Liesel: A Probabilistic Programming Framework for Developing Semi-Parametric Regression Models and Custom Bayesian Inference Algorithms

Abstract

Liesel is a new probabilistic programming framework developed with the aim of supporting research on Bayesian inference based on Markov chain Monte Carlo (MCMC) simulations in general and semi-parametric regression specifications in particular. Its three main components are (i) an R interface (RLiesel) for the configuration of an initial semi-parametric regression model, (ii) a graph-based model building library, where the initial model graph can be manipulated to incorporate new research ideas, and (iii) an MCMC library for designing modular inference algorithms combining multiple types of well-tested and possibly customized MCMC kernels. The graph builder as well as the MCMC library are implemented in Python, relying on JAX as a numerical computing library, and can therefore benefit from the latest machine learning technology such as automatic differentiation, just-in-time (JIT) compilation, and the use of high-performance computing devices such as tensor processing units (TPUs). Liesel provides all required tools for efficient and reliable statistical research on complex models and estimation algorithms. Its modular design allows users to expand the model library and inference algorithms, offering the flexibility and customization options to tailor the software to any specific research needs.

Keywords
Bayesian models · Markov chain Monte Carlo · probabilistic graphical models · Python · R · semi-parametric regression

1 Introduction

Developing advanced semi-parametric regression models with Bayesian inference often proceeds as follows: Starting from an established base model, certain components of the model are modified or extended, followed by required adaptations to the inferential scheme. This is conceptually supported by the modularity of Bayesian inference based on Markov chain Monte Carlo (MCMC) simulations, where the organisation of observation model and priors in a hierarchically structured directed acyclic graph (DAG) induces conditional independencies that can be exploited both for deriving full conditionals and for applying different updating schemes to blocks of parameters. Unfortunately, this
In this article, we introduce Liesel, a probabilistic programming framework developed with the aim of supporting research on Bayesian semi-parametric regression, while taking full advantage of the conceptual modularity of Bayesian inference with MCMC on the software side. The framework, named after a fountain in its birth city Göttingen, Germany, consists of three main components: (i) an R interface (RLiesel) for the configuration of an initial semi-parametric regression model, (ii) a graph-based model building library (Liesel-Model), where the initial model graph can be manipulated to incorporate new research ideas, and (iii) an MCMC library (Goose) for designing modular inference algorithms combining multiple types of well-tested MCMC kernels. The graph builder as well as the MCMC library are implemented in Python, relying on JAX (Bradbury et al., 2022) as a numerical computing library, and can therefore benefit from the latest machine learning technology such as automatic differentiation, just-in-time (JIT) compilation, and the use of high-performance computing devices such as tensor processing units (TPUs).

The components of Liesel and their relationships are illustrated in Figure 1. A standard workflow with Liesel involves the following steps: First, a semi-parametric regression model is configured with RLiesel, returning a Liesel-Model object. Second, the Liesel-Model object is modified for the research question at hand if required. Third, MCMC estimation is performed with Goose, potentially exploring different or new sampling schemes. In the end, Liesel’s utility functions can be used for model and estimation diagnostics.

Most available statistical software for Bayesian inference can be classified into software for a specific model class on the one hand and general probabilistic programming languages (PPLs) on the other hand. Liesel and RLiesel cover a middle ground between these two approaches: RLiesel facilitates the definition of semi-parametric models, while Liesel-Model and Goose are capable of expressing and estimating a broad range of statistical models. Hence, Liesel has similar capabilities as general-purpose PPLs like Stan (Stan Development Team, 2022), JAGS (Plummer, 2022), NIMBLE (the successor to BUGS, de Valpine et al. 2017) or PyMC (Salvatier et al. 2016). Unlike these programs, however, Liesel features a graph representation that allows users to modify a model in-memory before estimation.

https://liesel-project.org
Furthermore, with Liesel, users have full control of the estimation algorithm, while most alternatives provide only limited options for customization. For example, in contrast to Stan, Liesel offers the possibility to integrate user-defined samplers, supports blocked updates, and can handle discrete parameters. Compared to NIMBLE, which allows for a more detailed configuration of the MCMC algorithm than Stan, Liesel can wrap code of other JAX-based libraries and therefore avoids NIMBLE’s restriction to a subset of the R programming language. PyMC also offers some options to customize the MCMC algorithm but is more limited in this regard than Liesel and, similar to most other general-purpose PPLs, does not feature a mutable model object.

For complex models or large datasets, general-purpose PPLs may be slow or unable to sample the model at all. In these situations, model-specific software remains important, and modeling frameworks with customizable MCMC algorithms like Liesel or PyMC may serve as a basis for the implementation of model-specific solutions. Its flexible model building library sets Liesel apart from other more specialized software. Similar to brms (Bürkner, 2017), which provides an interface for various types of multi-level and additive regression models in Stan, R.Liesel provides an interface for semi-parametric regression models in Liesel. R.Liesel’s features are comparable to other software in the field like mgcv (Wood, 2022), gamlss (Stasinopoulos et al., 2017), GJRM (Marra and Radice, 2022), BayesX (Brezger et al., 2005) and bamless (Umlauf et al., 2021). Its approach is different, however, in that the intermediate graph-based model representation can be modified and extended, allowing for the implementation of new models that are derived from a base model.

This is also a particular feature of Liesel compared to BayesX, for example, which cannot be extended easily and therefore restricts the user to the pre-defined predictor components (i.e. linear, non-linear, spatial covariate effects, etc.). In bamless, the inference procedure offers more options for configuration, but a comprehensive collection of MCMC kernels as in Goose is missing, and automatic differentiation and high-performance computing hardware are also not supported. Finally, the packages mgcv and GJRM are not primarily focused on Bayesian inference, although mgcv offers an interface to JAGS using the jags() function. In contrast to Liesel, both packages have an exclusive focus on semi-parametric regression using basis function approaches.

Summarizing its major advantages, Liesel

- makes full use of the DAG structure of Bayesian model specifications for both model building and model manipulation for all its components,
- provides access to various well-established components of semi-parametric regression such as design matrices for various types of basis expansions, the construction of spatial effects, etc., via the R.liesel interface facilitating the model building process,
- implements various well-tested MCMC kernels that can be combined in a modular and flexible way, and
- enables access to the latest machine learning technology such as automatic differentiation, just-in-time (JIT) compilation, and the use of high-performance computing devices such as tensor processing units (TPUs).

Essentially, Liesel provides many default components for Bayesian inference in semi-parametric regression, which are easy to extend and liberate the researcher from the time-consuming duty of re-implementing the basic components of their models and inference algorithms, giving them the opportunity to focus on the novel aspects of their research. This way, Liesel meets the requirements of many computational statisticians working on new methods or extensions of existing ones. Currently, the framework is particularly useful for developing semi-parametric regression models, since it includes all components required for this model class, but it can easily be extended beyond these models. More specifically, Liesel’s modular design allows users to expand the model library and inference algorithms providing customization options for users to tailor the software to their specific research needs.

The remainder of this article is organized as follows: In Section 2, the Liesel-Model library is discussed. Section 3 describes Liesel’s MCMC library Goose, its main design goals, and the interfaces that allow the user to implement their own MCMC kernels and warmup schemes. R.Liesel, the R interface for semi-parametric and distributional regression is covered in Section 4, together with some theoretical background on these model classes. Finally, Sections 5 and 6 highlight the advantages of Liesel in two case studies illustrating the flexibility in combining and comparing different sampling schemes, on the one hand, and the construction of a complex model specification from simple building blocks, on the other hand. The article concludes with a discussion in Section 7.

2 Liesel-Model: Converting a statistical model into a software representation

The model library of Liesel aims at enabling the user to convert a statistical model into a software representation as smoothly and error-free as possible. Users have the flexibility to construct a model from scratch or modify an existing one – such as a model created by RLiesel. Regardless of the approach, the primary objective is to offer a fast
evaluating function tailored for sampling. More precisely, the model provides access to the point-wise evaluation of
the unnormalized log-posterior density of the model parameters or, equivalently, the joint log-density of the model
parameters and the observations. To make use of JAX’s just-in-time compilation and auto-differentiation, the function
must be written in a JAX compatible manner which implies in particular purity. A pure function’s value, similar to a
mathematical function, can only depend on the arguments but no other state.

Liesel employs probabilistic graphical models (PGM) as a bridge to transmute a statistical model into a computer
representation of the joint distribution of model parameters. Like a Bayesian model hierarchy composed of a likelihood
distribution and prior distributions, a PGM explicitly models the relationship between the random variables and
their conditional distributions as a graph. Resembling a Bayesian model hierarchy – which consists of a likelihood
distribution and prior distributions – a PGM explicitly models the relationship among random variables and their
conditional distributions as graph. The density of the joint distribution evaluated for a specific realization is simply
accessible via the product of the conditional densities. This makes the transition from a PGM to a computational model
quite intuitive.

In Liesel, the computational model is represented as a computational graph. This graph is a directed acyclic graph
(DAG) where nodes symbolize functions or computations. The connecting edges define the data flow, signifying
how the value from one node serves as an input to another. Nodes without inputs represent data (or pre-specified
hyperparameters).

With these foundational concepts, Liesel offers its users both a high-level view of the statistical model and a low-level
view of the computational model. The high-level view offers user-friendliness similar to frameworks like PyMC, Stan,
or NIMBLE, allowing for a direct transformation of the model hierarchy into its software analog. This perspective
further offers the visualization of the graph that aid in pinpointing any discrepancies between the model and its software
representation. Conversely, the low-level view is simply the computational graph, stripping away the semantic layers.
However, it gives the user access to computational details, offering room for precise tuning.

To fully grasp the capabilities and nuances of Liesel’s modeling approach, we commence with Liesel’s unique benefits
followed by a straightforward example, core design principles, and implementation details.

2.1 Benefits of using Liesel-Model

Liesel’s MCMC library, Goose, possesses the flexibility of being usable independent of the model-building library. This
allows compatibility with external tools such as PyMC or even custom-written log-probability functions. However, we
recognize the following distinct benefits of using Liesel’s model approach:

Correctness. The graph representation introduces a natural modularization. Each node stands independent, allowing
for isolated testing, which is considerably easier than evaluating a convoluted function in its entirety. In many
instances, the graph can partly comprise the well-tested implementation of specific nodes.

Computational efficiency. Liesel’s graph structure allows gains in computational efficiency. The design enables nodes
within the computational graph to cache results of expensive computations. This feature is especially valuable
for efficient MCMC sampling with multiple parameter blocks, a capability inherently supported by Goose.
Liesel’s architecture facilitates partial graph updates, potentially unlocking further performance enhancements.

Hackability. Liesel grants users full access to the computational graph. Thus, users can tweak the model for further
computational efficiency and extend the model or implement a new one. The design of the classes is simple
and follows the principle of least astonishment – prioritizing less surprising behavior over mere convenience.

Graph manipulations. The graph of a Liesel model can be modified, allowing for a workflow with a base model,
which can be customized to implement new model variants. RLiesel synergizes with this workflow by offering
models tailored for semi-parametric regression.

2.2 Example: The Bayesian linear model

A Bayesian linear model (BLM) is a statistical model that employs Bayesian inference to estimate the parameters of
a linear regression model. Within this model, the coefficients of the linear regression equation are treated as random
variables, each governed by a prior probability distribution. This principle extends to the scale of the error term. In this
section, we demonstrate how the BLM can be set up using Liesel. While the linear model is relatively straightforward,
it allows us to focus on the application of Liesel. Moreover, the BLM can be easily extended to more complex models
such as hierarchical models, shrinkage models, additive models, and generalized additive models for location, scale,
and shape (GAMLSs) with additive predictors (refer to Sections 4 to 6 for more advanced models). Overall, the goal is
to build a model for the BLM such that the unnormalized log-posterior can be evaluated point-wise.
The BLM assumes a hierarchical structure where the prior distributions for the model parameters are specified at different levels. At the lowest level, the distribution for the response variable, or likelihood, is specified as:

\[ y|\beta, \sigma^2 \sim N(X\beta, \sigma^2 I) \]  

where \( y \) is the response vector, \( \beta \) is the vector of regression coefficients, \( \sigma^2 \) is the variance of the error term, \( X \) is the design matrix, and \( I \) is the identity matrix. At the next level, the prior distribution for the regression coefficients \( \beta \) is specified as:

\[ \beta|\sigma^2 \sim N(\mu_0, \sigma^2 \Sigma_0) \]  

where \( \mu_0 \) is the prior mean vector and \( \sigma^2 \Sigma_0 \) is the prior covariance matrix. In this example, we use an uninformative prior with \( \mu_0 = 0 \) and \( \Sigma_0 = 100I \). Finally, the prior distribution for \( \sigma \) is specified as half-Cauchy with zero mean and unit scale.

A Liesel model is constructed in a top-down manner, starting with parameters that do not rely on other parameters as inputs, and then proceeding downward to the likelihood. The created objects are of the type \( \text{Var} \) – to which we refer as variables. These objects can either represent a random variable with an associated distribution (e.g., model parameters as \( \beta \) and \( \sigma \) or an observed random variable such as the response \( y \)) or they can represent deterministic calculations like \( \mu = X\beta \). Moreover, they can also be used to define the value of the parameters associated with the distribution of another variable. A graphical visualization of the variables in the example and their relations is displayed in Figure 2.

![Figure 2: Visualization of the DAG in the high-level view.](image)

In the BLM, we start by initializing an object of type \( \text{Var} \) representing \( \sigma \), whose distribution relies solely on constant hyperparameters. To create this object, the value and the distribution must be specified. Additionally, the user can assign a unique name for convenience. The name of the variable is for example used when visualizing the DAG as in Figure 2. The value set is the value at which the log-posterior should be evaluated and can be changed later, either manually or by an MCMC algorithm. Among the blue nodes, model parameters are highlighted with round contour lines.

Py> sigma = lsl.param(  
    1.0,  
    lsl.Dist(tfd.HalfCauchy, loc=0.0, scale=1.0),  
    name="sigma"  
)

The method \( \text{lsl.param} \) creates an instance of the \( \text{Var} \) class and sets a flag indicating that this variable is a model parameter. The value of the variable is then set in the next line. Following that, a distribution is specified by wrapping a class that conforms to the Distribution interface defined in TensorFlow Probability together with the arguments required for its instantiation. Here, we create a Half-Cauchy distribution with location zero and unit-scale.

After defining a variable object for \( \sigma \), we proceed creating objects representing the regression coefficients \( \beta \), the predicted values \( \mu = X\beta \), and the response \( y \). The prior for \( \beta \) involves a transformation of the variables \( \sigma \), leading to a slightly more complicated setup. Once again, the function \( \text{lsl.param} \) is used to create the object representing a model parameter. In the first argument the value of the parameter is specified where \( k \) refers to the dimension of \( \beta \). The functions \( \text{np.zeros} \) and \( \text{np.ones} \) create a vector of zeros and ones of specified length, respectively.

Py> beta = lsl.param(  
    np.zeros(k),  
)
The specification of the prior distribution is more involved. Akin to the creation of \( \sigma \), the class \( \text{lsl.Dist} \) is used. However, instead of specifying a distribution class and its parameters directly, an anonymous function indicated by the keyword \( \lambda \) is supplied as the first argument. The function must return an object of a type compatible with the Distribution interface defined in TensorFlow Probability. Within the function, however, variables can be transformed as demonstrated here with taking the square of \( s \). The other arguments to \( \text{lsl.Dist} \) match the arguments of the lambda-function, here \( s \). Notably, the object created above \( \sigma \) is employed as the argument for \( s \), signifying to Liesel to use the value stored in the \( \sigma \) object when creating the multivariate normal distribution.

Next, we create another object of type \( \text{lsl.Var} \) to represent the predicted value of \( y \), namely \( \mu = X \beta \). This time, there is no distribution associated with the value and furthermore the value is deterministically defined when conditioning on \( \beta \). Therefore, we supply an object of type \( \text{lsl.Calc} \) as the value and no \( \text{lsl.Dist} \) object to the constructor. Similar to the last code chunk, we use an anonymous function to specify how the value should be calculated and supply the object representing \( \beta \) as an argument to \( \text{lsl.Calc} \). The code assumes that the design matrix \( X \) is stored in \text{data.design_matrix}.

```python
Py> mu = lsl.Var(
    + lsl.Calc(
        + lambda b: data.design_matrix @ b,
        + b=beta,
        + ),
        + name="mu",
        + )
```

Finally, to create a variable for the response with the value stored in the variable \text{data.response}, one can use the following code:

```python
Py> lsl.obs(
    + data.response,
    + lsl.Dist(tfd.Normal, loc=mu, scale=sigma),
    + name="y",
    + )
```

This process is akin to the model parameters created above. This time, however, the function \( \text{lsl.obs} \) indicates that this is not a model parameter but an observed random variable. The identifiers \( \mu \) and \( \sigma \) refer to values that do not require transformation before being supplied to the normal distribution; thus, an anonymous function is unnecessary.

When using nodes (here objects of the type \( \text{Var} \)) as arguments, Liesel creates a connection between the nodes and passes the nodes value to the function. These relationships are visualized in Figure 2.

2.3 Main concepts and implementation details

Liesel’s model library follows an object-oriented design. We limit ourselves to a simplified version of the actual code to make understanding manageable while communicating the main concepts. In the following part, we introduce design concepts and describe implementation details.

2.3.1 The computational graph

As discussed before, the computational graph is a DAG in which nodes correspond to functions and edges indicate data flow. In Liesel, the class \( \text{Node} \) and its subclasses build the core of the computational graph. Here, we limit the discussion to the subclasses \( \text{Data} \) and \( \text{Calc} \), which are sufficient to describe the implementation of computational graphs in Liesel. As its name suggests, the first class describes a node without inputs representing a value assigned to
The graph in Liesel has the invariant that no dangling function arguments exist. The expression ‘not dangling’ means that at all times, each function argument wrapped in a \texttt{Calc} node must be linked to an input node via a reference in the field \texttt{inputs}. Therefore, the graph has to be built top-down in build mode, starting with data nodes and working the way down so that inputs are well-defined functions of data nodes. Moreover, the graph can be in two different modes. The graph is structurally mutable in the build mode. In contrast, the graph is structurally immutable in the computation mode; i.e., the relationship between nodes and the functions assigned to \texttt{Calc} nodes are immutable. Casting the finished graph to the computation model allows us to take advantage of its structural immutability.

Each node has a corresponding value. For a \texttt{Data} node, it is the assigned value; for a \texttt{Calc} node, it is the result of the computation. The naive implementation of calculating a node’s value on the fly can be inefficient, e.g. if a node serves as input to more than one node, its value and thus the value of all recursive inputs is calculated more than once. To avoid this overhead, a node in Liesel has three more fields: \texttt{value}, \texttt{ outdated}, and \texttt{outputs}. The field \texttt{outputs} stores references to all nodes whose input this node is. In the field \texttt{value}, a node stores the last result from computing its value, and \texttt{ outdated} indicates if the value stored in \texttt{value} is outdated, i.e. if any of the recursive inputs of a node has changed its value since the last time \texttt{value} was updated. Therefore, a node returns the stored value instead of recalculating it when the field \texttt{ outdated} is false. Otherwise, it calculates its value, stores the result in the field, and sets \texttt{ outdated} to false. The update mechanism is recursively triggered should one of the input nodes be outdated. A data node always returns its value since the outdated flag of a data node is always false.

This mechanism has the advantage that only nodes flagged as outdated compute their value. However, it has the disadvantage that each node needs to keep track of changes to nodes in the recursive input set. Nodes of the \texttt{Calc} class correspond to pure function. Therefore, it is sufficient when data nodes set the outdated flag in their recursive output set whenever a new value is assigned. For efficiency, Liesel updates the nodes flagged as outdated in topological order and can perform partial updates, i.e. updating only specific nodes and their recursive input set in topological order. Even after partial updates, the graph remains consistent due to the outdated flags and the graph’s structural immutability.

The computational graph can be viewed as a function mapping the value of the data nodes to the set of values of all nodes. The graph can also be used to construct functions that map only a subset of the data nodes to a subset of all nodes. Internally, these functions assign their arguments to the data nodes, which triggers the propagation of outdated flags and then requests and returns the value of the nodes in the output set, which triggers the update mechanism.

To make a connection to a Bayesian statistical model, consider a computational graph in which data nodes represent model parameters and data observed. Furthermore, one of the \texttt{Calc} nodes corresponds to the joint log-density. A function that takes the model parameter as an argument, assigning them to the corresponding data nodes and returning the node value representing the joint log-density can be considered the unnormalized log-posterior density function.

We aim to compile functions constructed with the graph using JAX and derive derivatives using JAX’s autodifferentiation toolchain. Both require purity of the function. However, functions derived from the graph as it is are not pure. The impureness arises from the state held by each node in terms of the tuple comprised of value and outdated flag. Jointly, the nodes’ states form the graph’s state. The functions constructed with the graph gain purity by supplementing the arguments and the return value by the state and updated state, respectively.

Some remarks on differences to the actual implementation: Some \texttt{Calc} nodes might not hold a state to lower the memory requirements. These nodes must recalculate the value on each request. We have introduced the state as the tuple of value and outdated flag. In the actual implementation, the state can be any python object or, in the case of JAX-compiled code, any PyTree. The broader definition of state enables the implementation of stateful nodes, e.g. for more advanced caching. At first glance, the computational graphs described here do not support randomness via pseudo-random number generation (PRNG). However, they do when modeling the state of the PRNG as a data node.

### 2.3.2 The statistical model

The statistical model in Liesel builds on the computational graph. It gives statistical semantics to the graph by introducing the concept of random variables. A random variable in Liesel has a value and an associated probability distribution represented by the class \texttt{Var}. Internally, the variable creates two nodes: a node representing the variable’s value and a node corresponding to the probability or density of the associated conditional distribution. The first node can either be a data node or the result of a calculation. The second node is of the type \texttt{Calc} and has as inputs the node holding the variable’s value and inputs for all distribution parameters. When constructing a variable, the specified
distribution must follow the distribution interface of TensorFlow Probability (TFP). Thus, all of TFP’s distributions can be used with Liesel, and new ones can be implemented. Furthermore, the class `Var` has a field to describe the role of this variable in the model, e.g. whether the quantity is a model parameter or corresponds to observed data. This information is used when creating an object of the `Model` class to automatically create nodes for the model’s log-likelihood, log-prior, or joint log-density.

An object of class `Model` represents a statistical model in Liesel. It gives the user easy access to values such as log-likelihood, log-prior, or joint log-density. The class also provides convenience functions, e.g. for creating pure functions based on the computational graph, as described in the last section. The user can set the model to REPL (read-evaluate-print-loop) mode, which keeps the model automatically in a consistent state in terms of node values. Furthermore, it can plot the statistical model as a PGM or the computational as a DAG. Under the hood, roughly speaking, a model object comprises a collection of nodes forming the computational graph and variables to allow for a statistically meaningful interpretation.

As part of a statistical model, the computational graph is always in computation mode. However, the model can be cast to the build mode. The graph builder (see next section) can cast the nodes and variables back to a model object. While in build mode, the model can be extended, and variables can be changed. The graph builder also supports more advanced manipulations of the graph and the statistical model.

### 2.3.3 Graph manipulations

For the construction of the computational graph and statistical model, Liesel offers a helper - implemented as the class `GraphBuilder` - that allows users to gradually implement the model before creating an object of type `Model`. In addition, the graph builder automatically creates nodes to calculate the model’s log-likelihood, log-prior density, and joint log-density. The builder also helps to manage the state of a PRNG in the graph by creating the required data nodes and distributing the PRNG state to nodes that require it. Using pseudo-randomness in the graph can come in handy when, for example, predictive checks are of interest.

Besides building the computational graph, the graph builder supports the user with more complex operations. These include transforming parameters from a restricted to an unrestricted space, e.g. allowing sampling with Hamiltonian Monte Carlo (HMC). Liesel has sensible defaults for these transformations but lets the user, in contrast to many popular software tools, overwrite the defaults. To continue with the running example from above, we transform \( \sigma \) to the unconstrained space using a log transformation. This transformation allows us to sample \( \sigma \) using an HMC-based sample in the next section. Afterwards, we add the remaining variables and build the model. Note, that we only need to add \( y \) and Liesel discovers the remaining variables. A visualization of the model with transformed parameter is shown in Figure 3.

```python
Py> gb = lsl.GraphBuilder()
Py> gb.transform(sigma, tfp.bijectors.Exp)
Py> gb.add(y)
Py> model = gb.build_model()
```

Other graph manipulations allow joining graphs, splitting graphs, replacing sub-graphs, or carrying out bulk commands like renaming nodes and variables according to a pattern. These graph manipulations are conceptually relatively simple but allow the customization of one or more base models. The internal operations boil down to simple substitutions. Recall that a `Calc` node holds references to its inputs. In this list, the reference to the old node can be replaced by referencing the replacement node and updating the output references accordingly. The substitution upholds the invariant requirement concerning no dangling inputs. For example, a sub-graph can be removed by replacing a `Calc` node with a `Data` node.

We keep the description of the builder short here and refer the reader to the project’s website where the API of the graph builder is documented. The case study in Section 6 features a more extended code example using the graph builder.

### 3 Goose: A toolbox for modular MCMC algorithms

The Liesel framework introduces a specialized library, Goose, dedicated to optimizing MCMC algorithms for the estimation problem at hand. Goose equips statisticians with the tools to craft custom MCMC algorithms, providing a tailored fit to their models, that way giving users the potential to outperform generic samplers. Goose supports the user in three pivotal ways:

**Building the MCMC transition.** Goose lets users decide how to transition model parameters between MCMC iterations by choosing one kernel or a combination of kernels. These kernels, the core elements of an MCMC
algorithm, facilitate the transition of the parameter vector, either in its entirety or segmented in a blocked sampling scheme, during one MCMC iteration. Notably, kernels can institute warmup processes, allowing them to automatically calibrate hyper-parameters, thus bypassing the need for manual adjustments. Furthermore, Goose’s capabilities extend to both continuous and discrete model parameters. Goose aims to incorporate well-established MCMC algorithms from existing libraries, like BlackJAX’s NUTS and HMC implementation. Drawing from the strength of the community, Goose can circumvent redeveloping intricate algorithms, ensuring accuracy while also bolstering open-source libraries and their community.

**Combining convenience with full control.** Central to Goose’s philosophy is ensuring that users maintain full control over the entire MCMC algorithm. This encompasses the ability to modify default configurations for every kernel and, crucially, to integrate specialized user components. Goose’s architecture is inherently modular, thus ensuring that researchers can seamlessly expand upon the framework. The well-documented interface grants users the flexibility to integrate custom, problem-specific kernels with the kernels provided or use only their own kernels. The former is often a convenient and robust solution when generic kernels are insufficient for the estimation challenge and users can improve estimation by integrating custom kernels only for parameters for which sampling is especially challenging. While Liesel models integrate naturally with Goose, the framework’s versatility is evident in its compatibility with any JAX-based model, be it set up with the PyMC library or a custom implementation.

**Streamlining the MCMC workflow.** Utilizing Goose alleviates statisticians from administrative chores often faced when setting up MCMC algorithms. This includes tracking the parameter values to form the MCMC chain, handling the PRNG state, parallelizing code for running multiple chains in concurrently, tracking errors, and logging debug messages. It also helps with calling tuning algorithms of the kernels and creating a summary of the results, which includes by default diagnostic statistics such as Rhat and the estimated number of effective samples.

Moreover, Goose strives to be convenient to use and fast. To achieve these goals, it provides pre-implemented components of popular MCMC algorithms like HMC and NUTS. Furthermore, Goose makes heavy use of JAX’s capabilities for automatic differentiation (sparing the user the implementation of derivatives) and just-in-time compilation (speeding up the repeated evaluation of the log-probability of the model). For this reason, the models and the components of the MCMC algorithms need to be expressed in JAX.

However, some aspects remain beyond Goose’s scope. For instance, it does not validate the mathematical accuracy of sampling schemes. Users bear the responsibility of crafting valid MCMC algorithms. While Goose’s results are generally consistent on the same system, exact reproducibility across varied hardware remains elusive due to slight discrepancies in floating-point computations. Over numerous MCMC iterations using cutting-edge algorithms, these minute differences might accumulate and become noticeable.

In essence, Goose offers a dual advantage: it empowers users to innovate new algorithms using the kernels provided by Goose while also granting the flexibility to go beyond existing components to cater to specific estimation needs. By streamlining the implementation with Goose, statisticians can focus on optimizing the MCMC algorithm. The remainder of this section delves deeper into Goose, outlining its intricate design considerations and shedding light on

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3 Many contemporary computational tools face challenges with exact reproducibility. Refer to Stan’s reference manual (https://mc-stan.org/docs/reference-manual/reproducibility.html) or the corresponding section in Liesel’s tutorial book (https://docs.liesel-project.org/en/stable/tutorials/md/05-reproducibility.html) for more insights.
certain implementation details. However, we start by showing how Goose can be used in the BLM example introduced in Section 2.2.

3.1 Continued example: Estimating the Bayesian linear model

To estimate the Bayesian linear model, we utilize a dual-kernel approach: a Gibbs kernel updates the regression coefficient vector $\beta$, and an HMC kernel manages $\log(\sigma)$. While various MCMC algorithm configurations could be employed here – including a sole HMC or NUTS kernel – we opt for the two-kernel method to demonstrate the blend of a default kernel with a user-defined sampler.

With Goose, constructing the sampler, which we also refer to as the engine, becomes easy using the EngineBuilder class. In a basic configuration, users connect the sampler to the model, set parameters such as sample quantity and initial values, add the chosen kernels, and finally, after building the engine, the sampler is ready for execution.

```python
Py> import liesel.goose as gs
Py> import jax.numpy as jnp
Py> builder = gs.EngineBuilder(seed=1, num_chains=4)
Py> interface = lsl.GooseModel(model)
Py> builder.set_model(interface)
```

The initial lines import the goose module and jax.numpy, which we alias as gs and jnp. The latter is needed for crafting the JAX-compatible Gibbs sampler in subsequent steps. Next, we initiate an engine builder configured to operate four parallel chains, mandating a specified seed for reproducibility. Due to the model-agnostic nature of Goose, an interface object is used for communicating with the model. Subsequently, we determine the initial values. For this illustration, we utilize the values present in the model’s strong nodes. Nevertheless, more intricate initialization strategies can be adopted.

```python
Py> builder.set_initial_values(model.state)
Py> builder.set_duration(warmup_duration=1000, posterior_duration=1000)
Py> builder.positions_included = ["sigma"]
```

The call set_duration specifies the number of MCMC steps for both the warmup and subsequent period. Concluding, we direct Goose to monitor the node labeled sigma.

Constructing the Gibbs sampler for $\beta$ necessitates the user to code a function that draws from its full conditional distribution. Specifically, this is given by $\beta | y, \sigma \sim N(\mu^*, \sigma^2 \Sigma^*)$ where $\Sigma^* = (X^T X + \Sigma_0^{-1})^{-1}$ and $\mu^* = \Sigma^*(X^T y + \Sigma_0^{-1} \mu_0)$. In our choice, the prior of $\beta$ is given by $\mu_0 = 0$ and $\Sigma_0 = I$.

The function implementing the draw should have a signature comprising an object of type PRNGKey – corresponding to the pseudo-random number generator’s state – and another representing the model state. It returns a dictionary with parameter names as keys and their updated values as entries. We employ the interface object within the function’s body to extract relevant values from the model state. Subsequently, we instantiate a multivariate normal distribution from which a sample is drawn.

```python
Py> def draw_beta(prng_key, model_state):
+     position = interface.extract_position(["y", "sigma"], model_state)
+     y = position["y"]
+     sigma = position["sigma"]
+     sigma_star = jnp.linalg.inv(
+         data.design_matrix.T @ data.design_matrix + jnp.eye(data.design_matrix.shape[1])
+     )
+     mu_star = sigma_star @ data.design_matrix.T @ y
+     dist = tfd.MultivariateNormalFullCovariance(mu_star, sigma**2 * sigma_star)
+     new_beta = dist.sample(seed=prng_key)
+     return {"beta": new_beta}
```

The function draw_beta is then wrapped by a Gibbs kernel and added to the builder.

```python
Py> builder.add_kernel(gs.GibbsKernel(["beta"], draw_beta))
```
Finally, we add the kernel for the transformed value of $\sigma$. Notably, the HMC sampler functions in the unconstrained real space. As a preparatory measure, we incorporated the log-transformed value into the model, as detailed in Section 2.3.3.

In order to add the HMC kernel, it can simply be created by providing a list of the keys that this kernel will sample.

```python
Py> builder.add_kernel(gs.HMCKernel(["sigma_transformed"]))
Py> engine = builder.build()
Py> engine.sample_all_epochs()
Py> results = engine.get_results()
Py> gs.Summary(results)
```

The subsequent steps create the engine, execute the sampler, and present a summary of the outcomes, partly displayed in Table 1.

Table 1: Parameter summary table for the Bayesian linear model as generated by Goose rounded to two decimal places.

| Parameter | Index | Kernel | Mean  | SD   | q0_0.05 | q0_0.5 | q0_0.95 | Sample Size | ESS Bulk | ESS Tail | $\hat{R}$ |
|-----------|-------|--------|-------|------|---------|--------|---------|-------------|----------|----------|----------|
| $\beta$ (0,) | kernel_00 | 1.04  | 0.12 | 0.84 | 1.03    | 1.24   |         | 4000        | 3874     | 3711     | 1.00     |
| $\beta$ (1,) | kernel_00 | 1.97  | 0.11 | 1.78 | 1.97    | 2.16   |         | 4000        | 3924     | 3773     | 1.00     |
| $\beta$ (2,) | kernel_00 | 2.90  | 0.12 | 2.70 | 2.90    | 3.10   |         | 4000        | 3947     | 3812     | 1.00     |
| $\sigma$ | () | kernel_01 | 1.13 | 0.08 | 1.01 | 1.13 | 1.27 | 4000 | 11611 | 2377 | 1.00 |
| $\sigma_{\text{transformed}}$ | () | kernel_01 | 0.12 | 0.07 | 0.01 | 0.12 | 0.24 | 4000 | 11610 | 2376 | 1.00 |

3.2 Main components of Goose

Goose is composed of many classes and interfaces. The design boils down to a few central pieces users must understand to successfully use Goose as their tool to create MCMC algorithms in a few steps. A deeper understanding is required to write extensions. The most important building blocks and their relationships are illustrated in Figure 4. We describe their roles here. Note that we sometimes refer to the model parameters as the “position”.

**Engine** The Engine class is the central part of Goose and acts as a coordinating entity, hiding a big part of the complexity from the user. In particular, after the user has decided how the transitions should be executed, it makes sure that the right functions and methods are called at the right time guaranteeing that the transitions of the position happen as requested. Moreover, the engine keeps track of the sampling history and advances through the different sampling phases (e.g. the warmup and posterior phase). It also coordinates the PRNG state and provides the top-level user interface.

**Kernel** A kernel object performs a single MCMC transition, i.e. an update of the position or some elements of the position. The update must be a valid MCMC transition, for example based on the Metropolis-Hastings algorithm. The Kernel interface describes how the engine can interact with the kernels. The user can either use pre-implemented kernels or implement new kernel classes adhering to the kernel interface.

**Epoch** An epoch is a series of MCMC iterations. The EpochConfig class describes an epoch. Epochs are used to communicate to the kernels which phase of the MCMC algorithm they are in and which operations they are allowed to perform in this phase. More specifically, we divide the sampling process into a warmup and a posterior phase. Samples from the posterior phase are expected to be valid MCMC samples. In contrast, during the warmup phase, the chain may not yet have converged, and during the so-called adaptation epochs, the Markov property may be violated. This way, we allow the kernels to learn their hyperparameters during the adaptation epochs in the warmup phase. If done right, this can spare the user the manual tuning of the kernel hyperparameters, and it can lead to more efficient sampling in the posterior phase.

The simplest setup would contain only two epochs: a burn-in epoch (part of the warmup phase) and a posterior epoch (part of the posterior phase), each containing multiple MCMC iterations. On the other hand, a more complex setup can include multiple adaptation epochs in the warmup phase.

**ModelInterface** The ModelInterface describes how the components of Goose can communicate with the model. Most importantly, it describes how the unnormalized log-posterior can be evaluated for a given position. By defining the model interface as an abstraction layer, Goose can easily be used with different model backends.

To set up an MCMC algorithm using Goose, the user can employ the EngineBuilder class for a simplified process. As we have demonstrated in Section 3.1, this class provides a step-by-step interface to configure the Engine object which handles the communication among the different Goose components used.
3.3 Standard kernels in Goose

Goose provides several kernels that can be used directly with many models. We discuss some of them here:

**RandomWalkKernel** The RandomWalkKernel implements a Gaussian proposal distribution and a Metropolis-Hastings acceptance step. The kernel is self-tuning and uses the dual average algorithm to adjust the step size (i.e. to scale the proposal distribution) during fast and slow adaptation epochs, such that a user-defined target acceptance rate, by default of 0.234 (Gelman et al., 1997), is reached.

**HMCKernel and NUTSKernel** The HMCKernel and NUTSKernel use the gradient of the log-posterior to generate MCMC chains with a low autocorrelation. The implementation of the transition() method is based on BlackJAX’s implementations of the HMC (Neal, 2011) and NUTS (Hoffman and Gelman, 2014; Lao et al., 2020; Phan et al., 2019) algorithms. Both kernels are able to tune the step size during fast and slow adaptation epochs using the dual averaging algorithm. After slow adaptation epochs, the mass vector or matrix of the impulse is adjusted based on the empirical variance-covariance of the samples from the previous epoch.

**IWLSKernel** The IWLSKernel is named after the method proposed by Gamerman (1997), which is often used for Bayesian distributional regression models (Brezger et al., 2005). However, Liesel’s implementation is also inspired by the roughly equivalent Metropolis-adjusted Langevin algorithm (MALA) with the Riemann metric (Girolami and Calderhead, 2011). This approach allows us to add a step size parameter in a straightforward way, which can then be tuned with the dual averaging algorithm during fast and slow adaptation epochs. More precisely, the IWLSKernel employs a Metropolis-Hastings correction and a Gaussian proposal density, where the mean vector $\mu$ and the covariance matrix $\Sigma$ depend on the gradient (score) and the Hessian (Hess) of the log-posterior, i.e.

$$\mu = \theta + s^2/2 \mathrm{Hess}(\theta)^{-1} \text{score}(\theta), \quad \Sigma = s^2 \mathrm{Hess}(\theta)^{-1},$$

where $s$ denotes the step size and $\theta$ the position vector. The factor $1/2$ that is multiplied with $s^2$ in the mean vector comes from the Langevin diffusion, which is the basis of the MALA algorithm.
The kernel can change its state and prepare for the following tuning. To invoke the tuning, the kernel method `transition()` is called informing the kernel about the new epoch and allowing it to modify the kernel state. The kernel state is a data structure used to store parameters defining the behavior of the kernel. It may be modified during the warmup. The scale of the proposal distribution (also known as the step size) of a random walk kernel serves as an example in this section. The kernel state can also include a cache required to calculate the actual parameters that affect the transitions. Allowing the kernel to change its state at the beginning of an epoch enables it to prepare for the subsequent operations.

Afterwards, the control is handed back to the engine, and it calls the kernel method `transition()` for each MCMC iteration in the current epoch. The transition method is supposed to move the position and return the new position together with additional information (which would typically include whether the position changed, how large the acceptance probability was, whether an error occurred, etc.) to the engine. The engine takes care of storing the position and the additional information. Note that during the warmup phase, the kernels are allowed to change their state in the transition method, which allows for on-the-fly tuning of kernel parameters and updates of the cache. This is required, for example, for the dual averaging algorithm (Nesterov, 2009; Hoffman and Gelman, 2014, Section 3.2) or for Welford’s online algorithm for calculating the empirical variance of an element of the position (Welford, 1962).

Once all transitions defined in the current epoch have been carried out, the kernel method `end_epoch()` is called. Again, the kernel can change its state and prepare for the following tuning. To invoke the tuning, the kernel method `tune()` is called if the current epoch is an adaptation epoch. In the adaptive random walk kernel, this method would be the place to calculate the new step size based on Welford’s algorithm and update it in the kernel state. The kernel is allowed to request the history of the positions visited in the current epoch. Having the history available facilitates the implementation of certain tuning algorithms.

The outlined process is repeated for each epoch. As soon as the first epoch of the posterior phase is encountered, the kernel method `end_warmup()` is called before the call to `start_epoch()`. It informs the kernel that the warmup phase is over, and subsequent to this call, the kernel must respect the Markov property.

Finally, the user can request the sampling results from the engine and inspect them. The results do not only contain the chain of the visited positions but also meta-information and an error log (e.g. an error is reported if the log-posterior evaluates to $-\infty$). Liesel also provides some utilities for the inspection of the chains.

A more interactive approach is also possible. The user can always add more epochs to continue sampling. One restriction is that Goose does not allow posterior epochs to be followed by epochs of any other type. The interactive approach is facilitated by the engine methods `append_epoch()` and `sample_next_epoch()`. The user can run a few
Figure 5: Sequence diagram of the communication between the engine and a kernel. For simplification, we show only one kernel here. However, the extension to multiple kernels is natural by calling the kernel methods in a sequence, which can be achieved by wrapping the kernels in a KernelSequence object. The engine provides additional methods to run the epochs one by one and to append epochs, which are not shown here. These methods allow for an interactive use of the engine, while the diagram illustrates a “one-shot” run of an already configured engine.
warmup epochs, inspect the chains, decide if they have reached the typical set and converged, add more warmup epochs if necessary or move on to the posterior epoch otherwise.

Everything that has been said so far can easily be generalized to multiple kernels. In that case, each method call is carried out in a loop over the sequence of kernels defined by the user. Note that the kernels cannot share their state.

If users want to work with custom MCMC transition or tuning methods or extend Goose’s collection of kernels, they have to implement a new class that is required to follow the `KernelInterface`. The two most important methods to do so are `transition()` and `tune()`. We describe them in more detail and also provide more information on the implementation of the engine, which is useful to understand the requirements for the kernel methods.

**The engine.** As described above, the engine orchestrates the sampling process and provides the top-level user interface. It also hides some complexity that arises from using JAX and just-in-time (JIT) compiled functions. Using JAX comes with many benefits, e.g. automatic differentiation and JIT compilation. Furthermore, JAX programs can be executed on high-performance devices like GPUs and TPUs. For efficient sampling, the engine automatically groups multiple MCMC iterations into one compilation unit and uses JAX’s `jit()` function to compile them together. Thus, the MCMC iterations are performed together on the computing device without the need for communication with the host. This ensures a better performance, especially if the computing device is not the CPU.

One drawback, or rather one limitation, is the requirement of “purity” for functions to be compiled with JAX. Purity is not necessarily a disadvantage, because pure functions are easier to reason about for humans and for the compiler. This can result in faster execution times compared to non-pure functions.

Goose needs to guarantee that the compiled functions are pure. This implies that the engine must manage the PRNG state – we use JAX’s splittable Threefry counter-based PRNG – as well as the kernel states. Goose requires all kernel methods called within the compiled functions (e.g. `transition()` and `tune()`) to be pure, meaning that the kernels cannot store values changing over time in fields but must pass them back to the engine via a `KernelState` object, and receive them again from the engine together with the PRNG state for the next transition.

**The transition method.** The two most important methods every kernel needs to implement are the `transition()` and the `tune()` method. These methods are called by the engine and need to be pure and jittable.

The purpose of the transition method is to move the position or parts of it using a valid MCMC step, e.g. a Metropolis-Hastings algorithm. The position is a subset of the model state. Through the standardized model interface, the kernel can extract the position from the model state.

The signature of the `transition()` method is as follows:

```python
Py> class Kernel:
    + ...
    +
    +     def transition(
    +         self,
    +         prng_key: KeyArray,
    +         kernel_state: KernelState,
    +         model_state: ModelState,
    +         epoch: EpochState,
    +     ) -> TransitionResult[KernelState, TransitionInfo]:
    +         ...
    +     ...
```

Since the `transition()` method must be pure and MCMC transitions generally involve the generation of random numbers, the state of the PRNG needs to be provided as an argument. In addition, the `transition()` method receives the kernel state, the model state and the epoch state as arguments, and returns a `TransitionResult` object, which wraps the new kernel state, the new model state and some meta-information about the transition, e.g. an error code or the acceptance probability (in a `TransitionInfo` object). An error code of zero indicates that the transition did not produce an error.

---

4 A pure function is a function whose value depends solely on the values of its arguments and which furthermore has no side effects. In JAX and Goose, the concept of purity is a bit weaker. A function may depend on variables in the environment. However, the values of those variables are then compiled into the function, and therefore, the behavior of the function does not change if the variables are updated later. Consequently, the compiled function is pure.
All inputs and outputs must be valid “pytrees” (i.e. arrays or nested lists, tuples or dicts of arrays). The structure of these objects, e.g. the shape of the arrays in the kernel state, must not change between transitions. This allows the kernels to have specialized `KernelState` and `TransitionInfo` classes.

**Tuning a kernel.** The sampling process can be divided into epochs of four types: fast and slow adaptation epochs, burn-in epochs and posterior epochs. The adaptation and burn-in epochs are so-called warmup epochs. During the adaptation epochs, the kernels are allowed to learn their hyperparameters from the history. Samples from the adaptation epochs are usually invalid as MCMC samples, because the Markov property of the chain is violated. In contrast, during a burn-in epoch, the kernels should no longer adjust their hyperparameters and the Markov property should be respected, but the chain may still require some more time to converge. Finally, when reaching the first posterior epoch, the chain should have converged, all transitions should be valid, e.g. there should be no divergent transitions, and hence, the samples should approximate the target distribution appropriately.

The kernel method `tune()` is supposed to update the kernel hyperparameters at the end of an adaptation epoch. The method receives the PRNG state, the model state, the kernel state, the epoch state and optionally the “history”, i.e. the samples from the previous epoch, as arguments. It returns a `TuningResult` object that wraps the new kernel state and some meta-information about the tuning process, e.g. an error code. As for the transition, the `TuningInfo` class can be kernel-specific but must be a valid pytree.

The signature of the `tune()` method is as follows:

```
def tune(
    self,
    prng_key : KeyArray,
    kernel_state : KernelState,
    model_state : ModelState,
    epoch : EpochState,
    history : Position | None,
) -> TuningResult[KernelState, TuningInfo]:
```

**Debugging.** The engine can be configured to store more information about the sampling process, e.g. for debugging purposes. The extra information can include the log-posterior, log-likelihood, log-prior or any other quantity that can be computed from the model state by a quantity generator. Debugging is further facilitated with the option to store the kernel states for each iteration. Moreover, the engine can store information about the transitions and the tuning such as the acceptance probabilities or the proposals. In any case, the `transition()` and `tune()` methods of the kernels need to return an error code and inform the engine about non-fatal errors and warnings. The engine keeps a log and warns the user about potential problems. Goose’s diagnostic tools can further aid the detection of potential sampling issues.

4 **RLiesel: An R interface for semi-parametric distributional regression**

4.1 **Semi-parametric distributional regression**

The linear regression model is limited in terms of its Gaussian response distribution, the restrictive linear functional form that is assumed in the relationship between the covariates and the regression predictor, and its focus on the conditional expectation of the response variable. In contrast, semi-parametric distributional regression models combine various types of covariate effects in an additive way (including parametric linear and non-linear spline-based specifications as special cases, but also spatial and random effects, etc.), as well as flexible response distributions and the possibility to model different response parameters; see [Kneib et al., 2023] for an overview of the model framework. Since the model class can be represented in a hierarchical form, it is well-suited for the Liesel-Model software, but the implementation of these types of models from scratch can be a tedious task. To facilitate the development of semi-parametric distributional regression models, RLiesel provides an interface between R and Liesel-Model that integrates all required model components based on existing software packages, e.g. spline-based predictor components from the `mgcv` package for R and response distributions from TensorFlow Probability.
In a stylized fashion, the hierarchical specification of semi-parametric distributional regression looks as follows:

\[ y \mid x, \theta \sim \mathcal{D}(\theta(x)), \text{ where } \theta(x) = (\theta_1(x), \ldots, \theta_K(x))^T, \]
\[ \theta_k(x) = h_k(\eta_k(x)), \]
\[ \eta_k(x) = f_{k_1}(x; \beta_{k_1}) + \cdots + f_{k_L}(x; \beta_{k_L}), \]
\[ \beta_{kl} \mid \tau^2_{kl} \sim \mathcal{N}(0, \tau^2_{kl} K_{kl}), \]
\[ \tau^2_{kl} \sim I\mathcal{G}(a, b). \]

On the first level, the parametric distribution \( \mathcal{D} \) is assumed for the response variable \( y \) given covariates \( x \), where \( \theta(x) \) denotes the \( K \)-dimensional, covariate-dependent parameter vector. The elements \( \theta_k(x) \) are related to semi-parametric regression predictors \( \eta_k(x) \) via known response functions \( h_k \) that ensure restrictions on the parameter space. The regression predictors themselves are additively composed of parametric and non-parametric covariate effects \( f_{kl}(x; \beta_{kl}) \), which are expressed as basis expansions with the regression coefficients \( \beta_{kl} \). To regularize the estimation of these potentially high-dimensional vectors, multivariate normal priors are assumed for \( \beta_{kl} \), where the precision matrices \( K_{kl} \) are chosen to reflect the desired regularization purpose (smoothness, shrinkage, etc.). The variances \( \tau^2_{kl} \) of the multivariate normal distributions determine the importance of the prior (or equivalently, the amount of regularization), and are themselves assigned a hyperprior, e.g. an inverse gamma prior with parameters \( a > 0, b > 0 \).

### 4.2 Continued example: Building two types of advanced regression models with RLiesel

Expanding on the example from Section 2.2, assume that we observe binary instead of Gaussian data, and therefore want to construct a logistic regression model. In this case, only \( K = 1 \) distributional parameter is considered, so we can drop the index \( k \) for simplicity. The logistic regression model can be implemented using the \texttt{tfd.Bernoulli} distribution from TensorFlow Probability instead of \texttt{tfd.Normal}. When replacing the response distribution of the regression model, we need to map the conditional expectation (i.e. the success probability) to the real line using an appropriate link function \( h^{-1} \), e.g. the logit function in the case of the logistic regression model. In TensorFlow Probability, this can be achieved by initializing the \texttt{tfd.Bernoulli} distribution with the \texttt{logits} instead of the \texttt{probs} argument, or with the \texttt{tfb.Sigmoid} bijector.

Moreover, assume that in addition to the covariates \( x_1, x_2 \) and \( x_3 \), we observe a fourth covariate \( x_4 \) with a non-linear effect on the success probability of \( y \). If we want to model the non-linear effect of \( x_4 \) with a spline-based basis expansion, e.g. a thin plate or B-spline, manually adapting the Bayesian linear model from Section 2.2 would require us to construct the corresponding design and penalty matrices. Depending on the desired basis and regularization, an implementation might or might not be available in Python, or might require substantial effort otherwise. To accelerate the model development, we can use RLiesel instead and construct the complete model with this R command:

```r
R> model <- liesel(
+   response = y,
+   distribution = "Bernoulli",
+   predictors = list(
+     logits = predictor(~x1 + x2 + x3 + s(x4))
+   )
+ )
```

The specification of the semi-parametric regression predictor \( \sim x1 + x2 + x3 + s(x4) \) indicates that the covariates \( x_1, x_2 \) and \( x_3 \) are modeled with linear effects and \( x_4 \) with a non-linear effect. As the predictor specification is passed on to \texttt{mgcv}, RLiesel uses the same defaults, i.e. thin plate splines for non-linear effects. Other bases can be selected using the \texttt{bs} argument of the \texttt{s()} function, e.g. \texttt{s(x4, bs = "ps")} for P-splines. Finally, note that the predictor specifications are passed to the \texttt{liesel()} function as a list. The names of the list need to match the names of the parameters of the selected TensorFlow Probability distribution, in this case the Bernoulli distribution as indicated by the string "Bernoulli".

In contrast to similar commands in R, RLiesel does not estimate the model automatically, but only constructs the model graph and the required design and penalty matrices. Due to the different priors of the parametric and non-parametric covariate effects, the hierarchy and graph of the logistic regression model (Figure 6) contain more variables than the Bayesian linear model in Section 2.2. If necessary, the user can modify the model graph, or the design or penalty matrices according to their requirements before estimating the model with Goose (or another JAX-compatible software). A real-world example of a model that is constructed from an existing RLiesel graph is provided in the case study in Section 6.
Figure 6: Model graph of the **logistic regression model**. Blue variables are strong (constant or sampled), orange variables are weak (computed from other variables). Double contour lines highlight variables with an associated probability distribution, and round contour lines highlight the model parameters.

Another direction in which the Bayesian linear model from Section 2.2 can be extended is the addition of more than one linear or semi-parametric regression predictor for further parameters of the response distribution. Assuming a Gaussian response distribution, the second response parameter would either be the standard deviation or the variance, depending on the parameterization of the model. If we observe heteroscedastic data, where in addition to the covariates $x_1, x_2$ and $x_3$ with an effect on the mean, a fourth covariate $x_4$ has a non-linear effect on the standard deviation, the appropriate Gaussian location-scale regression model can be set up with RLiesel using the following command:

```r
R> model <- liesel(
+   response = y,
+   distribution = "Normal",
+   predictors = list(
+     loc = predictor(~x1 + x2 + x3, inverse_link = "Identity"),
+     scale = predictor("s(x4)", inverse_link = "Exp")
+   )
+ )
```

In comparison to the command for the logistic regression model, we now have two predictor specifications, for which we need to provide appropriate inverse link functions. The inverse link functions are defined as strings, where the corresponding classes need to exist as bijectors in TensorFlow Probability. The graph of the Gaussian location-scale regression model (Figure 7) has a tree-like structure that is similar to the logistic regression model but splits into two branches right above the response variable: The left branch describes the regression predictor (and inverse link function) for the location parameter (the mean), while the right branch describes the scale parameter (the standard deviation).
In summary, RLiesel combines the tools from R allowing the user to set up semi-parametric and distributional regression models using an extremely concise syntax with the expressive and customizable model representation of Liesel-Model in Python. As RLiesel works at the interface of two programming languages, some configuration guidelines are provided in the following section.

4.3 Technology stack and workflow recommendations for RLiesel

RLiesel is implemented as a thin wrapper around the mgcv package for R [Wood, 2022]. The entry point to the package is the liesel() function, which requires the user to pass in the response data and distribution as well as the regression predictors as arguments. The regression predictors are specified as R formulas with the extensions from mgcv to define non-parametric predictor components. The formulas are then passed on to the gam() function from mgcv, which is used to initialize the design and penalty matrices. Finally, the model graph is constructed using the Liesel-Model library and filled with the matrices that are extracted from the gam object.

mgcv is the state-of-the-art package for semi-parametric regression in R. It is extremely powerful, supports a variety of response distributions and predictor components, and is one of the “recommended” packages that are installed with R by default. Other notable features of mgcv are the automatic smoothness selection [Wood, 2004] and several multivariate predictor components. To the best of our knowledge, no comparable package exists for Python. Most other R packages for semi-parametric regression build on mgcv, and RLiesel follows the same approach, leveraging the features of mgcv for the use with JAX, TensorFlow Probability, Liesel-Model and Goose, avoiding the need to re-implement most predictor components in Python.

To provide access to a wide range of response and prior distributions as well as link functions, RLiesel relies on TensorFlow Probability [Dillon et al., 2017]. Among other features, TensorFlow Probability comes with large collections of probability distributions and bijectors with standardized interfaces that can be combined to build complex models. TensorFlow Probability can use JAX [Bradbury et al., 2022] as a backend, which allows the user to employ any JAX-compatible software for the estimation of models from RLiesel, especially Liesel’s own MCMC library Goose.
Figure 8: The log-ratio of the LIDAR signals for each range on top of an MCMC sample of 4000 estimated mean functions (left) and 4000 estimated standard deviation functions (right). The red lines mark the posterior mean, the MCMC sample was obtained with the IWLS-Gibbs scheme described in Section 5.1.

As RLiesel provides an interface between two programming languages, R and Python, the user needs to configure an environment where both languages are installed and able to communicate with each other. To assist the user with the installation, the Liesel developers offer a template for such an environment that works on different operating systems. For a seamless integration, we recommend Quarto (Scheidegger et al., 2022) and reticulate (Ushey et al., 2022). Quarto allows the user to write and render dynamic documents in Markdown with embedded R and Python code cells, and using reticulate, objects can be shared between R and Python processes at runtime. With this setup, a model can be configured using RLiesel in an R code cell, then exchanged with a Python process, before an MCMC algorithm is developed in a Python code cell. Finally, the estimation results can be visualized in either R or Python, depending on the user’s preferences.

5 Case study I: Comparing different sampling schemes

In this first case study, we illustrate how the modularity of Goose can facilitate the design of efficient sampling schemes for a given model specification. More precisely, we show how different sampling blocks can be easily combined with each other and how the algorithm for an individual block can be replaced without interfering with the rest of the model. As a consequence, it gets very easy to try out and compare multiple sampling schemes, including the possibility to implement own sampling algorithms (kernels) for specific parameters and integrating them into an existing scheme.

For illustration, we use a dataset of LIDAR measurements, which was collected to determine the mercury concentration in the atmosphere (Holst et al., 1996). Two lasers with different wavelengths were emitted by the LIDAR device, and the log-ratio between the signals (the amount of reflected light, $y_i$) was recorded for each range (the distance the light traveled, $x_i$). The data is shown in Figure 8 suggesting that a semi-parametric Gaussian location-scale regression model

$$y_i \sim \mathcal{N}(\beta_0 + f(x_i), \exp(\gamma_0 + g(x_i))^2)$$  \hspace{1cm} (3)$$

might be a good fit for the data. Here, $\beta_0$ and $\gamma_0$ are the intercepts, and $f(x_i)$ and $g(x_i)$ are P-splines representing non-linear effects of the range on the mean and the variance. We use a cubic B-spline basis and a second-order random walk prior on the P-spline coefficients, see Lang and Brezger (2004) for details. The model belongs to the distributional regression framework as defined in Section 4.1 using a Gaussian response distribution and a log-link for the standard deviation.

https://github.com/liesel-devs/liesel-template
5.1 Sampling schemes with different kernels in Goose

Different sampling schemes are conceivable for Bayesian inference in Model (3), and we aim at evaluating the performance of five sampling schemes combining IWLS, Gibbs, NUTS and HMC kernels for different parameter blocks, see Table 2 for an overview of their configuration.

Table 2: Sampling schemes for Model (3). The IWLS kernel was used with the observed Fisher information as a metric (obtained through automatic differentiation). The NUTS kernel was configured with a maximum tree depth of 10 and a diagonal metric (tuned based on the empirical variances of the warmup samples). The HMC kernel was used with 64 integration steps and a diagonal metric. A smaller number of integration steps would have resulted in an insufficient exploration of the posterior distribution. The step size of the IWLS, NUTS and HMC kernels was calibrated with the dual averaging algorithm during the warmup epochs.

| Scheme               | β₀  | β₁  | τ₂ or log(τ₂) | γ₀  | γ₁  | τ₂ or log(τ₂) |
|----------------------|-----|-----|---------------|-----|-----|---------------|
| IWLS-Gibbs           | IWLS| Gibbs| IWLS          | NUTS| NUTS| Gibbs         |
| NUTS-Gibbs           | NUTS| NUTS| Gibbs         | IWLS| NUTS| Gibbs         |
| NUTS1                |     |     |               |     |     |               |
| NUTS2                |     |     |               |     |     |               |
| HMC2                 |     |     |               |     |     |               |

The IWLS-Gibbs sampling scheme is the default in RLiesel, following the suggestions in [Klein et al., 2015]. It combines IWLS kernels for the regression coefficients β with Gibbs kernels for the smoothing parameters τ². The IWLS kernel involves second derivatives to determine the Fisher information. For this reason, it is interesting to compare its performance with gradient-based MCMC approaches such as HMC or NUTS that avoid second derivatives. HMC and NUTS have been popularized with software like Stan [Stan Development Team, 2022] and PyMC [Salvatier et al., 2016], and are known to work well in many applications [MacKay, 2003, Chapter 30]. The smoothing parameters τ² need to be log-transformed if sampled with HMC or NUTS to guarantee an unconstrained parameter space. As Table 2 indicates, we are considering different blocking strategies involving HMC or NUTS, e.g. the first NUTS scheme, which combines all parameters in one large block, while the second NUTS scheme splits the mean and standard deviation parameters into two separate blocks.

Setting up and combining sampling schemes for parameter blocks is straightforward with Goose. To facilitate the configuration of an MCMC engine, a builder class can be used. Through the builder, kernels can be assigned to one or more parameters, the model and initial values can be set, as well as the number of MCMC iterations. Finally, the engine can be built and run. The following code snippet illustrates the procedure for the second NUTS scheme, but the setup of the other schemes works analogously:

```python
Py> builder = gs.EngineBuilder(seed=1337, num_chains=4)
Py> k1 = ["loc_p0_beta", "loc_np0_beta", "loc_np0_tau2_transformed"]
Py> k2 = ["scale_p0_beta", "scale_np0_beta", "scale_np0_tau2_transformed"]
Py> builder.add_kernel(gs.NUTSKernel(k1))
Py> builder.add_kernel(gs.NUTSKernel(k2))
Py> builder.set_model(gs.LieselInterface(model))
Py> builder.set_initial_values(model.state)
Py> builder.set_duration(warmup_duration=1000, posterior_duration=1000)
Py> engine = builder.build()
Py> engine.sample_all_epochs()
```

5.2 Run time and effective sample size

All sampling schemes from Table 2 converged to the same posterior distribution, leading to results of the form shown in Figure 8. We therefore focus on comparing their efficiency rather than the parameter estimates themselves. The MCMC algorithms were compiled and run on an Intel i7-1185G7 CPU with 8 cores and 3 GHz, using Liesel 0.2.7, BlackJAX 1.0.0 and JAX 0.4.20. The compilation was generally much more expensive than the generation of one chain with 1000 warmup and 1000 posterior iterations (see Figure 9). The IWLS-Gibbs and NUTS-Gibbs schemes were
Figure 9: The compile and run times of the sampling schemes from Table 2. The timings were obtained on an Intel i7-1185G7 CPU with 8 cores and 3 GHz, using Liesel 0.2.7, BlackJAX 1.0.0 and JAX 0.4.20, for one MCMC chain with 1000 warmup and 1000 posterior iterations. The IWLS-Gibbs and NUTS-Gibbs schemes were most expensive to compile (because they combine two types of kernels), while the first and second NUTS scheme were most expensive to execute (due to the high tree depth).

particularly slow to compile, presumably because combining two types of kernels means more work for the compiler, while the first and second NUTS scheme required most time to generate the chain.

The reason for the performance issues with NUTS was that the maximum tree depth of 10 was reached in about 90% of the posterior iterations for the first NUTS scheme, and in 75% for the second NUTS scheme. The problem did not occur with the NUTS-Gibbs scheme, where we split the regression coefficients and smoothing parameters into separate blocks. We tried to improve the performance of the first and second NUTS scheme with a non-centered parameterization as recommended by the Stan Development Team (2022, User’s Guide, Section 25.7) by diagonalizing the penalty matrices of the P-splines as described by Wood (2017, Section 5.4), but did not achieve an efficiency improvement. Other reparameterizations or the use of a Riemann metric (Girolami and Calderhead, 2011) might help to speed up the NUTS kernels, but we did not explore these options further in this case study.

The efficiency of an MCMC algorithm cannot be assessed based on the run time alone, but the quality of the samples needs to be taken into account as well. We use the effective sample size (ESS, Gelman et al., 2013) for this purpose. The ESS estimates the size an independent sample would need to have to contain the same amount of information as the correlated MCMC sample. An MCMC chain with a higher autocorrelation generally has a lower ESS. For the LIDAR model, the NUTS-Gibbs scheme had the highest ESS with a median of 318.67 per 1000 iterations, and the scheme with two HMC kernels had the lowest ESS with a median of 25.56 (Table 3). The table also shows the ESS per second, which takes both the quality of the samples and the run time into account. By that measure, the two schemes involving a Gibbs kernel performed best, with a median of 869.05 for NUTS-Gibbs and 325.21 for IWLS-Gibbs.

6 Case study II: Building a Multi-Species Count Model with Liesel

In this section, we illustrate how the different components of Liesel can be used to develop complex statistical models and perform Bayesian inference, building on the development of the multi-species count model (MSCM) in Kebl et al. (2023). Most importantly, we will see how components of a statistical model generated via RLiesel can be combined to a complex hierarchical model specification, Bayesian inference can be implemented via the different MCMC kernels provided by Goose, and how Bayesian inference for derived quantities is facilitated by including them into the model graph such that they can be tracked automatically through the MCMC samples.

The MSCM has been developed with the aim of assessing biodiversity across different taxa based on data collected at multiple field sites, accounting for the heterogeneity of the field sites based on covariates. The response data in this case are given in terms of an \( M \times N \) response matrix \( Y \), where the count variable in the \( i \)-th row and the \( j \)-th column records how often species \( j = 1, \ldots , M \) was observed on experimental plot \( i = 1, \ldots , N \), while the covariates \( x_{ij} \)
Table 3: The bulk ESS and bulk ESS per second of the sampling schemes from Table 2. 30 MCMC chains were generated per scheme, and the summary statistics were computed pooling all 22 parameters of the LIDAR model. The ESS per second was computed based on the run time of the posterior iterations alone, not taking the compilation and the warmup iterations into account. The NUTS-Gibbs scheme was the most efficient, both in terms of ESS and ESS per second.

|                  | 5%  | 25% | Median | 75%  | 95%  |
|------------------|-----|-----|--------|------|------|
| **Bulk ESS**     |     |     |        |      |      |
| IWLS-Gibbs       | 27.08 | 61.40 | **85.16** | 118.37 | 255.19 |
| NUTS-Gibbs       | 113.23 | 211.31 | **305.66** | 506.64 | 906.94 |
| NUTS1            | 8.80 | 46.33 | **95.97** | 340.33 | 921.96 |
| NUTS2            | 36.96 | 68.24 | **135.66** | 484.75 | 886.56 |
| HMC2             | 1.58 | 6.66 | **26.24** | 310.78 | 1157.11 |
| **Bulk ESS/s**   |     |     |        |      |      |
| IWLS-Gibbs       | 115.57 | 262.07 | **363.45** | 505.21 | 1089.17 |
| NUTS-Gibbs       | 253.79 | 473.64 | **685.11** | 1135.60 | 2032.83 |
| NUTS1            | 2.61 | 13.77 | **28.52** | 101.14 | 274.00 |
| NUTS2            | 21.78 | 40.22 | **79.95** | 285.70 | 522.51 |
| HMC2             | 6.13 | 25.78 | **101.50** | 1202.06 | 4475.50 |

contain information on the experimental plots. Given these data, the MSCM can be represented in hierarchical form as

\[
\text{the number of observations per species on plot } i, \quad y_i \sim \text{Multinomial}(n_i, p_i),
\]

\[
\text{the relative expected abundances per species on plot } i, \quad p_i = \frac{1}{\sum_{j=1}^{M} z_{ij} \mu_j} \times (z_{i1} \mu_1, \ldots, z_{iM} \mu_M),
\]

\[
\text{the total number of observations on plot } i, \quad n_i \sim \text{CountDistribution}(z_{ij}, \mu_j),
\]

\[
\text{the expected abundance of species } j, \quad \mu_j \sim \text{HalfNormal}(0, 10),
\]

\[
\text{the unobserved indicator whether species } j \text{ occupies plot } i, \quad z_{ij} \sim \text{Bernoulli}(\psi_{ij}),
\]

\[
\text{the probability that species } j \text{ occupies plot } i, \quad \psi_{ij} = \text{InvLogit}(\gamma_j + \eta_i),
\]

\[
\text{the occupancy intercept of species } j, \quad \gamma_j \sim \text{Normal}(0, 10).
\]

See also Figure 10 that shows the corresponding model graph (including prior specifications to be discussed below). In the model, the responses are assumed to be multinomially distributed with the total number of observations \(n_i\) and the relative expected abundances per species \(p_i\) on plot \(i\). The total number of observations is associated with a count data distribution (with \(\text{CountDistribution}(z_{ij}, \mu_j) = \text{Poisson}(\sum_j A_{ij})\) as a common default), which depends on the occupancy indicators \(z_{ij}\) and the expected abundances \(\mu_j\). The occupancy indicators and the expected abundances are normalized to obtain the relative expected abundances \(p_i\) representing the probabilities of the multinomial response distribution. The occupancy indicators are latent binary variables following Bernoulli distributions with occupancy probabilities \(\psi_{ij}\). Finally, \(\eta_i\) is a plot-specific semi-parametric regression predictor combining different covariate effects computed from the covariate vectors \(x_i\), implying a hyperprior structure as displayed in Figure 10.

While the model itself encodes valuable information on the distribution of species across sites, one is often interested in an overarching assessment of biodiversity, for example, to study the loss of biodiversity due to human overuse of natural resources. Based on the information in MSCMs, biodiversity can, among other indices, be quantified in terms of species richness,

\[
R_i = \sum_{j=1}^{M} z_{ij},
\]

i.e. the total number of species that are present at a site, or the Shannon index \(H'_i\),

\[
H'_i = -\sum_{j=1}^{M} p_{ij} \log(p_{ij}),
\]

that also takes abundances into account, in addition to the number of species. Both measures can be included in the graph representation of the model as derived quantities (i.e. quantities that are computed from other variables in the model graph as indicated in Figure 10), such that they can be tracked automatically during the MCMC sampling process, enabling statistical inference for the biodiversity indices of interest.

RLiesel, Liesel-Model and Goose facilitate the work with MSCMs in two important regards: (1) the configuration of the semi-parametric regression predictor, and (2) the implementation of a modular MCMC scheme. RLiesel can be used to
Figure 10: The graph of the multi-species count model (MSCM) used in Riebl et al. (2023). The semi-parametric regression predictor $\eta$ combines two parametric covariate effects (the species-specific intercepts and the composition of tree species) and a non-parametric spatial effect for the experimental plots (modeled as a Gaussian process based on the geographical distance of the plots).

configure a dummy model with the semi-parametric regression predictor $\eta_i$ for experimental plot $i$. In Riebl et al. (2023) (and Figure 10), the predictor combines parametric covariate effects (species-specific intercepts and the composition of tree species) with a non-parametric spatial effect. The spatial effect is modeled as a Gaussian process, requiring the corresponding design and penalty matrices as described in Fahrmeir et al. (2013) Section 8.2.3). The matrices are computed by RLiesel, and the graph of the complete predictor (including parametric and non-parametric effects) as returned by RLiesel can be combined with the response structure of the model (manually defined in terms of another Liesel-Model graph) using the lsl.GraphBuilder class in a straightforward way. The usage of the graph builder is illustrated step by step in the following code snippet. For the sake of simplicity, some details on the specification of the predictor and response structure are omitted:

```r
R> gb <- liesel(..., builder = TRUE)  # graph builder with the regression predictor
Py> pdt_vars = {var.name: var for var in r.gb.vars}  # extract predictor variables
Py> model = mscm.make_model(...)  # model with the mscm response structure
Py> _, mscm_vars = model.pop_nodes_and_vars()  # extract response variables
Py> gb = lsl.GraphBuilder().add(  # add root variables to new graph builder
          + mscm_vars["n"], mscm_vars["y"], mscm_vars["richness"], mscm_vars["shannon"],
          + mscm_vars["richness_landscape"], mscm_vars["shannon_landscape"]
)```
After the configuration of the model, Goose can be used to implement the following modular MCMC scheme for efficient Bayesian inference in MSCMs:

1. Initialize the model parameters as $z = 1(y > 0)$, where $1$ is the indicator function, $\mu = [\sum_{i=1}^{N} y_i \times 1(y_i > 0)]/[\sum_{i=1}^{N} 1(y_i > 0)]$, i.e. the mean of the non-zero counts for one species over the sites, $\gamma = 0$, $\beta = 0$ and $\tau^2 = 10.000$.

2. For each iteration of the algorithm:
   - Sample the occupancy states $z$ from the binary full conditional in a Gibbs update.
   - Update the species-specific expected abundances $\log(\mu)$ using NUTS.
   - Update the species-specific occupancy intercepts $\gamma$ using NUTS.
   - Update the site-specific parametric regression coefficients $\beta$ using NUTS.
   - For each site-specific non-parametric covariate effect:
     - Update the non-parametric regression coefficients $\beta$ using NUTS.
     - Sample the smoothing parameter $\tau^2$ from the inverse gamma full conditional in a Gibbs update.

3. Repeat step 2 for a great number of iterations to obtain a representative sample from the posterior distribution of the model parameters.

Riebl et al. (2023) use MSCMs to assess the diversity of communities of various taxa within the flora, fauna and microorganisms in pure and mixed forest stands located in Lower Saxony, Germany, based on data collected in the Research Training Group (RTG) 2300 “Enrichment of European Beech Forests with Conifers”. The data comprises information on tree species and associated organisms at eight field sites and 40 experimental plots located in even-aged, state-owned forests; see also Glatthorn et al. (2023). With the flexible MSCM specification and the inclusion of a spatial effect in particular, Riebl et al. (2023) can show that for all taxa, species richness and Shannon index are consistently estimated to be higher in southern Lower Saxony than in the north. Concerning the composition of tree species on the plots, a higher share of coniferous trees is associated with a higher species richness and Shannon diversity. We refrain from reproducing the complete results here, since our main aim is to highlight the flexible model building procedure with Liesel, and refer the interested reader to Riebl et al. (2023).

7 Discussion

In this article, we introduced the probabilistic programming framework Liesel, which allows the user to express Bayesian models as directed acyclic graphs and to build custom MCMC algorithms. With our software, established MCMC algorithms can be combined in new ways, and the user can implement problem-specific kernels and warmup schemes. Goose, Liesel’s MCMC library, is independent of Liesel’s graph-based model representation and can also be used with other JAX-compatible software, for example PyMC or user-defined log-posterior functions.

Models expressed in Liesel can be modified through a programmer-friendly API. A base model can be generated with RLiesel, a tool to configure semi-parametric regression models, and new ideas can be explored with little effort by modifying the base model. Using state-of-the-art technology like just-in-time compilation, automatic differentiation and cluster computing, which is possible through JAX, Liesel allows for a fast development and testing cycle in Python while maintaining good computational performance.

The development of Liesel will be continued in the coming years. Liesel uses many libraries that are under active development and whose API changes must be reflected in our software. We also plan to integrate new features and other enhancements of these libraries into Liesel. Based on JAX’s experimental module for sparse linear algebra, for example, we will improve the performance of different models using efficient decomposition algorithms for matrices with band structures or more general sparsity patterns.

Liesel will also be extended with more model components and new MCMC kernels. The new building blocks in the modeling library will facilitate the rapid development of new types of models, thus speeding up research. In particular, RLiesel will be extended with the functionality to build non-linear models that overcome the typical additive predictor structure of semi-parametric regression, or models that involve covariates that are themselves assigned a
model specification such as measurement error models or more general structural equation models. These extensions will also serve as a demonstration of the functionality and flexibility that Liesel offers for the development of Bayesian (regression) models.

Liesel’s technology stack facilitates the implementation of gradient-based methods. Having automatic differentiation available allows us to use general optimization algorithms to implement variational inference methods. Stochastic gradient MCMC (SG-MCMC) is a relatively new class of Monte Carlo algorithms that scale well to large datasets. Compared to traditional MCMC, these algorithms reduce the computational cost by using subsamples of the original dataset, while maintaining a high accuracy of the parameter estimates. Tools like Stan, PyMC and NIMBLE that enabled the broad success of Bayesian methods in many application areas are still missing SG-MCMC methods, although the first steps have been made (e.g. in the R package sgmcmc). We plan to implement SG-MCMC kernels and non-traditional tuning methods for SG-MCMC in Liesel in the near future.

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