Response to Comments from Reviewer 2

amt-2019-200 Total variation of atmospheric data: covariance minimization about objective functions to detect conditions of interest Nicholas Hamilton

There is some good content and work here, with a generalized method to find conditions of interest for multivariate timeseries; and (perhaps more importantly) inclusion of responsible application of a metric (Mahalonbis distance) to evaluate sensitivity of the method to outliers.

Thank you for taking the time to review my submission. I appreciate your concise and direct comments and, in addressing them, I think you will see that the manuscript has been greatly improved. It pleases me that the intended message of the work has been clearly understood and well received. I have provided a brief response to each of the points you raised in the review of my work and, where appropriate, also included any additions or subtractions from the manuscript.

The title is perhaps not quite appropriate; "Total variation of atmospheric data" is rather vague and somewhat grandiose, not accurately capturing the essence of the work and connoting more results/applicability than demonstrated.

I think that your suggestion is correct. The title never felt like it was perfectly suited to the content of the manuscript. Accordingly, the title has been changed to, "Atmospheric condition identification in multivariate data through a metric for total variation", which I believe more concisely conveys the intent of the work and communicates its scope as the development of an analysis and quality control method.

Some significant items of note, as a list:

In the abstract, 'periods' of interest is better expressed as 'conditions', both for the sake of validation and for getting conditional statistics (and towards making fair comparisons of statistics given some conditions).

I think that the suggested change from 'periods' to 'conditions' is appropriate. While the method is designed to quantify the total variability within a continuous time period, it is the identification of atmospheric events or conditions of interest that is the real objective.

Stationarity and conditional statistics underpin this written work; these concepts should be integrated (and referenced, as found in various texts for atmospheric flows), at least starting with the literature review.

The reviewer is correct to point out that the concept of statistical stationarity is one of the main concepts driving the current work. From the fundamental turbulence perspective, the term stationarity is not really expected to apply to data from an

inherently dynamical system (the atmosphere) over periods of this duration. However, the term 'stationary' is also familiar to the atmospheric science community, and has now been mentioned explicitly, as suggested by the reviewer. A statement has been added to Section 4 to underpin the importance of stationarity, "Statistical stationarity (i.e. time-independence of statistical quantities) is a common consideration in turbulence and atmospheric science (Chenge and Brutsaert, 2005; Metzger et al., 2007; Vincent et al., 2010, 2011; Guala et al., 2011). Stationarity is not often assumed for wind energy research and modeling applications, although it is rarely quantified or even considered in validation data."

In your literature review, a key method/scheme for event detection (beyond wavelets) appears to be missing: i.e., reference-signal (or ideal signal) approaches based on Hilbert transform, as in Hristov et al (1998, PRL 81 no.23), used in various literature (e.g. Kelly, Wyngaard & Sullivan 2009).

I would like to thank the reviewer for pointing out this method for detection of atmospheric conditions. A statement has been added to the introduction including the above references.

"Another method for parsing atmospheric conditions found in the literature leverages the Hilbert transform, which convolves time series signals with the Cauchy kernel and results in a phase-shifted set of Fourier components. This method has been used successfully to relate ocean wave conditions to atmospheric conditions through the use of a reference signal (Hristov et al., 1998) and has successfully been extended to turbulence modeling (Sullivan et al., 2000; Kelly et al., 2009) and to relate turbulent motions of various scales within the atmospheric boundary layer (Mathis et al., 2009). Previous use of the reference-signal method (Kelly et al., 2009) required the use of a periodic reference signal, which does not lend itself easily to the detection of nonperiodic atmospheric events, and strongly-correlated ocean wave and turbulent velocity data, which are not available for the majority of wind plant data sets."

When you mention "direct comparison of statistical quantities", it appears that you are trying to refer to statistics based on marginal distributions (or marginal statistics), are you not? In statistical parlance, one contrasts between marginal and conditional statistics.

The reviewer is correct, and that sentence was intended to describe comparison of marginal statistical quantities. The sentence in the introduction has been changed to read,

"Consideration of these variables independently may not provide a complete picture of the state of the atmosphere, as they are inherently correlated (Holtslag and Nieuwstadt, 1986; Kaimal et al., 1976); each variable offers a limited range of insights as to the dynamical state of the atmosphere relevant to the operation of wind energy assets. Direct comparison of the marginal distributions of atmospheric variables aggregates observations without regard to the value of other, potentially correlated variables. Even the use of conditional statistical distributions or measures discounts any dynamic coupling between them and may not fully describe the nature of the atmospheric physics (Hannesdóttir and Kelly, 2019; Preston et al.,

2009;Shahabi and Yan, 2003)."

The premise "In lieu of a time series of Richardson number or the Monin-Obukhov stability parameter, turbulence intensity (TI) is used in the current demonstration as a proxy for stability" is fundamentally problematic. That is, the balance of mechanical (shear) production, buoyant production or destruction, and dissipation ε (defining the 'simple' conditions where Monin-Obukhov similarity applies) results in TI being a proxy for stability only for flows/conditions with the same dissipation rate (Kelly, Larsen, Dimitrov & Natarajan, 2014). So your results per TI are conditional on ε , and do not act as such a proxy unless further constrained (e.g. via U assuming surface-layer similarity for ε .) Since stability is not really used in the paper, I suggest that you simply keep TI, and change the justification for its use: σ u and TI are important for driving turbine loads (e.g. Dimitrov, Kelly, Vignaroli & Berg 2018).

Thank you for your concise description of the issue of regarding TI as a proxy for metrics of atmospheric stability. This is an important point to consider when making decisions as to how one should quantify the state of the atmosphere considering the data available. In the current case, as noted by the reviewer, stability is not discussed outside of the referenced section, given that temperature and/or heat flux information are not available for the data used in the current demonstration, it would probably be better to focus the narrative around TI as a relevant quantity of interest for wind turbine loads and wake modeling. The previous framing of the discussion arose from the intent to state that stability is an important factor in describing the state of the atmosphere, while conceding that TI is the quantity considered in many wind energy applications. The relevant excerpt has been changed to read,

"Data used in the current work does not contain any observations of the temperature or heat flux between the atmosphere and the ocean surface, and thus no estimate for the traditional stability metrics are available. Turbulence intensity (TI), although an imperfect proxy of atmospheric stability from a fluid mechanical or atmospheric perspective, provides some sense of the energy contained in the fluctuating flow field, and is well-suited for presenting the utility of the total variation method below. Additionally, TI is a quantity frequently used in the wind energy community to characterize wind plant operating conditions and structural loading of wind turbines (Kelly et al., 2014; Dimitrov et al., 2018) and is often accessible through instrumentation on met masts or wind turbine nacelles making it an appropriate choice for the current demonstration."

In section 3, where you write "without explicitly considering the evolution of atmospheric variables" you should mention stationarity as well. In the atmospheric sciences and boundary-layer meteorology this is typically considered, whereas it is often neglected in wind energy applications.

A similar point from the reviewer regarding the discussion of statistical stationarity has been addressed above. A brief statement has been added to Section 3, noted by the reviewer, reading,

"Considering atmospheric variables in terms of either their marginal distributions (as in Fig. 2 or their conditional distributions (as in Figs. 3 and 5) falls short of saying anything about the dynamics embedded in those observations. Steady-state wake models are defined to represent the timeaveraged flow behind a wind turbine and higher-fidelity models assume that the bulk flow speed and direction do not change in time. Effective validation of numerical modeling tools for wind energy requires that observations conform to stationary atmospheric flow (Chenge and Brutsaert, 2005; Metzger et al., 2007; Vincentet al., 2010, 2011; Guala et al., 2011) or represent a dynamic event of interest."

Figure 5: missing axis values/scales

I must apologize for the rendering of the figure. I believe that the axis labels were not included in the typeset document for some reason. In the revised version of the manuscript, Section 3, describing the statistical view of atmospheric conditions, has been reduced in length. Because the 3D histogram did not add significantly to the discussion of the distributions of atmospheric variables beyond the 2D histograms, the figure and associated discussion has been removed.

Section 4: can you interpret the total variation in terms of the multivariate components, to avoid obfuscation? Section 4.0 (p.8) is essentially taken from PCA; you should include reference to appropriate PCA text(s) and try to explain V for the reader. E.g., for readers not as 'fluent' in statistics, if the PC's (P) are orthogonal, then how are the covariances accounted for?

The formulation leading to the total variation does include an eigendecomposition of the covariance matrix and is in fact related derived from PCA. The method was defined this way because PCA was one of the methods originally considered during the analysis. Because the principal components are not identical to the original variances, they must include information from the covariances. That said, the sum of the principal components is also equal to the trace of the covariance matrix, which remains difficult to relate to the covariances between variables. In subsequent work, I found that the determinant of the covariance matrix also reduces the covariance matrix to a single metric that quantifies its variability. In fact, for the current study, the determinant method and the PCA method rank the variability of continuous time periods in the same order, although the numerical value is a bit different. The formulation has been updated using the determinant method, which also happens to be a more direct means at arriving at \$\mathcal{V}\$.

"The total variation, V, of a given regularized data block, D, is expressed as the determinant of the respective correlation matrix,

$V = det(C) \tag{6}$

Larger values of Vindicate that the data points are more dispersed in the condition space. In the observational data of the atmosphere discussed here, V>0. The case of V= 0 would indicate that the full n-dimensional condition space is not occupied and some of the variables are perfectly correlated with, i.e. linearly dependent on, some of the others. Metrics of the variation of a multivariable dataset have some history in the literature. Notable past contributions include the pooled10variance method to estimate population variance from those of distinct samples Ruxton (2006), and the 'total' or 'overall' variability Goodman (1968); Anderson (1962) which combine variances of individual variables either linearly or in a sum of squares sense. The generalized variance (Wilks, 1932; Sengupta, 2004), shares a common formulation withV, but has historically been applied to a p-dimensional

random vector. In contrast, the total variation merges n distinct variables, whose relationship need not be known a priori, and seeks the determinant of the associated correlation matrix"

Is your V different than the 'overall' or 'total' variability found in literature? It could help also to point out the difference between summative variance and V.

These are good points and, given their similarity, I have decided to answer together. I take it that the reviewer is suggesting that the total variation method be more clearly related or disambiguated from other statistical measures of variability. The metrics total variability, overall variability, and summative variance in common use have slightly definitions and interpretations from the total variation introduced in the current work. Briefly,

Total variability is defined as the sum of squares total of difference between expected or mean value and observed qualities.

Overall variability refers generally to the variance or standard deviation of a population (i.e. a group of samples considered together).

Summative or **pooled variance** refers to the inferred variance of a population of observations from the collection of sample variances.

In contrast, the total variation used in the current work reduces the covariance between normalized variables to a single value through the determinant of the covariance matrix.

A close analog to this method is the generalized variance of a multi-dimensional random vector. Generalized variance was introduced by Wilks as a scalar measure of overall multidimensional scatter. However, in most formulations of generalized variance, the data are considered as a p-dimensional vector. The current work uses the same mathematical operations but applies them to distinct variables that have been merged into a matrix. Mechanically, the same operations are being applied to the data, but given the distinction in formulation, I have elected to maintain the current jargon of 'total variability'. A statement has been added to the introduction with references to some other metrics of variability.

"The metric used to quantify the overall variability of the atmosphere within any given time period is closely related to the generalized variance as per Wilks (1932); Sengupta (2004), but is distinct in that it is applied to a collection of variables rather than a multi-dimensional vector."

Figure 8: suggestion: use logarithmic scale on y-axis to compare more sensibly I thank the reviewer for the suggestion, although I'm not sure I entirely understand what the purpose of logarithmic scaling would be. The figure displays the atmospheric variables considered during time periods with minimum or maximum values of V Given that the data do not span multiple orders of magnitude, rescaling the axes is not expected to add to the interpretation of the data.

Fig.9c: which "dimensionless slope" are you using here?

The dimensionless slope referenced in the caption of Figure 9c refers to the coefficient c_0 in eq. (7). While all of the coefficients in relationships seen in eqs. (7) - (9) are dimensionless due to the normalization of the variables, the phrasing is a bit difficult to follow. All of the subplots captions have been updated accordingly.

Fig.11: captions are swapped between (c) and (d).

Thanks for catching this oversight. The figure captions have been updated.

Please also note the supplement to this comment:

Additional (minor) comments found in the marked-up document have all been addressed in the manuscript. Thank you for the detailed review of the work. I feel that it is substantially improved due to your thoughtful comments.