

Probabilistic Numerics for Uncertainty Quantification

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Introduction

The landscape of numerical analysis is undergoing a fundamental transformation, with increasing emphasis on quantifying uncertainty. A pivotal area in this evolution is Probabilistic Numerical Linear Algebra (PNLA), which reimagines traditional tasks like solving linear systems as sophisticated inference problems. This approach, as highlighted in a comprehensive overview, aims to move beyond mere single point estimates by rigorously quantifying the inherent uncertainty within numerical computations. The outcome is the provision of richer, more reliable insights into numerical solutions across a wide array of applications, empowering practitioners with a deeper understanding of computational reliability [1].

Similarly, the integration of uncertainty quantification into deep learning models represents a significant advancement, especially when applied to numerical simulations. A key review in this domain surveys the array of uncertainty-aware deep learning methods, underscoring their capacity to deliver more dependable predictions for complex engineering and scientific problems. This shift moves beyond deterministic outputs, offering crucial insights into the confidence levels of simulation results, which is vital for real-world decision-making [2].

Neural networks are also adapting to this probabilistic paradigm, demonstrating efficacy in generating forecasts for numerical time series, particularly within fields such as hydrology. This work reviews how these networks can provide not just single point estimates but full predictive distributions, effectively quantifying the uncertainty in future numerical outcomes. This capability allows for more robust decision-making in sectors heavily reliant on sequential numerical data, enhancing forecast utility [3].

For complex 'black-box' numerical models, especially those prevalent in engineering, the application of various Bayesian methods for uncertainty quantification proves invaluable. A comparative study evaluates techniques like Gaussian processes and Bayesian neural networks, emphasizing their crucial role in providing reliable uncertainty estimates. These estimates are essential for informed decision-making, particularly when dealing with models whose internal workings are not fully transparent [4].

The inherent randomness of systems modeled by stochastic differential equations (SDEs) presents a unique challenge, which probabilistic numerical methods address directly. These advanced algorithms are designed to not only approximate SDE solutions but also precisely quantify the uncertainty stemming from both numerical approximations and the stochastic nature of the equations themselves. This provides robust insights into inherently uncertain numerical dynamics, fostering a more complete understanding of system behavior [5].

The quantification of uncertainty in deep learning models is gaining significant

traction, particularly for scientific and engineering applications where reliability is paramount. A comprehensive review examines modern approaches, highlighting how probabilistic deep learning offers vital insights into the reliability of numerical predictions and simulations. This method moves beyond deterministic model outputs to provide a clearer picture of their confidence and limitations, aiding in critical application areas [6].

Probabilistic Graphical Models (PGMs) offer another structured framework instrumental in machine learning tasks that involve numerical data and require robust uncertainty quantification. A review of PGMs demonstrates their effectiveness in representing complex dependencies and propagating uncertainty throughout a model. This leads to more robust and interpretable numerical predictions across diverse domains by explicitly modeling stochastic relationships inherent in the data [7].

Extending probabilistic numerical methods to the challenging domain of partial differential equations (PDEs) marks another significant advance. This research treats PDE solving as an inference problem, yielding solutions accompanied by a quantification of approximation uncertainty. This approach provides a principled way to incorporate prior knowledge and rigorously quantify numerical errors in complex scientific computations, enhancing the trustworthiness of results [8].

Bayesian Deep Learning (BDL) provides a principled and robust framework for quantifying uncertainty within deep neural networks. A thorough review delves into various BDL techniques and their applications, especially in regression tasks involving numerical predictions. The emphasis is on BDL's crucial ability to output confidence intervals alongside point estimates, a feature critical for the development of truly trustworthy Artificial Intelligence systems [9].

Finally, in the realm of control theory, Probabilistic Model Predictive Control (PMPC) offers a sophisticated strategy for managing dynamic systems with inherent uncertainties. This control methodology explicitly accounts for system dynamics and disturbance uncertainties, utilizing probabilistic models to optimize numerical control actions. PMPC ensures constraint satisfaction with a high probability, thereby establishing a robust framework for managing dynamic numerical systems under unpredictable conditions [10].

Description

The landscape of modern numerical analysis is increasingly focusing on the critical aspect of uncertainty. Traditional deterministic approaches often fall short in providing a complete picture, prompting a shift towards methods that quantify inherent ambiguities. For instance, Probabilistic Numerical Linear Algebra (PNLA) reframes fundamental numerical tasks, such as solving linear systems, as inference problems [1]. This allows for moving beyond single point estimates by actively

quantifying the uncertainty present in numerical computations, offering richer and more reliable insights across diverse applications. Expanding on this, probabilistic numerical methods have also been specifically developed for inherently random systems, like stochastic differential equations (SDEs) [5]. These algorithms not only approximate solutions but precisely quantify uncertainty stemming from both numerical approximations and the stochastic nature of the equations, providing robust insights. The principles extend to highly complex scientific computations involving partial differential equations (PDEs), where treating PDE solving as an inference problem yields solutions with associated quantification of approximation uncertainty. This principled approach incorporates prior knowledge and rigorously quantifies numerical errors [8].

Uncertainty quantification is becoming paramount in the realm of Artificial Intelligence, especially within deep learning for numerical simulations. Research highlights how integrating uncertainty quantification into deep learning models leads to more reliable predictions for complex engineering and scientific problems, providing crucial insights into the confidence of simulation results rather than just deterministic outputs [2]. Further reinforcing this, a comprehensive review examines modern approaches for quantifying uncertainty in deep learning models specifically tailored for scientific and engineering applications [6]. Probabilistic deep learning offers vital insights into the reliability of numerical predictions and simulations, moving beyond simple outputs to present a clearer picture of confidence and limitations. Bayesian Deep Learning (BDL) offers a principled framework for quantifying uncertainty in deep neural networks, with various techniques explored, especially for regression tasks involving numerical predictions [9]. The emphasis here is on outputting confidence intervals alongside point estimates, which is crucial for building trustworthy Artificial Intelligence systems.

Beyond general deep learning applications, probabilistic forecasting with neural networks addresses the challenges of sequential numerical data. This is particularly relevant in areas like hydrology, where neural networks generate probabilistic forecasts for time series data. These techniques provide not just single point estimates but full predictive distributions, effectively quantifying the uncertainty in future numerical outcomes and supporting more robust decision-making [3].

For complex 'black-box' numerical models prevalent in engineering, Bayesian methods offer a powerful comparative framework for quantifying uncertainty. A study evaluates techniques such as Gaussian processes and Bayesian neural networks, emphasizing their essential role in delivering reliable uncertainty estimates [4]. These estimates are fundamental for informed decision-making based on the often opaque outputs of these models. Similarly, Probabilistic Graphical Models (PGMs) present a structured framework for machine learning tasks dealing with numerical data and uncertainty. PGMs are effective at representing complex dependencies and propagating uncertainty, leading to more robust and interpretable numerical predictions across various domains by explicitly modeling stochastic relationships [7].

In control systems, accounting for uncertainty is critical for effective operation. Probabilistic Model Predictive Control (PMPC) is a control strategy that explicitly considers system dynamics and disturbance uncertainties. By leveraging probabilistic models, PMPC optimizes numerical control actions while ensuring constraint satisfaction with a high probability [10]. This offers a robust and reliable framework for managing dynamic numerical systems even in the presence of inherent uncertainties. Collectively, these advancements illustrate a broad and impactful movement across scientific and engineering disciplines towards robustly handling and quantifying uncertainty in numerical computations.

Conclusion

This collection of papers highlights a significant shift in numerical computations, moving beyond deterministic point estimates to embrace probabilistic methods and uncertainty quantification. A core theme is framing numerical tasks, like solving linear systems and differential equations, as inference problems to quantify inherent computational uncertainty, offering richer and more reliable insights. This probabilistic approach extends to deep learning, where uncertainty-aware models provide reliable predictions for complex scientific and engineering problems. Neural networks are shown to generate probabilistic forecasts for numerical time series, especially in hydrology, allowing for robust decision-making by providing full predictive distributions.

Various Bayesian methods, including Gaussian processes and Bayesian neural networks, are explored for quantifying uncertainty in black-box numerical models. Probabilistic Numerical Linear Algebra (PNLA) is a key area, alongside probabilistic numerical methods tailored for stochastic and partial differential equations, which inherently model randomness or complex physical phenomena. These methods quantify uncertainty arising from both numerical approximations and the underlying stochastic nature of the systems.

Deep learning specifically benefits from this paradigm, with methods like Bayesian Deep Learning providing confidence intervals for numerical predictions, critical for trustworthy Artificial Intelligence. Probabilistic Graphical Models offer a structured framework for propagating uncertainty in machine learning tasks. Finally, in control theory, Probabilistic Model Predictive Control (PMPC) leverages probabilistic models to optimize actions under uncertainties, ensuring high-probability constraint satisfaction in dynamic numerical systems. Overall, these works underscore the importance of understanding and quantifying uncertainty for more informed, reliable, and robust numerical outcomes across diverse scientific and engineering applications.

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Conflict of Interest

None.

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