Gaussian Processes for simulating complex quantum systems

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Abstract

Supervised machine learning algorithms have proven to be robust algorithms capable of accurately predicting physical properties, e.g., the energy of a system, identifying different systems, to mention a few. In this talk, we present the use of Gaussian Process (GP) and Bayesian optimization to solve problems that are considered unsolvable in the field of quantum dynamics and increase the accuracy of computational quantum chemistry methods and density functional models. Also, we illustrate that GP, with a combination of simple kernels, can extrapolate physical properties beyond the training data regime to discover quantum systems with novel physical properties and new phases of matter.

1 Introduction

In recent years, machine learning (ML) algorithms have emerged as state-of-the-art tools to study quantum systems. For example, the classification of quantum states, the manipulation/control of quantum systems with external fields, the prediction of physical properties, to mention a few of the most common applications. So far, all the applications of ML to study physical systems are the interpolation of physical properties within the volume space of the training data. This research-line is extremely useful since could lead to discovering molecules with desired properties or a more accurate simulation of quantum systems with fewer data. However; what if we could push the boundaries of physics by using ML to answer "what is out there?" or tackle problems that are considered unsolvable, i.e., the inverse scattering problem for quantum reaction dynamics. In this talk, we illustrate by using Gaussian Processes (GPs) one can discover quantum systems with novel properties and solve the inverse scattering problem for quantum reaction dynamics.

GP is a probabilistic regression model which assumes that any collection of function values, $f(\mathbf{x_i})$, has a joint Gaussian distribution,

$$f(\mathbf{x}) \sim \mathcal{G}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')). \tag{1}$$

The mean and standard deviation of the GP predictive distribution is the conditional distribution of a test point, $\mathbf{x}_*$, given the training data, $\mathcal{D} = [X, \mathbf{y}]$,

$$\mu(\mathbf{x}_*) = K(\mathbf{x}_*, X)^\top K(X, X)^{-1}\mathbf{y}, \quad \sigma(\mathbf{x}_*) = K(\mathbf{x}_*, \mathbf{x}_*) - K(\mathbf{x}_*, X)^\top K(X, X)^{-1}K(\mathbf{x}_*, X), \tag{2}$$

where $K(\cdot, \cdot)$ is the covariance matrix and its matrix elements for all pairs of training and/or test points are given by the kernel function $k(\mathbf{x}_i, \mathbf{x}_j)$. In GP, the kernel function describes the similarity between points.

2 Main results

To extrapolate with GPs, the kernel function must learn the similarities of the data beyond the training data-space. We iteratively increase the complexity of the kernel function by combining simple kernel

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functions and selecting the kernel combination with the highest Bayesian Information Criteria (BIC) [1]. The first system we studied is a chain of electrons described by the Heisenberg model. The Heisenberg model is used to study the transition between the ferromagnetic phase (electrons are aligned) and the paramagnetic phase (electrons are aligned randomly). The transition between both phases is characterized by the change in the energy of the system as a function of the temperature, T. If we could simulate a physical system beyond the training regime, for example, $T > T_C$ for the Heisenberg model (colored area in Figure 1), we could discover the paramagnetic phase [2,3]. Figure 1 (a) illustrates that GPs can predict the transition between the ferromagnetic and paramagnetic phases by extrapolating the energy of the system at different temperatures. We also predict the entire phase diagram for a polaron system, an electron moving through atoms vibrating, with only the properties from a single-phase using GPs with kernel combination, Figure 1 (b) [2,3].

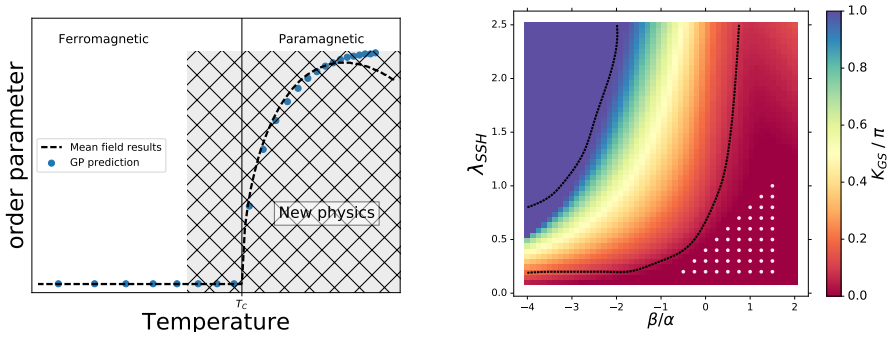

Figure 1: Predicted physical properties with GP with combination of kernels beyond the training data regime. (a) Order parameter for a chain of electrons as a function of the temperature. (b) Phase diagram of an electron moving through atoms vibrating, white dots reprensent the training data.

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One of the most common applications of GP is in the Bayesian optimization (BO) algorithm. We illustrate that BO can be used to optimize physical models, i.e., density functional (DF) models, widely used in material science. While DF theory is in principle an exact theory, most of the DF models contain empirical parameters which are commonly tuned to reproduce target physical properties, e.g., energy barriers and atomization energies, to mention few. We use BO to efficiently optimize the free parameters of DF models and select the density functional form that best describes the target physical properties [5]. In this talk, we will also illustrate that by combining GP to learn the solution of the electronic Schrödinger equation and BO one can solve the inverse scattering problem for quantum reaction dynamics, which has never been done [4]. We refer to the inverse scattering problem for quantum reaction dynamics as the possibility to predict the solutions of the electronic Schrödinger equation only using the output of the quantum dynamic calculations.

References

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