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- Surrogate modelling is seeing uptake in a wide variety of domains (including model-based design optimization).
- The notions of "sampling efficiency" and "surrogate efficiency" appear in the literature, but there does not seem to be a standardized way of expressing these notions precisely.

• Propose and test a standardized surrogate model efficiency metric.

$$\eta_{\rm SM} \sim \frac{\text{surrogate utility}}{\text{surrogate cost}}$$

Methodology (Proposition)

Consider standard benchmark problems of the form

$$y : \mathbb{R}^D \to \mathbb{R}$$

$$\vec{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_D \end{bmatrix}^\mathsf{T} \mapsto y(\vec{x})$$

namely: Rastrigin, Rosenbrock, Griewank, and Styblinski-Tang.

• <u>Define</u> surrogate utility as inverse of surrogate error, where surrogate error is

surrogate error =
$$\mu_{d-APE} + IQR_{d-APE}$$

- Assume surrogate cost is dominated by sampling cost (i.e., is proportional to number of samples N).
- Proposition:

$$\eta_{\text{SM}} = \exp\left[-\sqrt[D]{N}(\mu_{\text{d-APE}} + \text{IQR}_{\text{d-APE}})\right]$$

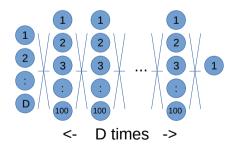
Methodology (Testing)

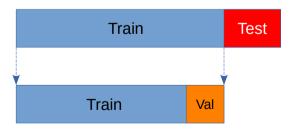
- Full factorial experiment considering combinations of
 - Benchmark problem [4
 - Sampling scheme (simple random vs latin hypercube)
 - Dimensionality 2 thru 6 [5]
 - Number of samples up to 10⁵ [16]
- Monte Carlo trials for each combination considered. [50]
- Each Monte Carlo trial consists of
 - Sample objective
 - Split sample data (train, validate, test)
 - Train surrogate
 - Test surrogate, compute efficiency

- ← some randomness here
- ← some randomness here
- ← some randomness here

Methodology (Testing)

- Neural networks are commonly used as surrogate models in the literature, so the same is done here.
- Surrogate is a dense network with D hidden layers of 100 neurons (ReLU) each.
- Train/test split is 85/15, and then train is further split 85/15 into train/validation.

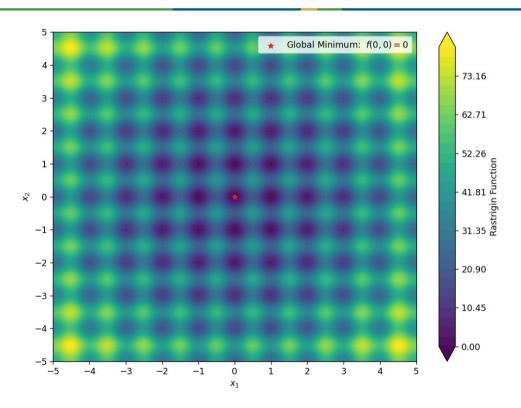




	Rastrigin (R ⁴ → R)	Rosenbrock (R ⁴ → R)
Simple Random	0.0 2 2.5 5.0 7.5 10.0 12.5 13.0 17.3	0.8 Monte Carlo data point stack means 0.0 0.0 0.0 2.5 3.0 7.5 10.0 12.5 15.0 17.5 17.5 17.5 17.5 17.5 17.5 17.5 17.5
Latin Hypercube	0.6 Moore Carlo data point stack means 0.6	0.0 Monte Carlo data point stack means



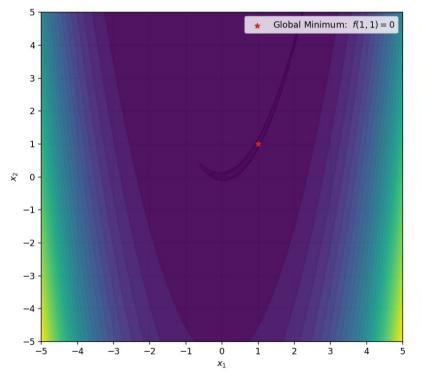


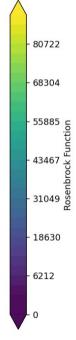


The Rastrigin function:

$$y(\vec{x}) = AD + \sum_{i=1}^{D} [x_i^2 - A\cos(2\pi x_i)]$$

where A = 10.

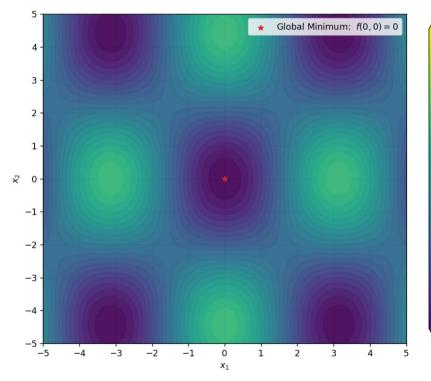


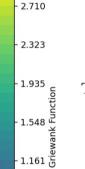


The Rosenbrock function:

$$y(\vec{x}) = \sum_{i=1}^{D-1} \left[A(x_{i+1} - x_i^2)^2 + (1 - x_i)^2 \right]$$

where A = 100.





- 0.774

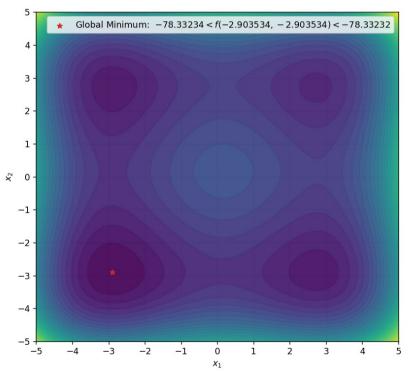
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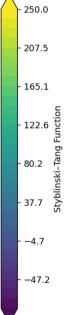
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The Griewank function:

$$y(\vec{x}) = 1 + \frac{1}{A} \sum_{i=1}^{D} x_i^2 - \prod_{i=1}^{D} \cos\left(\frac{x_i}{\sqrt{i}}\right)$$

where A = 4000.





The Styblinski-Tang function:

$$y(\vec{x}) = \frac{1}{2} \sum_{i=1}^{D} \left[x_i^4 - Ax_i^2 + Bx_i \right]$$

where A = 16 and B = 5.