Uncertainty and Parameter Space Analysis in Visualization

Session 4: Structural Uncertainty
Analyzing the effect of uncertainty on the appearance of structures in scalar fields

Rüdiger Westermann and Tobias Pfaffelmoser
Computer Graphics & Visualization

Uncertain scalar fields
• Uncertain scalar field \( Y : M \rightarrow \mathbb{R} \) on compact domain \( M \subset \mathbb{R}^n \)
• Discretely sampled on nodes \( \{x_i\}_{i=1}^n \) with values \( \{Y_i\}_{i=1}^n \)
• We assume a stochastic uncertainty model:
  \( Y \) are (correlated) Gaussian distributed random variables

\[
Y(x_i) = \mu_i + \mathcal{N}(0, \Sigma)
\]

Described by a multivariate Gaussian distribution

\[
\mu = \left( \mu_1, \ldots, \mu_n \right)
\]

with mean \( \mu = (\mu_1, \ldots, \mu_n) \)
and covariance matrix \( \Sigma \)

\[ Y(x_i) = \mu_i \] is the most likely configuration

Part 1: Structural uncertainty

Uncertainty parameters in the multivariate case
• The degree of uncertainty is modeled by the Covariance Matrix \( \Sigma \)

\[
\Sigma = \begin{pmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{12} & \sigma_{22} & \sigma_{23} \\
\sigma_{13} & \sigma_{23} & \sigma_{33}
\end{pmatrix}
\]

\[
\sigma_{ij} = \text{Var}(Y_i) = E[(Y_i - \mu_i)^2]
\]

\[
\sigma_{ij} = \text{Cov}(Y_i, Y_j) = E[(Y_i - \mu_i)(Y_j - \mu_j)]
\]

Specific literature
Multivariate Gaussian distribution

- Compute $\mu, \sigma_{ij}$ from a given ensemble of data sets
  - Ensemble members are treated as realizations of a corresponding multivariate random variable
- Specify $\mu, \sigma_{ij}$ and map independent normally distributed random number vectors to a corresponding realization

Variance as uncertainty indicator

- Example: an ensemble of 2D seismic tomography wave velocities
  - Relative velocities are color coded from blue (negative) to red (positive)
- Two prominent circular features are observed in the mean values
- Mapping the standard deviations to colors shows low, and almost constant uncertainty in both regions

Gaussian covariance matrix

- Variance information is often used as primary indicator of the uncertainty (square of the standard deviation $\sigma$)
  $$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_2^2 & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_3^2 \end{pmatrix}$$
  - Measure of the amount of variation of the values of a random variable
  - Often visualized directly via confidence regions, uncertainty glyphs, or specific color or opacity mappings

Variance as uncertainty indicator

- Uncertainty mapping in 3D via Stochastic Distance Functions
  - Mahalanobis distance: in numbers of standard deviation to the level-$i$ surface in the mean field
    $$\Psi_i(x) = \frac{\mu(x) - \mu_i}{\max(\sigma(x), \sigma_{\text{min}})}$$
  - SDF surfaces are level-sets in the Mahalanobis distance field, enclosing the volume which contains the uncertain surface with a certain probability
    - For Gaussian distributions, the less standard deviations an observation is from the mean, the higher the probability of this observation

Variance as uncertainty indicator

- Uncertainty visualization for an iso-surface in the mean values of a 3D temperature ensemble
- Uncertainty visualization for an iso-surface in the mean values of a 3D temperature ensemble

Iso-surface in the mean values of a 3D temperature ensemble
- Positional variability of the surface due to uncertainty
Limitations of variance as uncertainty indicator

- The standard deviation describes the local uncertainty but does not allow inferring on possible variations at different positions relative to each other:
  - e.g., if mean values and standard deviations at two adjacent points are identical, but the realizations of the random variables at both points behave independently. It cannot be predicted whether there is a positive, zero, or negative derivative of the data between the two points.
  - In general, the effect of uncertainty on structures which depend on random values at multiple points cannot be predicted from the mean values and standard deviations alone.
    - The effect is to a large extent arbitrary if the realizations of the random values are stochastically independent, while a structure’s shape can be assumed stable if the realizations are stochastically dependent.

Limitations of variance as uncertainty indicator

- Variations of an uncertain curve due to uncertainty:
  - Curve points \( y_i = f(x_i) \) are modeled via a multivariate Gaussian random variable with smoothly varying mean values (green curve) and a constant standard deviation (blue curves show corresponding confidence interval).

In a) and b), high and low stochastic dependence between the values at adjacent \( x \) was modeled.

Limitations of variance as uncertainty indicator

- Variations of an iso-surface in an uncertain 3D scalar field:
  - Stochastic dependence between scalar values was modeled explicitly via a respective covariance matrix \( \Sigma \).

(a) Low stochastic dependence:

(3) along \( y \)
(4) along \( x \) and \( y \)
(5) along \( z \)

(b) High stochastic dependence:

(1) along \( x \)
(2) along \( x \) and \( y \)
(3) along \( y \)

Limitations of variance as uncertainty indicator

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(b) High stochastic dependence:

(1) along \( x \)
(2) along \( x \) and \( y \)
Limitations of variance as uncertainty indicator

- Variations of an iso-surface in an uncertain 3D scalar field
  - Stochastic dependence between scalar values was modeled explicitly via a respective covariance matrix $\Sigma$

Low stochastic dependence:

1. High stochastic dependence
2. Along x
3. Along y
4. Along x and y
5. Along z
Limitations of variance as uncertainty indicator

- Random values in the 3D scalar field shown before were generated using a multivariate Gaussian distribution with constant standard deviation and linearly increasing mean (along z).

(a) Iso-surface in the mean values.
(b) Confidence volume containing all points that belong to the surface with a certain probability.
(c) Occurrence of the surface in (a) for one possible realization of the random values.

Structural uncertainty

- We call the effect of uncertainty in the data values on structures depending on the values at multiple points a structural uncertainty.
  - It is associated with the occurrence of particular structures in the data which are affected by the degree of dependence between the values at two or more data points.
- Indicators for structural uncertainty are given by the sub-diagonals of $\Sigma$, which contain covariance information on relative uncertainties between random variables:

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} & \sigma_{13} \\ \sigma_{12} & \sigma_2^2 & \sigma_{23} \\ \sigma_{13} & \sigma_{23} & \sigma_3^2 \end{pmatrix}$$

Stochastic dependence

- Variability of a scalar value around its mean position:

Conclusion: just by looking at the standard deviation it is impossible to infer on the stability (or confidence) of structures in the mean values.
- A structure is very likely to change its shape due to uncertainty, if the stochastic dependence between the data values making up the region is low.
- A structure is rather unlikely to change (it is stochastically stable), if the stochastic dependence between the data values making up the structure is high, even if the standard deviations are high.
- Thus, one important goal in uncertainty visualization is to convey the stochastic dependence and conclude on the stability of structures in the data.
Stochastic dependence

- Variability of a scalar value around its mean position:

Correlation describes relative variability of one or more random variables:

- Positive Correlation
- Negative Correlation

Confidence Interval
- Standard Deviation
- Mean Position
Stochastic dependence

- Correlation describes relative variability of one or more random variables.

Positive Correlation

Negative Correlation

Part 2: Local and global correlation visualization

2.1 Local Correlation Visualization

Structural uncertainty

- Remember the example in Part 1: locally varying structural variations of an iso-surface in different realizations of an uncertain 3D scalar field:
  - Caused by different correlation structures
  - Resulting in stochastically stable and unstable surface parts
  - Cannot be revealed by mean and standard deviation values

Low structural uncertainty

High structural uncertainty

Structural uncertainty

- Problems addressed in this part of the tutorial:
  1. How can one visualize correlations to analyze the structural uncertainty of particular features in 2D and 3D scalar fields, given a set of realizations or a (Gaussian based) stochastic uncertainty model?
  2. Two different approaches will be discussed, both aim at conveying correlation structures in the data:
     1. Local correlation analysis using characteristic correlation tensors
     2. Global correlation analysis showing long-range dependencies such as inverse correlations via correlation clusters
Local correlation analysis

- Assumption of a **distance dependent** correlation model: higher correlations between the data values at points with shorter Euclidean distance.

### Domain of a 2D scalar data set

- **Weak correlation**
- **Strong correlation**

### Distance dependent correlation model

- The Gaussian correlation function relates correlation to spatial distance:
  \[ \rho (Y(x_i), Y(x_j)) = \exp(-\tau \|x_i - x_j\|^2) \]

- Correlation strength parameter \( \tau \) relates correlation to distance and is independent of grid resolution for local correlation analysis.

### Correlation anisotropy

- Problem: Correlation values—and thus correlation strength parameters—depend on direction, yielding a **directional correlation distribution** at each grid point.

- A single correlation value can not represent the stochastic dependences!

### Correlation strength tensor

- Idea: The (anisotropic) distribution of the correlation strength parameter is modelled by a rank-2 tensor \( T \):
  - The correlation strength tensor \( T \) models the correlation strength to 8 (2D) or 26 (3D) neighbors.
  - Given \( T \), correlation strength \( \tau \) at position \( x \) into direction \( r \) can be computed via tensor-vector multiplication:

\[ \tau(x, r) = r^T T(x) r \]
Correlation strength tensor

- Given the tensor $T$, the distance and direction dependent correlation becomes
  \[ \rho(Y(x_i), Y(x_j)) = \exp\left(-\frac{(x_i - x_j)^T T (x_i - x_j)}{||x_i - x_j||^2}\right) \]

- At every grid point a correlation tensor is computed
  - i.e., correlation data is transformed into a distance dependent tensor model
  - Reduces memory requirements because it avoids storing (global) correlation values explicitly

Correlation visualization on iso-surfaces

- **Goal**: Visualizing the structural uncertainty of specific features in the mean data, i.e. an iso-surface
  - Requires correlation visualization with respect to the mean surface's geometric shape

- **Idea**: Distinguish between correlations in the surface's local tangent planes and normal direction, and visualize these correlations via glyphs

Correlation glyphs

- Correlation glyphs encode the correlation values in the first and second principal tangent and surface normal direction

  Glyph coloring wrt correlation in surface …

  (1) … normal direction
  (2) … first principal tangent direction
  (3) … second principal tangent direction

Correlation strength tensor computation

- $T$ is symmetric and has 3 (2D) or 6 (3D) free values to be determined
- $T$ models the correlation strength to 8 (2D) or 26 (3D) neighbors
- $T$ is obtained for every grid point by solving an over-determined linear system using a least squares approach

  \[ r^T \text{Tr} = -\log\left(\frac{1}{2}[\rho(Y(x_i), Y(n_k)) + \rho(Y(x_i), Y(-n_k))]ight) \]

  \[ r = \frac{n_k - n_0}{||n_k - n_0||}, \quad n_k \in N(x_i), \quad k \in \{1, 2, \ldots, 13\} \]

- $T$ is independent of the grid resolution, because correlation is set in relation to Euclidean distances

Correlation visualization on iso-surfaces

- **Approach**: Correlation values are extracted for the two principal correlation directions in the surface's tangent plane (highest and lowest strength) and normal direction [4]
  - Basis transformation is necessary to obtain correlation strength parameters in principal tangential directions ($\tau_{\tan_{\max}}$) and ($\tau_{\tan_{\min}}$) and normal direction ($\tau_{\normal}$) at every surface point
  - By interactively specifying an Euclidean radius of correlation values along the three principal directions are computed as
    \[ \tau_{\tan_{\max}} = \exp(-\tau_{\normal}) \]
    \[ \tau_{\tan_{\min}} = \exp(-\tau_{\normal}) \]
    \[ \tau_{\normal} = \exp(-\tau_{\normal}) \]
  - and used to model the appearance of circular correlation glyphs

Correlation glyphs

- **Correlation ratio** between first and second tangent direction is encoded in the shape of the elliptic zone (2)

  Glyph coloring wrt correlation in surface …

  (1) … normal direction
  (2) … first principal tangent direction
  (3) … second principal tangent direction
Correlation glyphs

- **Absolute** and **relative** correlation anisotropy in the surface tangent plane are encoded via color differences

\[
\begin{align*}
\rho = 1 & \quad \rho = 0.8 \\
\rho = 0.5 & \quad \rho = 0.0 \quad 0 \rightarrow \text{Correlation} \rightarrow 1
\end{align*}
\]

Structural uncertainty analysis

- Surface realization and glyph based correlation visualization on mean surface

High and low correlation in vertical and horizontal direction

Low correlation in both vertical and horizontal direction

Low correlation especially in normal direction
Structural uncertainty analysis

Mean surface in a simulated temperature ensemble

Glyph based correlation visualization

Local correlation analysis summary

- No integration of absolute uncertainty information (e.g. standard deviations)
- Global dependences are ignored
- Inverse correlation cannot be visualized as correlation model only accounts for correlation strengths (magnitudes)

Part 2: Local and global correlation visualization

2.2 Global correlation visualization
Global correlation analysis

• To analyze long-range spatial dependencies between the data values in uncertain scalar fields, in principle the full covariance matrix needs to be visualized.

• This is problematic due to the following reasons:
  – For a spatial grid points it requires $O(n^2)$ memory.
  – Entries in $\mathbf Z$ are not in a spatial context, making it difficult to infer on spatial dependencies.
  – Uncertainty information has to be visually separated from correlation information.

Example data set

• 2D temperature ensemble simulated by the European Centre for Medium-Range Weather Forecasts.

Correlation strength indicator

• Definitions:
  
  Correlation neighborhood:
  
  \[ n_{\rho_1}(x_i) = \{ x_j \in D \mid \rho(Y(x_i), Y(x_j)) \geq \rho^* \} \]
  
  $D$: data domain
  
  $\rho_1$: correlation level

  Cardinal number: \( |n_{\rho_1}(x_i)| \)

Global correlation analysis

• Requirements due to the aforementioned problems:
  – The correlation information first has to be condensed.
  – Requires to define and seek for the most prominent short- and long-range dependencies.
  – Correlation structures have to be embedded into standard visualizations providing spatial relationships.

• Approach:
  – Definition of a measure for the degree of dependency of a random variable to its local and global spatial surrounding.
  – Spatial clustering of random variables based on this measure.
  – Color coding of data points wrt. cluster IDs.

Correlation strength indicator

• Assumption: the more “correlation partners” a particular point in the domain has to which the correlation is larger than a given level, the more important this point is:
  – The sets of partners spread anisotropically across the domain.
  – The expansion in different directions is directly related to the correlation distribution in the respective region.

• For a given level and point $x_i$, the number of partners indicates the degree of dependency between the random variable $Y(x_i)$ to its local and global spatial surrounding:
  – It counts the most prominent partners of $x_i$, independent of their position in the domain.
  – The number of partners is used as the correlation strength indicator.

Correlation strength indicator

• Example showing relation between correlation neighborhoods and cardinal numbers.
Spatial correlation clustering

- **Basic idea**: use correlation neighborhoods as clusters
- **Problem**: correlation neighborhoods of different points can overlap
  - Results in ambiguities in the assignment of points to clusters
- **Solution**: process correlation neighborhoods sequentially and exclude those neighborhoods which overlap any previously processed neighborhood
- The strategy avoids overlapping clusters but, depending on selection order, will exclude large clusters which overlap small cluster
- Thus, neighborhoods are selected in descending order of cardinality such that the largest clusters are always selected first

Correlation clustering algorithm

- **Step 1**: Select correlation level \( \rho^+ \)
- **Step 2**: Compute cardinal numbers for all points in the 2D domain
- **Step 3**: Select domain point with largest cardinal number as first cluster center
- **Step 4**: Create cluster (correlation neighborhood)

Correlation clustering results

- **Visualization of correlation clusters and cluster centers on the mean height surface for a particular correlation level \( \rho^+ \)**

Correlation clustering results for varying levels

- **Inverse stochastic dependencies typically exist between spatially separated regions**, i.e., pairs which are inversely correlated to each other
  - **Inverse correlation structures** are global features and cannot be modeled by distant dependent correlation models
Inverse dependencies

- Inverse stochastic dependencies typically exist between spatially separated regions; i.e., pairs which are inversely correlated to each other.

  - Inverse correlation structures are global features and cannot be modeled by distant dependent correlation models.

Inverse correlation clustering algorithm

- Step 1: Select negative correlation level $\rho^-$
- Step 2: Compute correlation neighborhoods $\{Y(x_i), Y(x_j)\} \leq \rho^-$ and corresponding cardinal numbers for all points
- Step 3: Select point with largest cardinal number as first cluster center
- Step 4: Assign negatively correlated points to first cluster
- Step 5: Select point in cluster with largest number of inversely correlated points
Inverse correlation clustering algorithm

- Step 1: Select negative correlation level $\rho^-$
- Step 2: Compute correlation neighborhoods $\{i, j\} \leq \rho^-$ and corresponding cardinal numbers for all points
- Step 3: Select point with largest cardinal number as first cluster center
- Step 4: Assign negatively correlated points to first cluster
- Step 5: Select point in cluster with largest number of inversely correlated points
- Step 6: Assign both clusters to one pair

Inverse correlation clustering algorithm

- Step 1: Select negative correlation level $\rho^-$
- Step 2: Compute correlation neighborhoods $\{i, j\} \leq \rho^-$ and corresponding cardinal numbers for all points
- Step 3: Select point with largest cardinal number as first cluster center
- Step 4: Assign negatively correlated points to first cluster
- Step 5: Select point in cluster with largest number of inversely correlated points
- Step 6: Assign both clusters to one pair
- Step 7: Proceed with Step 3, taking into account that clusters do not overlap

Inverse dependencies

- Each pair of inversely correlated spatial regions gets assigned one distinct color
- Clusters in each pair are distinguished by differently oriented stripe patterns

Inverse dependencies for varying negative levels $\rho^-$
Global correlation analysis results

- Example: An uncertain 2D scalar field with constant means and standard deviations. Specific correlation structures have been enforced:
  - Strong positive correlation within the sets of points colored blue.
  - Zero correlation between these sets.
  - Inverse correlation between the two sets in the upper left region.

Confidence volume around mean surface

Covariance Matrix

Gaussian Random Number Generator

Global correlation analysis results

- Correlations
- Standard Deviations

Random realization

Confidence volume around mean surface

Covariance Matrix

Gaussian Random Number Generator

Global correlation analysis results

- Correlations
- Standard Deviations

Random realization

Confidence volume around mean surface

Covariance Matrix

Gaussian Random Number Generator

Global correlation analysis results

- Correlations
- Standard Deviations

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Global correlation analysis results

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Global correlation analysis results

- Covariance Matrix
- Gaussian Random Number Generator
- Standard Deviations
- Random realization
- Confidence volume around mean surface

Global correlation analysis results
Global correlation analysis results

- Correlation clustering algorithm identifies **positively correlated regions** correctly

Global correlation analysis results

- Correlation clustering algorithm identifies **inversely correlated regions** correctly

Global correlation analysis summary

- Correlation clustering allows analyzing **global correlation structures** such as inverse correlations, requiring an amount of memory that is linear in the number of data points
- The clusters’ distributions reveal **anisotropic correlation effects**
- **Uncertainty information** can be integrated easily, for instance, by extruding clusters depending on standard deviation [5]
- Extension to 3D is possible, but special projection or restriction schemes are required when used to analyze correlation structures on iso-surfaces

Future work and challenges in correlation visualization

- Approaches for visualizing correlation structures in 3D
- Correlation analysis/visualization for other data types (e.g. vector fields)
- Integration of correlation information in existing uncertainty visualization approaches (e.g. positional uncertainty of features)
- Quantification of the effect of correlation on the occurrence of differential quantities and higher order features, like critical points
- Modeling and interpretation of stochastic dependencies in non-Gaussian distributed random fields