Chapter 9
Mathematical Foundations of Uncertain Field Visualization

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Abstract Uncertain field visualization is currently a hot topic as can be seen by the overview in this book. This article discusses a mathematical foundation for this research. To this purpose, we define uncertain fields as stochastic processes. Since uncertain field data is usually given in the form of value distributions on a finite set of positions in the domain, we show for the popular case of Gaussian distributions that the usual interpolation functions in visualization lead to Gaussian processes in a natural way. It is our intention that these remarks stimulate visualization research by providing a solid mathematical foundation for the modeling of uncertainty.

9.1 Introduction

The visualization of uncertain field data has attracted a lot of attention in recent time. As practically no measured or simulated data is exact, visualization research attempts to incorporate uncertainty in the images presented to the user. Despite this undebated need, there has been only slow progress towards this goal. There are many field visualization methods without an extension taking uncertainty into account. We think that a major reason for this fact is a lack of knowledge regarding the necessary mathematical description of uncertainty in the case of fields. As we argue in this article, stochastic processes are a viable tool to describe uncertain functions over continuous domains. Since stochastic processes are usually not part of the standard curriculum in computer science and sometimes even mathematics, visualization researchers are not very familiar with this non-trivial subject.

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In many cases, the field visualization problem consists of a finite set of given positions where the field value is known. It shall be noted that this holds for scalar, vector, and tensor fields. Before most field visualization methods are applied, an interpolation of these values is defined creating a continuous field over the whole continuous domain. The uncertain field visualization problem is very similar: One is given a finite set of positions with a (known or estimated) distribution of the (unknown) field value at each position. We consider the prominent case of Gaussian distributions in this article and show that all the well-known interpolation methods in visualization can be used in this case to define the uncertain field over the continuous domain as a Gaussian process. This rarely known fact emphasizes the potential of stochastic processes as model for uncertain fields in visualization research.

9.2 Stochastic Processes

We want to describe a (scalar, vector or tensor) field over some closed domain $D \subset \mathbb{R}^d, d = 1,2,$ or 3, that depends on some unknown (typically high dimensional) parameter $\omega \in \Omega$. The whole uncertainty is contained in this parameter: If we know the parameter ω, we know the field. To keep things simple, we assume that $\Omega = \mathbb{R}^u$, but that is not necessary[1]. In addition, **we assume that Ω, is known** i.e. the number and type of parameters that determine our field.

In a first step, we need a probability measure on Ω. As Ω contains an uncountable number of elements, we use a σ-algebra $\mathbb{S}$ on Ω. Because of $\Omega = \mathbb{R}^u$, the Borelalgebra $\mathbb{B}(\mathbb{R}^u)$ is a natural choice[2]. Furthermore, we need a probability measure $\mathbb{P} : \mathbb{S} \to [0,1]$. As usually, this means that the probability for $\omega \in A \subset \Omega$ is $\mathbb{P}(A) \in [0,1]$. Again, **we assume that this probability measure is known**.

In our second step, we define a **random variable**

$$X : \Omega \to \mathbb{R}^v$$

as measurable[3] map where the σ-algebra on $\mathbb{R}^v$ is the Borelalgebra $\mathbb{B}(\mathbb{R}^v)$. Essentially, this is a usual (i.e. deterministic) function, assigning each (unknown) parameter $\omega \in \Omega$ a value[4]. If the parameter ω is known, the random variable has a fixed value. From the probability measure $\mathbb{P}$ on Ω, we can derive a probability distribution of X on $\mathbb{R}^v$: For any set $A \subset \mathbb{R}^v$ in the Borelalgebra $\mathbb{B}(\mathbb{R}^v)$, we set

[1] In general, we only need a complete probability space, i.e. some set Ω with a σ-algebra and a probability measure on this σ-algebra. Completeness means that any subset of a set with measure zero must be in the σ-algebra. One can construct a complete probability space from an arbitrary probability space by adding elements to the σ-algebra and defining the measure on these elements accordingly [4, Suppl. 2] without any change of practical relevance.

[2] The Borelalgebra is the smallest σ-algebra that contains all open and closed subsets. This ensures in our case that we can measure the probability for all subsets of interest in practical cases.

[3] A map is measurable if each preimage of a measurable set is measurable

[4] The case $v = 1$ means a scalar, $v = d, d = 2,3$ means a vector and the case $v = d \times d = d^2, d = 2,3$ describes a second order tensor.

$$P(X \in A) := \mathbb{P}(X^{-1}(A)).$$

As final step, we will define uncertain fields now. Basically, we need to define a random variable at every position $x \in D$. However, there has to be some strong correlation between the random variables at close positions because, in visualization, we are usually dealing with continuous or even differentiable fields. Following Adler and Taylor [2], we define an **uncertain field** depending on our uncertain parameter $\omega \in \Omega$ over the domain D as a measurable, separable[5] map

$$f : \Omega \to (\mathbb{R}^v)^D.$$

In perfect analogy to random variables, each parameter $\omega \in \Omega$ gets assigned a deterministic function $f_\omega : D \to \mathbb{R}^v$, here denoted as an element of $(\mathbb{R}^v)^D$. Furthermore, for each position $x \in D$, we have a random variable $f_x : \Omega \to \mathbb{R}^v$ that assigns a fixed value at point $x \in D$ to the parameter $\omega \in \Omega$. We will use the notations

$$f_\omega(x) := f_x(\omega) := f(\omega, x) := (f(\omega))_x \in \mathbb{R}^v$$

for the value of the uncertain field f at position $x \in D$ given parameter $\omega \in \Omega$. The measure on $(\mathbb{R}^v)^D$ can be defined by a consistent description of distributions on arbitrary finite subsets of positions in D[6].

If we consider the situation at a single point $x \in D$ and a measurable subset of values $V \subset \mathbb{R}^v$, e.g. V is closed or open, we have the probability

$$P(f(\omega, x) \in V) = \mathbb{P}(\{\omega | f(\omega, x) \in V\}).$$

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[5] This condition removes subtle measurement problems without imposing restrictions of practical relevance, see Adler and Taylor [2, p. 8]. The concept was originally introduced by Doob [4] in his book on stochastic processes. In essence, it demands a dense countable subset $D \subset P$, and a fixed null set $N \in \mathbb{S}$ with $\mathbb{P}(N) = 0$ such that for any closed $B \subset \mathbb{R}^d$ and open $I \subset P$

$$\{\omega | f(x, \omega) \in B \forall x \in I\} \Delta \{\omega | f(x, \omega) \in B \forall x \in I \cap D\} \subset N$$

with symmetric set difference Δ.

[6] According to Doob [4, I.5,II.1] and going back to theorems by Kolmogorov, one needs to define probability distribution functions

$$F_{x_1,\ldots,x_n}(a_1, \ldots, a_n) = \mathbb{P}(|x_1| \leq a_1, \ldots, |x_n| \leq a_n)$$

for arbitrary finite tuples $(x_1, \ldots, x_n)$ of points in D, such that the following rather obvious two consistency conditions hold for all finite subsets of points $\{x_1, \ldots, x_n\}$ and value bounds $a_1, \ldots, a_n \in \mathbb{R}$:

$$F_{x_1,\ldots,x_n}(a_1, \ldots, a_n) = F_{x_{\alpha_1},\ldots,x_{\alpha_n}}(a_{\alpha_1}, \ldots, a_{\alpha_n}) \forall \text{ permutations } \alpha$$

and

$$F_{x_1,\ldots,x_m}(a_1, \ldots, a_m) = \lim_{\lambda_j \to \infty, j=m+1,\ldots,n} F_{x_1,\ldots,x_n}(a_1, \ldots, a_n) \forall m < n$$

We will use multivariate Gaussian distributions for this purpose in the next sections. This footnote illustrates that other distributions are possible.

As an example for the probability space $(\Omega, \mathbb{S}, \mathbb{P})$, we assume that we have a set of positions $\{p^1, \ldots, p^N\} \in \mathbb{R}^2$ in the plane. At these positions, we have uncertain scalar values $\{v^1, \ldots, v^N\} \in \mathbb{R}$ with normal distributions[7] $W_i \sim N(\mu_i, \sigma_i)$. We may assume that these values are not independent with covariances

$$C_{ij} = E((v_i - \mu_i)(v_j - \mu_j)) \text{ with } \sigma_i = \sqrt{C_{ii}}.$$

Then, we have $(\Omega, \mathbb{S}, \mathbb{P}) = (\mathbb{R}^N, \mathbb{B}(\mathbb{R}^n), N(\mu, C))$. This means that our probability space is N-dimensional real space with an N-dimensional normal distribution with mean vector $\mu \in \mathbb{R}^N$ and (symmetric) covariance matrix $C \in \mathbb{R}^{N \times N}$. It shall be noted that it is possible to derive a space with independent Gaussian variables with potentially smaller dimension $M < N$ by spectral decomposition of C and using the eigenvectors with eigenvalue different from 0. In the following sections, we will see how we can define an uncertain scalar field from these data.

9.3 Gaussian Processes

The previous section introduced stochastic processes without referring to a specific type of distribution at every position. A careful look at the footnotes or intuition tells that the distributions at the different points have to be somehow consistent, and that a simple solution might be to use distributions of the same type everywhere. Looking at the literature, it can be said that Gaussian distributions are the most often used case. If one uses them, one arrives at the special topic of Gaussian processes. They have been analyzed in detail with respect to geometric properties by Adler and Taylor [1, 2, 3] in a mathematically rigorous fashion. But Gaussian processes have also been applied in other areas of computer science. A nice example is provided by machine learning as described in the book by Rasmussen and Williams [7]. This section and the rest of the article will focus on Gaussian processes.

As before, let $(\Omega, \mathbb{S}, \mathbb{P})$ be a known probability space. Let $D \subset \mathbb{R}^d, d = 1, 2,$ or 3 be the known domain of our field and let $\mathbb{R}^v$ be the set of potential values of our field, i.e. $v = 1$ means a scalar field, $v = d$ means a vector field, and $v = d \times d$ means a tensor field of second order. A measurable, separable map

$$f : \Omega \to (\mathbb{R}^v)^D$$

is called **Gaussian random field** on D if for all finite tuples $(x_1, \ldots, x_n)$ of points in D the random variable $(f_{x_1}, \ldots, f_{x_n})$ is a $v \times n$-dimensional Gaussian random variable. The function

[7] A normal distribution on $\mathbb{R}$ is defined by a probability density function

$$\phi(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp^{-\frac{(x-\mu)^2}{2\sigma^2}}.$$

μ is the mean of the distribution and σ the standard deviation.

$$\mu : D \to \mathbb{R}^v, \quad \mu(x) = E(f_x)$$

with expectation E is called **expectation function**. The map

$$C : D \times D \to \mathbb{R}^{v \times v} \quad C(x,y) := E((f_x - E(f_x))(f_y - E(f_y)))$$

is called **covariance function**. For any function $\mu : D \to \mathbb{R}^v$ and any non-negative definite function $C : D \times D \to \mathbb{R}^{v \times v}$, there is a unique Gaussian process with expectation function μ and covariance function C, see Adler and Taylor [2, p.5]! This statement is the basis behind the design and use of Gaussian processes in machine learning as described by Rasmussen and Williams [7]. However, we think that an approach starting with interpolation is more appropriate to visualization, as this is the usual way of defining continuous fields from discrete data in our discipline.

9.4 Linear Interpolation on the Line as a Gaussian Process

This section considers a very simple example. We take the real line as domain, i.e. $D = \mathbb{R}$. We assume that we are given two uncorrelated Gaussian distributions of scalar values

$$W_1 \sim N(\mu_1, \sigma_1) \text{ and } W_2 \sim N(\mu_2, \sigma_2)$$

at the points $x_1 = 0$ and $x_2 = 1$ as data. We want to describe a simple linear interpolation. Since the two values are uncorrelated, we take $\Omega = \mathbb{R}^2$ as parameter space, the Borelalgebra $\mathbb{B}(\mathbb{R}^2)$ as σ-algebra and the 2-dimensional normal distribution $\mathbb{P} = N(\mu, C)$ with

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \quad C = \begin{pmatrix} \sigma_1 & \\ & \sigma_2 \end{pmatrix}$$

as probability distribution. This means that we assume two normally distributed, independent real parameters that will determine our uncertain field. In this simple case, the two random variables

$$W_1 : \Omega \to \mathbb{R}, W_1(\omega) = \omega_1, \quad W_2 : \Omega \to \mathbb{R}, W_2(\omega) = \omega_2$$

determine the values at the two given positions x_1 and x_2, respectively. It is natural to define the linearly interpolated uncertain field f on the real line by

$$f : \Omega \to (\mathbb{R})^{\mathbb{R}}, \quad (f(\omega))_x := \omega_1(1-x) + \omega_2 x.$$

With the notation

$$f_\omega(x) = \omega_1(1-x) + \omega_2 x,$$

it becomes pretty clear that we are really defining a linear interpolation of the values at 0 and 1 on the real line for each given ω. However, the whole point of the chapter is that we are really defining a Gaussian process! The short argument is that this follows from slightly more abstract arguments of Adler and Taylor [3, pp. 17–19].

However, some basic computations might improve understanding of this point: At every position $x \in D$, we have the random variable

$$f_x(\omega) = \omega_1(1-x) + \omega_2 x.$$

As ω_1, ω_2 are independent Gaussian variables, this is a Gaussian variable with expectation

$$\mu(x) = E(f_x(\omega)) = \mu_1(1-x) + \mu_2 x$$

and variance

$$\sigma^2(x) = E((f_x(\omega) - \mu(x))^2) = \sigma_1^2(1-x)^2 + \sigma_2^2 x^2.$$

For the covariance function $C : D \times D \to \mathbb{R}$, we have

$$\begin{aligned} C(x,y) &= E((f_x(\omega) - \mu(x))(f_y(\omega) - \mu(y))) \\ &= E(((\omega_1 - \mu_1)(1-x) + (\omega_2 - \mu_2)x)((\omega_1 - \mu_1)(1-y) + (\omega_2 - \mu_2)y)) \\ &= (1-x)(1-y)E((\omega_1 - \mu_1)^2) + xyE((\omega_2 - \mu_2)^2) \\ &= (1-x)(1-y)\sigma_1^2 + xy\sigma_2^2 \end{aligned}$$

because of the independence of ω_1, ω_2, i.e. $E((\omega_1 - \mu_1)(\omega_2 - \mu_2)) = 0$. For $\sigma_1 = \sigma_2$, this coincides with the construction by Pöthkow and Hege [5].

9.5 General Interpolation

We turn now to a realistic interpolation scenario. We consider some closed domain $D \subset \mathbb{R}^d$. We assume that we are given N positions $p^1, \ldots, p^N \in D$. At these positions, we are given N uncertain v-dimensional values with normal distributions, say

$$W^i \sim N_v(\mu^i, C^i), \forall i = 1, \ldots, N$$

where $C^i \in \mathbb{R}^(v \times v)$ denotes the covariances between the dimensions at a single position. We still assume that the N values are independent. Our interpolation method is given by N (deterministic) weight functions

$$\phi_i : D \to \mathbb{R}, \forall i = 1, \ldots, N \text{ with } \phi_i(p^j) = \delta_{ij}$$

with Kronecker δ. This is the typical case in finite element formulations and for almost all grid based field data in visualization.

We define our probability space via $\Omega = \mathbb{R}^{N \times v}$, Borelalgebra $\mathbb{B}(\Omega)$ and

$$\mathbb{P} \sim N(\mu, C), \quad \mu = \begin{pmatrix} \mu^1 \\ \vdots \\ \mu^N \end{pmatrix}, \quad C = \begin{pmatrix} C^1 & & \\ & \ddots & \\ & & C^N \end{pmatrix}$$

as probability measure. Our uncertain field f is defined as

$$f : \Omega \to (\mathbb{R}^v)^D, \quad f(\omega,x) = f_\omega(x) = f_x(\omega) = (f(\omega))_x = \sum_{i=1}^{N} \omega^i \phi_i(x).$$

Fixing position $x \in D$, we get a random variable

$$f_x : \Omega \to \mathbb{R}^v$$

that describes the distribution of values at that position as a Gaussian distribution

$$f_x \sim N(\mu(x), C(x)), \quad \mu(x) = \sum_{i=1}^{N} \mu^j \phi_j(x), \quad C(x) \in \mathbb{R}^{v\times v}, C_{kl}(x) = \sum_{i=1}^{N} C_{kl}^i \phi_i^2(x).$$

Looking at the whole uncertain field again, we have the expectation function

$$\mu : D \to \mathbb{R}^v, \quad \mu(x) = \sum_{i=1}^{N} \mu^j \phi_j(x)$$

and the covariance function

$$C : D \times D \to \mathbb{R}^{v\times v}, \quad C_{kl}(x,y) = \begin{cases} 0 & k \neq l \\ \sum_{i=1}^{N} \sum_{j=1}^{N} \phi_i(x)\phi_j(y) C_{ij}^k & k = l \end{cases}$$

because of the independence of ω_k, ω_l. It should be noted that the definition of an interpolation as above and the definition of a covariance function as usually done in machine learning, see Rasmussen and Williams [7], is actually equivalent, see Adler and Taylor [3, pp. 17–19].

Finally, we describe the case of dependent data at given N positions. To simplify notation, we formulate only the scalar case. We consider a closed domain $D \subset \mathbb{R}^d$ and N positions $p^1, \ldots, p^N \in D$. At these positions, we are given N uncertain scalar values with normal distributions

$$W^i \sim N(\mu_i, C_{ii}) \quad \forall i = 1, \ldots, N$$

with covariances[8]

$$C_{ij} = E((W^i - E(W^i))(W^j - E(W^j))).$$

The interpolation is again given by N deterministic weight functions

$$\phi_i : D \to \mathbb{R}, \forall i = 1, \ldots, N \text{ with } \phi_i(p^j) = \delta_{ij}$$

[8] In praxis, the covariances are either given or have to be estimated from several given sample fields. Obviously, this estimation might be a challenge in its own right as the number of positions is almost certainly larger than the number of sample fields. Pöthkow et al. [6] made some comments in this direction.

with Kronecker δ. The interesting point is that the dependence of the uncertain values typically reduces the number of independent uncertain parameters. Mathematically, this means that the (symmetric) covariance matrix C has only $M <= N$ independent rows. One can find them by principal component analysis[9]. Let $\lambda_1, \ldots, \lambda_M \in \mathbb{R}$ be the non-zero eigenvalues of C, $e^1, \ldots, e^M \in \mathbb{R}^N$ the corresponding eigenvectors. Let $\Lambda \in \mathbb{R}^{M \times M}$ be the diagonal matrix of the non-zero eigenvalues $\lambda_1, \ldots, \lambda_M$. We model our probability space via $\Omega = \mathbb{R}^M$, Borelalgebra $\mathbb{B}(\Omega)$ and $\mathbb{P} \sim N(0, \Lambda)$ as probability measure. This probability space consists of M independent normally distributed scalar parameters with mean 0. The uncertain field f is defined as

$$f : \Omega \to (\mathbb{R}^v)^D, \quad (f(\omega))_x = \sum_{i=1}^{N} \left(\mu_i + \sum_{k=1}^{M} \omega_k e_i^k \right) \phi_i(x).$$

The Gaussian distribution at each position x, mean function and expectation function can be derived from here as before.

9.6 Conclusion

We have shown that stochastic processes provide a suitable mathematical foundation for the definition of uncertain fields in visualization. In the case of given Gaussian distributions, we have demonstrated how the well-known interpolation methods allow to define Gaussian processes from uncertain field data. We hope that these remarks will stimulate and simplify research on the visualization of uncertain field data. Of course, there is much more to say on the topic that would require more space than available here. For further reading, we recommend the cited literature below.

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[9] In praxis, there will be eigenvalues very close to zero in the estimated covariance matrix which one might want to set to zero. Again, this is an obvious challenge outside the scope of this article.