Negative Event Weights

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Outline

- Where do negative weights come from?
- Why are negative weights a problem?
- How to handle negative weights?

[References at the end]

Where do negative weights come from?

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Monte Carlo events

Predict (integrated) differential cross section for $PP \to X$:

$$\int_{\mathcal{D}} d\sigma_{PP\to X} = \frac{1}{F} \int_{\mathcal{D}} d\phi \, |\mathcal{M}_{PP\to X}(p)|^2$$

phase space selection
e.g. histogram bin

flux factor

scattering amplitude

Where do negative weights come from?

Monte Carlo events

Predict (integrated) differential cross section for $PP \to X$:

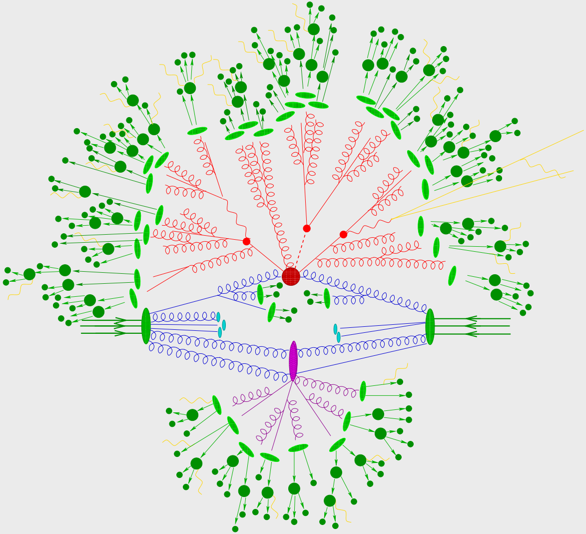
$$\int_{\mathcal{D}} d\sigma_{PP\to X} = \int_{\mathcal{D}} d\phi \, |\mathcal{M}_{PP\to X}(p)|^2 \xrightarrow{\text{Monte Carlo}} \sum_{i=1}^{N} \underbrace{\frac{\mathcal{D}}{FN} |\mathcal{M}_{PP\to X}(p_i)|^2}_{\text{weight } w_i}$$

Exact weights w_i

- are non-negative: proportional to modulus square
- indicate relative probability of event

Where do negative weights come from?

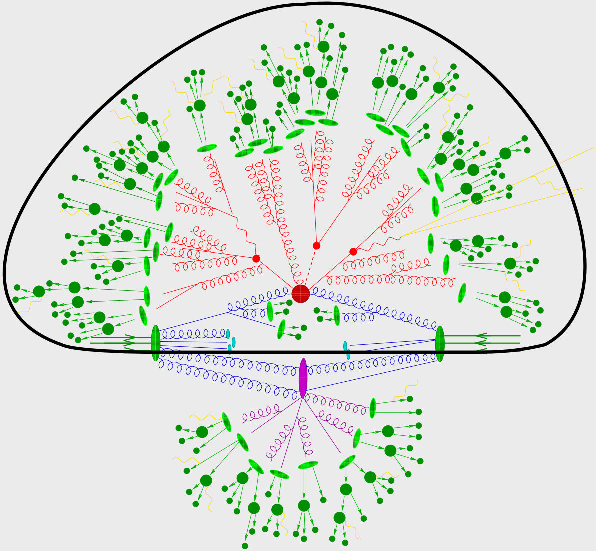
Standard theory picture



[Sherpa collaboration]

Where do negative weights come from?

Standard theory picture



[Sherpa collaboration]

Where do negative weights come from?
PDFs

$$\int_{\mathcal{D}} d\sigma_{PP\to X} \approx \int dx_a\, dx_b \int_{\mathcal{D}} d\sigma_{ab\to X}\, f_a(x_a) f_b(x_b)$$

- Factorisation not unique, PDFs are scheme dependent beyond leading order
  $\to$ physical interpretation not obvious
- PDFs can be negative, but [References]
  - Universality: same PDFs have to reproduce many positive cross sections
  - Naturalness: leading-order PDFs are non-negative, higher-order corrections should be small
- Can impose PDF positivity, e.g. NNPDF4.0MC

Partonic cross section generally main source of negative weights

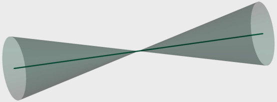
Where do negative weights come from?

Partonic cross section

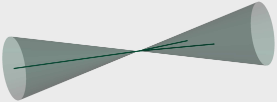
Consider simple scenario:

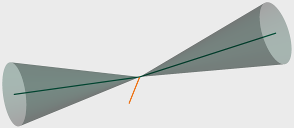
- exclusive dijet production
- no parton shower ← similar discussion, but more involved

$$\int_{\mathcal{D}} d\sigma_{ab\to 2j} = \quad d\sigma_{ab\to 2j} \text{ (2 partons)}$$



$$+ d\sigma_{ab\to 2j} \text{ (3 partons)}$$





$$+ \ldots$$

Separation unphysical, not InfraRed & Collinear safe

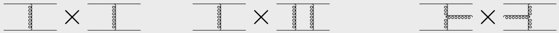
Where do negative weights come from?

NLO partonic cross section

Truncate at NLO:

$$\int_{\mathcal{D}} d\sigma_{ab\to 2j}\Big|_{\text{NLO}} = \int d\phi_2\,(B+V) + \int d\phi_3\,R$$

Born Virtual Real



- Terms on right-hand side diverge individually
- Introduce subtraction (Catani-Seymour, FKS, . . .)

Where do negative weights come from?

NLO partonic cross section

$$\int_{\mathcal{D}} d\sigma_{ab\to 2j}\Big|_{\text{NLO}} = \int d\phi_2\,(B + V + C_{\text{int}}) + \int d\phi_3\,(R - C)$$

$$\xrightarrow[\text{up to normalisation}]{\text{Monte Carlo}} \sum_{i=1}^{N_2}[B(p_i) + V(p_i) + C_{\text{int}}(p_i)] + \sum_{i=1}^{N_3}[R(p_i) - C(p_i)]$$

Where do negative weights come from?

NLO partonic cross section

$$\int_{\mathcal{D}} d\sigma_{ab\to 2j}\Big|_{\text{NLO}} = \int d\phi_2\,(B+V+C_{\text{int}}) + \int d\phi_3\,(R-C)$$

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Sources of negative weights:

1. $R(p_i) - C(p_i)$ negative
2. $B(p_i)+V(p_i)+C_{\text{int}}(p_i)$ negative
3. Split up

$$\sum_{i=1}^{N_2}[B(p_i)+V(p_i)+C_{\text{int}}(p_i)] \to \sum_{i=1}^{N_B} B(p_i) + \sum_{i=1}^{N_V}[V(p_i)+C_{\text{int}}(p_i)]$$

and $V(p_i)+C_{\text{int}}(p_i)$ negative

Where do negative weights come from?

Negative Born + Virtual

$$\underbrace{B(p_i)}_{\geq 0} + \underbrace{V(p_i) + C_{\text{int}}(p_i)}_{\mathcal{O}(\alpha_s \times B)} < 0$$

Where do negative weights come from?

Negative Born + Virtual

$$\underbrace{B(p_i)}_{\geq 0} + \underbrace{V(p_i) + C_{\text{int}}(p_i)}_{\mathcal{O}(\alpha_s \times B)} < 0$$

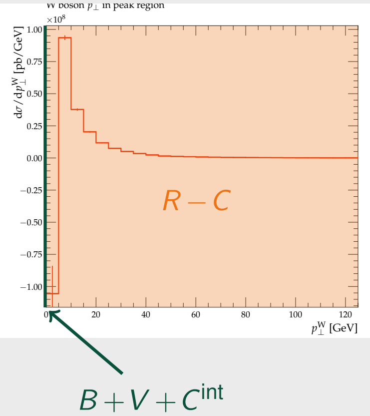
- Suggests oversubtraction or local breakdown of perturbation theory
  - Expect physical result when including (all) higher orders
  - Possible pragmatic solution:
    1. Carefully identify phase-space region where prediction breaks down
    2. Discarding complete "bad" phase-space region is formally $>$NLO change

Just discarding all negative weights is wrong

Where do negative weights come from?

Negative Born + Virtual

Example: W boson production at vanishing transverse momentum



- Cause of breakdown: Sudakov logarithms $\ln^2 \frac{m_W}{p_\perp^W}$
- Discard $B + V + C^{\text{int}}$?
  - Wrong prediction for small $p_\perp^W > 0$
  - Loose NLO accuracy in total cross section
- Discard region $[0, p_\perp^{\text{min}}]$ with $\int_0^{p_\perp^{\text{min}}} dp_\perp \frac{d\sigma}{dp_\perp} = 0$
  - Preserves total NLO cross section
  - Differential cross section suddenly drops to 0

Why are negative weights a problem?

Why are negative weights a problem?

Negative weights are

- "unphysical", but needed to cancel "unphysical" positive weights!
  - Wrong cross section prediction $\int_{\mathcal{D}} d\sigma_{PP\to X}$ for small enough $\mathcal{D}$
  - At odds with $|\mathcal{M}_{PP\to X}(p_i)|^2 \geq 0$
  - No clear interpretation as probabilities
- problematic for machine learning
- bad for statistical convergence: state-of-the-art predictions become computationally extremely expensive or even infeasible

Why are negative weights a problem?

Statistical convergence

Assume unweighted sample of $N \gg 1$ events:

- N_- events with weights $w_i = -W < 0$
- $N_+ = N - N_-$ events with weights $w_i = W > 0$

Why are negative weights a problem?

Statistical convergence

Assume unweighted sample of $N \gg 1$ events:

- N_- events with weights $w_i = -W < 0$
- $N_+ = N - N_-$ events with weights $w_i = W > 0$

$$\sigma = \sum_{i=1}^{N} w_i = -N_- W + (N - N_-)W = \Bigg(1 - 2\underbrace{\frac{N_-}{N}}_{\text{negative weight fraction } r_-}\Bigg) NW$$

Why are negative weights a problem?

Statistical convergence

Assume unweighted sample of $N \gg 1$ events:

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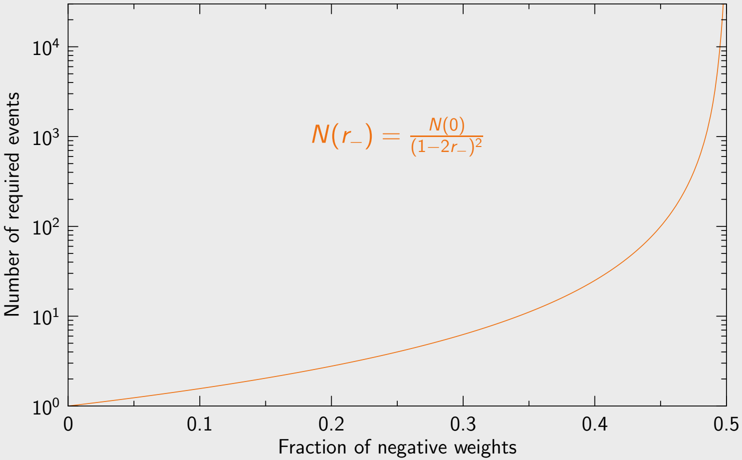
For uncorrelated events: $\Delta\sigma = \sqrt{\sum_{i=1}^{N} w_i^2} = \sqrt{N}W$

$$\frac{\Delta\sigma}{\sigma} = \frac{1}{(1 - 2r_-)\sqrt{N}}$$

Why are negative weights a problem?

Statistical convergence

Number of required events to reach given statistical accuracy:



Summary I

Negative weights come from

- Splitting the cross section into unphysical parts & introducing subtraction terms
  - Example: $R(p_i) - C(p_i)$
  - Details depend on formalism
- Local breakdown of perturbation theory
- Potentially negative PDFs
- …

They are a problem because they

- hinder statistical convergence
- are bad for machine learning
- do not have a physical interpretation

How to handle negative weights?

How to handle negative weights?

Many approaches for cancelling negative weights:

- Independent of event generation method
  - Cell resampling
  - Neural reweighting/refining
  - Folding
- Origin in additive parton shower matching
  - Born spreading
  - MC@NLO-Δ
  - ARCANE reweighting
- Origin in multiplicative parton shower matching
  - ESME
  - KrkNLO matching
- …

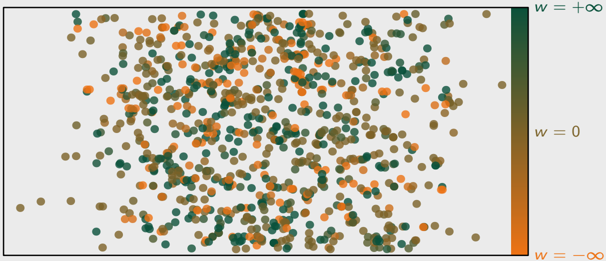
+ combinations of complementary methods

How to handle negative weights?

Cell resampling

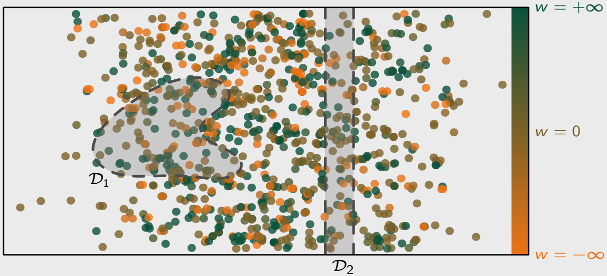
Cell resampling

Events in 2D projection of phase space:



Cell resampling

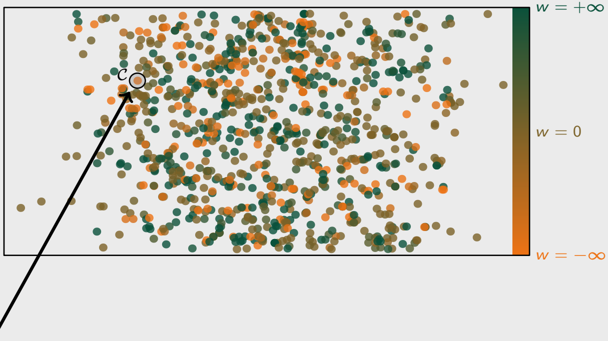
Integrated differential cross sections: $\int_{\mathcal{D}} d\sigma = \sum_{i \in \mathcal{D}} w_i$



- $\int_{\mathcal{D}} d\sigma = \sum_{i \in \mathcal{D}} w_i \geq 0$, provided
  - Theory can be trusted
  - Enough statistics
- Analysis has finite resolution $\Rightarrow$ minimum size for $\mathcal{D}$

Idea: redistribute weights over small distances

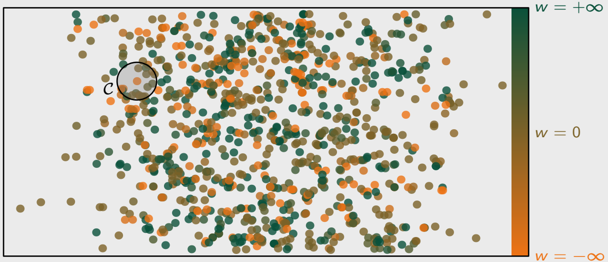
Cell resampling



Cell resampling:

1. Choose seed event with negative weight for cell $\mathcal{C}$

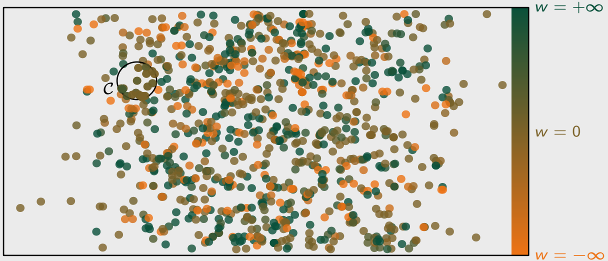
Cell resampling



Cell resampling:

1. Choose seed event with negative weight for cell $\mathcal{C}$
2. Iteratively add nearest event to cell until $\sum_{i \in \mathcal{C}} w_i \geq 0$ or radius exceeds $r_{\max}$

Cell resampling



Cell resampling:

1. Choose seed event with negative weight for cell $\mathcal{C}$
2. Iteratively add nearest event to cell until $\sum_{i \in \mathcal{C}} w_i \geq 0$ or radius exceeds r_{max}
3. Redistribute weights, e. g. average over cell: $w_i \to w = \frac{\sum_{j \in \mathcal{C}} w_j}{\text{\# events in } \mathcal{C}}$
4. Repeat

Cell resampling

Subsampling

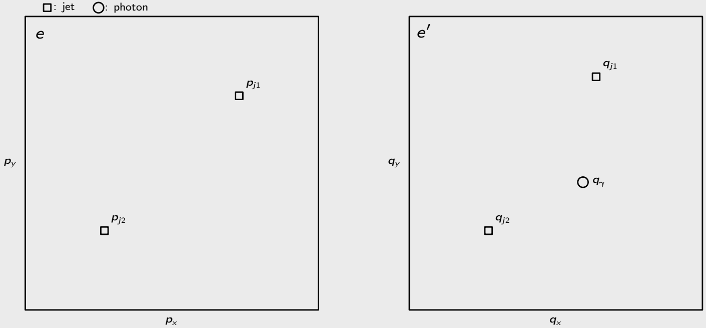
Generate more events inside cells with incomplete cancellation:

Cell resampling

Distance in phase space

Need distance that measures similarity between events

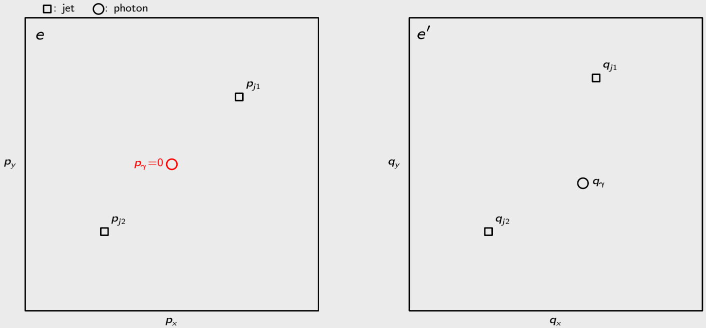
Example:



Cell resampling

Distance in phase space

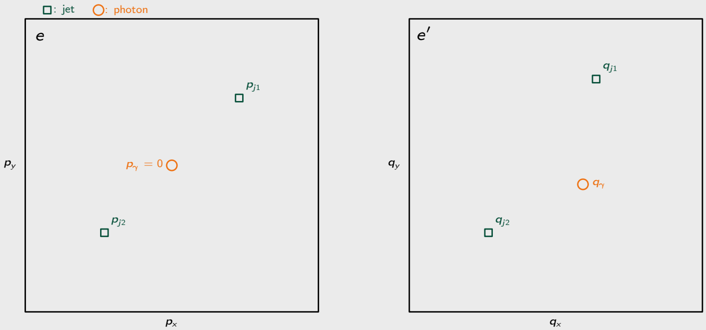
Ensure same multiplicities



Cell resampling

Distance in phase space

Compare physics objects of same type

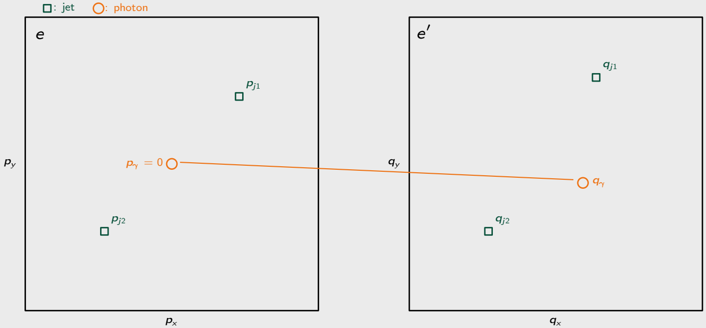


$$d(e,e') = d(s_j, s'_j) + d(s_\gamma, s'_\gamma)$$

Cell resampling

Distance in phase space

Compare photons

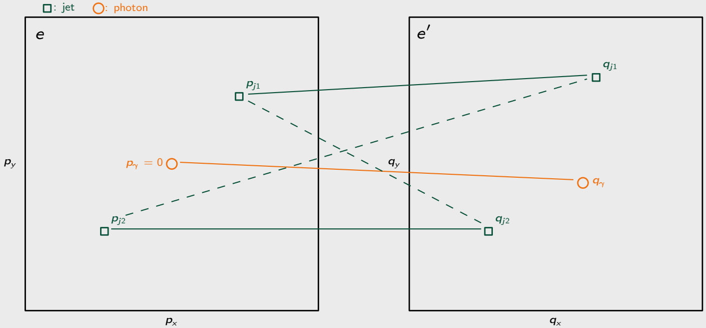


$$
\begin{aligned}
d(e, e') &= d(s_j, s_j') + d(s_\gamma, s_\gamma') \\
&= d(s_j, s_j') + d(p_\gamma, q_\gamma)
\end{aligned}
$$

Cell resampling

Distance in phase space

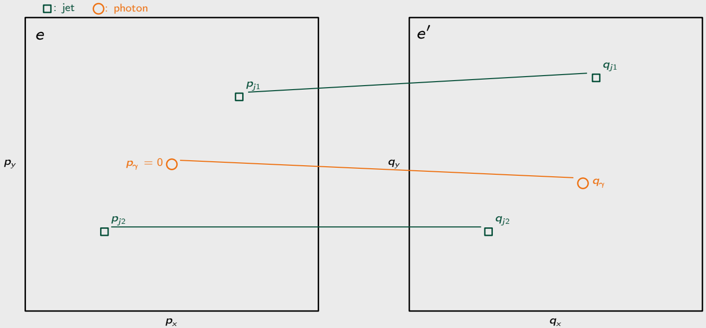
Compare jets: find pairs of most similar jets



$$d(e, e') = d(s_j, s'_j) + d(s_\gamma, s'_\gamma)$$
$$= \min\left[d(p_{j1}, q_{j1}) + d(p_{j2}, q_{j2}), d(p_{j1}, q_{j2}) + d(p_{j2}, q_{j1})\right] + d(p_\gamma, q_\gamma)$$

Cell resampling

Distance in phase space

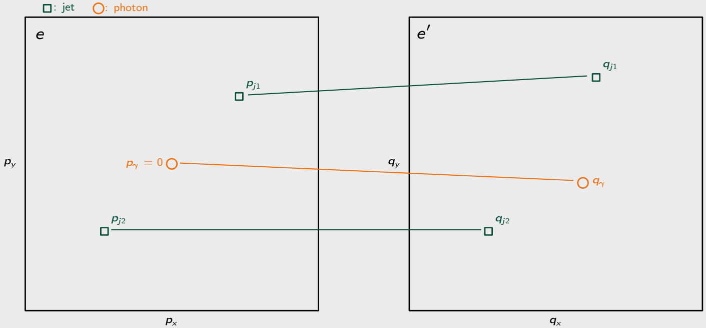


$$d(e, e') = d(s_j, s_j') + d(s_\gamma, s_\gamma')$$
$$= d(p_{j1}, q_{j1}) + d(p_{j2}, q_{j2}) + d(p_\gamma, q_\gamma)$$

Cell resampling

Distance in phase space

Compare momenta



$$d(e, e') = d(s_j, s_j') + d(s_\gamma, s_\gamma')$$
$$= |\vec{p}_{j1} - \vec{q}_{j1}| + |\vec{p}_{j2} - \vec{q}_{j2}| + |\vec{p}_\gamma - \vec{q}_\gamma|$$

How to handle negative weights?

Neural reweighting/refining

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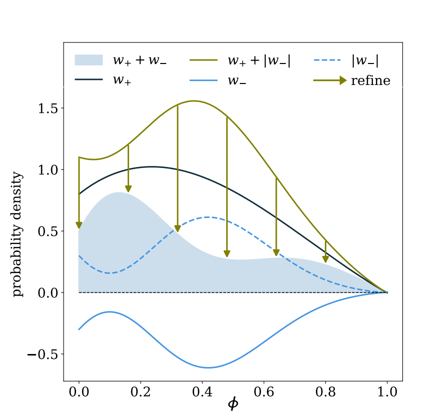
Idea: train neural network to replace weight w_i at phase space point ϕ_i

- Neural reweighting: replace by average weight $w'(\phi_i)$
- Neural refining: replace by rescaled weight $r(\phi_i)|w_i|$
  - Preserves weights in purely positive samples
  - Better behaviour in negative phase space regions



How to handle negative weights?

Folding

Folding

Assume $\int d\phi \, \mathcal{I}(p) \geq 0$

$$\sum_i \mathcal{I}(p_i) \longrightarrow \sum_i \underbrace{\frac{1}{K} \sum_k \mathcal{I}(p_i + k\Delta p)}_{w_i}$$

+ w_i is better estimate of integral $\Rightarrow$ $w_i \geq 0$ more likely
+ general technique, straightforward to use as ingredient in others
− each w_i requires multiple evaluations of $\mathcal{I}$ $\longrightarrow$ more computing time

Additive parton shower matching

Additive parton shower matching

NLO

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{NLO}} = \int d\phi_B \left[B + V + \int d\phi_r \, C\right] + \int d\phi_B d\phi_r \, [R - C]$$

Evaluate analytically

Additive parton shower matching

MC@NLO

Modify to subtract shower approximation of real emission

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{MC@NLO}} = \int d\phi_B \left[B + V + \int d\phi_r\ C_{\text{PS}}\right] \mathcal{F}^{(B)}_{\text{PS}} + \int d\phi_B d\phi_r\ [R - C_{\text{PS}}]\mathcal{F}^{(R)}_{\text{PS}}$$

Evaluate numerically
$\rightarrow$ negative weights

Shower evolution

How to handle negative weights?

Born spreading

Born spreading

𝕊tandard evolution events:

$$\int d\phi_B \, d\phi_r \left[\frac{B(\phi_B)}{\int d\phi_r} + \frac{V(\phi_B)}{\int d\phi_r} + C_{\text{PS}}(\phi_B, \phi_r) \right] \mathcal{F}^{(B)}_{\text{PS}}$$

Born spreading

Standard evolution events:

$$\int d\phi_B \, d\phi_r \, \left[\frac{B(\phi_B)}{\int d\phi_r} + \frac{V(\phi_B)}{\int d\phi_r} + C_{\mathrm{PS}}(\phi_B, \phi_r) \right] \mathcal{F}_{\mathrm{PS}}^{(B)}$$

Idea: “spread out” large + positive Born contribution to cancel negative weights:

$$\frac{B(\phi_B)}{\int d\phi_r} \to \frac{B(\phi_B) F(\phi_r)}{\int d\phi_r \, F(\phi_r)}$$

1. Sample integrand with original Born function $B(\phi_B)$
2. Define spreading function $F(\phi_r)$ via grid in ϕ_r to make integrand non-negative

How to handle negative weights?

MC@NLO-Δ

MC@NLO-Δ

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{MC@NLO}} = \int d\phi_B\ \underbrace{\left[B+V+\int d\phi_r\ C_{\text{PS}}\right]\mathcal{F}_{\text{PS}}^{(B)}}_{\mathbb{S}\text{tandard}} + \int d\phi_B d\phi_r\ \underbrace{[R-C_{\text{PS}}]\mathcal{F}_{\text{PS}}^{(R)}}_{\mathbb{H}\text{ard}}$$

MC@NLO-Δ

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{MC@NLO}} = \int d\phi_B \underbrace{\left[B + V + \int d\phi_r\, C_{\text{PS}}\right] \mathcal{F}_{\text{PS}}^{(B)}}_{\mathbb{S}\text{tandard}} + \int d\phi_B d\phi_r \underbrace{[R - C_{\text{PS}}]\mathcal{F}_{\text{PS}}^{(R)}}_{\mathbb{H}\text{ard}}$$

Idea:

- Born term B in $\mathbb{S}$ good for cancelling negative weights
- Move contributions from $\mathbb{H}$ to $\mathbb{S}$
- Preserve shower accuracy:
  can only move Born-like (soft, collinear) contributions

MC@NLO-Δ

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{MC@NLO-}\Delta} = \int d\phi_B \left[B + V + \int d\phi_r \, [C_{\text{PS}} - (1-\Delta)(R - C_{\text{PS}})]\right] \mathcal{F}^{(B)}_{\text{PS}} + \int d\phi_B d\phi_r \, \Delta[R - C_{\text{PS}}]\mathcal{F}^{(R)}_{\text{PS}}$$

- $0 \leq \Delta \leq 1$
- Must not move hard wide-angle emissions: $\Delta \to 1$
- Move all soft and collinear contributions: $\Delta \to 0$

$\Rightarrow$ construct Δ from Sudakov form factors

How to handle negative weights?

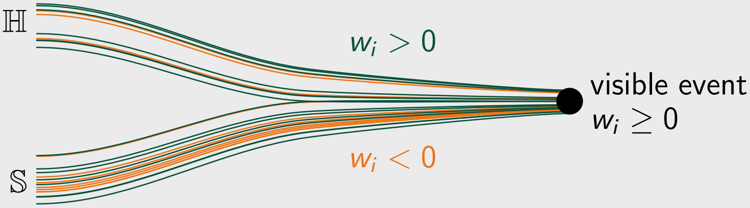
ARCANE reweighting

ARCANE reweighting

- Negative weights come from separating cross section into unphysical parts
- Adding up all parts would result in non-negative weight

ARCANE reweighting

- Negative weights come from separating cross section into unphysical parts
- Adding up all parts would result in non-negative weight
- In parton shower Monte Carlo: sum over all possibilities to generate event (impractical)



Idea: redistribute weights between history strands

How to handle negative weights?

Multiplicative shower matching

Multiplicative shower matching

POWHEG

Starting point: leading order + parton shower

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\mathrm{LOPS}} = \int d\phi_B \; B\mathcal{F}_{\mathrm{PS}}$$

Multiplicative shower matching

POWHEG

Starting point: leading order + parton shower

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{LOPS}} = \int d\phi_B \; B\mathcal{F}_{\text{PS}}$$

Needed for NLO + PS:

1. NLO normalisation
2. Hardest emission distribution must be NLO-accurate

Multiplicative shower matching

POWHEG

Starting point: leading order + parton shower

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{LOPS}} = \int d\phi_B \; B\mathcal{F}_{\text{PS}}$$

Needed for NLO + PS:

1. NLO normalisation

$$B \to B + V + C_{\text{int}} + \int d\phi_r (R - C)$$

   - Parton-shower evolution $\mathcal{F}_{\text{PS}}$ unitary $\Rightarrow$ correct NLO normalisation
   - Only Born kinematics passed on, so far all real emissions from parton shower

2. Hardest emission distribution must be NLO-accurate

Multiplicative shower matching

POWHEG

Starting point: leading order + parton shower

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{LOPS}} = \int d\phi_B \; B\mathcal{F}_{\text{PS}}$$

Needed for NLO + PS:

1. NLO normalisation
2. Hardest emission distribution must be NLO-accurate

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{NLOPS}} = \int d\phi_B \; \left[B + V + C_{\text{int}} + \int d\phi_r (R - C)\right] \mathcal{G}_{\text{PS}}$$

With modified shower $\mathcal{G}_{\text{PS}}$:

- unitary $\Rightarrow$ preserves NLO normalisation
- generates hardest emission according to R (or no emission)

Multiplicative shower matching

POWHEG

Starting point: leading order + parton shower

$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{LOPS}} = \int d\phi_B \; B\mathcal{F}_{\text{PS}}$$

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$$\int_{\mathcal{D}} d\sigma_{ab\to X}\Big|_{\text{NLOPS}} = \int d\phi_B \; \left[B + V + C_{\text{int}} + \int d\phi_r (R - C)\right] \mathcal{G}_{\text{PS}}$$

Monte Carlo estimate of $\int d\phi_r (R - C)$ only source of negative weights

assuming perturbation theory holds

How to handle negative weights?

ESME

Exponentiated Subtraction for Matching Events

Goal: better way to evaluate $\int d\phi_r (R - C)$

Sudakov algorithm to compute n_B with $\langle n_B \rangle = 1 + \int d\phi_r \frac{R-C}{B}$:

- Start with $n_B = 1, p_\perp = p_\perp^{\text{max}}$
- While $p_\perp > p_\perp^{\text{min}}$
  1. Sample next $p_\perp$ from $e^{-\frac{M}{B} \ln p_\perp}, M = \max(R, C)$
  2. Generate random number $0 < r < 1$
  3. If $r > \frac{|R-C|}{M}$ keep current n_B
  4. otherwise, if $R > C$ set $n_B = n_B + 1$
  5. otherwise, if $R < C$ set $n_B = n_B - 1$

Each step away from $n_B = 1$ suppressed by $\mathcal{O}(\alpha_s)$

$\Rightarrow$ negative n_B beyond NLO, can be discarded

How to handle negative weights?

KrkNLO

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- PDFs have to absorb collinear divergences in partonic cross section
- Shift additional finite collinear remnant into PDFs: Krk PDF scheme
- PDFs in Krk scheme remain positive in most regions

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KrkNLO algorithm

For each parton-showered Born-level event

1. If there is a first emission, reweight by positive factor for NLO accuracy
2. Reweight by factor $1 + \frac{V}{B} + \frac{C_{\text{int}}}{B} + \Delta^{\text{FS}}$
   Δ^{FS}: from change of PDF scheme, positive and large

Summary II

Various approaches for cancelling negative weights:

- Redistribute weights between similar/indistinguishable events: local cancellations between negative and excess positive weights
- Modified formulations to facilitate internal cancellations
- Alternative formalisms to avoid unphysical separations and Monte Carlo outliers

Many better methods than just discarding negative weights

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