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.

Keywords: uncertainty, critical points, stability, scalar topology

11. Introduction

Scalar ensembles consist of several scalar fields, where evs ery field or instance indicates a possible occurrence of the phe-4 nomenon represented by the data values. Ensembles are of-5 ten generated numerically via multiple simulation runs with 6 slightly perturbed input parameter settings. The rationale stems 7 from the observation that the result of every run is affected by a 8 certain degree of uncertainty, for instance, due to model simpli-9 fications or approximations inherent to the numerical schemes 10 employed. Generating multiple instances helps predict and quan-11 tify the range of outcomes and, thus, allows us to classify fea-12 tures with respect to their stability across instances.

An important class of features in scalar fields is based on 14 level-sets or iso-contours, i.e., the set of all points in the domain 15 where the scalar field takes on a prescribed value, also called 16 an iso-value. The effect of uncertainty on level-sets has been 17 treated in several works [1], [2], or [3], which investigate the 18 positional variations of level-sets due to uncertainty. Such an 19 analysis, however, does not allow making reliable estimates of 20 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 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 techon niques to classify critical points in scalar ensemble fields with

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³¹ respect to different notions of stability. Interesting features of-³² ten relate to critical points, since these indicate prominent sur-³³ face components and their topological changes. Depending on ³⁴ the position and type of the critical points, the spatial locations ³⁵ where changes in the surface topology take place and the nature ³⁶ of these changes can be identified: Surface components emerge ³⁷ 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 at 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 demonst strated on two synthetic and two real world data sets in Section 56. We conclude the paper with a summary of the contributions.

56 2. Related Work

⁵⁷ Uncertainty is a topic relevant to many research domains, ⁵⁸ and has been classified among the top research areas in visual-⁵⁹ ization. Overviews of uncertainty visualization approaches are ⁶⁰ given, for instance, in Griethe and Schumann [5], Thomson et ⁶¹ al. [6], or Potter et al. [7]. 62 ⁶³ tities such as mean and standard deviation, which have been ¹²⁰ by uncertainty. Investigating different aspects of the stability of e4 encoded together with the actual data by means of color maps, 121 critical points and how uncertainty affects them would be ben-65 opacity, texture, animation, glyphs, etc., in, for example Wit-66 tenbrink et al. [8], Djurcilov et al. [9], Rhodes et al. [10], 67 Lundstrom et al. [11], and Sanyal et al. [12]. Although such 68 methods indicate the amount of uncertainty affecting the data, ⁶⁹ they do not allow drawing conclusions on the way uncertainty ⁷⁰ affects specific features of the data, such as level-sets.

Several approaches have been proposed to visualize the ef-71 72 fect of uncertainty on the position and structure of such fea-⁷³ tures: Pang et al. [13] and Zehner et al.[14] use confidence 74 envelopes containing an isosurface with a certain confidence, 75 Grigoryan and Rheingans [15] displace each point on a sur-76 face along its surface normal to an extent proportional to the 77 local uncertainty, while Brown [16] uses surface animation to 78 illustrate the uncertainty of the values within different areas of 79 the surface. Pfaffelmoser et al. [1] examine the positional and ⁸⁰ geometrical variation of level-sets, whereas Pfaffelmoser and ⁸¹ Westermann [17], [18] incorporate correlation to offer insight ⁸² into possible structural variations. Pöthkow and Hege [2] use 83 the concept of numerical condition - the sensitivity of the out-84 put of a function to perturbations of the input data - to extract 85 features in uncertain scalar fields, and apply it to visualize the 86 positional uncertainty of level-sets. The proposed method was 87 extended to include spatial correlation in Pöthkow et al. [19].

Further approaches to gain insight into salient features and 88 89 their structure are based on topology. Overviews of methods ⁹⁰ dealing with topological features for both static and dynamic 91 scalar fields, and especially for steady and time-dependent vec-⁹² tor fields, are given in Theisel et al. [20], Laramee et al. [21], 93 and Scheuermann and Tricoche [22]. For ensembles of uncer-⁹⁴ tain scalar fields, Thompson et al. [23] introduce hixels - per 95 sample histograms of values - to approximate topological struc-⁹⁶ tures of down-sampled data. Then, Wu and Zhang [3] enhance 98 scalar fields and the position of the contours, as well as the vari-⁹⁹ ability of the contour trees themselves.

For uncertain vector fields, Otto et al. [24] generalize the 100 101 concepts of stream lines and critical points to uncertain (Gaus-¹⁰² sian) vector field topology, in order to segment the topology by ¹⁰³ integrating particle density functions. Probabilistic local fea-104 tures, such as critical points, are extracted from Gaussian dis-105 tributed vector fields using Monte Carlo sampling in Petz et 106 al. [25], where the mathematical model for uncertainty consid-107 ers the effect of spatial correlations. The method was extended 108 to several types of non-parametric models for uncertainty in ¹⁰⁹ Pöthkow and Hege [26]. A fuzzy topology is proposed in Bhatia 110 et al. [27], where the topological decomposition is performed 111 by growing streamwaves, based on a representation for vector 112 fields called edge maps. In the context of tractography, Schultz 167 the uncertainty in the data, which causes variations in the posi-113 et al. [28] interpret critical points and other topological con-114 cepts based on probabilistic fiber tracking.

Numerous techniques have been introduced to assess dif-115 116 ferent types of variations that uncertainty induces on level-sets 117 and other such data features. To the best of our knowledge, 118 however, no methods have been proposed to analyze and vi-

Uncertainty information has often been summarized by quan- 119 sualize the possible variations of critical points that are caused 122 eficial, since critical points are indicative of prominent features 123 and their topological changes, and such an analysis could serve 124 as a starting point for further insight into the effects of uncer-125 tainty on level-sets and other related features.

> 126 While such studies have not been performed for uncertain 127 data sets, critical points have been classified before according to 128 different measures of stability and importance, for various pur-129 poses. For scalar fields, Edelsbrunner et al. [29] introduce the 130 notion of homological persistence to assign importance mea-¹³¹ sures to critical points and use it for topology simplification. 132 Dey and Wenger [30] extend this notion to interval persistence, 133 to assess which critical points are stable under perturbations of 134 the scalar fields. Reininghaus et al. [31] use the persistence at 135 multiple scales in scale space, to distinguish between minima 136 and maxima with hill-, ridge-, or outlier-like spatial extent.

> 137 Topological persistence is used in the context of MS com-138 plexes, which decompose manifolds into regions of uniform 139 gradient flow behavior to investigate the topology of the sur-140 faces. Segmenting the surface into cells of uniform flow helps 141 identify its various features and the way they are connected. 142 Critical points, connected by lines of steepest descent, are the 143 nodes of the MS complex. Successively eliminating critical 144 points with an importance measure under a certain threshold re-145 sults in a hierarchy of MS complexes. e.g., Bremer et al. [32] or 146 Edelsbrunner et al. [33]. The methods require nonetheless a se-147 ries of assumptions, as well as numerical integration. For these 148 reasons and because we are interested exclusively in stability 149 aspects of the critical points themselves, we do not compute ¹⁵⁰ MS complexes, even though we also use the gradient vector 151 fields and Hessian matrices in our analysis.

152 For vector fields, various measures have been used to clas-153 sify the importance of critical points, such as the Euclidean dis-97 contour trees to represent uncertainty in the data values of the 154 tance between critical points in Tricoche et al. [34] or the area 155 of their corresponding flow regions in the topology graph in De 156 Leeuw and Van Liere [35]. Wang et al. [36] use the topological 157 notion of robustness to quantify the stability of critical points ¹⁵⁸ with respect to perturbations for stationary and time-varying 159 vector fields.

160 3. Critical Points in Ensembles

Critical points of scalar fields are those points where the 161 162 gradient vector vanishes. Several methods can be applied to lo-163 cate critical points in scalar data sets: finding the crossings of $_{164}$ the zero-contours of the x- and y-components of the gradient 165 vector field, or the grid points with non-zero Poincaré indices, 166 etc. The locations of critical points, however, are affected by 168 tions and types of critical points throughout the ensemble. We 169 are therefore interested to indicate how likely it is that a critical 170 point occurs around a given location and, if so, whether a cer-171 tain kind of behavior should be expected there. In the following, 172 we use two notions of stability: Positional stability refers to lo-173 cations around which critical points occur repeatedly in the en¹⁷⁴ semble members, while *type stability* is used to characterize the ¹⁷⁵ positions near which critical points of the same nature emerge ¹⁷⁶ 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 ted confidence intervals and use them to derive the indicators.

185 3.1. Confidence Intervals

186 For scalar data sets given at the vertices of a 2D Cartesian 187 grid structure, the data uncertainty is modeled by a multivariate ¹⁸⁸ random variable *X*, with components $X_{i,j}$ at each grid point $x_{i,j}$. 189 We express the range of possible data values at each vertex us-¹⁹⁰ ing intervals, $[\mu(X_{i,j}) - \sigma(X_{i,j}), \mu(X_{i,j}) + \sigma(X_{i,j})]$, where $\mu(X_{i,j})$ ¹⁹¹ is the mean value and $\sigma(X_{i,j})$ the standard deviation - a measure 192 of the data variability at the grid point. For specific probabil-¹⁹³ ity distributions of the random variables, confidence intervals 194 of various confidence levels can be constructed. The aforemen-¹⁹⁵ tioned interval corresponds to a 68% confidence level for a 1D Gaussian distributed variable, i.e., there is a 68% probability 196 that the true value lies in the confidence interval. In the fol-198 lowing, we call $[\mu(X_{i,j}) - \sigma(X_{i,j}), \mu(X_{i,j}) + \sigma(X_{i,j})]$ a confidence ¹⁹⁹ interval irrespective of the probability distribution, although we 200 assign confidence levels only for Gaussian distributions.

The uncertainty in the data also affects the variability of de-²⁰² rived quantities that depend on the values at neighboring grid ²⁰³ points, such as partial derivatives. To quantify the latter, we ex-²⁰⁴ press the derived quantities in terms of functions of the random ²⁰⁵ variables at neighboring vertices, and propagate the uncertainty ²⁰⁶ from the input variables to the outputs. We thus obtain confi-²⁰⁷ dence intervals for the derived quantities. The exact procedure ²⁰⁸ depends on the function relating the input to the output.

Propagating the uncertainty for first-order partial derivatives, 209 ²¹⁰ where the functions approximating the output quantities are lin-211 ear combinations of the values at the neighboring points of a grid vertex, has been treated before by Pfaffelmoser et. al [4]. 212 The paper assesses the variability of gradients in 2D uncertain 213 scalar fields and derives confidence intervals for the gradient 214 magnitude and orientation. We follow their approach to obtain 215 confidence regions for quantities that can be modeled using linear combinations of the input variables, such as the gradient, 217 ²¹⁸ the Hessian matrix, and the trace of the Hessian matrix. For ²¹⁹ non-linear combinations, such as the determinant of the Hessian ²²⁰ matrix, we propagate the uncertainty by linearizing the function 221 by a first-order Taylor approximation.

222 3.2. Confidence Intervals for Gradients

To propagate the uncertainty for the gradient, we first approximate the gradient $\nabla X_{i,j}$ using the central differences kernel A_{∇} on a stencil $s_1(X_{i,j})$ holding the four random variables at the non-diagonal neighbors of the vertex (cf. Figure 1),

$$\nabla X_{i,i} = A_{\nabla} s_1(X_{i,i}). \tag{1}$$

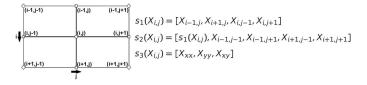


Figure 1: Stencils of random variables used in approximations.

²²⁷ The linear operator A_{∇} can then be applied to obtain a mean ²²⁸ $\mu_{\nabla}(X_{i,j})$ and covariance matrix $\Sigma_{\nabla}(X_{i,j})$ at every grid point

$$\mu_{\nabla}(X_{i,j}) = A_{\nabla}\mu(s_1(X_{i,j})), \tag{2}$$

$$\Sigma_{\nabla}(X_{i,j}) = A_{\nabla}\Sigma(s_1(X_{i,j}))A_{\nabla}^{\mathrm{T}}.$$
(3)

The input variables are $\mu(s_1(X_{i,j}))$, a four-element vector comprising the mean values $\mu(s_1(X_{i,j})_k)$ at each element of the stencil, and $\Sigma(s_1(X_{i,j}))$, a 4x4 covariance matrix, with the squared covariances $\sigma(s_1(X_{i,j})_k)\sigma(s_1(X_{i,j})_k)^2$ as diagonal elements, and the pair of elements of the stencil as non-diagonal elements. The non-diagonal elements consider the correlations between neighboring random variables $\rho(s_1(X_{i,j})_k, s_1(X_{i,j})_l)$. The output variables are the gradient mean $\mu_{\nabla}(x_{i,j})$, consisting of the mean values of the first-order partial derivatives in the *x*- and *y*-directions, and the covariance matrix $\Sigma_{\nabla}(x_{i,j})$ of dimension 2x2, holding the squared standard deviations and the covariances of the firstorder partial derivatives.

Note that, while standard deviations are sufficient to indi-243 cate the uncertainty in the scalar data, a 2x2 covariance matrix 244 is now necessary to express the variability in the two directions 245 of the gradient, as well as their correlation. Consequently, in-246 stead of two confidence intervals for each of the two directions, 247 we derive a confidence region corresponding to the covariance 248 matrix $\mu_{\nabla}(X_{i,j})^{T}\Sigma_{\nabla}(X_{i,j})^{-1}\mu_{\nabla}(X_{i,j}) \leq 1$.

249 3.3. Confidence Intervals for the Hessian Matrix

Derivations are similar for the second-order derivatives, ex-²⁵¹ cept that the central differences kernel A_H is now applied on ²⁵² a nine-point stencil $s_2(x_{i,j})$, holding the point itself and all of ²⁵³ its neighbors (cf. Figure 1). Uncertainty is propagated for the ²⁵⁴ Hessian matrix according to the following equations

$$\mu_H(X_{i,j}) = A_H \mu(s_2(X_{i,j})), \tag{4}$$

$$\Sigma_H(X_{i,j}) = A_H \Sigma(s_2(X_{i,j})) A_H^{\mathrm{T}}.$$
(5)

The output variables are $\mu_H(X_{i,j})$, a three-element vector holding the mean values of the second-order partial derivatives, Σ_{77} and $\Sigma_H(X_{i,j})$, the covariance matrix of dimension 3x3. We do the use these uncertainty parameters to derive a confidence region, but regard them as inputs to other scalar output quantities, the trace and the determinant of the Hessian matrix.

For the trace of the Hessian, $tr(H) = X_{xx} + X_{yy}$, the equations

$$\mu_{\rm tr}(X_{i,j}) = A_{\rm tr}\mu(s_3(X_{i,j})),\tag{6}$$

$$\sigma_{\rm tr}(X_{i,j}) = \sqrt{A_{\rm tr}\Sigma(s_3(X_{i,j}))A_{\rm tr}^{\rm T}},\tag{7}$$

261

262 yield a mean $\mu_{tr}(X_{i,j})$ and a standard deviation $\sigma_{tr}(X_{i,j})$ at every 263 grid vertex. The linear operator $A_{tr} = [1, 1, 0]$ is applied on the ²⁶⁴ three-element stencil $s_3(X_{i,j})$ holding the second-order deriva-265 tives, to obtain $[\mu_{\rm tr} - \sigma_{\rm tr}, \mu_{\rm tr} + \sigma_{\rm tr}]$ as a confidence interval for 266 the trace of the Hessian matrix.

The same procedure cannot be applied directly to propa-267 268 gate the uncertainty for the determinant of the Hessian ma-²⁶⁹ trix, det(H) = $X_{xx} \cdot X_{yy} - X_{xy}^2$, which is a non-linear combi-²⁷⁰ nation of random variables. Instead, we linearize the function $_{271} F(X_{xx}, X_{yy}, X_{xy}) = X_{xx} \cdot X_{yy} - X_{xy}^2$ by a first-order Taylor se-272 ries approximation, $F \approx c + Js_3^{-1}$. Here, c is a constant that $_{273}$ is disregarded in the propagation and J is the Jacobian matrix, $_{274}$ containing the first-order partial derivatives of the function F, $_{275} J = [X_{yy}, X_{xx}, -2X_{xy}]$. The uncertainty can now be propagated 276 as in the linear case, applying the Jacobian matrix to derive the 277 standard deviation of the determinant

$$\sigma_{\text{det}}(X_{i,j}) = \sqrt{J\Sigma(s_3(X_{i,j}))J^{\text{T}}},$$
(8)

²⁷⁸ associated with the mean $\mu_{det}(X_{i,j}) = F(\mu(s_3(X_{i,j})))$. The corre-279 sponding confidence interval for the determinant of the Hessian 280 matrix is then $[\mu_{det} - \sigma_{det}, \mu_{det} + \sigma_{det}]$.

281 3.4. Indicator Functions

Notice that, as long as statistical parameters can be obtained 282 ²⁸³ for the multivariate random variable characterizing the data val-284 ues at the grid points, uncertainty can be propagated to yield similar parameters for the gradient, and the trace and determinant of the Hessian matrix, irrespective of the probability distribution of the random variables. 287

We use the derived confidence region of the gradient at each 288 ²⁸⁹ grid vertex to indicate whether a critical point can occur around ³²¹ 290 the respective grid location. For scalar data given at the vertices 322 tex, but irrespective of the probability distribution that the gra-²⁹¹ of a Cartesian grid, critical points can occur anywhere within a ²⁹² grid cell and are characterized by a zero gradient. We therefore ²⁹³ derive positional indicators to relate the confidence region of ²⁹⁴ the gradient to a zero magnitude. Then, as the Hessian matrix ²⁹⁵ can be used to determine the type of a critical point, we use the 296 confidence intervals of the trace and determinant of the Hessian to infer on the nature of the critical point at the given position. 297

Throughout the investigations, we use confidence intervals 298 and avoid computing probabilities, because in this way we are 299 independent of any probability distribution of the random vari-300 ables. Furthermore, the applied procedures are deterministic 302 and computationally inexpensive, needing neither the large com-303 puting times, nor the individually tailored number of trials to 304 achieve a prescribed numerical tolerance that Monte Carlo in-305 tegrations do.

306 3.4.1. Positional Indicator Functions

The mean and covariance matrix of the gradient vector at 332 contains the origin or not 307 $_{308}$ a grid vertex state, for the x and y gradient components, their 309 means, dispersion around these means, and their coupling. The 310 covariance matrix can define the shape of several confidence

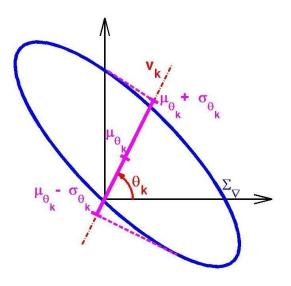


Figure 2: Projection of covariance matrix Σ_{∇} on a direction v_k corresponding to angle θ_k , to yield a mean μ_{θ_k} and standard deviation σ_{θ_k} .

311 regions, which, depending on the desired confidence level, con-312 tain a certain percentage of the total probability distribution. A 313 critical point can be considered to occur around a grid location ³¹⁴ if the origin falls within a prescribed confidence region. If no 315 specific distribution is assumed, the confidence ellipse corre-³¹⁶ sponding to the covariance matrix, $\mu_{\nabla}^{T} \Sigma_{\nabla}^{-1} \mu_{\nabla} \leq 1$, can be used 317 to test whether the origin is a possible realization or not. In 318 particular cases, such as the Gaussian distribution, confidence 319 regions for arbitrary confidence levels can be considered, for ₃₂₀ instance, $\mu_{\nabla}^{T} \Sigma_{\nabla}^{-1} \mu_{\nabla} \leq 6.17$ for a 95.4% confidence level.

Based on the confidence region of the gradient at a grid ver-323 dient vector may follow, we have thus derived a binary indicator 324 for the possibility of a critical point occurring at the grid vertex

$$\operatorname{ind1}(x_{i,j}) = \begin{cases} 1 & \text{if } \mu_{\nabla}^{\mathrm{T}} \Sigma_{\nabla}^{-1} \mu_{\nabla} \leq 1, \\ 0 & \text{otherwise.} \end{cases}$$
(9)

Because in Equation 9 we use the inverse of the covariance 326 matrix, ill-conditioned matrices will cause spurious results. In 327 such cases, instead of computing the Mahalanobis distance for 328 the origin, we project the covariance matrix on every direction ³²⁹ of a discretization of the unit circle $θ_k$ ∈ [0, 2π] (cf. Figure 2). 330 The projection yields a mean and a standard deviation

$$\mu_{\theta_k} = v_k^{\mathrm{T}} \mu_{\nabla}, \tag{10}$$

$$\sigma_{\theta_k} = \sqrt{\nu_k^{\mathrm{T}} \Sigma_{\nabla} \nu_k}, \qquad (11)$$

³³¹ which are then used to test whether every confidence interval

$$\operatorname{ind1}(x_{i,j}) = \begin{cases} 1 & \text{if } |\mu_{\theta_k}| \le \sigma_{\theta_k}, \forall \theta_k \in [0, 2\pi], \\ 0 & \text{otherwise.} \end{cases}$$
(12)

Depending on the amount of information the user has on the 333 ³³⁴ data, the positional indicator can be refined, by considering the 335 likelihood of the origin with respect to the covariance ellipse.

¹For a highly non-linear function, other probabilistic approaches, such as a Monte Carlo simulation, would be preferred to a linearization of the function.

We illustrate this for the particular case of a Gaussian distribution, where the mean is the most likely value of the gradient. For the grid vertices where the origin falls inside the confidence ellipse, we compute the Mahalanobis distance to yield how far from the mean the origin lies in terms of the width of the ellipse in the direction of the origin. We then take its complement

$$\operatorname{ind1}(x_{i,j}) = \begin{cases} 1 - \sqrt{\mu_{\nabla}^{\mathrm{T}} \Sigma_{\nabla}^{-1} \mu_{\nabla}} & \text{if } \mu_{\nabla}^{\mathrm{T}} \Sigma_{\nabla}^{-1} \mu_{\nabla} < 1, \\ 0 & \text{otherwise.} \end{cases}$$
(13)

The values of the indicator can vary from one - the origin 343 lies at the center of the confidence region, to zero - the origin 344 lies on the boundary of the confidence region or outside of it.

The refined indicator assesses the likelihood of the origin, depending on its position with respect to the confidence ellipse. Azero mean indicates that the origin is the most probable realization of the gradient vector. Critical points are thus likely to semble members. The likelihood of the origin as a realization of the gradient decreases as the origin drifts from the center of the ellipse. Consequently, critical points occur less frequently around this location across the ensemble.

The indicator functions characterize the locations of the crit-354 ical points and can be regarded as a measure of the positional 355 stability of the critical points. Indicators have positive values in 356 those regions where, according to the uncertainty analysis, criti-357 cal points occur repeatedly throughout the ensemble. Neverthe-³⁵⁹ less, a grid vertex where the positional indicator has a zero value 360 does not mean that a critical point cannot appear around the grid vertex. While a critical point may still emerge, it is less likely 361 ³⁶² to occur, e.g., it may be a transitory state or noise. Conversely, ³⁶³ indicators may have positive values at grid points around which ³⁶⁴ no critical point appears in any ensemble member. These reveal 365 locations where critical points could have occurred in ensemble ³⁶⁶ members that have not been realized. Furthermore, for specific ³⁶⁷ distributions, the indicators may be refined to suggest, in addi-368 tion to whether a critical point can occur around a vertex, the 369 qualitative likelihood of an occurrence.

370 3.4.2. Type Indicator Functions

The previously derived indicators point out the possible lo-37 372 cations where critical points occur frequently in the ensemble 373 members. They do not, however, provide any information on whether a certain type of critical point could be expected around 374 375 these positions. To obtain this kind of information, we need ³⁷⁶ to go an order higher than the gradient, to the Hessian matrix 377 and its associated eigenvalues: Only positive eigenvalues im-378 ply a local minimum, only negative eigenvalues a local maximum, whereas both positive and negative eigenvalues indicate 380 a saddle. The nature of the critical points can be character-³⁸¹ ized statistically by summarizing either the eigenvalues of the 382 Hessian matrix, or its trace and determinant. Because the func-383 tion relating the second-order derivatives to the determinant is ³⁸⁴ simpler than the function for the eigenvalues, we use the con-385 fidence intervals of the trace and determinant. From them, we 386 derive type indicators showing the tendency of critical points

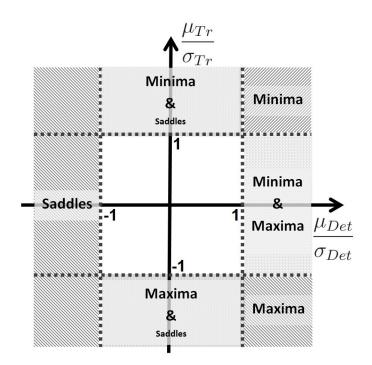


Figure 3: Classification of critical points showing stable behavior, depending on confidence intervals of trace and determinant.

³⁸⁷ appearing around a grid location to behave like a maximum, a³⁸⁸ minimum, or a saddle repeatedly throughout the ensemble.

³⁸⁹ Critical points can be classified according to the trace and ³⁹⁰ determinant of the Hessian as follows: Depending on the sign of ³⁹¹ the determinant, we can distinguish between saddles, det(*H*) < ³⁹² 0, and minima or maxima, det(*H*) > 0. For the latter, the sign ³⁹³ of the trace will further distinguish between minima, tr(*H*) > 0, ³⁹⁴ and maxima, tr(*H*) < 0. According to this classification and ³⁹⁵ the uncertainty analysis, critical points displaying a stable type ³⁹⁶ of the behavior can occur around the grid vertices where the ³⁹⁷ trace and the determinant of the Hessian can be considered as ³⁹⁸ clearly positive or negative based on their confidence intervals ³⁹⁹ (cf. Figure 3). We consider the trace (determinant) as *distinctly* ⁴⁰⁰ *positive* if the lower endpoint of its confidence interval is greater ⁴⁰¹ than zero, $\mu - \sigma > 0$ (or $\mu/\sigma > 1$), and as *distinctly negative* if ⁴⁰² the upper endpoint is less than zero, $\mu + \sigma < 0$ (or $\mu/\sigma < -1$).

We begin with an analysis based on the trace of the Hessian 404 matrix, for which the propagation of uncertainty necessitates no 405 linearization and is unbiased. The trace of the Hessian matrix is ⁴⁰⁶ simply the divergence of the gradient vector field; a clearly pos-407 itive (negative) value of the divergence indicates that a critical 408 point occurring around the given position tends to behave like 409 a minimum (maximum) or, potentially, a saddle. More specif-410 ically, a divergence deemed as distinctly positive at a certain 411 location indicates that, if a critical point appears at the loca-412 tion, it is unlikely that it is a maximum. A minimum has both 413 eigenvalues positive and thus a positive divergence of the gra-414 dient, whereas a maximum has both eigenvalues negative and a 415 negative divergence. Saddles, on the other hand, have both pos-416 itive and negative eigenvalues, and the divergence can take both 417 positive and negative values, depending on which eigenvalue is 418 larger in absolute value. Because saddles may display negative

to be able to distinguish between minima and saddles, we need 476 gether with various related surface components. to take the sign of the determinant into account. Depending on 477 422 424 negative, the critical point will most likely be a minimum or a 479 face, the used colormap consisting of shades of blue (for low 425 saddle. Otherwise, a clear distinction is not possible, although 426 minima are more likely. A similar analysis can be performed 427 for a critical point around a position showing a clearly negative 428 divergence: The critical point is expected to be a maximum, a 429 saddle, or both, depending on the determinant of the Hessian.

An analysis based solely on the trace of the Hessian in-430 431 dicates locations where predominantly minima (maxima) and ⁴³² possibly saddles emerge. Taking the determinant into account 433 can further differentiate between minima (maxima) and sad-434 dles. Vice-versa, an analysis based only on the determinant 435 of the Hessian points out locations with either saddle or min-436 imum/maximum behavior. The trace of the Hessian is in this 437 case used to potentially distinguish between stable minima and 491 4.1. Visualization of Positional Indicators 438 maxima.

439 440 ability distributions. In the case of a Gaussian distribution, we 494 avoid clutter, the circular glyphs have radii equal to half of the 441 can identify locations with an almost zero divergence, where 442 only saddle points should be expected. A grid point is consid-⁴⁴³ ered to have a very small divergence if zero is less than a certain 444 threshold τ away from $\mu_{\rm Tr}$ in terms of $\sigma_{\rm Tr}$, i.e., $|\mu_{\rm Tr}|/\sigma_{\rm Tr} < \tau$.

445 446 critical points appear in the ensemble, the type indicators point 500 the locations where critical points occur. In the following, we 447 out whether a stable behavior can be expected at any of these 501 denote the connected areas where the indicators take positive 448 locations. At grid points where a stable sign can be assumed 449 for both the trace and the determinant of the Hessian, critical 450 points of the same type are likely to occur. The user can ex-451 pect a specific type of critical point and of surface behavior 452 around the grid points throughout the ensemble. If just one 506 points occur repeatedly around the grid vertex throughout the 453 of the quantities shows a stable sign, certain variations in type 507 ensemble. Both types of positional indicators are illustrated 454 can be expected. While minima (maxima) are still more likely 508 in Figures 4(a) and (b), showing the mean field of a tempera-455 than saddles for a stable sign of the trace, no distinction be-456 tween maxima and minima can be made for a stable sign of the 510 Range Weather Forecast (ECMWF) for a forecast period of nine 457 determinant. If no exact statement can be made on the sign of 511 days above Europe. The general indicators are displayed in Fig-458 any of the two quantities, according to the uncertainty analysis, 512 ure 4(c), along with every critical point of the ensemble. It can ⁴⁵⁹ any type of critical point may appear around the location. This 460 indicates a highly unstable surface behavior at the given spatial 514 cur in the ensemble agree with those marked by the indicators. 461 location in the ensemble.

462 ⁴⁶³ ods are presented for the 2D case, the extension to 3D is straight-464 forward. Due to space considerations, however, we do not give 465 the mathematical derivations for 3D, but only briefly illustrate 466 possible 3D visualizations in Section 4.

467 4. Visualization

In the following, we present techniques to illustrate the in-468 ⁴⁶⁹ troduced indicators together with the scalar fields of the ensem-⁴⁷⁰ ble. We occasionally display the critical points, even though 471 they are not relevant to computing the indicator functions, in 472 order to contribute to the validation of the proposed techniques. 528 bers that have not been realized. Conversely, regions that have 473 Furthermore, the concurrent visualization allows us to place the 529 not been marked and still contain critical points, suggest that

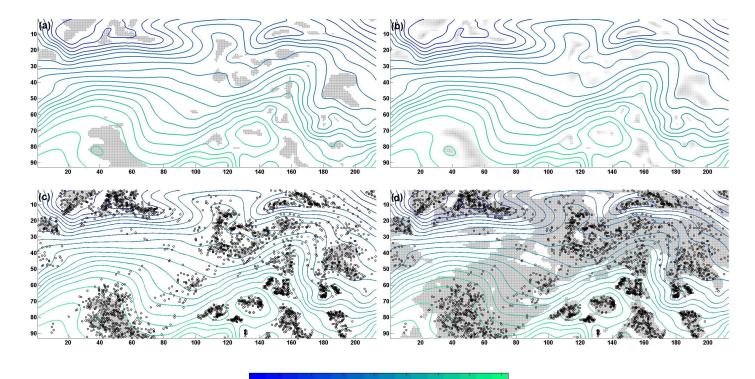
⁴¹⁹ or zero divergence, they are less likely to occur near locations ⁴⁷⁴ indicators and the critical points in space, and observe the poswith clearly positive divergence than minima are. Nevertheless, 475 sible occurrences of critical points and their type stability to-

Visual outputs have the scalar fields in the background, eiwhether the determinant can be regarded as clearly positive or 478 ther as contour plots or texture maps on a zero-elevation sur-⁴⁸⁰ values) and green (for high values). We use a rather low number 481 of shades, in order to avoid smooth transitions between colors 482 and thus convey to a certain extent different surface compo-483 nents when using texture maps. Depending on the interests of 484 the user, the visualization techniques can be extended to inte-485 grate further surface components, but, since these are specific 486 to the user's needs, we do not do so here. Critical points, if 487 shown, are drawn as circles, colored either in black, when the ⁴⁸⁸ type information is not relevant, or depending on the type of the 489 critical points: Saddles maintain their black color, maxima are ⁴⁹⁰ colored in orange, and minima in pink.

Positional-related indicators are encoded via gray-colored 100 The type indicators can also be refined for particular prob- 493 circular glyphs, centered at every vertex of a Cartesian grid. To ⁴⁹⁵ length of a grid cell's side. We prefer a glyph-based to a point-496 based representation, because it reflects better the fact that criti-⁴⁹⁷ cal points occur around and not exactly at the grid vertices. The 498 visualization is more dense and thus more likely to cover the ac-If the positional indicators suggest the spatial positions where 499 tual positions of the critical points. It also serves to emphasize 502 values as emphasized or marked regions.

> For the refined positional indicators, we encode the comple-503 ⁵⁰⁴ ment of the Mahalanobis distance in the opacity of the glyph: ⁵⁰⁵ The more opaque the glyph, the more likely it is that critical ⁵⁰⁹ ture ensemble, simulated by the European Center for Medium-⁵¹³ be observed that the locations where critical points actually oc-

Representing the possible locations of critical points via the 515 It is worth mentioning that, even though the proposed meth- 516 positional indicators has several benefits over simply displaying 517 the critical points of the ensemble. Firstly, deriving and display-⁵¹⁸ ing the indicators is a computationally inexpensive technique 519 to highlight the regions where critical points tend to occur pre-520 dominantly in the ensemble and requires no tailoring compared 521 to various clustering algorithms. It also needs little to no effort 522 on the user's side. Furthermore, the indicators reflect the vari-⁵²³ ability induced by uncertainty on the positions of critical points, 524 marking locations around which critical points are expected to ⁵²⁵ appear consistently in the ensemble. Thus, regions that are em-526 phasized, but contain no critical points, indicate locations where 527 critical points could have occurred in further ensemble mem-



255 260 265 270 275 290 280 285

Figure 4: Iso-contours of mean scalar field with positional indicator functions: (a) General and (b) refined indicators for confidence ellipse given by covariance matrix. (c) General indicators with all critical points. (d) General indicators for confidence level of 95.4% with all critical points.

so such unstable critical points are less likely to occur. Moreover, 559 to least stable by means of a slider functionality: As α varies ⁵³¹ in particular cases, e.g., a Gaussian distribution, we can further ⁵⁶⁰ in the right hand side of $\mu_{\nabla}(x_{i,i})^T \Sigma_{\nabla}(x_{i,i})^{-1} \mu_{\nabla}(x_{i,i}) \leq \alpha$ from 0 ⁵³² improve the stability assessment and distinguish between the ⁵⁶¹ to 9.21 (corresponding to a confidence level of 99%), more and 534 critical points occur only occasionally. 535

536 is useful when the occurrence of certain events or features is 537 strictly related to the existence of critical points. It is also rel-538 evant as a first step to rapidly identify the locations and iso-539 values that deserve further investigation. 540

54 542 emphasized regions may occupy larger areas when confidence regions with higher confidence levels are considered. Figure 543 4(d) shows the positional indicators for a confidence level of 544 95.4%. Just a few critical points are outside of the covered re-546 in unmarked areas. Moreover, critical points that appear in re-547 548 consistently than those in regions marked in both figures. 549

Figures 4(a)-(d) have the mean scalar field as a background. 550 We could have nonetheless used any other ensemble member 551 instead, since the mean scalar field is only relevant to illustrate 552 the ensemble behavior for particular distributions of the random variables, such as the Gaussian distribution. In fact, displaying 554 ⁵⁵⁵ the circular glyphs representing the indicators over the individ-

most stable regions - where critical points are likely to occur in 562 more circular glyphs cover the critical points of the ensemble most ensemble members, and the least stable regions - where 563 member; the lower the value of α that first results in a critical ⁵⁶⁴ point being covered, the more stable the critical point. Criti-Finding the regions holding the most stable critical points $_{565}$ cal points left uncovered for $\alpha \ge 9.21$ are classified as unstable ⁵⁶⁶ according to the uncertainty analysis.

Illustrating the possible locations of the critical points via ⁵⁶⁸ the indicators is more revealing than simply displaying critical 569 points of individual ensemble members or of their mean scalar Assuming a Gaussian distribution for the current example, 570 field. While in particular cases the mean field is illustrative 571 of the ensemble behavior, its critical points do not provide the 572 same insight as that offered by the indicators. First of all, the 573 critical points of the mean data set do not necessarily occur in ⁵⁷⁴ every region emphasized by the indicators (cf. Figure 5). Secgions or, vice-versa, critical points are not expected to occur 575 ondly, while these critical points reveal locations around which 576 critical points may be expected, they indicate neither the shape, gions marked in (d), but not in (c), are less likely to emerge 577 nor the extent of the regions where critical points may occur.

Similar techniques can be applied to visualize the potential ⁵⁷⁹ locations of critical points in 3D. We illustrate this in Figure 6 580 for the 3D temperature ensemble for which the aforementioned 581 2D data set is the slice at the highest pressure level. Spheri-⁵⁸² cal glyphs, the direct extension of the circular glyphs in 2D, are ⁵⁸³ shown immersed in the partly transparent volume data in Figure ⁵⁸⁴ 6(a). Then, from a volume data containing at each grid vertex $_{556}$ ual ensemble members and their critical points classifies criti- $_{585}$ the Mahalanobis distance $\mu_{\nabla}^{T} \Sigma_{\nabla}^{-1} \mu_{\nabla}$ of the origin from the gradi-557 cal points as stable or unstable. Moreover, in the Gaussian case, 586 ent mean, we extract in Figure 6(b) the iso-surface of iso-value 558 the user can interactively classify the critical points from most 587 1, which we color depending on the values of the scalar field at

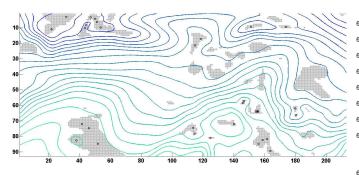


Figure 5: Critical points of the mean scalar field with positional indicators for confidence ellipse given by covariance matrix.

⁵⁸⁸ the vertices of the iso-surface. The most representative critical ⁵⁸⁹ points of the ensemble are shown as red spheres.

590 4.2. Visualization of Type Indicators

The type indicators are encoded via colored circular glyphs: ⁵⁹² Glyphs for grid points where only the determinant of the Hessian matrix fulfills the specified criteria for a certain type are colored in purple, while those where only the trace of the Hes-594 sian fulfills the criteria are colored in brown, unless the deter-595 minant suggests saddle behavior when the trace indicates maxi-596 mum (minimum) behavior. Such grid points are colored in gray. 597 Finally, the glyphs where the criteria hold for both the determinant and the Hessian matrix, i.e., where critical points with the 599 most stable behavior emerge, are colored in red. 600

60. colored according to their type. Figure 7(b) emphasizes regions 602 where critical points tend to behave like maxima. Notice that 603 regions with stable behavior are indicated mostly in the areas 604 where critical points of the same type cluster together, as opposed to those comprising a mixture of critical points of different types. The type indicators offer nevertheless additional ⁶⁰⁸ insight compared to the naive display of critical points colored according to their nature. For instance, both regions numbered and 2 in Figure 7(b) appear to consist of three clusters of maxima and saddle points, for which a visual inspection would indi-611 cate stable maximum behavior in the middle of the first region, 612 and the left and right thirds of the second region. According to 613 the uncertainty analysis, however, only the second region shows both positive determinant and negative trace values, and thus 615 more likely maximum behavior. Nonetheless, both regions show clearly negative trace values, pointing out that minima are unlikely to occur, whereas maxima and potentially saddle 618 points can be expected around the indicated regions. 619

Compared to regions 1 and 2, a clear separation between 620 critical points of different types is more difficult to do visually 621 622 in region 3. The type indicators suggest that maxima and, possi-623 bly, saddles are likely to appear in the upper half of the region, 624 while maxima and minima can be expected in the lower half. 679 625 Critical points occurring around three grid vertices display stable maximum behavior. 626

Spatial positions suggesting critical points with predomi-627 628 nantly saddle behavior are displayed in Figure 7(c). Although 629 critical points of different types occur in both regions numbered

630 1 and 2, the type indicators reveal locations around which sad-631 dle points can be expected to occur frequently. Figure 7(d) 632 shows grid vertices around which primarily minima are expected 633 to emerge. Notice that, even though grid points in regions num-634 bered 1 and 2 have distinctively positive trace values, their clearly 635 negative determinant values suggest saddle points instead of 636 minima as more likely to occur there. Figure 7(a) indicates that 637 saddle points indeed prevail in the two areas.

638 5. Validation

In the previous sections we introduced and visualized two 640 types of functions to indicate, at each grid vertex, whether criti-641 cal points can be assumed to emerge nearby and display a stable 642 behavior. Depending on the indicators, critical points have been 643 classified as more or less stable in location and type.

According to this classification, critical points occurring near 645 grid vertices where positional indicators have positive values 646 are stable, i.e., they are more likely to appear frequently around 647 the same position in the ensemble members. The so-called un-648 stable points are less likely to occur, i.e., they may be numer-649 ical noise or a transitory configuration. Furthermore, positive 650 indicator values for those grid vertices around which no crit-651 ical points appear suggest locations where critical points may 652 appear in further realizations of the ensemble.

653 To validate our techniques, we want to relate the number of 654 occurrences of a critical point around a certain position with its 655 classification as stable or unstable. This is nonetheless difficult, All critical points of the ensemble are shown in Figure 7(a), 656 since critical points do not generally occur at the same spatial 657 location. Even assigning critical points to grid points does not 658 typically result in a significant increase in the number of ensem-659 ble members where a grid vertex gets assigned at least one crit-660 ical point, because critical points may be assigned to different 661 neighboring grid points. We alleviate this problem by assigning 662 a critical point to all the vertices at the corners of the grid cell ⁶⁶³ where the critical point resides. Then, we build a 2D histogram 664 that counts, for each grid vertex, the number of ensemble mem-665 bers where at least one critical point was assigned to the vertex. 666 Starting with the peak of the histogram in descending order, 667 we check, for all the grid points having the given histogram 668 value, the percentage of points that do not have positive indica-669 tor values, i.e., the grid points to which critical points have been 670 assigned, but have not been marked by the indicators as well. 671 This yields, for each histogram value, the percentage of false ⁶⁷² negatives. We can perform a similar analysis for false positives, 673 computing the percentage of points that have positive values 674 of the indicators, but zero histogram values, i.e., the grid points 675 that have been marked by the indicators, but to which no critical 676 points have been assigned. Note that the grid points considered 677 in the false negative and false positive analysis do not sum up 678 to the total number of grid points.

The false negative error rates for the previous 2D example 680 are shown in Table 1. Figure 8 shows the mean scalar field with 681 the positional indicators and the six grid points that have the five ⁶⁸² highest histogram values, numbered from 1 to 5 in decreasing 683 order. The grid point numbered 1, at the peak of the histogram, 684 is marked in 56% of the ensemble members and has a positive

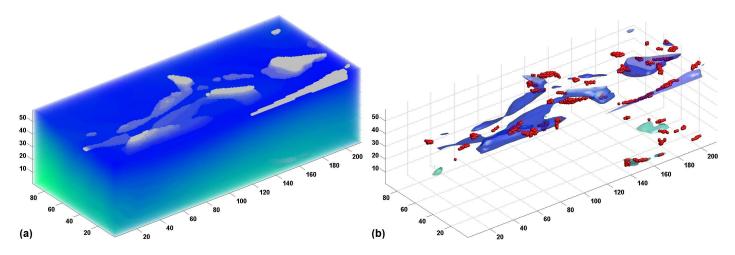


Figure 6: 3D temperature ensemble showing positional indicators via (a) gray-colored spherical glyphs and (b) iso-surface of iso-value 1, along with critical points shown as red spheres in the latter figure.

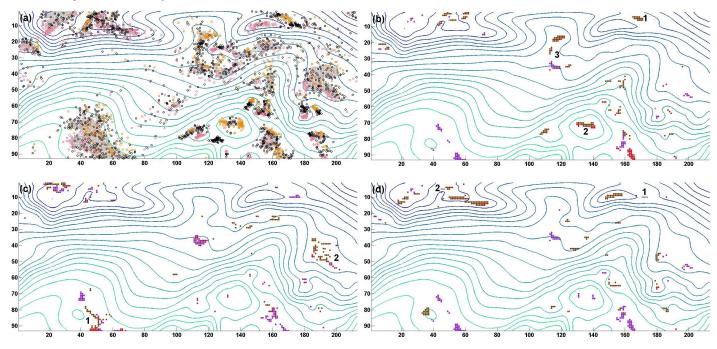




Figure 7: Iso-contours of mean scalar field of temperature ensemble with type indicator functions and critical points. (a) Critical points of the ensemble. Indicators only for (b) maxima, (c) saddle points, and (d) minima.

600 tices also have high histogram values, although only grid points 600 rates increase towards the end of the table, revealing the grid 687 numbered 4 and 5 have positive indicator values. Critical points 700 points around which critical points appear less frequently. The 688 in the grid cell given by the four vertices can be assumed stable, 701 shown error rates are in fact upper bounds of the actual values, ⁶⁰⁹ i.e., they occur frequently in the cell within the ensemble mem-⁶⁹⁰ bers, but the frequency can be expected to decrease in the lower ⁷⁰³ points, but not every grid point is marked by the indicators. ⁶⁹¹ right direction. Comparable observations can be made for the 704 ⁶⁹² two grid points numbered 3: Both vertices are marked in 46% 693 of the ensemble members, but only the lower grid point (black-694 colored in Figure 8) shows a positive indicator value. Critical 707 tive indicator values did not get any critical points assigned. For ⁶⁹⁵ points are thus less likely to emerge in the upper direction. Such 708 specific distributions, increasing the confidence level would reese grid points, with zero indicator values, but neighboring vertices 709 sult in a larger coverage of the indicators, i.e., lower false neg-⁶⁹⁷ with positive indicator values, cause the positive false negative 710 ative rates, but higher false positive rates.

685 indicator value. Notice that three other of its neighboring ver- 688 error rates at the beginning of the table. False negative error

The results show that grid vertices around which critical 705 points occur most often are also marked by the indicators. Re-706 garding the false positives, 12% of the 2019 vertices with posi-

Н	n	r	Н	n	r
0.56	1	0	0.22	15	0.33
0.5	1	1	0.2	19	0.58
0.46	2	0.5	0.18	27	0.52
0.4	1	0	0.16	33	0.3
0.38	1	0	0.14	62	0.21
0.34	2	0	0.12	105	0.29
0.32	3	0	0.1	183	0.36
0.3	2	0.5	0.08	352	0.41
0.28	3	0.67	0.06	676	0.54
0.26	5	0.4	0.04	1344	0.66
0.24	12	0.17	0.02	2868	0.84

Table 1: False negative analysis for temperature ensemble. H - histogram value, normalized by number of ensemble members; n - number of grid points holding histogram value; r - error rate.

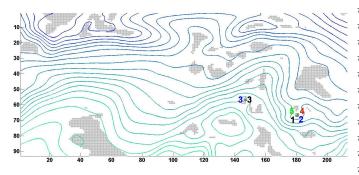


Figure 8: Mean scalar field with positional indicators and the grid points holding the five highest histogram values, numbered from 1 to 5.

711 6. Further Results

We apply the introduced techniques for analysis, visualiza-713 tion, and validation to three other data sets, two synthetic en-714 sembles and another ECMWF ensemble.

The first synthetic data set, of dimensions 100 x 100, was respectively assigning the three parameters *a*, *b*, and *c* in $-x^4/4$ respectively $y^4/4 - x^2y^2/2 + ax^2/2 + bxy + cy^2/2$, $(x, y) \in [-2, 2]X[-2, 2]$, ranrespectively respectively respective respectively respectively respectively respectively resp

$$\mu = \begin{bmatrix} 0.5\\1\\0.5 \end{bmatrix}, \ \Sigma = \begin{bmatrix} 1 & -0.5 & 0.5\\-0.5 & 1 & -0.5\\0.5 & -0.5 & 1 \end{bmatrix}.$$

When the parameters take on the values in the mean vec-720 $_{721}$ tor, there are three critical points, a saddle at (0,0) and two maxima at $(\sqrt{0.75}, \sqrt{0.75})$ and $(-\sqrt{0.75}, -\sqrt{0.75})$. Figure 9 722 illustrates the results for the first 50 members of an ensemble 723 724 comprising 5000 members, where the considered confidence ellipse was that corresponding to the covariance matrix. The 725 refined positional indicators, shown in Figure 9(a) (assuming a 727 Gaussian distribution fits the data), cover many of the critical 728 points, especially around the critical points of the mean. In Fig-729 ure 9(b), several grid points situated around the maxima of the 730 mean show clearly positive determinant and negative trace val-731 ues, i.e., stable maximum behavior. The rest of the grid points

Η	1	0.04	0.02
n	4	50	476
r	0.5	0.48	0.40

Table 2: False negatives for first synthetic data set (50 ensemble members).

Ν	50	100	500	1000	2500	5000
R	0.84	0.71	0.33	0.15	0.02	0.001

Table 3: False positives for first synthetic data set. N - number of ensemble members; R - false positive error rate.

⁷³² display only definitely negative trace values, which means that ⁷³³ saddles should not be excluded around these locations, although ⁷³⁴ maxima are more likely. No vertex with a dominant minimum ⁷³⁵ behavior is found, since the clearly positive determinant values ⁷³⁶ shown in Figure 9(c) only exclude saddles and, according to ⁷³⁷ Figure 9(b), indicate maximum behavior. Minima appear occa-⁷³⁸ sionally only around the origin. Even though critical points are ⁷³⁹ present around the origin in every ensemble member and the ⁷⁴⁰ positional indicators show positive values there, no stable type ⁷⁴¹ behavior can be identified in the region. This happens because ⁷⁴² saddle points also occur around the origin, although neither fre-⁷⁴³ quently enough to cause distinctly negative determinant values, ⁷⁴⁴ nor with predominantly positive trace values. Grid points with ⁷⁴⁵ small trace values ($\tau = 0.1$), around which saddle points are ⁷⁴⁶ expected to occur, are shown in Figure 9(d).

Table 2 shows the results of the false negative analysis. The 747 748 four grid points that make the peak of the histogram, two of 749 which have positive indicator values, are located around the ori-750 gin. Notice that critical points are identified around the origin 751 in all ensemble members. Furthermore, these critical points ap-752 pear mostly on the secondary diagonal of the square, near the 753 two grid points with positive indicator values. The other two 754 grid points with maximum histogram values have non-positive 755 indicator values, since critical points do not occur around them. Their high histogram value is due to the critical points having been assigned to all neighbors. Except for these critical points, 757 758 however, all other critical points are rather scattered, reason for 759 which no other grid point is marked in more than two ensemble 760 members. According to the false negative error rate, nonethe-761 less, the grid points near which more critical points appear have 762 positive indicator values.

⁷⁶³ Due to the low number of critical points and their scatter-⁷⁶⁴ ing, the false positive error rate is very high (84%). Never-⁷⁶⁵ theless, the grid points around which no critical points occur, ⁷⁶⁶ but which display positive indicator values, suggest locations ⁷⁶⁷ where critical points may appear in further realizations of the ⁷⁶⁸ ensemble. To illustrate this, we consider all the 5000 ensem-⁷⁶⁹ ble members. At the peak of the histogram the situation is un-⁷⁷⁰ changed, showing that the tendency of critical points to occur ⁷⁷¹ on the secondary rather than main diagonal of the square had ⁷⁷² been captured well previously. While critical points are still ⁷⁷³ scattered (except for the grid points in the vicinity the origin, ⁷⁷⁴ no other vertex is marked in more than 64 ensemble members), ⁷⁷⁵ they cover more densely the regions emphasized by the indi-

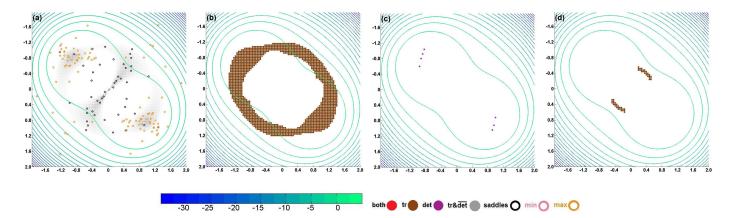


Figure 9: Iso-contours of mean scalar field of first synthetic data set with indicators. (a) Refined positional indicators with all critical points. (b) Type indicators for maxima. (c) Type indicators for minima. (d) Type indicators for saddle points.

Н	n	r	Н	n	r
0.24	1	0	0.12	9	0.44
0.22	1	0	0.1	15	0.87
0.2	3	0.67	0.08	38	0.76
0.18	1	0	0.06	47	0.81
0.16	3	0	0.04	46	0.89
0.14	1	0	0.02	97	0.99

Table 4: False negative analysis for second synthetic data set.

⁷⁷⁶ cators. Consequently, the false positive rate decreases dramati-⁷⁷⁷ cally to 0.1%. The decreasing trend of the error rate for increas-⁷⁷⁸ ing numbers of ensemble members is shown in Table 3.

A second synthetic data set, also of dimensions 100 x 100, was generated by assigning the parameter ω in $x^3 + y^3 - \omega xy - x - x^{-1}$ $y = 0, (x, y) \in [-2, 2]X[-2, 2]$, random numbers generated from a normal distribution with a zero mean and standard deviation of 2. Depending on the value of ω , there should be either four reading on the value of ω , there should be either four a saddle for $\omega = \pm 2$), or two critical points (a node and a saddle reading for $\omega < -2$ or $2 < \omega$).

The mean scalar field, together with the positional and type 787 ⁷⁸⁸ indicators, and all critical points, is shown in Figures 10(a)-(c). The badly-scaled covariance matrices of the gradients cause 789 spurious results for the positional indicators (cf. Figure 10 (a)), 790 which now cover the whole domain with no distinct pattern, 791 even though critical points occur mostly on the main diagonal. Nonetheless, it does not affect the type indicators (cf. Figures 793 10 (b) and (c)), which still identify the maximum behavior in 794 the upper triangular part and the minimum behavior in the lower 795 triangular part. Projecting the covariance matrix (cf. Figures 10(d)-(f)) results in positional indicators that cover mostly ar- $_{798}$ eas where critical points are identified. Both false positive (13%) ⁷⁹⁹ for 45 marked grid points) and negative error rates (cf. Table 4) are correspondingly low. 800

For our last example we use data from the ECMWF Ensemble Prediction System (EPS), ECMWF's operational ensemble weather forecast system. The EPS produces forecasts twice daily and includes 50 members and a control run. For more

⁸⁰⁵ details on the system, we refer the reader to, for instance, [37]. ⁸⁰⁶ Here we use the forecast initialized on October 17, 2012. The ⁸⁰⁷ data has been interpolated horizontally from the model grid to ⁸⁰⁸ a regular latitude/longitude grid with a grid spacing of 0.3 de-⁸⁰⁹ grees in both dimensions, and vertically to levels of constant ⁸¹⁰ pressure. The selected scalar field is the 60 hour forecast of the ⁸¹¹ geopotential height field at a pressure level of 1000 hPa, valid ⁸¹² on October 19, 2012.

Figure 11 shows the geolocated mean scalar field, where B14 low altitudes of the pressure surface are colored in shades of B15 blue and high altitudes in shades of green. A distinct low pres-B16 sure system is visible south of Greenland, several critical points B17 appearing there. Critical points are useful in this context to help B18 identify features related to adverse weather conditions, such as B19 cyclonic centers. Cyclonic features can be located by using B20 a mixture of techniques, among which the detection of well-B21 defined geopotential minima. Since data is inherently affected B22 by uncertainty, it is relevant to point out the spatial locations B23 around which pressure minima are to be expected and which B24 should be further investigated.

Positional indicators are shown in Figure 11(a) for a confience ellipse corresponding to a 95.4% confidence level. The indicators cover the majority of areas where critical points ocence cur, including the region displaying the low pressure. False negative error rates are therefore low, many of them under 20%, while the false positive rate is 37%. Type indicators showing stable minimum behavior are shown in Figure 11(b). The upence per left corner of the region has several grid points with clearly positive trace values, but no definitely positive determinant values and even five grid points with clearly negative determinant values, i.e., while minima are the most likely type of critical points to appear in the region, saddle points should not be exsor cluded, especially around the five grid points.

838 7. Conclusion

Prominent features display variations across ensembles, po-⁸⁴⁰ tentially changing their location and shape. In this paper, we ⁸⁴¹ developed several indicator functions to give insight into the

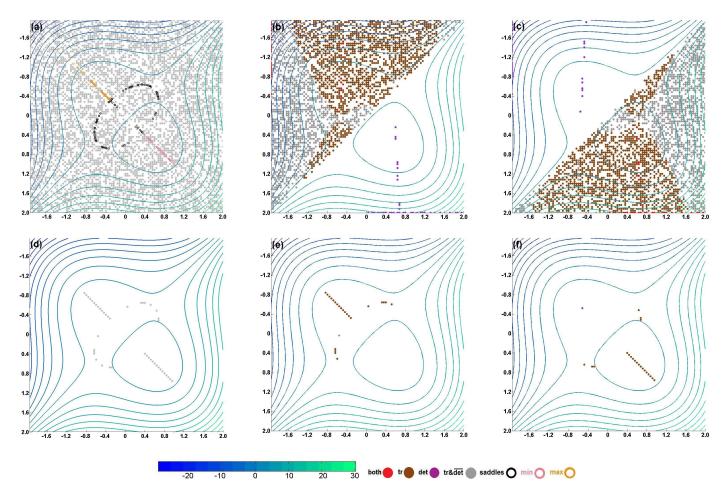


Figure 10: Iso-contours of mean scalar field of second synthetic data set with indicators. (a) Positional indicators and all critical points. (b) Type indicators for maxima. (c) Type indicators for minima. (d) Modified positional indicators. (e) Type indicators for maxima after modification. (f) Type indicators for minima after modification.

843 ing their associated critical points. We summarized ensembles 865 according to the uncertainty analysis. Depending on the size 845 ciated gradient fields and the determinant and trace of the Hes-846 whereas the latter reveal whether the critical point tends to be- 870 for ensemble members that have not been realized. 848 have consistently like a minimum, a maximum, or a saddle. 871 849 850 852 853 synthetic and two real world data sets, to illustrate how the pro-⁸⁵⁴ posed methods emphasize the possible critical points and their ⁸⁷⁶ structure, in the sense that the critical point, the region grown stability in behavior in ensembles of uncertain scalar fields. 855

856 ⁸⁵⁷ dients show the locations where critical points tend to occur ⁸⁷⁹ other hand, a spatial position with no specific type behavior 858 repeatedly within ensemble members. Critical points already 880 indicates a potentially unstable structure, whose shape inverts 860 861 components emerge at minima, disappear at maxima, split or 883 the associated features are harder to draw when the uncertainty merge at saddles. The positional indicators can be regarded as analysis allows the clear exclusion of only one type of critical and fast and computationally inexpensive method to point out the and point behavior. The type indicators are also useful in appli-

842 salient features of scalar fields and their stability, by investigat- 864 locations and iso-values that are significant for the ensemble statistically and computed corresponding moments for the assosian matrices. The first were used to derive quantities indicating 800 grid points with no critical points occurring in the immediate the likelihood of existence of a critical point at a given location, 869 vicinity. However, such locations were shown to be suggestive

The type indicators characterize the behavior of critical points We then presented techniques to visualize the proposed indica- 872 and suggest the manner in which interesting associated surface tors simultaneously with the scalar fields and several of their 873 components (iso-contours and various regions grown around surface components. Finally, we applied the methods on two 874 critical points) develop. For instance, a location indicating a 877 around it, and the topological event of a surface component Positional indicators based on confidence intervals of gra- 878 emerging persist throughout the ensemble members. On the indicate within one ensemble member the relevant iso-values ⁸⁸¹ across the ensemble, even though the structure may be present where topological changes of the iso-contours occur: Contour 882 in most ensemble members. Conclusions on the stability of

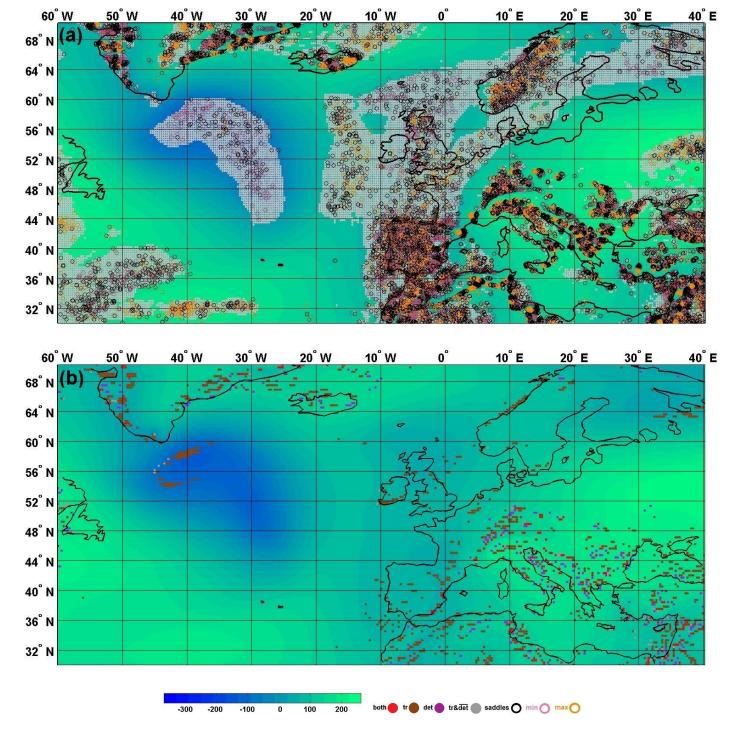


Figure 11: Mean scalar field of temperature ensemble with indicator functions. (a) Positional indicators with all critical points. (b) Type indicators for minima.

886 cations where locating stable critical points of a certain type 946 [13] Pang AT, Wittenbrink CM, Lodha SK. Approaches to uncertainty visual-⁸⁸⁷ is relevant to the detection and tracking of various features, 888 e.g., pressure minima are used in meteorological applications 889 to identify cyclonic features.

There are several possible directions for future work: Firstly, 951 890 891 the notion of stability of critical points could be extended, to al-⁸⁹² low tracking critical points (and associated features) from one ⁸⁹³ ensemble member to another. Furthermore, similar investiga-894 tions could be performed for uncertain vector fields. It would ⁸⁹⁵ be interesting to develop the analysis to assess the stability of ⁸⁹⁶ the entire topology of the vector fields, in addition to the critical 897 points.

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