Machine Learning for Scattering Amplitudes

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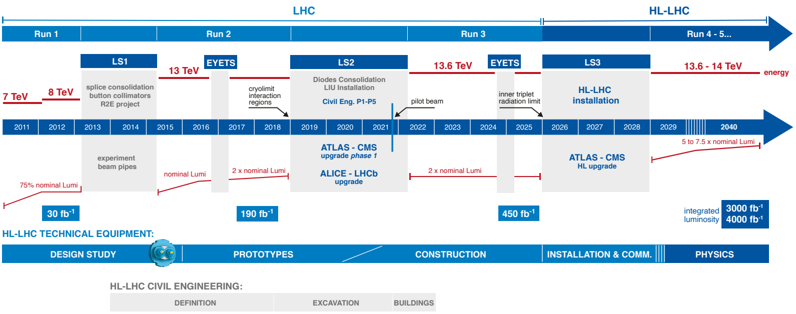
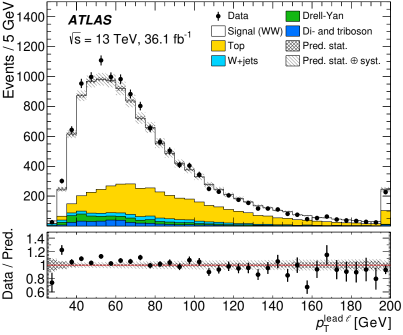
HELMHOLTZ

LHC / HL-LHC Plan

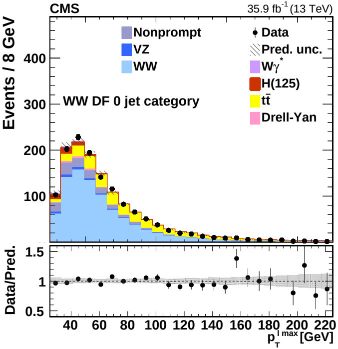


An example: di-bosons

[1905.04242]



[2009.00119]



$$\chi^2 = \frac{(O-E)^2}{\Delta^2} \approx \left(\frac{N_{\mathsf{BSM}}}{N_{\mathsf{SM}}}\right)^2 \left[\frac{1}{N_{\mathsf{SM}}} + \varepsilon^2_{\mathsf{TH}} + \varepsilon^2_{\mathsf{EXP}}\right]^{-1}, \qquad \begin{aligned} E &= N_{\mathsf{SM}} + N_{\mathsf{BSM}} \\ O &= N_{\mathsf{SM}} \end{aligned}$$

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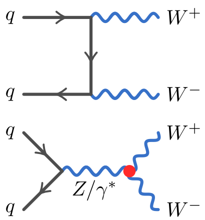

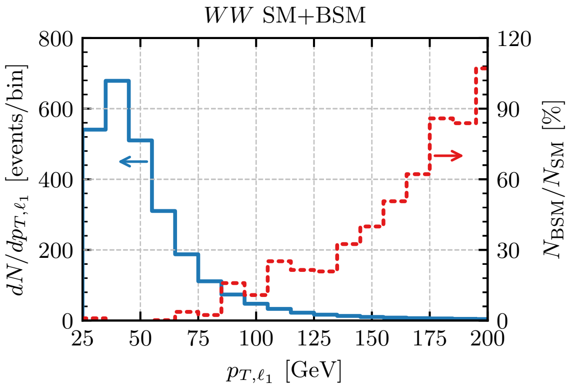

$$N_{\mathsf{SM}} = 100,\ \varepsilon_{\mathsf{EXP}} = 3\%,\ \varepsilon_{\mathsf{TH}} = \{15\%, 3\%\} \Rightarrow \frac{N_{\mathsf{BSM}}}{N_{\mathsf{SM}}} < \{46\%, 18\%\} @\, 95\% \text{ C.I.}$$

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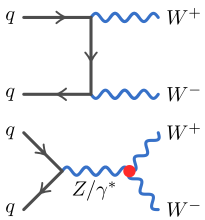

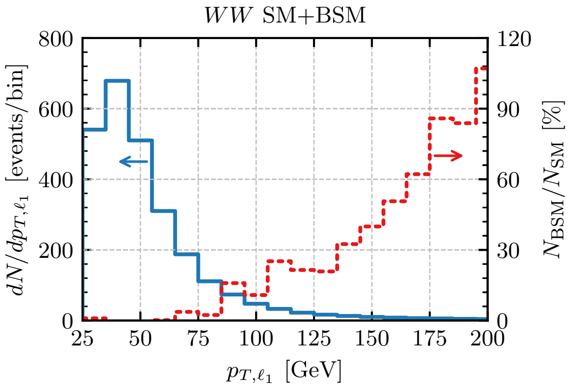

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Better precision $\rightarrow$ better ability to discover or exclude BSM

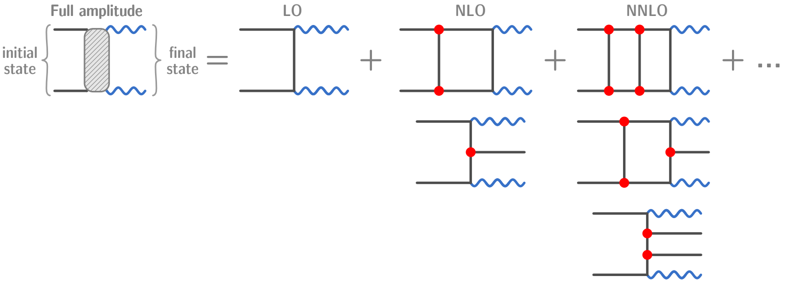
Precision $\rightarrow$ compute higher orders in expansion

Exact value $= \underline{0.142857143}$

$$\frac{1}{7} = \frac{1}{10}\left[1 - \frac{3}{10}\right]^{-1} \approx \frac{1}{10}\left[1 + \underbrace{0.3}_{\text{NLO}} + \underbrace{0.09}_{\text{NNLO}} + \underbrace{0.027}_{\text{N3LO}} + \dots\right]$$

	LO	NLO	NNLO	N3LO
Cumulative sum:	0.1	0.13	0.139	0.1417
Relative error:	30%	9%	3%	1%

Perturbative expansion in QFT (but, series is asymptotic)

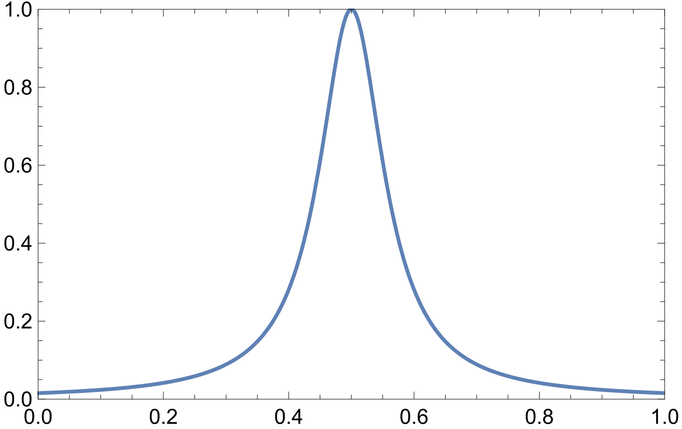


- Need Monte Carlo events @ higher orders in α

- Higher-order matrix elements are slow to evaluate numerically

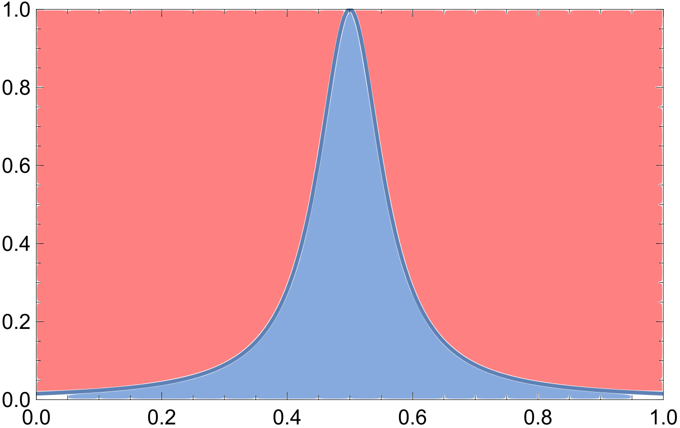
- Moreover, need to evaluate these matrix elements **many** times

The Monte Carlo method



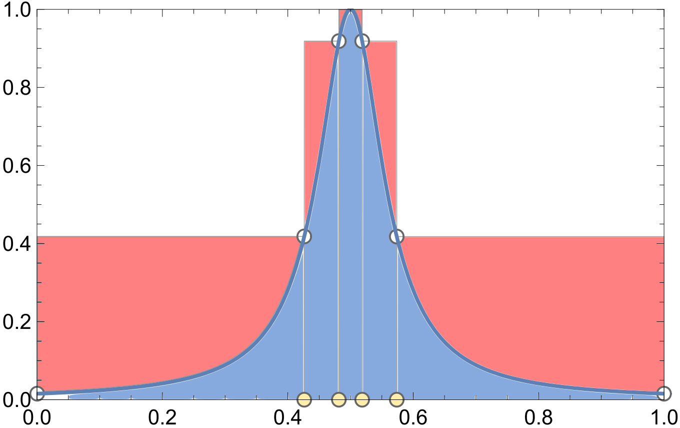
Cauchy-Lorentz dist'n $\propto \dfrac{\gamma}{\pi\left[\gamma^2 + (x-\mu)^2\right]}$ with $\mu = \frac{1}{2}, \gamma = \frac{1}{16}$

The Monte Carlo method



$$\text{un-weighting efficiency} \equiv \frac{\#\,\text{accepted}}{\#\,\text{thrown}} = 18\%$$

The Monte Carlo method



$$\text{un-weighting efficiency} \equiv \frac{\#\ \text{accepted}}{\#\ \text{thrown}} = X\%$$

For instance, time to generate 1 million events s.t. MC statistical error $1/\sqrt{N} \sim 10^{-3}$

time/point $[s]$	unwgt. efficiency	CPU time
1	100%	12 days
10	100%	116 days
10	1%	32 years
1000	1%	**3170 years**

This is not just about speeding up – **it's about making the impossible possible** (1% eff. is quite optimistic)

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Upshot: neural network CPU time $\mathcal{O}(10^{-3})$ s $\sim$ indep.[‡] of amplitude!

process (${process_id})	LO runtime estimate for 10^{-3} uncertainty	NLO runtime estimate for 10^{-3} uncertainty	NNLO runtime estimate for 10^{-3} uncertainty	
$pp \to H$ (pph21)	2 CPU seconds	1 CPU minute	19 CPU days	Higgs
$pp \to Z$ (ppz01)	4 CPU seconds	1 CPU minute	11 CPU days	DY
$pp \to W^-$ (ppw01)	2 CPU seconds	1 CPU minute	10 CPU days	
$pp \to W^+$ (ppwx01)	5 CPU seconds	2 CPU minutes	11 CPU days	
$pp \to e^- e^+$ (ppeex02)	28 CPU seconds	12 CPU minutes	22 CPU days	
$pp \to \nu_e \bar{\nu}_e$ (ppnenex02)	1 CPU minute	4 CPU minutes	18 CPU days	
$pp \to e^- \bar{\nu}_e$ (ppenex02)	1 CPU minute	16 CPU minutes	21 CPU days	
$pp \to e^+ \nu_e$ (ppexne02)	1 CPU minute	15 CPU minutes	24 CPU days	
$pp \to \gamma\gamma$ (ppaa02)	1 CPU minute	19 CPU minutes	6 CPU days	diphoton
$pp \to e^- e^+ \gamma$ (ppeexa03)	9 CPU minutes	4 CPU hours	167 CPU days	
$pp \to \nu_e \bar{\nu}_e \gamma$ (ppnenexa03)	1 CPU minute	1 CPU hour	17 CPU days	
$pp \to e^- \bar{\nu}_e \gamma$ (ppenexa03)	13 CPU minutes	9 CPU hours	232 CPU days	Wγ
$pp \to e^+ \nu_e \gamma$ (ppexnea03)	17 CPU minutes	1 CPU day	443 CPU days	
$pp \to ZZ$ (ppzz02)	1 CPU minute	4 CPU minutes	25 CPU days	
$pp \to W^+ W^-$ (ppwxw02)	1 CPU minute	3 CPU minutes	13 CPU days	
$pp \to e^- \mu^- e^+ \mu^+$ (ppemexmx04)	2 CPU minutes	20 CPU minutes	45 CPU days	
$pp \to e^- e^- e^+ e^+$ (ppeeexex04)	6 CPU minutes	1 CPU hour	193 CPU days	
$pp \to e^- e^+ \nu_\mu \bar{\nu}_\mu$ (ppeexnmnmx04)	3 CPU minutes	29 CPU minutes	31 CPU days	
$pp \to e^- \mu^+ \nu_\mu \bar{\nu}_e$ (ppemxnmnex04)	7 CPU minutes	3 CPU hours	119 CPU days	
$pp \to e^- e^+ \nu_e \bar{\nu}_e$ (ppeexnenex04)	10 CPU minutes	4 CPU hours	52 CPU days	
$pp \to e^- \mu^- e^+ \bar{\nu}_\mu$ (ppemexnmx04)	3 CPU minutes	26 CPU minutes	19 CPU days	
$pp \to e^- e^- e^+ \bar{\nu}_e$ (ppeeexnex04)	6 CPU minutes	1 CPU hour	39 CPU days	
$pp \to e^- e^+ \mu^+ \nu_\mu$ (ppeexmxnm04)	4 CPU minutes	1 CPU hour	21 CPU days	
$pp \to e^- e^+ e^+ \nu_e$ (ppeexexne04)	6 CPU minutes	3 CPU hours	44 CPU days	

MATRIX CPU budget (total runtime)

[Grazzini, Kallweit, MW '17]

from seconds at LO
to minutes at NLO
to days at NNLO

(MATRIX not optimized for simple processes)

diphoton fastest NNLO process

Wγ slowest NNLO process

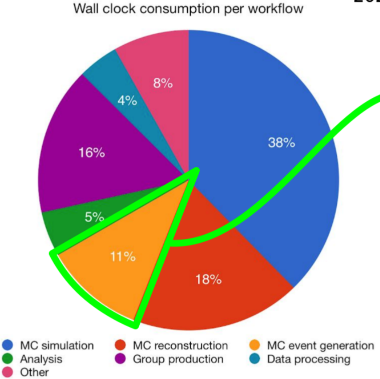
(dependents on fiducial cuts!)

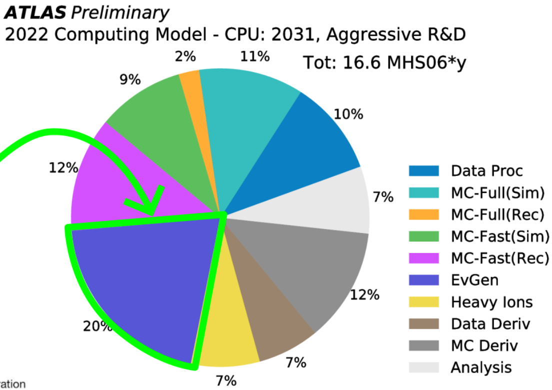
off-shell diboson processes

from minutes at LO
to hours at NLO
to days at NNLO

Slide by Marius Wiesemann

ATLAS Computing Budget, e.g.





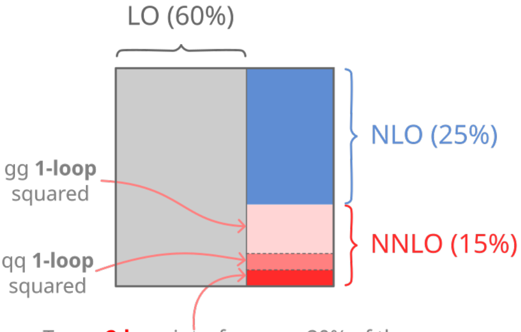
But remember the goal: impossible $\rightarrow$ possible

Why is it reasonable to approximate?

- There are many sources of error:
  - Experimental: statistics, JES/JER, tagging, …,
  - Theoretical: PDF, α_s, …,
  - Monte Carlo statistics $\sim \mathcal{O}(10^{-3})$,
- this guides the approximation precision requirement
- and …

process (${process_id})	σ_{LO}	σ_{NLO}	σ_{loop} $(\sigma_{\mathrm{loop}}/\Delta\sigma^{\mathrm{ext}}_{\mathrm{NNLO}})$	$\sigma^{r_{\mathrm{cut}}}_{\mathrm{NNLO}}$	$\sigma^{\mathrm{extrapolated}}_{\mathrm{NNLO}}$	K_{NLO}	K_{NNLO}
$pp \to ZZ$ (ppzz02)	$9.845(1)^{+5.2\%}_{-6.3\%}$ pb	$14.10(0)^{+2.9\%}_{-2.4\%}$ pb	$1.361(1)^{+25\%}_{-19\%}$ pb (52.9%)	$16.68(1)^{+3.2\%}_{-2.6\%}$ pb	$16.67(1)^{+3.2\%}_{-2.6\%}$ pb	+43.3%	+18.2%
$pp \to W^+W^-$ (ppwxw02)	$66.64(1)^{+5.7\%}_{-6.7\%}$ pb	$103.2(0)^{+3.9\%}_{-3.1\%}$ pb	$4.091(3)^{+27\%}_{-19\%}$ pb (29.5%)	$117.1(1)^{+2.5\%}_{-2.2\%}$ pb	$117.1(1)^{+2.5\%}_{-2.2\%}$ pb	+54.9%	+13.4%

Grazzini, Kallweit, Wiesemann [1711.06631]



Tree x **2-loop** interference ~20% of the NNLO contribution...

... but O(**100-1000**) times slower than 1-loop amplitudes

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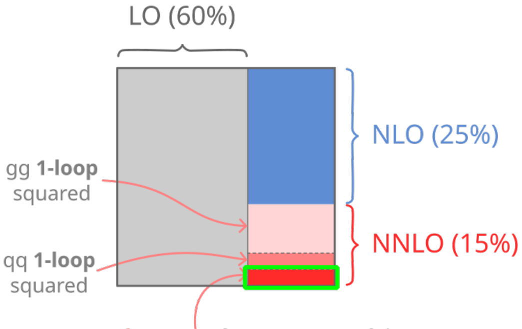

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Machine Learning

- Universal Approximation Theorem: "…any multivariate continuous function can be represented as a superposition of one–dimensional functions" (Neural Networks/sigmoid)
  [From Braun, J. & Griebel, M. Constr Approx (2009)]

- In practice, convergence is non-trivial (and not guaranteed)

- ✓ Gradient boosting machines perform extremely well

- ✓ Deep neural networks with special architectures do even better for higher dimensions

Definition of Machine Learning

The basic concept of machine learning in data science involves using statistical learning and optimization methods that let computers analyze datasets and identify patterns (view a visual of machine learning via R2D3). Machine learning techniques leverage data mining to identify historic trends and inform future models.

The typical supervised machine learning algorithm consists of roughly three components:

1. **A decision process:** A recipe of calculations or other steps that takes in the data and "guesses" what kind of pattern your algorithm is looking to find.
2. **An error function:** A method of measuring how good the guess was by comparing it to known examples (when they are available). Did the decision process get it right? If not, how do you quantify "how bad" the miss was?
3. **An updating or optimization process:** A method in which the algorithm looks at the miss and then updates how the decision process comes to the final decision, so next time the miss won't be as great.

[https://ischoolonline.berkeley.edu/blog/what-is-machine-learning/]

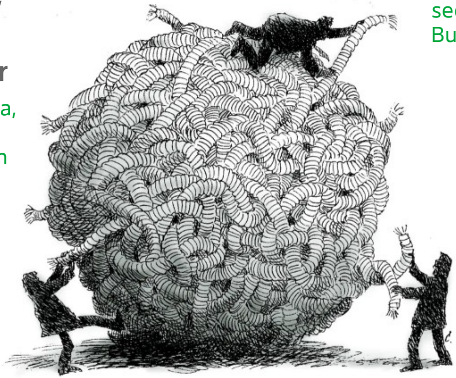
Lots of machine learning activity in HEP theory

Numerical stability by well-chosen integration contour

Winterhalder, Magerya, Villa, Jones, Kerner, Butter, Heinrich, Plehn [2112.09145]

Symbolic simplification of polylogs using language models

Dersy, Schwartz, Zhang [2206.04115]



Approximating amplitudes

see also Badger & Bullock [2002.07516]

Hadronization

Ilten, Menzo, Youssef, Zupan [2203.04983]

And much more…

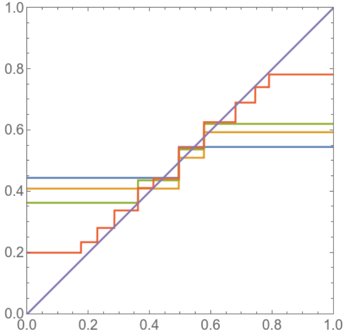
Integration and sampling efficiency

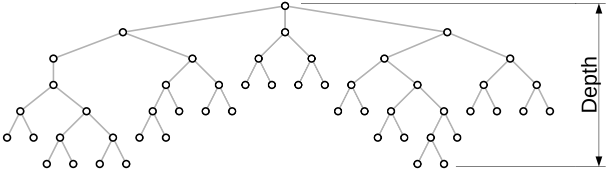
see e.g., Bendavid [1707.00028]; Klimek, Perelstein [1810.11509]; Gao, Isaacson, Krause [arXiv:2001.05486]; Gao, Höche, Isaacson, Krause, Schulz [2001.10028], Maitre, Santos-Mateos [2211.02834]

Boosted decision trees with XGBoost

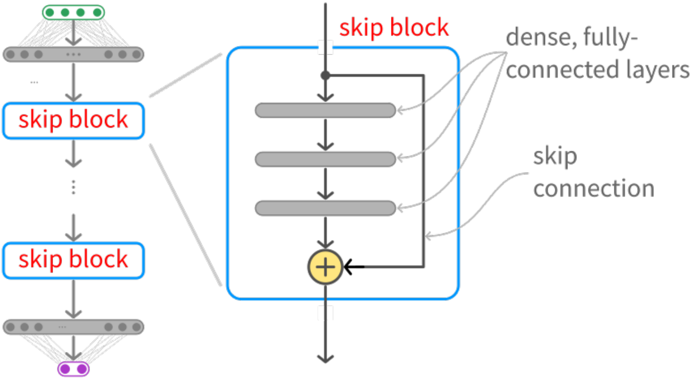
Sequential, additive corrections to previous result

$$\hat{y}_i^{(0)} = 0$$
$$\hat{y}_i^{(1)} = f_1(x_i) = \hat{y}_i^{(0)} + f_1(x_i)$$
$$\hat{y}_i^{(2)} = f_1(x_i) + f_2(x_i) = \hat{y}_i^{(1)} + f_2(x_i)$$
$$\dots$$
$$\hat{y}_i^{(t)} = \sum_{k=1}^{t} f_k(x_i) = \hat{y}_i^{(t-1)} + f_t(x_i)$$





Neural network with skip connections



Physics guidance and considerations

- Functions span many orders of magnitude, transform

$$f(x) = \begin{cases} \log(1+x) & x > 0 \\ -\log(1-x) & x < 0 \end{cases}$$

- Symmetries of the amplitudes $\rightarrow$ reduce number of functions needed and necessary calls, even
- Improve NN performance by constructing linear combinations of functions with nicer properties (e.g. even more symmetry)
- How to generate a training sample over the domain?
  - Generally, sample uniformly
  - Some variables need to be sampled log-uniformly – **need to invert transformation s.t. point density is uniform!**

- *High-Precision Regressors for Particle Physics*
  F. Bishara, A. Paul, J. Dy. Paper submitted to Nature Scientific Reports for peer-review (now in 2nd round) [arXiv:2302.00753]

- *Skip Connections for High Precision Regressors*
  F .Bishara, A. Paul, J. Dy. Machine Learning and the Physical Sciences, Workshop at the 36th Conference on Neural Information Processing Systems (NeurIPS 2022)

- *Machine Learning Amplitudes for Faster Event Generation*
  F. Bishara and M. Montull. Phys. Rev. D 107 (2023) no.7, L071901 [arXiv:1912.11055]

Proof of Principle

$gg \to ZZ$

[FB & Marc Montull [1912.11055]]

- $[2m_Z \oplus p_{T,Z} > 1\ \mathrm{GeV}, 3\ \mathrm{TeV}] \mapsto [0,1]^2$
  - the p_T cut regulates an integrable singularity @ $\cos\theta = \pm 1$ as in `MCFM` and `MG5_aMC@NLO` otherwise **no cuts** on P.S.!
  - extending $\sqrt{\hat{s}}$ to the full 14 TeV is trivial

- Phase-space is 2-dimensional: $\{\sqrt{\hat{s}}, \cos\theta\}$
  - squared/averaged matrix element $\langle|\mathcal{M}|^2\rangle : \mathbb{R}^2 \mapsto \mathbb{R}_{>0}$
  - for on-shell Z's, invariant under $\cos\theta \to -\cos\theta$

- It is important to normalize $\langle|\mathcal{M}|^2\rangle$ because of loss function
  - simple sol'n: divide by max. value in large sample
  - better: divide by std. deviation of large sample
  - even better: take the $\log$

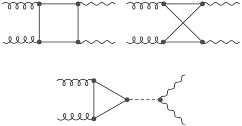
- Populate full phase-space uniformly
  - Training: 1.5M points
  - Validation: 15M points (10$\times$ to catch rare events)

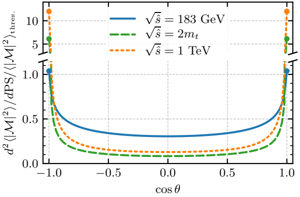
- Compute $\langle|\mathcal{M}|^2\rangle$ using `OpenLoops2`
  [Buccioni, Lang, Lindert, Maierhöfer, Pozzorini, Zhang, Zoller [1907.13071]]

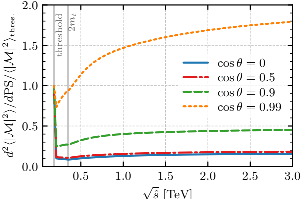
- Approximation error defined as

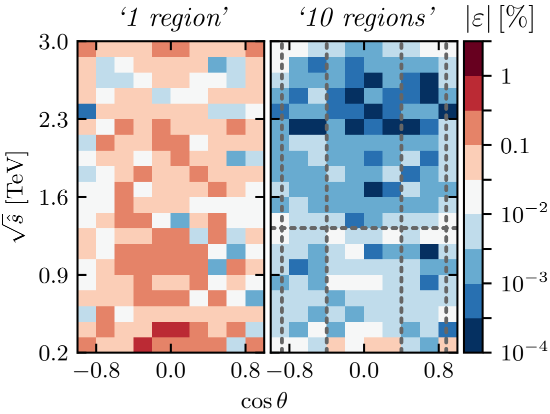
$$\varepsilon = 1 - \frac{\texttt{approx.}}{\texttt{exact}}$$

Proof of principle: loop-induced matrix element









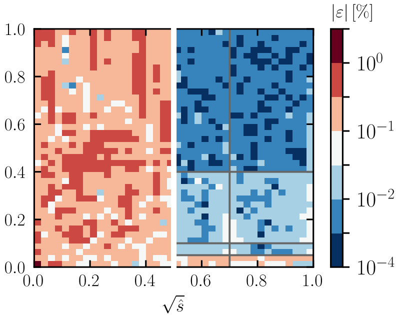
Exact (`OpenLoops2`): $\sim$ 10s / 1k point

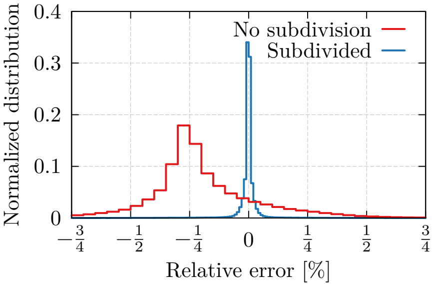
Approximate: $\sim$ 10s / **1M** points

Relative approximation error $< 10^{-3}$, speed gain $1000\times$

$qq \to ZZ$ @2L (on-shell)

- Two-loop form-factors from `VVAMP` (finite remainder) [Gehrmann, von Manteuffel, Tancredi [1503.04812]]
- Compute and approximate $\mathcal{T}^{(2)}$ (full or 2L$\times$ Born)

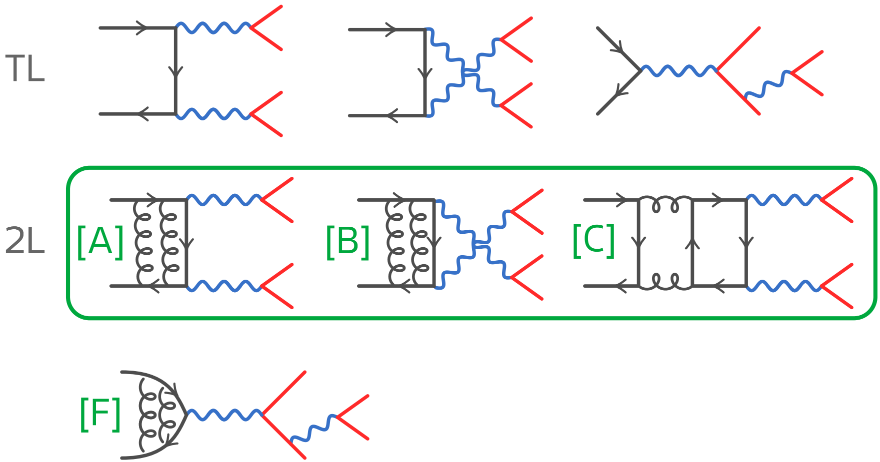




Exact:	$\sim$ 16s / point
Approximate:	$\sim$ 16s / **1M** points

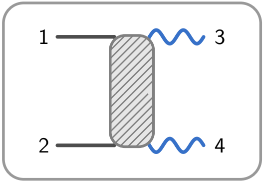
The $\mathbf{qq} \to 4\ell$ Amplitudes

$\mathbf{pp \to 4\ell}$ @ NNLO (double virtual)

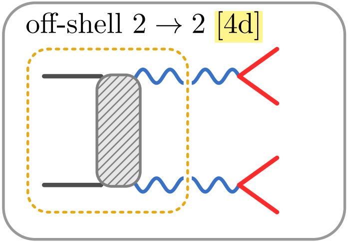


The phase space

on-shell $2 \to 2$ [2d]



on-shell $2 \to 4$ [8d]



- The resonant-propagator numerators can be rewritten as

$$\Delta_{\mu\nu} = -g_{\mu\nu} + (1-\xi)\frac{q_\mu q_\nu}{q^2 - m^2} \xrightarrow{\text{e.o.m.}} -g^{\mu\nu} = \sum_\lambda \epsilon_\mu^\lambda \epsilon_\nu^{\lambda *}$$

Two-loop matrix element

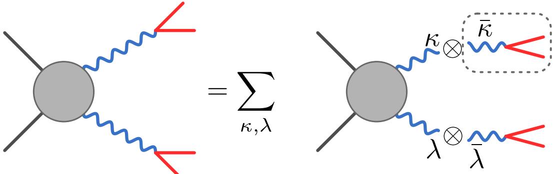
10 tensor structures
@LO only 4: $T_7, \ldots, T_{10}$

form factors = scalar
functions of kinematic vars.

Squared amplitude:

$$\mathcal{T}\left(s,t,p_3^2,p_4^2\right) = \sum_{\text{pols,cols}} \left| \sum_{j=1}^{10} A_j\left(s,t\right) T_j^{\mu\nu}\, \varepsilon_\lambda^\mu\left(p_3\right) \varepsilon_{\lambda'}^\nu\left(p_4\right) \right|^2$$

Gauge and Lorentz invariant sub-amplitudes



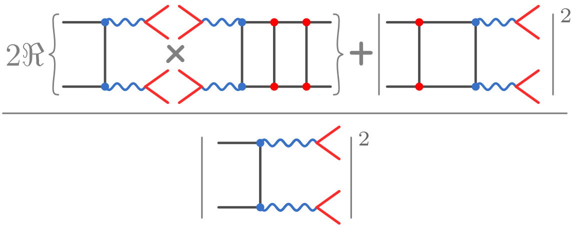
lepton amps. are simple:
$\propto \langle 3 \not{\epsilon}_{\bar{\kappa}} 4] \text{ and } [3 \not{\epsilon}_{\bar{\kappa}} 4\rangle$

8d P.S.

4d P.S. + 2 × 2d P.S.

Two paths to approximation

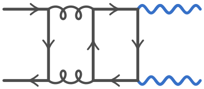
k-factor



- Couplings cannot be factored out (frozen-in)
- Phase-space is 8-dim.
- Can sum over helicities → only one function per process

(sub)-amplitudes

[A]  [B]

[C] 

- Couplings can be factored out (at least when sum of Qi=0)
- Phase-space is 4-dim.
- Can be recycled for different vector boson combinations

[Work in progress with Ayan Paul]

- Goal: **implement into MC generators**, many details to consider
  - want functions that can be recycled $\to$ couplings factored out
  - and for this, approximate **amplitudes** (i.e. not squared)
  - amplitudes are complex objects $f : \mathbb{R}^d \mapsto \mathbb{C}$
  - want V_1 and V_2 **off-shell** but don't want leptons so **4d**

- Therefore, have $2 \times 3 \times 3 = 18$ amplitudes in principle
  - ✔ Amplitudes have symmetries $\to$ reduced set

- Nice choice of reference momenta $\to$ more symmetry
  - simultaneous light-cone decomposition of p_3 and p_4 leads to

$$\epsilon^-_{3,\mu} = \frac{\langle 4\gamma_\mu 3]}{\sqrt{2}\langle 43\rangle}, \quad \epsilon^+_{3,\mu} = \frac{\langle 3\gamma_\mu 4]}{\sqrt{2}[34]}, \quad \epsilon^-_{4,\mu} = \frac{\langle 3\gamma_\mu 4]}{\sqrt{2}\langle 34\rangle}, \quad \epsilon^+_{4,\mu} = \frac{\langle 4\gamma_\mu 3]}{\sqrt{2}[43]}$$

  - in C.M. frame with p_3 and p_4 pointed along $\pm\hat{z}$ direction and with appropriate choice of spinor phases, $\langle 34\rangle = [43]$

- Only **4** / 18 amplitudes can generate the full set

- $\Re$ and $\Im$ parts of the amplitudes are correlated $\rightarrow$ natural to output them together (trivial for NNs)

- In the future, could be a good application for complex activation functions

- For now, ignore complications that arise if the two pairs of leptons have the same flavor

Populating the Phase Space

$qq \to Z^* Z^*$

[FB & A. Paul [work in progress]]

- Map full phase-space to unit hypercube

$$\begin{aligned} \sqrt{s_{12}} &\in [m_{34} + m_{56}, 14\ \mathrm{TeV}] \mapsto [0,1] \\ \cos\theta^* &\in [-1, 1] \mapsto [0,1] \\ m_{34}, m_{56} &\in [50, 130]\ \mathrm{GeV} \mapsto [0,1] \end{aligned}$$

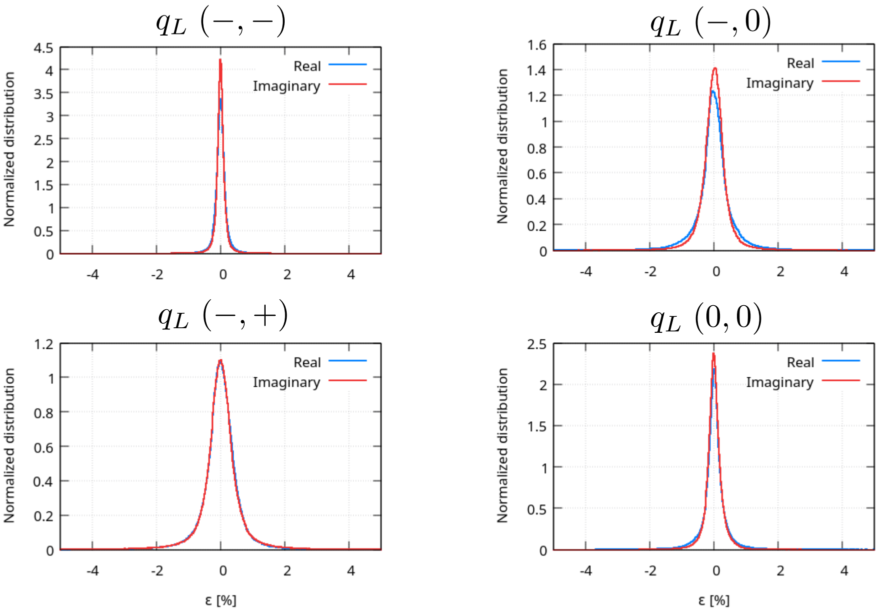
  - otherwise **no cuts** on P.S.!
  - two options to extend m_{ij} even up to 14 TeV to cover W boson

- The scattering angle of $Z(p_{34})$ is defined as

$$\cos\theta^* = \frac{t-u}{s\,\lambda}$$

where $s \equiv s_{12}$ and λ is the Källén function $\lambda(1, \frac{m_{34}}{\sqrt{s_{12}}}, \frac{m_{56}}{\sqrt{s_{12}}})$

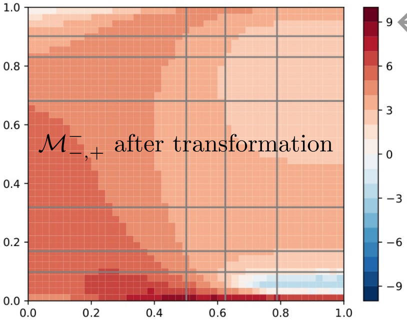
Early results: $\sqrt{s_{12}}$ up to 500 GeV



[FB & A. Paul [work in progress]]

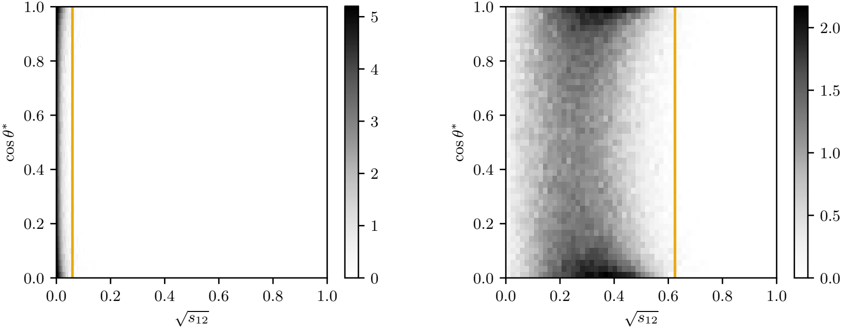
- Amplitudes span many order of magnitude (and can be negative of course) $\to$ transform according to

$$f(x) = \begin{cases} \log(1+x) & x > 0 \\ -\log(1-x) & x < 0 \\ 0 & \text{otherwise} \end{cases}$$



$e^9 \sim \mathcal{O}(10^4)$

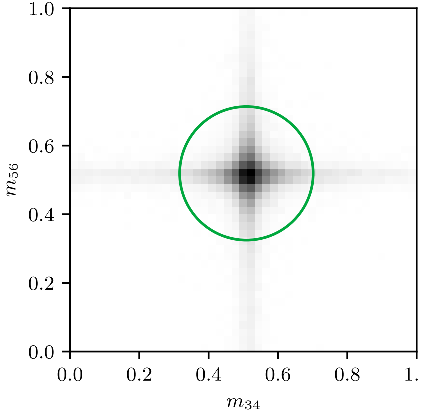
- Training the network is done on the full phase-space, uniformly populated except for s_{12} because...

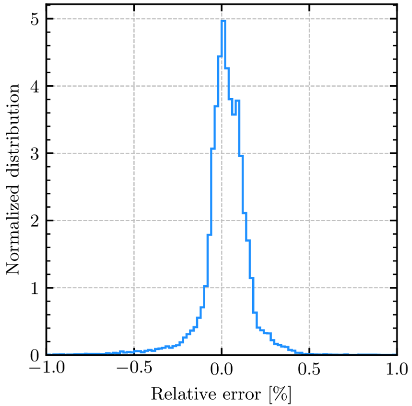


- Populate s_{12} log-uniformly

$$\mathsf{CDF}(x) = \frac{1}{p} \log\left\{1 + x\left(e^p - 1\right)\right\}$$

- The $m_{34} - m_{56}$ is also clearly sparse if PS is uniformly populated but, for now, keep it as is

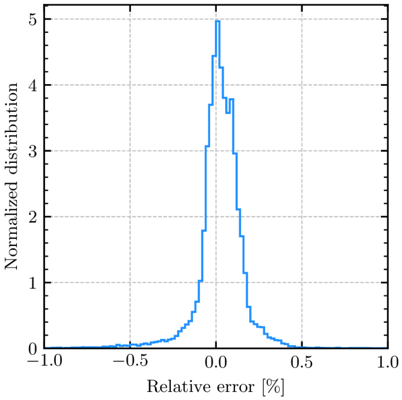




Trained on uniformly populated masses predictions in a very small region of PS!

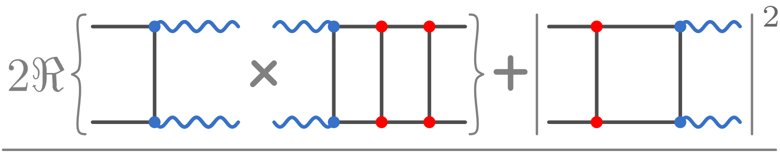
Of course can/should improve this i.e. by distributing according to a wide Cauchy dist.

- Approximation of $2\Re\{\mathcal{M}^{(0)}\mathcal{M}^{(2)*}\}$
- Relative error is **sub-percent** ($\sim 0.01\%$ on total)
- Runs in < 2 **milliseconds** per phase-space point
  compare with **2 seconds** for exact!
- Code to produce this:
  - `Fortran` prog. (no ext. dep.)
  - reads parameter files (a few MB)
  - takes in phase-space coords
  - outputs helicity amplitudes

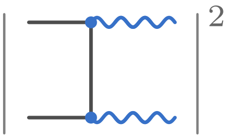


K-Factors

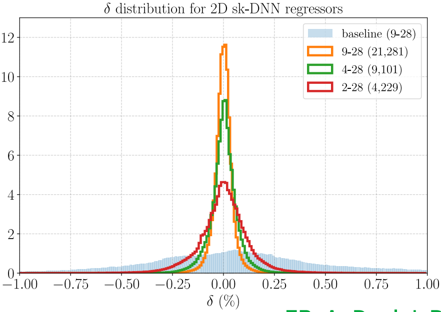
- “Toy” process just to establish generalization to higher dims.
  [FB, Ayan Paul, Jennifer Dy; `https://ml4physicalsciences.github.io/2022/files/NeurIPS_ML4PS_2022_164.pdf`]
  [FB, Ayan Paul, Jennifer Dy; [2301.XXXXX]]

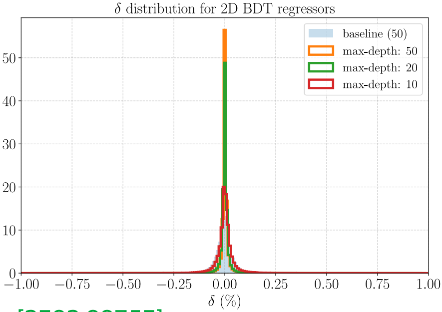


This study only includes classes [A] + [B]

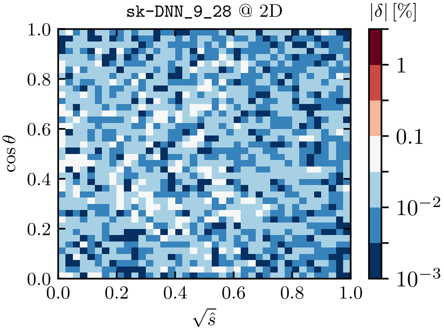


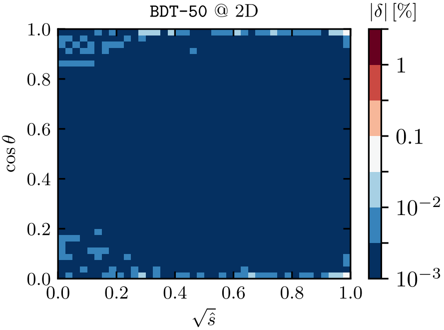
- Compute $\langle |\mathcal{M}|^2 \rangle$ for $qq \to ZZ(\to 4\ell)$ using `VVAMP`
  - Training: 4.8M points
  - Validation: 3.2M
  - Testing: 2M

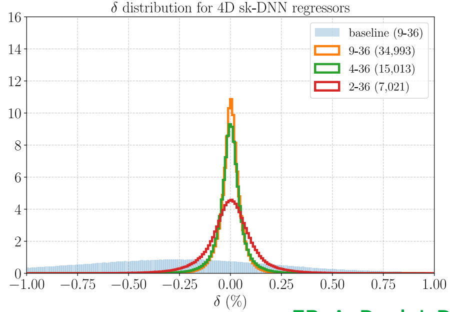


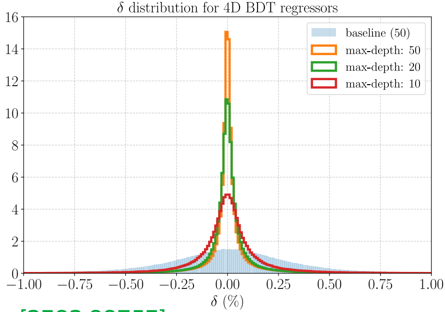


FB, A. Paul, J. Dy [2302.00753]

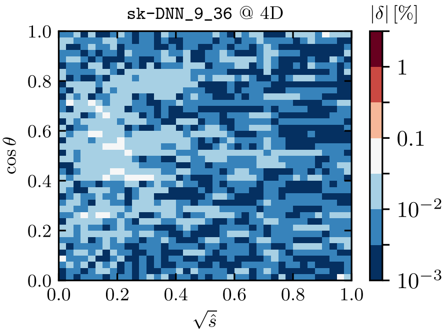


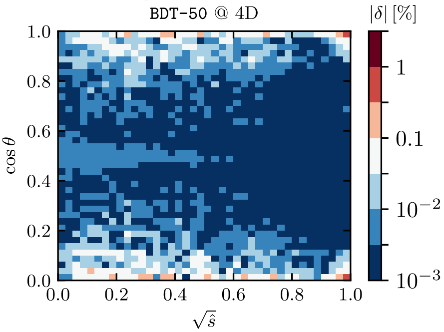


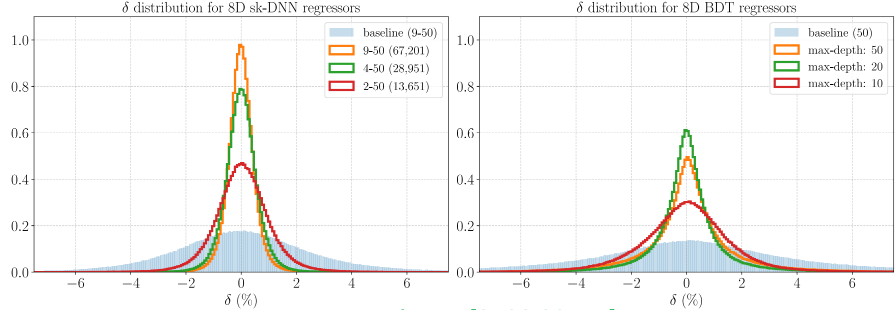




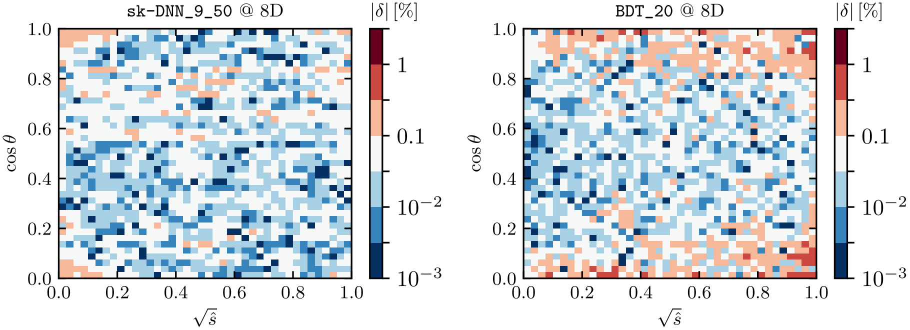
FB, A. Paul, J. Dy [2302.00753]







FB, A. Paul, J. Dy [2302.00753]



Summary and outlook

- Approximate double-virtual amplitudes can leapfrog MC generation times for some processes
- Implementation soon in `MCFM`, then in `GENEVA` and hopefully also `MATRIX`
- Many many future directions and application to other amplitudes, e.g., including gluon-induced di-bosons @NLO, top mass in the loop, 5-point 3-photon two loop amplitude, etc.