Bayesian optimization (BO) optimizes a black box objective function which is typically expensive to compute due to the amount of time required, monetary cost or an opportunity cost. This class of machine learning problem is suitable for solving problems in continuous domain of maximum 20 dimensions. This method builds a surrogate model for the objective function and quantifies the uncertainty in the surrogate using gaussian process regression. It then uses an acquisition function called expected improvement to decide the next sampling point.

The problem of finding an optimal global arrangement of Kevlar polymer chain in space (as shown in figure 1) is solved using BO technique. The feasible set space in the present problem is define as a set of 8 tuple values . The polymer chains are allowed to displace in the y and z directions. This problem can be solved using Bayesian optimization as the objective function and the feasible set space have following properties:

1. The input feasible set has dimension 8 which is less than 20 for usual BO applications

and it is a hyper-rectangle since , and therefore it is a simple set.

1. Objective function to be optimized i.e. the potential energy surface is continuous in nature and has no known special structure i.e. linearity, concavity etc. It is very expensive to evaluate since each evaluation takes 3-6 hours and hence it is intractable to do brute force search for global optimum.

The pseudo code for obtaining the optimal global arrangement of Kevlar using BO technique is described below:

1. Observe n data points {

2. Build a gaussian process prior on .

3. Bayesian optimization

{

a. Obtain next by optimizing acquisition function EI over GP as

b. Obtain the ground truth by running one round of black box vasp evaluation for obtaining the potential energy value.

c. Obtain a new augmented set

n = n+1

d. Update the gaussian process prior on .

}

4. Expected Improvement acquisition functionEI

{

a.

Here is a gaussian process prior obtained by fitting the n data points.

b. EI =

}

The initial n { distribution and the predicted data points are shown in figure 2. Since are a set of 4 values each, we combine them together using one-to-one mapping function having the following functional form,

yval = , here

zval = , here

A close up of a map

Description automatically generated

Figure 2: Distribution of feasible set distribution for initial ground truth and later BO predicted values.

A close up of a piece of paper

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Figure 3: Total distributed energy values for all the function evaluations done during the optimization process

The Gaussian process regression is fitted initially to ground truth values and augmented each step to include the new data point and newest evaluated values. The algorithm for BO optimization is described in the pseudo code above. The model converges to optimum in nearly 40 iterations as shown in figure 4 and successfully exploit as well as explore the function space as shown in figure 2 and 3.

A close up of a logo

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Figure 4: Bayesian optimization using expected improvement acquisition function shows convergence in 20 iterations.