

Sequential Sampling for Kriging

Adaptive Design of Experiments

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Non-Sequential Sampling:

(Monte Carlo, Latin Hypercube)

- All sample locations $\{x_1, \dots, x_n\}$ determined prior
- No adaptation based on observed responses

Sequential Adaptive Sampling:

- Choose i points using Monte Carlo or Latin Hypercube.
- Next $n-i$ points are chosen adaptively:
$$x_{i+1} = f(x_1, \dots, x_i, Y_1, \dots, Y_i)$$
- Main idea is to target locations with high uncertainty.

Criteria for Choosing the Next Sample Point

IMSE

Integrated Mean Squared Error

- Global approach: minimizes the **average** prediction variance over the whole domain.

MMSE

Maximum Mean Squared Error

- Local approach: targets the points where the **worst-case** prediction variance occurs.

Source: Sacks et al. (1989) - "Design and Analysis of Computer Experiments"

Simulation : Sequential vs Non-Sequential

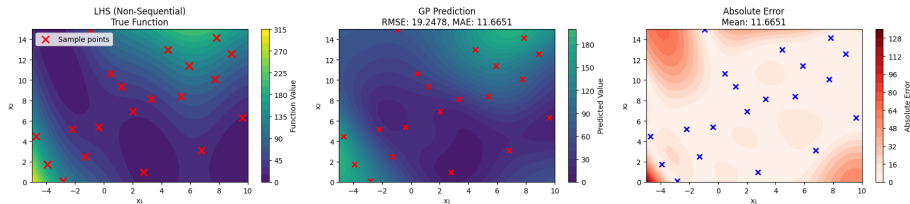


Figure: Kriging interpolation using LHS design.

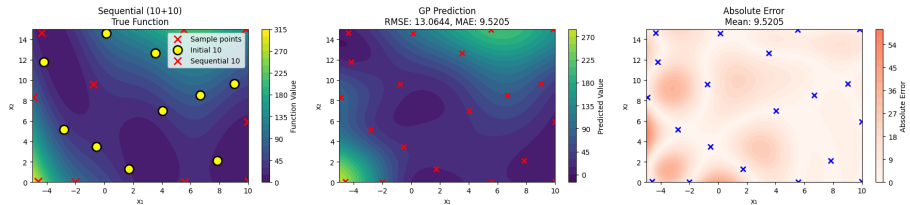


Figure: Kriging interpolation using Sequential design.

Advantages and Disadvantages

Advantages:

- **Better accuracy** with same budget
- **Adaptive exploration** of design space
- **Flexible** stopping criteria - can potentially reduce budget

Disadvantages:

- **Sequential nature**: no parallelization
- **Piling up Problem**: greedy selection may be suboptimal

Modified IMSE:

- Build global boxes and assign new points to box with highest uncertainty.
- Reduces effect of piling up.

Source: Sacks et al. (1989) - "Design and Analysis of Computer Experiments"