Max Integral Operator: A Probabilistic Numerical Approach

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Abstract

The Max Integral Operator is an expression of the form $\max_a \int f(a, s)ds$. Such expressions arise in many computational domains including machine learning, statistical inference, and optimization. Intuitively, maximizing over some variables and integrating out others is a useful operation to perform. In most practical settings, however, these integrals are non analytic and exact evaluation is computationally intractable. Much research has explored Bayesian quadrature, a method of numerical integration that provides estimates of uncertainty on an integral's value. In this work, we present a framework for efficiently evaluating the Max Integral Operation by incorporating this uncertainty information into the optimization procedure. We jointly optimize over the outer optimization variable and the selection of queries in estimating the inner integrals. As a result, our framework exhibits increased sample efficiency, allowing us to get accurate value estimates with fewer function evaluation queries. We investigate the effectiveness of our framework, the various applications, and the theoretical guarantees.

Introduction

Function maximization and numerical integration have received much focus from the optimization and applied mathematics communities, respectively. However, in performing these operations simultaneously there is added complexity and simply applying existing optimization and integration algorithms is computationally infeasible. We will take a deeper look at evaluation of the Max Integral Operator and,in particular, show how taking a probabilistic numerical perspective...

A reasonable method for evaluating an integral might be sampling-based Monte Carlo techniques, just as we would use to estimate an expectation in a discrete setting. However, in "Monte Carlo is Fundamentally Unsound", O'Hagan identified a series of inconsistencies with such methods. He then presents Bayes-Hermite quadrature, which treats the numerical integration problem as a statistical inference problem. By doing so, you may use the estimate of uncertainty of an integral's value as a convergence criterion and actively sample function evaluations that reduce uncertainty.

Bayesian quadrature involves fitting a Gaussian Process to the integrand and integrating the mean function of the GP. Under certain conditions of the kernel function and prior, this integral will have a closed form. Bayesian Monte Carlo and Gaussian Process Dynamic Programming state these closed forms and explore the applications of quadrature in computing marginal likelihood and RL action policies, respectively.

Other work on Bayesian quadrature has focused on cases where the integrand is non-negative (Osborne 2017) (Gunter 2016) and shown how using certain warping functions can induce cheap active learning schemes. Using these sampling procedures they show fast convergence compared to other numerical integration methods.

In both these works, however, they assume either a discrete optimization space or a relatively small continuous state space. We observe that if both these assumptions are violated, their methods of optimization over the integral are infeasible. In most use cases of the Max Integral Operator, we are interested in continuous high-dimensional spaces and therefore, it seems reasonable that our methods of evaluation should extend to these domains. For these reasons, we believe that methods for evaluating the Max Integral Operator merit further investigation.

The remainder of this paper is structured as follows: (1) We present the framework for optimization and three variants of implementation. Then, we do a thorough analysis of these variants on test functions. (2) We apply the optimization procedure to the Reinforcement Learning setting, specifically to Bellman Updates, and developed two extensions to existing algorithms for solving MDPs. The first is classical value iteration and the next is RTDP. We show how our Max Integral Optimization allows you to efficiently learn robust policies in stochastic continuous state-action domains. (3) We use our framework in computing maximum a posteriori estimates for a series of common Posterior Estimation problems (4) We investigate the theoretical guarantees we can make regarding optimality and convergence in Max Integral settings.

Preliminaries

In this section, we review Gaussian Process Regression, Bayesian Optimization and Quadrature, and Multi-armed Bandits. For further reference we recommend...

Gaussian Process Regression

A Gaussian process is a method of representing a distribution over functions. It can initially be defined by the prior mean function and a covariance function, which captures our smoothness assumptions on the functions we are modeling (see Rasmussen and Williams 2005). These priors can be engineered through existing domain knowledge, but in many cases the prior mean is assumed to be 0.

As we make additional function queries, we will condition on our set of observations using a Bayesian update method. By conditioning on our observation, we can derive the posterior distribution. This GP posterior is not a closed form function e.g. f(x) = sin(x), instead, at each input point the posterior is a Gaussian Distribution as follows:

$$\begin{aligned} & y|\mathbf{y}_* \sim \mathcal{N}(\mu, \sigma) \\ & \mu = m(X_*) + K(X_*, X)K_y^{-1}(y - m(X)) \\ & \sigma = m(X_*) + K(X_*, X)K_y^{-1}(y - m(X)) \end{aligned} \tag{1}$$

The core of a Gaussian process is the multivariate Gaussian. The model's assumption is that observed samples from the function are samples from a multivariate Gaussian. Then, for unobserved inputs we use the mean and covariance functions to infer a distribution. In a way, a Gaussian process is an extension of the multivariate Gaussian to the infinite-dimensional domain.

GPs are powerful tool in modeling unknown functions because the posterior distribution captures our uncertainty about the function's value. In the next subsection, we discuss how this can be leveraged in optimization and estimation procedures.

Bayesian Optimization

Bayesian optimization is a function optimization procedure that relies on priors and sequential updates of a posterior. The posterior will guide the queries made to the function, through an acquisition function. Bayesian Optimization is a black box optimizer beceause it relies on only the function inputs and outputs to create its' representation. Bayesian Optimization does not relate on derivatives, either.

In continuous domains, Gaussian processes are used as the posterior model because they allow us to easily condition on our previous observations and generalize to the infinite domain, according to our specificied prior mean and kernel function.

The key component of Bayesian Optimization is the acquisition function that defines how we select function evaluations. While there are many different acqusition functions used in practice, they all essentially balance what is commonly referred to as "exploration vs exploitation". Exploration is the tendency to query areas in the domain where there is uncertainty about value, while Exploitation is querying areas that have highest value.

The commonly used acquisition function is Upper Confidence Bound, because of its simplicity as well as it theoretical guarantees. The UCB function is as follow:

$$\begin{aligned} & UCB(x) = \mu + \beta\sigma \\ & argmax_x UCB(x) \end{aligned} \tag{2}$$

In UCB, as β tends to 0, the acquisition policy becomes exploitation and as it increases, the acquistion policy increasingly weights uncertainty.

Bayesian Quadrature

Just as Bayesian Optimzation takes a sequential query approach to optimizing a function, Bayesian quadrature takes a similar approach in estimating the integral of a black box function. These methods were first proposed as Bayes-Hermite quadrature (O'Hagan) and then reformulated in the Bayes Monte Carlo (Rasmussen). Most work has focused on integrals of the form:

$$\int f(x)p(x)dx$$

In Bayesian Quadrature, the acquisition function is chosen to prefer queries that can reduce the uncertainty about the value of the integral. This acquisition would be:

$$argminV(f|D) \tag{3}$$

An alternative acquistion function would be Uncertainty sampling

$$argminV(f|D) \tag{4}$$

Under certain conditions, the integral will have a closed form. One such case, is if the integrand f is modeled by a GP with an RBF kernel and the prior p is a Gaussian. For completeness we present the derivation of this closed form below:

$$\begin{aligned} & E_{f|\mathcal{D}}[f_p] = z^T K^{-1} f \\ & z = |A^{-1}B + I|^{-1/2}\, exp[-0.5(a-b)^T(A+B)^{-1}(a-b)] \end{aligned}$$

Multi Armed Bandits

In many real-world scenarios, we seek to maximize some reward or utility through our series of actions. These actions can, in addition to providing reward, give us more information about our problem scenario and inform following decision making. The multi armed bandits problem, originally presented by Robins, is a mathematical formalization of such a scenario. The problem has number of "arms" which when pulled give certain reward and over a series of "pulls" the player must maximize the reward gained.

...

Bayesian optimization is a variant of the multi armed bandits problem with an additional assumption on the dependence of arms. Though we have already presented an overview of Bayesian optimization, ...

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Robinson, A. L. 1980a. New Ways to Make Microcircuits Smaller. *Science* 208: 1019–1026.

Magazine Article
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Additional Resources

LaTeX is a difficult program to master. If you’ve used that software, and this document didn’t help or some items were not explained clearly, we recommend you read Michael Shell’s excellent document (testflow doc.txt V1.0a 2002/08/13) about obtaining correct PS/PDF output on LaTeX systems. (It was written for another purpose, but it has general application as well). It is available at www.ctan.org in the tex-archive.

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