# Removing negative weights in Monte Carlo event samples

Andreas Maier

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J. R. Andersen, A. Maier, D. Maître Eur.Phys.J.C 83 (2023) 9, 835
J. R. Andersen, A. Maier Eur.Phys.J.C 82 (2022) 5, 433
J. R. Andersen, C. Gütschow, A. Maier, S. Prestel Eur.Phys.J.C 80 (2020) 11, 1007
+ ongoing work with Ana Cueto, Ella Cole, Stephen Jones

# What are event weights?

## Leading-order cross sections

Example: prediction for dijet production cross section

1. Relate to partonic cross section

$$\sigma_{2\text{ jets}} \stackrel{\text{LO}}{=} \sigma_{2\text{ partons}}$$

2. Simulate partonic scattering events with weights $w_i$
   - Computed from scattering matrix elements + PDF + phase space factor
   - Weights proportional to probability: $w_i > 0$
   - Sum of weights gives the cross section:

$$\sigma_{2\text{ partons}} = \sum_i w_i$$

# What are negative event weights?

## Next-to-leading-order cross sections

Example: prediction for dijet production cross section

1. Relate to partonic cross section

$$\sigma_{2\text{ jets}} \overset{\text{NLO}}{=} \sigma_{2\text{ partons}} + \sigma_{3\text{ partons}}$$

2. Simulate partonic scattering events

$$\sigma_{2\text{ partons}} = \sum_i w_i$$

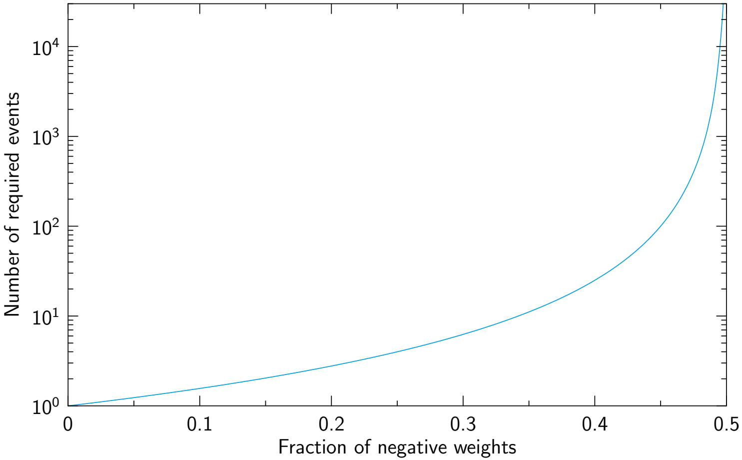
$$\sigma_{3\text{ partons}} = \sum_j w_j$$

$\sigma_{2\text{ partons}}, \sigma_{3\text{ partons}}$ not separately observable:

Events weights can be either positive or negative

# Why are negative event weights a problem?

Number of unweighted events to reach given accuracy:



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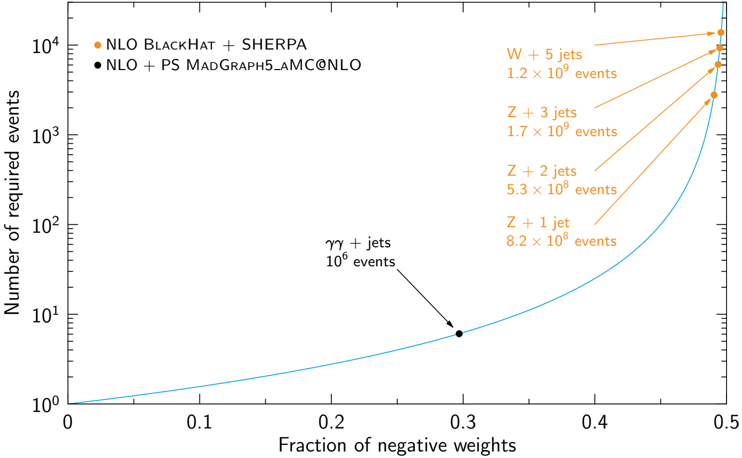
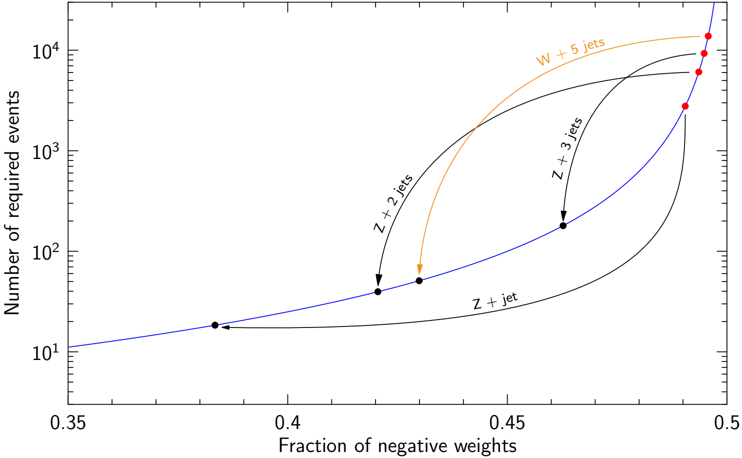



V + jets: Phys. Rev. D 88 (2013) 014025, Phys. Rev. D 97 (2018) 096010

$\gamma\gamma$ + jets: parameters from background modelling for ATLAS $H \to \gamma\gamma$ measurement arXiv:2306.11379

# Cell resampling for V + jets at NLO

## Negative weights

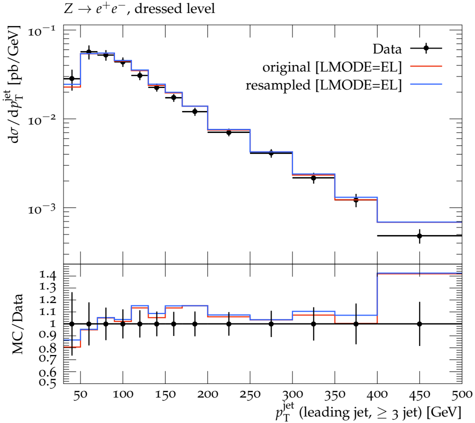


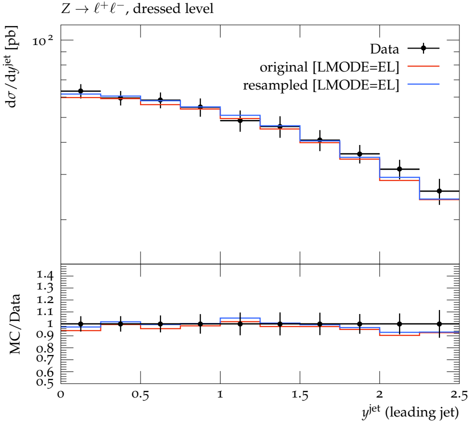

Cell resampling drastically reduces the number of required events

# Cell resampling for V + jets at NLO

## Predictions

Analysis from ATLAS, Eur. Phys. J. C77 (2017) 361:

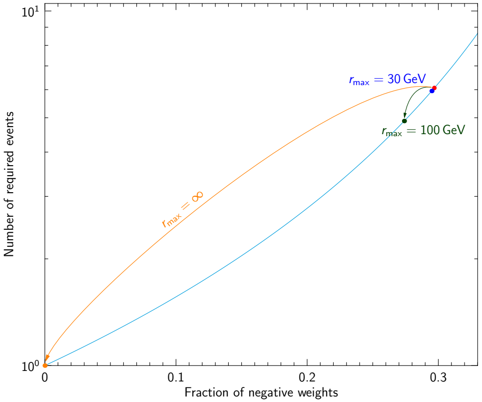


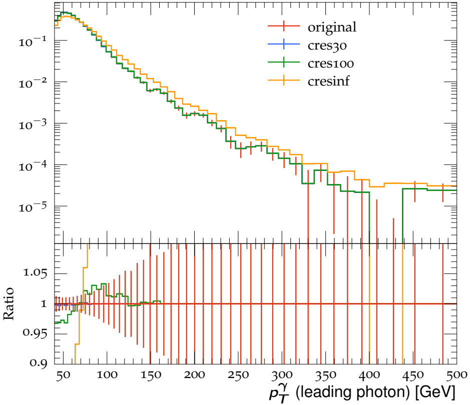




Cell resampling preserves predictions within a few per cent

# Work in progress: showered samples

$pp \to \gamma\gamma +$ jets, $10^6$ events:

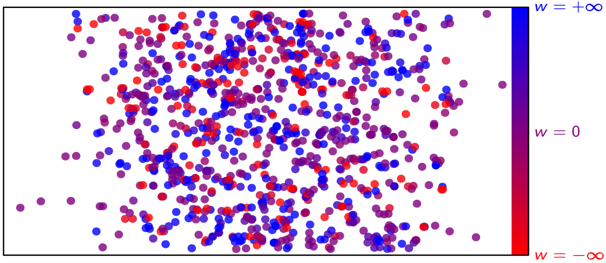



Negative-weight reduction more efficient for large weighted samples

# Observables

Weighted events in 2D projection of phase space:



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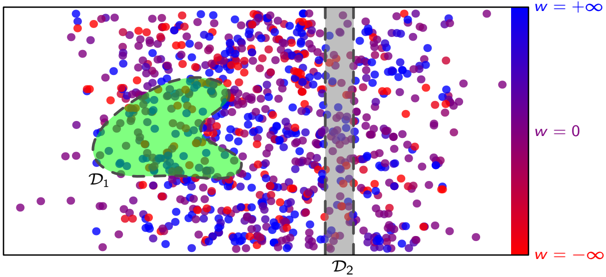



Observables $\mathcal{O}$:

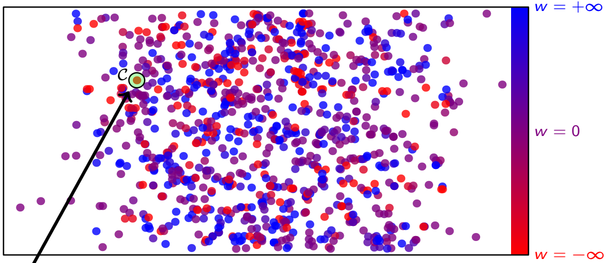
- Select region $\mathcal{D}$ in phase space $\geq$ experimental resolution
- $\mathcal{O} = \sum_{i \in \mathcal{D}} w_i \geq 0$ with sufficient statistics

e.g. histogram bins

Redistribute weights without affecting any observable

# Cell resampling

[Andersen, Maier 2021]




Cell resampling:

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

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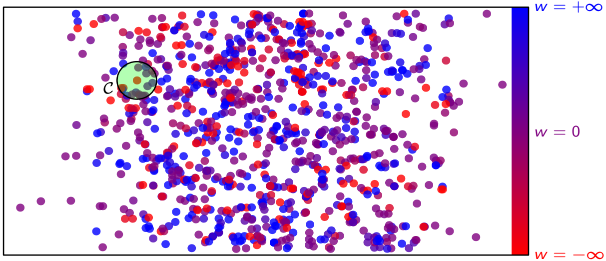


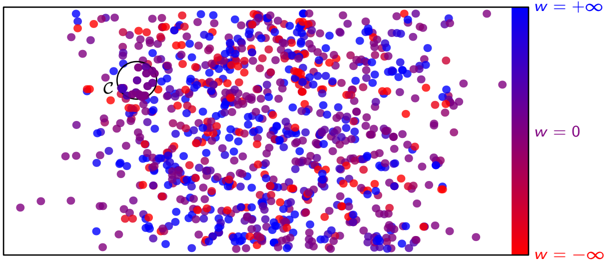

Cell resampling:

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 $r_{\text{max}}$

Cells get systematically smaller with increasing statistics

# Cell resampling

**[Andersen, Maier 2021]**

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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

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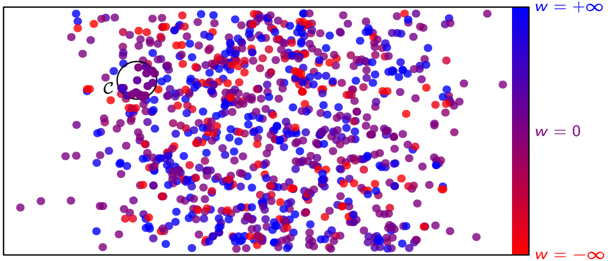


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1. Choose seed event with negative weight for cell $\mathcal{C}$
2. Iteratively add nearest event to cell until $\sum_{i \in \mathcal{C}} w_i \geq 0$ or radius exceeds $r_{\text{max}}$
   What does "nearest" mean?
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4.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

# Distances in phase space

Criteria for distance function:

- Small distance between events that look similar in detector or differ only in properties the event generator can't predict
- Large distance between events that look different in detector

Define distance in terms of infrared & collinear safe objects, e.g. jets

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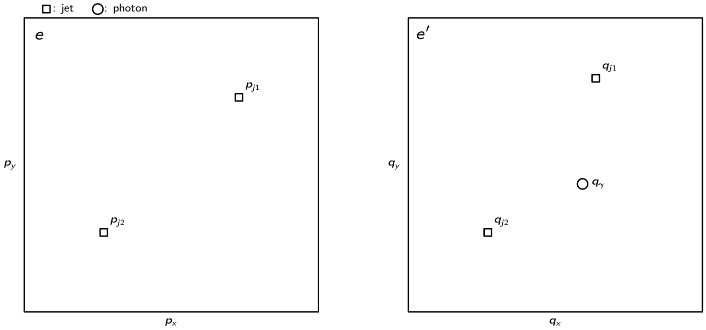
Define distance in terms of infrared & collinear safe objects, e.g. jets

Current choice:

1. Find optimal pairing between observable objects in both events
2. Sum up spatial momentum differences

# Distances in phase space

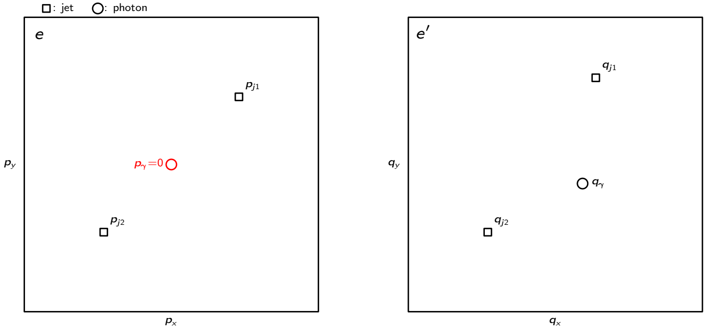
## Example



# Distances in phase space

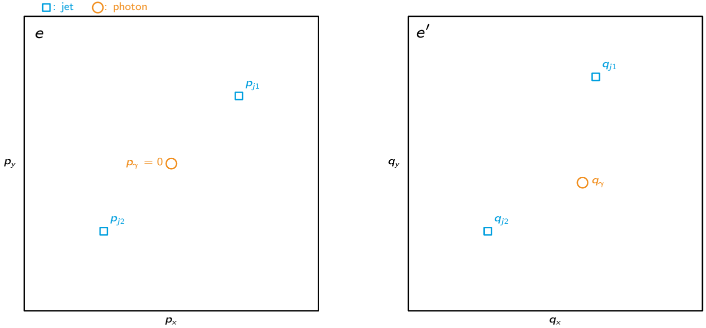
## Example

Ensure same multiplicities



# Distances in phase space
## Example

Compare physics objects of same type

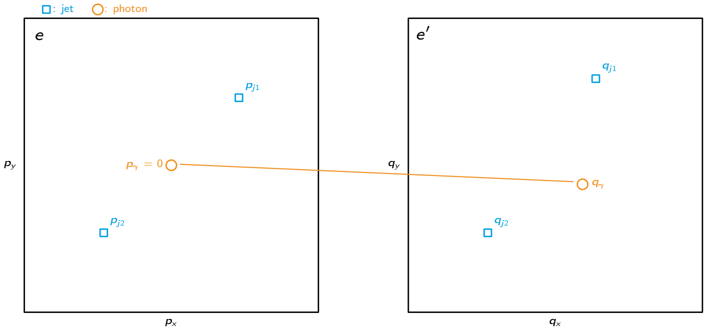



$$d(e, e') = d(s_j, s'_j) + d(s_\gamma, s'_\gamma)$$

# Distances in phase space

## Example

Compare photons

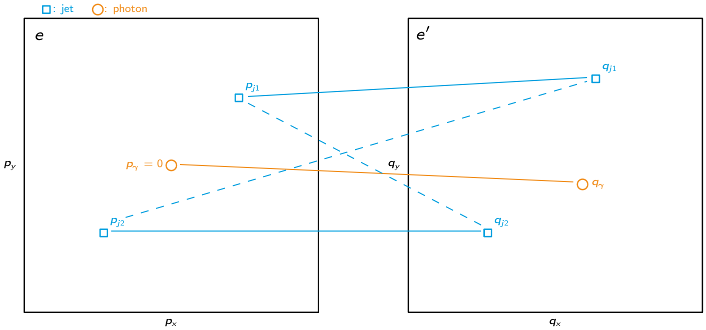



$$
\begin{aligned}
d(e, e') &= d(s_j, s_j') + d(s_\gamma, s_\gamma') \\
&= d(s_j, s_j') + d(p_\gamma, q_\gamma)
\end{aligned}
$$

# Distances in phase space

## Example

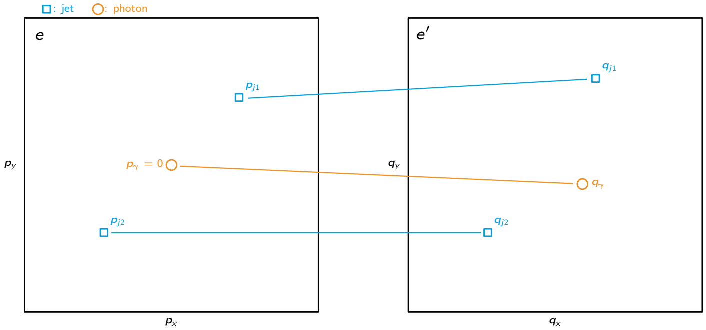
Compare jets: find pairs of most similar jets




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

# Distances in phase space

## Example

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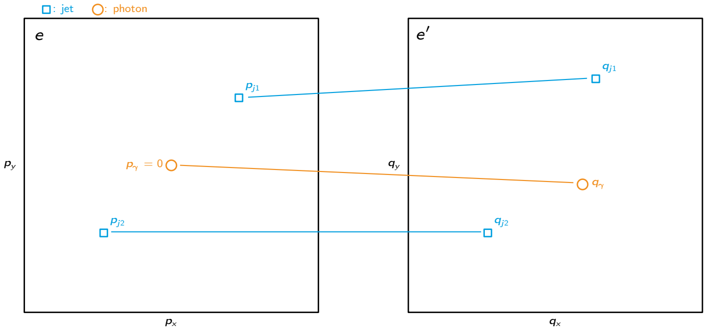
\end{aligned}
$$

# Distances in phase space

## Example

Compare momenta




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

# Distances in phase space

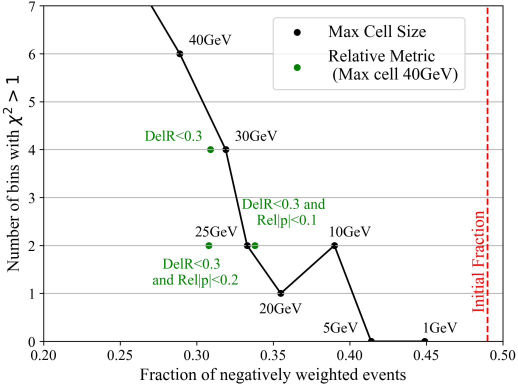
## Work in progress: relative distance

Alternative metric based on relative momentum differences:

- Closer to experimental sensitivity
- Amount of cancellation better aligned with statistical uncertainty

Initial exploration for W $p_\perp$ distribution in W + 1 jet:

[Plot by Ella Cole]



# Runtime scaling

- Runtime for generating $N$ events: $\mathcal{O}(N)$
- Naive cell resampling: $\mathcal{O}(N^2)$
  - Expect: $\#\text{cells} \propto (\#\text{events with } w < 0) \propto \#\text{events}$
  - Naive (k) nearest neighbour search: $\mathcal{O}(N)$

Need faster nearest-neighbour search

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  - Naive (k) nearest neighbour search: $\mathcal{O}(N)$

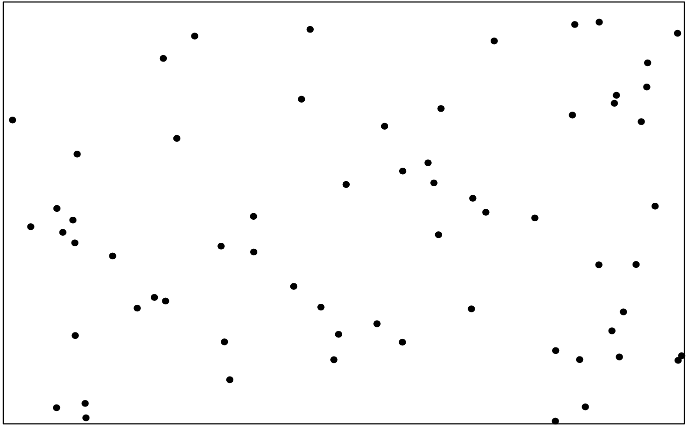
Need faster nearest-neighbour search

Small number of dimensions:

- Histograms
- Voronoi cells ($\to$ jet clustering in `fastjet`)

Here: vantage-point tree search

# Nearest-neighbour search



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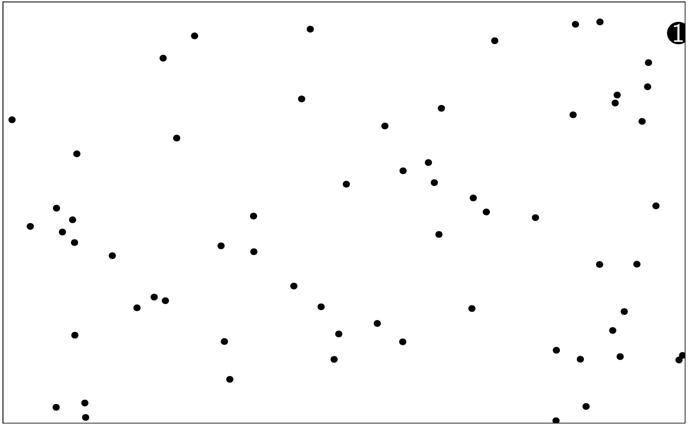
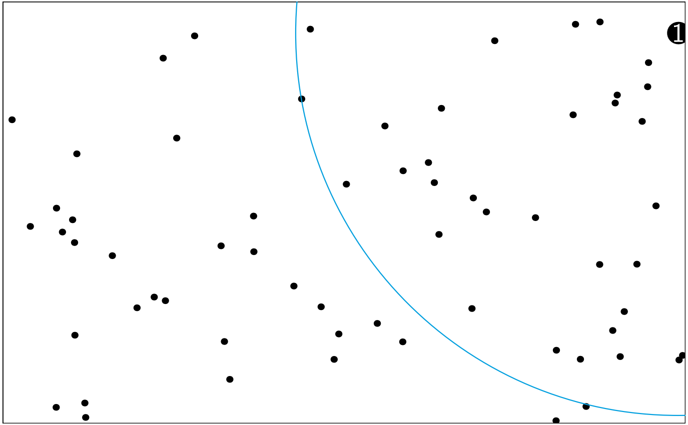



Vantage-point tree:

➊

# Nearest-neighbour search

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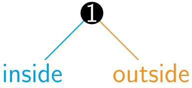

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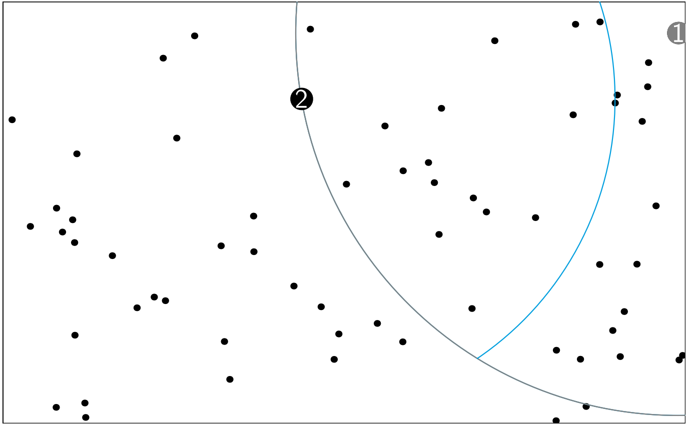


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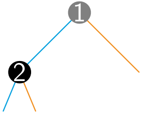

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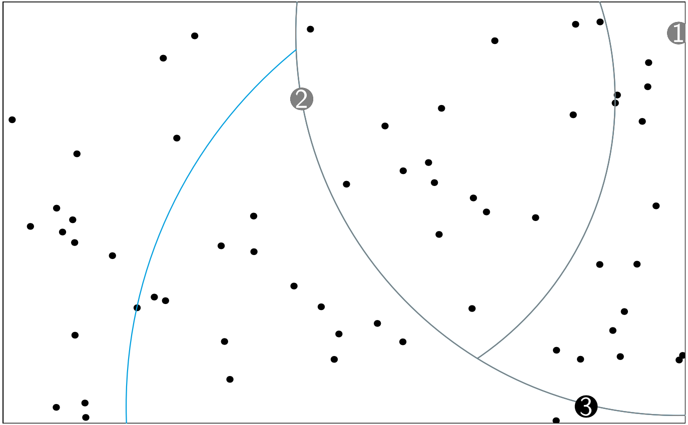


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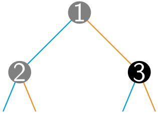

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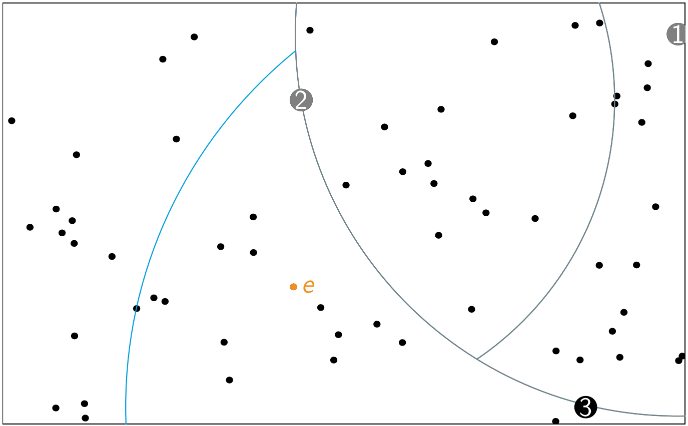


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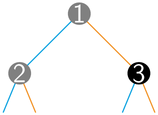


Search nearest neighbour for *e*:

- Find candidate in region containing *e*
- Search neighbouring regions only if better candidate may be found

# Summary

- Negative event weights lead to slow statistical convergence
- Idea: remove negative weights by smearing over small phase space regions
  - Potential to reduce the number of required events by orders of magnitude
  - Preserves predictions of observables
  - Agnostic with respect to process and observables
  - Automatic improvement with increasing statistics
  - Computationally efficient: $\sim 55$ CPU hours for one billion events (W + 5 jets)

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Outlook:

- Application to parton showered samples ✓ [Andersen, Cueto, Maier, Jones]
- IRC safety with electroweak corrections [Andersen, Maier, Schönherr]
- Systematic estimate of uncertainties
- Integrate into existing workflows
- Guide Monte Carlo event generation? [Andersen, Maier, Maître, Schönherr]

# Backup

# Why do we need many more events?

Consider $N$ uncorrelated unweighted events:

- $w_i = -w$ for $i \leq N_-$
- $w_i = +w$ for $i > N_-$

$\Rightarrow$ Negative weight fraction: $r_- = \frac{N_-}{N}$

Then

- $\sigma = \sum_i w_i = -N_- w + (N - N_-)w = (1 - 2r_-)Nw$
- $\Delta\sigma = \sqrt{\sum_i w_i^2} = \sqrt{N}w$

To reach given relative uncertainty $\frac{\Delta\sigma}{\sigma} = \frac{1}{(1-2r_-)\sqrt{N(r_-)}} = \frac{1}{\sqrt{N(0)}}$:

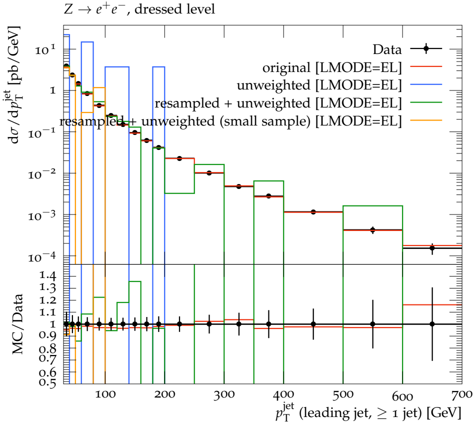
$$N(r_-) = \frac{N(0)}{(1 - 2r_-)^2}$$

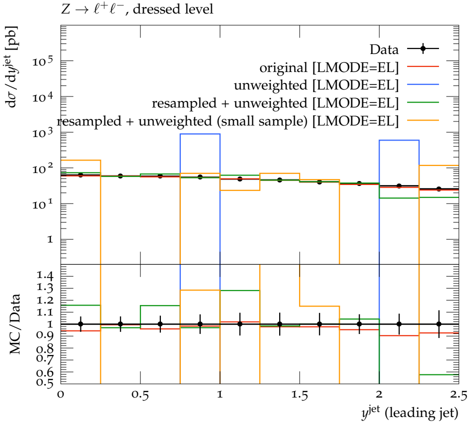
# Event samples

[BlackHat + Sherpa 2013 + 2017]

| Sample | Process | Centre-of-mass energy | # events |
|---|---|---|---|
| `Z1` | $pp \to (Z \to e^+e^-) + \text{jet}$ | 13 TeV | $8.21 \times 10^8$ |
| `Z2` | $pp \to (Z \to e^+e^-) + 2\ \text{jets}$ | 13 TeV | $5.30 \times 10^8$ |
| `Z3` | $pp \to (Z \to e^+e^-) + 3\ \text{jets}$ | 13 TeV | $1.65 \times 10^9$ |
| `W5` | $pp \to (W^- \to e^-\nu_e) + 5\ \text{jets}$ | 7 TeV | $1.17 \times 10^9$ |

# Unweighting for Z + jet



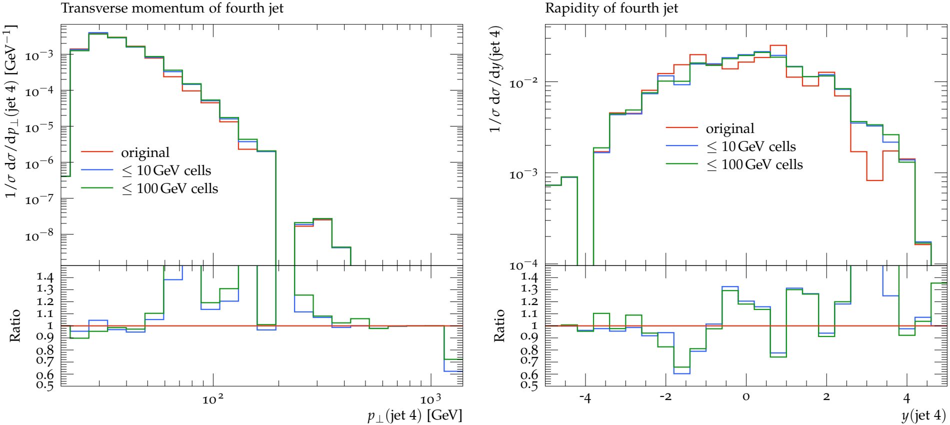

original: $8.21 \times 10^8$ events

unweighted: 320 events

resampled + unweighted: 11574 events

resampled + unweighted (small sample): 320 events

# Resampling for W + 5 jets



# Distances in phase space

Need distance function $d(e, e')$ between events $e, e'$

- Essential: $d(e, e')$ small $\Rightarrow$ $e, e'$ look similar in detector or differ only in properties the event generator can't predict
- Desirable: $d(e, e')$ large $\Rightarrow$ $e, e'$ look different in detector

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Example: infrared safety

- $d(e, e')$ unaffected by collinear splittings with $\Theta \to 0$
- $d(e, e')$ unaffected by soft particles with $p \to 0$

$\Rightarrow$ define distance in terms of infrared-safe physics objects, e.g. jets

Here: Example for fixed-order (QCD) event generator

# Distances in phase space

## Concrete implementation

1. Collect all infrared-safe objects in event $e$ into sets $\{\overset{\text{jets}}{s_1}, \overset{\text{electrons}}{s_2}, \ldots, s_T\}$

$$d(e, e') = \sum_{t=1}^{T} d(s_t, s'_t)$$

# Distances in phase space

## Concrete implementation

jets electrons

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$$d(e, e') = \sum_{t=1}^{T} d(s_t, s_t')$$

2. Objects in $s_t$ have four-momenta $( p_1, \ldots \ldots\ldots, p_P )$

Objects in $s_t'$ have four-momenta $( q_1, \ldots, q_Q, 0, \ldots, 0 )$

$$d(s_t, s_t') = \min_{\sigma \in S_P} \sum_{i=1}^{P} d_t(p_i, q_{\sigma(i)})$$

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Efficient minimisation: Hungarian algorithm [Jacobi 1890]

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   Objects in $s'_t$ have four-momenta $(\, q_1 \,, \ldots \,, q_Q, 0, \ldots, 0 \,)$

$$d(s_t, s'_t) = \min_{\sigma \in S_P} \sum_{i=1}^{P} d_t(p_i, q_{\sigma(i)})$$

3. Choose distance function between particle momenta
   Here: independent of particle type $t$, do not consider internal structure

$$d_t(p, q) = \sqrt{(\vec{p} - \vec{q})^2 + \tau^2 (p_\perp - q_\perp)^2} \qquad \tau\text{: tunable parameter}$$

# Computing requirements

## Memory

Fast + exact nearest-neighbour search: keep all events in memory

Need $\sim$ (byte size of event) GB for $\sim 10^9$ events

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Only store relevant event data: weights + momenta of outgoing analysis objects

Read + convert events $\longrightarrow$ Cell resampling $\longrightarrow$ Read + write events

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## Memory

Fast + exact nearest-neighbour search: keep all events in memory

Need $\sim$ (byte size of event) GB for $\sim 10^9$ events

Only store relevant event data: weights + momenta of outgoing analysis objects

Read + convert events → Cell resampling → Read + write events

Current requirements:

- Persistent event samples with reasonably fast sequential access
- 300 GB to 400 GB of memory per $10^9$ events,
  no huge increase from showering expected

# Computing requirements

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- Persistent event samples with reasonably fast sequential access
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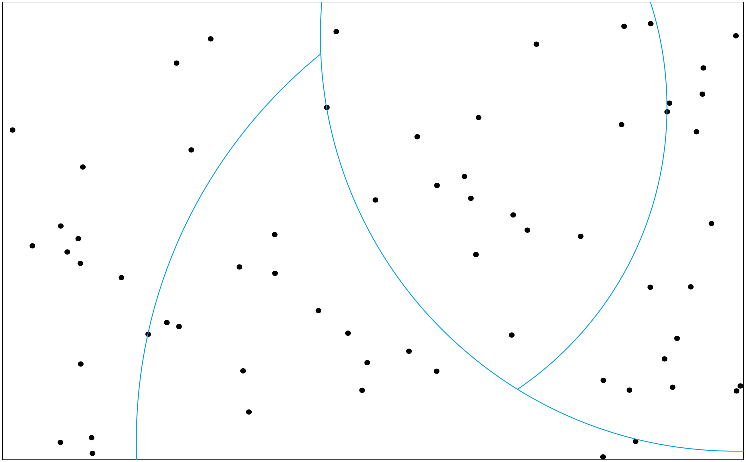
Can we go beyond $\sim 10^9$ events?

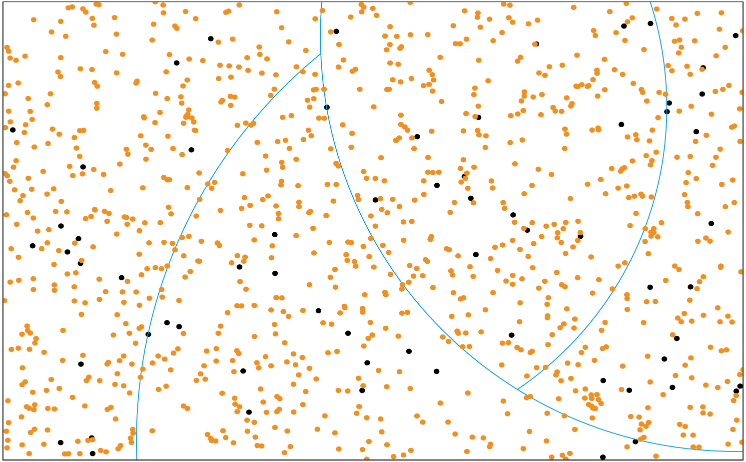
# Work in progress: memory efficiency

1. Partition phase space using vantage-point tree from small event sample



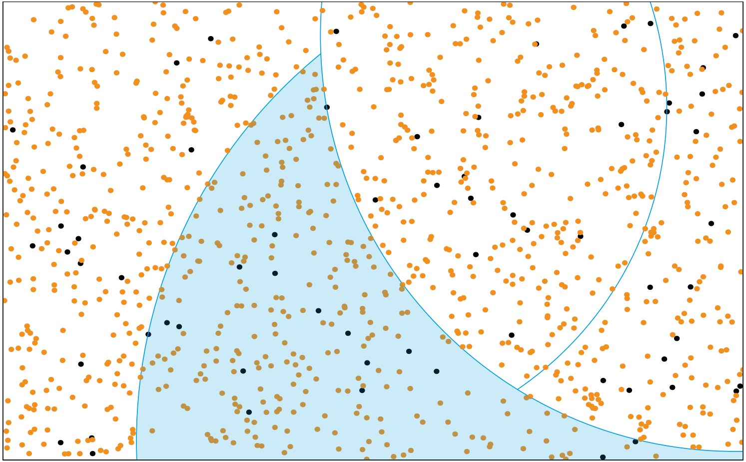
# Work in progress: memory efficiency

2. Identify region for each event in large sample



# Work in progress: memory efficiency

3. Independent cell resampling for each region



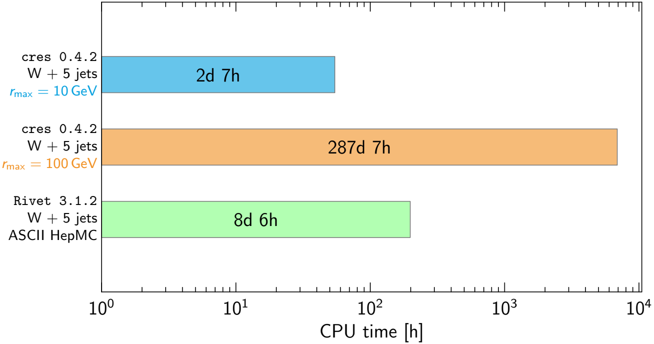
# Computing requirements

## CPU time

Benchmark machines:

| # Cores | CPU model | Memory | Age |
|---|---|---|---|
| 20 | XEON E5-2640 @ 2.40GHz | 400GB | ∼7 years |
| 12 | XEON E5-2643 @ 3.40GHz | 800GB | ∼6 years |

Local rotating disks, RAID 6



# Computing requirements

## Wall-clock time

Benchmark machines:

| # Cores | CPU model | Memory | Age |
|---|---|---|---|
| 20 | XEON E5-2640 @ 2.40GHz | 400GB | ∼7 years |
| 12 | XEON E5-2643 @ 3.40GHz | 800GB | ∼6 years |

Local rotating disks, RAID 6