Sequential Sampling for Kriging

Adaptive Design of Experiments

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Design Options for Kriging Method

Non-Sequential Sampling:
(Monte Carlo, Latin Hypercube)

- All sample locations $\{x_1, \ldots, x_n\}$ 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:
  $x_{i+1} = f(x_1, \ldots, x_i, Y_1, \ldots, Y_i)$
- Main idea is to target locations with high uncertainty.

Criteria for Choosing the Next Sample Point

$$IMSE = \int_{\mathcal{X}} s^2(x)\, dx$$

$$MMSE = \max_{x \in \mathcal{X}} s^2(x)$$

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

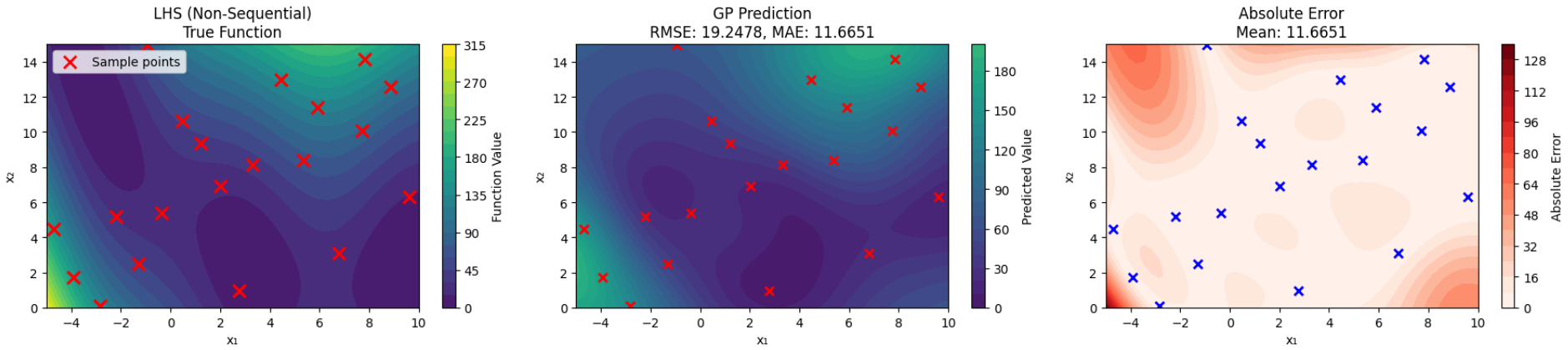

Figure: Kriging interpolation using LHS design.

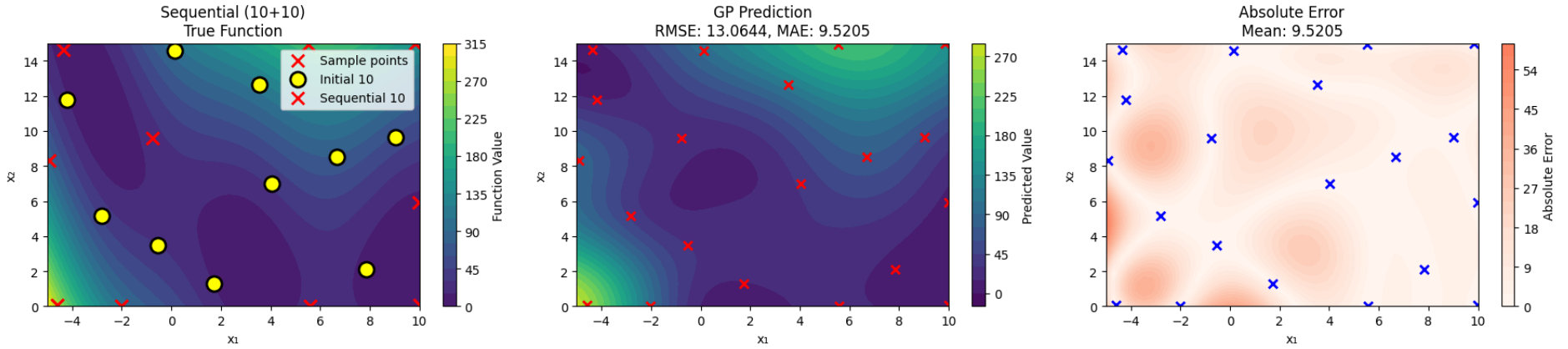

Figure: Kriging interpolation using Sequential design.

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 uncertainity.
- Reduces effect of piling up.

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