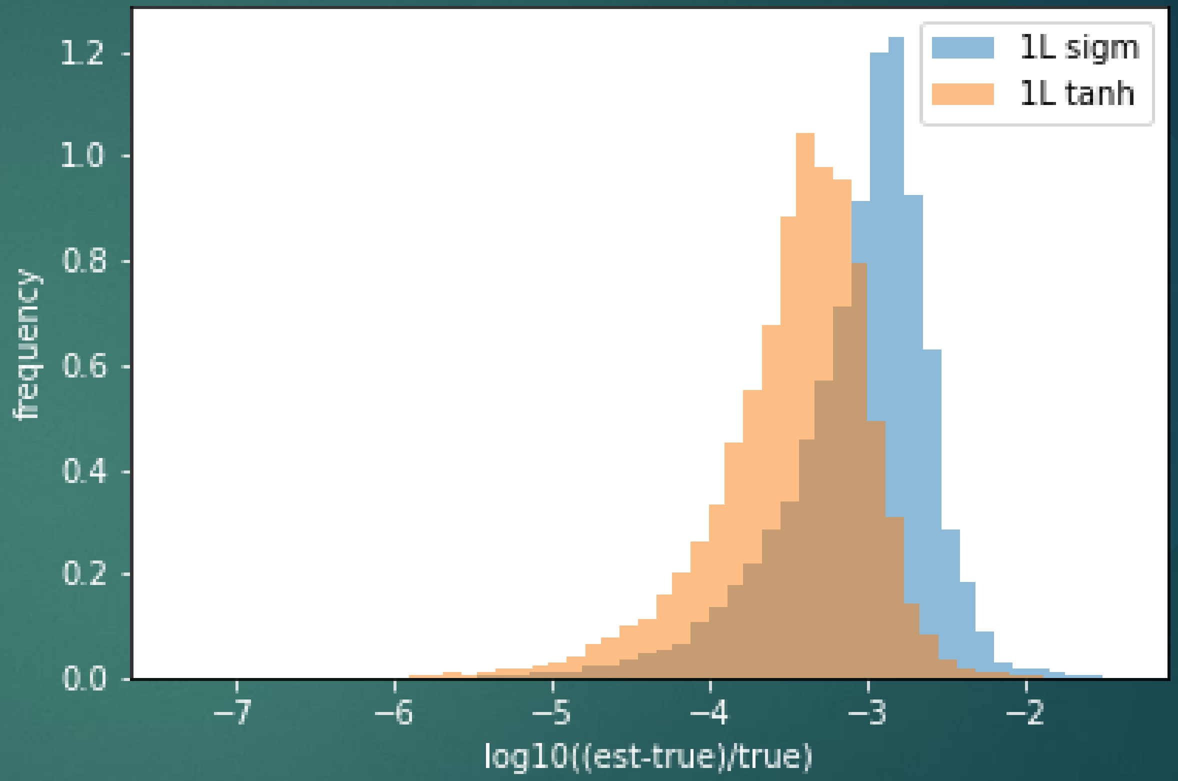
- 1-loop box for gg → HH
- Four physical parameters: m_t^2, m_H^2, s_{12}, s_{14}
- Three Feynman parameters x_1, x_2, x_3
- 3 sectors generated by pySecDec
- Euclidean region

$$-30 \leq s_{12}/m_t^2 \leq -3 \qquad -30 \leq s_{14}/m_t^2 \leq -3 \qquad -30 \leq m_H^2/m_t^2 \leq -3$$

Result

- 100 nodes
- 4 hidden layers
- 4M x 800 = 3.2B PS points

$$p = \log_{10}\left|\frac{e-t}{t}\right|$$

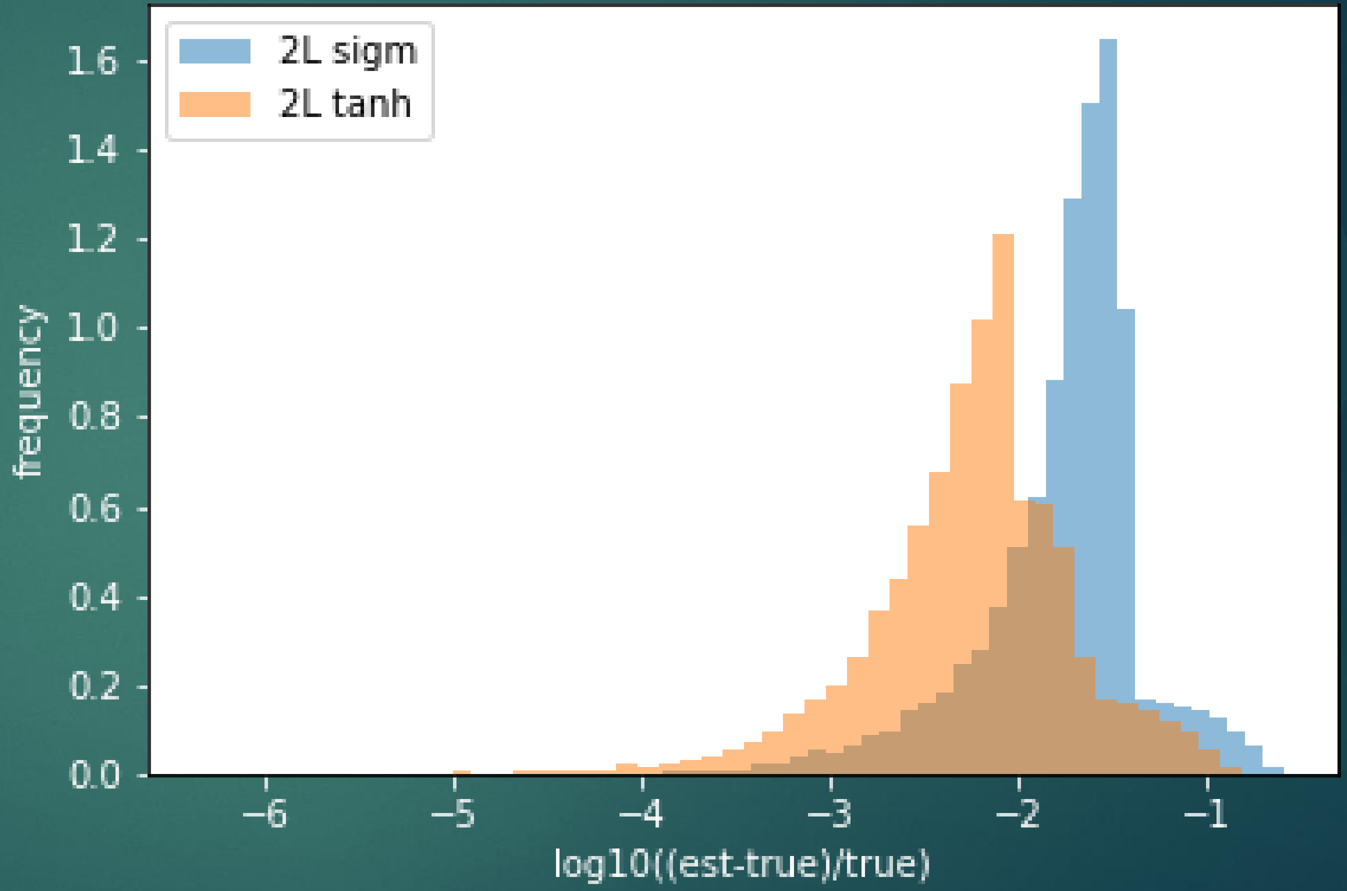


Example 2

- 2-loop box for gg→HH
- Same physical parameters
- 6 Feynman parameters
- 1 of 30 sectors from pySecDec

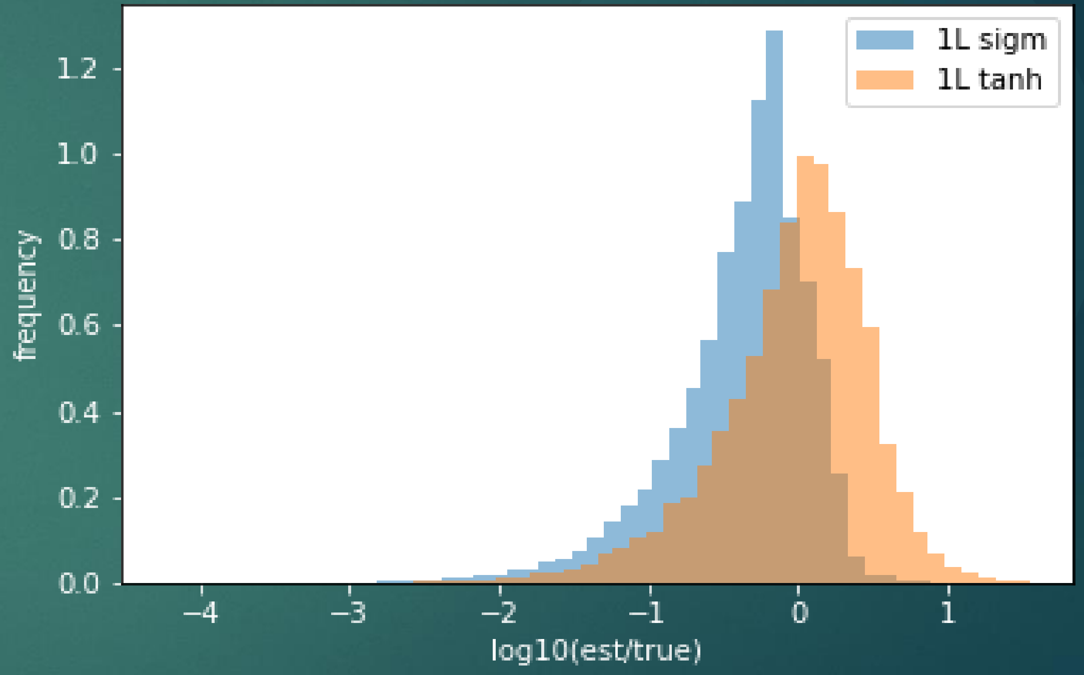
Results

- 30 nodes
- 4 hidden layers
- 800k x 200 PS points



Error estimate

- Use 4 replicas of the network
- Use average as the prediction
- Standard deviation as error estimate



Reducing variance

- Usual subtraction

$$\int_0^1 dx_1 \dots \int_0^1 dx_k \left(f(x_1, \dots, x_k) - s(x_1, \dots, x_k)\right) \quad + \quad S$$

$$S = \int_0^1 dx_1 \dots \int_0^1 dx_k\, s(x_1, \dots, x_k)$$

- Using our neural network

$$\int_0^1 dx_1 \dots \int_0^1 dx_k \left(f(x_1, \dots, x_k) - \frac{d^k \mathcal{N}}{dx_1 \dots dx_k}\right) \quad + \quad \sum_{b_i=0,1} \pm \mathcal{N}(b_i, \dots, b_k)$$

Reducing variance

- Usual subtraction

$$\int_0^1 dx_1 \ldots \int_0^1 dx_k \left(f(x_1, \ldots, x_k) - s(x_1, \ldots, x_k)\right) \quad + \quad S$$

$$S = \int_0^1 dx_1 \ldots \int_0^1 dx_k s(x_1, \ldots, x_k)$$

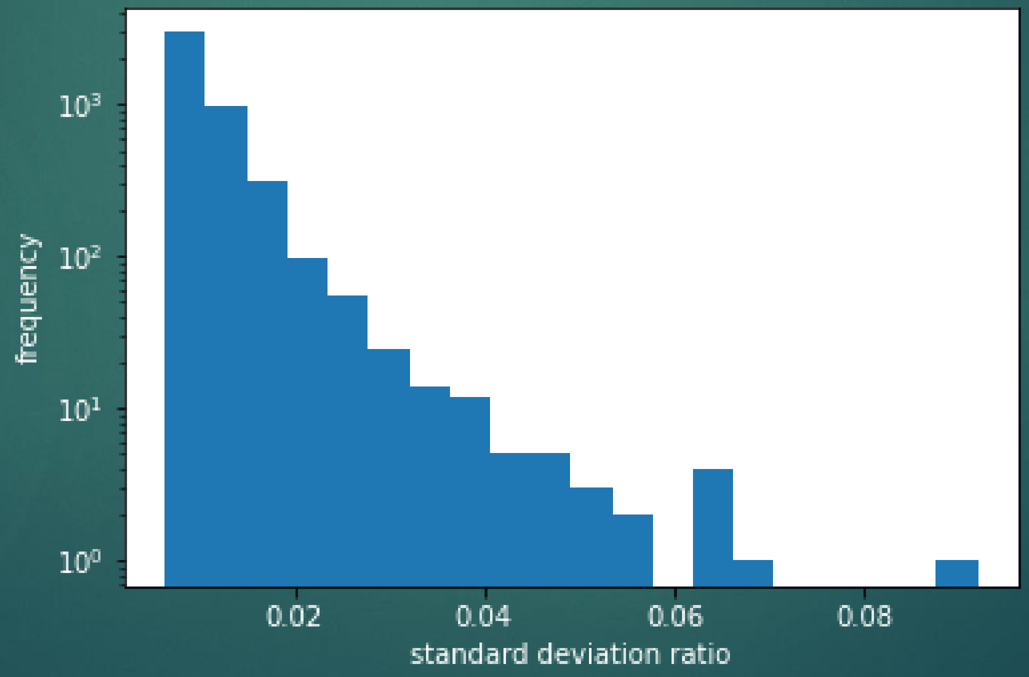
- Using our neural network

$$\int_0^1 dx_1 \ldots \int_0^1 dx_k \left(f(x_1, \ldots, x_k) - \frac{d^k \mathcal{N}}{dx_1 \ldots dx_k} \right) + \sum_{b_i = 0,1} \pm \mathcal{N}(b_i, \ldots, b_k)$$

Lower variance !

Reduce variance

- 1-Loop example
- Ratio of variance with NN subtraction wrt without subtraction



Outlook

- More work on training
  - Initialisation
  - Training data sequencing
- Size / depth of networks / number of replica
- More complicated examples
  - More integration variables
  - Combined sectors, combined integrals
  - Minkowsky space
- Use as a parametrized Gibbs sampler

Conclusion

- Proof of concept
- Integral from fitting integrand
- Lots to learn about the behaviour/training of network with derivative loss

Training

- Neural network training is similar to standard network but
  - Take care of initialization
  - Can choose our data
    - Random vs qmc grids
    - Size of sample
    - Re-use or generate new data
  - Pick activation function
    - Tanh/sigmoid in N: derivatives in Loss
    - Antiderivatives of tanh/sigmoid in N: tanh and sigmoid in loss (and lower antiderivatives)

Preprocessing

- Korobov transform

$$x = t^2(3-2t)\,, \qquad \int_0^1 dx\, f(x) = \int_0^1 dt\; 6t(1-t)\, f(x(t))$$

- Remove overall scaling

$$f \to \tilde{f}(s_1, \ldots, s_m; x_1, \ldots, x_k) \equiv \frac{f(s_1, \ldots, s_m; x_1, \ldots, x_k)}{f(s_1, \ldots, s_m; \frac{1}{2}, \frac{1}{2}, , \ldots, \frac{1}{2})}$$