# On the reduction of negative weights in MC@NLO

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Taming the accuracy of event generators, 03/07/2020

Based on
`Frederix, Frixione, Prestel, PT, 2002.12716`

# Outline

- Negative weights.
- Negative weights in MC@NLO.
- A new NLO+PS matching: MC@NLO-$\Delta$.
- Some results.
- Outlook / open issues.

# Negative weights (I)

- Cross section beyond LO not positive definite locally in phase space.

- Not a conceptual problem, just a reduction in generation efficiency.

- Main effect: larger event samples for a given target MC accuracy.

- Generate $N = N_+ + N_-$ unweighted (up to a sign) events

  $N_- = f\,N$ with negative weight, $N_+ = (1-f)N$ with positive weight, $0 \leq f < 0.5$.

$$\sigma = \omega\left(N_+ - N_- \pm \sqrt{N_+ + N_-}\right) = \omega\left((1-2f)N \pm \sqrt{N}\right).$$

- Same thing for positive-definite generation

$$\sigma = \omega'\left(M \pm \sqrt{M}\right).$$

# Negative weights (II)

$$\sigma = \omega \left( (1-2f)N \pm \sqrt{N} \right) = \omega' \left( M \pm \sqrt{M} \right).$$

- To reach the same MC error

$$N = \frac{M}{(1-2f)^2}.$$

- For example: with $f = 30\%$, which may occur for complicated processes, $N = 6.25 \times M$.

- In experiments a significant amount of time is spent after event generation (detector simulation, ...).

- Reduction of negative weights and sample size at the price of some increase in generation time can still be beneficial.

# MC@NLO

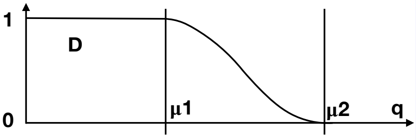
$$d\sigma_{\mathrm{MC@NLO}} = d\Phi_B \, d\Phi_{\mathrm{rad}} \left[ \frac{B+V}{\int d\Phi_{\mathrm{rad}}} + K_{PS} \right] \mathcal{F}_{PS}^{(n)} + d\Phi_B \, d\Phi_{\mathrm{rad}} \left[ R - K_{PS} \right] \mathcal{F}_{PS}^{(n+1)}$$

$$= d\sigma^{(\mathbb{S})}(\Phi_B, \Phi_{\mathrm{rad}}) \, \mathcal{F}_{PS}^{(n)} + d\sigma^{(\mathbb{H})}(\Phi_B, \Phi_{\mathrm{rad}}) \, \mathcal{F}_{PS}^{(n+1)}$$

- $\mathcal{F}_{PS}^{(j)}$ = shower spectrum starting from $j$- body kinematics
- $\mathbb{S}$ events. Showered by the PS starting from Born ($n$-body) kinematics $\mathcal{F}_{PS}^{(n)}$
  $\mathbb{H}$ events. Showered by the PS starting from real ($n+1$-body) kinematics $\mathcal{F}_{PS}^{(n+1)}$
- $K_{PS}$ = Monte Carlo counterterm: $\mathcal{O}(\alpha_{\mathrm{S}})$ expansion of the shower emission probability

$$d\Phi_{\mathrm{rad}} \, K_{PS} \;\propto\; D(q, \mu_1, \mu_2) \sum_c \sum_{\ell \in c} \frac{dq^2}{q^2} dz \frac{\bar{\alpha}_{\mathrm{S}}(q^2)}{2\pi} P(z)$$

$q^2, z$ shower variables (depend on colour flow $c$, line $\ell$); $D$ dampening profile.



# Negative weights in MC@NLO: $\mathbb{S}$ events

$$d\sigma^{(\mathbb{S})}(\Phi_B, \Phi_{\rm rad})\, \mathcal{F}_{PS}^{(n)} \quad = \quad d\Phi_B\, d\Phi_{\rm rad} \left[ \frac{B+V}{\int d\Phi_{\rm rad}} + K_{PS} \right] \mathcal{F}_{PS}^{(n)}$$

- $\mathbb{S}$ events have Born kinematics, but $d\sigma^{(\mathbb{S})}$ has support in the full $n+1$-body phase space.
- Locally in the $n+1$-body phase space their weight can be negative.
- Negative $\mathbb{S}$ weights can be reduced by folding [Nason, 0709.2085] (used in POWHEG-BOX [Alioli, et al., 1002.2581])
- First integrate $\mathbb{S}$ short-distance cross section over $d\Phi_{\rm rad}$, and then generate Born phase space, i.e.

$$d\sigma^{(\mathbb{S})}(\Phi_B, \Phi_{\rm rad})\, \mathcal{F}_{PS}^{(n)} \quad \to \quad \mathcal{F}_{PS}^{(n)} \int d\Phi_{\rm rad} \frac{d\sigma^{(\mathbb{S})}(\Phi_B, \Phi_{\rm rad})}{d\Phi_{\rm rad}}$$

# Negative weights in MC@NLO: $\mathbb{S}$-event folding

- In practice

$$\mathcal{F}_{PS}^{(n)} \int d\Phi_{\rm rad} \frac{d\sigma^{(\mathbb{S})}(\Phi_B, \Phi_{\rm rad})}{d\Phi_{\rm rad}} \quad \sim \quad \mathcal{F}_{PS}^{(n)} \sum_{i=1}^{n_\xi} \sum_{j=1}^{n_y} \sum_{k=1}^{n_\phi} \frac{w_{ijk}}{n_\xi n_y n_\phi} \frac{d\sigma^{(\mathbb{S})}(\Phi_B, \xi_i, y_j, \phi_k)}{d\Phi_{\rm rad}}$$

- At a fixed Born phase-space point ($\Phi_B$) one generates $n_\xi \times n_y \times n_\phi$ radiative configurations ($\xi$, $y$, $\phi$ are the FKS variables for the radiative phase space).

  Possible using the MINT integrator [Nason, 0709.2085].

- The more the one averages over radiative variables, the more the negative contributions are reduced (dominated by Born).

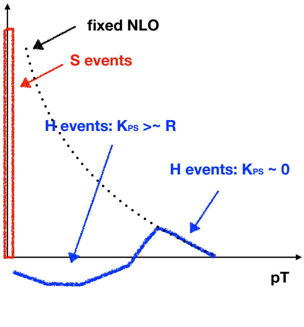
- Price to pay: increase running time in generation of $\mathbb{S}$ events (typically a factor up to $n_\xi \times n_y \times n_\phi$).

- This is a purely technical aspect, i.e. no change in the matching formula.

# Negative weights in MC@NLO: $\mathbb{H}$ events

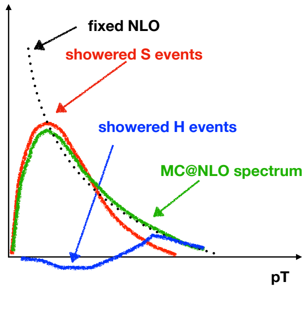
$$d\sigma^{(\mathbb{H})}(\Phi_B, \Phi_{\rm rad})\, \mathcal{F}_{PS}^{(n+1)} \quad = \quad d\Phi_B\, d\Phi_{\rm rad} \Big[ R - K_{PS} \Big]\, \mathcal{F}_{PS}^{(n+1)}$$

- Sketch for $p_T$ of the Born-level system



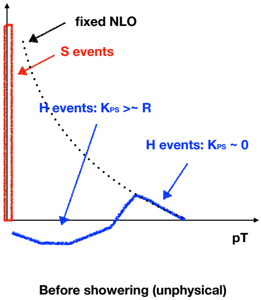
Before showering (unphysical)

$\Longrightarrow$

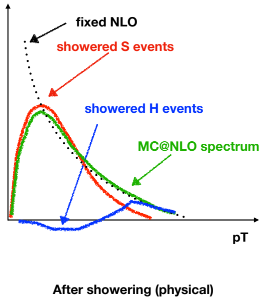


After showering (physical)

# Negative weights in MC@NLO: $\mathbb{H}$ events



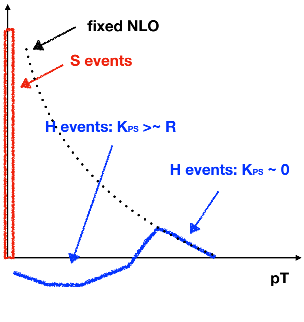

$\Longrightarrow$




- Negative $\mathbb{H}$ weights come mainly from small/intermediate $p_T$ configurations.
- This region is PS-dominated: efficiently filled by $\mathbb{S}$ events after showering.
- In this region, $\mathbb{H}$ events have little impact on shapes of distributions, mostly affect normalisation.
- MC@NLO is allowing many negative $\mathbb{H}$ events there at short-distance level, which are eventually totally compensated by the shower.
- A new matching scheme, MC@NLO-$\Delta$, to reduce this problem in the first place.

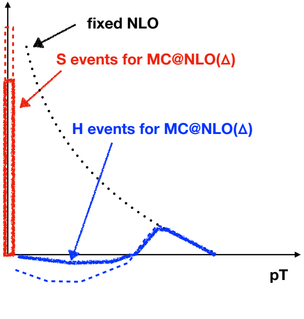
# MC@NLO-$\Delta$ (I)

- Main reasoning behind MC@NLO-$\Delta$: suppress $R - K_{PS}$ at small $p_T$.




Before showering (unphysical)

$\Longrightarrow$




Before showering (unphysical)

- Suppression factor $0 \leq \color{red}{\Delta} \leq 1$, with support in the $n+1$-body phase.
- $\Delta$ designed not to spoil any of the MC@NLO accuracy properties.
- $\Delta$ constructed with sole PS information, can be used to enrich the NLO – PS cross talk.

# MC@NLO-Δ (II)

$$d\sigma_{\text{MC@NLO}} = d\sigma^{(\mathbb{S})}(\Phi_B, \Phi_{\text{rad}})\, \mathcal{F}_{PS}^{(n)} + d\sigma^{(\mathbb{H})}(\Phi_B, \Phi_{\text{rad}})\, \mathcal{F}_{PS}^{(n+1)}$$

$$\rightarrow$$

$$d\sigma_{\text{MC@NLO}(\Delta)} = \left[d\sigma^{(\mathbb{S})}(\Phi_B, \Phi_{\text{rad}}) + d\sigma^{(\mathbb{H})}(\Phi_B, \Phi_{\text{rad}})\,(1-\Delta)\right] \mathcal{F}_{PS}^{(n)} + d\sigma^{(\mathbb{H})}(\Phi_B, \Phi_{\text{rad}})\; \Delta\; \mathcal{F}_{PS}^{(n+1)}$$

- $\Delta = 1 + \mathcal{O}(\alpha_S)$: difference w.r.t. MC@NLO starts at $\mathcal{O}(\alpha_S^2)$, preserving NLO accuracy.
- $\int d\sigma_{\text{MC@NLO}(\Delta)} = \int d\sigma_{\text{MC@NLO}} = \int d\sigma_{\text{NLO}}$.
- $\Delta \to 0$ in the S/C region, to dampen $\mathbb{H}$ events there.
- In the S/C region this enforces $d\sigma_{\text{MC@NLO}(\Delta)} \propto \mathcal{F}_{PS}^{(n)}$ in a stronger way than $d\sigma_{\text{MC@NLO}}$. The proportionality factor in the S/C region tends to $[B + V + \int d\Phi_{\text{rad}} R]$, PS-independent.
- MC@NLO-Δ much less sensitive than MC@NLO to showers with incorrect soft limit.
- $\Delta \to 1$ in the hard region, to preserve exact NLO matrix-element information there.

# Construction of $\Delta$ factor

- $\Delta$ is constructed as the product of no-emission probabilities associated with all QCD legs present at Born level

$$
\begin{aligned}
\Delta &= \prod_{i=1}^{n} \Pi_i(q,\mu) \\
&= \prod_{i=1}^{n} F_i \exp\left\{ -\frac{1}{N_{\ell_i}} \sum_{\ell_i} \sum_{j} \int_{q^2}^{\mu^2} \frac{dt}{t} \frac{\bar{\alpha_S}(t)}{2\pi} \int_{\epsilon(t,\ell_i)}^{1-\epsilon(t,\ell_i)} dz\, \frac{1}{2} P_{ji}(z) \right\}.
\end{aligned}
$$

- Suppression factors for all potential Born-level radiators.
- Stronger suppression where the PS is expected to radiate more.
- $F_i = f_i(x,q)/f_i(x,\mu)$ for $i$ in the initial state, $F_i = 1$ in the final state.
- Gluons enter two dipoles: we take a (PS-driven) weighted average of the two contributions where the contribution with the smaller scale $q$ has larger weight.
- One needs enforce $\Delta = 1$ if $q > \mu$, or in a PS dead zone.
- $\Delta$ provided numerically by the PS, for each phase-space point.

# Choice of scales entering the $\Delta$ factor (I)

$$\Delta = \prod_{i=1}^{n} \Pi_i(q, \mu)$$

- 'Starting' scales $\mu$ are typical hard scales associated with the kinematics of the process.
- Pick randomly a Born-level colour flow, depending on its relative contribution to $K_{PS}$.
- Compute reference scales $M_{ab}^2 = (\bar{k}_a + \bar{k}_b)^2$, with $\bar{k}$ = Born-level momenta

  *ab* colour-connected partons in the picked flow.
- One shower starting scale per dipole end: $\mu_{ab} = D^{-1}(r_{ab}, \mu_{1,ab}, \mu_{2,ab})$

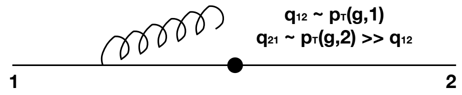
  $r_{ab}$ = flat random numbers, and $\mu_{i,ab} = f_i \, M_{ab}$

  $f_{1,2} = \mathcal{O}(1)$ factors to assess shower-scale systematics.

# Choice of scales entering the $\Delta$ factor (II)

$$\Delta = \prod_{i=1}^{n} \Pi_i(q, \mu)$$

- 'Stopping' scales $q$ must be $q \to 0$ for soft/collinear radiation ($\Delta \to 0$), and $q \simeq \mu$ for hard radiation ($\Delta \to 1$).
- We passe Born kinematics and colour flow + real kinematics to the PS.
- PS returns $q_{ab}$ = shower variable associated with the real radiation occurring from radiator $a$, colour-connected to $b$; in general $q_{ab} \neq q_{ba}$.



# Remarks

- Parton shower called at run time (and not only after event generation) to get information on
  - no-emission probabilities $\rightarrow$ pre-tabulated shower Sudakovs
  - target scales $q_{ij}$
- Cross-talk may become beneficial in MadGraph5_aMC@NLO: may lead to abandon hard-coded $K_{PS}$ and gain flexibility.
- LH events can be naturally endowed with two scales per colour dipole $\mu_{ij}$ for $\mathbb{S}$ events, $q_{ij}$ for $\mathbb{H}$ events.
- Especially relevant for complex multi-leg processes, where one shower starting scale per event may be suboptimal.

```
<event>
  ....
  <scales muf='1.0E+01' mur='1.0E+01' ... scalup_a_b='X' ...>
  </scales>
</event>
```

# Results - setup

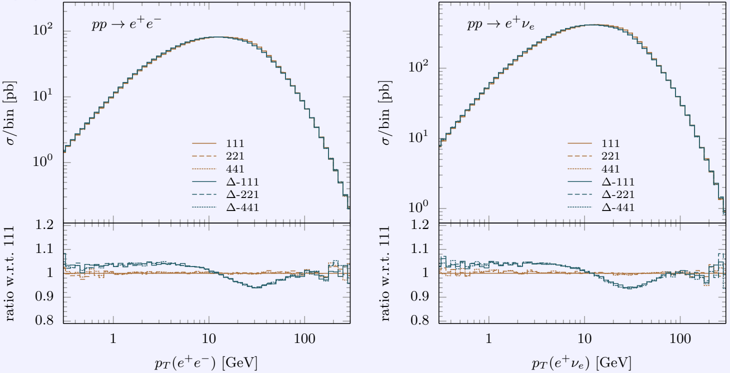
- LHC at 13 TeV.
- NNPDF2.3 with $\alpha_S(M_Z) = 0.119$.
- Central $\mu_R, \mu_F = H_T/2 = \frac{1}{2}\sum_i \sqrt{m_i^2 + p_{T,i}^2}$.
- MadGraph5_aMC@NLO interfaced with PYTHIA8.
- No hadronisation, no underlying event, no QED showers.

# Results (I)

| | MC@NLO | | | MC@NLO-Δ | | |
|---|---|---|---|---|---|---|
| | 111 | 221 | 441 | Δ-111 | Δ-221 | Δ-441 |
| $pp \to e^+e^-$ | 6.9% (1.3) | 3.5% (1.2) | 3.2% (1.1) | 5.7% (1.3) | 2.4% (1.1) | 2.0% (1.1) |
| $pp \to e^+\nu_e$ | 7.2% (1.4) | 3.8% (1.2) | 3.4% (1.2) | 5.9% (1.3) | 2.5% (1.1) | 2.3% (1.1) |
| $pp \to H$ | 10.4% (1.6) | 4.9% (1.2) | 3.4% (1.2) | 7.5% (1.4) | 2.0% (1.1) | 0.5% (1.0) |
| $pp \to Hb\bar{b}$ | 40.3% (27) | 38.4% (19) | 38.0% (17) | 36.6% (14) | 32.6% (8.2) | 31.3% (7.2) |
| $pp \to W^+j$ | 21.7% (3.1) | 16.5% (2.2) | 15.7% (2.1) | 14.2% (2.0) | 7.9% (1.4) | 7.4% (1.4) |
| $pp \to W^+t\bar{t}$ | 16.2% (2.2) | 15.2% (2.1) | 15.1% (2.1) | 13.2% (1.8) | 11.9% (1.7) | 11.5% (1.7) |
| $pp \to t\bar{t}$ | 23.0% (3.4) | 20.2% (2.8) | 19.6% (2.7) | 13.6% (1.9) | 9.3% (1.5) | 7.7% (1.4) |

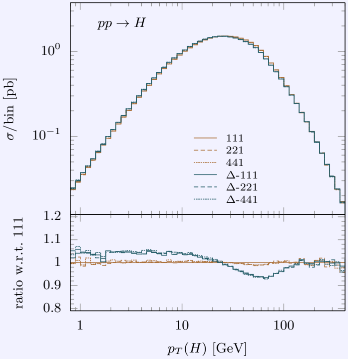
- 111, 221, 441, are the folding parameters $n_\xi$, $n_y$, $n_\phi$.
- Number in brackets is the 'relative cost' defined as $1/(1-2f)^2$.
- $\Delta$ + folding quite effective for $t\bar{t}$, or $Wj$.
- $Hb\bar{b}$ still challenging. Ongoing further investigation.

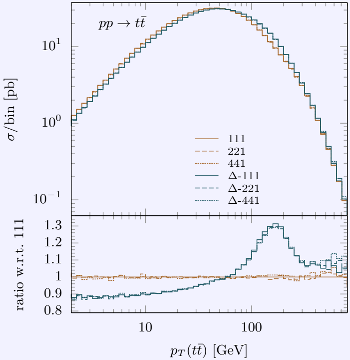
# Results (II)




- $p_T$(Born system) = maximally sensitive to matching systematics.
- Same shape at small $p_T$, $\mathcal{O}(5\%)$ difference in the matching region, same shape and normalisation at high $p_T$.
- Difference compatible with systematics effects from shower-scale variations (not shown).
- Folding does not affect distributions, just statistics.

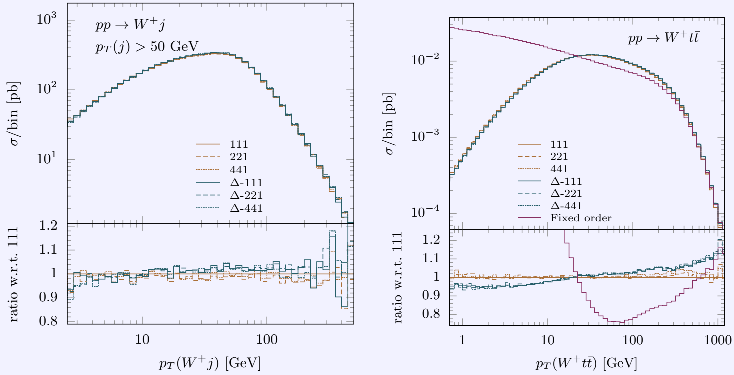
# Results (III)



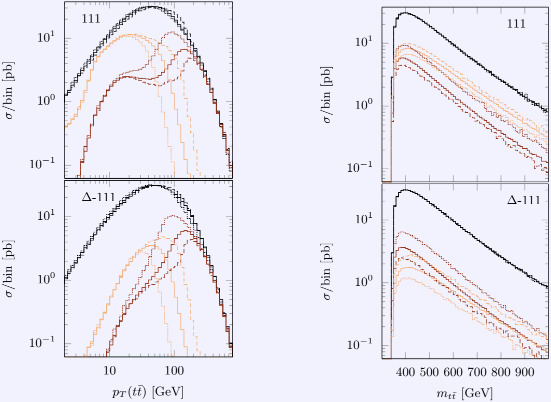

- Similar pattern for gluon fusion Higgs production as for DY.
- For $t\bar{t}$ up to 30% difference in the matching region.

# Results (IV)




- $Wt\bar{t}$: asymptotic regime approached very slowly, shower effects at hundreds of GeV.
- MC@NLO-Δ converges to NLO faster than MC@NLO.
- MC@NLO's single shower scale may be suboptimal w.r.t. multiple scales based on the kinematics of the single dipoles.

# Results (V)




- MC@NLO vs MC@NLO-Δ: positive (brown) and negative (orange) $\mathbb{H}$ events and showered results (black) in $t\bar{t}$ production.
- Solid: ($f_1 = 0.1, f_2 = 1.0$), dotted: ($f_1 = 0.1, f_2 = 0.55$), dashed: ($f_1 = 0.55, f_2 = 1.0$).

# Outlook

- Reduction of negative weights in MC@NLO achieved by folding for $\mathbb{S}$ events, by modifying matching prescription for $\mathbb{H}$ events: MC@NLO-$\Delta$.
- Some physics and technical benefits of MC@NLO-$\Delta$.
  - Reduction of negative weights and size of event samples
  - Better scale assignments (one scale per dipole end)
  - Reduced sensitivity to PS in the soft limit
  - Enhanced flexibility in the MadGraph5_aMC@NLO implementation
- Some drawbacks: folding and MC@NLO-$\Delta$ may increase the running time.
- I consider it as a first step of a more general revision of MC@NLO formalism, and of its implementation in MadGraph5_aMC@NLO.
- Work in progress / open questions.
  - Optimise implementation to reduce running times
  - Other ways to tackle the problem with less drawbacks? A couple of ideas to be investigated.
  - Revision of the matching scheme: a chance not only to reduce negative weights but also to include subleading terms?
  - What is the formal logarithmic accuracy of MC@NLO / MC@NLO-$\Delta$?

Thank you for your attention