How to use Bayesian optimization add-in using Gaussian processes

Note: This document is translated using Microsoft Translator.

About this add-in

This add-in allows you to perform Bayesian optimization using Gaussian process model in JMP.

1. Introduction

Bayesian optimization is one technique used when repeatedly performing sequential experiments and searching for an optimal solution. The main flow of Bayesian optimization is as follows:

A relationship between x and y is represented by $y = f(x)$.

where the function $f(.)$ is an unknown smooth function.

Define some acquisition function $A(.)$ and find x that maximizes $A(f(x))$.

Find the next experimental point by the following procedure.

(1) Establish a Space-Filling design (or other design) with an appropriate number of experiments.

(2) Conduct experiments run.

(3) Estimate the Gaussian process model from the observed data.

(4) Calculate the appropriate function $A(.)$ using the Gauss process model $g(x)$ (and its covariance matrix $\sum$) estimated from the data. Find the point $x *$ at which $A(g(x))$ is the largest.

(5) Add x* as an experimental point and return to (2).

In JMP, the Gaussian process model can be applied on the "Gaussian process" platform. The "Gaussian Process" platform also allows you to save prediction and variance formulas in a data table. You can perform the Bayesian optimization described above using these features,
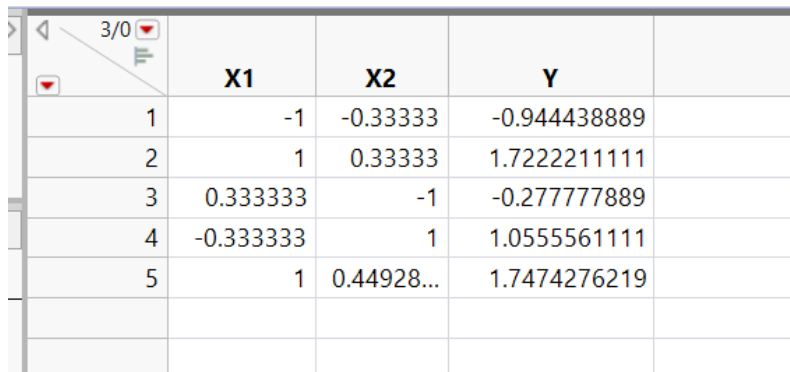
Before conducting a real experiment, it is highly recommended to check whether it works well with some pseudo data. There are cases where it is impossible to find the optimal point well with few experiments. Also, as the data grows, the computation time spent estimating the Gaussian process model could become very long. Also, please note that in some data, especially if the covariance structure is a Gauss, the estimation result may be strange if the experimental points are close.

2. System Requirements

- JMP 15 or JMP 16
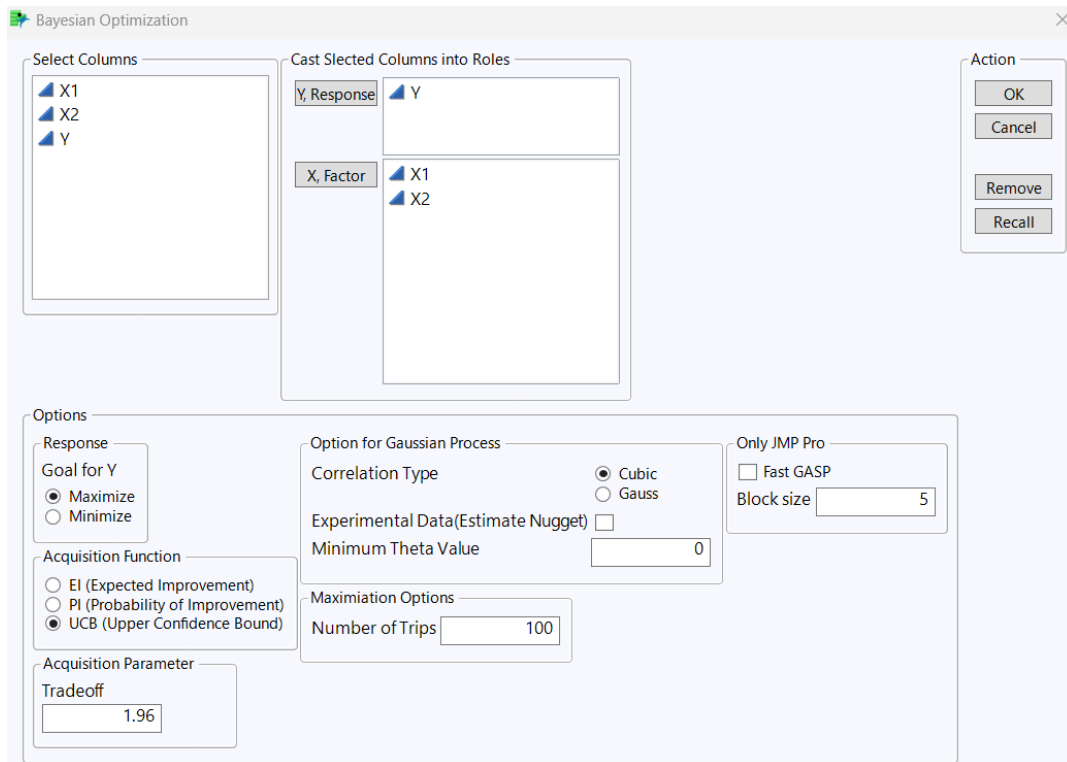- Display languages are English and Japanese only

3. How to use

1) Open the JMP data table where you entered the experimental data you have already done.

   * Note: The current version only supports cases where the response variable (Y) is one. Also, you can use only the continuous factor variable (X).

	X1	X2	Y
1	-1	-0.33333	-0.944438889
2	1	0.33333	1.7222211111
3	0.333333	-1	-0.277777889
4	-0.333333	1	1.0555561111
5	1	0.44928...	1.7474276219

2) Select Add-Ins > Bayesian Optimization.

3) Set columns and options.

- You can use the following acquisition functions: For more information about the acquisition function, see B. Shahriari et al. (2016).
  - PI (Probability of improvement)
  - EI (Expected Improvement)
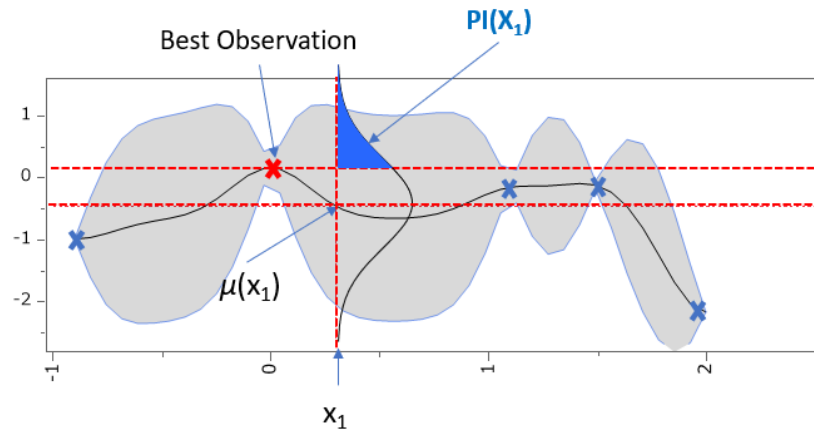 - UCB (upper confidence limit) / LCB (lower confidence limit)

Figure 1: PI

- The formula for each acquisition function is as follows (if the purpose of Y is maximization): Tradeoff and β parameters can be set in the launch dialog (parameters of the acquisition function).
  - PI = Normal distribution $((\mu(x)- Ybest- \text{trade-off})/\sigma(x))$
  - EI = $z1*$ Normal distribution $(z2) + \sigma(x)*$ Normal density $(z2)$

    where $z1 = \mu(x)-Ybest- \text{trade-off}$, $z2 = z1/\sigma(x)$
  - UCB = $\mu(x) + \beta*\sigma(x)$

- For more information on Gaussian process options, see the following online documentation: If you are using JMP Pro, you can also use the fast Gaussian process.

  https://www.jmp.com/support/help/en/16.2/#page/jmp/launch-the-gaussian-process-platform.shtml#

- The setting with the largest value of the acquisition function is the next experimental candidate point. Add-ins use the maximize desirability function of the prediction profiler to find candidate points. You can set the number of processes ("Number of trips") that randomly set the initial value so that it does not fall into a local solution when maximizing desirability.

  https://www.jmp.com/support/help/en/16.2/#page/jmp/maximization-options-window.shtml#

- For data with noise, such as experimental data, check the "Experimental Data (Estimate Nugget)" checkbox. A nugget parameter is useful if there is noise or randomness in the response, and you want the prediction model to smooth over the noise instead of perfectly interpolating.

4) When the analysis is finished, a window will be displayed. If you want to add candidate experimental points to the table, click the "Add the row to table" button.

5) The Profiler on the "Acquisition function" tab is a prediction profiler. The acquisition function and the predicted values by the Gaussian process are displayed. From the red triangle button next to the Profiler, you can also use "Optimization and desirability" > "Maximize desirability" to explore for other candidates. If you want to use the profile settings to be the next candidate experiment, click the "Use Prediction Profile Settings" button. After that, click the "Add the row to the table" button.

6) The "Gaussian Model" tab displays the results of the Gaussian Process Model.
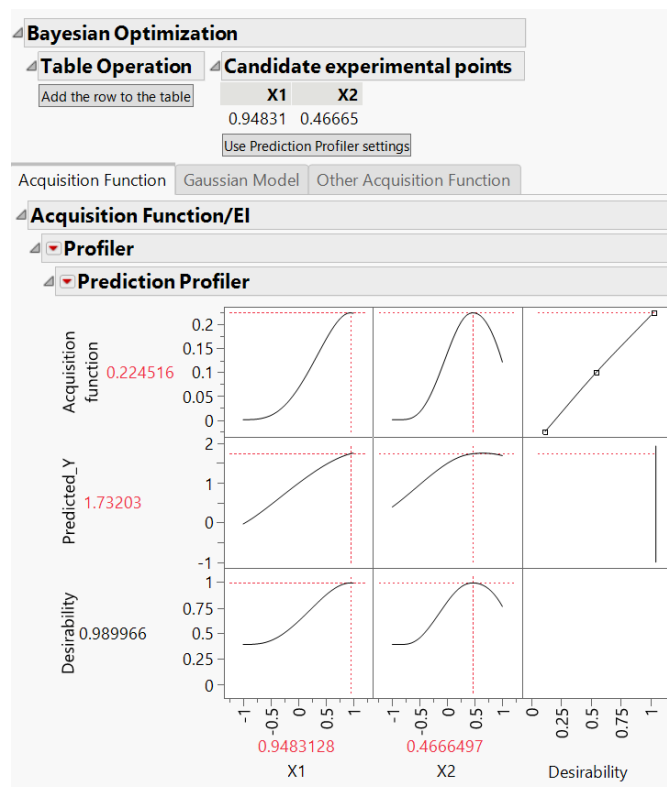
7) If you want to repeat the Bayesian optimization, click "Run Bayesian Optimization Add-in" in the table script.

■References

[1] B. Shahriari, K. Swersky, Z. Wang, R. P. Adams and N. de Freitas, "Taking the Human Out of the Loop: A Review of Bayesian Optimization," in Proceedings of the IEEE, vol. 104, no. 1, pp. 148-175, Jan. 2016, doi: 10.1109/JPROC.2015.2494218.