Abstract

Probabilistic numerical methods (PNMs) solve numerical problems via probabilistic inference. They have been developed for linear algebra, optimization, integration and differential equation simulation. PNM naturally incorporate prior information about a problem and quantify uncertainty due to finite computational resources as well as stochastic input. In this paper, we present ProbNum: a Python library providing state-of-the-art probabilistic numerical solvers. ProbNum enables custom composition of PNM for specific problem classes via a modular design as well as wrappers for off-the-shelf use. Tutorials, documentation, developer guides and benchmarks are available online at www.probnum.org.

Keywords: probabilistic numerics, machine learning, numerical analysis

1. Introduction

Mathematical models are used to explain and predict the behavior of complex systems in all fields of engineering and the physical sciences. In practice, their application relies heavily on numerical approximation. However, a finite computational budget or noise-corrupted inputs induce uncertainty over the quality of any computed approximation. For example, the accurate simulation of a tsunami model may take several hours [1], but operational needs require much faster approximate simulation [2]. Quantification of the induced error is crucial to any practitioner relying on the output of such a model.

Probabilistic numerics (PN) [3–5] quantifies uncertainty in computation by solving problems from numerical analysis with statistical inference. The probabilistic viewpoint provides a principled way to encode structural knowledge about a problem into the algorithm and gives rise to new functionality beyond the scope of non-probabilistic methods [6].
import probnum as pn

belief = pn.linalg.problinsolve(A, b)
belief.x  # <Normal with shape=(n,), dtype=float64>

(a) Solving a linear system with ProbNum.  
(b) Output belief of a PN method for ODEs.

Figure 1: ProbNum’s probabilistic numerical methods compute beliefs over the solution of a numerical problem. The example code in (a) shows how to solve a linear system, while (b) illustrates the uncertainty arising from approximating the solution of a differential equation.

Previously, implementations of PN algorithms have been either standalone, only available for a specific numerical problem, or not available at all. This lack of quality open-source software has inhibited the development of PN methods and their application. To promote the widespread adoption of PN in the scientific community, we introduce ProbNum, an open-source Python library implementing probabilistic numerical methods. Our library

- facilitates rapid experimentation with, and application of, state-of-the-art PN solvers;
- enables custom composition of solvers for specific problems from predefined components;
- simplifies and accelerates development of new methods via a unified API.

Finally, by implementing PN methods in a composable manner, ProbNum is an initial step towards the vision of PN of propagating uncertainty through chains of computations [3].

2. Core Functionality

ProbNum implements probabilistic numerical methods (PNMs) for solving linear systems, differential equations, and integration problems (see Figure 1 for an example). Table 1 lists all currently implemented solvers.

Table 1: Probabilistic numerical methods implemented in ProbNum.

| Area          | Problem      | s.t.       | QoI           | Solver                  | Ref. |
|---------------|--------------|------------|---------------|-------------------------|------|
| Linear Algebra| $Ax = b$     | $A \in \mathbb{R}^{n \times n}$ | $x, A^{-1}$ x | Prob. linear solver     | [7, 8] |
|               |              | $A$ spd    | $x$           | BayesCG                 | [9, 10] |
| ODEs          | $\dot{y}(t) = f(y(t), t)$ | $y(t_0) = y_0$ | $y(t)$         | ODE filter              | [11–14] |
|               |              |            |               | Perturbed solver        | [15] |
| Integration   | $F = \int_{\Omega} f(x) d\mu(x)$ | $\Omega \subseteq \mathbb{R}^n$ | $F$             | Bayesian Monte Carlo     | [16] |
|               |              |            |               | Bayesian quadrature      | [17] |

Linear Algebra  PNMs for linear algebra are focused on solving linear systems. ProbNum implements iterative solvers, which either compute a belief over the (pseudo-)inverse of the matrix [7, 8] or the solution directly [9, 10]. While these perspectives differ conceptually, they are inherently connected [18].
Ordinary Differential Equations  ProbNum’s stable implementation [11] of filtering-based ODE solvers and their variations [13, 14] enables uncertainty calibration, step-size adaptation, dense output, event handling and posterior sampling [11, 12]. ProbNum also provides perturbation-based ODE solvers [15].

Numerical Integration  The Bayesian quadrature implementation in ProbNum comprises both Bayesian Monte Carlo [16] and Bayesian quadrature with fixed user-specified points [e.g. 17]. Currently, integrals can be estimated with respect to the Lebesgue and Gaussian measure.

3. Library Design

ProbNum mainly targets two groups of users. Those, that either want to

(a) use PNM\ts out-of-the-box and explore their potential for their application of interest; or

(b) customize, develop and implement new PNM\ts for specific problems.

This focus on two different user groups is realized with a corresponding design pattern which reflects ProbNum’s core principles: usability, extensibility, and composability.

Out-of-the-Box PN methods  The widespread application of PN to scientific simulation problems necessitates that PN algorithms can be called without knowing the algorithmic details of each solver. Consequently, ProbNum provides user-friendly interface methods for standard PN algorithms. These take the numerical problem to be solved – and optionally known prior information – as input and return a belief over the quantities of interest. Interface methods often shadow the function signatures of their direct NumPy or SciPy equivalent, which makes them immediately usable inside more general simulation pipelines.

Plug-and-Play for Custom Problems  Often, specific problems require tailored numerical methods. Therefore, ProbNum allows the construction of PN methods from individual components. In fact, ProbNum’s interface methods merely call these lower-level, customizable implementations of PN methods. Each PNM is constructed from a set of components, for example, policies, information operators, belief updates, hyperparameter optimization routines, or perturbation strategies. An illustrative example is shown in Figure 2. This compositional structure makes PN methods extensible: a user only needs to implement single components of PN algorithms in order to build a novel, directly usable PN implementation. Finally, since all PN algorithm components act on random variables or random processes, their implementations are naturally composable with each other.
Supporting Subpackages  There are several ProbNum subpackages such as basic data structures given by random variables and processes, time- and memory-efficient matrix-free linear operators, as well as Bayesian filters and smoothers. These fundamentally enable and enhance the functionalities above, but may be of independent interest.

4. Project Development

ProbNum is an open-source, community-driven library hosted publicly on GitHub at

https://github.com/probabilistic-numerics/probnum,

which allows for the tracking of issues, bugs and feature requests, as well as code contributions via pull requests. ProbNum is distributed under the MIT license and available from the Python Packaging Index (PyPI) for all recent Python versions via pip install probnum. All contributors and community members are expected to adhere to the code of conduct.

Documentation  ProbNum’s documentation can be found at www.probnum.org. A range of tutorials showcasing PN methods, their applications, and how to use the library are also available. A detailed development guide promotes contributions to the library.

Dependencies  ProbNum fundamentally only depends on NumPy and SciPy, but includes the option to install additional packages to extend its functionality (such as automatic differentiation frameworks). All dependencies are kept up-to-date automatically via a bot.

Continuous Integration and Tests  The project’s documentation and tutorial notebooks are built for each commit to the main library and every pull request. Automatic linting preserves a high level of code quality and style. ProbNum’s extensive unit tests leverage pytest, and the test coverage is updated automatically whenever new changes occur. Finally, regular, automated benchmarks detect potential performance regressions.

5. Related Concepts and Libraries

ProbNum’s solvers may be used as a drop-in replacement for classic numerical solvers (such as those offered by SciPy [19]). While ProbNum does not implement any classical solvers, some PNM fundamentally recover these without incurring significant computational overhead to compute uncertainty. The field of PN can be seen as a subset of the broad research area of uncertainty quantification, which “is the end-to-end study of the reliability of scientific inferences” [20]. However, existing software libraries for uncertainty quantification [21, 22] do not implement any PN algorithms. ProbNum provides (approximate) inference algorithms for numerical tasks by casting them as statistical inference problems. It is therefore not a probabilistic programming framework [23–25], which automate general probabilistic inference. Nevertheless, ProbNum may serve as a low-level building block inside probabilistic programs, e.g. to add computational uncertainty. Finally, there are special-purpose packages implementing some PNM, e.g. for Bayesian optimization [26–28] and quadrature [27, 29].

6. Conclusion

We hope that ProbNum will increasingly be the home for algorithmic research in probabilistic numerics and grow to further be a practical tool for applied users who want to leverage
the functionality of probabilistic numerical methods. For developers and researchers alike, ProbNum offers the scaffold for efficient implementation of novel methods, as well as the repository of existing methods for comparisons. For applied users, ProbNum provides clean interfaces and a “one-stop-shop” for emerging new functionality.

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