Max Integral Operator: A Probabilistic Numeric Approach

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Max Integral Operator

In this work, we will explore techniques to evaluate expressions of the following form:

$$\max_{a} \int f(a, s)p(s)\ \mathrm{d}s$$

We find the Max Integral expression in a variety of computation problems.

- Optimization
- Reinforcement Learning
- Statistical Inference

Intuitively, maximizing over some parameters while integrating out others is a useful operation.

Method

Our method uses techniques of both Bayesian Optimization and Bayesian Quadrature to simultaneously estimate the inner integral and maximize over it.

We jointly optimize over the outer optimization variable and the selection of queries to estimate the inner integrals. As a result, our framework exhibits increased sample efficiency, allowing us to get accurate value estimates with fewer function evaluation queries.

Preliminaries

- Gaussian Process Regression
- Bayesian Optimization
- Bayesian Quadrature

Gaussian Process Regression

Quadrature techniques, first presented as Bayes-Hermite Quadrature [1], are used to actively sample function evaluations in order to reduce uncertainty about an integral's value. This is usually done by maintaining a Gaussian Process over the integrand and then integrating the GP.

Most work in BQ has focused on integrals of the form:

$$\int f(x)p(x)\ \mathrm{d}x$$

In our framework, we will use this distribution over the integral's value as a convergence criterion, which can guide the optimization (maximization) procedure.

Monte Carlo

But why not use Monte Carlo to sample from p and estimate the integral?

Of course, with sufficiently many samples this will work. However, with a limited number of samples, by randomly sampling we might not be accurately represnting f. Quadrature selects this samples in order reduce our uncertainty about the integral's value.

Basic Max Integral Optimization

We will first demonstrate our method on simple 2 dimensional functions:

$$f(s, a) = \mathcal{N}(s|3.0, 1.0) * \mathcal{N}(a|0.0, 1.0)$$
$$p(s) = \mathcal{N}(s|0.0, 10.0)$$

Now we will estimate:

$$\max_a \int f(a, s)p(s)\ \mathrm{d}s$$

Basic Max Integral Optimization

We take initial samples of $f(a, s)$ for each of actions. This gives us a rough estimate of the integral and serves as an initialization for the optimization.

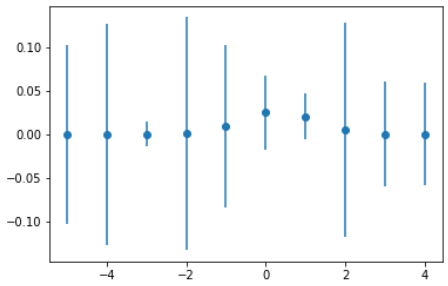
Then we will proceed in a multi armed bandits fashion according to an acquisition function. Here, we use the UCB acquisition function. We find the a^* that maximizes the acquisition function and then make queries to $f(\cdot, a^*)$. We combine this with the samples we already have (from previous iterations) in order to refind our estimate of the integral for that action.

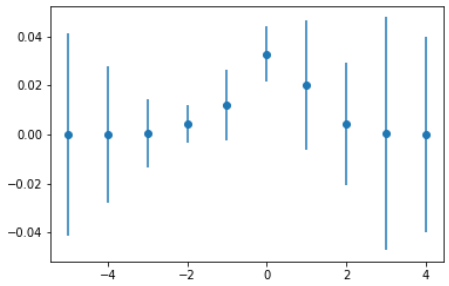
We repeat the above procedure until some convergence criterion is satisfied. For this setting we have just discretized the action space. Later, we will present how to generalize this procedure to the continuous action setting.

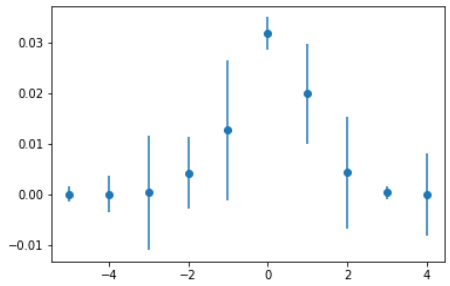
probabilistic convergence criterion is reached (action a^* is the argmax with probability p). Below is an animation showing execution of the optimization.

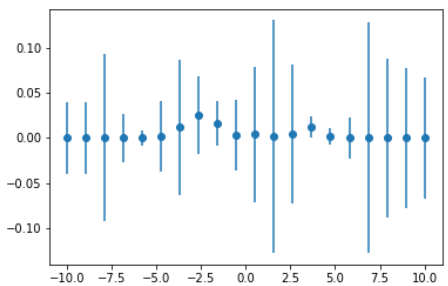
Basic Max Integral Optimization

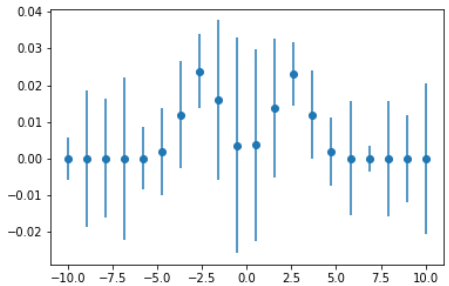
Here are images of the progression of the algorithm. Above is on simple gaussians and below is on mixtures of guassians.

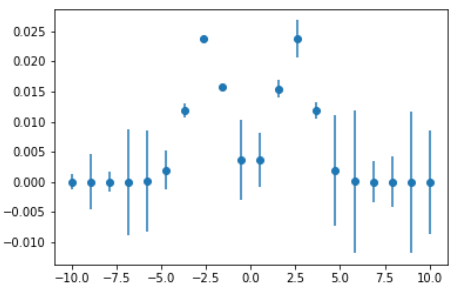












Efficient Optimization

In higher dimensions and larger spaces, quadrature (even in settings where there is a closed form solution) can be an expensive operation. By accounting for the distribution over value, we can focus on evaluating actions with potential of high value. As a result, the algorithm is sample efficient and feasible to implement in practice.

This type of optimization procedure is necessary for evaluating the Max Integral operator. Without it, you will either sacrifice accuracy of the integral estimate (by discretization or Monte Carlo methods) or accuracy of the maximization procedure.

Max Integral in RL

In Reinforcement Learning, the Bellman Update (in continuous state space) is:

$$V^{\pi}(s) = \max_{a \in A} \int_{s' \in S} p(s'|s,a)\big(R(s'|s,a) + \gamma^{\Delta t} V^{\pi}(s')\big)\ \mathrm{d}s'$$

If we use a GP to model the Value Function, and a Gaussain or mixture prior, then this integral will have a closed form and we will maximize over actions. From our experiments, however, we see that it is infeasible to fully compute this integral for each action (each update is slow). We will use our optimization procedure in order to allow for more efficient Bellman update. As a result, we are able to use GPs to model the value function and make more accurate value updates in each iteration.

Bibliography

[1] O'Hagan, A. (1991). Bayes–Hermite quadrature. Journal of Statistical Planning and Inference, 29(3), 245–260.
[2] M. P. Deisenroth, J. Peters, and C. E. Rasmussen, "Approximate dynamic programming with Gaussian processes," in Proc. of the IEEE American Control Conference (ACC), 2008, pp. 4480–4485.
[3] Rasmussen, C.E., Ghahramani, Z.: Bayesian Monte Carlo. In Becker, S., Obermayer, K., eds.: Advances in Neural Information Processing Systems. Volume 15. MIT Press, Cambridge, MA (2003)