Verkfræðilegar Bestunaraðferðir

Day 13 - Group 2

T-423-ENOP

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Exercise 1 - Multiobjective Evolutionary Algorithm

Description

Minimize the function f(x) of two variables implemented as exercise_1_function. The function domain is [-2 3] x [-1 2]. The function should be minimized using some sort of surrogate-based optimization. Hint: build a functional surrogate model (e.g., kriging) using sampled data from f; optimize the surrogate and refine the surrogate in the vicinity of this optimal solution. Perform a few iterations of this procedure. Try to use as small number of evaluations of f as possible. Visualize the search process.

Functionality

We decided to try two different approaches; Quadratic Regression optimized with ParticleSwarm from day 7 and Kriging (we used the Dace toolbox) with Differential Evolution from day 7 as well.

Quadratic Regression/RBF & Particle Swarm

We begin by constructing a model using basis functions $1, x_1, x_2, x_1^2, x_2^2, x_1^3, x_2^3, ..., x_1^j, x_2^j$. The number of function evaluations to be computed to construct the model is an input into the MATLAB script. Like in previous exercises we solve compute lambda by solving

$$X\lambda = Y$$

where Y is the function evaluations at points that are input into the basis functions. We then optimize the surrogate function using the particle swarm algorithm constructed in a previous exercise, and compute the real function value at the point that minimizes the surrogate function, and solve for lambdas again, refining the grid at the surrogate minima, optimizing the surrogate again and so on.

Kriging & Differantial Evolution

It begins with the initialization of the function domain and the generation of initial sample points. The domain is defined with lower bounds $[-2, -1]$ and upper bounds $[3, 2]$. The number of initial function evaluations is set. Initial sample points are generated using Latin Hypercube Sampling (LHS) to ensure a well-distributed set of points within the domain. These points are then evaluated using the function `exercise_1_function`.

After generating and evaluating the initial sample points, an initial Kriging model is created using the DACE toolbox. The model is fitted with initial guesses for the correlation parameters and their respective bounds.

The script then enters a surrogate-based optimization loop, which iterates multiple times to refine the surrogate model and search for the function's minimum. In each iteration, the following steps are performed:

- First, the surrogate model, represented by the Kriging model, is used to predict the minimum using Differential Evolution. The predicted minimum point is then evaluated using the real function `exercise_1_function`. This new evaluation point is added to the existing set of points, and the Kriging model is updated accordingly.

- Next, the script generates plots to visualize the surrogate model and the evaluated points. The plot includes the predicted surface from the surrogate model and highlights the evaluated points, the predicted minimum, and the real function value at the predicted minimum.

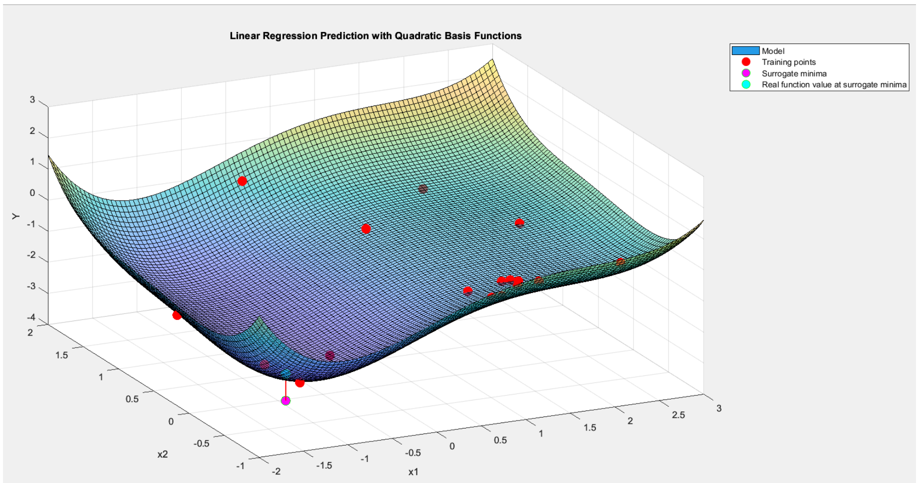
- Finally, the root mean square error (RMSE) between the surrogate model's prediction and the actual function value at the predicted minimum is calculated and displayed. This error metric provides a quantitative measure of the surrogate model's accuracy.

This process is repeated for a specified number of iterations (in our testing we used 4 iterations), continually refining the surrogate model and improving the accuracy of the predicted minimum. The script provides a robust approach for optimizing complex functions with potentially expensive evaluations.

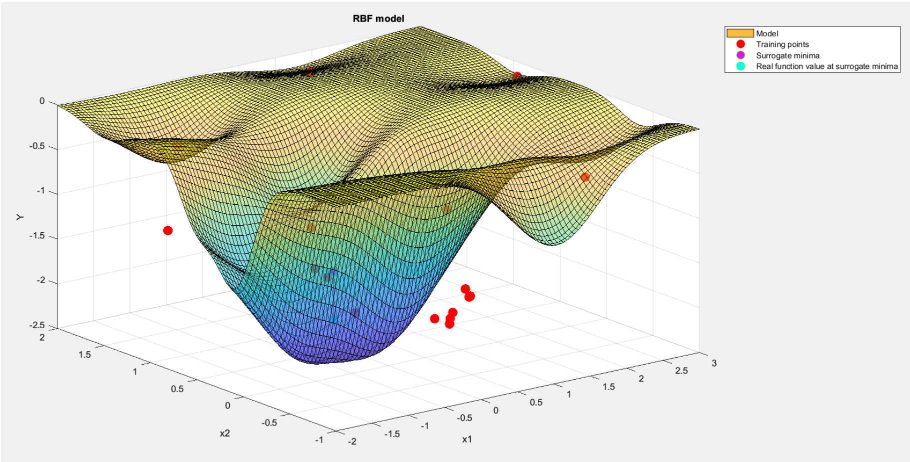
Results

Quadratic Regression/RBF & Particle Swarm

Using 8 initial function evaluations for the model construction, 10 iterations for the refinement and j =4 (basis functions are polynomials of order 4), we get the following result:
Minimum x_1, x_2 = [-1.188 -0.350], min y = -2.570270



Thereafter an attempt was made to use radial basis function models, with gaussian basis function, exactly as it was done in previous exercise, instead of linear regression. Using c = 4, we get the following results:
Minimum x_1, x_2 = [-0.334 0.329], min y = -2.055503



Kriging & Differantial Evolution

For 4 iteration of the surrogate-based optimization loop a total of 5 function evaluations are made, one at initialization and one per iteration of the loop. After all four iteration the coordinates of the minima is $[-0.759, 0.046, -2.831]$. The root mean square error for each iteration is:

1. Root mean square error at surrogate minima = 0.498813
2. Root mean square error at surrogate minima = 0.028779
3. Root mean square error at surrogate minima = 0.085431
4. Root mean square error at surrogate minima = 0.247295

Because the root mean square error is the best at the third iteration we decided to include the minima found there as well, $[-0.479, -0.415, -2.909]$.

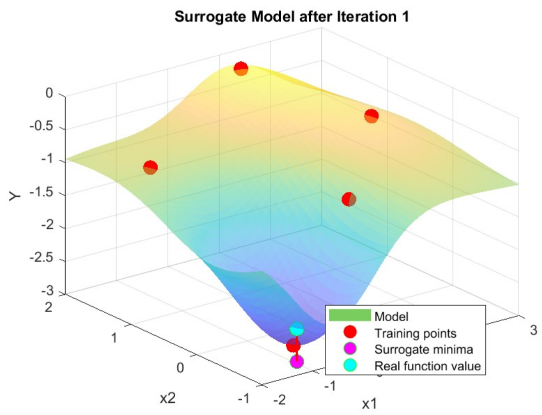


Figure 1: Model, training points, surrogate minima and real function value after 1 iteration

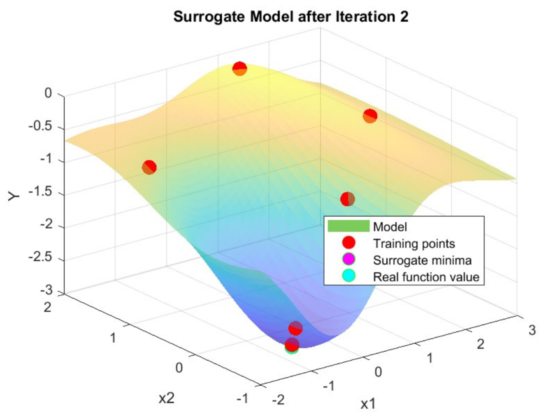


Figure 2: Model, training points, surrogate minima and real function value after 2 iteration

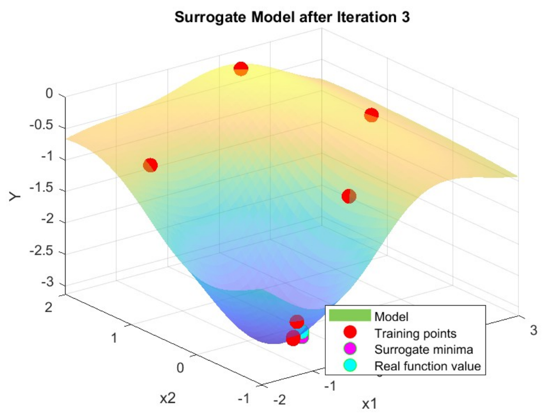


Figure 3: Model, training points, surrogate minima and real function value after 3 iteration

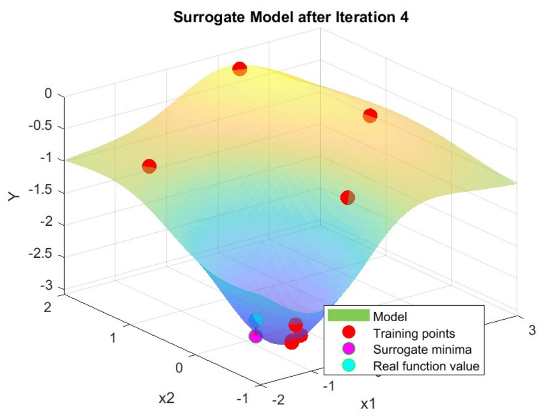


Figure 4: Model, training points, surrogate minima and real function value after 4 iteration