The Matrix Element Method at next-to-leading order QCD for single top-quark production at the LHC

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Matrix Element Method (MEM) in a nutshell [Kondo '88,'91]

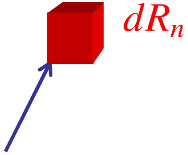
For the collision $\boxed{A + B \to a_1(p_1) + a_2(p_2) + \cdots + a_n(p_n)}$

the differential cross section

$$\frac{d\sigma_n}{d^4 p_1 \ldots d^4 p_n} \propto \frac{1}{2s} \left|\mathcal{M}(p_1, \ldots, p_n)\right|^2 dR_n$$

$$dR_n(p_1, \ldots, p_n) = (2\pi)^4 \delta(P - \sum_i p_i) \prod_j \frac{d^3 p_j}{(2\pi)^3 2E_j}$$

is a measure for the probability to observe the final state in the inf. phase space region dR_n located at $(p_1, \ldots, p_n)$



$\vec{p} = (p_1, \ldots, p_n)$

Matrix Element Method (MEM) in a nutshell [Kondo '88,'91]

Collecting generic partonic final state variables in $\vec{x}$:

e.g. $\vec{x} = (E_i, \theta_j, \ldots)$: $\boxed{\frac{d\sigma_n}{d^4p_1 \ldots d^4p_n} \rightarrow \frac{d\sigma_n}{d\vec{x}}}$

Experimentally we observe hadronic variables $\vec{y}$ instead of partonic variables $\vec{x}$.

Probability to measure $\vec{y}$:

$$\mathcal{P}(\vec{y}) = \frac{1}{\sigma} \int d\vec{x} \, \frac{d\sigma}{d\vec{x}} \, W(\vec{x}, \vec{y})$$

Transfer function $W(\vec{x}, \vec{y})$:

- Probability to experimentally observe a hadronic event $\vec{y}$ given a partonic event $\vec{x}$
- Determined by experiments through simulations
- δ-functions in the following

Matrix Element Method (MEM) in a nutshell [Kondo '88,'91]

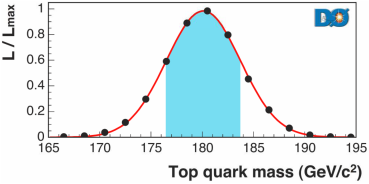
Extraction of model parameters Ω from data by maximizing a likelihood $\propto$ differential cross section ($\propto |\mathcal{M}^{\text{LO}}|^2$):

Likelihood as a function of Ω for event sample $\{\vec{x}_i\}$

$$\mathcal{L}^{\text{LO}}(\Omega) = \prod_i \frac{1}{\sigma^{\text{LO}}(\Omega)} \int d\vec{y}\, \frac{d\sigma^{\text{LO}}(\Omega)}{d\vec{y}} \underbrace{W(\vec{x}_i, \vec{y})}_{\substack{\text{transfer function,} \\ \text{here: } =\delta(\vec{x}_i - \vec{y})}} = \prod_i \frac{1}{\sigma^{\text{LO}}(\Omega)} \frac{d\sigma^{\text{LO}}(\Omega)}{d\vec{x}_i}$$

Maximizing wrt Ω yields estimator $\widehat{\Omega}$: $\mathcal{L}^{\text{LO}}(\widehat{\Omega}) = \sup_{\Omega} \mathcal{L}^{\text{LO}}(\Omega)$

All information from event used $\Longrightarrow$ most efficient estimator!



e.g. top mass measurement at Tevatron
[D0: Nature 429, 638], [CDF: PRD 50, 2966]
based on $O(70)$ events!

MEM beyond LO:

Experimental analysis so far restricted to LO

Steps towards MEM@NLO:

- Effects of real radiation [Alwall,Freitas,Mattelaer '11]
- Final states without strongly interacting particles [Campbell,Giele,Williams '12], [Campbell,Ellis,Giele,Williams '13]
- Steps towards final states with strongly interacting particles [Campbell,Giele,Williams '13]
- Complete algorithm [Martini,Uwer '15]

MEM beyond LO: NLO cross section at parton level

$$\sigma^{\text{NLO}} = \overbrace{\int dR_n \frac{d\sigma^{\text{B}}}{dR_n}}^{\text{Born}} + \underbrace{\overbrace{\int dR_n \frac{d\sigma^{\text{V}}}{dR_n}}^{\text{virtual}} + \overbrace{\int dR_{n+1} \frac{d\sigma^{\text{R}}}{dR_{n+1}}}^{\text{real}}}_{\text{separately IR divergent}}$$

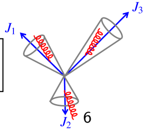
Jet Physics: observed final states are jets

partonic events $\longrightarrow$ "Jet events"

New in NLO:

- Infrared and collinear divergences in virtual and real corrections $\xrightarrow{\text{KLN theorem}}$ mutual cancelation
- $n+1$ particle phase space due to real corrections: Non-trivial mapping: parton momenta $\leftrightarrow$ jet momenta

Born and virtual: $J_i = p_i$ trivial but real: $J_i = \widetilde{J}_i(p_1, \ldots, p_{n+1})$



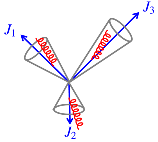
Likelihood at NLO: 3 major obstacles

$$\mathcal{L}^{\text{NLO}}(\Omega) = \prod_i \frac{1}{\sigma^{\text{NLO}}_{n\text{-jet}}(\Omega)} \left(\frac{d\sigma^{\text{B+V}}_{n\to n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n} + \frac{d\sigma^{\text{R}}_{n+1\to n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n} \right)\Bigg|_{\text{event } i}$$

- Born+virtual and real contribution separately IR divergent

  NEED: Point-wise cancelation in jet phase space

- Integration over jet cones in real contribution introduces δ-functions $\rightarrow$ numerically not feasible!



  NEED: factorisation of real phase space

- Born+virtual matrix elements only defined for 'Born kinematics'

  NEED: clustered jets obeying 'Born kinematics'

$\rightarrow$ not possible with $2 \rightarrow 1$ clustering/recombination

Proposal: $3 \to 2$ clustering

$3 \to 2$ clustering $p_i, p_j, p_k \to \widetilde{J}_{ij}, \widetilde{J}_k$
can meet all 3 requirements at the same time

$\Downarrow$

Using $3 \to 2$ jet algorithm instead of $2 \to 1$
allows to overcome the 3 obstacles

$3 \to 2$ clusterings inspired by Catani-Seymour dipole subtraction method [Catani, Seymour '97], [Catani, Dittmaier, Seymour, Trocsanyi '02]

Jet event weight at NLO

Phase space factorisation allows to define an event weight (differential jet cross section) at NLO

$$\frac{d\sigma^{\text{NLO}}_{n\text{-jet}}(\Omega)}{dJ_1 \dots dJ_n} = \underbrace{\underbrace{\frac{d\sigma^{\text{B+V}}(\Omega)}{dJ_1 \dots dJ_n}}_{\text{still IR divergent}} + \underbrace{\overbrace{\int dR_{\text{unres}}(\Phi)}^{\text{3dim integration}} \frac{d\sigma^{\text{R}}(\Omega)}{dp_1 \dots dp_{n+1}}}_{\text{still IR divergent}}}_{\text{finite through subtraction/slicing}}$$

Mutual cancelation of IR-divergences from the virtual and the real part has to be carried out by a suitable method (e.g. phase space slicing)

Validation

We consider the exclusive s–channel production of single top quarks in association with a light jet at the LHC

$$p + p \to t + j \quad @ \text{ NLO QCD}$$

Veto on additional jet emission, no resolved additional jet!

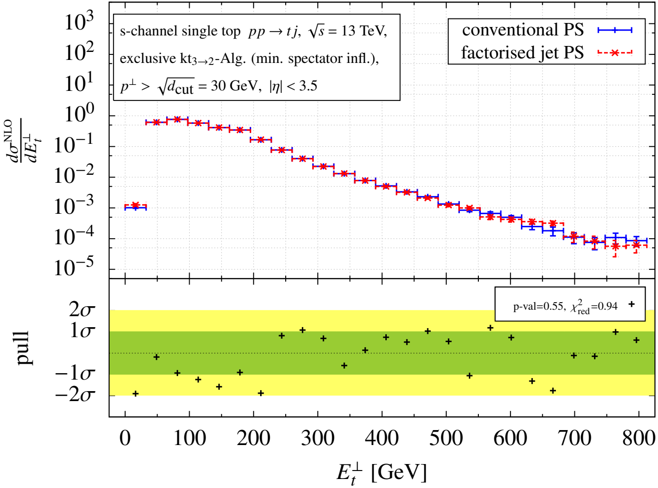
Note: top decay not included, tops are treated as tagged top jets

To Check:

1. Generation of real phase space
2. Generation of unweighted events (at NLO accuracy!)

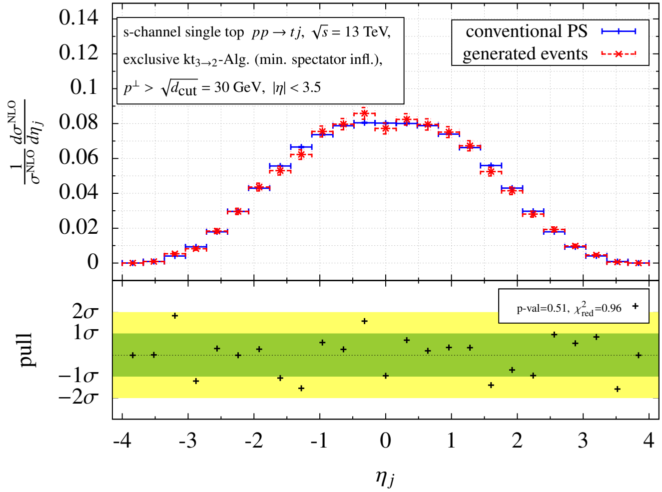
Validation 1: Phase space generation

Calculate jet distributions in NLO accuracy using conventional approach (parton level MC + 3 $\to$ 2 jet alg.) and compare with distributions obtained from $\frac{d\sigma^{\mathrm{NLO}}_{n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n}$ with factorised jet phase space



Validation 2: Unweighted events

Fill histograms with unweighted events generated according to $\rho = \frac{d\sigma^{\mathrm{NLO}}_{n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n}$ and compare with jet distributions in NLO accuracy obtained from conventional approach (parton MC + $3 \to 2$ clus.)



Application: Matrix Element Method at NLO

(example: $p + p \to t + j$ via s-channel @ NLO QCD)

Toy experiment: Generate sample of N unweighted NLO tj events

$$\vec{x}_i = (\eta_t, E_j, \eta_j, \phi_j)_i \quad \text{with } \Omega = m_t = m_t^{\text{true}} = 173.2 \text{ GeV}$$

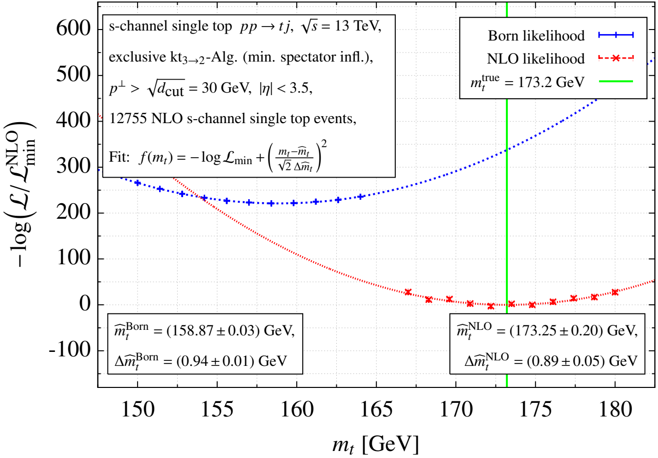
NLO likelihood function for event sample

$$\mathcal{L}^{\text{NLO}}(m_t) = \prod_i^N \mathcal{L}^{\text{NLO}}(\vec{x}_i | m_t) = \left(\frac{1}{\sigma^{\text{NLO}}(m_t)}\right)^N \prod_{i=1}^N \left(\frac{E_j^2 \cosh(\eta_t)}{2\, s\, E_t \cosh^3(\eta_j)} \frac{d\sigma^{\text{NLO}}}{d^4 J_t\, d^4 J_j}(m_t)\right)\Bigg|_i$$

Find minimum of negative logarithm of NLO likelihood
("Log-Likelihood") to obtain estimator $\widehat{m}_t$ for top mass

$$-\log \mathcal{L}^{\text{NLO}}(\widehat{m}_t) = \inf_{m_t} \left(-\log \mathcal{L}^{\text{NLO}}(m_t)\right)$$

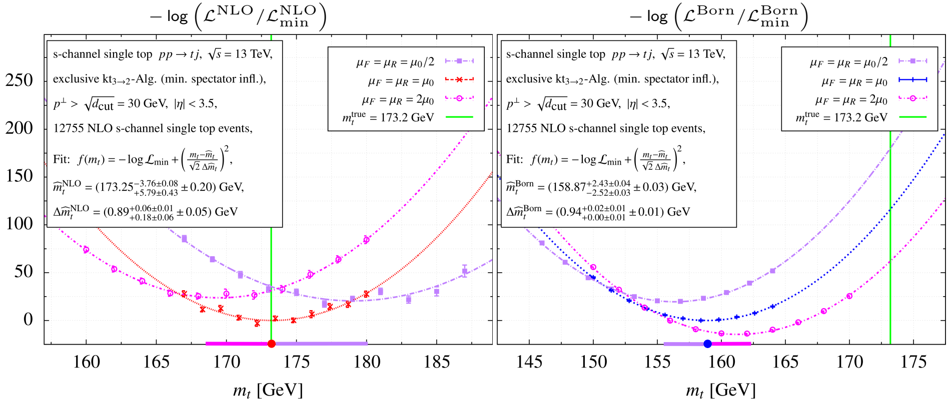
MEM at NLO: top-quark mass extraction via parabola fit



NLO analysis recovers m_t^{true} but significant difference if MEM@LO is used!

- $\approx 13k$ events allow already precise mass determination
- Mass definition unambigously defined through NLO calculation
- Large shift observed in LO analysis would require significant calibration with related uncertainties

MEM at NLO: scale dependence



- Impact of scale variation in NLO analysis bigger than in Born analysis (n.b.: LO is actually EW process, no μ_R dependence)
- Large shift in Born analysis with respect to NLO not covered by scale variation between $[\frac{\mu_0}{2}, 2\mu_0]$
- Scale variation between $[\frac{\mu_0}{2}, 2\mu_0]$ in Born analysis does not give reliable estimate of NLO effects

Conclusion

$3 \to 2$ jet clustering algorithm:

- Uniquely maps real corrections onto Born kinematics

Allows:

- Evaluation of event weights for jet events in NLO accuracy
- Generation of unweighted events at NLO
- Application of MEM at NLO
  - Extraction of m_t with NLO likelihood from NLO single top events: Perfect agreement with input value!
  - Extraction with Born likelihood: Large deviation from input value possible (not necessarily covered by scale variation)!
  - Renormalization scheme well-defined in MEM at NLO (allows for example unambiguous measurement of top-quark mass)

Outlook: MEM at NLO for t-channel, top-pair, including decay, top+Higgs...

BackUp: Likelihood at NLO: 3 major obstacles

$$\mathcal{L}^{\text{NLO}}(\Omega) = \prod_i \frac{1}{\sigma^{\text{NLO}}_{n\text{-jet}}(\Omega)} \left(\frac{d\sigma^{\text{B+V}}_{n \to n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n} + \frac{d\sigma^{\text{R}}_{n+1 \to n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n} \right) \Bigg|_{\text{event } i}$$

1) Born+virtual and real contribution separately IR divergent

NEED: Point-wise cancelation in jet phase space

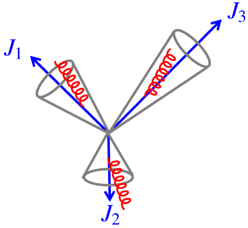
$\rightarrow$ both contributions must be evaluated for same jet momenta

BackUp: Real contributions – formal definition

(one recombination: $J_i = \widetilde{J}_i(p_1, \ldots, p_{n+1}),\ i = 1, \ldots, n$)

$$\frac{\sigma^{\mathrm{R}}_{n+1\to n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n} = \int dR_{n+1} \frac{d\sigma^{\mathrm{R}}(\Omega)}{dR_{n+1}} \prod_{i=1}^{n} \delta(\widetilde{J}_i(p_1, \ldots, p_{n+1}) - J_i)$$

2) Integration over δ-function numerically not feasible!



NEED: factorisation of phase space

→ Integration trivial:

$$dR_{n+1}(p_1, \ldots, p_{n+1}) = dR_n(\widetilde{J}_1, \ldots, \widetilde{J}_n) dR_{\text{unres}}(\Phi)$$

$$\Rightarrow \int dR_{n+1}(p_1, \ldots, p_{n+1}) \prod_{i=1}^{n} \delta(\widetilde{J}_i - J_i) = \int dR_{\text{unres}}(\Phi)\Big|_{\widetilde{J}_i = J_i,\ i=1,\ldots,n}$$

BackUp: Born+virtual contributions

(no recombination: $J_i = p_i = \widetilde{J}_i,\ i = 1, \ldots, n$)

$$\frac{\sigma^{B+V}_{n\to n\text{-jet}}(\Omega)}{dJ_1 \ldots dJ_n} = \int dR_n \frac{d\sigma^{\mathrm{B+V}}(\Omega)}{dR_n} \prod_{i=1}^{n} \delta(p_i - J_i) = \frac{\sigma^{\mathrm{B+V}}(\Omega)}{dJ_1 \ldots dJ_n}$$

3) Born+virtual matrix elements only defined for ‘Born kinematics’

NEED: clustered jets obeying ‘Born kinematics’

$\rightarrow$ on-shell condition and momentum conservation:

$$\widetilde{J}_i^2 = m_i^2 \quad \text{and} \quad p_1 + \ldots + p_{n+1} = \widetilde{J}_1 + \ldots + \widetilde{J}_n$$

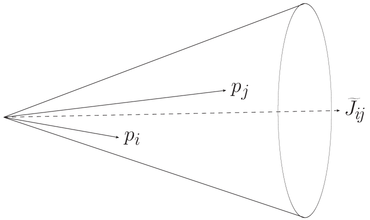
not possible with $2 \rightarrow 1$ clustering/recombination

BackUp: Ingredients of iterative $2 \to 1$ jet algorithms

1. Resolution:

e.g. $$y_{ij} = \min({p_i^\perp}^{2p}, {p_j^\perp}^{2p}) \frac{\Delta_{ij}}{R^2}, \qquad \Delta_{ij} = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

($p = 1$: "kt-algorithm", $p = -1$: "anti-kt-algorithm")



2. Recombination/Clustering:

If $y_{ij} < y_{\text{cut}}$:
p_i, p_j are clustered to jet $\widetilde{J}_{ij}$

e.g. $$\widetilde{J}_{ij} = p_i + p_j$$ $\to$ respects 4-momentum conservation, violates on-shell condition

or $$\vec{\widetilde{J}}_{ij} = \vec{p}_i + \vec{p}_j,\ \widetilde{J}^0_{ij} = \sqrt{\vec{\widetilde{J}}^2_{ij} + m^2_{ij}}$$ $\to$ respects on-shell condition, violates energy conservation

("p-scheme")

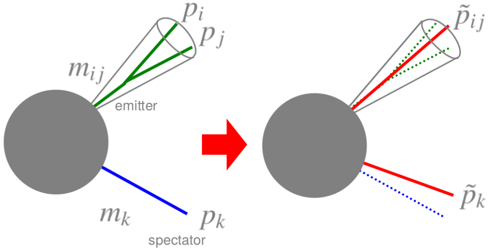
BackUp: $3 \to 2$ jet algorithm as an augmented $2 \to 1$ algorithm

- Use resolution criterium y_{ij} of the $2 \to 1$ algorithm to pick final state particle to be clustered with final state particle or beam ("emitter")
- Choose final state particle or beam as "spectator"
- 4 different types of mappings
  (emitter,spectator) = (final,final), (final,initial), (initial, initial), (initial,final)
- Respective clusterings for massless and massive particles already worked out in Catani-Seymour dipole subtraction method [Catani,Seymour '97], [Catani,Dittmaier,Seymour,Trocsanyi '02] (let's use those!)

BackUp: Modified clustering [Catani,Seymour '97], [Catani,Dittmaier,Seymour,Trocsanyi '02]

(example: massless final state clustering with final state spectator)

$$(p_i, p_j, p_k) \to \left(\tilde{p}_{ij} = p_i + p_j - \frac{y}{1-y} p_k,\ \tilde{p}_k = \frac{1}{1-y} p_k\right) \to (\widetilde{J}_{ij}, \widetilde{J}_k)$$



$$\widetilde{J}_{ij} + \widetilde{J}_k = p_i + p_j + p_k$$

and $\widetilde{J}_{ij}^2 = m_{ij}^2,\ \widetilde{J}_k^2 = m_k^2$

Phase space factorises: $dR_{n+1}(p_i, p_j, p_k) = dR_n(\widetilde{J}_{ij}, \widetilde{J}_k) dR_{\text{unres}}(\Phi)$

integrating over $dR_{\text{unres}}(\Phi = \{\phi, z, y\}) = \frac{\widetilde{J}_{ij} \cdot \widetilde{J}_k}{2(2\pi)^3}\, d\phi\, dz\, dy\, (1-y)$

generates all p_i, p_j, p_k with $(p_i, p_j, p_k) \stackrel{!}{\to} (\widetilde{J}_{ij}, \widetilde{J}_k)$

BackUp: Modified clustering: Generation of real phase space

(e.g. massless final-final clustering à la Catani-Seymour)

3→2 jet clustering: $(p_1, ..., p_{n+1}) \to (\widetilde{J}_1, ..., \widetilde{J}_n, \Phi)$

$$\widetilde{J}_{ij} = p_i + p_j - \frac{y}{1-y} p_k, \qquad \widetilde{J}_k = \frac{1}{1-y} p_k, \qquad \widetilde{J}_m = p_m, \; m \neq i, j, k$$

$$\Phi = \left\{ \phi, \; z = \frac{p_i \cdot p_k}{p_k \cdot (p_i + p_j)}, \; y = \frac{p_i \cdot p_j}{p_i \cdot p_j + p_k \cdot (p_i + p_j)} \right\}$$

Opposite direction required: $(\widetilde{J}_1, ..., \widetilde{J}_n, \Phi) \to (p_1, ..., p_{n+1})$

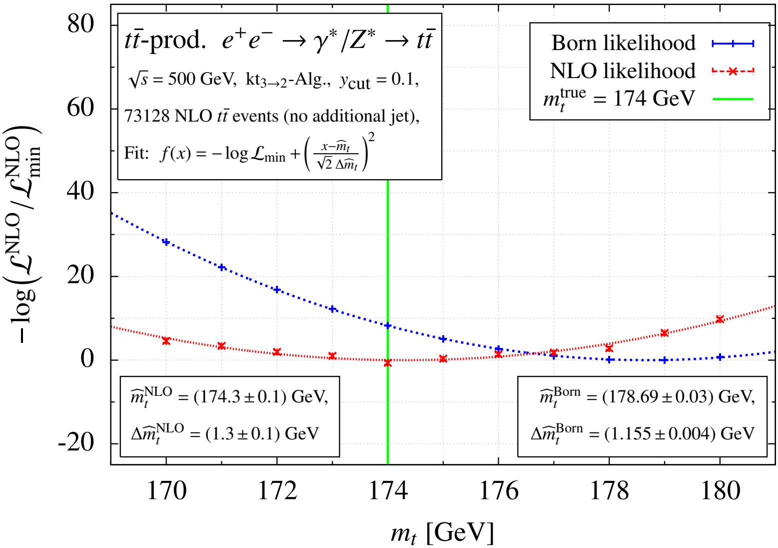
$$p_i + p_j = \widetilde{J}_{ij} + y \widetilde{J}_k, \qquad p_k = (1-y) \widetilde{J}_k, \qquad p_m = \widetilde{J}_m, \; m \neq i, j, k$$

$$\Phi = \left\{ \phi, \; z = \frac{p_i \cdot \widetilde{J}_k}{\widetilde{J}_{ij} \cdot \widetilde{J}_k}, \; y = \frac{p_i \cdot p_j}{\widetilde{J}_{ij} \cdot \widetilde{J}_k} \right\}$$

Phase space factorises: $dR_{n+1}(p_1, ..., p_{n+1}) = dR_n(\widetilde{J}_1, \ldots, \widetilde{J}_n) dR_{\text{unres}}(\Phi)$

$$\Longrightarrow \quad dR_{\text{unres}} \longrightarrow \left(p_1(\widetilde{J}_1, \ldots, \widetilde{J}_n, \Phi), \ldots, p_{n+1}(\widetilde{J}_1, \ldots, \widetilde{J}_n, \Phi) \right)$$

BackUp: MEM at NLO: top-quark mass extraction from $e^+e^- \to t\bar{t}$



NLO analysis recovers m_t^{true} but significant difference if MEM@LO is used!