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Special Section on Uncertainty and Parameter Space Analysis in Visualization

Visualizing the stability of critical points in uncertain scalar fields

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ABSTRACT

In scalar fields, critical points (points with vanishing derivatives) are important indicators of the topology of iso-contours. When the data values are affected by uncertainty, the locations and types of critical points vary and can no longer be predicted accurately. In this paper, we derive, from a given uncertain scalar ensemble, measures for the likelihood of the occurrence of critical points, with respect to both the positions and types of the critical points. In an ensemble, every instance is a possible occurrence of the phenomenon represented by the scalar values. We show that, by deriving confidence intervals for the gradient and the determinant and trace of the Hessian matrix in scalar ensembles, domain points can be classified according to whether a critical point can occur at a certain location and a specific type of critical point should be expected there. When the data uncertainty can be described stochastically via Gaussian distributed random variables, we show that even probabilistic measures for these events can be deduced.

1. Introduction

Scalar ensembles consist of several scalar fields, where every field or instance indicates a possible occurrence of the phenomenon represented by the data values. Ensembles are often generated numerically via multiple simulation runs with slightly perturbed input parameter settings. The rationale stems from the observation that the result of every run is affected by a certain degree of uncertainty, for instance, due to model simplifications or approximations inherent to the numerical schemes employed. Generating multiple instances helps predict and quantify the range of outcomes and, thus, allows us to classify features with respect to their stability across instances.

An important class of features in scalar fields is based on level-sets or iso-contours, i.e., the set of all points in the domain where the scalar field takes on a prescribed value, also called an iso-value. The effect of uncertainty on level-sets has been treated in several works [1,2], or [3], which investigate the positional variations of level-sets due to uncertainty. Such an analysis, however, does not allow making reliable estimates of the possible geometric or topological variations of level-sets.

Recently, Pfaffelmoser et al. [4] have looked into the effect of uncertainty on the variability of gradients in scalar fields. Indicators for the likelihood of geometric changes of level-sets were derived from confidence intervals of the gradient magnitude and orientation, resulting in a stability analysis of both the shape and the slope of level-sets. By using a similar technique to propagate uncertainty for derived quantities in scalar fields that are linear combinations of the input values, and by introducing a method for non-linear combinations, we propose techniques to classify critical points in scalar ensemble fields with respect to different notions of stability. Interesting features often relate to critical points, since these indicate prominent surface components and their topological changes. Depending on the position and type of the critical points, the spatial locations where changes in the surface topology take place and the nature of these changes can be identified: surface components emerge or vanish at minima and maxima, join or split at saddles.

Contribution: We investigate the associated gradient and Hessian matrix fields of the scalar ensemble members to identify the possible locations of the critical points, and assess their stability in type throughout the ensemble. We first summarize ensembles statistically and derive corresponding moments for the gradients. Since critical points occur where the gradients vanish, we use confidence intervals of the gradients to obtain quantities indicating the possibility of a critical point occurring around a given location. We then derive statistical summaries for the trace and determinant of the Hessian matrix, to give insight into the tendency of critical points to behave like minima, maxima, or saddles near a specified location in the ensemble.

The remainder of the paper is as follows: in the next section we review related work. We then introduce methods to analyze critical points in Section 3, which we visualize in Section 4. The proposed approaches are validated in Section 5 and demonstrated on two synthetic and two real world data sets in Section 6. We conclude the paper with a summary of the contributions.

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2. Related work

Uncertainty is a topic relevant to many research domains, and has been classified among the top research areas in visualization. Overviews of uncertainty visualization approaches are given, for instance, by Griethe and Schumann [5], Thomson et al. [6], or Potter et al. [7].

Uncertainty information has often been summarized by quantities such as mean and standard deviation, which have been encoded together with the actual data by means of color maps, opacity, texture, animation, glyphs, etc., by, for example Wittenbrink et al. [8], Djurcilov et al. [9], Rhodes et al. [10], Lundstrom et al. [11], and Sanyal et al. [12]. Although such methods indicate the amount of uncertainty affecting the data, they do not allow drawing conclusions on the way uncertainty affects specific features of the data, such as level-sets.

Several approaches have been proposed to visualize the effect of uncertainty on the position and structure of such features: Pang et al. [13] and Zehner et al. [14] use confidence envelopes containing an isosurface with a certain confidence, Grigoryan and Rheingans [15] displace each point on a surface along its surface normal to an extent proportional to the local uncertainty, while Brown [16] uses surface animation to illustrate the uncertainty of the values within different areas of the surface. Pfaffelmoser et al. [1] examine the positional and geometrical variation of level-sets, whereas Pfaffelmoser and Westermann [17,18] incorporate correlation to offer insight into possible structural variations. Pöthkow and Hege [2] use the concept of numerical condition – the sensitivity of the output of a function to perturbations of the input data – to extract features in uncertain scalar fields, and apply it to visualize the positional uncertainty of level-sets. The proposed method was extended to include spatial correlation in Pöthkow et al. [19].

Further approaches to gain insight into salient features and their structure are based on topology. Overviews of methods dealing with topological features for both static and dynamic scalar fields, and especially for steady and time-dependent vector fields, are given by Theisel et al. [20], Laramee et al. [21], and Scheuermann and Tricoche [22]. For ensembles of uncertain scalar fields, Thompson et al. [23] introduce hixels – per sample histograms of values – to approximate topological structures of down-sampled data. Then, Wu and Zhang [3] enhance contour trees to represent uncertainty in the data values of the scalar fields and the position of the contours, as well as the variability of the contour trees themselves.

For uncertain vector fields, Otto et al. [24] generalize the concepts of stream lines and critical points to uncertain (Gaussian) vector field topology, in order to segment the topology by integrating particle density functions. Probabilistic local features, such as critical points, are extracted from Gaussian distributed vector fields using Monte Carlo sampling in Petz et al. [25], where the mathematical model for uncertainty considers the effect of spatial correlations. The method was extended to several types of non-parametric models for uncertainty by Pöthkow and Hege [26]. A fuzzy topology is proposed by Bhatia et al. [27], where the topological decomposition is performed by growing streamwaves, based on a representation for vector fields called edge maps. In the context of tractography, Schultz et al. [28] interpret critical points and other topological concepts based on probabilistic fiber tracking.

Numerous techniques have been introduced to assess different types of variations that uncertainty induces on level-sets and other such data features. To the best of our knowledge, however, no methods have been proposed to analyze and visualize the possible variations of critical points that are caused by uncertainty. Investigating different aspects of the stability of critical points and how uncertainty affects them would be beneficial, since critical points are indicative of prominent features and their topological changes, and such an analysis could serve as a starting point for further insight into the effects of uncertainty on level-sets and other related features.

While such studies have not been performed for uncertain data sets, critical points have been classified before according to different measures of stability and importance, for various purposes. For scalar fields, Edelsbrunner et al. [29] introduce the notion of homological persistence to assign importance measures to critical points and use it for topology simplification. Dey and Wenger [30] extend this notion to interval persistence, to assess which critical points are stable under perturbations of the scalar fields. Reininghaus et al. [31] use the persistence at multiple scales in scale space, to distinguish between minima and maxima with hill-, ridge-, or outlier-like spatial extent.

Topological persistence is used in the context of MS complexes, which decompose manifolds into regions of uniform gradient flow behavior to investigate the topology of the surfaces. Segmenting the surface into cells of uniform flow helps identify its various features and the way they are connected. Critical points, connected by lines of steepest descent, are the nodes of the MS complex. Successively eliminating critical points with an importance measure under a certain threshold results in a hierarchy of MS complexes, e.g., Bremer et al. [32] or Edelsbrunner et al. [33]. The methods require nonetheless a series of assumptions, as well as numerical integration. For these reasons and because we are interested exclusively in stability aspects of the critical points themselves, we do not compute MS complexes, even though we also use the gradient vector fields and Hessian matrices in our analysis.

For vector fields, various measures have been used to classify the importance of critical points, such as the Euclidean distance between critical points in Tricoche et al. [34] or the area of their corresponding flow regions in the topology graph in De Leeuw and Van Liere [35]. Wang et al. [36] use the topological notion of robustness to quantify the stability of critical points with respect to perturbations for stationary and time-varying vector fields.

3. Critical points in ensembles

Critical points of scalar fields are those points where the gradient vector vanishes. Several methods can be applied to locate critical points in scalar data sets: finding the crossings of the zero-contours of the x- and y-components of the gradient vector field, or the grid points with non-zero Poincaré indices, etc. The locations of critical points, however, are affected by the uncertainty in the data, which causes variations in the positions and types of critical points throughout the ensemble. We are therefore interested to indicate how likely it is that a critical point occurs around a given location and, if so, whether a certain kind of behavior should be expected there. In the following, we use two notions of stability: *positional stability* refers to locations around which critical points occur repeatedly in the ensemble members, while *type stability* is used to characterize the positions near which critical points of the same nature emerge consistently throughout the ensemble.

To this purpose we do not use the actual critical points of the individual ensemble members. Instead, we derive two types of indicator functions at every vertex of a Cartesian grid and show the chances of a critical point of a certain type occurring close to the vertices, i.e., the stability in position and type. As gradients and Hessian matrices are fundamental to finding critical points and their types, we summarize these quantities statistically via confidence intervals and use them to derive the indicators.