We need to evaluate Feynman integrals

\[
\int \frac{d^Dk}{i\pi^{D/2}} \frac{1}{k^2 (k+p_1)^2 (k+p_1+p_2)^2 (k+p_1+p_2+p_3)^2}
\]

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

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

Most powerful tool for analytic computation of Feynman integrals

Neat connection with study of special functions

Growing interest for semi-numerical solution with generalised power series
How do we solve the DEs?

- Analytical
- Numerical
Outline

• Quick review of the method of DEs

• Analytic method: “pentagon functions” = basis of special functions

  Chicherin, Sotnikov, SZ (2110.10111)
  Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ (2306.15431)

• Numerical method: “physics-informed deep learning”

  Calisto, Moodie, SZ (23XX.XXXXX)
Method of differential equations
Integral families and master integrals

Scalar Feynman integrals with the same propagator structure = \textbf{integral family}

\[ I_{\vec{a}}(s, t; \epsilon) = \int \frac{d^{D}k}{i\pi^{D/2}} \frac{1}{D_{1}^{a_{1}}\ldots D_{4}^{a_{4}}} \]

\[ \{ I_{\vec{a}}(s, t; \epsilon) \mid \forall \vec{a} \in \mathbb{Z}^{4} \} \]

\[ D_{1} = -k^{2} \]
\[ D_{2} = -(k + p_{1})^{2} \]
\[ D_{3} = -(k + p_{1} + p_{2})^{2} \]
\[ D_{4} = -(k - p_{4})^{2} \]
Integral families and master integrals

Scalar Feynman integrals with the same propagator structure = integral family

\[
I_{\vec{a}}(s, t; \epsilon) = \int \frac{d^Dk}{i\pi^{D/2}} \frac{1}{D_1^{a_1} \cdots D_4^{a_4}}
\]

\[
\{ I_{\vec{a}}(s, t; \epsilon) | \forall \vec{a} \in \mathbb{Z}^4 \}
\]

\[
D_1 = -k^2
\]
\[
D_2 = -(k + p_1)^2
\]
\[
D_3 = -(k + p_1 + p_2)^2
\]
\[
D_4 = -(k - p_4)^2
\]

Identities among the \( I_{\vec{a}} \)'s

\[
\frac{3 - D}{p^2} \times \quad \text{e.g. Integration-By-Parts relations}
\]

[Chetyrkin, Tkachov '81; Laporta 2000]
Integral families and master integrals

Scalar Feynman integrals with the same propagator structure = integral family

$$I_{\vec{a}}(s, t; \epsilon) = \int \frac{d^{D}k}{i\pi^{D/2}} \frac{1}{D_{1}^{a_{1}} \ldots D_{4}^{a_{4}}}$$

$$D_{1} = -k^{2}$$
$$D_{2} = -(k + p_{1})^{2}$$
$$D_{3} = -(k + p_{1} + p_{2})^{2}$$
$$D_{4} = -(k - p_{4})^{2}$$

{\(I_{\vec{a}}(s, t; \epsilon) \mid \forall \vec{a} \in \mathbb{Z}^{4}\)}

Identities among the \(I_{\vec{a}}\)'s

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

\[ \Rightarrow \]

e.g. Integration-By-Parts relations

[Chetyrkin, Tkachov '81; Laporta 2000]

Finite-dimensional basis:

master integrals \(\mathbf{F}(s, t; \epsilon)\)
Integrating by differentiating

\[ \frac{\partial}{\partial s_{12}} \vec{F}(s; \epsilon) = \sum \bar{c}_\bar{a} \bar{I}_\bar{a} \]

IBP reduction

\[ = A_{s_{12}}(s; \epsilon) \cdot \vec{F}(s; \epsilon) \]

\[
D = 4 - 2\epsilon
\]

⇒ System of 1\textsuperscript{st} order linear PDEs for the MIs \( \vec{F} \)

- How do we solve it?

\[ \vec{F}(s; \epsilon) = \sum_w e^w \vec{F}^{(w)}(s) \]

- What is a “good” choice of MIs?
Solution made simple by the canonical form

Choose MIs such that the DEs take the canonical form

\[ \text{d} \vec{F}(s; \epsilon) = \epsilon \text{ d} \vec{A}(s) \cdot \vec{F}(s; \epsilon) \]
Solution made simple by the canonical form

Choose MIs such that the DEs take the canonical form

\[ d\vec{F}(s; \epsilon) = \epsilon \ d\tilde{A}(s) \cdot \vec{F}(s; \epsilon) \]

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

\[ \tilde{A}(s) = \sum_i a_i \log W_i(s) \]

**Letters**: algebraic functions of kinematics

- e.g. \{s, t, s + t\} for the box
Solution made simple by the canonical form

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

\[
d \vec{F}(s; \epsilon) = \epsilon \, d\tilde{A}(s) \cdot \vec{F}(s; \epsilon)
\]

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

\[
\tilde{A}(s) = \sum_{i} a_i \log W_i(s)
\]

**Letters**: algebraic functions of kinematics

- e.g. \( \{s, t, s + t\} \) for the box

**Constant matrices**

Best-case scenario! 🥳
Solution made simple by the canonical form

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

\[ d\vec{F}(s; \epsilon) = \epsilon d\tilde{A}(s) \cdot F(s; \epsilon) \]

Many “strategies”, but no general algorithm!

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

\[ \tilde{A}(s) = \sum_i a_i \log W_i(s) \]

**Letters:** algebraic functions of kinematics

- e.g. \{s, t, s + t\} for the box

Best-case scenario! 😃
Even the best-case scenario is challenging

If the letters $W_i(s)$ are rational $\Rightarrow$ solution in terms of multiple polylogarithms

$$G(z_1, \ldots, z_n; x) := \int_0^x \frac{dt_1}{t_1 - z_1} \int_0^{t_1} \frac{dt_2}{t_2 - z_2} \cdots \int_0^{t_{n-1}} \frac{dt_n}{t_n - z_n}$$

1. **Square roots** ruin the party: solution may be MPL, but difficult and not algorithmic

2. MPLs satisfy functional identities $\Rightarrow$ **Redundant representation**

$$\text{Li}_2(z) + \frac{1}{2} \log^2(-z) + \text{Li}_2 \left( \frac{1}{z} \right) + \frac{\pi^2}{6} = 0$$

Simplifications hidden, inefficient evaluation, complicated expressions…
The best-case scenario is not enough

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

• Obtaining the canonical form is very challenging
• Mathematical technology much less mature

Growing interest for semi-numerical solution based on series expansions

[Mo?iello 2019]

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

😄 Very flexible (canonical form not required)
😊 Long evaluation times
Two opposite methods

1. Write the solution in terms of a **basis** of special functions (“pentagon functions”)
   - Make the most out of the canonical DEs

2. Train a **neural network** to approximate solution to the DEs
   - Does not rely on a canonical form at all
1. Pentagon functions

Chicherin, Sotnikov, $SZ$ (2110.10111)

Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, $SZ$ (2306.15431)
The “pentagon functions” approach

Very successful for 2-loop 5-point amplitudes

Express MIs in terms of a basis of algebraically independent special functions

\[ \epsilon^3(1 - 2\epsilon)\sqrt{\Delta_3^{(1)}} \times \]

\[ = e^2 f_{23}^{(2)} + e^3 \left[ \frac{1}{4} (f_1^{(1)} - f_6^{(1)}) f_{23}^{(2)} + \frac{1}{2} f_3^{(3)} - \frac{1}{2} f_{29}^{(3)} \right] + e^4 f_{47}^{(4)} + \mathcal{O}(\epsilon^5) \]

Algorithmically!

Efficient numerical evaluation through one-fold integrals

[Gehrmann, Henn, Lo Presti 2018; Chicherin, Sotnikov 2020; Chicherin, Sotnikov, SZ 2021; Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ 2023]
2-loop 5-pt 1-mass master integrals

NNLO QCD corrections for
pp $\rightarrow H/V + 2 \text{ jets}/\gamma$, $e^+e^- \rightarrow 4 \text{ jets}$

[Abreu, Ita, Moriello, Page, Tschernow, Zeng 2020; Canko, Papadopoulos, Syrrakos 2020; Syrrakos 2020; Chicherin, Sotnikov, SZ 2021]

[Abreu, Ita, Moriello, Page, Tschernow 2021; Kardos, Papadopoulos, Smirnov, Syrrakos, Wever 2022]

[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ 2023]
1-mass pentagon alphabet: 204 letters

127 rational

\[ W_1 = p_1^2 , \]
\[ \{ W_2, \ldots, W_5 \} = \{ \sigma(s_{12}) : \sigma \in S_4/S_3[3,4,5] \} , \]
\[ \{ W_6, \ldots, W_{11} \} = \{ \sigma(s_{23}) : \sigma \in S_4/(S_2[2,3] \times S_2[4,5]) \} , \]
\[ \{ W_{12}, \ldots, W_{15} \} = \{ \sigma(2p_1 \cdot p_2) : \sigma \in S_4/S_3[3,4,5] \} , \]
\[ \{ W_{16}, \ldots, W_{27} \} = \{ \sigma(2p_2 \cdot (p_3 + p_4)) : \sigma \in S_4/S_2[3,4] \} , \]

77 algebraic

\[ \{ W_{186}, \ldots, W_{188} \} = \left\{ \sigma \left( \frac{\Omega_{-}^{--} \Omega_{++}^{+}}{\Omega_{-}^{--} + \Omega_{++}^+} \right) : \sigma \in S_4/(S_2[2,3] \times S_2[4,5] \times S_2[s_{23}, s_{45}]) \right\} , \]
\[ \{ W_{189}, \ldots, W_{194} \} = \left\{ \sigma \left( \frac{\tilde{\Omega}_{-}^{--} \tilde{\Omega}_{++}^{+}}{\tilde{\Omega}_{-}^{--} + \tilde{\Omega}_{++}^+} \right) : \sigma \in S_4/(S_2[3,4] \times S_2[2,5]) \right\} , \]

where

\[ \Omega^{\pm \pm} = s_{12}s_{15} - s_{12}s_{23} - s_{15}s_{45} \pm s_{34}\sqrt{\Delta_3^{(1)}} \pm \sqrt{\Delta_5} , \]
\[ \tilde{\Omega}^{\pm \pm} = p_3^2s_{34} \pm \sqrt{\Delta_5} \pm \sqrt{\Sigma_5^{(1)}} , \]

6 variables

\[ \Sigma_5 = (s_{12}s_{15} - s_{12}s_{23} - s_{15}s_{45} + s_{34}s_{45} + s_{23}s_{34})^2 - 4s_{23}s_{34}s_{45}(s_{34} - s_{12} - s_{15}) \]

10 square roots:

\[ \Delta_5 = \det G(p_1, p_2, p_3, p_4) \]
\[ = (s_{12}s_{15} - s_{12}s_{23} - p_3^2s_{34} - s_{15}s_{45} + s_{34}s_{45} + s_{23}s_{34})^2 \]
\[ - 4s_{23}s_{34}s_{45}(p_3^2 - s_{12} - s_{15} + s_{34}) . \]

Closed under permutations of the massless momenta

[Abreu, Ita, Moriello, Page, Tschernow 2021]

Algorithmic approach made necessary by the scale of the problem
Algorithmic construction of the function basis
Chen iterated integrals

\[ [w_i, \ldots, w_n]_{s_0}(s) = \int_{\gamma} d \log w_i(s') [w_i, \ldots, w_{i-1}]_{s_0}(s') \]

All functional relations become manifest in terms of iterated integrals

\[ \text{Li}_2(z) + \frac{1}{2} \log^2(-z) + \text{Li}_2 \left( \frac{1}{z} \right) + \frac{\pi^2}{6} = 0 \]
Chen iterated integrals

\[
[w_i, \ldots, w_n]_{s_0}(s) = \int_{\gamma} d \log w_i(s') [w_i, \ldots, w_{i-1}]_{s_0}(s')
\]

All functional relations become manifest in terms of iterated integrals

\[
\text{Li}_2(z) + \frac{1}{2} \log^2(-z) + \text{Li}_2\left(\frac{1}{z}\right) + \frac{\pi^2}{6} = 0
\]

\[
\text{Li}_2(z) = -[1 - z, z]_{-1} - \log 2 [z]_{-1} - \frac{\pi^2}{12}
\]

\[
\text{Li}_2\left(\frac{1}{z}\right) = [1 - z, z]_{-1} - [z, z]_{-1} + \log 2 [z]_{-1} - \frac{\pi^2}{12}
\]

\[
\frac{1}{2} \log^2(-z) = [z, z]_{-1}
\]
Chen iterated integrals

\[
[w_i, \ldots, w_n]_{s_0} (s) = \int_\gamma d \log w_i (s') [w_i, \ldots, w_{i-1}]_{s_0} (s')
\]

All functional relations become manifest in terms of iterated integrals

\[
\text{Li}_2 (z) + \frac{1}{2} \log^2 (-z) + \text{Li}_2 \left( \frac{1}{z} \right) + \frac{\pi^2}{6} = 0
\]

\[
\text{Li}_2 (z) = - [1 - z, z]_{-1} - \log 2 [z]_{-1} - \frac{\pi^2}{12}
\]

\[
\text{Li}_2 \left( \frac{1}{z} \right) = [1 - z, z]_{-1} - [z, z]_{-1} + \log 2 [z]_{-1} - \frac{\pi^2}{12}
\]

\[
\frac{1}{2} \log^2 (-z) = [z, z]_{-1}
\]
Chen iterated integrals

\[
[w_{i_1}, ..., w_{i_n}]_{s_0} (s) = \int_{\gamma} d \log w_{i_n} (s') [w_{i_1}, ..., w_{i_{n-1}}]_{s_0} (s')
\]

All functional relations become manifest in terms of iterated integrals

\[
\text{Li}_2 (z) + \frac{1}{2} \log^2(-z) + \text{Li}_2 \left( \frac{1}{z} \right) + \frac{\pi^2}{6} = 0
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\text{Li}_2 (z) = - [1 - z, z]_{-1} - \log 2 [z]_{-1} - \frac{\pi^2}{12}
\]

\[
\text{Li}_2 \left( \frac{1}{z} \right) = [1 - z, z]_{-1} - [z, z]_{-1} + \log 2 [z]_{-1} - \frac{\pi^2}{12}
\]

\[
\frac{1}{2} \log^2(-z) = [z, z]_{-1}
\]

\[ n = \text{transcendental weight} \]
Chen iterated integrals

$$[w_i, \ldots, w_n]_{s_0}(s) = \int_{\gamma} d \log w_i(s') [w_i, \ldots, w_{i-1}]_{s_0}(s')$$

$n = \text{transcendental weight}$

All functional relations become manifest in terms of iterated integrals

$$\text{Li}_2(z) + \frac{1}{2} \log^2(-z) + \text{Li}_2\left(\frac{1}{z}\right) + \frac{\pi^2}{6} = 0$$

$$\text{Li}_2(z) = -\left[1 - z, z\right]_{-1} - \log 2 \left[z\right]_{-1} - \frac{\pi^2}{12}$$

$$\frac{1}{2} \log^2(-z) = \left[z, z\right]_{-1}$$

$$\text{Li}_2\left(\frac{1}{z}\right) = \left[1 - z, z\right]_{-1} - \left[z, z\right]_{-1} + \log 2 \left[z\right]_{-1} - \frac{\pi^2}{12}$$
The solution to canonical DEs is uniform in the transcendental weight

Solution in terms of iterated integrals can be simply read off from the canonical DEs

\[ d\tilde{F}(s; \epsilon) = \epsilon \ d\tilde{A}(s) \cdot \tilde{F}(s; \epsilon) \]

\[ \tilde{A}(s) = \sum_i a_i \log W_i(s) \]

\[ \tilde{F}(s; \epsilon) = \frac{1}{\epsilon^{2\ell}} \sum_{w \geq 0} \epsilon^w \tilde{F}^{(w)}(s) \]

\( \mathbb{Q} \)-linear combination of weight-\( w \) iterated integrals

Uniform transcendentality
Important properties of iterated integrals

• \{ W_i(s) \} multiplicatively independent \Rightarrow [W_1, \ldots, W_n] \mathbb{Q}\text{-linearly independent}

• No \mathbb{Q}\text{-linear relations among iterated integrals with different weight}

• Shuffle product:

\[
[W_1, W_2]_{s_0} \times [W_3]_{s_0} = [W_1, W_2, W_3]_{s_0} + [W_1, W_3, W_2]_{s_0} + [W_3, W_1, W_2]_{s_0}
\]

(weight \(w_1\)) \times (weight \(w_2\)) = \mathbb{Q}\text{-linear combination of weight} (w_1 + w_2)
Extract function basis from MI coefficients

\[ \overline{\text{MI}}(s, \epsilon) = \sum_{w \geq 0} \epsilon^w \overline{\text{MI}}^{(w)}(s) \]

Written in terms of Chen iterated integrals
Up to required order (here, \( w = 4 \))

\[
\begin{align*}
\{ \text{MI}^{(1)}_i \} & \longrightarrow \{ f^{(1)}_k \} \\
\{ \text{MI}^{(2)}_i \} \cup \{ f^{(1)}_i \times f^{(1)}_j \} & \longrightarrow \{ f^{(2)}_k \} \\
\{ \text{MI}^{(3)}_i \} \cup \{ f^{(2)}_i \times f^{(1)}_j \} \cup \{ f^{(1)}_i \times f^{(1)}_j \times f^{(1)}_k \} & \longrightarrow \{ f^{(3)}_k \}
\end{align*}
\]

Algebraically independent
Irreducible

Solution of a linear system of equations

Linear algebra only 👍
Need to know relations among boundary values

We only know $\overrightarrow{MI}^{(w)}(s_0)$ numerically

Previous approach: high-precision evaluation of MPLs + PSLQ algorithm

\[ \text{MI}^{(2)}_1(s_0) = -1.644934067... \]
\[ \text{MI}^{(2)}_2(s_0) = 0.4060916335... \]
\[ \text{MI}^{(2)}_3(s_0) = 1.436746367... \]

\[ 3 \text{MI}^{(2)}_1(s_0) + 4 \text{MI}^{(2)}_2(s_0) - 2 \text{MI}^{(2)}_3(s_0) = 0 \]

- Very heavy from computational point of view (e.g. ~3000-digit precision in [Chicherin, Sotnikov, SZ 2021]) 😞
- Relies on MPL representation 😞
The new algorithm

[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ 2023]

1. Select MI coefficients for the basis at symbol level \( \{ f_i^{(w)} \} \)

Symbol = iterated integral stripped of boundary information

\[
\text{Li}_2(z) = -[1 - z, z]_1 - \log 2 [z]_1 - \frac{\pi^2}{12}
\]

\[
\delta \left[ \text{Li}_2(z) \right] = -[1 - z, z]
\]
The new algorithm

[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ 2023]

1. Select MI coefficients for the basis at symbol level \( \{ f_i^{(w)} \} \)

\( \text{Symbol} = \text{iterated integral stripped of boundary information} \)

\[
\begin{align*}
\text{Li}_2(z) &= - [1 - z, z] - \log 2 [z] - \frac{\pi^2}{12} \\
\delta \left[ \text{Li}_2(z) \right] &= - [1 - z, z]
\end{align*}
\]

2. **Ansatz**: all MI coefficients are polynomials in \( \{ f_i^{(w)} \} \) + \( \zeta_2 \) and \( \zeta_3 \) (up to weight 4)

\[
\text{MI}^{(2)} = \sum_i \alpha_i f_i^{(2)} + \sum_{i \leq j} \beta_{ij} f_i^{(1)} f_j^{(1)} + \gamma \zeta_2 \quad \alpha_i, \beta_{ij}, \gamma \in \mathbb{Q}
\]
The new algorithm

[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ 2023]

1. Select MI coefficients for the basis at symbol level \( \{ f_i^{(w)} \} \) [Goncharov, Spradlin, Vergu, Volovich 2010]

Symbol = iterated integral stripped of boundary information

\[
\text{Li}_2(z) = - \left[ 1 - z, z \right]_{-1} - \log 2 \left[ z \right]_{-1} - \frac{\pi^2}{12} \quad \Rightarrow \quad \delta \left[ \text{Li}_2(z) \right] = - \left[ 1 - z, z \right]
\]

2. Ansatz: all MI coefficients are polynomials in \( \{ f_i^{(w)} \} + \zeta_2 \) and \( \zeta_3 \) (up to weight 4)

\[
\text{MI}^{(2)} = \sum_i \alpha_i f_i^{(2)} + \sum_{i \leq j} \beta_{ij} f_i^{(1)} f_j^{(1)} + \gamma \zeta_2 \quad \alpha_i, \beta_{ij}, \gamma \in \mathbb{Q}
\]

Fixed by symbol-level analysis
The new algorithm

[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ 2023]

1. Select MI coefficients for the basis at symbol level \( \{ f_i^{(w)} \} \) [Goncharov, Spradlin, Vergu, Volovich 2010]

Symbol = iterated integral stripped of boundary information

\[
\text{Li}_2(z) = -[1 - z, z]_1 - \log 2 \left[ z \right]_1 - \frac{\pi^2}{12} \quad \delta [\text{Li}_2(z)] = -[1 - z, z]
\]

2. Ansatz: all MI coefficients are polynomials in \( \{ f_i^{(w)} \} \) and \( \zeta_2 \) and \( \zeta_3 \) (up to weight 4)

\[
\text{MI}^{(2)} = \sum_i \alpha_i f_i^{(2)} + \sum_{i \leq j} \beta_{ij} f_i^{(1)} f_j^{(1)} + \gamma \zeta_2 \quad \alpha_i, \beta_{ij}, \gamma \in \mathbb{Q}
\]

Fixed by symbol-level analysis

Fixed by evaluation at \( s_0 \) + rationalisation
Summary of the algorithm

Input:
- canonical DEs
- numerical boundary values \{ \text{MI}_i^{(w)}(s_0) \}

Only needed at the accuracy required for the evaluation (~70 digits)

Easy to obtain using AMFlow
[Liu, Ma 2022]

Output:
- function basis \{ f_i^{(w)} \} (written in terms of iterated integrals)
- relations among the boundary values
- expression of all MI coefficients as polynomials in \{ f_i^{(w)} \} and \zeta \) values
One-mass pentagon functions

All 1-mass 2-loop 5-pt integrals (2304 independent MIs)

Functions chosen to highlight analytic properties

E.g. letters expected to drop out, singularities... are isolated in the minimal number of functions

All 4! permutations of external massless legs → everything that is needed for any amplitude of this kind
Efficient numerical evaluation
Logs and dilogarithms up to weight 2

Explicit expressions by fitting ansätze

\[ f^{(1)} \sim \log + \tau^{(1)} \]
\[ f^{(2)} \sim \text{Li}_2 + \log^2 + \tau^{(1)} \log + \tau^{(2)} \]

Arguments guessed [Duhr, Gangl, Rhodes 2011] and chosen s.t. functions are well defined in a physical scattering region (s_{45} channel)

\[ f^{(1)}_2 = \log (-s_{34}) \]
\[ f^{(2)}_2 = \text{Li}_2 \left( \frac{s_{14}}{p_1^2} \right) + \log \left( -\frac{s_{14}}{p_1^2} \right) \log \left( 1 - \frac{s_{14}}{p_1^2} \right) + i\pi \log (s_{15} - s_{23} + s_{45}) - i\pi \log (p_1^2) \]

Can be evaluated numerically straightforwardly
One-fold integrals at weight 3 and 4

Path $\gamma : [0, 1] \rightarrow s$ entirely within the physical region

$$[W_{i_1}, W_{i_2}, W_{i_3}]_{s_0}(s) = \int_0^1 dt \frac{d \log W_{i_3}(s'(t))}{dt} [W_{i_1}, W_{i_2}]_{s_0}(s'(t))$$

Through integration by parts [Caron-Huot, Henn 2014]

$$f^{(4)} \sim \int_0^1 dt \log \times \frac{d \log}{dt} \times f^{(2)}$$

No analytic continuation required!

Numerical integration implemented in C++ library PentagonFunctions++

⇒ All functions evaluated in ~3 s (double precision, single core)!
Pentagon functions allowed for efficient amplitude computation

Massless pentagon functions
[Chicherin, Sotnikov 2020]
- $3\gamma$
- $2\gamma + j$
- $3j$
- $\gamma + 2j$

1-mass pentagon functions (planar)
[Chicherin, Sotnikov, SZ 2021]
- $W + b\bar{b}$ (planar)
- $W + 2j$ (planar)
- $H + b\bar{b}$ (planar)
- $W + \gamma + j$ (planar)

[Abreu, Page, Pascual, Sotnikov 2020; Chawdhry, Czakon, Mitov, Poncelet 2021; Abreu, De Laurentis, Ita, Klinkert, Page, Sotnikov, 2023]
[Abreu, Febres-Cordero, Ita, Page, Sotnikov 2021; De Laurentis, Ita, Klinkert, Sotnikov 2023; Agarwal, Buccioni, Devoto, Gambuti, von Manteuffel, Tancredi 2023]
[Badger, Czakon, Bayu Hartanto, Moodie, Peraro, Poncelet, SZ 2023]
[Badger, Bayu Hartanto, SZ 2021; Bayu Hartanto, Poncelet, Popescu, SZ 2022]
[Abreu, Febres Cordero, Ita, Klinkert, Page, Sotnikov 2022]
[Badger, Bayu Hartanto, Kryś, SZ 2021]
[Badger, Bayu Hartanto, Kryś, SZ 2022]
Ready for deployment in NNLO QCD phenomenology

Leading colour @ 2 loops

\( pp \rightarrow 3\gamma \) [Kallweit, Sotnikov, Wiesemann 2020; Chawdhry, Czakon, Mitov, Poncelet 2020]

\( pp \rightarrow 2\gamma + j \) [Chawdhry, Czakon, Mitov, Poncelet 2021; Badger, Gehrmann, Marcoli, Moodie 2021]

\( pp \rightarrow 3j \) [Czakon, Mitov, Poncelet 2021; Chen, Gehrmann, Glover, Huss, Marcoli 2022]

\( pp \rightarrow W + b\bar{b} \) [Bayu Hartanto, Poncelet, Popescu, \textcolor{red}{SZ} 2022; Buonocore, Devoto, Kallweit, Mazzitelli, Rottoli, Savoini 2023]

\( pp \rightarrow \gamma + 2j \) [Badger, Czakon, Bayu Hartanto, Moodie, Peraro, Poncelet, \textcolor{red}{SZ} 2023]

The pentagon functions meet the demands of phenomenological applications
What if we don’t have canonical DEs?
2. Physics-informed deep learning

Calisto, Moodie, **SZ (23XX.XXXXX)**

*Logo by Ryan Moodie*
Neural networks are universal function approximators

[Hornik, Stinchcombe, White '89]

Typical problem: approximate function \( f(x) \) from large dataset of values \( f(x_i) \)
Neural networks are universal function approximators

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```
Neural network diagram:
```

- **Input layer**: $x$
- **Weights**: $\theta$
- **Hidden layers**
- **Activation function**
- **Output layer**: $h(x; \theta)$

"Surrogate function"
Neural networks are universal function approximators

[Horik, Stinchcombe, White ’89]

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

Optimisation problem: find weights $\theta$ such that a loss function is minimised

$$L(D; \theta) = \frac{1}{N} \sum_{i=1}^{N} [f(x_i) - h(x_i; \theta)]^2$$
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: \( \frac{df(x)}{dx} = A(x)f(x) \)
Physics-informed deep learning

Idea: include the DEs in the loss function

\[ L(D; \theta) = \sum_i \left[ h(x_i; \theta) - f(x_i) \right]^2 + \sum_j \left[ \frac{dh(x; \theta)}{dx} \bigg|_{x=x_j} - A(x_j) h(x_j; \theta) \right]^2 \]

Small “boundary” dataset

Infinite dimensional “DE” dataset

Derivatives of the NN computed with automatic differentiation

Input: few boundary values + the analytic DEs

[Raissi, Perdikaris, Karniadakis 2017]

[Griewank, Walther 2008]
The canonical form of the DEs is not needed

We make mild assumptions to simplify the problem:

\[
\frac{\partial}{\partial v_i} \vec{F}(\vec{v}; \epsilon) = A_{v_i}(\vec{v}; \epsilon) \cdot \vec{F}(\vec{v}; \epsilon) \quad \forall \ i = 1, \ldots, n_v \quad \vec{v} : \text{kinematic variables}
\]
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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 \(\epsilon = 0\),

\[
A_{v_i}(\vec{v}; \epsilon) = \sum_{k=0}^{k_{\text{max}}} e^k A_{V_i}^{(k)}(\vec{v})
\]

\(\Rightarrow\) Simplifies the \(\epsilon\) expansion of the solution

\[
\vec{F}(\vec{v}; \epsilon) = e^{w*} \sum_{w=0}^{w_{\text{max}}} e^w \vec{F}^{(w)}(\vec{v})
\]
Dimensionless kinematic variables

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

Re or Im part of $\vec{F}^{(w)}$ up to a certain order in $\epsilon$
3 kinematic variables, 36 MIs
\[ \vec{v} = \{ s = (p_1 + p_2)^2, \ t = (p_1 - p_3)^2, \ m^2 \} \]

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]

[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

Mls (Re or Im)

36 x 5 = 180 outputs

$\epsilon$ orders

$$\overline{F}(\overline{v}; \epsilon) = \frac{1}{\epsilon^4} \sum_{w=0}^{4} \epsilon^w \overline{F}^{(w)}(\overline{v})$$
Heavy crossed box: kinematic region

$s$ channel: $s > -t > 0 \land m^2 > 0$

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]
Ensemble of 10 NNs

Iterations: $7.9 \times 10^4$

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)

Mean absolute difference: $1.6 \times 10^{-3}$

Mean magnitude of rel. diff.: $7.3 \times 10^{-3}$

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

Flatness of the performance with respect to

- Analytic complexity ($\epsilon$ orders, MI) within the same family
- Across different families

Instantaneous evaluation times 😍
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Only proof of concept!

Many ideas to improve!
Conclusion

New algorithm to construct solutions to canonical DEs

- Efficient computation of amplitudes
- Efficient numerical evaluation

All 2-loop 5-pt integrals with 1 external massive leg now available!

*Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, SZ (2306.15431)*

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

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Thank you!
One-mass pentagon functions

Avg. time per point: 3 s

Number of points

Fraction of points

$R$ (correct digits)

New non-planar feature: integrable (and genuine)
singularities in the $s_{45}$ channel at $\Sigma_5^{(i)} = 0$

Planar subset ~10 times better

Double accuracy
(quadruple and octuple also available)
One-mass pentagon functions
PentagonFunctions++

Avg. time per point: 9 s
Solving the canonical DEs in terms of iterated integrals is straightforward.

\[
\begin{align*}
\left\{ \begin{array}{l}
    d\left[w_{i_1}, \ldots, w_{i_n}\right]_s(s) = d\log w_{i_n}(s) \left[w_{i_1}, \ldots, w_{i_{n-1}}\right]_s(s) \\
    \left[w_{i_1}, \ldots, w_{i_n}\right]_s(s_0) = 0
\end{array} \right.
\end{align*}
\]

Chen’s iterated integrals

Canonical DEs

\[
\begin{align*}
\left\{ \begin{array}{l}
    d \overrightarrow{F}^{(w)}(s) = \sum_i a_i d\log w_i(s) \overrightarrow{F}^{(w-1)}(s) \\
    \overrightarrow{F}^{(w)}(s_0) = \overrightarrow{F}^{(w)}_0
\end{array} \right.
\end{align*}
\]

Insensitive to square roots!
Proof-of-concept implementation

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

\[ L_{DE}(D_{DE}, \theta) = \sum_{\tilde{x}^{(i)} \in D_{DE}} \sum_{j=1}^{n_F} \sum_{l=1}^{n_v-1} \sum_{w=0}^{w_{\text{max}}} \left[ \partial_{x(l)} h_j^{(w)}(\tilde{x}^{(i)}; \theta) - \sum_{k=0}^{\min(w,k_{\text{max}})} \sum_{r=1}^{n_F} A_{x(l),j,r}^{(k)}(\tilde{x}^{(i)}) h_r^{(w-k)}(\tilde{x}^{(i)}; \theta) \right]^2 \]

\[ L_b(D_b, \theta) = \sum_{\tilde{x}^{(i)} \in D_b} \sum_{j=1}^{n_F} \sum_{w=0}^{w_{\text{max}}} \left[ h_j^{(w)}(\tilde{x}^{(i)}; \theta) - g_j^{(w)}(\tilde{x}^{(i)}) \right]^2 \]
<table>
<thead>
<tr>
<th>Integral family</th>
<th>box</th>
<th>one-mass double box</th>
<th>heavy crossed box</th>
<th>top double box</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inputs</td>
<td>1</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Hidden layers</td>
<td>$3 \times 32$</td>
<td>$3 \times 256$</td>
<td>$3 \times 256$</td>
<td>$4 \times 128$</td>
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<tr>
<td>Outputs</td>
<td>15</td>
<td>90</td>
<td>180</td>
<td>99</td>
</tr>
<tr>
<td>Learning rate</td>
<td>$10^{-2}$</td>
<td>$10^{-3}$</td>
<td>$10^{-3}$</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>Batch size</td>
<td>64</td>
<td>256</td>
<td>256</td>
<td>256</td>
</tr>
<tr>
<td>Boundary points</td>
<td>2</td>
<td>6</td>
<td>10</td>
<td>20</td>
</tr>
<tr>
<td>$c_{n_v}$</td>
<td>$s = 10$</td>
<td>$s_{12} = 2.5$</td>
<td>$m^2 = 1$</td>
<td>$m_t^2 = 1$</td>
</tr>
<tr>
<td>Scale bound</td>
<td>—</td>
<td>—</td>
<td>$s \leq \sqrt{10}$</td>
<td>$s_{12} \leq 5$</td>
</tr>
<tr>
<td>Physical cut (%)</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Spurious cut (%)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Summary of hyperparameters
<table>
<thead>
<tr>
<th>Integral family</th>
<th>Final loss</th>
<th>Iterations</th>
<th>Time (minutes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>box</td>
<td>$2.7 \times 10^{-7}$</td>
<td>$2.5 \times 10^5$</td>
<td>16</td>
</tr>
<tr>
<td>one-mass double box</td>
<td>$3.4 \times 10^{-4}$</td>
<td>$1.1 \times 10^5$</td>
<td>53</td>
</tr>
<tr>
<td>heavy crossed box</td>
<td>$1.4 \times 10^{-5}$</td>
<td>$7.9 \times 10^4$</td>
<td>75</td>
</tr>
<tr>
<td>top double box</td>
<td>$7.1 \times 10^{-4}$</td>
<td>$5.2 \times 10^4$</td>
<td>32</td>
</tr>
</tbody>
</table>

Training statistics

<table>
<thead>
<tr>
<th>Integral family</th>
<th>MEU</th>
<th>MDE</th>
<th>MAD</th>
<th>MMRD</th>
<th>MLR</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>box</td>
<td>$2.8 \times 10^{-5}$</td>
<td>$3.6 \times 10^{-4}$</td>
<td>$2.9 \times 10^{-5}$</td>
<td>$2.2 \times 10^{-5}$</td>
<td>$3.9 \times 10^{-7}$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>one-mass DB</td>
<td>$8.1 \times 10^{-4}$</td>
<td>$1.1 \times 10^{-2}$</td>
<td>$2.0 \times 10^{-3}$</td>
<td>$1.1 \times 10^{-2}$</td>
<td>$-2.8 \times 10^{-4}$</td>
<td>$10^5$</td>
</tr>
<tr>
<td>heavy CB</td>
<td>$2.8 \times 10^{-4}$</td>
<td>$2.8 \times 10^{-3}$</td>
<td>$1.6 \times 10^{-3}$</td>
<td>$7.3 \times 10^{-3}$</td>
<td>$-4.5 \times 10^{-4}$</td>
<td>$10^2$</td>
</tr>
<tr>
<td>top DB</td>
<td>$1.9 \times 10^{-4}$</td>
<td>$1.7 \times 10^{-3}$</td>
<td>$9.0 \times 10^{-4}$</td>
<td>$3.9 \times 10^{-3}$</td>
<td>$1.8 \times 10^{-4}$</td>
<td>$10^2$</td>
</tr>
</tbody>
</table>

Uncertainty and testing errors