

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]

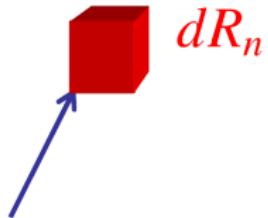
For the collision $A + B \rightarrow a_1(p_1) + a_2(p_2) + \cdots + a_n(p_n)$

the differential cross section

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

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

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



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

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

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

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

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]

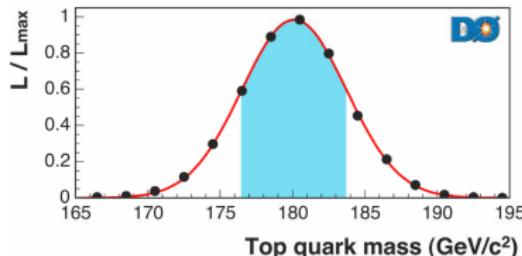
Extraction of model parameters Ω from data by maximizing a likelihood \propto differential cross section ($\propto |\mathcal{M}^{\text{LO}}|^2$):

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 $\hat{\Omega}$: $\mathcal{L}^{\text{LO}}(\hat{\Omega}) = \sup_{\Omega} \mathcal{L}^{\text{LO}}(\Omega)$

All information from event used \implies most efficient estimator!



e.g. top mass measurement at Tevatron
[D0: Nature 429, 638], [CDF: PRD 50, 2966
(1994)] based on $O(40)$ 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

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

separately IR divergent

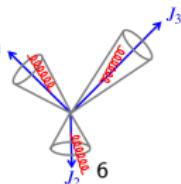
Jet Physics: observed final states are jets

partonic events → “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: $J_i = \tilde{J}_i(p_1, \dots, p_{n+1})$



Likelihood at NLO: 3 major obstacles

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

- 1) Born+virtual and real contribution separately IR divergent

NEED: Point-wise cancelation in jet phase space

→ both contributions must be evaluated for same jet momenta

Real contributions – formal definition

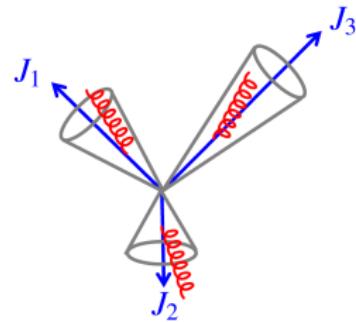
(one recombination: $J_i = \tilde{J}_i(p_1, \dots, p_{n+1})$, $i = 1, \dots, n$)

$$\frac{\sigma_{n+1 \rightarrow n\text{-jet}}^R(\Omega)}{dJ_1 \dots dJ_n} = \int dR_{n+1} \frac{d\sigma^R(\Omega)}{dR_{n+1}} \prod_{i=1}^n \delta(\tilde{J}_i(p_1, \dots, p_{n+1}) - J_i)$$

2) Integration over δ -function numerically not feasible!

NEED: factorisation of phase space

→ Integration trivial:



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

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

Born+virtual contributions

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

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

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

NEED: clustered jets obeying ‘Born kinematics’

→ on-shell condition and momentum conservation:

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

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

Proposal: $3 \rightarrow 2$ clustering

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



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

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

Modified clustering: Generation of real phase space

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

3→2 jet clustering:

$$(p_1, \dots, p_{n+1}) \rightarrow (\tilde{J}_1, \dots, \tilde{J}_n, \Phi)$$

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

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

Opposite direction required:

$$(\tilde{J}_1, \dots, \tilde{J}_n, \Phi) \rightarrow (p_1, \dots, p_{n+1})$$

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

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

Phase space factorises:

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

$$\implies dR_{\text{unres}} \rightarrow \left(p_1(\tilde{J}_1, \dots, \tilde{J}_n, \Phi), \dots, p_{n+1}(\tilde{J}_1, \dots, \tilde{J}_n, \Phi) \right)$$

Jet event weight at NLO

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

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

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 separately the exclusive s- or t-channel production of single top quarks in association with a light jet at the LHC

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

Veto on additional jet emission, no resolved additional jet!

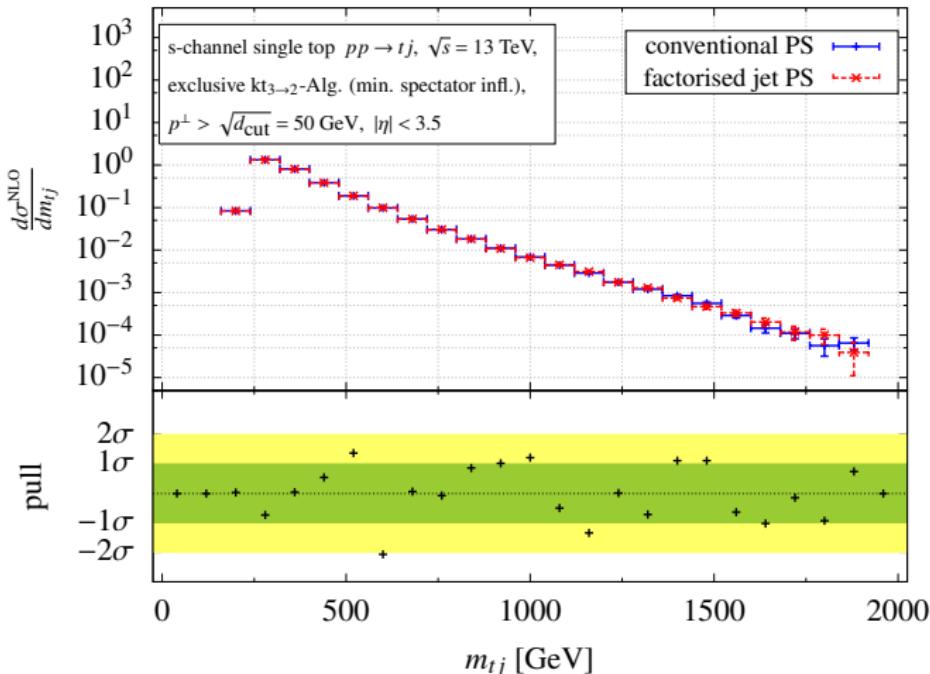
Note: top decay not included, tops are treated as tagged top jets

To Check:

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

Validation 1: Phase space generation (e.g. s-channel)

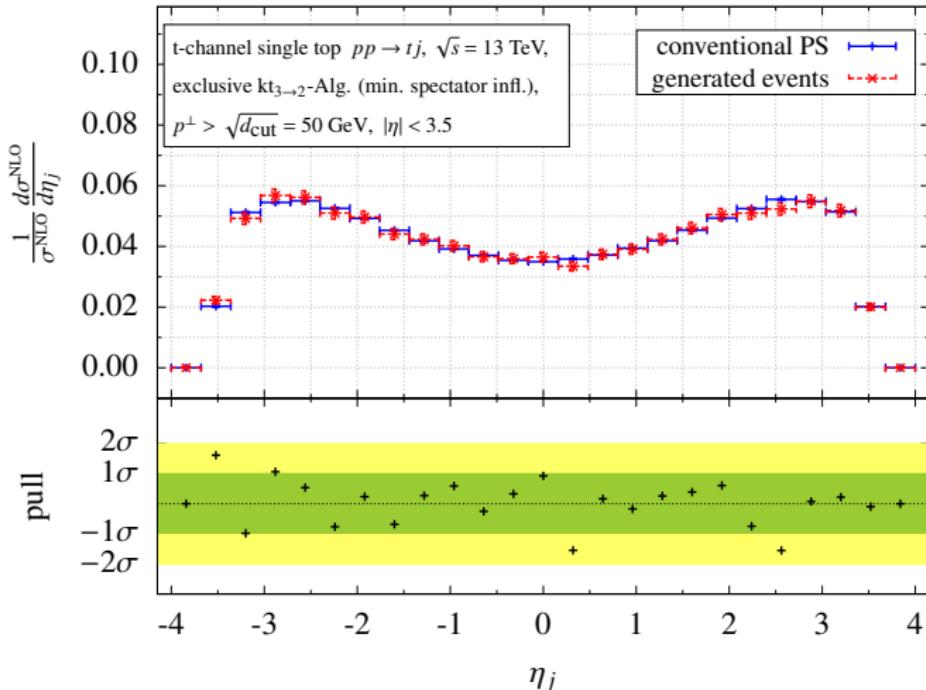
Calculate jet distributions in NLO accuracy using conventional approach (parton level MC + $3 \rightarrow 2$ jet alg.) and compare with distributions obtained from $\frac{d\sigma_{n\text{-jet}}^{\text{NLO}}(\Omega)}{dJ_1\dots dJ_n}$ with factorised jet phase space



Validation 2: Unweighted events (e.g. t-channel)

Fill histograms with unweighted events generated according to

$\rho = \frac{d\sigma_{n\text{-jet}}^{\text{NLO}}(\Omega)}{dJ_1 \dots dJ_n}$ and compare with jet distributions in NLO accuracy obtained from conventional approach (parton MC + 3 → 2 clus.)



Application: Matrix Element Method at NLO

(examples: $p + p \rightarrow t + j$ via s- or t-channel @ NLO QCD)

Toy experiment: Generate sample of N unweighted NLO tj events

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

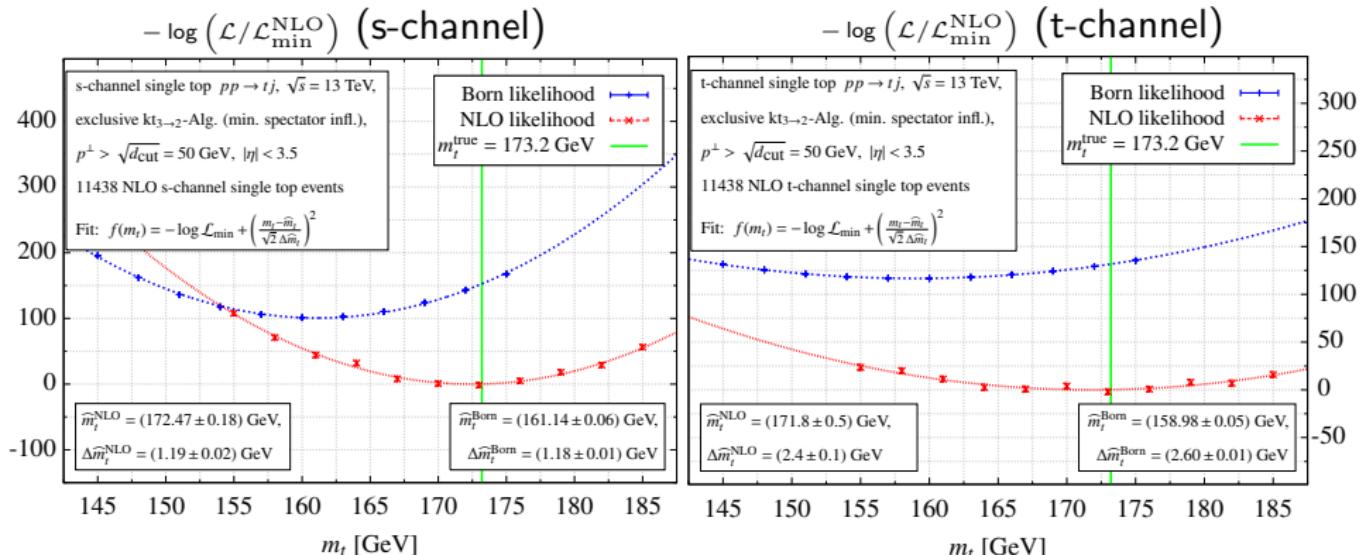
NLO likelihood function for event sample

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

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

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

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



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

- ▶ $\approx 10k$ events allow already precise mass determination (s-channel more precise!)
- ▶ Mass definition unambiguously defined through NLO calculation
- ▶ Large shift observed in LO analysis would require significant calibration with related uncertainties

Conclusion

$3 \rightarrow 2$ 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!**
 - ▶ Renormalization scheme well-defined in MEM at NLO
(allows for example unambiguous measurement of top-quark mass)

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

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

1. Resolution:

e.g.

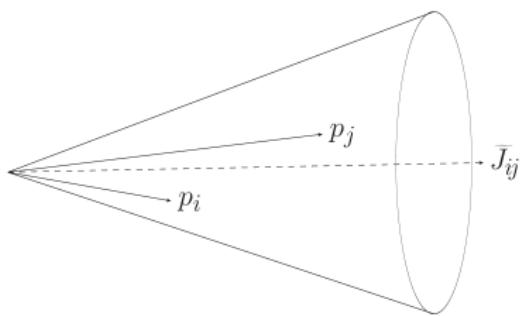
$$y_{ij} = \min(p_i^{\perp 2p}, p_j^{\perp 2p}) \frac{\Delta_{ij}}{R^2}, \quad \Delta_{ij} = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$$

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

2. Recombination/Clustering:

If $y_{ij} < y_{\text{cut}}$:

p_i, p_j are clustered to jet \tilde{J}_{ij}



e.g.

$$\tilde{J}_{ij} = p_i + p_j$$

→ respects 4-momentum conservation,
violates on-shell condition

or

$$\tilde{J}_{ij} = \vec{p}_i + \vec{p}_j, \quad \tilde{J}_{ij}^0 = \sqrt{\tilde{J}_{ij}^2 + m_{ij}^2}$$

→ respects on-shell condition,
violates energy conservation
("p-scheme")

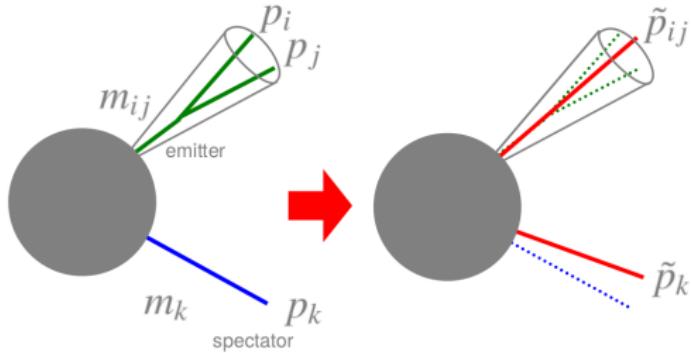
BackUp: $3 \rightarrow 2$ jet algorithm as an augmented $2 \rightarrow 1$ algorithm

- ▶ Use resolution criterium y_{ij} of the $2 \rightarrow 1$ 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
 $(\text{emitter}, \text{spectator}) = (\text{final}, \text{final}), (\text{final}, \text{initial}), (\text{initial}, \text{initial}), (\text{initial}, \text{final})$
- ▶ 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!)

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

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

$$(\mathbf{p}_i, \mathbf{p}_j, \mathbf{p}_k) \rightarrow (\tilde{\mathbf{p}}_{ij} = \mathbf{p}_i + \mathbf{p}_j - \frac{y}{1-y} \mathbf{p}_k, \tilde{\mathbf{p}}_k = \frac{1}{1-y} \mathbf{p}_k) \rightarrow (\tilde{\mathbf{J}}_{ij}, \tilde{\mathbf{J}}_k)$$



$$\tilde{\mathbf{J}}_{ij} + \tilde{\mathbf{J}}_k = \mathbf{p}_i + \mathbf{p}_j + \mathbf{p}_k$$

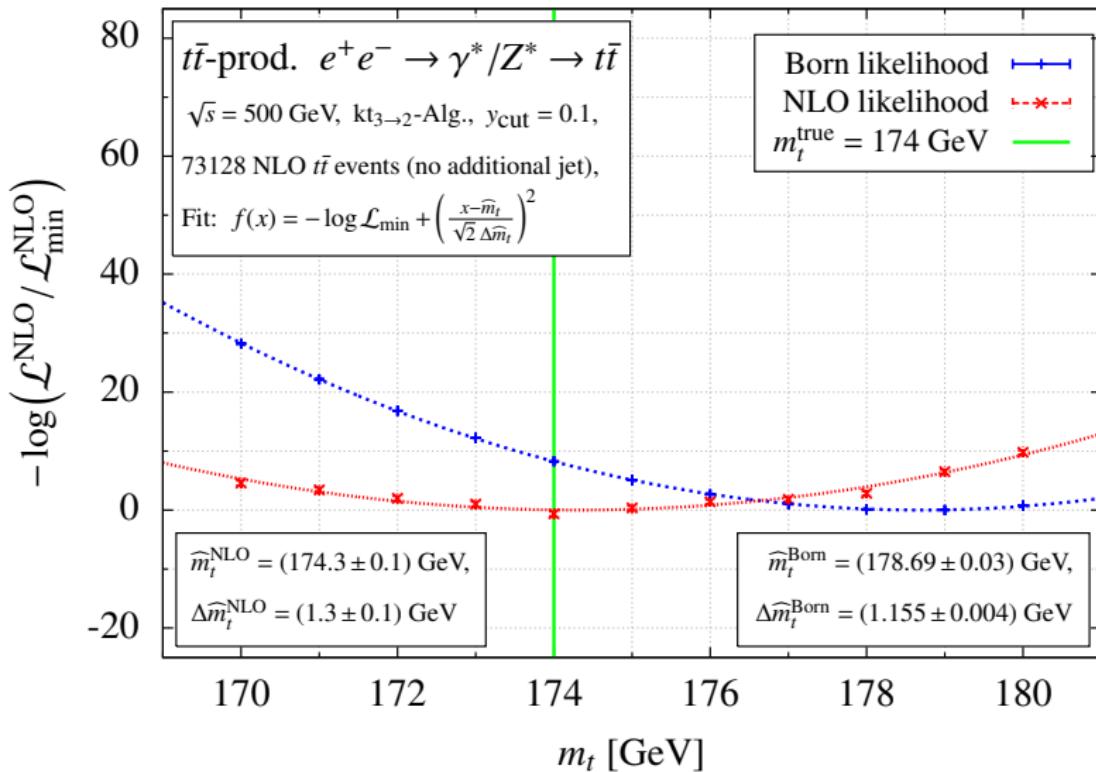
$$\text{and } \tilde{\mathbf{J}}_{ij}^2 = m_{ij}^2, \tilde{\mathbf{J}}_k^2 = m_k^2$$

Phase space factorises:

$$dR_{n+1}(\mathbf{p}_i, \mathbf{p}_j, \mathbf{p}_k) = dR_n(\tilde{\mathbf{J}}_{ij}, \tilde{\mathbf{J}}_k) dR_{\text{unres}}(\Phi)$$

integrating over $dR_{\text{unres}}(\Phi = \{\phi, z, y\}) = \frac{\tilde{\mathbf{J}}_{ij} \cdot \tilde{\mathbf{J}}_k}{2(2\pi)^3} d\phi dz dy (1-y)$
generates all $\mathbf{p}_i, \mathbf{p}_j, \mathbf{p}_k$ with $(\mathbf{p}_i, \mathbf{p}_j, \mathbf{p}_k) \xrightarrow{!} (\tilde{\mathbf{J}}_{ij}, \tilde{\mathbf{J}}_k)$

MEM at NLO: top-quark mass extraction via parabola fit ($t\bar{t}$ -prod.)



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