Treatment of non-positive definite integrands with Normalising Flows

Rene Poncelet

based on work together with Timo Janßen and Steffen Schumann [2505.xxxx]

THE HENRYK NIEWODNICZAŃSKI
INSTITUTE OF NUCLEAR PHYSICS
POLISH ACADEMY OF SCIENCES

The problem

- Numerical integration of highly dimensional integrands → Monte Carlo Sampling

Integral

$$I = \int_{\mathbf{x}\in\Omega} \mathrm{d}\mathbf{x} f(\mathbf{x})$$

MC estimate

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i) \,,$$

MC error estimate

$$\delta\hat{I} = \sqrt{\frac{1}{N-1}\left(\frac{1}{N}\sum_{i=1}^{N} f^2(\mathbf{x}_i) - \hat{I}^2\right)}$$

- Variance reduction techniques improve performance, mapping $\mathbf{H} : \Omega \to \Omega, \mathbf{x} \mapsto \mathbf{H}(\mathbf{x})$

$$I = \int_{\mathbf{H}(\mathbf{x})\in\Omega} \mathrm{d}\mathbf{H} \frac{f(\mathbf{x})}{h(\mathbf{x})}$$

$$h(\mathbf{x}) = \left|\det\left(\frac{\partial \mathbf{H}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

Find with $h(\mathbf{x})$ adaptive MC techniques: VEGAS [Lepage'78], Parni [Hameren'14],
ML techniques: Normalising Flows Iflow [Bothmann'20] Madnis [Heimel'22], ...

How to build $\mathbf{h}(\mathbf{x})$?

- by hand…
- ‘Standard’: VEGAS/Parni
  → essentially histograms, assuming integrand factorises wrt to integration variables
- Deep Learning approach: Normalising Flows
  - Coupling Layer (CL) Flows
  - Continuous (ODE) Flows

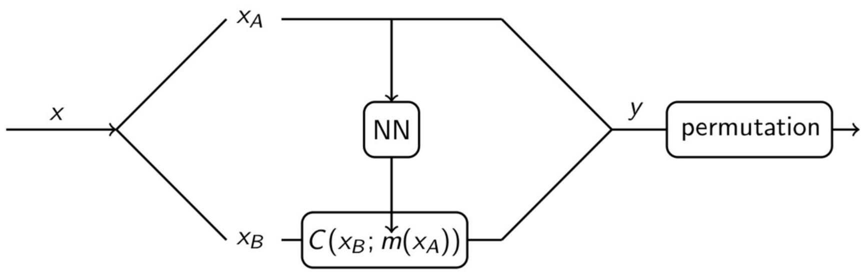
Coupling Layer Normalizing Flow

Based on the i-flow paper: 2001.05486

Series of bijections: $\vec{x}_K = c_K(c_{K-1}(\cdots c_2(c_1(\vec{x}))))$

Distribution: $$g_K(\vec{x}_K) = g_0(\vec{x}_0) \prod_{k=1}^{K} \left| \frac{\partial c_k(\vec{x}_{k-1})}{\partial \vec{x}_{k-1}} \right|^{-1}, \quad \text{where} \quad \begin{cases} \vec{x}_0 = \vec{x} \\ \vec{x}_k = c_k(\vec{x}_{k-1}) \end{cases}$$

Structure of a single coupling layer:



$$\begin{aligned} x'_A &= x_A, & A &\in [1, d]\ , \\ x'_B &= C(x_B; m(\vec{x}_A)), & B &\in [d+1, D]\ . \end{aligned}$$

The inverse map

$$x_A = x'_A \ ,$$
$$x_B = C^{-1}(x'_B; m(\vec{x}'_A)) = C^{-1}(x'_B; m(\vec{x}_A))$$

Inverse Jacobian: $\left|\frac{\partial c(\vec{x})}{\partial \vec{x}}\right|^{-1} = \left|\begin{pmatrix} \vec{1} & 0 \\ \frac{\partial C}{\partial m}\frac{\partial m}{\partial \vec{x}_A} & \frac{\partial C}{\partial \vec{x}_B} \end{pmatrix}\right|^{-1} = \left|\frac{\partial C(\vec{x}_B; m(\vec{x}_A))}{\partial \vec{x}_B}\right|^{-1}$

Derivative of the NN

Big advantage: $\frac{\partial m}{\partial x_A}$ not needed!
→ Performance

How many coupling layers you need?

$$\begin{array}{ll} 2\log_2 D & \text{for} \quad D > 5 \\ D & \text{for} \quad D \leq 5 \end{array}$$

Example: Masking to capture all correlations for D=12

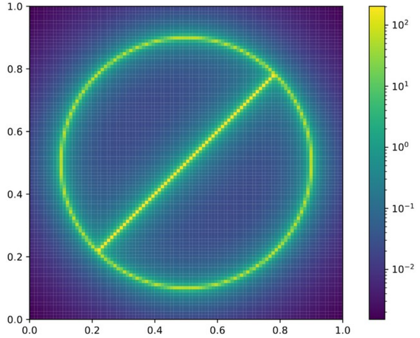
2x

Dimension	0	1	2	3	4	5	6	7	8	9	10	11
Transformation 1	0	1	0	1	0	1	0	1	0	1	0	1
Transformation 2	0	0	1	1	0	0	1	1	0	0	1	1
Transformation 3	0	0	0	0	1	1	1	1	0	0	0	0
Transformation 4	0	0	0	0	0	0	0	0	1	1	1	1

A toy example

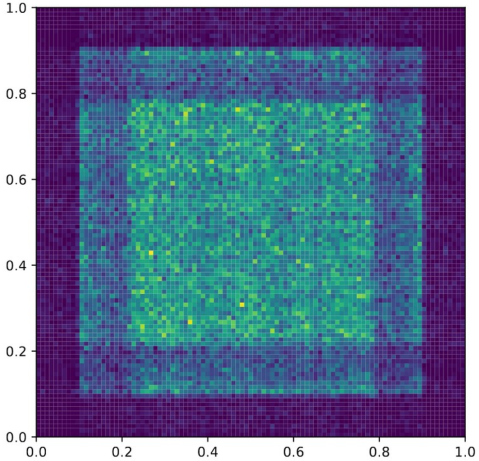
Multi-modular function ("stop-sign"):

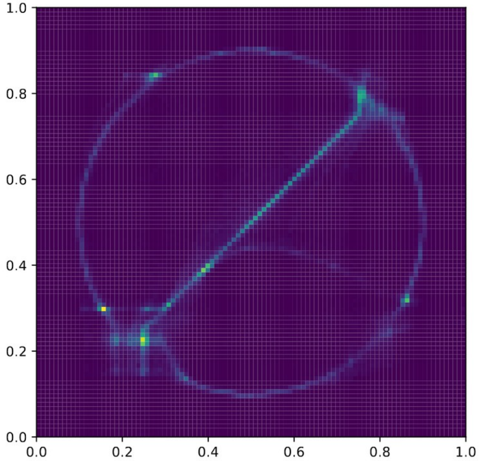
$$f(x,y) = \frac{1}{2\pi^2} \cdot \frac{\Delta r}{\left(\sqrt{(x-x_0)^2+(y-y_0)^2}-r_0\right)^2+(\Delta r)^2} \cdot \frac{1}{\sqrt{(x-x_0)^2+(y-y_0)^2}}$$
$$+\frac{1}{2\pi r_0} \cdot \frac{\Delta r}{((y-y_0)-(x-x_0))^2+(\Delta r)^2} \cdot \Theta\left(r_0 - \sqrt{(x-x_0)^2+(y-y_0)^2}\right).$$



Sampling densities:

VEGAS





Coupling-Layer Flow

Continuous Flows

"time"-dependent probability density function: $$\log q_t(\mathbf{y}_t) = \log q_0(\mathbf{y}_0) - \log\left|\det \frac{\partial \phi_t}{\partial \mathbf{y}_0}\right|$$

constructed from $$\frac{\mathrm{d}}{\mathrm{d}t}\phi_t(\mathbf{y}) = v_t(\phi_t(\mathbf{y}))\,, \quad \text{with} \quad \phi_0(\mathbf{y}) = \mathbf{y}$$

+continuity equation (preserve prob.)

vector-field is given by a trainable NN

The mapped point is the solution of a simple ODE: $$\mathbf{y}_1 = \phi_1(\mathbf{y}_0) = \int_0^1 v_t(\phi_t(\mathbf{y}_0))\,\mathrm{d}t$$

Jacobian by inverse ODE:

$$\frac{\mathrm{d}}{\mathrm{d}s}\begin{bmatrix}\phi_{1-s}(\mathbf{y})\\ f(1-s)\end{bmatrix} = \begin{bmatrix}-v_{1-s}(\phi_{1-s}(\mathbf{y}))\\ -\operatorname{div}\big(v_{1-s}(\phi_{1-s}(\mathbf{y}))\big)\end{bmatrix} \qquad \begin{bmatrix}\phi_1(\mathbf{y})\\ f(1)\end{bmatrix} = \begin{bmatrix}\mathbf{y}_1\\ 0\end{bmatrix}$$

$$\rightarrow \quad \log q_1(\mathbf{y_1}) = \log q_0(\mathbf{y_0}) - f(0)$$

Training and model parameters

Training target based on Kullback–Leibler (KL) divergence:

$$D_{\mathrm{KL}}(p \parallel q_\theta) = \sum_{i=1}^{N} p(\mathbf{y}_i) \log\left(\frac{p(\mathbf{y}_i)}{q_\theta(\mathbf{y}_i)}\right)$$

1) Generate sample & evaluate target function
   (1M points)

2) Do NN optimization step with gradient descend (ADAM)

3) Repeat 1)
   (10 times)

Size of neural networks depends on the dimension of the problem.

→ we investigated 4 to 13 dimensional problems + discrete parameters (conditional NNs):

~ 100k – 10M parameters for CL flows

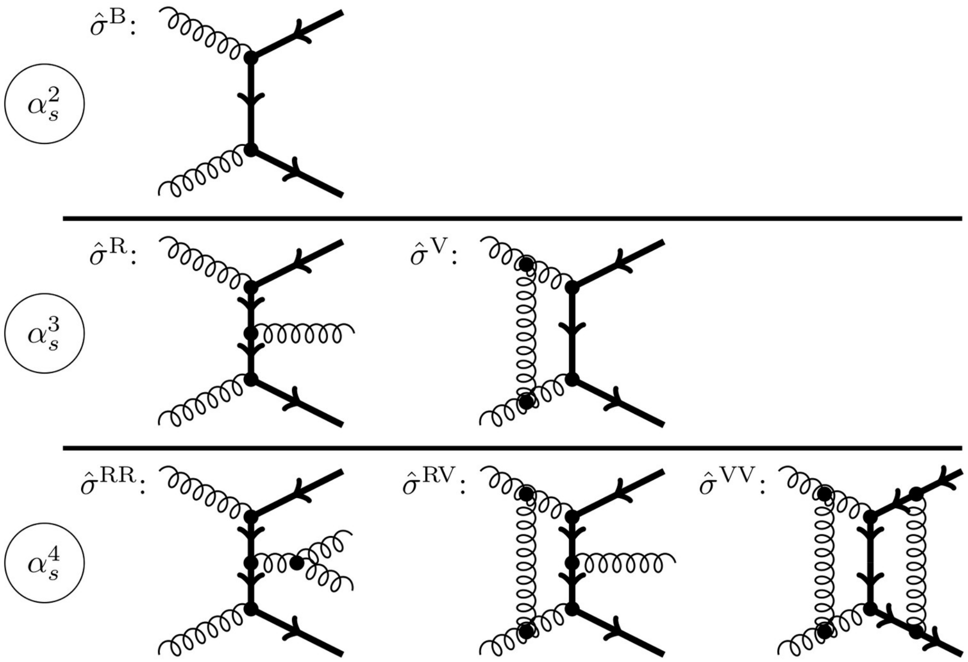
~ 1M parameter for ODE flows

The integrands

Cross sections in STRIPPER:

$$\sigma(h(P_1)h(P_2) \to X) = \sum_{ab} \iint_0^1 \mathrm{d}x_1\,\mathrm{d}x_2 \phi_a(x_1)\phi_b(x_2)\hat{\sigma}_{ab}(x_1P_1, x_2P_2)$$

Example diagrams top-pair production



NNLO pQCD: $\hat{\sigma}_{ab} = \hat{\sigma}_{ab}^{(0)} + \hat{\sigma}_{ab}^{(1)} + \hat{\sigma}_{ab}^{(2)}$

$$\hat{\sigma}_{ab}^{(0)} = \hat{\sigma}_{ab}^{\mathrm{B}}$$

$$\hat{\sigma}_{ab}^{(1)} = \hat{\sigma}_{ab}^{\mathrm{R}} + \hat{\sigma}_{ab}^{\mathrm{V}} + \hat{\sigma}_{ab}^{\mathrm{C}}$$

$$\hat{\sigma}_{ab}^{(2)} = \hat{\sigma}_{ab}^{\mathrm{RR}} + \hat{\sigma}_{ab}^{\mathrm{RV}} + \hat{\sigma}_{ab}^{\mathrm{VV}} + \hat{\sigma}_{ab}^{\mathrm{C1}} + \hat{\sigma}_{ab}^{\mathrm{C2}}$$

The integrands II

Matrix elements + measurement functions

Structure of partonic contributions:

different partonic channels $\hat{\sigma}^i_{ab} = \sum_{j \in \mathcal{C}^i_{ab}(ab \to X)} \hat{\sigma}^i_{ab,j}$ ➡ $\hat{\sigma}^i_{ab,j} = N_j \int \mathrm{d}\Phi_j \mathcal{F}_{ab,j}(\Phi_j)$

Subtraction for real-emission contributions
based on sector-decomposition + residue subtraction:

$$\hat{\sigma}^{(1)} \ni \int \mathrm{d}\Phi_j \sum_{kl} \mathcal{S}_{kl} |\mathcal{M}_j(\Phi_j)|^2 F(\Phi_j) \,.$$

$$\hat{\sigma}^{(i)} \ni \int_{[0,1]^m} \mathrm{d}^m \chi \int_{[0,1]^n} \mathrm{d}^n \mathbf{x} \frac{f^j_{\{k\}}(\chi, \mathbf{x}) - \sum f^j_{\{k\}}(\chi|_{\to 0}, \mathbf{x})}{\prod_i^m \chi_i}$$

But for the integration problem (in case of tot cross sections) it is enough to consider:

$$\boxed{\hat{\sigma}^{(i)} \ni \int_{[0,1]^n} \mathrm{d}\mathbf{y}\, g^j_{\{k\}}(\mathbf{y})}$$

$$\sum_{\{k\},h} \int_{[0,1]^n} \mathrm{d}\mathbf{y}\, g^j_{\{k\},h}(\mathbf{y}) = \sum_l \int_{[0,1]^n} \mathrm{d}\mathbf{y}\, g^j_l(\mathbf{y})$$

Sum of
Sectors, helicities, channels

Benchmarks

- To make life simple: Optimization goal is total integral (i.e. total cross section)
  → focusing on gluonic top-pair production (small number of channels)

- Three integrators: VEGAS (reference for the current default), CL, ODE
  each with standard absolute training and positive/negative stratified training

- Benchmark quantities

  - Weight variance

  - Unweighting efficiency

Results LO and NLO

Frozen integrators
1M points

Estimate + Error

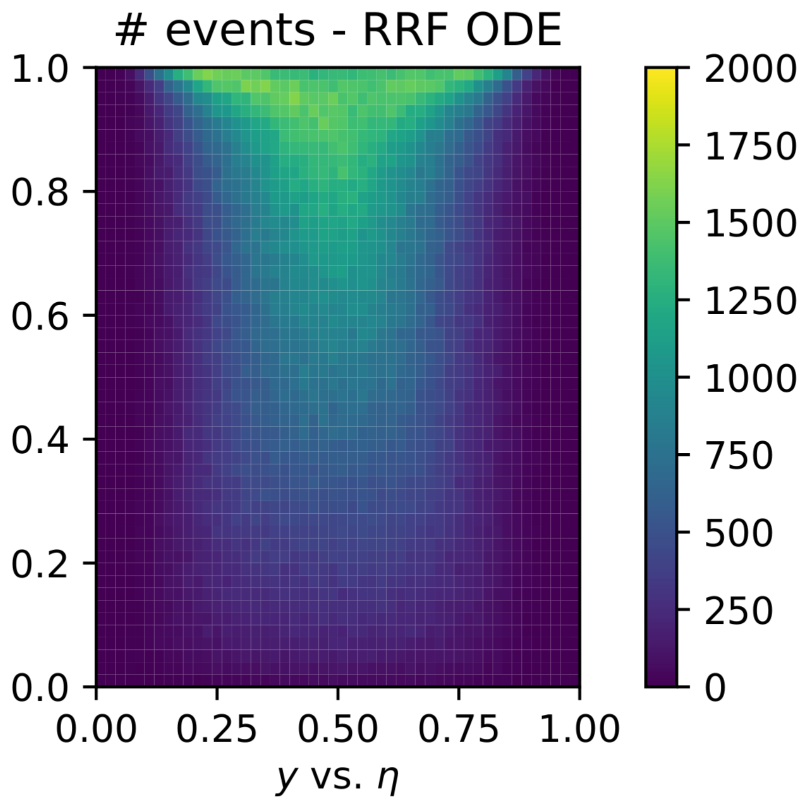
Observation #1: Saturation of lower bounds with flows, for VEGAS only in the simpler ones

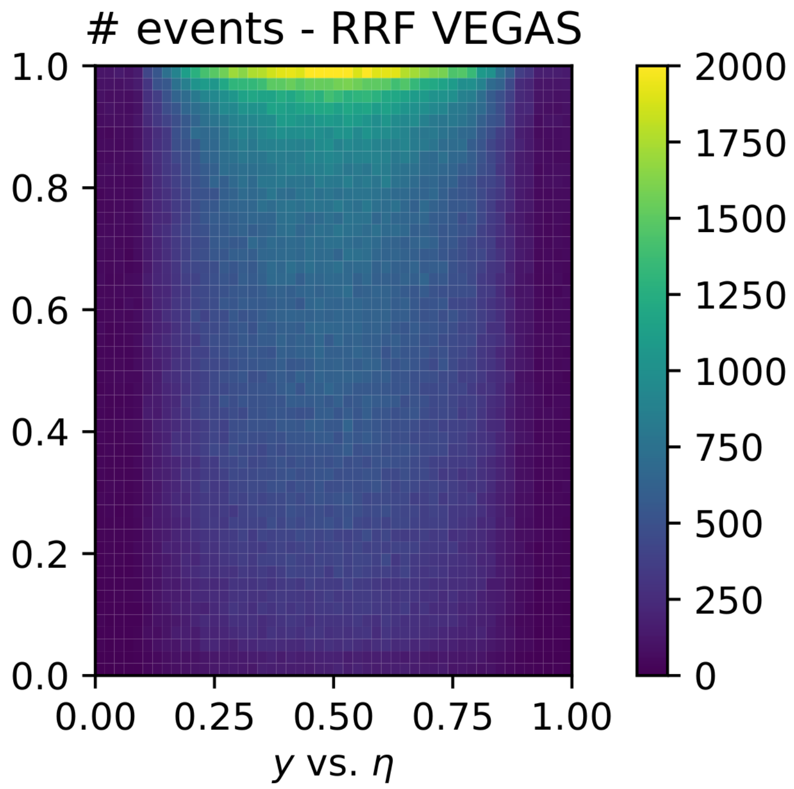
Contribution	$\sigma_{\mathrm{B}} \cdot 10^{-2}$	$\sigma_{\mathrm{RF}} \cdot 10^{-2}$	$\sigma_{\mathrm{RU}} \cdot 10^{-2}$	$\sigma_{\mathrm{VF}} \cdot 10^{-1}$
δ^{opt}	0.0001	0.008	0.01	0.006
CPU cost [a.u.]	1	6	1.5	1.3
VEGAS				
$\hat{\sigma} \pm \delta\hat{\sigma}$	5.3278 ± 0.002	6.967 ± 0.01	-5.378 ± 0.02	-4.487 ± 0.006
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	5.3284 ± 0.002	8.955 ± 0.01	4.432 ± 0.006	1.403 ± 0.0008
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	$-0.0006446 \pm 5e-07$	-1.981 ± 0.004	-9.8098 ± 0.008	-5.8939 ± 0.003
$\Sigma^{\pm}$	5.3278 ± 0.002	6.973 ± 0.01	-5.378 ± 0.01	-4.4909 ± 0.003
ϵ_{Φ}^+	0.99	0.728	0.639	0.808
ϵ_{Φ}^-	0.834	0.384	0.852	0.95
$\epsilon^+ (\epsilon^+_{0.1\%})$	0.13 (0.43)	0.048 (0.098)	0.02 (0.048)	0.082 (0.21)
$\epsilon^- (\epsilon^-_{0.1\%})$	0.016 (0.066)	0.013 (0.021)	0.049 (0.17)	0.12 (0.27)
ODE Flow				
$\hat{\sigma} \pm \delta\hat{\sigma}$	5.3279 ± 0.0005	6.98 ± 0.009	-5.394 ± 0.01	-4.483 ± 0.006
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	5.32872 ± 0.0004	8.9494 ± 0.002	4.4185 ± 0.002	1.4018 ± 0.0001
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	$-0.00064495 \pm 1e-07$	-1.9844 ± 0.0006	-9.802 ± 0.003	-5.89315 ± 0.0005
$\Sigma^{\pm}$	5.32808 ± 0.0004	6.965 ± 0.003	-5.3835 ± 0.004	-4.4914 ± 0.0006
ϵ_{Φ}^+	1.0	0.991	0.992	1.0
ϵ_{Φ}^-	0.997	0.99	0.987	0.999
$\epsilon^+ (\epsilon^+_{0.1\%})$	0.33 (0.7)	0.025 (0.3)	0.0059 (0.099)	0.11 (0.56)
$\epsilon^- (\epsilon^-_{0.1\%})$	0.055 (0.36)	0.028 (0.17)	0.02 (0.16)	0.12 (0.73)
Coupling Layer Flow				
$\hat{\sigma} \pm \delta\hat{\sigma}$	5.32795 ± 0.0003	6.972 ± 0.009	-5.39 ± 0.01	-4.492 ± 0.006
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	5.32807 ± 0.0003	8.949 ± 0.002	4.4101 ± 0.002	$1.40155 \pm 9e-05$
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	$-0.000644883 \pm 3e-08$	-1.9821 ± 0.0007	-9.8 ± 0.002	-5.89183 ± 0.0003
$\Sigma^{\pm}$	5.32742 ± 0.0003	6.9669 ± 0.003	-5.3899 ± 0.004	-4.49028 ± 0.0004
ϵ_{Φ}^+	1.0	0.989	0.988	1.0
ϵ_{Φ}^-	1.0	0.99	0.994	1.0
$\epsilon^+ (\epsilon^+_{0.1\%})$	0.53 (0.81)	0.028 (0.24)	0.0082 (0.046)	0.17 (0.63)
$\epsilon^- (\epsilon^-_{0.1\%})$	0.11 (0.79)	0.0074 (0.06)	0.009 (0.19)	0.4 (0.79)

Results NNLO

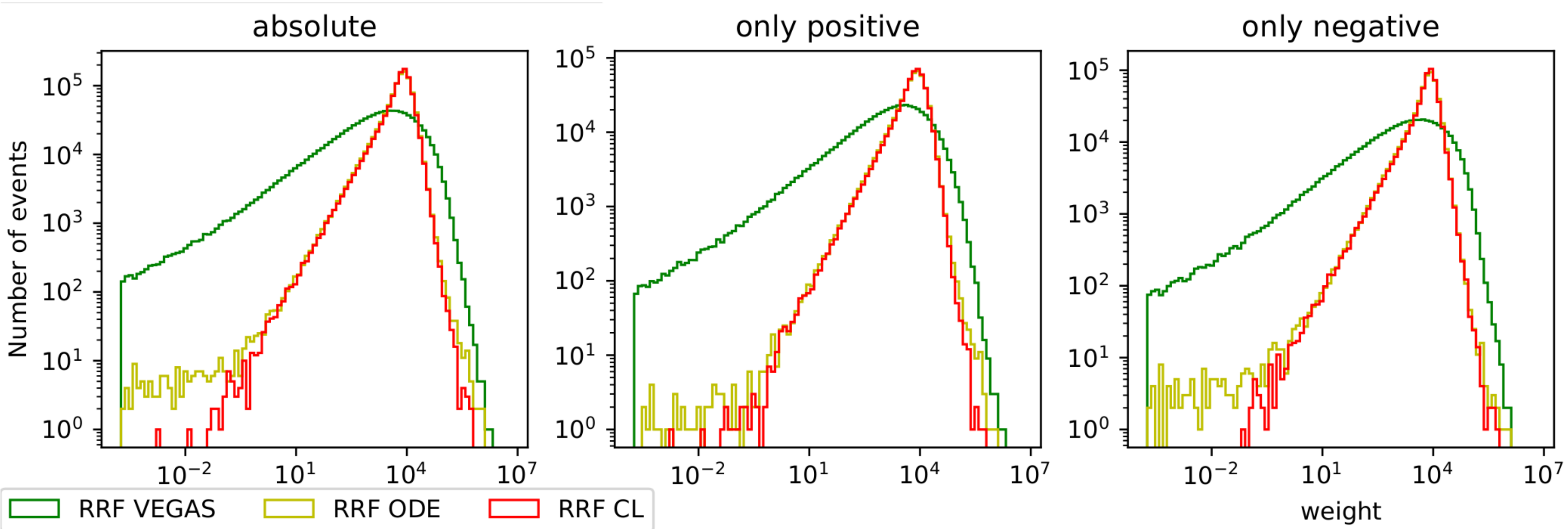
Contribution	$\sigma_{\mathrm{RRF}} \cdot 10^{-2}$	$\sigma_{\mathrm{RRSU}} \cdot 10^{-3}$	$\sigma_{\mathrm{RRDU}} \cdot 10^{-3}$	$\sigma_{\mathrm{RVF}} \cdot 10^{-2}$	$\sigma_{\mathrm{RVFR}} \cdot 10^{-2}$	$\sigma_{\mathrm{RVDU}} \cdot 10^{-3}$	$\sigma_{\mathrm{VVF}} \cdot 10^{-0}$
δ^{opt}	0.0079	0.0036	0.013	0.0081	0.0018	0.0045	0.011
CPU cost [a.u.]	53	26	8	1542	2.7	2.7	13
				VEGAS			
$\hat{\sigma} \pm \delta\hat{\sigma}$	-0.3 ± 0.02	2.835 ± 0.0069	-2.461 ± 0.017	-6.808 ± 0.022	0.2864 ± 0.0023	0.267 ± 0.0049	14.768 ± 0.014
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	3.823 ± 0.013	3.718 ± 0.0056	5.639 ± 0.0065	1.669 ± 0.0026	1.051 ± 0.0014	2.381 ± 0.0011	16.711 ± 0.0067
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	-4.135 ± 0.013	-0.8813 ± 0.0022	-8.078 ± 0.0085	-8.4539 ± 0.0068	-0.7635 ± 0.0012	-2.1114 ± 0.0012	-1.955 ± 0.0011
$\Sigma^\pm$	-0.312 ± 0.025	2.836 ± 0.0079	-2.439 ± 0.015	-6.785 ± 0.0094	0.2871 ± 0.0025	0.2696 ± 0.0023	14.756 ± 0.0078
ϵ_Φ^+	0.54	0.732	0.803	0.55	0.593	0.946	0.956
ϵ_Φ^-	0.513	0.402	0.8	0.871	0.501	0.916	0.816
$\epsilon^+(\epsilon_{0.1\%}^+)$	0.004 (0.0052)	0.0073 (0.017)	0.0018 (0.022)	0.013 (0.024)	0.025 (0.06)	0.029 (0.22)	0.015 (0.1)
$\epsilon^-(\epsilon_{0.1\%}^-)$	0.0041 (0.0053)	0.0035 (0.01)	0.0037 (0.019)	0.014 (0.038)	0.021 (0.05)	0.011 (0.11)	0.024 (0.17)
				ODE Flow			
$\hat{\sigma} \pm \delta\hat{\sigma}$	-0.333 ± 0.011	2.823 ± 0.0048	-2.421 ± 0.015	-6.784 ± 0.0081	0.2893 ± 0.0019	0.271 ± 0.0046	14.758 ± 0.012
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	3.812 ± 0.0063	3.7056 ± 0.0028	5.6439 ± 0.0036	1.6764 ± 0.00085	1.0495 ± 0.00038	2.3806 ± 0.00043	16.72 ± 0.0026
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	-4.142 ± 0.0057	-0.8848 ± 0.0045	-8.071 ± 0.0068	-8.4578 ± 0.0019	-0.76271 ± 0.00026	-2.1109 ± 0.0005	-1.9554 ± 0.00023
$\Sigma^\pm$	-0.33 ± 0.012	2.821 ± 0.0073	-2.427 ± 0.01	-6.7814 ± 0.0027	0.2868 ± 0.00064	0.2697 ± 0.00093	14.765 ± 0.0028
ϵ_Φ^+	0.855	0.945	0.977	0.988	0.981	0.998	0.999
ϵ_Φ^-	0.853	0.834	0.982	0.991	0.983	0.998	0.998
$\epsilon^+(\epsilon_{0.1\%}^+)$	0.0013 (0.0027)	0.0028 (0.022)	0.003 (0.023)	0.0029 (0.067)	0.0081 (0.099)	0.03 (0.27)	0.0086 (0.49)
$\epsilon^-(\epsilon_{0.1\%}^-)$	0.0019 (0.0053)	0.00025 (0.00025)	0.0018 (0.0096)	0.051 (0.25)	0.017 (0.095)	0.017 (0.18)	0.17 (0.49)
				Coupling Layer Flow			
$\hat{\sigma} \pm \delta\hat{\sigma}$	-0.317 ± 0.01	2.829 ± 0.0044	-2.414 ± 0.014	-6.778 ± 0.0079	0.285 ± 0.0019	0.276 ± 0.0045	14.771 ± 0.012
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	3.814 ± 0.0054	3.7038 ± 0.0025	5.6425 ± 0.0039	1.676 ± 0.0024	1.05 ± 0.00059	2.3799 ± 0.00043	16.718 ± 0.0021
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	-4.134 ± 0.0063	-0.8849 ± 0.0015	-8.0756 ± 0.0047	-8.456 ± 0.0026	-0.76256 ± 0.00055	-2.1091 ± 0.00036	-1.95479 ± 0.00011
$\Sigma^\pm$	-0.32 ± 0.012	2.819 ± 0.0041	-2.433 ± 0.0086	-6.7803 ± 0.005	0.2874 ± 0.0011	0.2708 ± 0.00079	14.763 ± 0.0022
ϵ_Φ^+	0.838	0.956	0.985	0.987	0.988	0.998	1.0
ϵ_Φ^-	0.852	0.836	0.988	0.991	0.985	0.999	1.0
$\epsilon^+(\epsilon_{0.1\%}^+)$	0.0022 (0.0056)	0.0096 (0.022)	0.0029 (0.011)	0.00076 (0.00076)	0.0024 (0.035)	0.01 (0.22)	0.02 (0.31)
$\epsilon^-(\epsilon_{0.1\%}^-)$	0.0034 (0.006)	0.0012 (0.0028)	0.0044 (0.011)	0.0054 (0.13)	0.0017 (0.018)	0.022 (0.22)	0.1 (0.68)

Non-factorizing phase space features





Weight distribution for double real



Non-positive definite integrands

- Non-definite integrands introduce new challenges

  → cancellation between +/- parts increase the variance

- Consider extreme case: $|f(x)|/h(x) = w = \text{const.}$

  MC estimate:

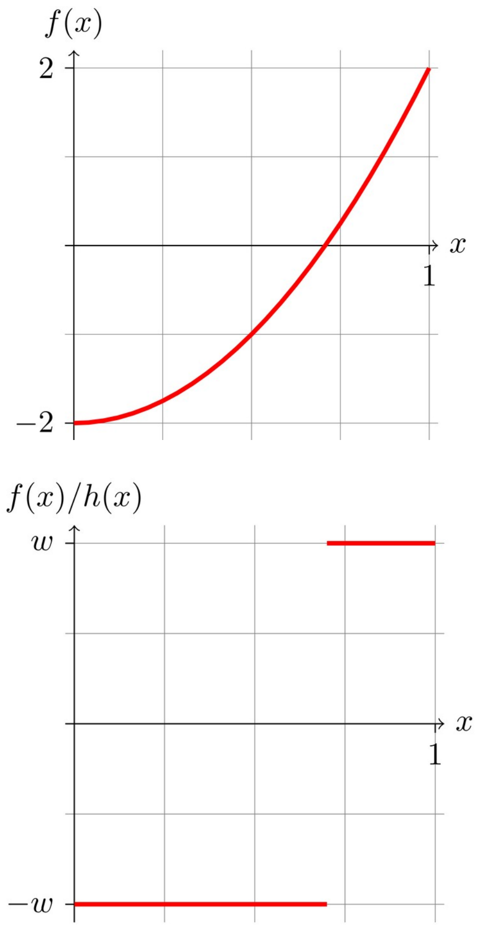
$$\hat{I} = w\frac{N_+ - N_-}{N} \equiv w(2\alpha - 1) \qquad \alpha = N_+/N$$

- Lower bound on variance:

$$\mathrm{Var}(\hat{I}) = w^2 - w^2(2\alpha - 1)^2 = w^2(4\alpha(1-\alpha))$$

→ relative uncertainty: $\frac{\delta\hat{I}}{\hat{I}} = \frac{1}{\sqrt{N-1}}\frac{\sqrt{\alpha(1-\alpha)}}{\alpha - \frac{1}{2}}$

Rephrased: at some point it doesn't matter any more how good your adaptive MC is...



Stratification of signed integrands

There are ways around:

1) Add a large constant

2) Stratification: $$f(\mathbf{x}) = f_+(\mathbf{x}) + f_-(\mathbf{x})\,, \quad \text{with} \quad f_\pm(\mathbf{x}) = \Theta(\pm f(\mathbf{x}))f(\mathbf{x})$$

$$\Rightarrow \quad I = \int_{\mathbf{H}_+(\mathbf{x})\in\Omega} \mathrm{d}\mathbf{H}_+ \frac{f_+(\mathbf{x})}{h_+(\mathbf{x})} + \int_{\mathbf{H}_-(\mathbf{x})\in\Omega} \mathrm{d}\mathbf{H}_- \frac{f_-(\mathbf{x})}{h_-(\mathbf{x})}$$

"two independent integrals"

$$\hat{I}_{\text{strat}} = \hat{I}_+ + \hat{I}_- = \frac{1}{N_+}\sum_{i=1}^{N_+}\frac{f_+(\mathbf{x}_i)}{h_+(\mathbf{x}_i)} + \frac{1}{N_-}\sum_{i=1}^{N_-}\frac{f_-(\mathbf{x}_i)}{h_-(\mathbf{x}_i)}$$

$$\delta\hat{I}_{\text{strat}} = \sqrt{\frac{1}{N-1}\left[\frac{N}{N_+}\mathrm{Var}(\hat{I}_+) + \frac{N}{N_-}\mathrm{Var}(\hat{I}_-)\right]}$$

$$\mathrm{Var}(\hat{I}_\pm) = \frac{1}{N_\pm}\sum_{i=1}^{N_\pm}\left(\frac{f_\pm(\mathbf{x}_i)}{h_\pm(\mathbf{x}_i)}\right)^2 - \hat{I}_\pm^2$$

+ The total variance is now bounded by the individual variances

- The mappings are more complicated (need high phase space efficiency)

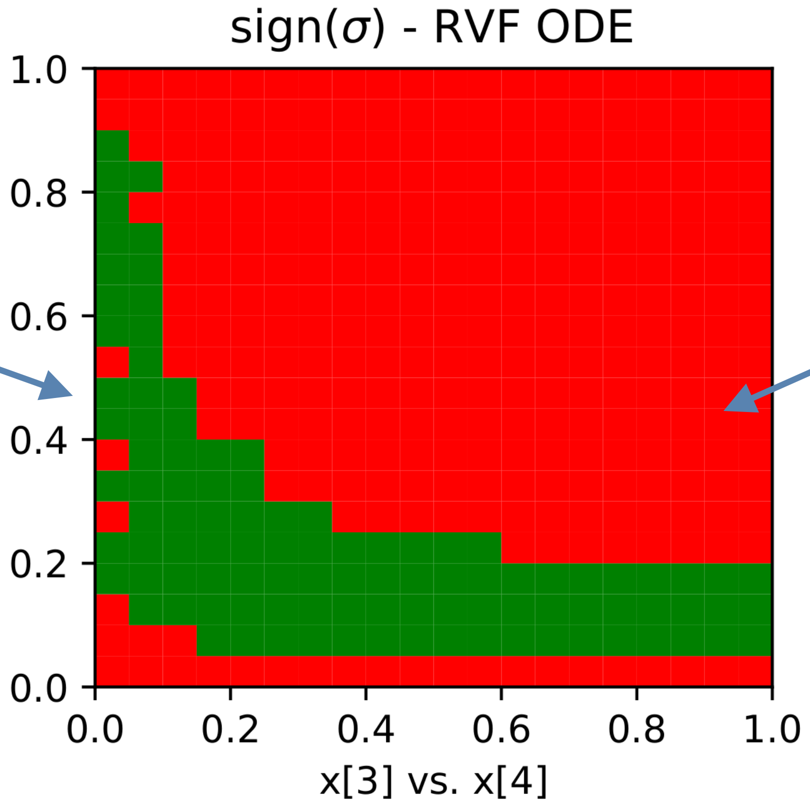
Results LO and NLO

Observation #2:
Splitting can give a significant performance gains for flow based integrators
→ requires high phase space eff.

Contribution	$\sigma_{\mathrm{B}} \cdot 10^{-2}$	$\sigma_{\mathrm{RF}} \cdot 10^{-2}$	$\sigma_{\mathrm{RU}} \cdot 10^{-2}$	$\sigma_{\mathrm{VF}} \cdot 10^{-1}$
δ^{opt}	0.0001	0.008	0.01	0.006
CPU cost [a.u.]	1	6	1.5	1.3
VEGAS				
$\hat{\sigma} \pm \delta\hat{\sigma}$	5.3278 ± 0.002	6.967 ± 0.01	-5.378 ± 0.02	-4.487 ± 0.006
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	5.3284 ± 0.002	8.955 ± 0.01	4.432 ± 0.006	1.403 ± 0.0008
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	$-0.0006446 \pm 5e-07$	-1.981 ± 0.004	-9.8098 ± 0.008	-5.8939 ± 0.003
$\Sigma^{\pm}$	5.3278 ± 0.002	6.973 ± 0.01	-5.378 ± 0.01	-4.4909 ± 0.003
ϵ_{Φ}^{+}	0.99	0.728	0.639	0.808
ϵ_{Φ}^{-}	0.834	0.384	0.852	0.95
$\epsilon^+ (\epsilon_{0.1\%}^+)$	0.13 (0.43)	0.048 (0.098)	0.02 (0.048)	0.082 (0.21)
$\epsilon^- (\epsilon_{0.1\%}^-)$	0.016 (0.066)	0.013 (0.021)	0.049 (0.17)	0.12 (0.27)
ODE Flow				
$\hat{\sigma} \pm \delta\hat{\sigma}$	5.3279 ± 0.0005	6.98 ± 0.009	-5.394 ± 0.01	-4.483 ± 0.006
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	5.32872 ± 0.0004	8.9494 ± 0.002	4.4185 ± 0.002	1.4018 ± 0.0001
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	$-0.00064495 \pm 1e-07$	-1.9844 ± 0.0006	-9.802 ± 0.003	-5.89315 ± 0.0005
$\Sigma^{\pm}$	5.32808 ± 0.0004	6.965 ± 0.003	-5.3835 ± 0.004	-4.4914 ± 0.0006
ϵ_{Φ}^{+}	1.0	0.991	0.992	1.0
ϵ_{Φ}^{-}	0.997	0.99	0.987	0.999
$\epsilon^+ (\epsilon_{0.1\%}^+)$	0.33 (0.7)	0.025 (0.3)	0.0059 (0.099)	0.11 (0.56)
$\epsilon^- (\epsilon_{0.1\%}^-)$	0.055 (0.36)	0.028 (0.17)	0.02 (0.16)	0.12 (0.73)
Coupling Layer Flow				
$\hat{\sigma} \pm \delta\hat{\sigma}$	5.32795 ± 0.0003	6.972 ± 0.009	-5.39 ± 0.01	-4.492 ± 0.006
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	5.32807 ± 0.0003	8.949 ± 0.002	4.4101 ± 0.002	$1.40155 \pm 9e-05$
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	$-0.000644883 \pm 3e-08$	-1.9821 ± 0.0007	-9.8 ± 0.002	-5.89183 ± 0.0003
$\Sigma^{\pm}$	5.32742 ± 0.0003	6.9669 ± 0.003	-5.3899 ± 0.004	-4.49028 ± 0.0004
ϵ_{Φ}^{+}	1.0	0.989	0.988	1.0
ϵ_{Φ}^{-}	1.0	0.99	0.994	1.0
$\epsilon^+ (\epsilon_{0.1\%}^+)$	0.53 (0.81)	0.028 (0.24)	0.0082 (0.046)	0.17 (0.63)
$\epsilon^- (\epsilon_{0.1\%}^-)$	0.11 (0.79)	0.0074 (0.06)	0.009 (0.19)	0.4 (0.79)

Non-trivial positive/negative structure

Negative



Positive

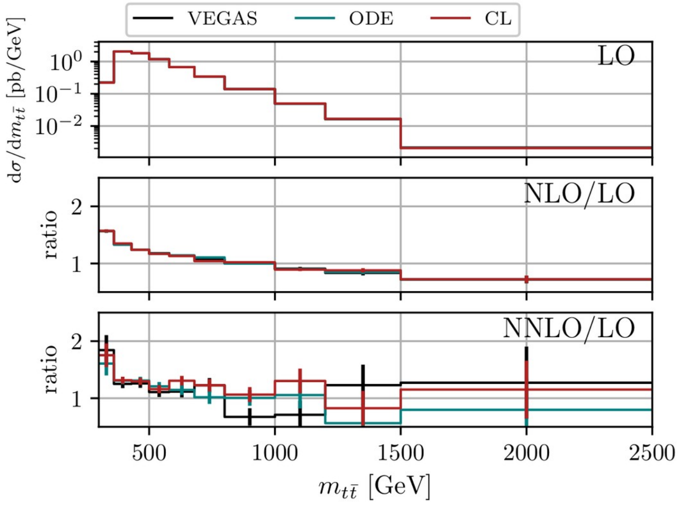
Results NNLO

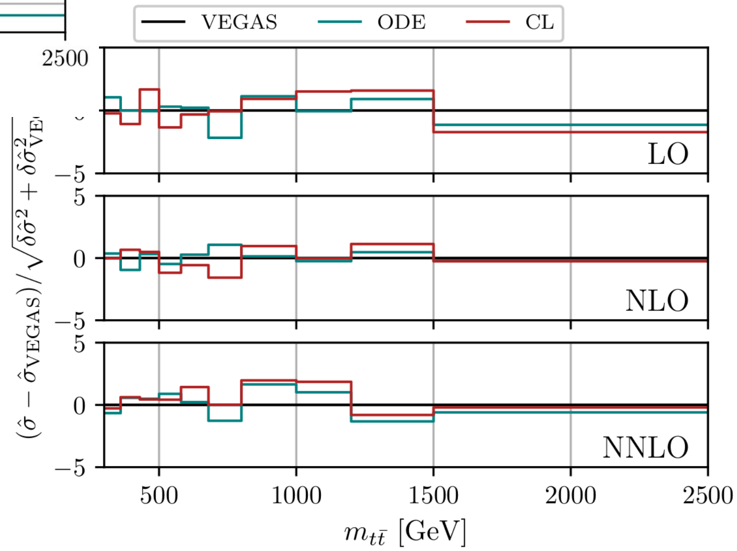
Contribution	$\sigma_{\rm RRF}\cdot 10^{-2}$	$\sigma_{\rm RRSU}\cdot 10^{-3}$	$\sigma_{\rm RRDU}\cdot 10^{-3}$	$\sigma_{\rm RVF}\cdot 10^{-2}$	$\sigma_{\rm RVFR}\cdot 10^{-2}$	$\sigma_{\rm RVDU}\cdot 10^{-3}$	$\sigma_{\rm VVF}\cdot 10^{-0}$
$\delta^{\rm opt}$	0.0079	0.0036	0.013	0.0081	0.0018	0.0045	0.011
CPU cost [a.u.]	53	26	8	1542	2.7	2.7	13
VEGAS							
$\hat\sigma \pm \delta\hat\sigma$	-0.3 ± 0.02	2.835 ± 0.0069	-2.461 ± 0.017	-6.808 ± 0.022	0.2864 ± 0.0023	0.267 ± 0.0049	14.768 ± 0.014
$\hat\sigma^+ \pm \delta\hat\sigma^+$	3.823 ± 0.013	3.718 ± 0.0056	5.639 ± 0.0065	1.669 ± 0.0026	1.051 ± 0.0014	2.381 ± 0.0011	16.711 ± 0.0067
$\hat\sigma^- \pm \delta\hat\sigma^-$	-4.135 ± 0.013	-0.8813 ± 0.0022	-8.078 ± 0.0085	-8.4539 ± 0.0068	-0.7635 ± 0.0012	-2.1114 ± 0.0012	-1.955 ± 0.0011
$\Sigma^\pm$	-0.312 ± 0.025	2.836 ± 0.0079	-2.439 ± 0.015	-6.785 ± 0.0094	0.2871 ± 0.0025	0.2696 ± 0.0023	14.756 ± 0.0078
ϵ_Φ^+	0.54	0.732	0.803	0.55	0.593	0.946	0.956
ϵ_Φ^-	0.513	0.402	0.8	0.871	0.501	0.916	0.816
$\epsilon^+(\epsilon^+_{0.1\%})$	0.004 (0.0052)	0.0073 (0.017)	0.0018 (0.022)	0.013 (0.024)	0.025 (0.06)	0.029 (0.22)	0.015 (0.1)
$\epsilon^-(\epsilon^-_{0.1\%})$	0.0041 (0.0053)	0.0035 (0.01)	0.0037 (0.019)	0.014 (0.038)	0.021 (0.05)	0.011 (0.11)	0.024 (0.17)
ODE Flow							
$\hat\sigma \pm \delta\hat\sigma$	-0.333 ± 0.011	2.823 ± 0.0048	-2.421 ± 0.015	-6.784 ± 0.0081	0.2893 ± 0.0019	0.271 ± 0.0046	14.758 ± 0.012
$\hat\sigma^+ \pm \delta\hat\sigma^+$	3.812 ± 0.0063	3.7056 ± 0.0028	5.6439 ± 0.0036	1.6764 ± 0.00085	1.0495 ± 0.00038	2.3806 ± 0.00043	16.72 ± 0.0026
$\hat\sigma^- \pm \delta\hat\sigma^-$	-4.142 ± 0.0057	-0.8848 ± 0.0045	-8.071 ± 0.0068	-8.4578 ± 0.0019	-0.76271 ± 0.00026	-2.1109 ± 0.0005	-1.9554 ± 0.00023
$\Sigma^\pm$	-0.33 ± 0.012	2.821 ± 0.0073	-2.427 ± 0.01	-6.7814 ± 0.0027	0.2868 ± 0.00064	0.2697 ± 0.00093	14.765 ± 0.0028
ϵ_Φ^+	0.855	0.945	0.977	0.988	0.981	0.998	0.999
ϵ_Φ^-	0.853	0.834	0.982	0.991	0.983	0.998	0.998
$\epsilon^+(\epsilon^+_{0.1\%})$	0.0013 (0.0027)	0.0028 (0.022)	0.003 (0.023)	0.0029 (0.067)	0.0081 (0.099)	0.03 (0.27)	0.0086 (0.49)
$\epsilon^-(\epsilon^-_{0.1\%})$	0.0019 (0.0053)	0.00025 (0.00025)	0.0018 (0.0096)	0.051 (0.25)	0.017 (0.095)	0.017 (0.18)	0.17 (0.49)
Coupling Layer Flow							
$\hat\sigma \pm \delta\hat\sigma$	-0.317 ± 0.01	2.829 ± 0.0044	-2.414 ± 0.014	-6.778 ± 0.0079	0.285 ± 0.0019	0.276 ± 0.0045	14.771 ± 0.012
$\hat\sigma^+ \pm \delta\hat\sigma^+$	3.814 ± 0.0054	3.7038 ± 0.0025	5.6425 ± 0.0039	1.676 ± 0.0024	1.05 ± 0.00059	2.3799 ± 0.00043	16.718 ± 0.0021
$\hat\sigma^- \pm \delta\hat\sigma^-$	-4.134 ± 0.0063	-0.8849 ± 0.0015	-8.0756 ± 0.0047	-8.456 ± 0.0026	-0.76256 ± 0.00055	-2.1091 ± 0.00036	-1.95479 ± 0.00011
$\Sigma^\pm$	-0.32 ± 0.012	2.819 ± 0.0041	-2.433 ± 0.0086	-6.7803 ± 0.005	0.2874 ± 0.0011	0.2708 ± 0.00079	14.763 ± 0.0022
ϵ_Φ^+	0.838	0.956	0.985	0.987	0.988	0.998	1.0
ϵ_Φ^-	0.852	0.836	0.988	0.991	0.985	0.999	1.0
$\epsilon^+(\epsilon^+_{0.1\%})$	0.0022 (0.0056)	0.0096 (0.022)	0.0029 (0.011)	0.00076 (0.00076)	0.0024 (0.035)	0.01 (0.22)	0.02 (0.31)
$\epsilon^-(\epsilon^-_{0.1\%})$	0.0034 (0.006)	0.0012 (0.0028)	0.0044 (0.011)	0.0054 (0.13)	0.0017 (0.018)	0.022 (0.22)	0.1 (0.68)

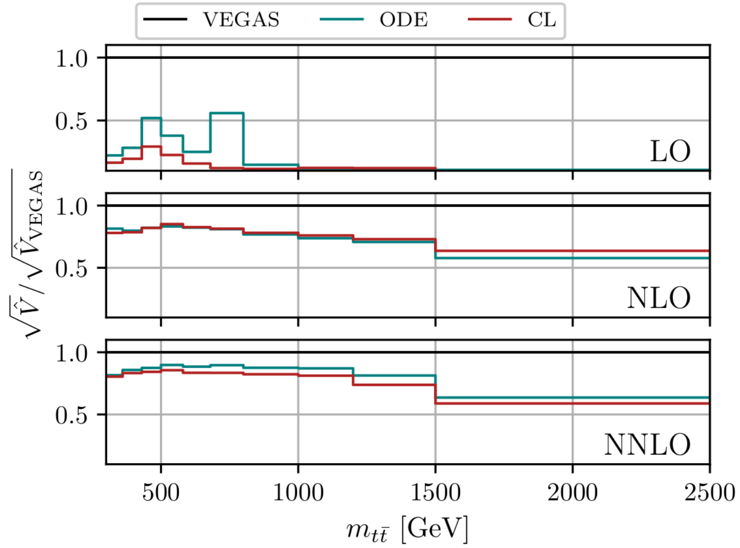
Results NNLO

Contribution	$\sigma_{\mathrm{RRF}} \cdot 10^{-2}$	$\sigma_{\mathrm{RRSU}} \cdot 10^{-3}$	$\sigma_{\mathrm{RRDU}} \cdot 10^{-3}$	$\sigma_{\mathrm{RVF}} \cdot 10^{-2}$	$\sigma_{\mathrm{RVFR}} \cdot 10^{-2}$	$\sigma_{\mathrm{RVDU}} \cdot 10^{-3}$	$\sigma_{\mathrm{VVF}} \cdot 10^{-0}$
δ^{opt}	0.0079	0.0036	0.013	0.0081	0.0018	0.0045	0.011
CPU cost [a.u.]	53	26	8	1542	2.7	2.7	13
VEGAS							
$\hat{\sigma} \pm \delta\hat{\sigma}$	-0.3 ± 0.02	2.835 ± 0.0069	-2.461 ± 0.017	-6.808 ± 0.022	0.2864 ± 0.0023	0.267 ± 0.0049	14.768 ± 0.014
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	3.823 ± 0.013	3.718 ± 0.0056	5.639 ± 0.0065	1.669 ± 0.0026	1.051 ± 0.0014	2.381 ± 0.0011	16.711 ± 0.0067
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	-4.135 ± 0.013	-0.8813 ± 0.0022	-8.078 ± 0.0085	-8.4539 ± 0.0068	-0.7635 ± 0.0012	-2.1114 ± 0.0012	-1.955 ± 0.0011
$\Sigma^\pm$	-0.312 ± 0.025	2.836 ± 0.0079	-2.439 ± 0.015	-6.785 ± 0.0094	0.2871 ± 0.0025	0.2696 ± 0.0023	14.756 ± 0.0078
ϵ_Φ^+	0.54	0.732	0.803	0.55	0.593	0.946	0.956
ϵ_Φ^-	0.513	0.402	0.8	0.871	0.501	0.916	0.816
$\epsilon^+(\epsilon^+_{0.1\%})$	0.004 (0.0052)	0.0073 (0.017)	0.0018 (0.022)	0.013 (0.024)	0.025 (0.06)	0.029 (0.22)	0.015 (0.1)
$\epsilon^-(\epsilon^-_{0.1\%})$	0.0041 (0.0053)	0.0035 (0.01)	0.0037 (0.019)	0.014 (0.038)	0.021 (0.05)	0.011 (0.11)	0.024 (0.17)
ODE Flow							
$\hat{\sigma} \pm \delta\hat{\sigma}$	-0.333 ± 0.011	2.823 ± 0.0048	-2.421 ± 0.015	-6.784 ± 0.0081	0.2893 ± 0.0019	0.271 ± 0.0046	14.758 ± 0.012
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	3.812 ± 0.0063	3.7056 ± 0.0028	5.6439 ± 0.0036	1.6764 ± 0.00085	1.0495 ± 0.00038	2.3806 ± 0.00043	16.72 ± 0.0026
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	-4.142 ± 0.0057	-0.8848 ± 0.0045	-8.071 ± 0.0068	-8.4578 ± 0.0019	-0.76271 ± 0.00026	-2.1109 ± 0.0005	-1.9554 ± 0.00023
$\Sigma^\pm$	-0.33 ± 0.012	2.821 ± 0.0073	-2.427 ± 0.01	-6.7814 ± 0.0027	0.2868 ± 0.00064	0.2697 ± 0.00093	14.765 ± 0.0028
ϵ_Φ^+	0.855	0.945	0.977	0.988	0.981	0.998	0.999
ϵ_Φ^-	0.853	0.834	0.982	0.991	0.983	0.998	0.998
$\epsilon^+(\epsilon^+_{0.1\%})$	0.0013 (0.0027)	0.0028 (0.022)	0.003 (0.023)	0.0029 (0.067)	0.0081 (0.099)	0.03 (0.27)	0.0086 (0.49)
$\epsilon^-(\epsilon^-_{0.1\%})$	0.0019 (0.0053)	0.00025 (0.00025)	0.0018 (0.0096)	0.051 (0.25)	0.017 (0.095)	0.017 (0.18)	0.17 (0.49)
Coupling Layer Flow							
$\hat{\sigma} \pm \delta\hat{\sigma}$	-0.317 ± 0.01	2.829 ± 0.0044	-2.414 ± 0.014	-6.778 ± 0.0079	0.285 ± 0.0019	0.276 ± 0.0045	14.771 ± 0.012
$\hat{\sigma}^+ \pm \delta\hat{\sigma}^+$	3.814 ± 0.0054	3.7038 ± 0.0025	5.6425 ± 0.0039	1.676 ± 0.0024	1.05 ± 0.00059	2.3799 ± 0.00043	16.718 ± 0.0021
$\hat{\sigma}^- \pm \delta\hat{\sigma}^-$	-4.134 ± 0.0063	-0.8849 ± 0.0015	-8.0756 ± 0.0047	-8.456 ± 0.0026	-0.76256 ± 0.00055	-2.1091 ± 0.00036	-1.95479 ± 0.00011
$\Sigma^\pm$	-0.32 ± 0.012	2.819 ± 0.0041	-2.433 ± 0.0086	-6.7803 ± 0.005	0.2874 ± 0.0011	0.2708 ± 0.00079	14.763 ± 0.0022
ϵ_Φ^+	0.838	0.956	0.985	0.987	0.988	0.998	1.0
ϵ_Φ^-	0.852	0.836	0.988	0.991	0.985	0.999	1.0
$\epsilon^+(\epsilon^+_{0.1\%})$	0.0022 (0.0056)	0.0096 (0.022)	0.0029 (0.011)	0.00076 (0.00076)	0.0024 (0.035)	0.01 (0.22)	0.02 (0.31)
$\epsilon^-(\epsilon^-_{0.1\%})$	0.0034 (0.006)	0.0012 (0.0028)	0.0044 (0.011)	0.0054 (0.13)	0.0017 (0.018)	0.022 (0.22)	0.1 (0.68)

Differential distributions







Summary

- Investigated the usage of flow-based methods for phase space sampling
- Reduction of weight distributions
  → Pos/Neg cancellation bottleneck in many cases → lower bound

- Pos/Neg splitting allows **to go beyond this bound**

- Performance gains of O(10) with pos/neg splitting + normalising flow can be achieved
  → **non-factorising model is crucial**!

Outlook:

→ fully fledged integration in STRIPPER & HighTEA

→ go beyond "simple" NNLO QCD top-pair

→ differential pos/neg splitting