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Hadronic recoil regression with deep neural networks

In the recent years a significant progress was achieved in the field of big datasets analysis. There is a number of principles available for solving a wide variety of tasks. In this thesis a deep neural network (DNN) was used for the regression of the 2-component hadronic recoil vector.

1.1 Deep neural networks

Normally a machine learning problem has a number of ingredients: a dataset $\mathbf{X}$, a set of parameters θ, a model $g(\theta)$ and a loss function $C(\mathbf{X})$ that tells us how well the model $g(\theta)$ describes the dataset. Finding the values of θ that would minimize the loss function we fit the model.

1.1.1 Gradient descent optimization

One of the most powerful and used class of methods in minimizing the loss function is called the *gradient descent*, [1] especially its sub-class, the stochastic gradient descent (SGD) [2], [3]. One of its modifications called ADAM [4] was used as an optimization algorithm in the work presented in this thesis.

Let's assume that a loss function $E(\theta)$ may be estimated as a sum over n data points:

$$E(\theta) = \sum_{i=1}^{n} e_i(x_i, \theta), \tag{1.1}$$

where x_i is a data point and e_i is an estimate of performance. In the simplest case of the gradient descent (GD) algorithm we start looking for the values of parameters θ such that the sum of functions $\sum_{i=1}^{n} e_i$ is minimal. We start with a certain value θ_0 and then iteratively perform the following:

$$
\begin{aligned}
v_t &= \eta_t \, \nabla_\theta \, E(\theta_t), \\
\theta_{t+1} &= \theta_t - v_t,
\end{aligned}
\tag{1.2}
$$

where $\nabla_\theta E(\theta_t)$ is the gradient of $E(\theta)$ with respect to θ; factor η_t is called the *learning rate* and defines the length of the step in the direction of θ performed with every iteration. Balancing learning rate is very important for learning process and convergence. A value too low can make the convergence

"stuck" in a local minimum, it also increases the number of iterations. Picking a very high learning rate we risk to miss the minimum so the algorithm would never converge to a minimum. Also, if the number of data points n is high, calculating the gradient is a costly task in terms of CPU time.

Some of the problems accompanying the use of GD are dealt with by using its modification - the SGD. The idea is the following: instead of using all the available data points n at each iteration of the GD, we split the data into k *minibatches*, each having M data points, such that $k = n/M$. Normally the size of the batch is few hundreds of data points, to provide a certain degree of variance and incorporating stochasticity. The transition to SGD algorithm is done in the following way:

$$\nabla_\theta E(\theta) = \sum_{i=1}^{n} \nabla_\theta e_i(x_i, \theta) \to \sum_{i \in B_l} \nabla_\theta e_i(x_i, \theta), \tag{1.3}$$

where B_l is a set of data points belonging to a minibatch $l \in 1, ..., n/M$. Now every next iteration of θ parameters update is performed over a different batch, consecutively running over all the batches:

$$\begin{aligned} \nabla_\theta E^{EM}(\theta) &= \sum_{i \in B_l} \nabla_\theta e_i(x_i, \theta), \\ v_t &= \eta_t \nabla_\theta E^{EM}(\theta_t), \\ \theta_{t+1} &= \theta_t - v_t. \end{aligned} \tag{1.4}$$

A full iteration over all the n/M batches is called an *epoch*. Now stochasticity prevents the gradient algorithm from getting stuck in a local minimum. Also computing the gradient over fewer data point notably decreases the CPU time spent.

The algorithm may be further improved, adding a "memory", that is to say making every next step t dependent on the direction of the previous step $t - 1$:

$$\begin{aligned} v_t &= \gamma v_{t-1} \eta_t \nabla_\theta E^{EM}(\theta_t), \\ \theta_{t+1} &= \theta_t - v_t. \end{aligned} \tag{1.5}$$

Because of an analogy from physics the parameter γ is called a *momentum*, having $0 \le \gamma \le 1$ [5], [6]. This parameter provides a certain "inertia" in the change of the direction of the gradient descent. Introduction of the momentum helps for quicker convergence in the case of a slow but steady change of a certain parameter during the gradient descent.

The convergence of the GD may be significantly improved if the learning rate could be different in different directions, depending on the landscape of the parameter space θ: the steeper the gradient in a certain direction - the smaller the corresponding step. The optimal step could be estimated by obtaining the *Hessian matrix* in the vicinity of a point θ_0, providing a description of the local curvature in a multidimensional space. Although calculating Hessian matrix is complicated and slow-converging process [7]. However, a number of methods use the second moment of the gradient to efficiently estimate the optimal learning rate. One of such methods is called ADAM (ADAptive Momentum) [4],

84 its iterative relations are the following:

$$
\begin{aligned}
g_t &= \nabla_\theta E(\theta_t) \\
m_t &= \beta_1 m_{t-1} + (1 - \beta_1) g_t \\
s_t &= \beta_2 s_{t-1} + (1 - \beta_2) g_t^2 \\
\hat{m}_t &= \frac{m_t}{1 - (\beta_1)^t} \\
\hat{s}_t &= \frac{s_t}{1 - (\beta_2)^t} \\
\theta_{t+1} &= \theta_t - \eta_t \frac{\hat{m}_t}{\sqrt{\hat{s}_t} + \epsilon}.
\end{aligned}
\tag{1.6}
$$

85 Here the parameters β_1 and β_2 set the memory lifetime for the first and second moment; η is the learning
86 rate and ϵ is a small regularization constant keeping the denominators from vanishing. Like in other
87 cases of the SGD here the iterations are performed batch-wise. Parameter s_t is linked to the variance of
88 the gradient size. This basically means that the learning rate is proportional to the first momentum of
89 the gradient and inverse proportional to its standard deviation.

1.1.2 DNN structure and training

91 A neural network is composed of single neurons, also called nodes, arranged in layers. The first layer is
92 called the input layer, the last one is called the output layer; all the layers in between are named hidden
93 layers (see Fig. 11).
94 A single node i takes a vector of k input features $\mathbf{x} = (x_1, x_2, ..., x_k)$ and produces a scalar input $a_i(\mathbf{x})$.
95 Function a_i may have a different form, although it normally can be decomposed into two steps. The
96 first step is a linear transformation of the inputs into a scalar value assigning each input a weight:

$$
z^i = w_k^i \cdot x_k + b^i,
\tag{1.7}
$$

97 where $\mathbf{w}^i = (w_1^i, w_2^i, ..., w_k^i)$ is a set of k weights assigned to corresponding inputs. The weights $\mathbf{w}^i$ are
98 specific to a neuron i, as well as the scalar bias b^i. The next step is where the non-linear function σ_i
99 comes into play: we can express the output function $a_i(\mathbf{x})$ as follows:

$$
a_i(\mathbf{x}) = \sigma_i(z^i).
\tag{1.8}
$$

100 There exists a number of options for the non-linear function σ; in current thesis a tanh is used. When
101 the neurons are arranged in layers in a feed-forward neural network - the outputs from neurons of
102 the previous layer serve as inputs for the succeeding layers neurons. The universal approximation
103 theorem states, that a neural network with a single hidden layer can approximate any continuous
104 multiparametric function with arbitrary accuracy [8], [9]. However, in practice it is easier to reach the
105 possible precision having more hidden layers.
106 So in terms of a DNN fitting the model means tuning the weights and biases $(\mathbf{w}^i, b^i)$ in such a way
107 that a loss function applied to the new dataset would be minimal. It is reached through iterative
108 process called *training*, that involves the GD with an algorithm called *backpropagation* [10]. The
109 backpropagation algorithm allows to calculate the gradients and adjust the corresponding parameters

110 in a very computation-efficient way.

Let us assume that there are L layers in the network $l = 1, ..., L$, that w_{jk}^l and b_j^l are the weight of an
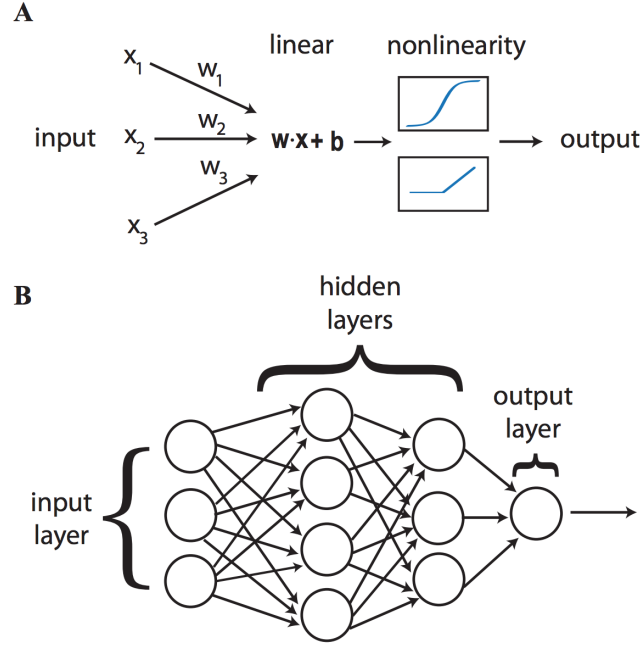
A

B

Figure 11: A: The nodes perform a linear transformation of the inputs, then apply a non-linear activation function. B: The architecture of a deep neural network: neurons are arranged into layers [11].

111
112 input parameter k and the bias for node k in layer l respectively. The layered structure of the neural
113 network ensures that the inputs for the nodes in layer l depend only on the outputs of the nodes from
114 layer $l-1$, hence:

$$a_j^l = \sigma\left(\sum_k w_{jk}^l a_k^{l-1} + b_j^l\right) = \sigma(z_j^l), \qquad (1.9)$$

115 where the linear weighted sum is denoted as:

$$\sigma(z_j^l) = \sum_k w_{jk}^l a_k^{l-1} + b_j^l. \qquad (1.10)$$

116 The cost function E is computed from the output of the neural network, so it directly depends only on
117 the values of a_j^L. Let us define the error Δ_j^L of the j-th node in the output (L-th) layer as a change in the
118 cost function with respect to the weighted output of the last layer:

$$\Delta_j^L = \frac{\partial E}{\partial z_j^L}. \qquad (1.11)$$

119 At the same time the loss depends indirectly on all the preceding layers, so keeping in mind eq. 1.9 we
120 can define the error of an arbitrary node j in arbitrary layer l as the change in the cost function E with
121 respect to the weighted input z_j^l:

$$\Delta_j^l = \frac{\partial E}{\partial z_j^l} = \frac{\partial E}{\partial a_j^l}\sigma'(z_j^l), \qquad (1.12)$$

122 where $\sigma'(z_j^l)$ is the derivative of the non-linear activation function σ with respect to its input at z_j^l. But
123 on the other hand we can also interpret the error function Δ_j^L in terms of bias partial derivatives:

$$\Delta_j^l = \frac{\partial E}{\partial z_j^l} = \frac{\partial E}{\partial b_j^l} \frac{\partial b_j^l}{\partial z_j^l} = \frac{\partial E}{\partial b_j^l} \cdot \mathbf{1}. \tag{1.13}$$

124 So starting from the output layer we can compute the error in any layer l, provided we know it for the
125 subsequent layer $l + 1$:

$$\begin{aligned} \Delta_j^l = \frac{\partial E}{\partial z_j^l} = \sum_k \frac{\partial E}{\partial z_j^{l+1}} \frac{\partial z_j^{l+1}}{\partial z_j^l} = \\ = \sum_k \Delta_j^l \frac{\partial z_j^{l+1}}{\partial z_j^l} \left(\sum_k \Delta_j^l w_{kj}^{l+1} \right) \sigma'(z_j^l). \end{aligned} \tag{1.14}$$

126 And finally we can get the gradient of the cost function E with respect to a weight of an arbitrary
127 neuron:

$$\frac{\partial E}{\partial w_{jk}^l} = \frac{\partial E}{\partial z_j^l} \frac{\partial z_j^l}{\partial w_{jk}^l} = \Delta_j^l a_k^{l-1}. \tag{1.15}$$

128 Using these four equations (1.11, 1.13, 1.14, 1.15) it is possible to "backpropagate" the error back from
129 the output layer and once we can compute the gradient - we know how we should tune the weights and
130 biases in order to minimize the loss function.

131 1.1.3 Batch normalization

132 Batch normalization is a regularization scheme that helps to improve the speed and stability of the
133 DNN training. The main idea behind the method is to prevent an *internal covariant shift* - a change in
134 the distribution of network activations due to the change in network parameters during training by
135 means of normalization of the parameters transferred from layer l to layer $l + 1$ [12]. So let us consider
136 a layer l that has d inputs $\mathbf{x} = (x^1, x^2, ..., x^d)$, then for every x^k we perform the following transformation:

$$\hat{x}^k = \frac{x^k - E[x^k]}{\sqrt{Var[x^k]}}, \tag{1.16}$$

137 where $E[x^k]$ and $Var[x^k]$ are the expectation and variance of the parameter x, calculated over the
138 training dataset, respectively. Although we have to be sure that we preserve the non-linearity of the
139 activation function output. In order to do this the two additional parameters are introduced:

$$y^k = \gamma \hat{x}^k + \beta^k, \tag{1.17}$$

140 where the parameters γ and β are trained just like the rest of the network parameters. Practically
141 if the training is performed within the mini-batch scheme with batch size $B = x_1, ..., x_m$ the batch
142 normalization layer is inserted between the DNN layers the transformations for the input x are the

following:

$$
\begin{aligned}
\frac{1}{m} \sum_{i=1}^{m} x_i &\to \mu_B \\
\frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_B)^2 &\to \sigma_B^2 \\
\frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} &\to \hat{x}_i \\
\gamma \hat{x}_i + \beta &\to y_i \equiv BN_{\gamma, \beta}(x_i),
\end{aligned}
\tag{1.18}
$$

where ϵ is a small regularization constant.

1.2 HR regression

Considering that hadronic recoil is an observable that uses many inputs from Inner Detector (ID), electromagnetic calorimeter (EMC) and hadronic calorimeter (HC) it is reasonable to expect improvement of the result using modern MultiVariate Analysis (MVA) techniques.

1.2.1 Input features and model

Training, testing and validation was performed using a simulated MC sample $W^+ \to \mu\nu$ at 13 TeV, following the selection presented in Section **??**. From the 3625136 events that have passed the selection 12 734 109 were used for training and 3 034 130 for testing the performance. Below is the list of 38 input features:

- **Vector sums** of charged Particle Flow Objects (PFO), neutral PFO (see Section **??**) and the vector sum of both. All three vector sums are included into the input features having two Cartesian components each, making 6 input features.

- **Transverse energy sum** $\sum E_T$ is also defined in three similar ways, adding three input features.

- Cartesian components of the two leading jets momenta in the transverse plane. The jets were demanded to have $p_T > 20$ GeV. If one or both jets don't make the cut or there is less than two jets in the event - the corresponding features were assigned zero value.

- Cartesian components of the five leading Neutral Particle Flow Objects (nPFOs) and five leading Charged Particle Flow Objects (cPFOs) momenta in the transverse plane.

- Number of primary vertices in the event.

- Pile-up value μ.

- Total number of jets in the event.

- Total number of nPFOs and cPFOs in the event.

167 All input features were pre-processed using the StandardScaler module from Scikit Learn package [13].
168 The model contains 3 dense layers with 256 neurons each, alternated with batch normalization layers
169 (see Fig. 12). Using batch normalization layers has allowed to reduce the training time by a factor
10. The model has used Adam optimizer with learning step 0.001 and batch size of 4000 data points.
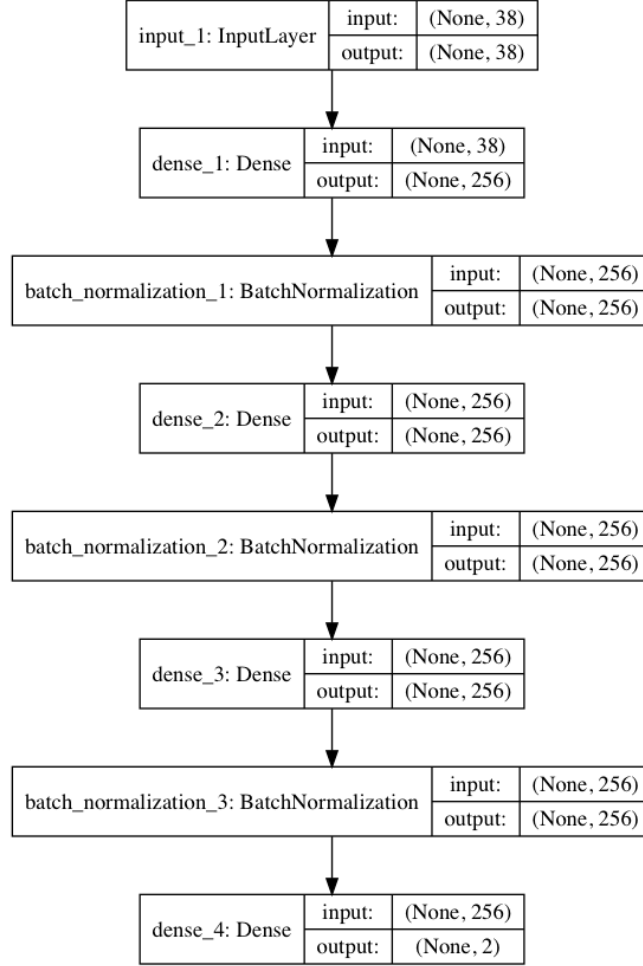

Figure 12: A model of the DNN used in the analysis.

170
171 Twenty percent of events were used for validation. The two target values were Cartesian components
172 of the truth p_T^W vector.
173 The loss function used is the mean square error, which means that for every batch of size B the loss is
174 defined as:

$$\mathcal{L} = \sum_{i=1}^{B} (x_i^{pred} - x_i^{target})^2, \tag{1.19}$$

175 where x_i^{target} and x_i^{pred} are the target (truth) and predicted values for the ith event respectively. For our
176 case of two target values, namely u_X and u_Y the loss takes the following form:

$$\mathcal{L} = \sum_{i=1}^{B} \left((x_i^{pred} - x_i^{target})^2 + (y_i^{pred} - y_i^{target})^2 \right). \tag{1.20}$$

177 Figure 13 shows dependence of loss on training epochs. Eventually the model with weights obtained after 38 epochs of training was used in the analysis.
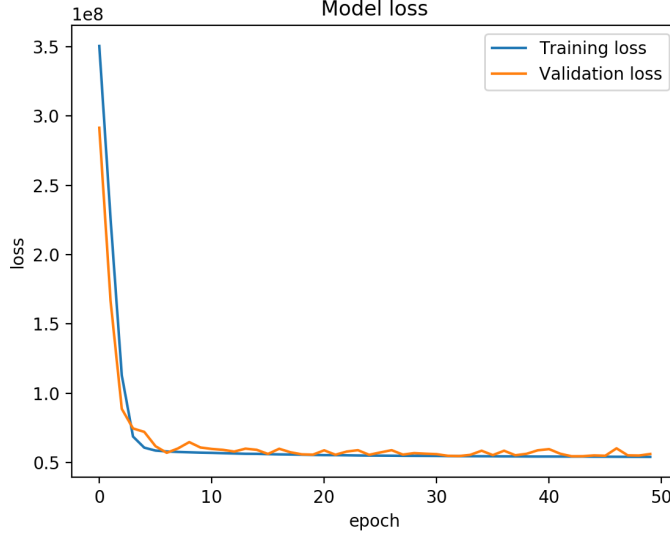
Figure 13: Learning curve of the model.

178

1.2.2 Kinematic distributions

180 The results presented here show the regression plots obtained with the trained DNN. The regression
181 was tested for the four W channels in MC and for the two Z channels in both data and MC. Below the
182 plots for $W^- \to \mu\nu$ channel are presented, the rest of the results are presented in Appendix B.
183 In Figure 14 the difference between the reconstructed hadronic recoil and truth distributions (targets)
184 are shown. For the two target components u_X and u_Y a sharper peak centred at zero is observed in the
185 MVA-reconstructed recoil comparing to the standard algorithm. Similar comparison is shown in Fig.
186 **??** for HR vector components in polar coordinates. The polar angle u_ϕ of the HR vector shows a very
187 small, nearly negligible improvement from the MVA. The u_T vector magnitude demonstrates a shift
188 from zero for the u_T^{MVA}, indicating a bias. Figure 16 shows that the MVA-reconstructed recoil has a
189 softer spectrum comparing to both p_T^{truth} and standard recoil spectra.
190 The bias is shown in Fig. **??** together with the u_{perp} component. Indeed the u_T^{MVA} demonstrates a
191 larger bias as compared to the standard algorithm. At the same time the standard deviation of the $u_\perp$
192 component indicates an improvement in the resolution.
193   The dependence of the bias and $u_\perp$ on the momentum is studied in Fig. 18. The u_T^{MVA} recoil
194 demonstrates improvement in the resolution and a larger bias in the region of $p_T < 80\text{GeV}$. However,
195 for a quantitative resolution comparison we need to make sure that $u_\perp$ and $u_\perp^{MVA}$ are on the same scale.
196 A possible way to achieve this is to normalize them to average recoil $< u_T >$. The resulting normalized
197 curves on Fig. 19 show that the MVA provides 5-10% resolution improvement at $p_T < 10\text{GeV}$ and a bit

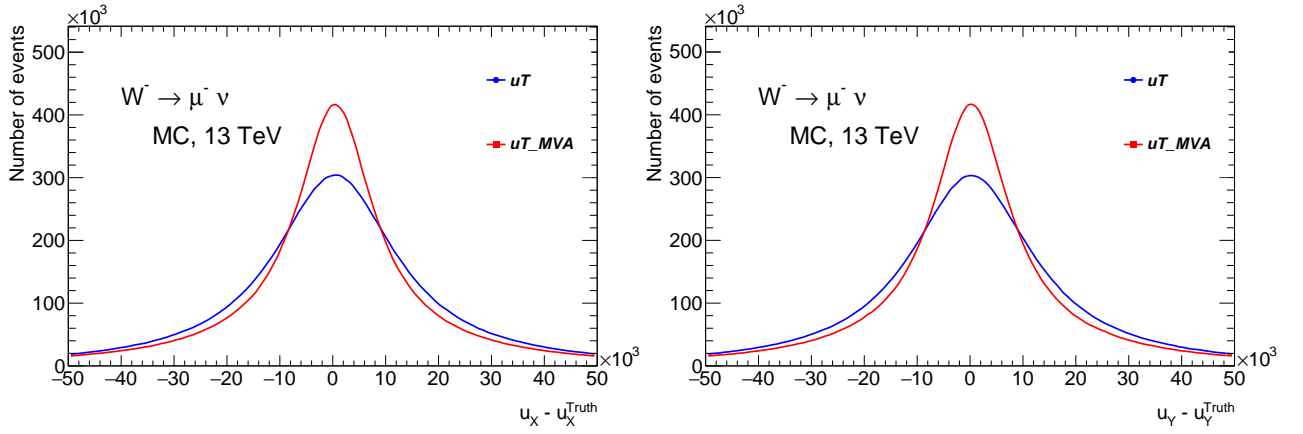**Figure 14:** The difference between the Cartesian components of the HR vector for the standard u_T and u_T^{MVA}.
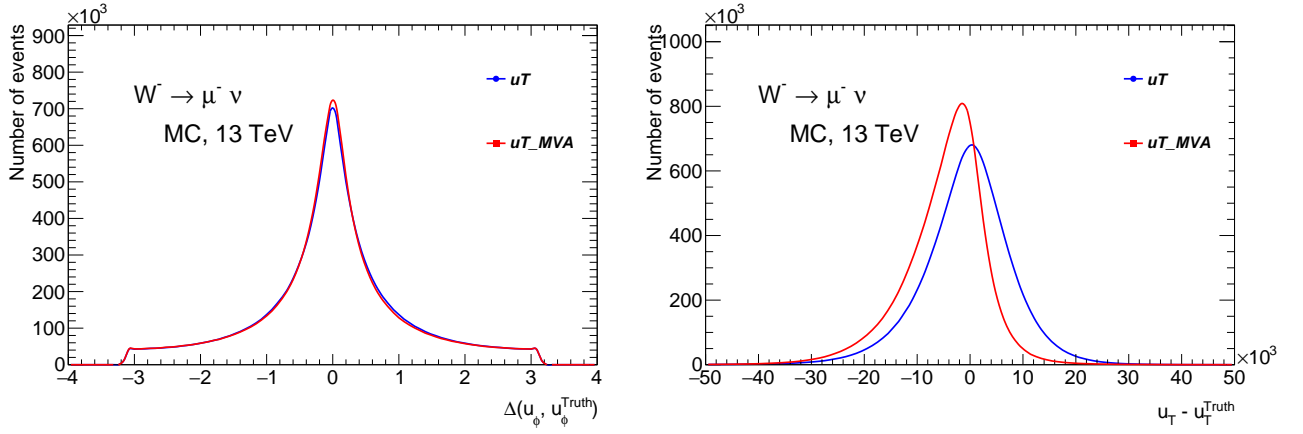

Figure 15: The difference between the polar components of the HR vector for the standard u_T and u_T^{MVA}.
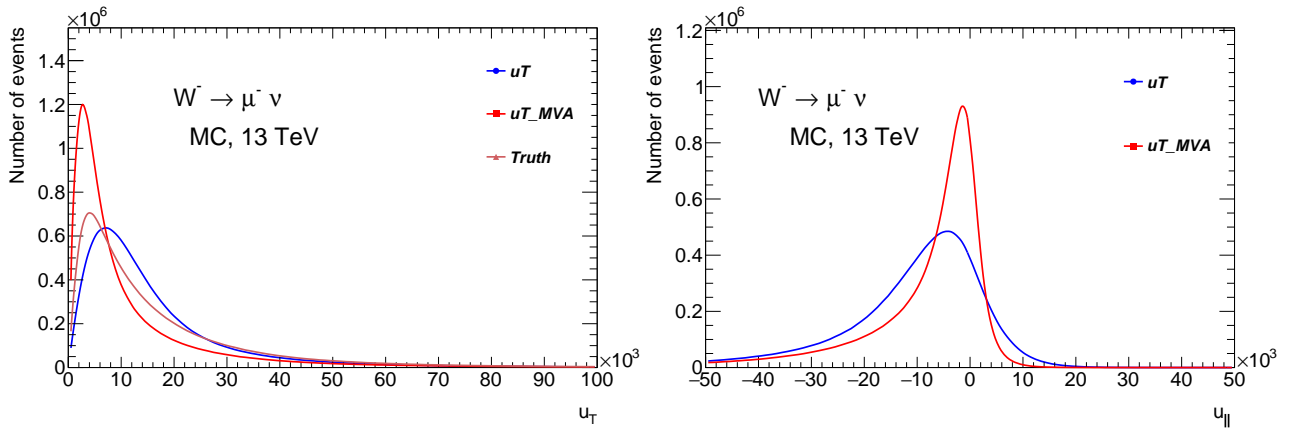

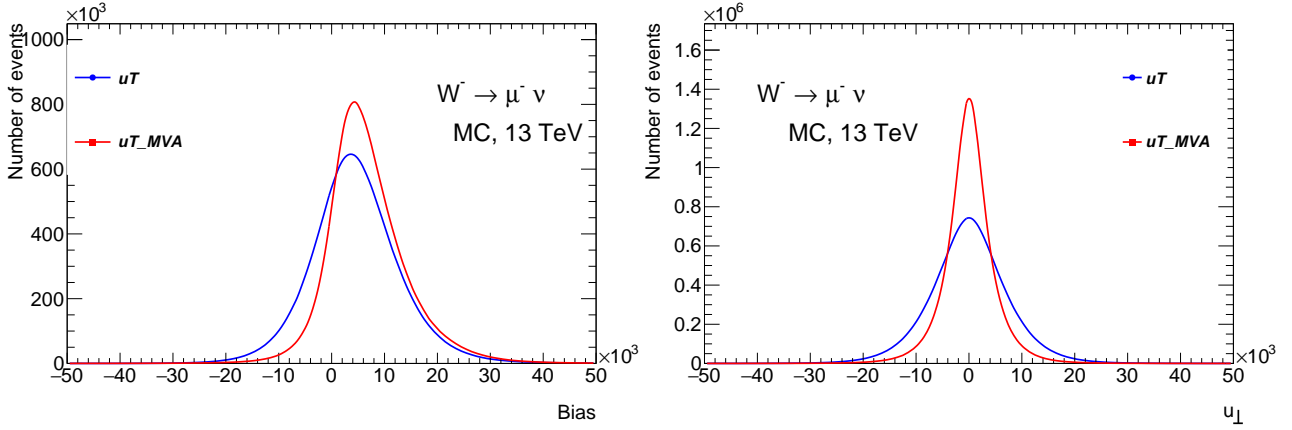**Figure 16:** Comparison of u_T and u_T^{MVA} spectra and response.

Figure 17: Bias and $u_\perp$ for the standard u_T and u_T^{MVA}.

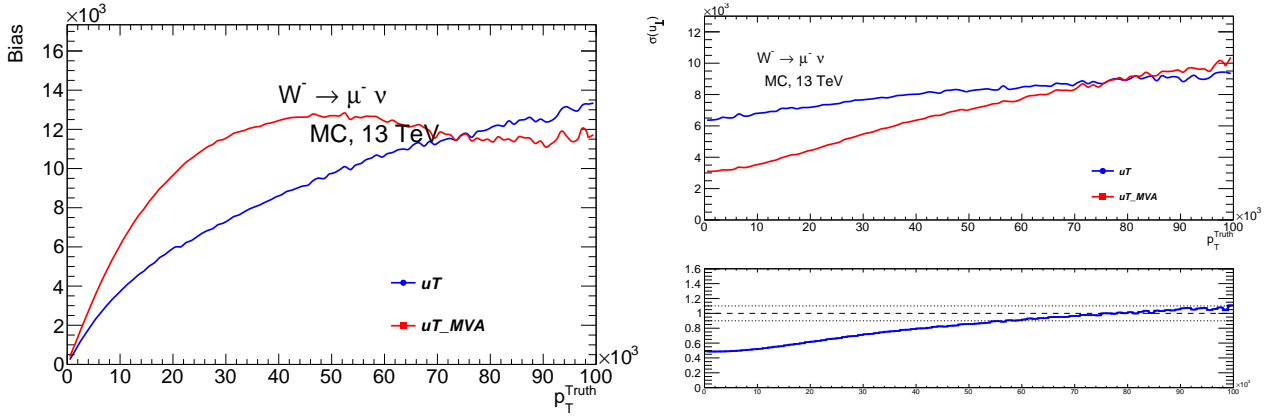more than 10% in $10 < p_T < 30$GeV transverse momentum region.

Figure 18: Bias and $u_\perp$ as a function of p_T^{truth}.

The same neural network was applied for the HR regression for both Z channels, for data and MC events. In case of data the p_T^{truth} vector was replaced with $p_T^{\ell\ell}$. A qualitatively similar picture holds for both Z channels, confirming recoil universality for W and Z events (see Fig. 110). The complete set of u_T vs u_T^{MVA} comparison plots for all W and Z channels can be found in Appendix B.

1.3 Conclusions

The application of contemporary analysis methods like the regression using DNNs shows a promising potential for improving the measurements precision.
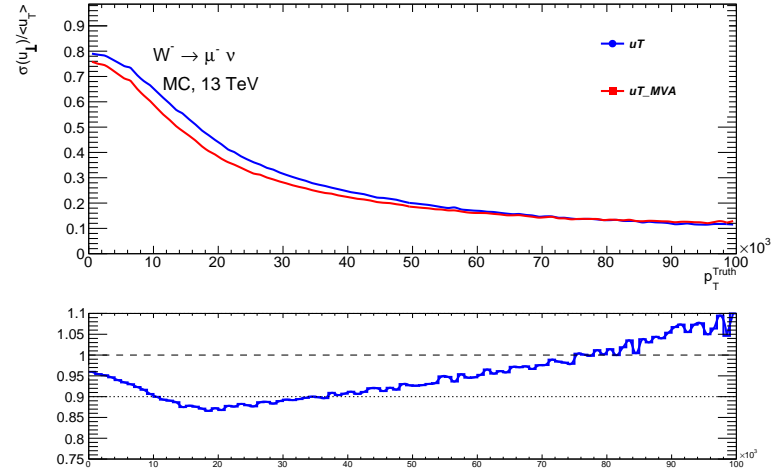
Figure 19: Normalized $\frac{u_\perp}{\langle u_T \rangle}$ as a function of p_T^{truth}.
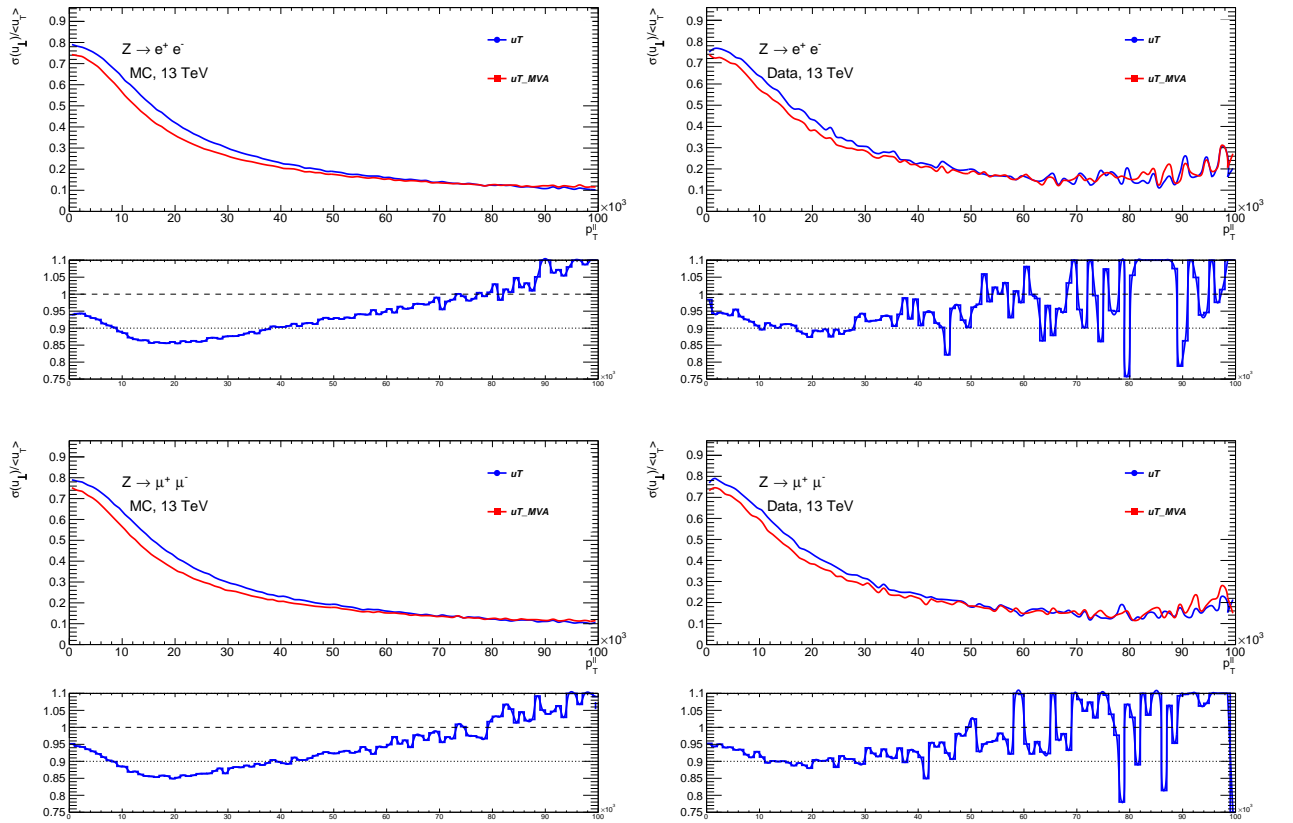
Figure 110

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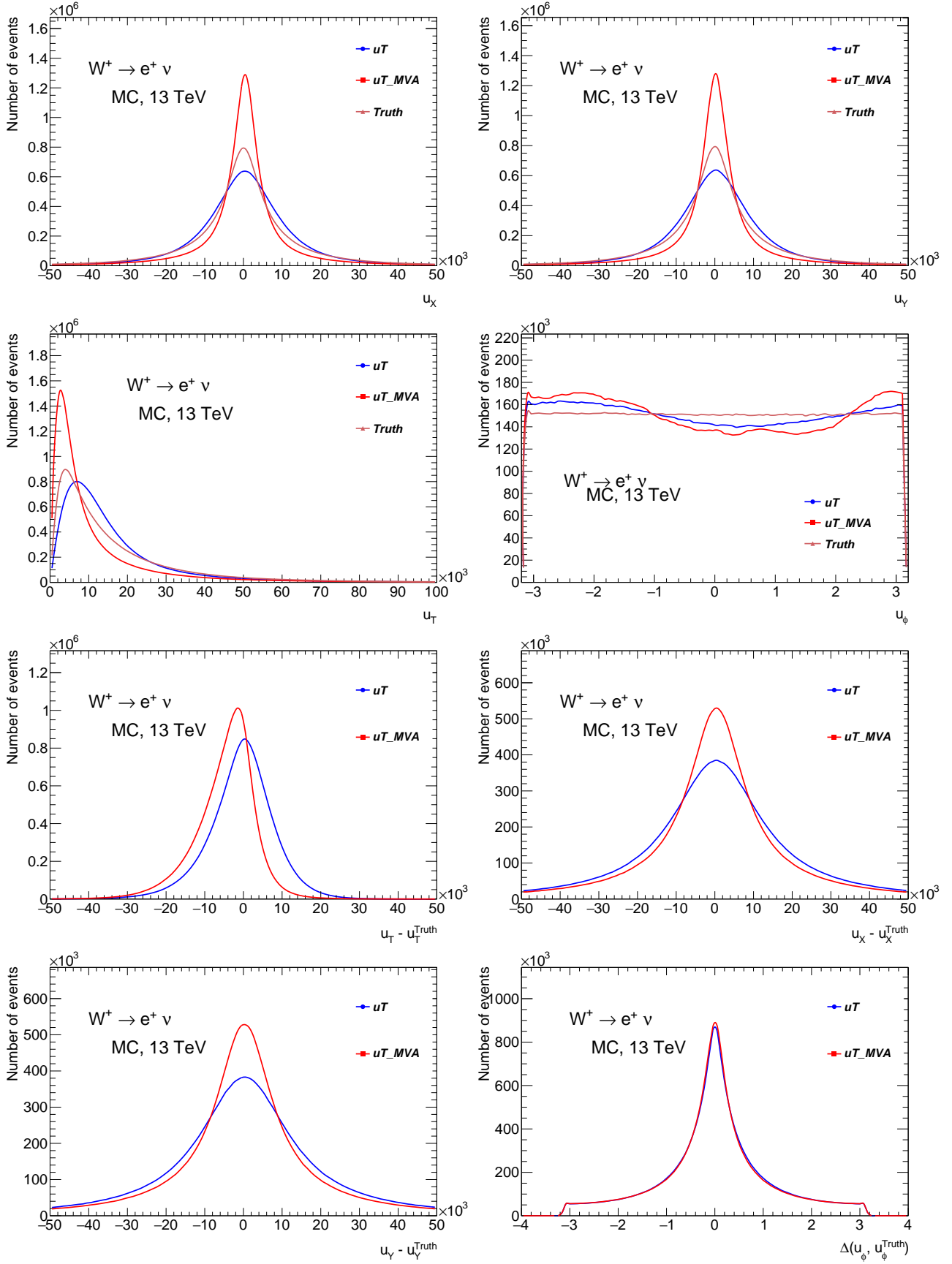
2
Appendix B

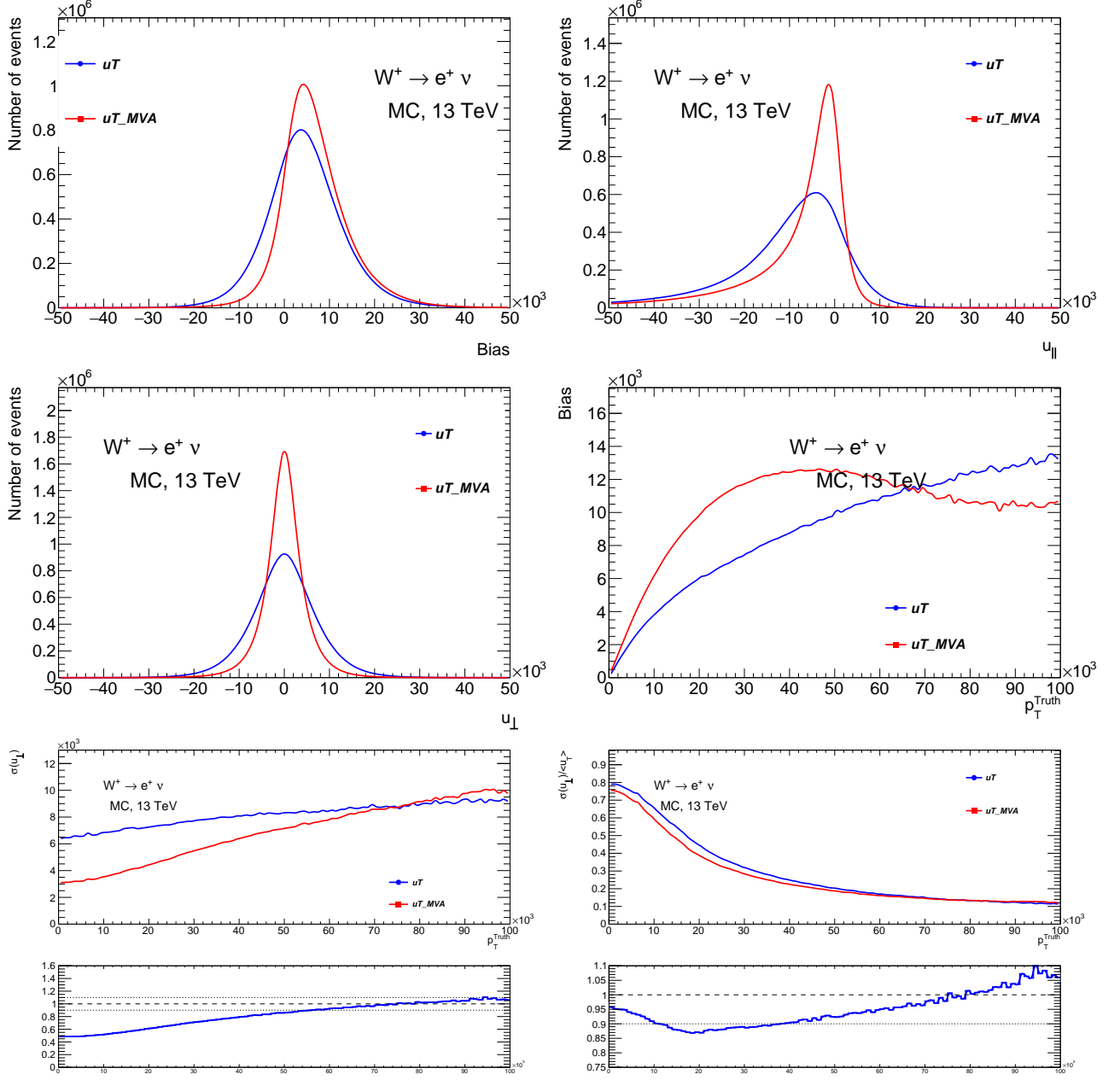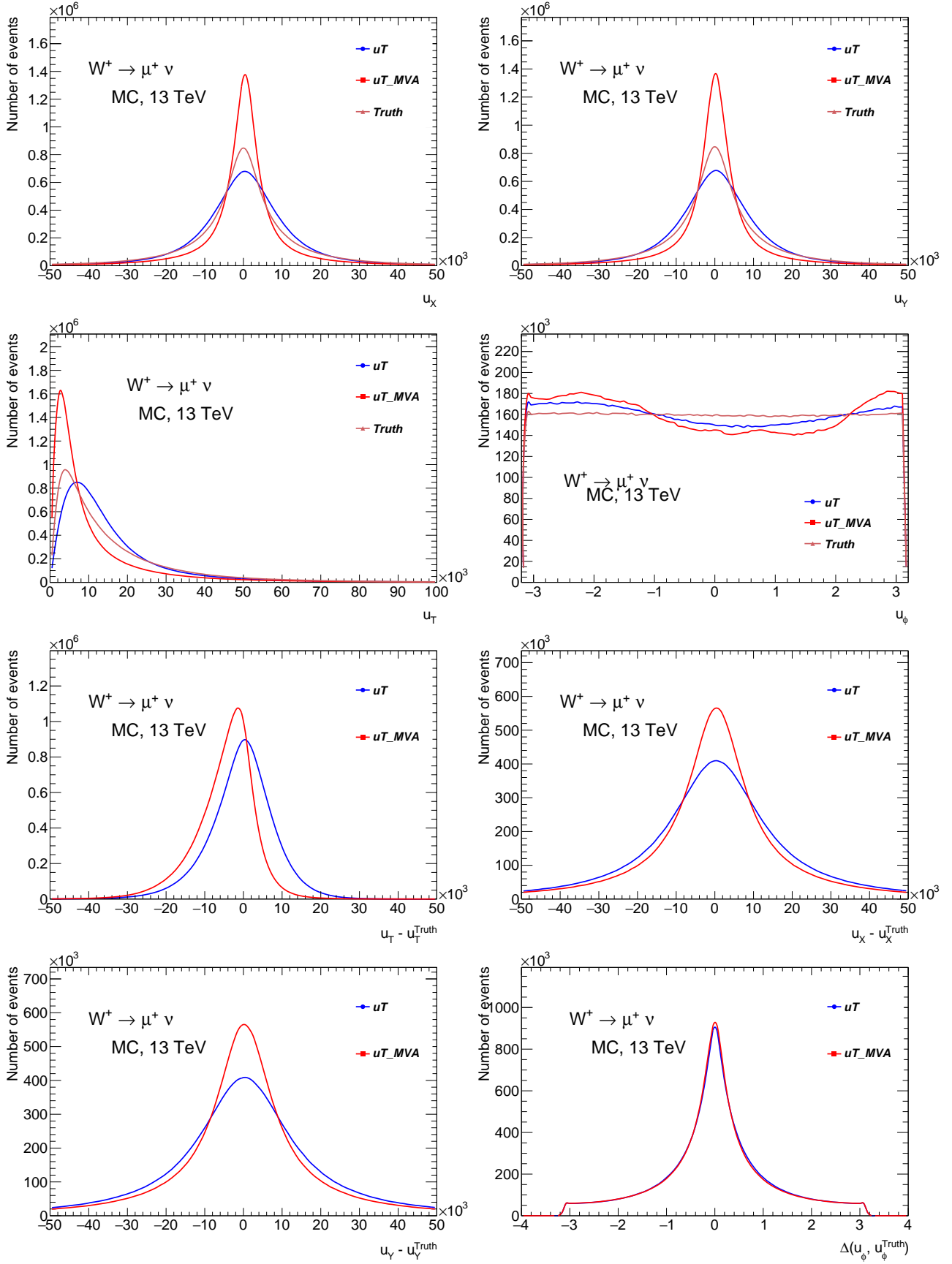245 Current appendix contains the comparison of all the kinematic distributions for all W and Z channels.

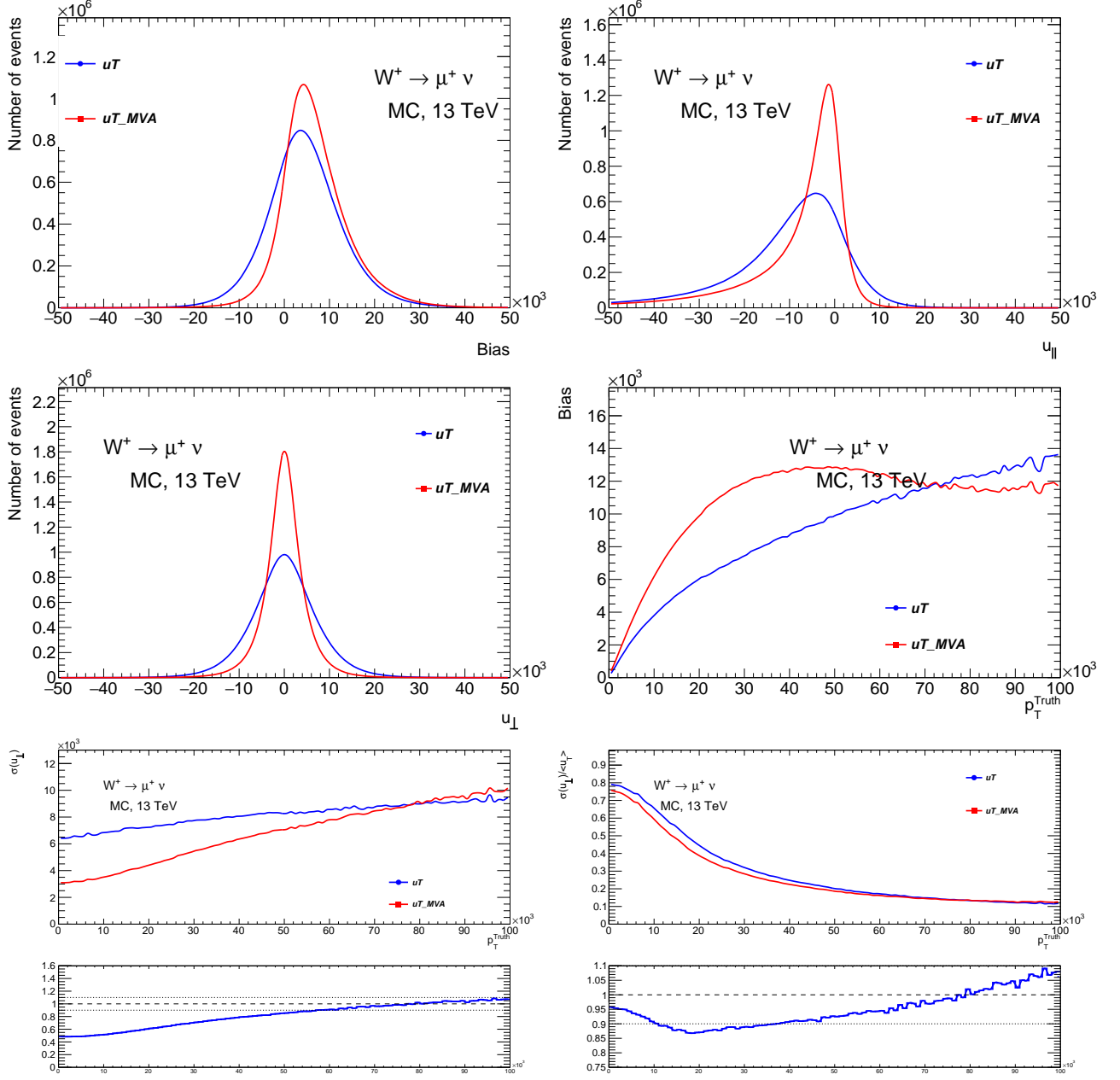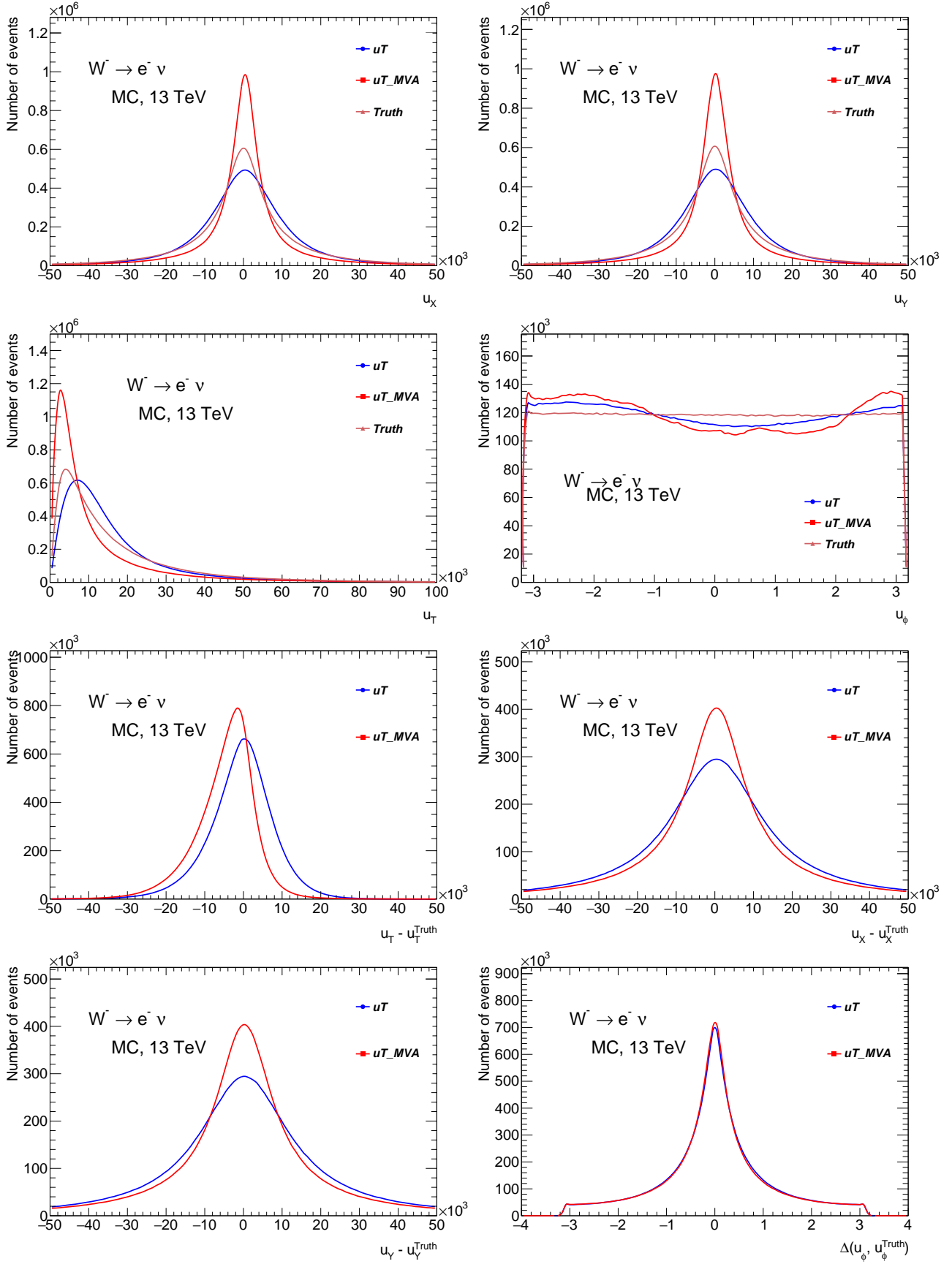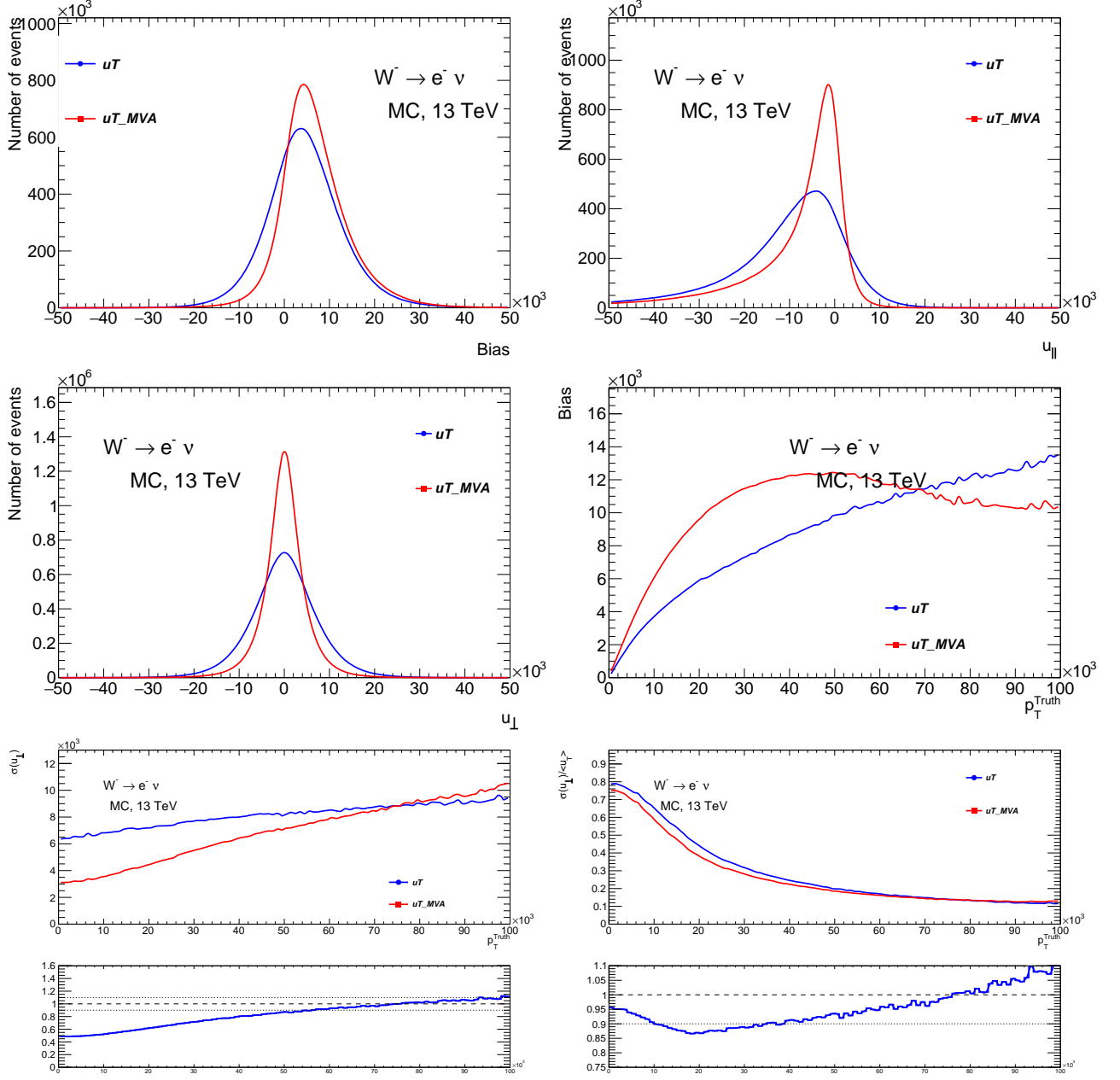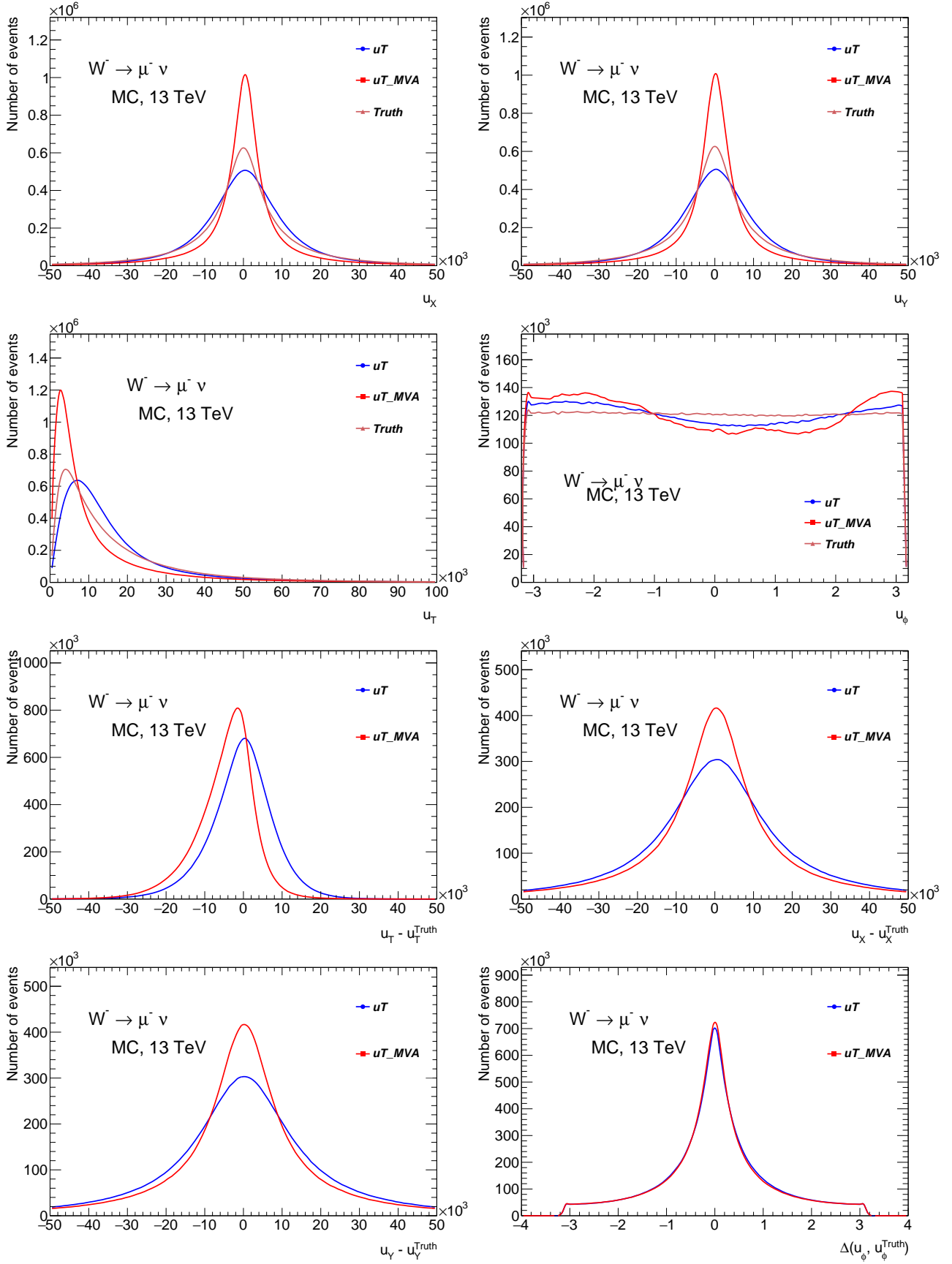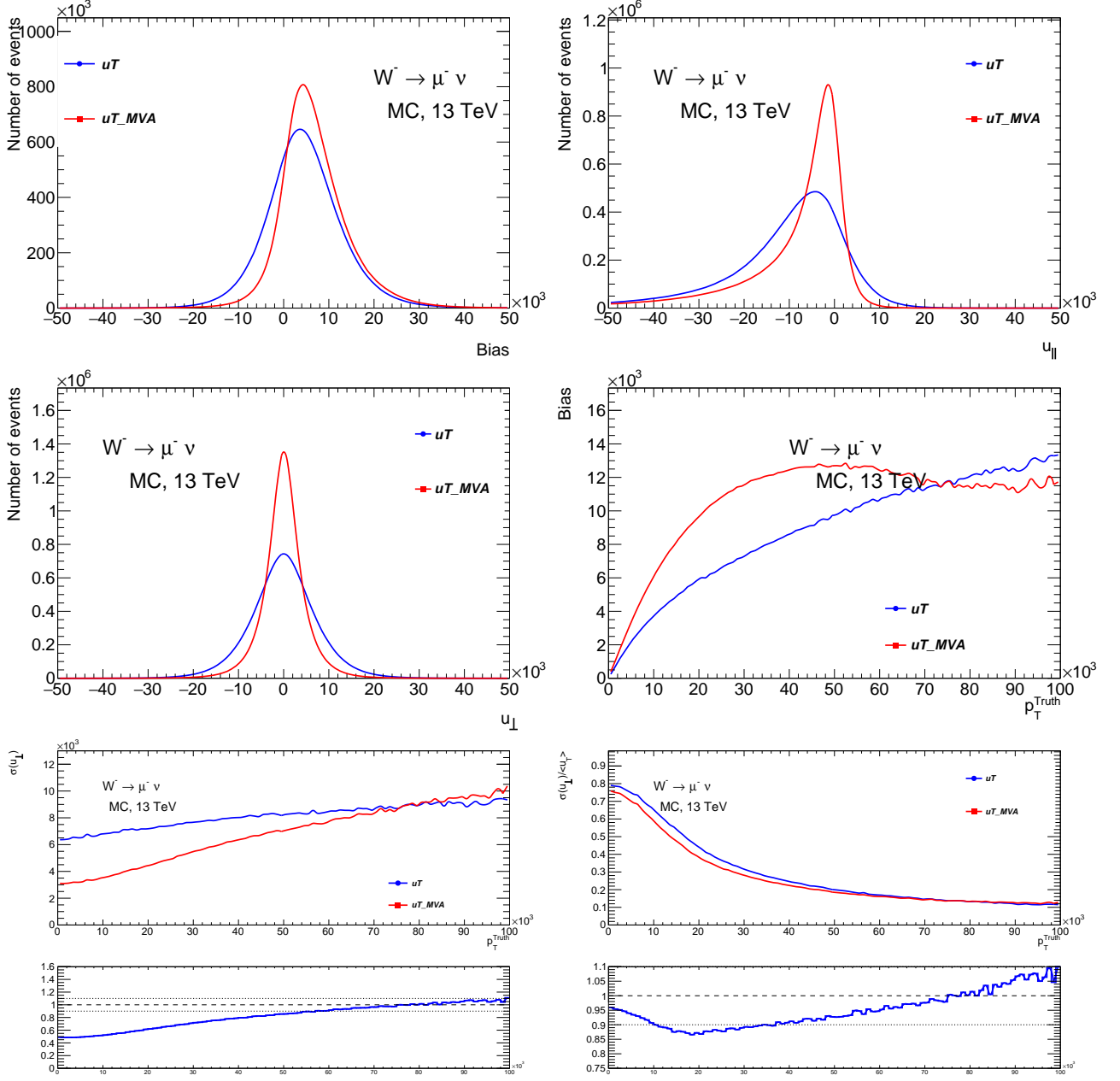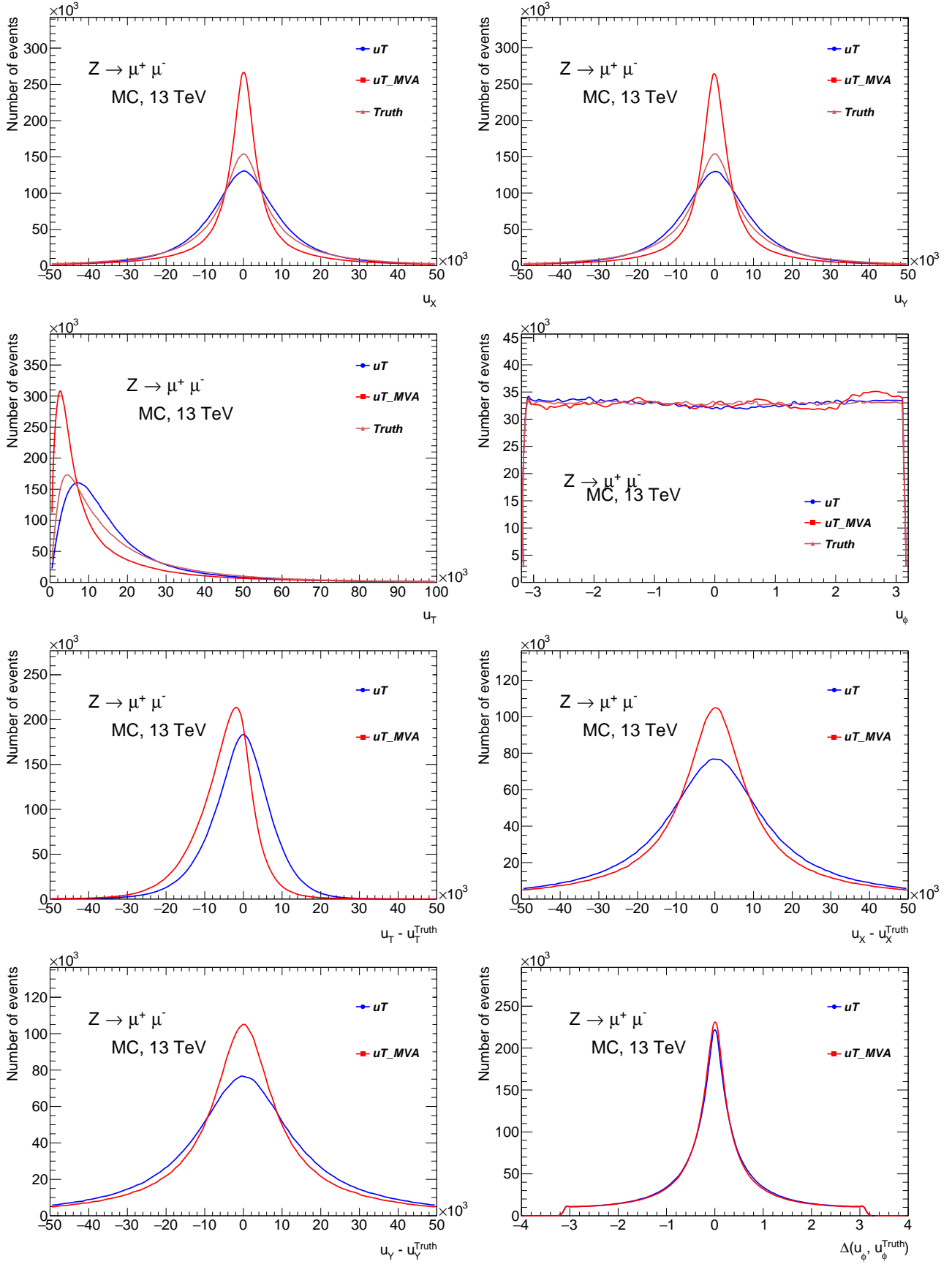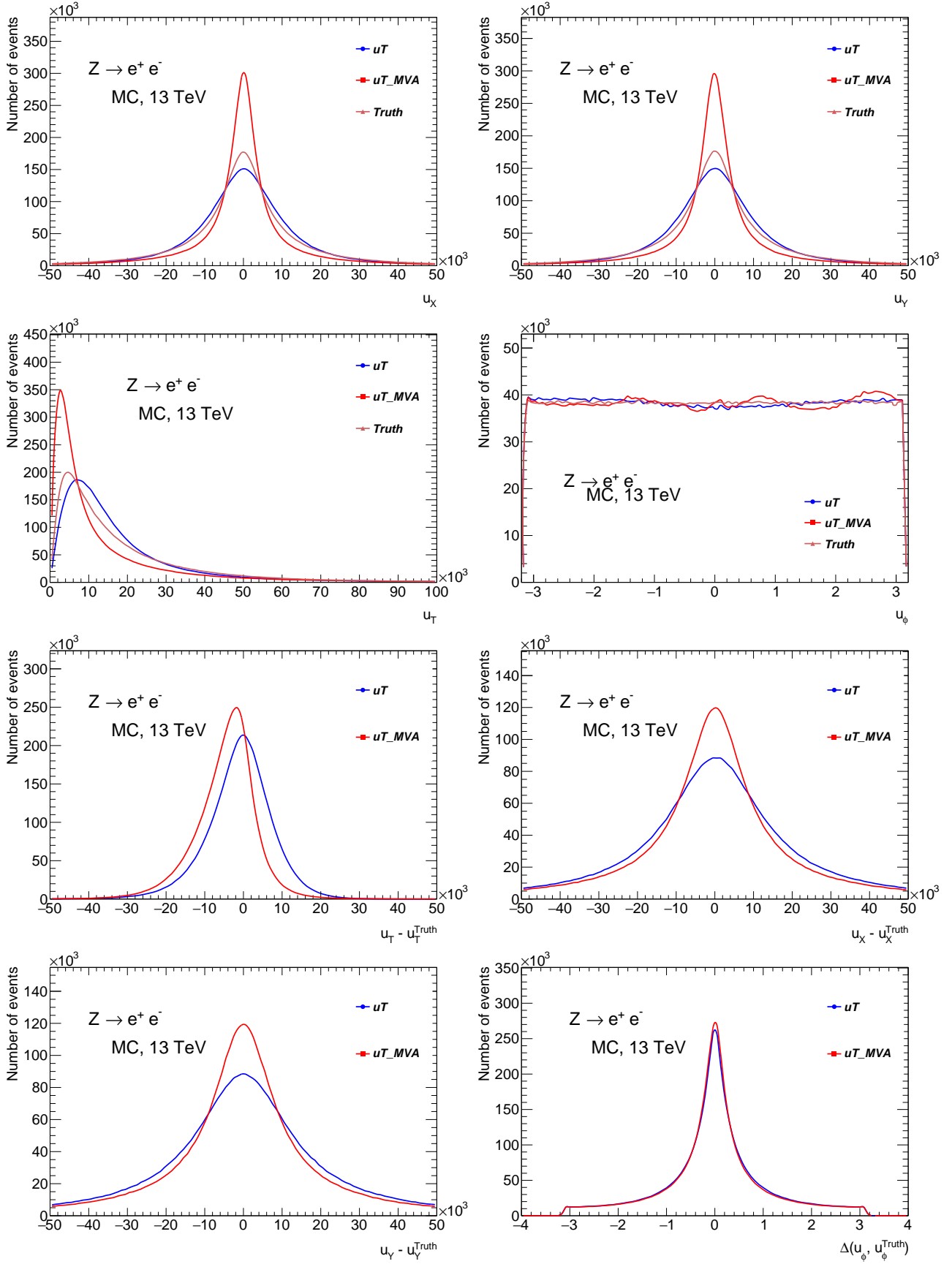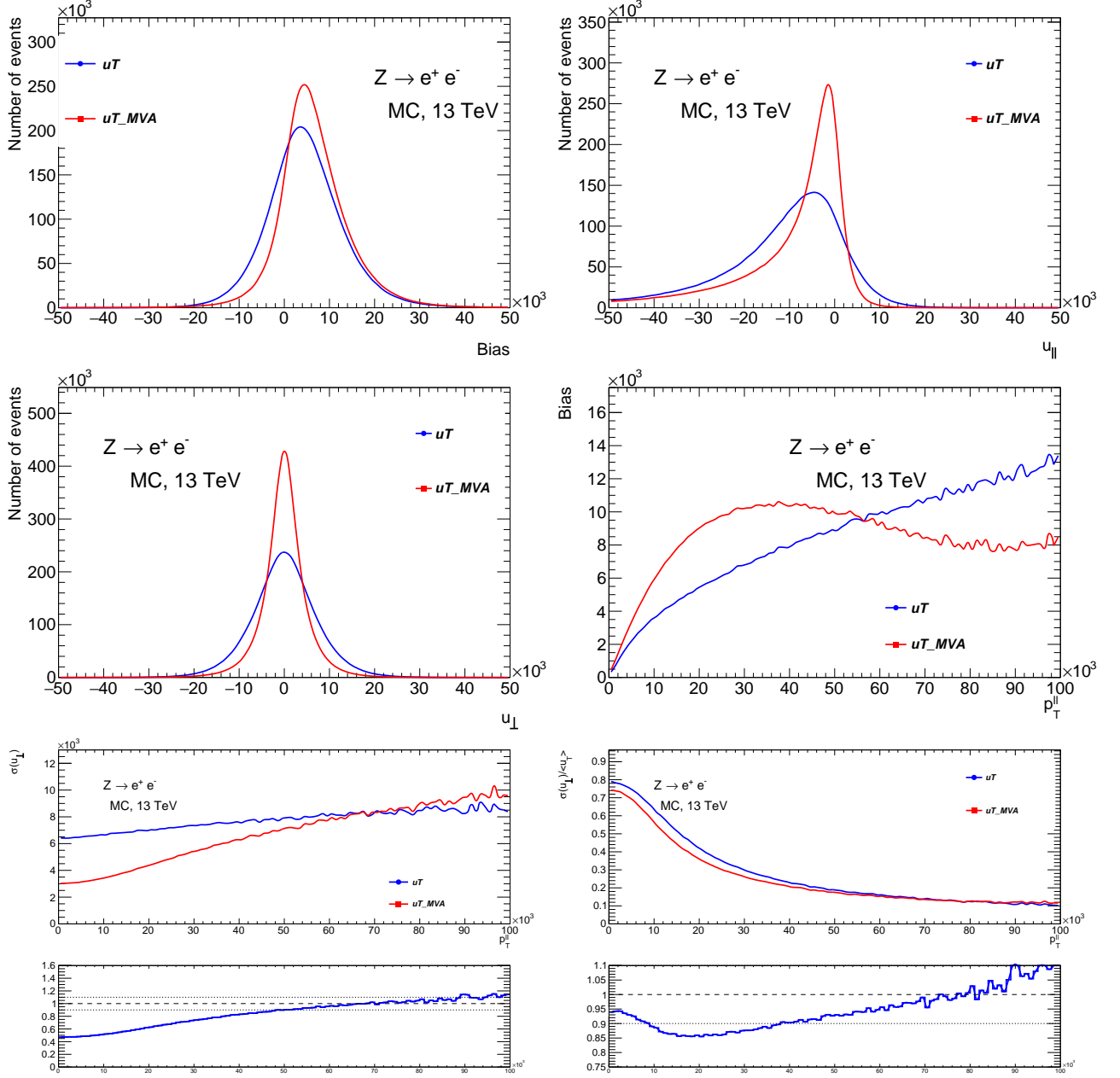**Figure 21:** Comparison of kinematic distributions of u_T vs u_T^{MVA} for $W^+ \rightarrow e^+ \nu$ data sample.

Figure 22: Comparison of kinematic distributions of u_T vs u_T^{MVA} for $W^- \rightarrow e^- \nu$ data sample.

Figure 23: Comparison of kinematic distributions of u_T vs u_T^{MVA} for $W^+ \to \mu^+ \nu$ data sample.

Figure 24: Comparison of kinematic distributions of u_T vs u_T^{MVA} for $W^- \to \mu^- \nu$ data sample.
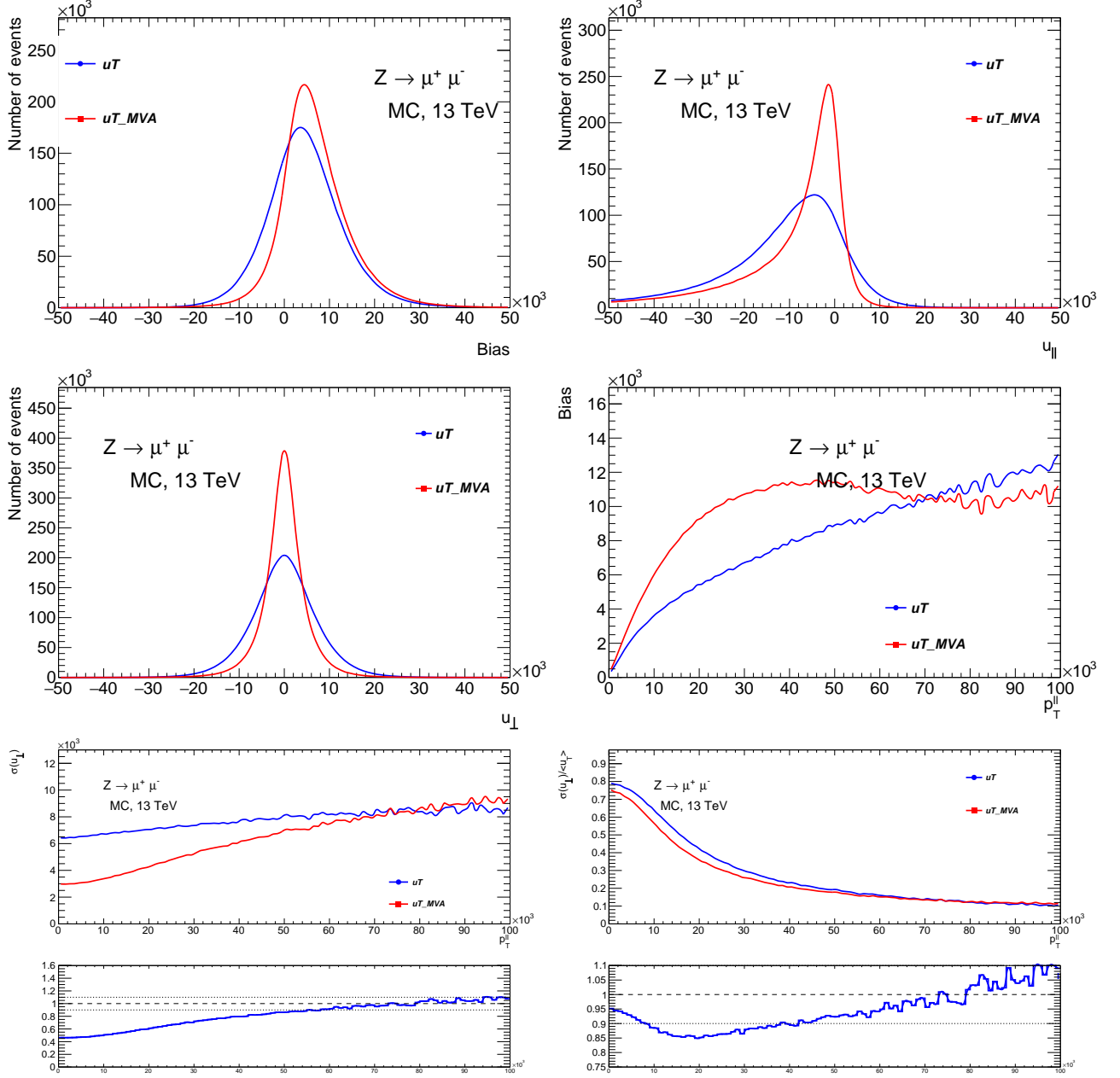
Figure 25: Comparison of kinematic distributions of u_T vs u_T^{MVA} for $Z \to \mu\mu$ MC sample.

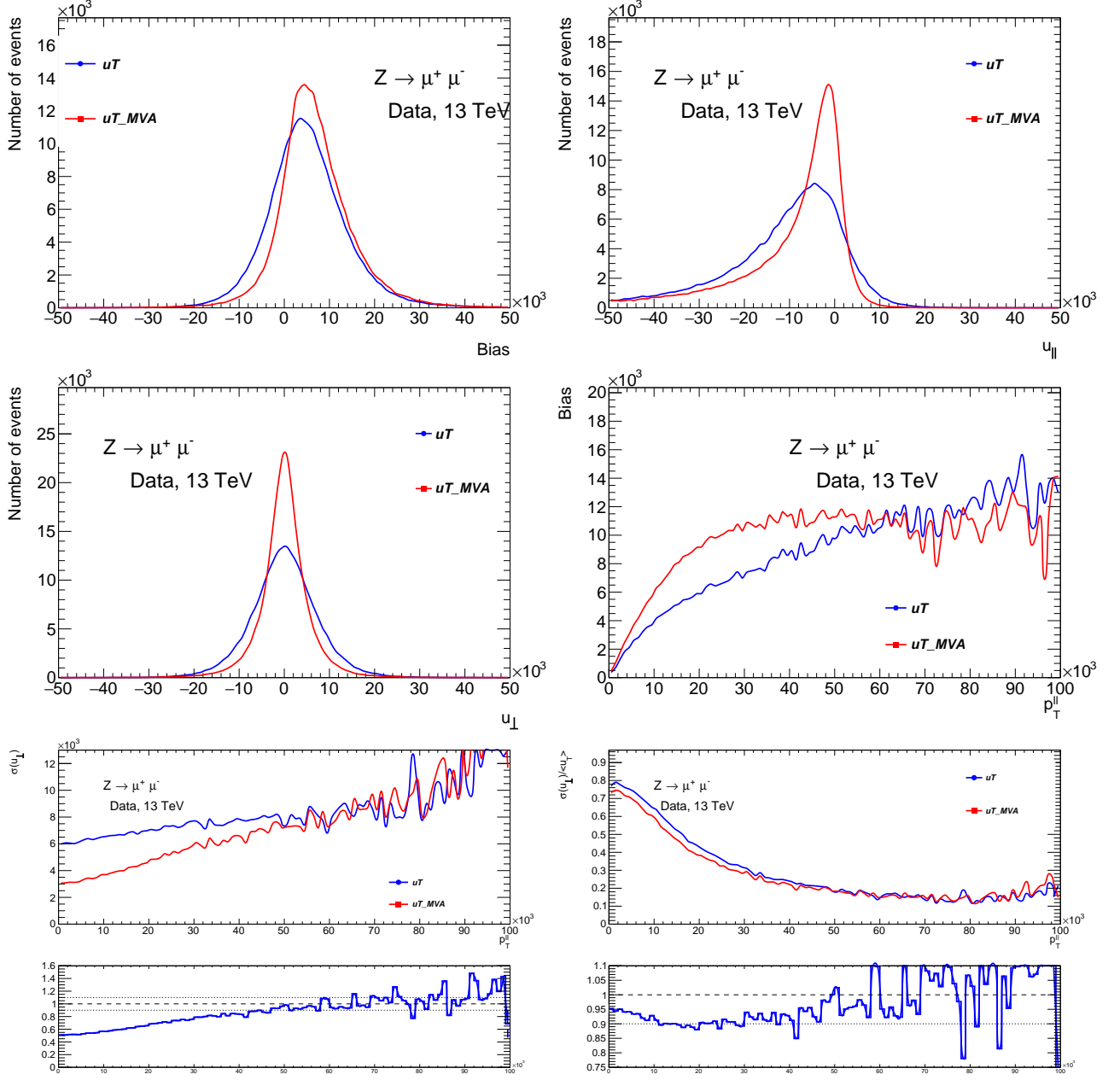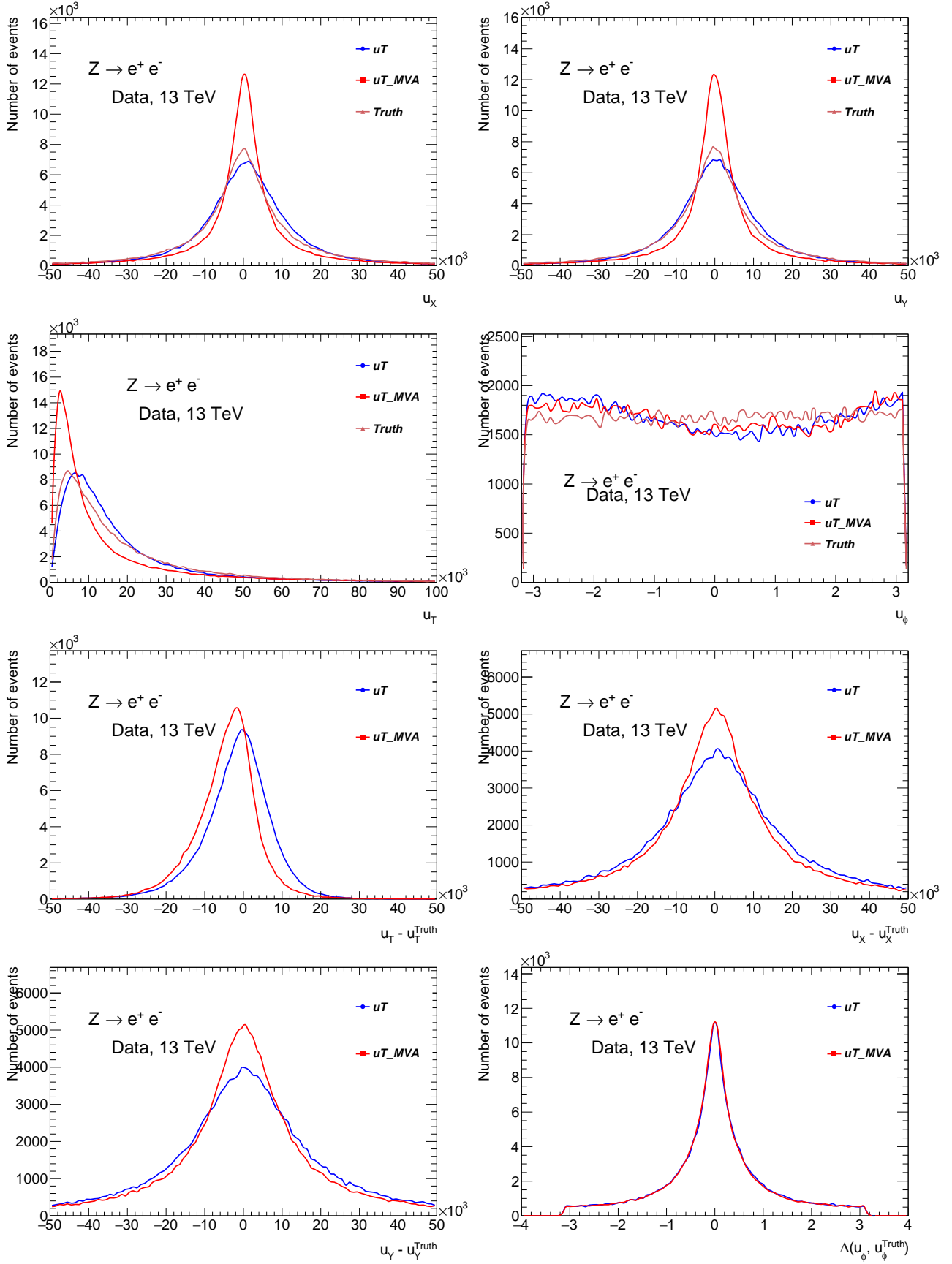**Figure 26:** Comparison of kinematic distributions of u_T vs u_T^{MVA} for $Z \to ee$ MC sample.
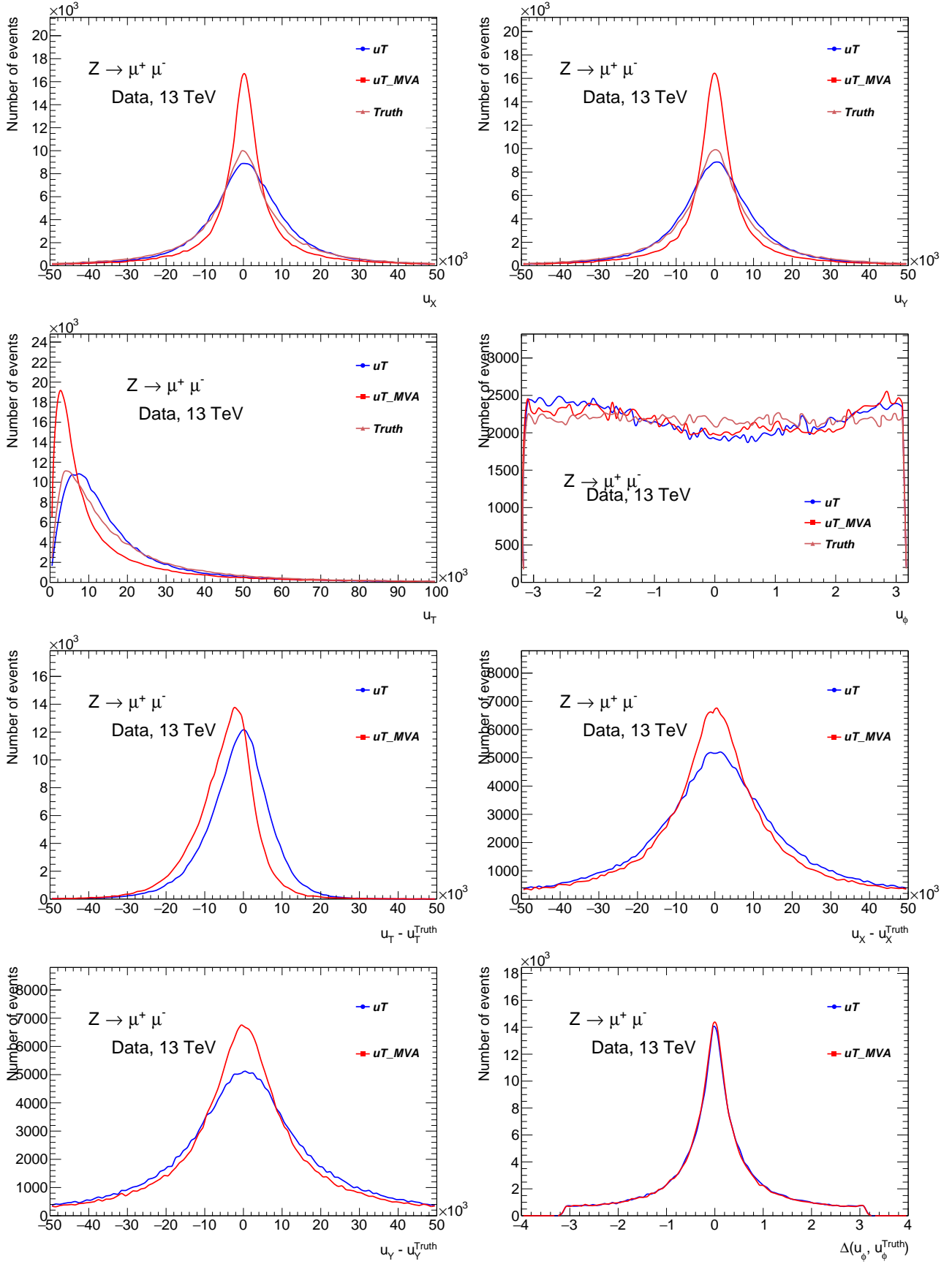
Figure 27: Comparison of kinematic distributions of u_T vs u_T^{MVA} for $Z \to \mu\mu$ data sample.
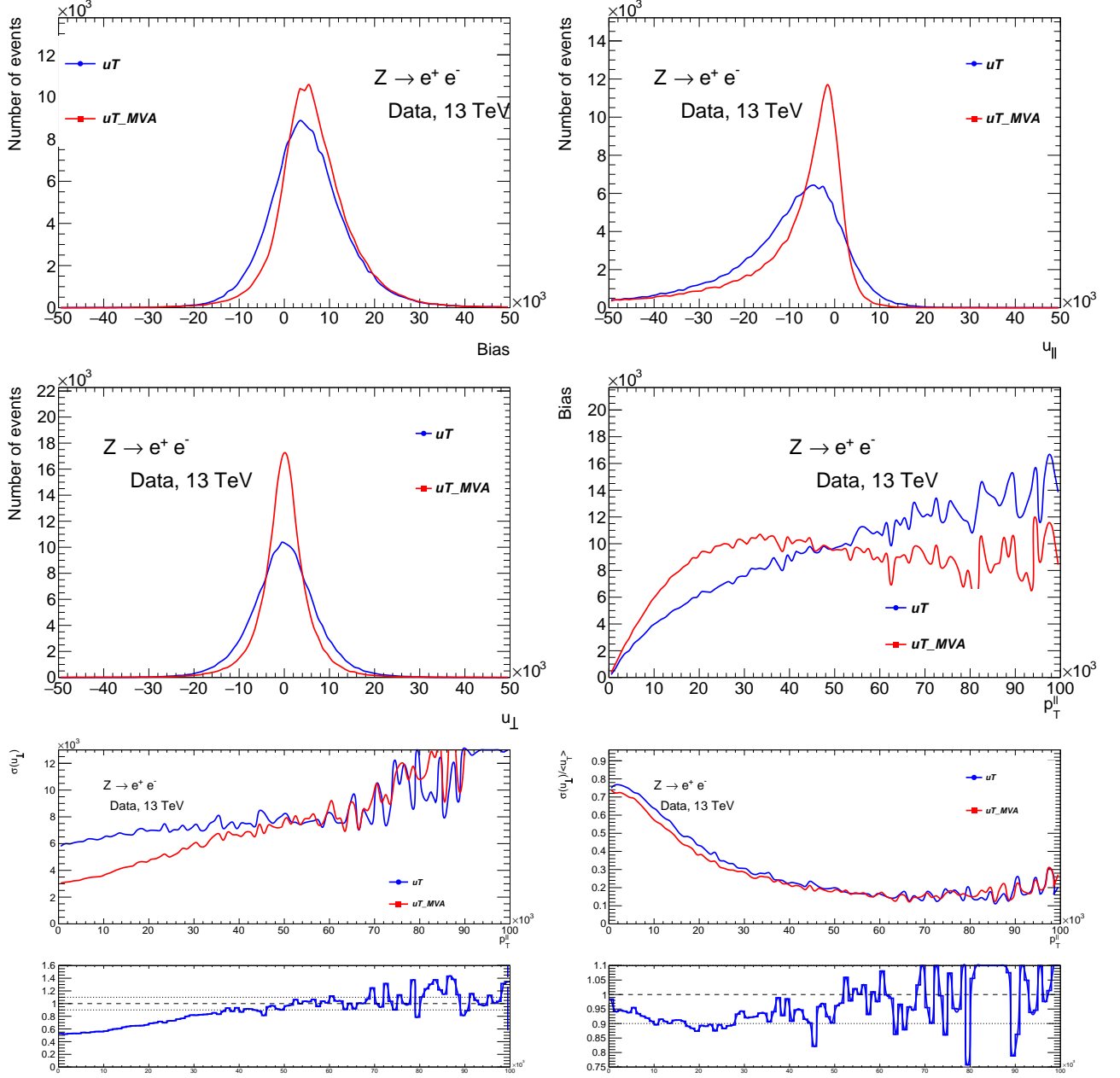
Figure 28: Comparison of kinematic distributions of u_T vs u_T^{MVA} for $Z \to ee$ data sample.