Linearly Constrained Gaussian Processes with Boundary Conditions

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Abstract
One goal in Bayesian machine learning is to encode prior knowledge into prior distributions, to model data efficiently. We consider prior knowledge from systems of linear (partial and ordinary) differential equations together with their boundary conditions. We construct multi-output Gaussian process priors with realizations dense in the solution set of such systems, in particular any solution (and only such solutions) can be represented to arbitrary precision by Gaussian process regression. The construction is fully algorithmic via Gröbner bases and it does not employ any approximation. It builds these priors combining two parametrizations via a pullback: the first parametrizes the solutions for the system of differential equations and the second parametrizes all functions adhering to the boundary conditions.

1. Introduction
Gaussian processes (Rasmussen & Williams, 2006) are very data efficient. Hence, they are the prime regression technique for small datasets and applied when data is rare or expensive to produce. Applications range, among many others, from robotics (Lima et al., 2018), biology (Honkela et al., 2015), global optimization (Osborne et al., 2009), hyperparameter search (Thornton et al., 2013), astrophysics (Garnett et al., 2015) to engineering (Thewes et al., 2015).

Roughly, a Gaussian process can be viewed as a suitable probability distribution on a set of functions, which we can condition on observations using Bayes’ rule. This avoids overfitting. Due to the self-conjugacy of the Gaussian distribution, the posterior is again Gaussian. The mean function of the posterior is used for regression and the variance quantifies uncertainty. When choosing a suitable covariance function of the prior, the posterior can approximate any behavior present in data, even in noisy or unstructured data.

Any prior knowledge about the regression problem should be incorporated into the prior. Then, the precisely rare measurement data can be used to refine and improve on this prior knowledge, instead needing to learn it. The prior knowledge is usually encoded into the covariance structure of the Gaussian process, cf. (Rasmussen & Williams, 2006, §4) or (Duvenaud, 2014). Gaussian process regression differs in philosophy from deep learning, where the latter thrives on extracting knowledge from a lot of data but struggles with one-shot learning and encoding prior knowledge.

Prior knowledge is often given by physical laws. In particular, it is important to include linear differential equations into machine learning frameworks. Gaussian processes that adhere to such a set of linear differential equations were constructed several times in the literature (Macedo & Castro, 2008; Särkkä, 2011; Scheuerer & Schlather, 2012; Wahlström et al., 2013; Solin et al., 2018; Jidling et al., 2017; 2018). All realizations and the mean function of the posterior strictly adhere to these physical laws. Such Gaussian processes exist if and only if the set of linear differential equations describes a controllable system. Their construction can be completely automatized by symbolic algorithms from algebraic system theory, which again strongly build on Gröbner bases (Lange-Hegermann, 2018).

Usually, differential equations turn up together with boundary conditions. Hence, a description of boundary conditions in a machine learning framework is highly desirable. For ODEs, boundary conditions behave as data points, which are trivially included into a Gaussian process (cf. Example 4.1). For PDEs, one would need functions (with infinite dimensional data) to describe the boundary conditions. Graepel (2003) approximated these functions by finite dimensional data. Solving this problem exactly is the main contribution of this paper: the construction of Gaussian process priors combining differential equations and general boundary conditions. This construction is based on symbolically building parametrizations using Gröbner bases.

Using the results of this paper, one can add information to Gaussian processes by

(i) conditioning on data points (Bayes’ rule),

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2For notational simplicity, we refrain from using the phrase “almost surely” in this paper, e.g. by assuming separability.
(ii) restricting to solutions of linear operator matrices (Lange-Hegermann, 2018), and

(iii) adding boundary conditions (this paper).

Since these constructions are compatible, we can combine strict, global information from equations and boundary conditions with noisy, local information from observations. This paper is an example in how symbolic techniques can help data driven machine learning. All results are mathematically proven and the algorithms are demonstrated on toy examples with only one or two data points, an extreme form of one-shot learning. The code for reproduction of the results is given in Appendix B and the (very small amount of) data is completely given in the text.

We recall Gaussian processes and their connection to linear operators in Section 2 and summarize the construction of Gaussian processes adhering to linear operators in Section 3. Describing boundary conditions as parametrizations is surprisingly simple (Section 4). Theorem 5.2 describes the core construction of this paper, which allows to check whether two parametrizations are combinable and computes the combination in the positive case. In Section 6 we construct boundary conditions with non-zero right hand sides.

2. Operators and Gaussian Processes

This section gives a short exposition of Gaussian process regression and their connection to linear operators.

2.1. Gaussian processes

A Gaussian process \( g = \mathcal{GP}(\mu, k) \) describes a probability distribution on the evaluations of functions \( \mathbb{R}^d \to \mathbb{R}^d \) such that the function values \( g(x_1), \ldots, g(x_n) \) at \( x_1, \ldots, x_n \in \mathbb{R}^d \) have a joint Gaussian distribution. It is specified by a mean function

\[
\mu : \mathbb{R}^d \to \mathbb{R}^d : x \mapsto E(g(x))
\]

and a positive semidefinite covariance function

\[
k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d_{\geq 0} : (x, x') \mapsto E ((g(x) - \mu(x))(g(x') - \mu(x'))^T) .
\]

All higher moments exist and are uniquely determined by \( \mu \) and \( k \), all higher cumulants are zero. We often restrict the domain of a Gaussian process to a subset \( X \subseteq \mathbb{R}^d \).

Assume the regression model \( y_i = g(x_i) \) and condition on \( n \) observations

\[
\{(x_i, y_i) \in \mathbb{R}^{1 \times d} \times \mathbb{R}^{1 \times d} | i = 1, \ldots, n\} .
\]

Denote by \( k(x, X) \in \mathbb{R}^{1 \times n} \) resp. \( k(X, X) \in \mathbb{R}^{n \times n} \) the (covariance) matrices obtained by concatenating the matrices \( k(x, x_j) \) resp. the positive semidefinite block partitioned matrix with blocks \( k(x_i, x_j) \). Write \( \mu(X) \) resp. \( y \in \mathbb{R}^{1 \times n} \) for the row vector obtained by concatenating the rows \( \mu(x_i) \) resp. \( y_i \). The posterior is the Gaussian process

\[
\mathcal{GP} \left( x \mapsto \mu(x) + (y - \mu(X))k(X, X)^{-1}k(x, X)^T, (x, x') \mapsto k(x, x') - k(x, X)k(X, X)^{-1}k(x', X)^T \right).
\]

Its mean function can be used as regression model and its variance as model uncertainty.

2.2. Linear operators on Gaussian processes

Roughly, Gaussian processes are the linear objects among stochastic processes and there is a rich interplay of Gaussian processes and linear operators, which is present everywhere in this paper. In particular, the class of Gaussian processes is closed under linear operators once mild assumptions hold. This subsection formalizes and generalizes the following well-known example of differentiating a Gaussian process.

Example 2.1. Let \( g = \mathcal{GP}(0, k(x, x')) \) be a scalar univariate Gaussian process with differentiable realizations. Then,

\[
\left[ \frac{\partial}{\partial x} \right] g := \mathcal{GP} \left( 0, \frac{\partial^2}{\partial x \partial x'} k(x, x') \right)
\]

is the Gaussian process of derivatives of realizations of the Gaussian process \( g \). One can interpret this Gaussian process \( \left[ \frac{\partial}{\partial x} \right] g \) as taking derivatives as measurement data and producing a regression model of derivatives. Taking a one-sided derivative \( \frac{\partial}{\partial x} k(x, x') \) yields the cross-covariance between a function and its derivative. See (Cramér & Leadbetter, 2004, §5.2) for a proof and (Wu et al., 2017) resp. (Cobb et al., 2018) for applications in Bayesian optimization resp. vector field modeling.

Recall the mathematical definition of a pushforward. Given a set of functions \( G \subseteq \{ f : X \to Y \} \) and \( b : Y \to Z \), then

\[
b_* G = \{ b \circ f \mid f \in G \} \subseteq \{ f : X \to Z \} .
\]

Similarly, we can define the pushforward of any stochastic Process \( g : \Omega \to (X \to Y) \) by

\[
b_* g : \Omega \to (X \to Z) : \omega \mapsto (b \circ g(\omega)) .
\]

Lemma 2.2. Let \( \mathcal{F} \) and \( \mathcal{G} \) be spaces of functions defined on \( D \subseteq \mathbb{R}^d \) with product σ-algebra of function evaluations. Let \( g = \mathcal{GP}(\mu(x), k(x, x')) \) be a Gaussian process with realizations in \( \mathcal{F} \) and \( B : \mathcal{F} \to \mathcal{G} \) a linear, measurable operator which commutes with expectation w.r.t. the measure induced from \( g \) on \( \mathcal{F} \) and by \( b_* g \) on \( \mathcal{G} \). Then, the pushforward \( B_* g \) of \( g \) under \( B \) is again a Gaussian process with

\[
B_* g = \mathcal{GP}(B\mu(x), Bk(x, x')(B')^T) .
\]
where \( B' \) denotes the operation of \( B \) on functions with argument \( x' \).

Call \( B, g \) the pushforward Gaussian process of \( g \) under \( B \).

We postpone the proof to Appendix A. Lemma 2.2 is often stated without assuming that \( B \) commutes with expectation, but also without proof. If such a more general version of Lemma 2.2 holds, I would like a reference. Special cases have been discussed in the literature, often only for mean square differentiability, cf. e.g. (Papoulis & Pillai, 2002, discussion after (9.87) (or (10.78) in the third edition)), (Adler, 1981, Thm 2.2.2), (Agrell, 2019), (Da Veiga & Marrel, 2012, §2.3), (Bertinet & Agnan, 2004, Thm. 9).

Consider change points and change surfaces as first relevant application of Lemma 2.2, following ideas from (Garnett et al., 2009; 2010; Lloyd et al., 2014; Herlands et al., 2016).

**Example 2.3.** Let \( \rho_1, \rho_2 : \mathbb{R}^d \to [0,1] \) a partition of unity, i.e., \( \rho_1(x) + \rho_2(x) = 1 \) for all \( x \in \mathbb{R}^d \). Usually, both \( \rho_1 \) and \( \rho_2 \) are close to being 0 or close to being 1 over most of \( \mathbb{R}^d \). Such a partition of unity induces a linear operator

\[
\rho = [\rho_1, \rho_2] : \mathcal{F}^2 \times 1 \to \mathcal{F}^1 \times 1 : \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \mapsto [\rho_1 \rho_2] \begin{bmatrix} f_1 \\ f_2 \end{bmatrix},
\]

where \( \mathcal{F} \) is a space of functions \( \mathbb{R}^d \to \mathbb{R} \). Given two Gaussian processes \( g_1 = \mathcal{GP}(0, k_1), g_2 = \mathcal{GP}(0, k_2) \) with realizations in \( \mathcal{F} \), we have

\[
\rho_* g := \begin{bmatrix} \rho_1 & \rho_2 \end{bmatrix} \begin{bmatrix} g_1 \\ g_2 \end{bmatrix} = \mathcal{GP}(0, \rho_1 k_1(x,x') \rho_1(x') + \rho_2(x) k_2(x,x') \rho_2(x'))
\]

Thereby, we can model a change point (for \( d = 1 \)) or a change surface (for \( d > 1 \)) at a position where \( \rho_1 \) changes from being close to 0 to being close to 1.

This example is the basis for boundary conditions in Section 4: when setting \( g_2 \) to zero, \( \rho_* g \) is close to zero where \( \rho_2 \approx 1 \) and close to \( g_1 \) where \( \rho_1 \approx 1 \).

**3. Solution Sets of Operator Equations**

We consider linear ordinary and partial differential equations defined on the set of smooth functions. Consider the real vector space \( \mathcal{F} = C^\infty(X, \mathbb{R}) \) of smooth functions from \( X \subseteq \mathbb{R}^d \) to \( \mathbb{R} \) with the usual Fréchet topology. The squared exponential covariance function

\[
k_\mathcal{F}(x_i, x_j) = \exp\left(-\frac{1}{2} \sum_{a=1}^d (x_{i,a} - x_{j,a})^2 \right)
\]

induces a Gaussian process prior \( g_\mathcal{F} = \mathcal{GP}(0, k_\mathcal{F}) \) with realizations dense in the space of functions \( \mathcal{F} = C^\infty(X, \mathbb{R}) \).

The following three rings of linear operators \( R \) model operator equations. These rings are all \( \mathbb{R} \)-algebras such that \( \mathcal{F} \) is a topological \( R \)-left-module, i.e., \( \mathcal{F} \) is a topological \( \mathbb{R} \)-vector space of functions \( X \to \mathbb{R} \) for \( X \subseteq \mathbb{R}^d \) that also is an \( R \)-left-module such that the elements of \( R \) operate continuously on \( \mathcal{F} \).

**Example 3.1.** The polynomial ring \( R = \mathbb{R}[\partial_{x_1}, \ldots, \partial_{x_d}] \) models linear differential equations with constant coefficients, as \( \partial_{x_i} \) acts on \( \mathcal{F} = C^\infty(X, \mathbb{R}) \) via partial derivative w.r.t. \( x_i \), making \( \mathcal{F} \) into an \( R \)-module.

**Example 3.2.** The polynomial ring \( R = \mathbb{R}[x_1, \ldots, x_d] \) models algebraic equations via multiplication on \( \mathcal{F} \). This ring is relevant for boundary conditions.

**Example 3.3.** To combine linear differential equations with constant coefficients with boundary conditions or to model linear differential equations with polynomial coefficients, consider the Weyl algebra \( R = \mathbb{R}[x_1, \ldots, x_n][\partial_{x_1}, \ldots, \partial_{x_n}] \). It has the non-commutative relation \( \partial_{x_i} x_j = x_j \partial_{x_i} + \delta_{ij} \) representing the product rule of differentiation, where \( \delta_{ij} \) is the Kronecker delta. Operators defined over these three rings satisfy the assumptions of Lemma 2.2: Since the realizations of \( g_\mathcal{F} \) are continuously differentiable, it is an easy exercise in the dominated convergence theorem that taking expectation commutes with taking derivatives and multiplication obviously commutes with taking expectations.

These three rings also operate continuously on \( \mathcal{F} \). The Fréchet topology is constructed to make derivation continuous. If \( X \) is bounded away from infinity, then the multiplication is bounded and hence continuous, as \( \mathcal{F} \) is Fréchet.

**3.1. Parametrizations**

For \( A \in R^d \times \ell \) define the solution set

\[
sol_\mathcal{F}(A) := \{ f \in \mathcal{F}^\ell \mid A f = 0 \}
\]

as a nullspace of an operator matrix \( A \). We say that a Gaussian process is in a function space, if its realizations are contained in said space. The following tautological lemma

\[
\text{for} \quad f \in \mathcal{F}^\ell \Rightarrow \sup_{i} \sup_{z \in [-1,1]^d} \left| \frac{\partial}{\partial z_i} f(z) \right| \leq \sup_{i} \sup_{z \in [-1,1]^d} \left| \frac{\partial}{\partial z_i} f(z) \right|
\]

of seminorms for \( a, b \in \mathbb{Z}_{\geq 0} \) on \( \mathcal{F} \) (Treves, 1967, §10).
is a version of the fundamental theorem of homomorphisms. It describes the interplay of Gaussian processes and solution sets of operators.

Lemma 3.4 (Lange-Hegermann (2018, Lemma 2.2)). Let $g = GP(\mu, k)$ be a Gaussian process in $\mathcal{F}^\ell \times 1$. Then $g$ is a Gaussian process in the solution set $\text{sol}_\mathcal{F}(A)$ of $A \in \mathbb{R}^{\ell \times \ell}$ if and only if both $\mu$ is contained in $\text{sol}_\mathcal{F}(A)$ and $A_*(g - \mu)$ is the constant zero process.

To construct Gaussian processes with realizations in the solution set $\text{sol}_\mathcal{F}(A)$ of an operator matrix $A \in \mathbb{R}^{\ell \times \ell}$, one looks for a $B \in \mathbb{R}^{\ell \times \ell}$ with $AB = 0$ (Jidling et al., 2017). If $g = GP(0, k)$ is a Gaussian process in $\mathcal{F}^\ell \times 1$, then the realizations of $B_*g$ are contained in $\text{sol}_\mathcal{F}(A)$ by Lemma 3.4, as $B_*(g - \mu) = (AB)_*g = 0$. $g = 0$.

In practice, one would like that any solution in $\text{sol}_\mathcal{F}(A)$ can be approximated by $B_*g$ to arbitrary precision, i.e., that the realizations of the Gaussian process $B_*g$ are dense in $\text{sol}_\mathcal{F}(A)$. To this end, we call $B \in \mathbb{R}^{\ell \times \ell}$ a parametrization of $\text{sol}_\mathcal{F}(A)$ if $\text{sol}_\mathcal{F}(A) = B\mathcal{F}^\ell \times 1$.

Proposition 3.5. Let $B \in \mathbb{R}^{\ell \times \ell}$ be a parametrization of $\text{sol}_\mathcal{F}(A)$ for $A \in \mathbb{R}^{\ell \times \ell}$. Take the Gaussian process $g_B^{(\ell)} \in \mathcal{F}^\ell \times 1$ of $\ell$ i.i.d. copies of $g_A$, the Gaussian process with squared exponential covariance function $k_\ell$, from Eq. (1). Then, the realizations of $B_*g_B^{(\ell)}$ are dense in $\text{sol}_\mathcal{F}(A)$.

Proof. The realizations of $g_B^{(\ell)}$ are dense in $\mathcal{F}^\ell \times 1$ by construction. The operator $B$ induces a surjective map, which is continuous, as $\mathcal{F}$ is a topological $\mathbb{R}$-module. Surjective continuous maps send dense sets to dense sets.

3.2. Algorithmically constructing parametrizations

We summarize the algorithm which decides whether a parametrization of a system of linear differential equations exists and compute it in the positive case.

To construct the parametrization $B$, we are lead to just compute the nullspace of $\mathcal{F}^\ell \times 1 \hookrightarrow \mathcal{F}^{\ell \times 1}$.

This is not feasible, as $\mathcal{F}$ is too “big” to allow computations. Instead, we compute the nullspace of $\mathbb{R}^{\ell \times 1} \hookrightarrow \mathcal{F}^{\ell \times 1}$, a symbolic computation, only using operations over $\mathbb{R}$ without involvement of $\mathcal{F}$.

Theorem 3.6. Let $A \in \mathbb{R}^{\ell \times \ell}$. Let $B$ be the right nullspace of $A$ and $A'$ the left nullspace of $B$. Then $\text{sol}_\mathcal{F}(A')$ is the largest subset of $\text{sol}_\mathcal{F}(A)$ that is parametrizable and $B$ parametrizes $\text{sol}_\mathcal{F}(A')$.

A well-known and trivial special case of this theorem are linear equations in finite dimensional vector spaces, with $R = \mathcal{F} = \mathbb{R}$ the field of real numbers. In that case, $\text{sol}_\mathcal{F}(A)$ can be found by applying the Gaussian algorithm to the homogeneous system of linear equations $AB = 0$ and write a base for the solutions of $b$ in the columns of a matrix $B$. This matrix $B$ is the (right) nullspace of $A$. There are no additional equations satisfied by the above solutions, i.e. $A = A'$ generates the (left) nullspace of $B$.

In general, the left nullspace $A'$ of the right nullspace $B$ of $A$ is not necessarily $A$. E.g., for the univariate polynomial ring $R = \mathbb{R}[x]$ and the matrix $A = \begin{bmatrix} x \end{bmatrix}$ we have $B = \begin{bmatrix} 0 \end{bmatrix}$ and $A' = \begin{bmatrix} 1 \end{bmatrix}$.

Corollary 3.7. In Theorem 3.6, $\text{sol}_\mathcal{F}(A)$ is parametrizable if and only if the rows of $A$ and $A'$ generate the same row-module. Since $AB = 0$, this is the case if all rows of $A'$ are contained in the row module generated by the rows of $A$. In this case, $\text{sol}_\mathcal{F}(A)$ is parametrized by $B$.

For a formal proof we refer to the literature. Luckily, there is a high level description of the parametrizable systems.

Theorem 3.8 (Oberst (1990, §7.21)). A system $\text{sol}_\mathcal{F}(A)$ is parametrizable if it is controllable.

The intuition for controllability is that one can partition the functions of the system into state and input, such that any chosen state can be reached by suitably manipulating the inputs. If $A$ is not parametrizable, then the solution set $\text{sol}_\mathcal{F}(A')$ is the subset of controllable behaviors in $\text{sol}_\mathcal{F}(A)$.

Reduced Gröbner bases generalize the reduced echelon form from linear systems to systems of polynomial (and hence linear operator) equations, by bringing them into a standard form. They are computed by Buchberger’s algorithm, which is a generalization of the Gaussian and Euclidean algorithm and a special case of the Knuth-Bendix completion algorithm. The generalization of Gröbner bases to vectors of polynomials is straightforward.

Gröbner bases make the above theorems algorithmic. Similar to the reduced echelon form, Gröbner bases allow to compute all solutions over $\mathbb{R}$ of the homogeneous system and compute, if it exists, a particular solution over $\mathbb{R}$ for an inhomogeneous system. Solving homogeneous systems is the same as computing its right resp. left nullspace (of $A$ resp. $B$). Solving inhomogeneous equations decides whether an element (the rows of $A'$) is contained in a module (the row module of $A$).

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7The nullspace is also called kernel; we do not use this name to avoid confusion with symmetric positive semidefinite functions.

8FD vector spaces are naturally isomorphic to their bi-dual.

9(Zerz et al., 2010, Thm. 2). (Zerz, 2000, Thm. 3, Alg. 1, Lemma 1.2.3), (Oberst, 1990, §7.24), (Quadrat, 2013; 2010; Barakat, 2010; Seiler & Zerz, 2010; Chyzak et al., 2005; Robertz, 2015)

10depending only on the choice of a so-called monomial order.
A formal description of Gröbner bases exceeds the scope of this note. We refer to the excellent literature\textsuperscript{11}. In addition to polynomial rings, Gröbner bases exist for the Weyl algebra\textsuperscript{12} and many further rings. They are implemented in various computer algebra systems (Decker et al., 2019; Grayson & Stillman).

Gröbner bases solve problems of high complexity like EXPSPACE completeness (Mayr, 1989; Mayr & Meyer, 1982; Bayer & Stillman, 1988). In practice, this is less of a problem, as the Gröbner basis computations only involve the operator equations, but no data, hence we view the complexity of the Gröbner basis computations in $O(1)$. In particular, every example in this paper terminates instantaneously.

The next example is extended over the course of this paper.

**Example 3.9 (Lange-Hegermann (2018, Example 4.4)).** We construct a prior for smooth tangent fields on the sphere without sources and sinks using the polynomial Weyl algebra $R = \mathbb{R}[x, y, z](\partial_x, \partial_y, \partial_z)$. I.e., we are interested in $\text{sol}_A(\mathcal{F}) = \{v \in C^\infty(S^2, \mathbb{R}^3) \mid A \cdot v = 0\}$ for

$$A := \begin{pmatrix} x & y & z \\ \partial_x & \partial_y & \partial_z \end{pmatrix}.$$  

The right nullspace

$$B := \begin{pmatrix} -z \partial_y + y \partial_z \\ z \partial_z - x \partial_x \\ -y \partial_x + x \partial_y \end{pmatrix}.$$  

can be checked to yield a parametrization of $\text{sol}_F(A)$. For a demonstration of this covariance functions, see Figure 1.

![](Figure 1. The posterior mean of the conditioning the prior in Example 3.9 at two opposite points on the equator with tangent vectors pointing north (displayed artificially bigger). Without sources and sinks, the tangent vectors flow south away from the data.

\[ \begin{aligned} + (-2xy + x + y - 1) \left( e^{x+y-2} + e^{-1} \right) \\ + (xy - y + 1)e^{y-2} + (xy - x + 1)e^{x-2} \\ + (y - x - 2)e^{y-1} + (x - y - 2)e^{x-1} \end{aligned} \]

which is zero if $x$ or $y$ are in $\{0, 1\}$.

We now create priors for homogeneous boundary conditions for PDEs (for the inhomogeneous case see Section 6). Such boundary conditions fix the function values and/or their derivatives at a subset of the domain $X$.

Denote by $\mathcal{F} = C^\infty(X, \mathbb{R})$ the set of smooth functions defined on $X \subset \mathbb{R}^d$ compact. Let $R' \subset \mathbb{R}^X$ be a Noetherian ring of functions and subring of $R$, and $M \subset X$ implicitly defined by an ideal $I \trianglelefteq R'$ of equations, i.e.,

$$M = \text{V}(I) := \{m \in X \mid f(m) = 0 \text{ for all } f \in I\}.$$  

An important example for this setting is the Weyl algebra $R = \mathbb{R}[x_1, \ldots, x_d](\partial_{x_1}, \ldots, \partial_{x_d})$ and its subring $R'$ the polynomial ring $R' = \mathbb{R}[x_1, \ldots, x_d]$.

All solutions of a homogenous boundary condition $f|_M = 0$ for a single function $f \in \mathcal{F}$ can be parametrized by $\mathcal{F} \leftrightarrow \mathcal{F}^\ell \times \mathbb{R}^\ell$ where $B' = \begin{bmatrix} f_1 & \ldots & f_{\ell} \end{bmatrix}$ is a row whose entries generate $I$. When there are $\ell > 1$ functions with boundary conditions, $B' \in (R')^{\ell \times \ell} \times \mathbb{R}^\ell$ is a direct sum matrix, e.g.,

$$B' = \begin{bmatrix} B'_1 & 0 \\ 0 & B'_2 \end{bmatrix}$$  

for $\ell = 2$ where $B'_1, B'_2$ are rows over $R'$.

**Example 4.2.** Functions $\mathcal{F} = C^\infty([0, 1]^2, \mathbb{R})$ with Dirich-
let boundary conditions
\[ f(0, y) = f(1, y) = f(x, 0) = f(x, 1) = 0 \]
are parametrized by \( B' = [x(x - 1)y(y - 1)] \).

**Example 4.3.** Functions \( F = C^\infty(\mathbb{R}^3, \mathbb{R}) \) with boundary condition \( f(0, 0, z) = 0 \) are parametrized by \( B' = [x \ y] \).

Generalized boundary conditions with derivatives vanishing can be achieved by multiplicities in the ideal \( I \).

**Example 4.4.** Consider \( F = C^\infty(\mathbb{R}^2, \mathbb{R}) \) with boundary conditions \( f(0, y) = (\frac{\partial}{\partial x} f(x, y)) |_{x=0} = 0 \). Such functions are parametrized by \( B = [x^2] \).

Parametrizations using the the indeterminates \( x_i \) have the drawback of a big global influence on the prior. Example 4.4 leads to the covariance function \( k_b = x_1 x_2 : k \) of the Gaussian process with the boundary condition, where \( k \) is the covariance function of the parametrizing Gaussian process. This covariance function \( k_b \) has strongly changing variance, depending on proximity to the boundary \( x = 0 \).

**Remark 4.5.** To localize the shifting variances to the boundary, consider a pair of uncorrelated Gaussian processes \( (GP(0, k), GP(0, 0)) \), where \( GP(0, 0) \) is constant zero. Now, take a pushforward under a partition of unity \( \rho_1, \rho_2 : \mathbb{R}^d \rightarrow [0, 1] \) as in Example 2.3, where \( \rho_1(x, y) \) should be close to 1 over most of the domain, except at the boundary. Of course, the ring \( R \) needs to be enlarged to include \( \rho_1 \) and its derivatives.

We now can construct a parametrization \( B \in R^{\ell \times \ell'} \) of the solutions of a differential equation \( A \in R^{\ell \times \ell} \) and a parametrization \( B' \) of boundary conditions. Sadly, they are not combinable by iterating pushforwards. Consider e.g. \( B' \) created via a partition of unity \( \rho_1, \rho_2 \). Then \( (\rho_1)_*(B_2 g) \) is no longer a solution of the differential equation defined by \( A \) and \( B_2 ((\rho_1)_*, g) \) no longer adheres to the boundary conditions defined by \( \rho_1 \). Worse, \( B' B' \) or \( BB' \) is not even defined in general.

**5. Intersecting parametrizations**

We have seen how to parametrize certain solutions of differential equations and boundary conditions. Now, given two parametrizations, \( B_1 \in R^{\ell \times \ell'} \) and \( B_2 \in R^{\ell \times \ell''} \), we intersect their images to get \( B_1 F_{\ell' \ell''} \cap B_2 F_{\ell'' \ell} \).

**Example 5.1.** Actually, the Dirichlet boundary condition of Example 4.2 is an intersection of the images of the boundary conditions parametrized by \( [x], [x - 1], [y], \) and \( [y - 1] \).

The following theorem constructs a parametrization of intersections of parametrizations algorithmically.

**Theorem 5.2 (Intersecting parametrizations).** Let \( B_1 \in R^{\ell \times \ell''} \) and \( B_2 \in R^{\ell \times \ell''} \). Denote by
\[ C := \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} \in R^{(\ell'' + \ell') \times m} \]
the right-nullspace of the matrix \( B := \begin{bmatrix} B_1 & B_2 \end{bmatrix} \in R^{\ell \times (\ell' + \ell'')} \). If \( B \) generates the left-nullspace of \( C \), then \( B_1 C_1 = -B_2 C_2 \) parametrizes \( B_1 F_{\ell' \ell''} \cap B_2 F_{\ell'' \ell} \).

The computations are again Gröbner basis computation in the ring \( R \).

**Sketch of a proof of Theorem 5.2.** By Corollary 3.7, the assumptions of this theorem ensure that we have a parametrization \( C \) of the system defined by \( B \). As \( C \) is the nullspace of \( B \), we have \( B_1 C_1 = -B_2 C_2 \). The parametrization follows, as the cospan \( R^{\ell''} \xrightarrow{C_1} R \xrightarrow{C_2} R^{\ell'} \) defines a free hull of the pushout of the span \( R^{\ell''} \xrightarrow{B_1} R^{\ell \times \ell} \xrightarrow{B_2} R^{\ell' \ell''} \). After dualization, this leads to a free cover of a pullback, and pullbacks are the abstraction of intersections. □

**Example 5.3.** We rephrase the computation of divergence free fields on the sphere from Example 3.9. This is the intersection of divergence free fields, the zero set of \( A := [\partial_x \ \partial_y \ \partial_z] \) parametrized by
\[ B_1 := \begin{bmatrix} 0 & \partial_z & -\partial_y \\ -\partial_z & 0 & \partial_y \\ \partial_y & -\partial_x & 0 \end{bmatrix} \]
and the fields on the sphere, the zero set of \( A_2 := [x \ y \ z] \) parametrized by
\[ B_2 := \begin{bmatrix} 0 & z & -y \\ -z & 0 & x \\ y & -x & 0 \end{bmatrix} \]
The right-nullspace of \( [B_1 \ \ B_2] \) is
\[ C = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} x & \partial_z & 0 \\ y & \partial_y & 0 \\ z & \partial_z & 0 \end{bmatrix} \begin{bmatrix} x & \partial_z & 0 \\ 0 & 0 & x \\ 0 & y & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & z \\ 0 & 0 & 0 \end{bmatrix} \]
The matrix \( [B_1 \ \ B_2] \) is the left nullspace of \( C \). Now,
\[ B_1 C_1 = -B_2 C_2 = \begin{bmatrix} z\partial_y - y\partial_z & 0 & 0 \\ -z\partial_x + x\partial_z & 0 & 0 \\ y\partial_x - x\partial_y & 0 & 0 \end{bmatrix} \]
is equivalent\(^\text{13}\) to the matrix \( B \) from Example 3.9.

\(^{13}\)The matrices \( B_1 \) and \( B_2 \) each have a non-zero nullspace, which correspond to the two trivial columns in \( B_1 C_1 \).
Whereas Corollary 3.7 gives a necessary and sufficient condition whether a parametrization exists, this theorem only gives a sufficient condition. The reason is that parametrizations are a more general concept than parametrizations of controllable systems, e.g., no example in Section 4 is the parametrization of a controllable system, as the left-nullspace of any parametrizing matrix $B'$ is zero. In practice, this means that we might even get a suitable parametrization, even if the left nullspace of $C$ is bigger than $B$.

**Example 5.4.** We continue with the divergence free fields on the sphere from Examples 3.9 and 5.3. These are parametrized by

$$B_1 := \begin{bmatrix} -z\partial_y + y\partial_z \\ z\partial_x - x\partial_z \\ -y\partial_x + x\partial_y \end{bmatrix}.$$ \[\text{The solutions of the boundary condition } f(x,y,0) = 0, \text{ i.e., functions vanishing at the equator, are parametrized by} \]

$$B_2 := \begin{bmatrix} z & 0 & 0 \\ 0 & z & 0 \\ 0 & 0 & z \end{bmatrix}.$$ \[\text{The nullspace of } [B_1 \ B_2] \text{ is} \]

$$C := \begin{bmatrix} C_{1,1} \\ C_{2,1} \\ C_{2,2} \\ C_{2,3} \end{bmatrix} = \begin{bmatrix} -z^2 \\ z^2\partial_y - y\partial_x - 2y \\ -z^2\partial_x + xz\partial_z + 2x \\ yz\partial_x - xz\partial_y \end{bmatrix}.$$ \[\text{The left nullspace of } C \text{ is not only generated by } [B_1 \ B_2], \text{ but by the additional relation} \]

$$D := \begin{bmatrix} 0 & x & y & z \end{bmatrix}.$$ \[\text{This relation } D \text{ tells us, that the parametrized solutions of } C_2 \text{ are a vector field on a sphere around the origin, which they remain after being multiplied by the scalar matrix } B_2. \text{ We gladly accept this additional condition.} \]

Now,

$$B_1C_1 = -B_2C_2 = \begin{bmatrix} -z^3\partial_y + yz\partial_x + 2yz \\ z^3\partial_x - xz^2\partial_z - 2xz \\ -yz^2\partial_x + xz^2\partial_y \end{bmatrix}$$ \[\text{parametrizes the divergence free fields on the sphere vanishing at the equator. This is demonstrated in Figure 2.} \]

### 6. Inhomogenous boundary conditions

So far, we have only considered homogeneous equations and boundary conditions, i.e., with right hand sides zero. The fundamental theorem of homomorphisms (cf. Lemma 3.4) extends this to the inhomogeneous case, by taking a particular solution as mean function. While this is simple theoretically, finding a particular solution can be quite hard in practice. We restrict ourselves to an example.

**Example 6.1.** Consider again smooth divergence free fields on the 2-sphere $X = S^2$, i.e., $f \in \mathbb{R}^{3 \times 1}$ with

$$Af = \begin{bmatrix} x \\ y \\ z \end{bmatrix} f = 0$$ \[\text{and inhomogeneous boundary condition } f_3(x, y, 0) = y. \]

The function $\mu = [0 \ -z \ y]^T$ is a particular solution. Hence, we take it as mean function. The matrix $B_1C_1 = -B_2C_2$ from Example 5.4 parametrizes all functions with the corresponding homogeneous boundary condition $f_3(x, y, 0) = 0$ of functions vanishing at the equator.

Hence, assuming mean zero and squared exponential covariance $k_x$, the Gaussian process $GP (\mu, (B_1C_1)k((B_1C_1)'T))$ is a prior distribution dense in the solutions of the equations and boundary conditions by Lemma 3.4, which we demonstrate in Figure 2.

### 7. Conclusion

This paper incorporates prior knowledge into machine learning frameworks. It presents a novel framework to

1. describe parametrizations for boundary conditions,
2. combine parametrizations by intersecting their images, and
3. build Gaussian process priors with realizations dense in the solution set of a system of linear differential equations with boundary conditions.

All this works without any assumptions or approximations. These priors have been demonstrated on geometric problems and lead to reasonable models with one (cf. Figure 2) or two (cf. Figure 1) data points. The next steps are to

a. reduce the need of data in applications like Bayesian optimization, active learning, or design of experiments,
b. allow for stronger extrapolation in robotics,
c. estimate parameters in differential equations via maximum likelihood,
d. construct neural networks, which approximate these Gaussian process priors, reverting the current trend of approximating neural networks via Gaussian processes, cf. (Neal, 1996; Lee et al., 2018; Garriga-Alonso et al., 2019; Arora et al., 2019) and references therein.

The author is interested in further work on encoding physical or system-theoretic properties in Gaussian process priors.
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Figure 2. On the left, the posterior mean from Example 5.4 of a divergence free tangent field on the sphere which is zero at the equator (red) and conditioned at a single observation (plotted artificially bigger) at the north pole. Notice the flow parallel to the equator in middle latitudes, orthogonal to the observation, avoids sinks or sources. On the right, the posterior mean from Example 6.1 of a divergence free tangent field on the sphere with the given boundary condition (red) at the equator being conditioned at a single observation (plotted artificially bigger) at the north pole.

A. Proof of Lemma 2.2

Before giving the proof of Lemma 2.2, we recall the definition (if it exists) of the $\ell$-th cumulant function $\kappa_\ell(g)$

$$\kappa_\ell(g) \left( x^{(1)}, \ldots, x^{(\ell)} \right) = \sum_{\pi \in \text{part}(\ell)} (-1)^{|\pi|-1} (|\pi|-1)! \prod_{\tau \in \pi} E \left( \prod_{i \in \tau} g \left( x^{(i)} \right) \right)$$

of a stochastic process $g$, where $\text{part}(\ell)$ is the set of partitions of $\ell$ and $|\pi|$ denotes the cardinality of $\pi$. In particular, the first two cumulant functions $\kappa_1$ resp. $\kappa_2$ are equal to the mean resp. covariance function. Furthermore, $g$ is Gaussian iff all but the first two cumulant functions vanish.

The stochastic process $B_* g$ exists, as $F$ is an $R$-module and the realizations of $g$ are all contained in $F$. The compatibility with expectations proves the following formula for the cumulant functions of $\kappa(B_* g)$ of $B_* g$, where $B^{(i)}$ denotes the operation of $B$ on functions with argument $x^{(i)} \in \mathbb{R}^d$:

$$\kappa_\ell(B_* g) \left( x^{(1)}, \ldots, x^{(\ell)} \right) = \sum_{\pi \in \text{part}(\ell)} (-1)^{|\pi|-1} (|\pi|-1)! \prod_{\tau \in \pi} E \left( \prod_{i \in \tau} (B_* g) \left( x^{(i)} \right) \right)$$

As $g$ is Gaussian, the higher ($\ell \geq 3$) cumulants $\kappa_\ell(g)$ vanish, hence the higher ($\ell \geq 3$) cumulants $\kappa_\ell(B_* g)$ vanish, which implies that $B_* g$ is Gaussian. The formulas for the mean function resp. covariance function follow from the above computation for $\ell = 1$ resp. $\ell = 2$. \qed
B. Code

The following computation have been performed in Maple with the OreModules package (Chyzak et al., 2007).

```maple
> # code for GP
regressionGP:=proc(Kf, points, yy, epsilon)
local n, m, kf, K, s1, s2, alpha, KStar;
    n:=nops(points);
m:=RowDimension(Kf); s1:=map(a->[x1=a[1], y1=a[2], z1=a[3]], points);
s2:=map(a->[x2=a[1], y2=a[2], z2=a[3]], points);
kf:=convert(Kf,listlist);
    K:=convert(evalf(map( a->map( b->convert(subs(a,subs(b,kf)), Matrix), s2), s1)), Matrix):
alpha:=yy.(K+epsilonˆ2)ˆ(-1);
    KStar:=map( a->subs(a,kf), s1): KStar:=subs([x2=x, y2=y, z2=z], KStar):
    KStar:=convert(map(op, KStar), Matrix): return alpha.KStar;
end:
```

Example B.1 (General Code for GP regression).

```maple
> restart;
> with(OreModules):
> with(LinearAlgebra):
> Alg:=DefineOreAlgebra(diff=[Dx,x], diff=[Dy,y], diff=[Dz,z], diff=[Dx1,x1], diff=[Dy1,y1], diff=[Dz1,z1], diff=[Dx2,x2], diff=[Dy2,y2], diff=[Dz2,z2], polynom=[x,y,z,x1,x2,y1,y2,z1,z2]):
> A:=<<x,Dx>|<y,Dy>|<z,Dz>>;
> # combine
> B:=Involution(
>   SyzygyModule(B, Alg), Alg):
>  _syzygy:=SyzygyModule(B, Alg):
>   reduce:=ReduceMatrix(A, _syzygy):
>   reduce:=ReduceMatrix(_syzygy, A):
>   # check parametrization
>   A1:=SyzygyModule(B, Alg):
>   ReduceMatrix(A, A1, Alg):
>   ReduceMatrix(A1, A, Alg):
```

Example B.2 (Code for Example 3.9).

```maple
A :=
[ x  y  z ]
[ Dx Dy Dz ]
>
> # prepare covariance
> SE:=exp(-1/2*(x1-x2)^2 -1/2*(y1-y2)^2 -1/2*(z1-z2)^2):
> Kg:=apply( DiagonalMatrix([SE]), [x1,y1,z1,x2,y2,z2]):
```

```maple
P2:=ApplyMatrix(B, Alg, Alg);
> l1:=[x=x1, y=y1, z=z1, Dx=Dx1, Dy=Dy1, Dz=Dz1];
> l2:=[x=x2, y=y2, z=z2, Dx=Dx2, Dy=Dy2, Dz=Dz2];
```

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Example B.3 (Code for Example Code for Example 4.1)

\[ k := (x, y) \mapsto e^{-1/2(x-y)^2} \]

\[ k := \exp(-1/2*(x-y)^2); \]

\[ K := \begin{bmatrix} 1 & 0 & e^{-1/2} & -e^{-1/2} \\ 0 & 1 & e^{-1/2} & 0 \\ e^{-1/2} & e^{-1/2} & 1 & 0 \\ -e^{-1/2} & 0 & 0 & 1 \end{bmatrix} \]
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\[ e^{-\frac{1}{2}(x-y)^2} - e^{-\frac{1}{2}x^2 - \frac{1}{2}y^2} \]
\[ (x^2 - 3e^{-1} + 1) \]
\[ (xy - x - y + 2)e^{x^2 + y^2} + (xy + 1) \]
\[ + (-2xy + x + y - 1)(e^{x+y} + e^{-1}) \]
\[ + (xy - y + 1)e^{y^2} + (xy - x + 1)e^{-2} \]
\[ + (y - x - 2)e^{y-1} + (x - y - 2)e^{x-1} \]

\[ B2 := \begin{bmatrix} 0 & z & -y \\ -z & 0 & x \\ y & -x & 0 \end{bmatrix} \]

Example B.4 (Code for Example 5.3).

\[ A1 := \begin{bmatrix} Dz & Dy & 0 \\ 0 & -Dx & Dz \\ -Dx & 0 & -Dy \end{bmatrix} \]

\[ B1 := \begin{bmatrix} y*Dz-z*Dy, -x*Dz+z*Dx, -y*Dx+x*Dy \end{bmatrix} \]
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\[ B_{old} := \begin{bmatrix} -zDy + Dz y \\ Dx z - Dz x \\ -Dx y + Dy x \end{bmatrix} \]

\[ B_2 := \begin{bmatrix} z \\ 0 \\ 0 \\ 0 \end{bmatrix} \]

\[ \overset{\text{ReduceMatrix}(BB,B,Alg);} {\text{# new relation!}} \]

\[ \begin{bmatrix} 0 & x & y & z \end{bmatrix} \]

Example B.5 (Code for Example 5.4).

\[ B1 := \begin{bmatrix} y^*Dz-z^*Dy, -x^*Dz+z^*Dx, -y^*Dx+x^*Dy \end{bmatrix} \]

\[ \overset{\text{# the new parametrization}} {\text{# div-free fields on } S^2} \]

\[ B2 := \begin{bmatrix} z(-Dy z^2 + Dz yz + 2y) \\ z(Dx z^2 - xDz - 2x) \\ (-Dx y + Dy x)z^2 \end{bmatrix} \]

\[ P := \begin{bmatrix} 0 & x & y & z \end{bmatrix} \]

\[ \overset{\text{# check parametrization}} {\text{# new relation!}} \]

\[ \overset{\text{# parametrize}} {\text{# the new parametrization}} \]

\[ \text{equator=0B2:=DiagonalMatrix([z$3])}; \]

\[ \overset{\text{Example B.5 (Code for Example 5.4).}} {\text{# parametrize}} \]

\[ \text{SE} := \exp(-1/2*(x1-x2)^2 -1/2*(y1-y2)^2-1/2*(z1-z2)^2); \]

\[ Kg := \unapply(\text{DiagonalMatrix([SE]}), (x1,y1,z1,x2,y2,z2)); \]

\[ \overset{\text{prepare covariance}} {\text{# parametrizing function}} \]

\[ P2 := \text{ApplyMatrix}(P, [x(x,y,z)], Alg); \]

\[ \overset{\text{# prepare covariance}} {\text{# covariance for \ parametrizing function}} \]

\[ \overset{\text{# prepare covariance}} {\text{# parametrizing function}} \]

\[ \overset{\text{# check parametrization}} {\text{# prepare covariance}} \]

\[ BB := \text{SyzygyModule}(C, Alg); \]

\[ \overset{\text{# prepare covariance}} {\text{# prepare covariance}} \]

\[ BB := \text{SyzygyModule}(C, Alg); \]

\[ \overset{\text{# check parametrization}} {\text{# prepare covariance}} \]

\[ \overset{\text{# prepare covariance}} {\text{# check parametrization}} \]
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> # construct covariance
> # apply from one side
> Kf:=convert(
> map(
> b->subs(
> [xi(x1,y1,z1)=b[1]],
> subs(l1,P2)),
> convert(
> Kg(x1,y1,z1,x2,y2,z2),
> listlist)),
> Matrix):
> # apply from other side
> Kf:=convert(
> expand(
> map(
> b->subs(
> [xi(x2,y2,z2)=b[1]],
> subs(l2,P2)),
> convert(
> Transpose(Kf),
> listlist))),
> Matrix):
> gp:=unapply(
> piecewise(z<0,[0,0,0],
> evalf(convert(
> GP(Kf,[[0,0,1]],<1|0|0>,1e-5),
> list))),
> (x,y,z)):
> gp(x,y,z) assuming z>0:
> factor(simplify(%));

\[
\begin{align*}
-0.6065 & z(-z^2 + y^2 + 2y^2) e^{-0.5x^2 - 0.5y^2 - 0.5z^2}, \\
0.6065 & xyz(z+2) e^{-0.5x^2 - 0.5y^2 - 0.5z^2}, \\
-0.6065 & xy^2 e^{-0.5x^2 - 0.5y^2 - 0.5z^2}.
\end{align*}
\]

> Alg:=DefineOreAlgebra(diff=[Dx,x],
> diff=[Dy,y], diff=[Dz,z],
> diff=[Dx1,x1], diff=[Dy1,y1],
> diff=[Dz1,z1], diff=[Dx2,x2],
> diff=[Dy2,y2], diff=[Dz2,z2],
> polynom=[x,y,z,x1,x2,y1,y2,z1,z2]):
> B1:=<<y*Dz-z*Dy,-x*Dz+z*Dx,-y*Dx+x*Dy>>;

Example B.6 (Code for Example 6.1).

\[
B1 := \begin{bmatrix}
-zy + Dz y \\
z Dx - Dz x \\
-Dx y + Dy x
\end{bmatrix}
\]

> mu:=[0,-z,y];

\[
\mu := \begin{bmatrix}
0 \\
-z \\
y
\end{bmatrix}
\]

> #check:
> A1:=Matrix(1,3,[[Dx,Dy,Dz]]):
> A2:=Matrix(1,3,[[x,y,z]]):
> ApplyMatrix(A1,mu,Alg);
> ApplyMatrix(A2,mu,Alg);

\[
\begin{bmatrix}
0 \\
0
\end{bmatrix}
\]

> # the new parametrization
> P:=Mult(B1,[[z^2]],Alg);

\[
P := \begin{bmatrix}
z(-Dy z^2 + Dz yz + 2y) \\
z(Dx z^2 - x Dz z - 2x) \\
(-Dx y + Dy x) z^2
\end{bmatrix}
\]

> # covariance for
> # parametrizing function
> SE:=exp(-1/2*(x1-x2)^2
> -1/2*(y1-y2)^2-1/2*(z1-z2)^2):
> Kg:=unapply(
> DiagonalMatrix([SE]),
> (x1,y1,z1,x2,y2,z2)):
> # prepare covariance
> P2:=ApplyMatrix(P,
> [xi(x,y,z)], Alg):
> P2:=convert(P2,list):
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\[
\begin{align*}
    &l1 := [x=x1, y=y1, z=z1, \\
    &Dx=Dx1, Dy=Dy1, Dz=Dz1]: \\
    &l2 := [x=x2, y=y2, z=z2, \\
    &Dx=Dx2, Dy=Dy2, Dz=Dz2]: \\
    &\text{# construct covariance} \\
    &\text{# apply from one side} \\
    &Kf := \text{convert(} \\
    &\text{map(} \\
    &b \rightarrow \text{subs(} \\
    &[xi(x1,y1,z1)=b[1]], \\
    &\text{subs(l1,P2))}, \\
    &\text{convert(} \\
    &Kg(x1,y1,z1,x2,y2,z2), \\
    &\text{listlist)}), \\
    &\text{Matrix):} \\
    &\text{# apply from other side} \\
    &Kf := \text{convert(} \\
    &\text{expand(} \\
    &\text{map(} \\
    &b \rightarrow \text{subs(} \\
    &[xi(x2,y2,z2)=b[1]], \\
    &\text{subs(l2,P2))}, \\
    &\text{convert(} \\
    &\text{Transpose(Kf),} \\
    &\text{listlist)}), \\
    &\text{Matrix):} \\
    &p := [0,0,1]: \\
    &mu_p := \text{Transpose(} \\
    &\text{subs(} \\
    &[x=p[1], y=p[2], z=p[3]], \\
    &mu)) : \\
    &gp := \text{unapply(} \\
    &\text{factor(simplify(} \\
    &\text{convert(} \\
    &\text{GP(Kf, [p], <1|0|0>-mu_p, le-5),} \\
    &\text{list))} \\
    &\text{+convert(mu, list),} \\
    &\text{GP(x, y, z)):} \\
    &gp(x, y, z); \\
\end{align*}
\]

\[
\begin{align*}
    &0.6065 \times yz(z + 2) \times e^{-0.5 \times x^2 - 0.5 \times y^2 + 0.5 \times z^2 - z,} \\
    &-0.6065 \times x^2 \times e^{-0.5 \times x^2 - 0.5 \times y^2 + 0.5 \times z^2 + y}.
\end{align*}
\]

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