# <span id="page-0-0"></span>Reconstruction of Semi-Leptonic Top Anti-top Pair Production with Deep Learning

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- **Heaviest known fundamental** particle  $(m_t \approx 172.5 \text{GeV})$ 
	- $\blacktriangleright$  First place a new particle could be observed, particularly if it couples to mass
- Extremely short lifetime  $({\sim 5 \times 10^{-25}} s)$ 
	- $\triangleright$  Decays semi-weakly (t→Wb), before hadronization can occur
	- $\triangleright$  Only place to study properties of a "bare" quark
- Precise measurements enhance our sensitivity to possible beyond SM effects



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#### Background Top-Antitop Pair Production (ttbar)



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- $\bullet$  *W* decays hadronically with ∼70% branching ratio and leptonically with ∼30%
- Focus on semi-leptonic decays (∼30% branching ratio)



## **Objective**

#### Algorithms:

- **Currently well-established and** widely used
- Determines the best permutation of detector-level jets to particle-level jets by:
	- Employing kinematic constraints
	- $\blacktriangleright$  Sometimes aiming to maximize a likelihood or minimize a chi-squared
	- $\blacktriangleright$  Assuming a four-jet system
- Reconstruct the top and anti-top 4-vectors from this permutation
- E.g. Kinematic Likelihood Fitter (KLFitter), TtresChi2 (Chi2), and PseudoTop (PT)

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#### Deep Neural Networks:

- Determines weights and functions (through training) that will map the typical detector-level objects to the expected parton-level objects
- Could be more precise, more efficient, and less model dependant
- 3 slight variations we're working on: TRecNet, TRecNet+ttbar, and TRecNet+ttbar+JetPretrain

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#### Goal:

Design a deep neural network to reconstruct  $t\bar{t}$  better than current algorithms!

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- Detector response simulated by Geant4 (detector/reco-level)
	- I Jets:  $(p_{\tau}, \eta, \phi, E)$ ,  $b_{\tau a\sigma}$
	-
	- **I** Lepton:  $(p_{T_{lep}}, \eta_{lep}, \phi_{lep})$ <br>**I** Missing Transverse Energy:  $E_T, \phi_{E_T}$

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#### "Predictions"/"Reco Output"

- Previous fitting algorithms vs. Top Reconstruction Neural Networks
	- $\blacktriangleright$  Hadronic Top:
		- $(p_{\mathcal{T}_{t_h}}, \eta_{t_h}, \phi_{t_h}, m_{t_h})$
	- **Leptonic Top:**  $(p_{\tau_{t_i}}, \eta_{t_i}, \phi_{t_i}, m_{t_i})$
	- In ttbar:  $(p_{\tau_{t\bar{t}}}, \eta_{t\bar{t}}, \phi_{t\bar{t}}, m_{t\bar{t}})$

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### **Architectures**

Model #1: TRecNet



- $\bullet$  Input: pre-processed jets  $(6)$  and other (lep, met) variables
- First attempts to learn which jets are relevant to  $t\bar{t}$  process
- Predicts leptonic 4-vectors  $(t_l, W_l)$ first, since their classification is easier, and then uses this information to help inform predictions on the hadronic 4-vectors  $(t_h, W_h)$

### **Architectures**

Model #2: TRecNet+ttbar



- $\bullet$  Input: pre-processed jets  $(6)$  and other (lep, met) variables
- First attempts to learn which jets are relevant to  $t\bar{t}$  process
- Predicts leptonic 4-vectors  $(t_l, W_l)$ first, since their classification is easier, and then uses this information to help inform predictions on the hadronic 4-vectors ( $t_h$ ,  $W_h$ ) and  $t\bar{t}$  variables

### Architectures

#### Model #3: TRecNet+ttbar+JetPretrain



## Hadronic Top Results

#### Response Matrices



TRecNet+ttbar+JP is more diagonal than KLFitter  $\implies$  improved precision!

## Hadronic Top Results

Resolutions and Residuals



TRecNet+ttbar+JP is more narrow and less skewed than KLFitter  $\implies$  improved precision!

# Hadronic Top Results

 $p_T$  Resolutions at Different Momenta



- Neural networks completely remove the extra bump at high  $p_T!$ 
	- $\blacktriangleright$  Jets become more difficult to resolve at high  $p_T$  (events occur with more or less than jets)
	- $\blacktriangleright$  Neural networks use all jet info, but algorithms use only best permutation of 4 out of 6



### Leptonic Top Results

 $p_T$  Resolutions at Different Momenta



- No extra bump at high  $p<sub>T</sub>$  on leptonic side!
	- $\triangleright$  Only one b-jet to resolve
- But neural networks still have better resolution over range of  $p_T$



## $t\bar{t}$  Results

#### $m_{t\bar{t}}$  Resolutions at Different Momenta



- Neural networks improve upon reconstruction of mass of  $t\bar{t}$  system
- Adding  $t\bar{t}$  variables to the neural network helped improve precision for  $m_{t\bar{t}}$



- Advantages of the neural networks:
	- $\triangleright$  Appear to improve upon results of from likelihood-based algorithms
	- $\blacktriangleright$  Perform more efficiently
	- Flexibility to handle events with more or less than 4 jets (and thus performs better than previous methods in the boosted topology)
- Future possibilities and outlook:
	- $\triangleright$  Widen model to consider more jets (e.g. 7 or 8)
	- Unfreeze the jet pre-training weights to fine-tune TRecNet+ttbar+JetPretrain model
	- Measure model dependency
	- Include systematics to obtain a more quantitative measure of the neural network's improvement

### Thanks to . . .

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- Tao Zhang
- The ATLAS Collaboration
- NSERC



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#### Background Parton-level vs. Particle-level vs. Detector-level



- Parton-level: Only includes perturbative matrix element calculations
	- $\blacktriangleright$  E.g. hard scattering events generated by POWHEG
- **Particle-level**: Includes both perturbative and non-perturbative matrix element calculations
	- E.g. parton shower/hadronization components handled by  $Pythia8$
- **Q.** Detector-level: What we measure
	- $\blacktriangleright$  E.g. data or simulated data from Geant4
	- $\blacktriangleright$  The top reconstruction algorithms we're using are at this level





#### **Increasing Transverse Momentum**





# Reconstruction Algorithms

Kinematic Likelihood Fitter (KLFitter)

Best permutation of jets determined using kinematics and likelihood calculations:

$$
\mathcal{L} = \beta(m_{q_1q_2q_3}|m_t, \Gamma_t) \cdot \beta(m_{q_1q_2}|m_W, \Gamma_W) \cdot \beta(m_{q_4\ell_{\nu}}|m_t, \Gamma_t) \cdot \beta(m_{\ell_{\nu}}|m_W, \Gamma_W) \cdot \prod_{i=1}^4 W_{\text{jet}}(E_{\text{jet},i}^{\text{meas}}|E_{\ell}) \cdot W_{\ell}(E_{\ell}^{\text{meas}}|E_{\ell}) \cdot W_{\text{miss}}(E_{\text{x}}^{\text{miss}}|p_X^{\nu}) \cdot W_{\text{miss}}(E_{\text{y}}^{\text{miss}}|p_Y^{\nu})
$$

- **►** Breit-Wigner terms  $(B)$   $\rightarrow$  quantify agreement of known masses with measured decay products
- **If Transfer function terms**  $(W) \rightarrow$  quantify agreement of fitted energies and missing transverse momentum components with measured values (detector-specific and representative of experimental resolutions)
- Likelihood calculated for each possible association of detector-level jets to particle-level jets, where  $m_t$ ,  $E_{jet,i}$ ,  $E_\ell$ , and  $\vec{p}_\nu$  are treated as parameters varied to maximize the likelihood
- Retain permutation with highest likelihood (called the "best permutation")
- $\bullet$  Can make cuts on log  $\mathcal L$  to separate well- and poorly-reconstructed events

### Reconstruction Algorithms

Breit-Wigner Functions and Transfer Functions

#### Breit-Wigner Function:

$$
\mathcal{B}(E|M,\Gamma)=\frac{k}{(E^2-M^2)^2+M^2\Gamma^2}
$$

where,

$$
k = \frac{2\sqrt{2}M\Gamma\gamma}{\pi\sqrt{M^2 + \gamma}}
$$

and

$$
\gamma = \sqrt{M^2(M^2+\Gamma^2)}
$$

Transfer Function:

$$
W(E) = \left. \frac{Y(E)}{X(E)} \right|_{initial conditions = 0}
$$

where,

$$
Y =
$$
 laplace transform of output

and

 $X =$  laplace transform of input

### Reconstruction Algorithms TtresChi2

• Best permutation of jets determined using kinematics and chi-squared calculation:

$$
\chi^2 = \left[\frac{m_{jj} - m_{W_h}}{\sigma_{W_h}}\right]^2 + \left[\frac{m_{jjb} - m_{jj} - m_{t_h - W_h}}{\sigma_{t_h - W_h}}\right]^2 + \left[\frac{m_{b\ell\nu} - m_{t_\ell}}{\sigma_{t_\ell}}\right]^2
$$

$$
+ \left[\frac{(p_{\tau, jjb} - p_{\tau, b\ell\nu}) - (p_{\tau, t_h} - p_{\tau, t_\ell})}{\sigma_{p_{\tau, t_h} - p_{\tau, t_\ell}}}\right]^2
$$

- Constraint on dijet mass to form hadronic W
- $\triangleright$  Constraint on three jets to form hadronic top contribution of hadronic W subtracted to decouple first two terms, since  $m_{ii}$  and  $m_{iib}$  are highly correlated
- $\triangleright$  Constraint on remaining jet, lepton and neutrino (met) to form leptonic top
- **In** Constraint on transverse momentum balance between the two top quarks ( $p_T$ ) should be similar, as expected in a resonance)
- Expected values of parameters  $m_{W_h}, m_{t_h-W_h}, m_{t_\ell}, p_{T,t_h} p_{T,t_\ell}$  as well as their uncertainties  $\sigma_{W_h}$ ,  $\sigma_{t_h-W_h}$ ,  $\sigma_{t_\ell}$ ,  $\sigma_{p_{T,t_h}-p_{T,t_\ell}}$  are obtained from the simulated Z' events by matching reconstructed objects to truth partons
- Can make cuts on  $\chi^2$  to separate well- and poorly-reconstructed events

## Reconstruction Algorithms

PseudoTop

- Uses lepton, jet, and missing transverse energy measurements, as well as known mass of W boson
- $\bullet$  Only two b-tagged jets with highest  $p<sub>T</sub>$  are considered part of the system

#### Algorithm:

- 1. Reconstructs neutrino 4-momentum
	- $\blacktriangleright$  p<sub>x</sub> and p<sub>v</sub> obtaining from met
	- $\blacktriangleright$   $p_z$  calculated by conservation of momentum
- 2. Reconstruct leptonic W from lepton and neutrino
- 3. Reconstruct leptonic top from leptonic W and b-tagged jet closest in  $\Delta R = \sqrt{\Delta \phi^2 + \Delta \eta^2}$  to lepton
- 4. Reconstruct hadronic W from the two light-flavoured jets whose invariant mass is closest to mass of W boson
- 5. Reconstruct hadronic top from hadronic W and remaining b-tagged jet

# Neural Networks

Pre-Processing Trials

- Model performance was evaluated on validation data using mean-squared error  $(mse = \langle truth - prediction \rangle^2)$
- Mean/variance scaling  $\left(x_i^{\text{scaled}} = \frac{x_i \bar{x}}{\sigma(x)}\right)$  vs. mean/max scaling  $\left(x_i^{\text{scaled}} = \frac{x_i \bar{x}}{\max(|x|)}\right)$
- $\blacktriangleright$  Standard procedure for allowing the network to focus on each variable equally **Encoding**  $\phi$  with sin( $\phi$ ) and cos( $\phi$ ) vs. triangle wave of sin( $\phi$ ) and cos( $\phi$ ) vs.  $p_x$  and  $p_y$ 
	- $\triangleright$  Former two produced edge peaks that the network has trouble predicting
- Boxcox transformation of  $p_T$   $\left(p_T = \frac{p_T^2 1}{\lambda}\right)$  vs.  $\left(p_x, p_y\right)$  vs.  $p_T$ 
	- Boxcox did better on average, but poorly reconstructed low  $p_T$  events
	- $p_x$  and  $p_y$  difficult to predict, resulting in large compounding error for  $p_{\overline{1}}$



Pre-Processing Procedure



#### Final procedure:

- Encode  $\phi_{\tau}$  with sin( $\phi_{\tau}$ ), cos( $\phi_{\tau}$ ) and all other  $\phi$  with  $p_{x}$  and  $p_{y}$
- All inputs (except  $b_{tag}$ ) undergo mean/max scaling
- Model predicts  $(p_{\tau}, p_{x}, p_{y}, \eta, m)$  for top quarks and Ws in mean/max scale
- Invert mean/max scaling and  $\phi$  encoding to return predictions to original scale

## Training Features

Loss Function



- **Loss function: quantifies error for current state of model want to change** weights to reduce this loss on next evaluation
- E.g. Binary cross entropy loss function:
	- $\triangleright$  Default loss function for binary classification problems
	- $\triangleright$  Calculates a score between [0, 1] that summarizes average difference between true and predicted, and tries to minimize this score through training
	- $\blacktriangleright$  Used for jet-pretraining model
- E.g. Mean absolute error (MAE) loss function:
	- $\blacktriangleright$  Calculates average absolute difference between true and predicted
	- Often most appropriate in regression problems where target distributions are mostly Gaussian but may have outliers, since it punishes larger mistakes from outliers less harshly than, for example, MSE
	- I Used for TRecNet models

**Optimizer** 



- **Optimizer:** Method or algorithm by which we change weights of network in order to locate minima of loss function
- E.g. Stochastic gradient descent (SGD):
	- $\blacktriangleright$  Estimates gradient of loss function with randomly selected subset of data
	- $\triangleright$  Uses estimated gradient to choose direction to move in search space (with step size determined by learning rate)
- E.g. Adam:
	- $\triangleright$  Particular type of SGD where learning rate is non-static individual adaptive learning rates are computed for different parameters from estimates of first and second moments of the gradients
	- Used for TRecNet models and jet pre-training

Learning Rate



- **Learning rate: Step size that optimization algorithm uses at each iteration to** move towards the minima
	- $\blacktriangleright$  Parameter that can be fine-tuned to optimize model performance
	- Can modulate how learning rate changes over training

#### E.g. Polynomial decay rate:

- Begin with larger learning rate  $\rightarrow$  take larger steps and train faster
- Gradually move to smaller learning rate  $\rightarrow$  take smaller steps and fine-tune optimization
- ▶ Used for TRecNet and jet pre-training (which slight differences)

# Training Features

Activation Function



- Activation function: Defines how weighted sum of input to a node is transformed to output from that node
	- Allows network to handle more complex patterns and non-linear problems  $\rightarrow$ large impact on capability and performance of network
	- $\blacktriangleright$  Can have different activation functions for different layers
- E.g. ReLU (Rectified Linear Function):  $max(0, x)$ 
	- **Popular for hidden layers**
	- Easy to implement, quick, computationally light, and less susceptible to the vanishing gradient problem
	- $\blacktriangleright$  Used for almost all of our hidden layers
- E.g. Sigmoid (or Logistic) Function:  $1/(1 + e^{-x})$ 
	- **I** Popular for hidden and output layers
	- Use for output from jet classifier

Regularization



- Regularization: Techniques to prevent over- or under-fitting
- $\bullet$  E.g. Early stopping (monitor=val\_loss,patience=10):
	- $\triangleright$  End training after 10 epochs of no improvement in loss for the validation data
	- $\blacktriangleright$  Used for TRecNet and jet pre-training



#### **Events: 33 million**

- $\blacktriangleright$  70% to training
- $\blacktriangleright$  15% to validation
- $\blacktriangleright$  15% to testing
- **Batch Size: Number of events processed before model is updated** 
	- I Used batch size  $= 1000$  for all models

# Neural Networks

**Training** 



# Jet Pre-Training

Jet Matching Algorithm

- For a match (matched jet tag  $= 1$ ) between detector-level jet and parton-level decay product:
	- $\blacktriangleright$  Require jet has the same flavour as the decay product
	- Require  $\Delta R = \sqrt{\Delta \phi^2 + \Delta \eta^2} < 0.4$
- 85% of detector-level jets were matched to a parton-level decay product, with  $\sim$ 100% having a reasonable fractional  $\Delta p_T$



### <span id="page-43-0"></span>Jet Pre-Training

Jet Pre-Training Response Matrices

