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LDRD Project Summary: Incorporating physical constraints into Gaussian process surrogate models

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ABSTRACT

This report summarizes work done under the Laboratory Directed Research and Development (LDRD) project titled "Incorporating physical constraints into Gaussian process surrogate models." In this project, we explored a variety of strategies for constraint implementations. We considered bound constraints, monotonicity and related convexity constraints, Gaussian processes which are constrained to satisfy linear operator constraints which represent physical laws expressed as partial differential equations, and intrinsic boundary condition constraints. We wrote three papers and are currently finishing two others. We developed initial software implementations for some approaches. This report summarizes the work done under this LDRD.

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CONTENTS

1. INTRODUCTION

This report summarizes work done under a two-year Laboratory Directed Research and Development (LDRD) project titled "Incorporating physical constraints into Gaussian process surrogate models." In this project, we explored a variety of strategies for constraint implementations. We considered bound constraints, monotonicity and related convexity constraints, Gaussian processes which are constrained to satisfy linear operator constraints which represent physical laws expressed as partial differential equations, and intrinsic boundary condition constraints. We wrote three papers and currently are finishing two others. We developed initial software implementations for some approaches. This report summarizes the work done under this LDRD.

The various constraint implementation strategies are extensively described in our papers. We do not reproduce the entire papers here but instead give an annotated bibliography. This report is divided into two subsequent chapters: Chapter 2 lists the publications and Chapter 3 describes our software. The final Chapter presents a summary.

2. PAPERS

The papers produced as part of this LDRD research program are listed below with annotations.

2.1. Constrained Gaussian Processes

The literature on constrained Gaussian processes (GPs) is extensive and growing rapidly. There are many different approaches: some methods relax the global constraints to constraints at a finite set of "virtual" points; others transform the output of the GP to guarantee the predictions satisfy constraints, or construct a sample space of predictions in which every realization satisfies the constraints; some methods involve a modification or transformation of the likelihood function or covariance kernel while others do not.

A major contribution of this LDRD is a 40 page survey paper which describes the main areas of constrained GP research and provides readers an overview of the approaches. We completed this survey paper in June, 2020 and submitted it to the *Journal of Machine Learning for Modeling and Computing*. It was reviewed internally by Khachik Sargsyan who provided detailed comments which helped tighten and improve the manuscript.

The GP survey paper discusses bound contraints, monotonicity and convexity constraints, "physics-informed" approaches where the GP is constained to satisfy linear operator constraints which represent physical laws expressed as partial differential equations (PDEs), and boundary condition constraints. A main goal of the paper is to aid readers in selecting methods appropriate for their applications. In addition to presenting a survey of existing approaches, this paper identified common themes in constraint implementation approaches and suggests a categorization of strategies for enforcing constraints. The addition of constraints typically adds computational cost and complexity to the formulation and training process, so strategies to address these computational challenges such as low rank methods were provided.

The paper is titled: "A Survey of Constrained Gaussian Process Regression: Approaches and Implementation Challenges", with authors Laura Swiler, Mamikon Gulian, Ari Frankel, Cosmin Safta, and John Jakeman. [12]. It is available on arXiv (SAND2020-6086J):

- https://arxiv.org/abs/2006.09319

2.2. Tensor Basis Gaussian Processes

Ari Frankel led the development of a Gaussian process regression model for hyperelastic material behavior. This work is described in the paper titled "Tensor Basis Gaussian Process Models of Hyperelastic Materials" by Ari Frankel, Reese Jones, and Laura Swiler. [1]. This paper was accepted by the *Journal of Machine Learning for Modeling and Computing* and will be published in the inaugural issue. It is available at the following sites:

- doi:10.1615/.2020033325
- https://arxiv.org/abs/1912.10872

In this paper, we developed an approach to model the components of the Cauchy stress tensor as a function of the components of the Finger stretch tensor using a Gaussian process. Then, we presented an improvement on this approach that embeds the rotational invariance of the stress-stretch constitutive relation in the GP representation. Finally, we considered an approach that recovers the strain-energy density function and derives the stress tensor from this potential. The paper demonstrated the efficacy of the GP regression on a synthetic dataset corresponding to the Mooney-Rivlin hyperelastic constitutive relation. The GP regression approach that embeds rotational invariance attained orders of magnitude improved accuracy compared to a standard GP regression approach.

The "tensor basis" GP developed for hyperelastic materials is a good example of physics-informed machine learning, in which knowledge of the material laws and physics at hand yields a substantial improvement over a naive implementation of popular machine learning models. This particular approach is of immediate use to researchers in computational material science who wish to develop robust and accurate models for the macroscale behavior of complex materials. In addition, the embedding of the physics in a GP framework enables the calculation of uncertainty in predictions, which is an important part of building confidence in a machine learning model.

2.3. Optimal Sampling

The question of how to select samples to best inform a Gaussian process has been a long-standing research question. Typically, this is done by choosing points (often from a candidate set) that minimize the average predictive variance of the GP over the domain. [8, 9, 10] or which minimize the predictive variance at a particular location of interest [3].

John Jakeman led an investigation of optimal experimental design for Gaussian process models. This work is documented in the article titled "Weighted greedy-optimal design of computer experiments for kernel-based and Gaussian process model emulation and calibration" by H. Harbrecht, J.D. Jakeman, and P. Zaspel [5]. The paper has been submitted to *Communications in Computational Physics* and the authors are addressing the reviews.

This paper focuses on the approximation of high dimensional functions by kernel-based methods, with the goal of constructing approximations that are accurate with respect to to a probability

density function of random variables. The paper presents a nested greedy sampling strategy based upon a weighted modification of the pivoted Cholesky factorization which successively generates samples with the goal of minimizing error in regions of high probability. The approximation error is defined with respect to a weighted L^p-norm.

A major contribution of this paper is to allow the specification of a probability density function (PDF) over the input random variables which is then incorporated in the approximation and optimal experimental design. Typically, the optimal designs assume independent uniform inputs and are not tailored to the input PDFs. Numerical experiments validate that this new importance sampling strategy is superior to other sampling approaches, especially when used with non-product probability density functions. The paper demonstrates how to use the proposed algorithm to efficiently generating surrogates for inferring unknown model parameters from data.

2.4. Boundary constraints

As mentioned in the survey article [12], when a GP is expected to satisfy a linear operator constraint, it is possible to develop covariance operators that satisfy those constraints explicitly and even perform co-kriging. [7] [6] developed covariance operators that embed linear differential operators between function observations to enforce satisfaction of ordinary and partial differential equations.

One special case is that of a differential equation subject to boundary condition constraints: a boundary value problem. This situation can arise in a number of physical processes of interest, including prominent examples of the Poisson equation for electrostatics, advection-diffusion of a scalar (such as temperature or species concentration), wave propagation (as in spectral analysis of acoustics), or elastic deformation of materials. In these cases there is a known linear differential equation with additional information associated with the behavior of the function of interest at the domain. Enforcing the boundary conditions explicitly would require adding fictitious data points to the training data and increase the cost of inference. Requiring the data points to satisfy the differential operator would complicate the formulation and estimation of the Gaussian process. If the observed data were noisy, then there would also be no guarantee that the boundary conditions would be satisfied exactly.

In a recent work, [11] demonstrated that by projecting the observed data to an orthonormal eigenbasis that goes to zero at the boundaries, the resulting GP will also satisfy those boundary conditions since any linear combination of GPs is also a GP. The eigenbasis derived in that work was determined by approximating the spectrum associated with the Laplacian operator. In summary, [11] derived a GP that satisfies the Poisson equation subject to Dirichlet boundary conditions. The reduction of the regression to a finite eigenbasis also represented a compression of the dataset and led to a large speed-up due a much smaller matrix inversion.

Ari Frankel and Mamikon Gulian have combined the linear operator GP approach for PDEs with the boundary condition approach. Their paper (in draft, to be submitted by Sept. 30) shows that this spectral expansion can be used to solve other boundary value problems with different

governing equations and boundary conditions with similar computational speed-up. The paper provides the derivation of the covariance matrix for a "co-kriging" GP for a PDE operator based on the spectral expansion formulation. The methodology is demonstrated on two example problems: a 1-D Poisson equation with noise in both the solution observations and the forcing function, and a 2-D Helmholtz problem.

2.5. Stochastic parameter treatment within GP-PDE approaches

The fifth paper involves explicitly including stochastic parameters in the formulation of Gaussian processes for PDEs. That is, the paper starts with a formulation where a Gaussian processes may be constrained to satisfy linear operator constraints of the form

$$\mathscr{L}u = f \tag{2.5.1}$$

given data on f and u. When $\mathscr{L}$ is a linear partial differential operator, equation 2.5.1 can be used to constrain GP predictions to satisfy known physical laws expressed as linear partial differential equations. This formulation requires forming the joint Gaussian process $[u; f]$ where observations on both the forcing function (or source term) and on the solution at various points in the domain are used to inform the overall GP. [7] [6] The covariance matrix of the resulting GP is a four block matrix assembled from the covariance matrix of the GP for the solution u, the covariance of the GP for the forcing function, and the cross terms.

This fifth paper extends a GP formulation based on 2.5.1 to allow for stochastic parameters within the PDE such as diffusivity coefficients or material properties. For example, the goal is to develop a GP framework to model the following simple PDE with a stochastic parameter ξ:

$$\xi \frac{\partial^2 u}{\partial x^2} = -1 \tag{2.5.2}$$

The objective is to treat inherent randomness in parameters such as a diffusion coefficient within the GP formulation. This requires another co-kriging layer to be added to the Gaussian process and formulating the GP over both $[x, \xi]$. There are some issues with ensuring that the GP properly incorporates the uncertainty in the stochastic parameter when calculating the mean and variance predictions from the joint GP. This is the topic of the last paper.

3. SOFTWARE

In this section, we summarize the software developed under this LDRD. We have created a repository on Sandia's gitlab site:

- `https://gitlab.sandia.gov/lpswile/ConstrainedGP`

Contact Laura Swiler for access to this repository. There are example scripts in the directory `code_sept20`. We have annotated these scripts but emphasize this is prototype code, not production code. All the code is written in Python. The scripts that we currently have include:

- `spline_boundGP.py` This implements bound constraints with a spline approach for a 1-D problem.
- `spline_boundGP_multi.py` This implements bound constraints with a spline approach for multiple dimensions.
- `sample_boundDer.py` This implements monotonicity constraints with a four-block covariance matrix using an MCMC approach.
- `pde_constraints_example.py` This implements a simple example of the linear operator four block covariance for a GP which satisfies a PDE.
- `lagp` There is an entire directory for lagp. This directory has a revised version of the Local Approximation GP developed by Gramacy et al. [2, 3] This code is written in Python, not R, and is a new implementation to allow users who have large data sets to construct and evaluate GPs efficiently.

4. SUMMARY

In this Laboratory Directed Research and Development (LDRD) project, we investigated a wide variety of approaches for incorporating physical constraints into Gaussian process models. We explored bound constraints, monotonicity, and convexity constraints. We also explored Gaussian processes which are constrained to satisfy linear operator constraints which represent physical laws expressed as partial differential equations, and intrinsic boundary condition constraints. We examined approaches which employ various transformations on the output to guarantee the predictions satisfy the constraints, approaches which involve truncated multivariate Gaussians, and a formulation involving splines, where a multivariate Gaussian prior is placed on a class of spline functions and the constraints are incorporated through constraints on the coefficients of the spline functions. We examined the idea of relaxing the global constraints to constraints at a finite set of "virtual" points. We examined methods that involve a modication or transformation of the likelihood function or covariance kernel. Because the addition of constraints increases the computational cost of building and training the Gaussian process, we investigated approaches to improve computational efficiency of GPs.

We developed two special formulations for particular problems: a tensor basis GP to handle the types of rotational invariance constraints found in materials modeling problems and a GP for PDEs which incorporates boundary conditions through a spectral expansion. We demonstrated the tensor basis GP on a hyperelastic materials model and the spectral expansion GP on boundary value problems for a Poisson equation and for a Helmholtz equation.

Finally, this work has led to more communication and awareness of constrained Gaussian processes across Sandia. Mamikon Gulian presented the work at the Machine Learning and Deep Learning 2020 Workshop [4]. Laura Swiler plans to present it at SIAM CSE 2021. Further, our team members are involved in subsequent projects which will leverage these contributions.

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