Targeting Multi-Loop Integrals with Neural Networks

Ramon Winterhalder

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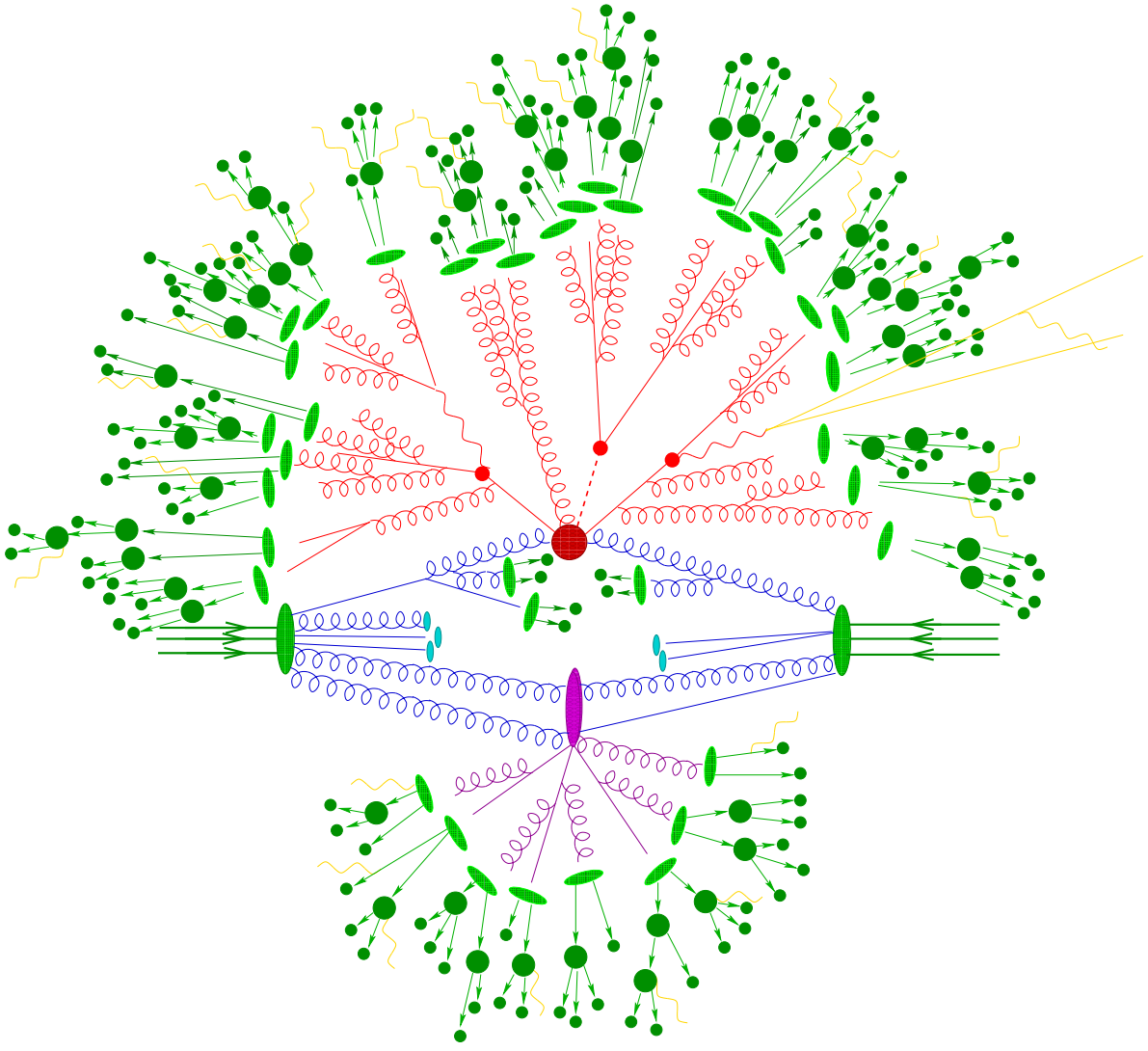
5th IML Workshop – CERN 2022

Based on [2112.09145], SciPost Phys. 12, 129 (2022)

in collaboration with Vitaly Magerya, Emilio Villa, Stephen P. Jones, Matthias Kerner, Anja Butter, Gudrun Heinrich, and Tilman Plehn

UCLouvain

Data analysis in HEP



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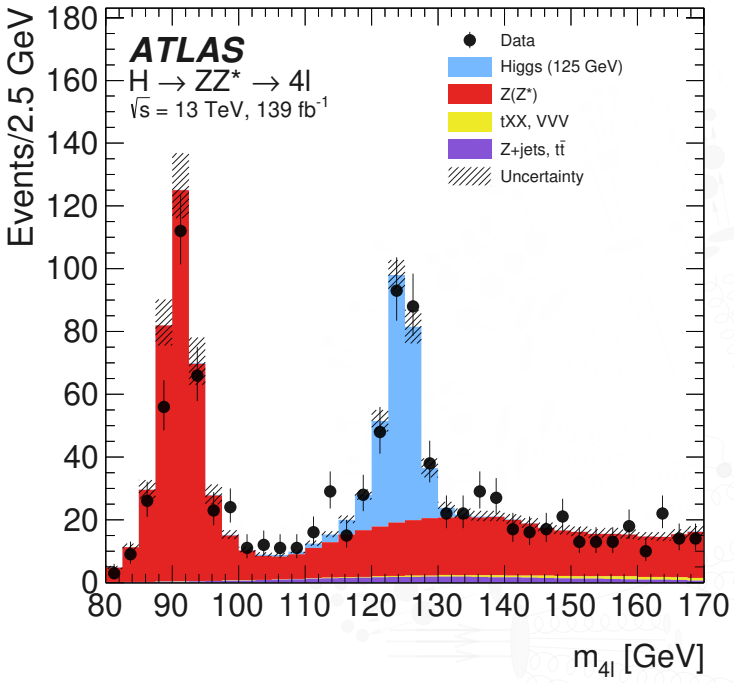

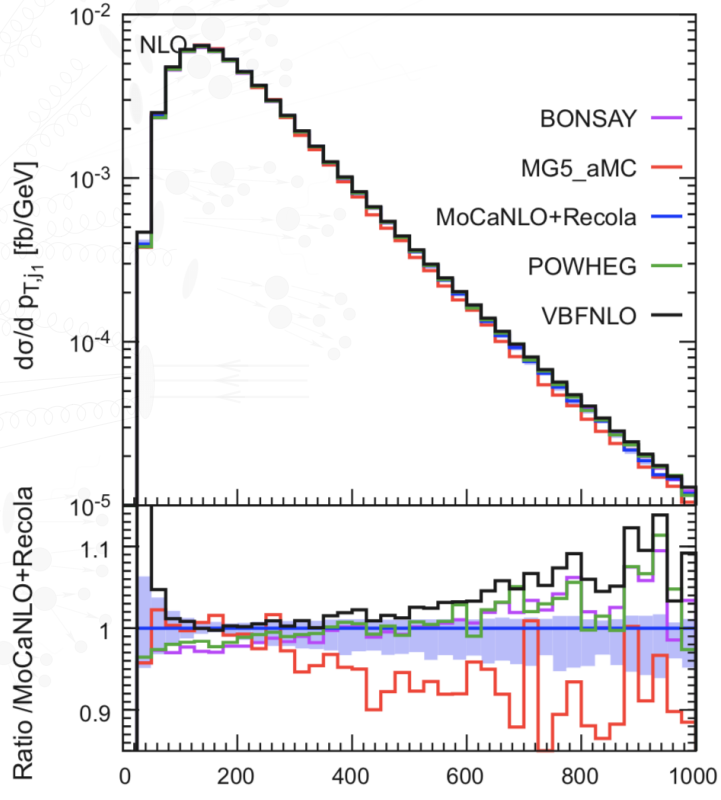

Theory predictions in HEP

$$\mathcal{A}_{n,\{\lambda,c,\dots\}}(p_a, p_b | p_1, \dots, p_n) : \mathbb{M} \to \mathbb{C}$$

Quantum numbers:
spin, colour charge etc.

Kinematics:
Momenta in Minkowski space, masses, etc.

$$\sigma_n = \frac{1}{\text{flux}} \sum_{a,b} \int \mathrm{d}x_a \mathrm{d}x_b \, f(x_a) f(x_b) \int \mathrm{d}\Phi_n \, \left\langle |\mathcal{A}_n(p_a, p_b | p_1, \dots, p_n)|^2 \right\rangle$$

Cross section:
more generally, differential observables*

PDFs:
convolution over all possible initial state configurations

Phase-space integral:
over final state kinematics

Squared amplitude:
summed over final states, averaged over initial states

Theory predictions in HEP

Outline for today

→ Focus on **calculation of amplitudes**

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Towards high precision

Fixed-order perturbative expansion

$$\mathcal{A}_n = \mathcal{A}_n^{(0)} + \underbrace{\mathcal{A}_n^{(1)} + \mathcal{A}_n^{(2)} + \dots}_{\text{loop amplitudes}}$$

Theory predictions in HEP

Outline for today

→ Focus on **calculation of amplitudes**

Towards high precision

Fixed-order perturbative expansion

$$\mathcal{A}_n = \mathcal{A}_n^{(0)} + \underbrace{\mathcal{A}_n^{(1)} + \mathcal{A}_n^{(2)} + \dots}_{\text{loop amplitudes}}$$

Calculation of loop amplitudes

For complicated integrals

analytic solution impractical

→ numerical evaluation in Feynman parameter space

Multi-loop integral

Feynman parametrization

$$G = \frac{(-1)^\nu\,\Gamma(\nu - LD/2)}{\prod_{j=1}^{N}\Gamma(\nu_j)} \int \left(\prod_{j=1}^{N} \mathrm{d}x_j\, x_j^{\nu_j - 1}\right) \delta\left(1 - \sum_{l=1}^{N} x_l\right) \frac{\mathcal{U}^{\nu-(L+1)D/2}}{\mathcal{F}^{\nu-LD/2}}$$

with $\mathcal{U} \equiv \det(M)$ and $\mathcal{F} \equiv \det(M)\left[\sum_{i,j=1}^{L} Q_i \left(M^{-1}\right)_{ij} Q_j - J - \mathrm{i}\delta\right]$.

$\mathcal{U}$: polynomial in x_i only

$\mathcal{F}$: depends on x_i and kinematic invariants s_{ij}, m_i^2

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Caveats

Careful treatment of singularities in the integral!

Singularity structure

UV and IR singularities

show up as poles $1/\epsilon^{\alpha}$

(1a) Overall UV poles: $\Gamma(\nu - LD/2) \propto \Gamma(n\epsilon)$

(1b) UV subdivergencies: arise from $\mathcal{U}(\vec{x}) = 0$ for some $x_i = 0$.

(2) IR divergencies (soft and collinear):
arise from $\mathcal{F}(x, s_{ij}, m_i^2) = 0$ for some $x_i = 0$.

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(3) $\mathcal{F}(x, s_{ij}, m_i^2) = 0$ inside integration region

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Sector decomposition

algorithm to isolate and subtract poles

→ public tool pySecDec [Heinrich et al, '10,'17,'19, '21]

and expand integral

$$G = \sum_{j=-2L}^{n} C_j \epsilon^j$$

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numerical integration of finite C_j

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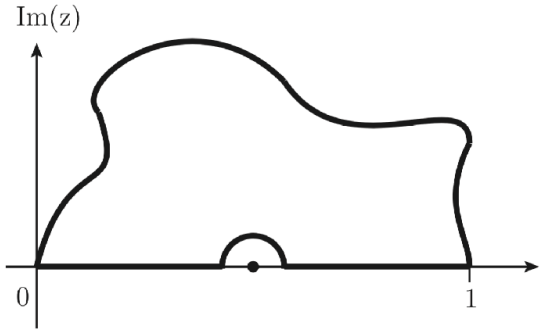
→ needs procedure to avoid poles!

Contour Deformation

Neural Contour Deformation

Standard contour deformation



Cauchy theorem:

$$\oint_c \prod_{j=1}^{N} \mathrm{d}z_j \, \mathcal{I}(\vec{z}) = \int_0^1 \prod_{j=1}^{N} \mathrm{d}x_j \, \mathcal{I}(\vec{x}) + \int_\gamma \prod_{j=1}^{N} \mathrm{d}z_j \, \mathcal{I}(\vec{z})$$

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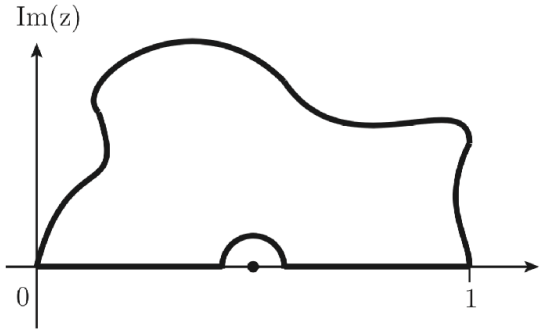

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Transformation: $x_j \to z_j(\vec{x}) = x_j - \mathrm{i}\tau_j(\vec{x})$

Deformation parameter: λ_j

$$\tau_j = \lambda_j x_j (1 - x_j) \frac{\partial \mathcal{F}(\vec{x})}{\partial x_j}$$

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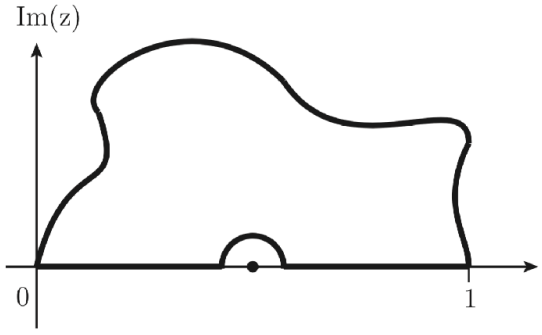

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$$+ \frac{\mathrm{i}}{6} \sum_{j,k,l} \tau_j \tau_k \tau_l \frac{\partial^3 \mathcal{F}(\vec{x})}{\partial x_j \partial x_k \partial x_l} + \cdots$$

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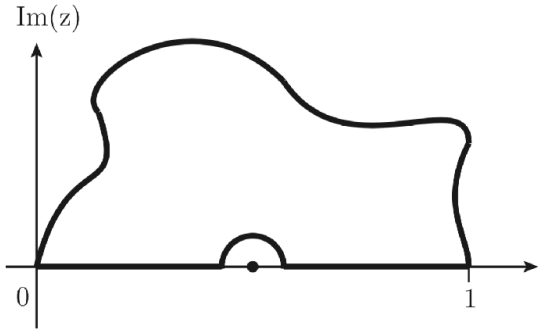

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always positive

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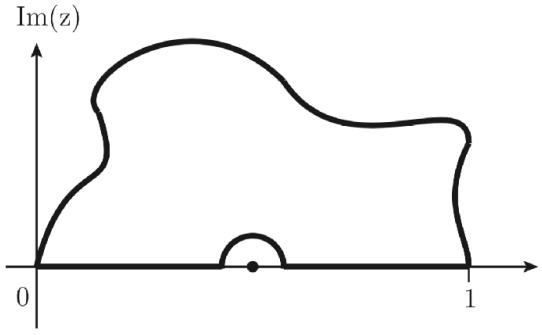

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Does **not** spoil sign for small enough λ

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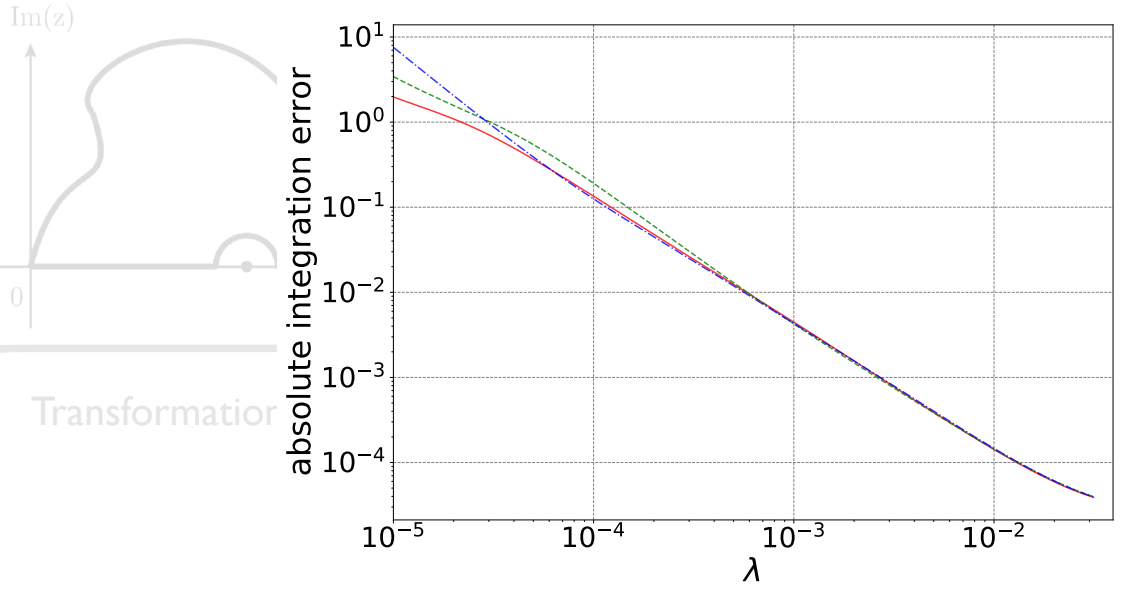

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Λ-Glob algorithm

Complex shift

$$x_j \to z_j(\vec{x}) = x_j - \mathrm{i}\tau_j(\vec{x}),$$

$$\tau_j = \lambda_j x_j(1-x_j)\frac{\partial F(\vec{x})}{\partial x_j}, \qquad \rho(\vec{z}(\vec{x})) = \left|\frac{\partial \vec{z}(\vec{x})}{\partial \vec{x}}\right|^{-1}$$

$$I = \int_\gamma \prod_{j=1}^{N} \mathrm{d}z_j(\vec{x})\,\frac{\mathcal{I}(\vec{z})}{\rho(\vec{z})} \quad \Rightarrow I \simeq I_m = \frac{1}{m}\sum_{i=1}^{m}\frac{\mathcal{I}(\vec{x}_i)}{\rho(\vec{x}_i)} = \langle \mathcal{I}/\rho \rangle_x$$

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Note II: The integrand is a complex-valued function!

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Caution!

Careful treatment of complex derivatives!

Complex derivatives in TensorFlow

Consider the Jacobian matrix

$$J = \begin{pmatrix} 1 + \mathrm{i}\lambda_0 & 0 \\ 0 & 1 + \mathrm{i}\lambda_1 \end{pmatrix}$$

Check GitHub and Colab for details!

Next we calculate its determinant

$$\det J = (1 + \mathrm{i}\lambda_0)(1 + \mathrm{i}\lambda_1) = (1 - \lambda_0\lambda_1) + \mathrm{i}(\lambda_0 + \lambda_1)$$

And afterwards its absolute square

$$L = \det J \cdot (\det J)^* = (1 - \lambda_0\lambda_1)^2 + (\lambda_0 + \lambda_1)^2$$

And finally we take the gradient with respect to $\vec{\lambda}$ and obtain

$$\nabla_\lambda L = \left(2\lambda_0(1 + \lambda_1)^2, 2\lambda_1(1 + \lambda_0)^2\right)$$

Now evaluating this gradient at $\vec{\lambda} = (2, 1)$ yields $\nabla_\lambda L\Big|_{\vec{\lambda}=(2,1)} = (10, 8)$.

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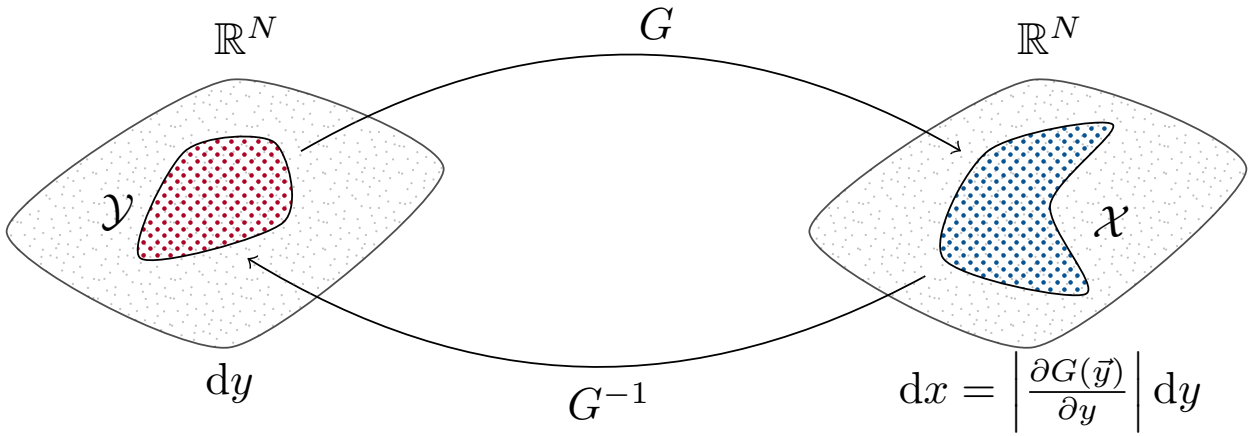
However: Tensorflow obtains $\nabla_\lambda L\Big|_{\vec{\lambda}=(2,1)} = (-14, -8.8)$

Normalizing flow

Neural importance sampling Gao et al. [2001.05486, 2001.10028], Bothmann et al. [2001.05478]



$$x_j \to x_j(\vec{y}) = G_j(\vec{y}), \qquad g(\vec{x}(\vec{y})) = \left|\frac{\partial G(\vec{y})}{\partial y}\right|^{-1}$$

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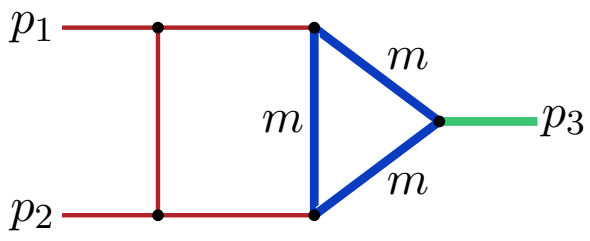
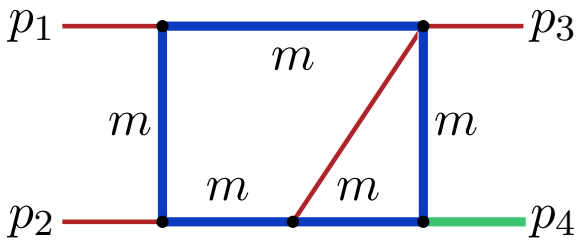
Results – Two-loop integrals

Example diagrams



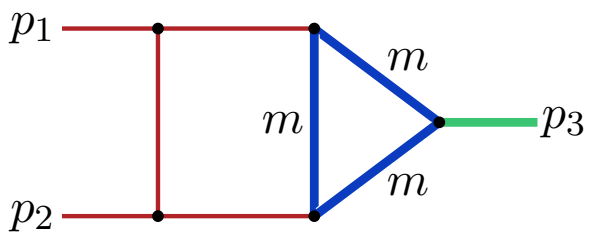
- NLO correction to $gg \to h$
- 5 feynman parameters
- 2 kinematic invariants: s, m^2

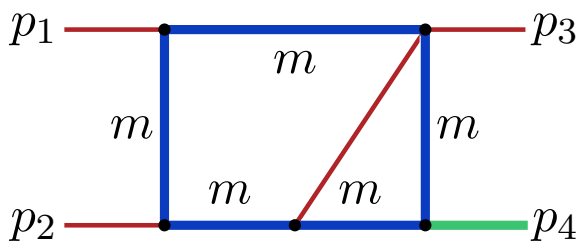


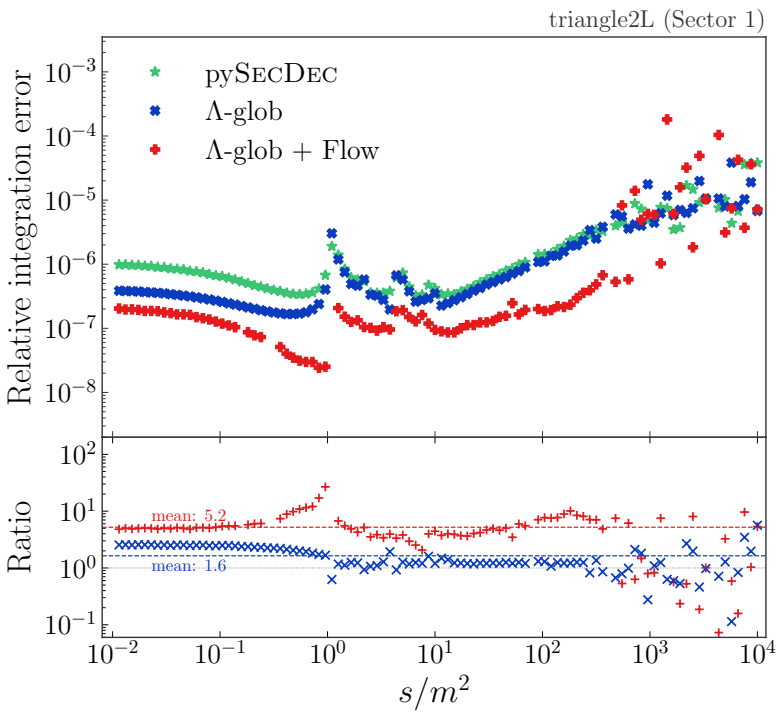
- $gg \to hj$ at two loops
- 5 feynman parameters
- 4 kinematic invariants: s, t, p_4^2, m^2

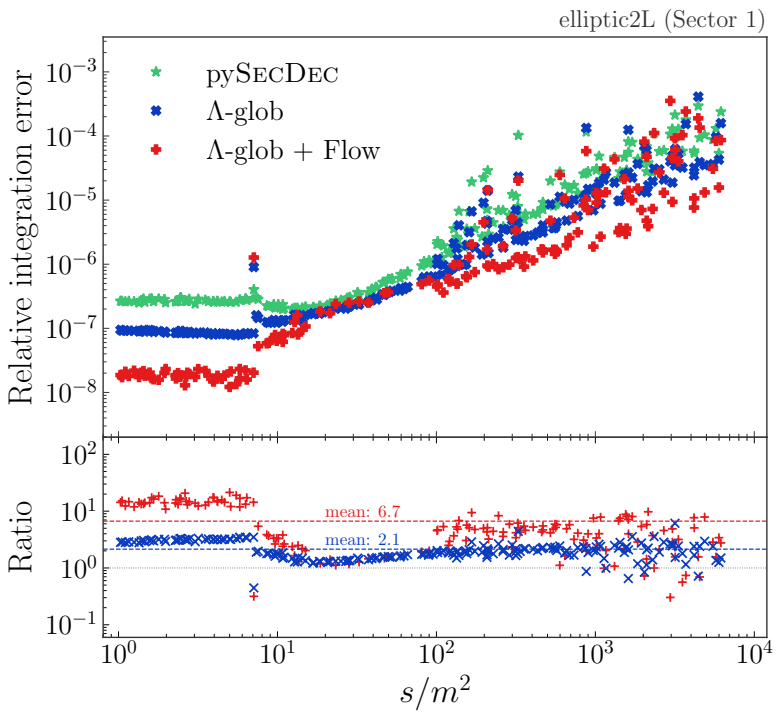
Results – Two-loop integrals

Example diagrams









Conclusion and Outlook

Summary

- Improved precision of numerical loop integrals!
- Two-step procedure:
  (a) Λ-Glob: complex shift
  (b) Normalizing Flow: importance sampling reals

Outlook

- Further investigation of more complicated integrals
- Possibly check integrals for which standard pySecDec fails.
- Integrate into full workflow of pySecDec