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Simultaneous Unbinned Differential Cross-Section Measurement of Twenty-Four $Z +$ jets Kinematic Observables with the ATLAS Detector

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Z boson events at the Large Hadron Collider can be selected with high purity and are sensitive to a diverse range of QCD phenomena. As a result, these events are often used to probe the nature of the strong force, improve Monte Carlo event generators, and search for deviations from standard model predictions. All previous measurements of Z boson production characterize the event properties using a small number of observables and present the results as differential cross sections in predetermined bins. In this analysis, a machine learning method called OMNIFOLD is used to produce a simultaneous measurement of twenty-four $Z +$ jets observables using 139 fb^{-1} of proton-proton collisions at $\sqrt{s} = 13$ TeV collected with the ATLAS detector. Unlike any previous fiducial differential cross-section measurement, this result is presented unbinned as a dataset of particle-level events, allowing for flexible reuse in a variety of contexts and for new observables to be constructed from the twenty-four measured observables.

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The production of Z bosons is a standard candle process at the Large Hadron Collider (LHC), used for various purposes, such as precision tests of the standard model, detector calibration, and testing new analysis methods. The large $pp \to Z + X$ cross section, in combination with the easily identifiable $Z \to \ell\ell$ decay (with $\ell \in \{e, \mu\}$), makes it possible to collect event samples with high purity and efficiency. When the Z boson is produced at large transverse momentum, it is usually accompanied by an associated hadronic recoil that is collimated into one or more jets. Measurements of $Z +$ jets production are crucial for many purposes, including powerful tests of perturbative quantum chromodynamics (QCD) [1–5] and improvements of the parameters used in parton shower Monte Carlo calculations [6,7] and tunes of the underlying event [8,9].

Numerous measurements of $Z +$ jets production that probe the kinematic properties of the Z boson and the associated jets were performed at the Tevatron [10,11] and at the LHC [12–20], including several dedicated measurements of the internal structure of the associated jets [21–24]. Each of these measurements takes the form of a binned fiducial differential cross section at the particle level by fully correcting for detector effects using *unfolding* methods [25–27].

The most widely used unfolding methods employ forms of regularized matrix inversion [28–30]. This analysis presents developments that address four features of traditional unfolding techniques that potentially limit the future utility of the published data. First, the target observables must be specified prior to unfolding and cannot be changed after the measurement. Second, the binning of the observables must be fixed at the start of the measurement. Third, due to the binned nature of existing techniques, most measurements are done as a function of a single observable, and only occasionally in bins of two or three observables (e.g., Refs. [31–34]). Finally, existing methods can have large uncertainties associated with biases in the detector response due to mismodeling by the Monte Carlo simulation of observables other than the ones directly measured.

Recently proposed machine learning methods address these challenges directly [35,36]. Such methods use discriminative [35,37–42] or generative [43–51] neural networks (NNs) to readily process dozens of input observables in an unbinned manner. One discriminative approach is OMNIFOLD [39,40], an iterative method that generalizes to unbinned data the widely used Lucy-Richardson deconvolution approach [52,53] (also known as iterative Bayesian unfolding or IBU [28]). This method has recently been applied to perform the first unbinned studies [54] of hadronic final states with data from H1 [55,56], LHCb [57], CMS [58], and STAR [59]. OMNIFOLD learns a correction (assigned as event weights) to an initial set of simulated events instead of the more difficult task of learning to produce new events, as is done in generative approaches. As these methods are multidimensional, they

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can better account for variable dependency of the detector response that improves the measurement precision.

This Letter presents unbinned differential cross sections for $Z+$jets events in the dimuon channel $Z/\gamma^* \to \mu\mu$ using the OMNIFOLD method. The result constitutes a precision measurement in its own right, with multiple novel use cases as described below, and also serves as a proof-of-principle application of the OMNIFOLD method to provide an unbinned, high-dimensional measurement with full covariance for public use. The analysis is performed using the full Run 2 proton-proton dataset collected by the ATLAS detector [60] at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of $\mathcal{L} = 139\ \mathrm{fb}^{-1}$. The measurements are at the particle level, defined by final-state stable particles with mean lifetime satisfying $c\tau > 10$ mm. The fiducial volume requires two muons not originating from the decay of hadrons that each satisfy transverse momenta $p_{\mathrm{T}} > 25$ GeV and $|\eta| < 2.5$ [61]. The final-state muon is "dressed," such that collinear radiation of photons within a cone of $\Delta R = 0.1$ are added to its four momentum. The muons are further required to have opposite charges, dimuon invariant mass $m_{\mu\mu} \in (81, 101)$ GeV, and $p_{\mathrm{T}}^{\mu\mu} > 200$ GeV. The last criterion selects an unbiased sample of high-p_{T} jets, allowing jet properties to be probed in a previously underexplored kinematic regime, and reduces the size of the dataset, which simplifies the computational challenge for the unfolding method. The jets are reconstructed from charged particles with $p_{\mathrm{T}} > 0.5$ GeV and $|\eta| < 2.5$ using the anti-k_t algorithm [62,63] with $R = 0.4$; charged particles corresponding to prompt leptons, such as muons from $Z \to \mu\mu$, are excluded from the jet finding. Charged particles are used due to the precision with which they can be measured and the availability of full uncertainties. No additional acceptance requirements are placed on the jets, as these are implicitly set by the charged particle selection criteria. The 24 measured event observables are (i) $p_{\mathrm{T}}^{\mu\mu}$ and $y_{\mu\mu}$ of the dimuon system that probe the Z boson production kinematics; (ii) the kinematics of the two muons defined by $p_{\mathrm{T}}^{\mu 1}$, $p_{\mathrm{T}}^{\mu 2}$, $\eta_{\mu 1}$, $\eta_{\mu 2}$, $\phi_{\mu 1}$, $\phi_{\mu 2}$, which probe the Z boson decay kinematics; (iii) the kinematics of the two leading charged particle jets defined by $p_{\mathrm{T}}^{\mathrm{j1}}$, $p_{\mathrm{T}}^{\mathrm{j2}}$, y_{j1}, y_{j2}, ϕ_{j1}, and ϕ_{j2}; and (iv) the masses (m_{j1}, m_{j2}), charged particle multiplicities (n_{ch}^{j1}, n_{ch}^{j2}) and N-subjettiness quantities τ_1^{j1}, τ_1^{j2}, τ_2^{j1}, τ_2^{j2}, τ_3^{j1} and τ_3^{j2} [64,65] that probe the substructure of the two leading charged particle jets.

There is a significant overlap in observables between the OMNIFOLD analysis and the ones used to produce the ATLAS A14 parameter set (tune) [8] of the PYTHIA event generator [66,67]. A natural application of this measurement would hence be to create precise event generator tunes improving the modeling of the parton showers, hadronization and the underlying event. Other uses could include studies of jet substructure and jet flavor; for example, selecting jets back to back with the Z boson should yield quarklike jets, while wide angle radiation would give more gluonlike jets. Since the measurement is unbinned and probes a wide p_{T} range of jets, it is straightforward to switch between observables and study various quantities as a function of other quantities (e.g., jet m vs p_{T}, n_{ch}^{j1} vs y_{j1}, etc.).

The ATLAS detector has forward-backward symmetric cylindrical geometry and a near 4π coverage in solid angle. It includes an inner detector (ID) for charged particle tracking covering $|\eta| < 2.5$ surrounded by a thin solenoid providing an axial field of 2 T, electromagnetic and hadron calorimeters, and a muon spectrometer (MS). A two-level trigger system is used to select events [68]. An extensive software suite [69] is used for all aspects of data collection, curation, and analysis.

Data events are collected using single-muon triggers [70]. Muons are reconstructed by matching charged particle tracks in the ID and MS, accounting for energy loss in the calorimeters [71]. They are required to fulfill *medium* identification criteria and *PflowLoose* isolation [71], and must satisfy $|d_0|/\sigma_{d_0} < 3$ and $|z_0 \sin(\theta)| < 0.5$ mm for their transverse and longitudinal distances to the point of closest approach to the beam spot, ensuring that they originate from the interaction vertex, i.e., the primary vertex with the highest sum of associated track p_{T}^2. Charged particle tracks used for jet building are required to fulfill *loose* quality criteria, a *tight* track-to-vertex matching criterion [72], and must not be used by the selected muons. Identical kinematic requirements are applied to the reconstructed quantities as those used to define the particle-level fiducial volume.

Monte Carlo (MC) simulated samples are used to provide theoretical predictions both at the reconstructed and particle level, and to perform the unfolding. Most $Z+$jets events that satisfy the selection originate from the Drell-Yan process. Two MC samples are used to model this process: a nominal prediction is provided by MADGRAPH5_AMC@NLO2.6.5 [73–75] interfaced to PYTHIA8.240 (denoted MADGRAPH in the following), and SHERPA2.2.11 [75,76] provides an alternative. Both samples use the NNPDF3.0NNLO parton distribution functions (PDF) set [77]; additional details for these samples are given in Ref. [75]. Contributions from electroweak production of $Z+$jets are provided using HERWIG7.2 [78,79] interfaced with VBFNLO v3.0.0 [80] using the MMHT2014LO PDF set [81]. Diboson $ZV \to Zjj$ production is modeled at NLO accuracy by SHERPA2.2.1 or 2.2.2 [76] using NNPDF3.0NNLO. Background contributions from top processes ($t\bar{t}$, tV, single top) are modeled by POWHEGv2 [82] interfaced to PYTHIA8.230. The detector response is simulated using a dedicated GEANT4-based model [83] of the ATLAS detector [84]. Simulated inelastic minimum-bias events are overlaid to model additional pp collisions in the same and neighboring bunch crossings ("pileup") [84]. Simulated events are reconstructed using the same procedure as for data.

After the event selection, a pure $Z+$ jets signal sample is obtained with a composition of about 95% Drell-Yan, 3% diboson (primarily $ZV \to \mu\mu jj$), and 2% electroweak Zjj. The fraction of non-Drell-Yan $Z+$ jets increases with $p_{\mathrm{T}}^{\mu\mu}$ and reaches about 10% at $p_{\mathrm{T}}^{\mu\mu} > 500$ GeV. The fraction of diboson events is also sensitive to m_{j1}, and reaches ~8% for $m_{j1} > 45$ GeV. The analysis measures inclusive $Z+$ jets production and makes no attempt to separate these processes. Only the Drell-Yan production is used in the simulation for the unfolding itself, and the full difference between this and the result in which all $Z+$ jets are included is found to be small and taken as a conservative estimate of the process composition uncertainty. Backgrounds of about 0.2% arise due to the top processes (mostly $t\bar{t} \to \mu\mu\nu\nu jj$ and $tW \to \mu\mu\nu jj$). Contributions from events without two muons from the hard scatter are found to be negligible. The top background increases in regions with significant jet activity and is estimated to be ~2% for both $p_{\mathrm{T}}^{\mathrm{j1}} > 300$ GeV and $n_{\mathrm{ch}}^{j1} > 25$. As the background is small, it is not subtracted in the measurement; an estimate of its contribution is instead assigned as an uncertainty.

The OMNIFOLD-based unfolding produces event weights that are applied to the MADGRAPH Drell-Yan $Z+$ jets sample at particle level (see the Appendix). The number of iterations was fixed to five following a dedicated study that found unfolding performance plateaued around that number. The analysis is performed in a phase space slightly larger ($p_{\mathrm{T}}^{\mu\mu} > 190$ GeV) than the fiducial volume ($p_{\mathrm{T}}^{\mu\mu} > 200$ GeV) in order to reduce migration uncertainties, which also includes the final normalization of the results such that it provides fiducial cross sections, σ_{fid}. During this step, all OMNIFOLD weights are scaled by a constant to fulfill the relation $\mathcal{L}\sigma_{\mathrm{fid}}\varepsilon/f_{\mathrm{fid}} = n_{\mathrm{data}}$, where the overall efficiency ε and fiducial factor f_{fid} is evaluated using the same MC as used for unfolding, and n_{data} is the data count. After normalization, the sum of weights in any subset of the OMNIFOLD dataset can be interpreted as an estimate of its associated cross section. The final output of OMNIFOLD is the original particle-level simulated event sample with additional event weights that can be used to define measurements of the cross section of fiducial subregions (bins) defined by the 24 observables subject to the precision of the measurement. This includes differential cross sections of any of the 24 input variables or any combinations of those observables.

All NNs are constructed in TensorFlow [85,86], with three hidden layers of 200 nodes each with rectified linear unit (ReLU) [87] activation functions and a sigmoid final activation function. Two main challenges were faced regarding obtaining reliable and accurate NN outputs. The first is regarding MC event weights of the input samples, which initially had a large spread and often were negative that causes issues for the performance. This is addressed by preprocessing the MC sample such that negative weights are removed and the spread of weights is reduced as described in Ref. [88]. The second challenge is intrinsic to the NNs themselves, as the classifier output can vary slightly due to the randomly initialized starting weights. To stabilize the result, an ensemble of 100 NNs are created for each training, and the weight is taken as the median of the 100 NN weights.

Uncertainties on the unfolded result are evaluated using error propagation. Perturbations are introduced to the input samples by an amount commensurate with the uncertainty variation in question, and the full analysis (unfolding and normalization) is repeated, resulting in OMNIFOLD weights that differ from the nominal weights. The measurement central value is obtained with the nominal weight, and a total of 250 variation weights, each used to estimate the uncertainty.

Systematic uncertainties are split into 25 components that are each treated as independent. Experimental sources of uncertainty include systematic bias due to the following: the muon efficiency and calibration [71], track reconstruction [72], pileup modeling, and the luminosity measurement [89]. Theoretical uncertainties are evaluated for variations of PDF and α_s choices [75], QCD scales [75], and the generator tune [9]. Imperfections inherent to the choice of Monte Carlo simulation contribute to two sources of systematic uncertainty: the sensitivity to differences in the underlying truth distribution of the measured observables and the sensitivity to mismodeling of detector effects by the Monte Carlo generator that are not captured by the chosen input variables. The uncertainty ("unfolding prior") for the imperfect particle-level shape of the initial MC sample is assessed by reweighting the nominal MC sample at particle level such that it approximately agrees with data for the 24 observables. This reweighting function is constructed using a sequence of one-dimensional Gaussian-kernel functions, iteratively obtained from the data-to-MC ratio. The obtained data-driven correction is applied to the MC to obtain an "Asimov dataset" used as the input to the measurement, and the difference between the resulting measurement and the corresponding reweighted particle level MC is taken as the uncertainty. An uncertainty in the top-quark background is assessed as the full difference between measurements performed using two Asimov datasets constructed from MC predictions with and without the top-quark contribution. To assess the dependence on the detector response from modeling of features not included in the unfolding ("hidden variable uncertainty"), the measurement is performed with the alternative Drell-Yan MC sample with the particle-level shape of the 24 observables adjusted to match the nominal MC sample (see also [90–92] for similar procedures). Similarly, modeling of the non-Drell-Yan components (EW Zjj and ZV) are assessed as the full difference by performing the measurement with

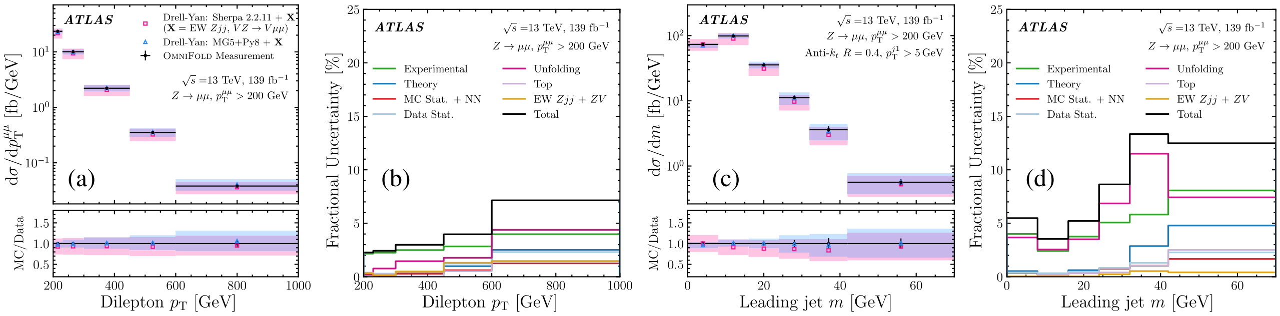

FIG. 1. Measured differential cross sections compared with particle-level predictions from SHERPA and MADGRAPH for two of the 24 directly measured observables: (a) $p_{\mathrm{T}}^{\mu\mu}$ with its (b) associated uncertainty breakdown, and (c) m_{j1} with its (d) associated uncertainty breakdown. For display purposes, binned (marginal) distributions are shown, though the measurement itself is unbinned and 24 dimensional.

and without these components added. Both of these variations are provided as separate event datasets that provided varied measurements (two-point uncertainties).

Four types of stochastic uncertainties are assessed: statistical uncertainties on the data and the MC training sets are each assessed by bootstrapping [93] (100 and 25 weights, respectively); an uncertainty due to the NN stability is calculated from the standard error on the median of weights of the 100 individual NNs; and an additional uncertainty is assigned for the limited statistics of the nominal event dataset. Overall, the total uncertainty in most bins chosen to illustrate the final measurement is between 3% and 5%, but can grow as large as 15% in tails of distributions. The unfolding uncertainty from the unfolding prior and hidden variables tends to be the dominant contributor for many observables, in particular for the ten jet substructure variables [see Fig. 1(d)].

The measured differential cross sections of $p_{\mathrm{T}}^{\mu\mu}$ and m_{j1}, in comparison with two MC predictions, are shown in Fig. 1 along with breakdowns of the associated measurement uncertainties. Plots of the measured spectra, associated uncertainty breakdown, and correlation matrices for all of the 24 directly measured observables are provided as Supplemental Material [94]. The total fiducial measured cross section is 1808 ± 42 fb. The differential measurements are significantly more precise than the predictions, in particular with respect to SHERPA. MADGRAPH generally models the data better than SHERPA, except for τ_1^{j2}, τ_2^{j2} and τ_3^{j2}. The measurement is publicly available as event datasets that contain the 24 observables and a series of event weights that define the measurement and systematic uncertainties via Refs. [95,96].

Figure 2 presents additional results constructed from the nominal measurement that highlight its flexibility of use. Figures 2(a)–2(c) show the differential cross sections of "derived" variables that were not directly unfolded, namely $\tau_{21} = \tau_2/\tau_1$ (the most widely used observable for hadronic W/Z boson identification [64,65]) and $\Delta R(\ell\ell, j1)$ (sensitive to higher-order effects). These observables are functions of two and eight of the 24 input variables, respectively. In the inclusive region, τ_{21} is not infrared and collinear (IRC) safe and therefore has no fixed-order perturbative expansion in α_S. It has been shown [97] that τ_{21} becomes IRC safe when applying a requirement on τ_1, and Fig. 2(b) shows an unprecedented measurement of τ_{21} in an IRC-safe fiducial volume defined by $\tau_1^{j_1} > 0.1$. Figure 2(d) shows a measurement of the average m_{j1} in bins

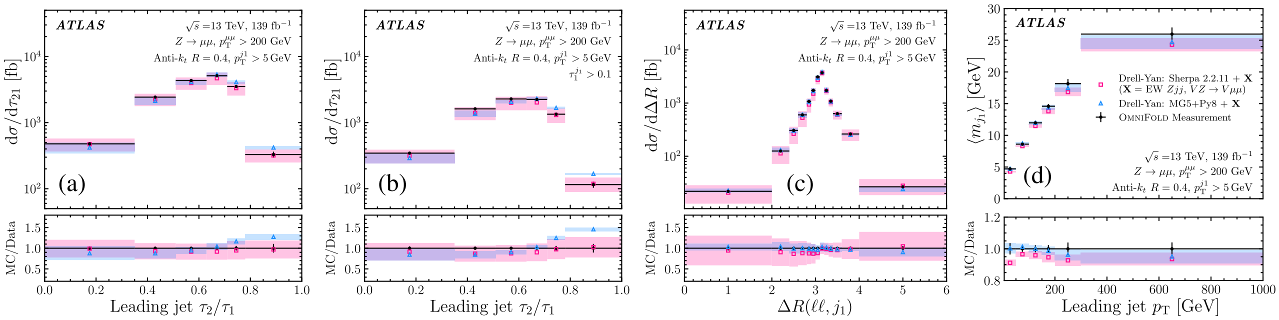

FIG. 2. Four measurements of quantities constructed from several of the 24 input observables, along with particle-level predictions from SHERPA and MADGRAPH: the jet substructure observable $\tau_{21}^{j1} = \tau_2^{j1}/\tau_1^{j1}$ in (a) the inclusive region and (b) the reduced region defined by $\tau_1^{j1} > 0.1$; (c) ΔR between the dilepton system and the leading jet; and (d) the average m_{j1} as a function of p_{T}^{j1}.

of $p_{\mathrm{T}}^{\mathrm{j1}}$, providing an example of a distribution useful for MC tuning. All of the derived observables can be calculated from the OMNIFOLD data event by event and be used to define bins with associated cross sections and uncertainties, just as for any of the 24 input variables.

The analysis was validated using a "pseudodata" sample constructed by reweighting the particle-level quantities in the alternative MC sample to resemble the real reconstruction-level data. Two such samples were generated: a high-statistics sample with weighted events and a datalike sample with unit weights obtained by bootstrapping the former sample. The full analysis was performed on the unit-weight pseudodataset, and the unfolding bias uncertainty was evaluated by assessing the closure between the OMNIFOLD result with the particle-level target. Chi-squared compatibility tests between the obtained measurements and the known underlying particle-level distributions for each of the $24 + 2$ observables all yielded p values > 0.07, except for $p_T^{j_1}$, with a p value of 0.038. A full analysis of the pseudodataset was also performed using IBU, where each observable was measured individually with the same binning and input data. The central values of the IBU measurements agree well within precision with the OMNIFOLD result. The IBU experimental, theoretical, unfolding, and statistical uncertainty components are also similar to those of the OMNIFOLD measurement in magnitude, shape, and resulting covariance. IBU also demonstrates a very similar performance in the closure test against the target. The total uncertainty was found overall to be similar, but tends to be somewhat larger for the OMNIFOLD measurement, primarily due to the NN initialization uncertainty that does not apply to IBU. The average bin uncertainty across all 24 observables was found to be 3.0% for IBU and 3.9% for OMNIFOLD. The uncertainty due to hidden variables does decrease for certain variables, but not generally, which is likely an indication that the detector response is not strongly covariate with the variables used for this measurement.

The OMNIFOLD result was then validated by performing χ^2 tests of differential spectra in dedicated kinematic subregions: high $p_{\mathrm{T}}^{\mu\mu}$ ($p_{\mathrm{T}}^{\mu\mu} > 250$ GeV), electroweak-enhanced ($m_{jj} > 200$ GeV, $\Delta y_{jj} > 2$), and diboson-enhanced ($m_{j1} > 32$ GeV). Chi-squared tests were performed against the pseudodata target within each subregion for all measured and several derived observables. All results yielded p values greater than 0.05, except for one observable (m_{j1}) in the electroweak-enhanced region, which had a p value of 0.02. The result was also validated in two-dimensional kinematic subregions, e.g., for $p_{\mathrm{T}}^{\mu\mu}$ vs $y_{\mu\mu}$, with p values > 0.05. Ablation studies on the input variables were performed to understand the effect of removing one or two variables from the unfolding procedure. These tests indicated that apart from a small number of cases in which critical variables including m_{j1}, m_{j2}, $p_{\mathrm{T}}^{\mathrm{j1}}$, and $p_{\mathrm{T}}^{\mathrm{j2}}$ were removed, removing almost any of the other twenty-four input variables still yielded excellent agreement within the quoted unfolding uncertainties. Stress tests were also performed to ensure the result is robust to nontrivial distortions. These included randomly and deterministically shifting and stretching the input spectra. No significant bias in the final result was observed.

The results of the validation tests were used to define a set of recommendations on how to use the provided datasets based on phase space coverage in data and simulation. The OMNIFOLD results are entirely unbinned, so the chosen binning is for presentation purposes only and is configurable. When choosing bins, certain best practices are recommended to help ensure that the number of MC and data events per bin yield sufficient support for the unfolding and stable uncertainties. These recommendations are detailed in the User Guide found in Supplemental Material [94], and examples of use are provided in the interactive PYTHON notebooks associated with the published unbinned datasets [95].

In conclusion, this Letter presents an unbinned unfolded cross-section measurement of $Z +$ jets events using $139\ \mathrm{fb}^{-1}$ of proton-proton collisions at $\sqrt{s} = 13$ TeV collected with the ATLAS detector at the LHC. The 24 observables treated in this analysis are simultaneously unfolded using the machine learning method OMNIFOLD. These results demonstrate that collider data can be unfolded in an unbinned manner and that the result can be reanalyzed at the event level, allowing researchers significant increased utility such as adjusting binning and constructing new observables from the 24 provided ones. This flexibility makes it possible to probe kinematic regimes and observables not originally foreseen, which can enable numerous physics use cases including strong tests of QCD and detailed tuning of MC event generators.

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End Matter

Appendix—The OMNIFOLD method [39,40] is illustrated in Fig. 3 and briefly reviewed here. The approach takes two event samples as input: (1) an MC sample containing events with both particle-level ($\vec{x}_\mathrm{p}$) and detector-level ($\vec{x}_\mathrm{r}$) information, and (2) the reconstructed data, where $\vec{x}$ is a list of the 24 event-level observables: $\vec{x} = (p_\mathrm{T}^{\mu\mu}, \ldots, \tau_3^{j2})$. The MC sample encodes information about the detector response such as energy and momentum resolution, particle and selection inefficiencies. The method is based on a multidimensional reweighting: at each step, a smooth weighting function is obtained using the event observables $\vec{x}$. First, it corrects reconstructed-level MC to match data with weights $\omega(\vec{x}_\mathrm{r})$. Next, an improved MC prediction is achieved by propagating $\omega(\vec{x}_\mathrm{r})$ to the particle level $\vec{x}_\mathrm{p}$. Then, a new reweighting function $\nu(\vec{x}_\mathrm{p})$ is obtained by reweighting the particle-level prediction to the improved one from the previous step. It should be noted that $\nu(\vec{x}_\mathrm{p})$ itself does not rely on the detector level input, even if this was crucial in the derivation of it. Event weights defined by $\nu(\vec{x}_\mathrm{p})$ is then propagated back through the MC to the detector level, resulting in an improved prediction to the data compared to the initial MC. The method is repeated iteratively; the updated reweighting function becomes a product of the previous one until a predefined number of iterations are performed, when the method stops.

The reweighting functions used in OMNIFOLD are based on the output $f(\vec{x})$ of NNs trained with a weighted binary cross-entropy loss function:

$$\mathcal{L}[f(\vec{x})] = -\sum_{i\in A} w_i \log[f(\vec{x}_i)] - \sum_{i\in B} w_i \log[1 - f(\vec{x}_i)], \quad \text{(A1)}$$

where the w_i are event weights for datasets A and B, with associated (joint) probability densities $p_A(\vec{x})$ and $p_B(\vec{x})$. With this choice of loss function, the produced NN classifier $f(\vec{x})$ can be used to define the quantity $\omega(\vec{x}) \equiv f(\vec{x})/[1 - f(\vec{x})]$, which is known to asymptotically approach the likelihood ratio $p_A(\vec{x})/p_B(\vec{x})$ [99,100], assuming A and B are normalized to unity ($\sum_A w_i = \sum_B w_i = 1$). This quantity is used to perform the 24-dimensional shape reweighting in the first and third step of the OMNIFOLD method. The correction in the second and fourth step is applied to each event i in sample B by updating the event weights by $w_i \mapsto w_i \omega(\vec{x}_i)$.

In the first reweighting step of OMNIFOLD, Sample A is data and Sample B is detector-level MC simulation. Each event weight $w_i = 1$ for data, while for MC simulation, w_i

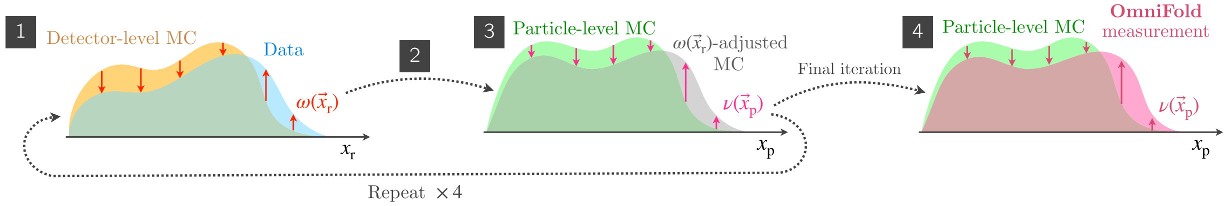

FIG. 3. Illustration of the OMNIFOLD method. First, MC is corrected to match data at the detector level. Second, particle-level MC is adjusted by propagating the learned correction through the MC using a weighting function $\omega(\vec{x}_\mathrm{r})$. Third, a new correction $\nu(\vec{x}_\mathrm{p})$ is learned based on particle-level quantities only. Finally, $\nu(\vec{x}_\mathrm{p})$ is propagated through the MC back to the detector level achieving an improved agreement to data. The method proceeds iteratively four more times, achieving a combined function $\nu(\vec{x}_\mathrm{p})$ that reweights the MC such that the event yields and kinematics match those observed in the data.

is initialized as the nominal MC sample weights. Both samples are normalized such that $\sum_i w_i = 1$, and the MC event weights are updated for each iteration as described above. In the second reweighting step of OMNIFOLD, Samples A and B both have the same events and kinematics $\vec{x}_\mathrm{p}$, but the weights for A are taken as $\omega(\vec{x}_r)$ from the previous step. The reweighting then takes place using only particle-level quantities.

This analysis does not subtract the background as it is small ($< 0.25\%$). A natural way to subtract backgrounds as part of the OMNIFOLD procedure with nontrivial backgrounds would be to add negatively weighted MC events to the A dataset, such that in total, A corresponds to data with background subtracted [40]. The differential acceptance and efficiency are accounted for naturally by events satisfying one of the detector-level or particle-level event selections, but not both. Events that do not carry an updated weight from the previous step are assigned the average weight in their region of phase space x using Eq. (A1) [40].

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