Blackbox Optimization using LSTMs

Felix Sattler, Pattarawat Chormai, Raphael Holca-Lamarre

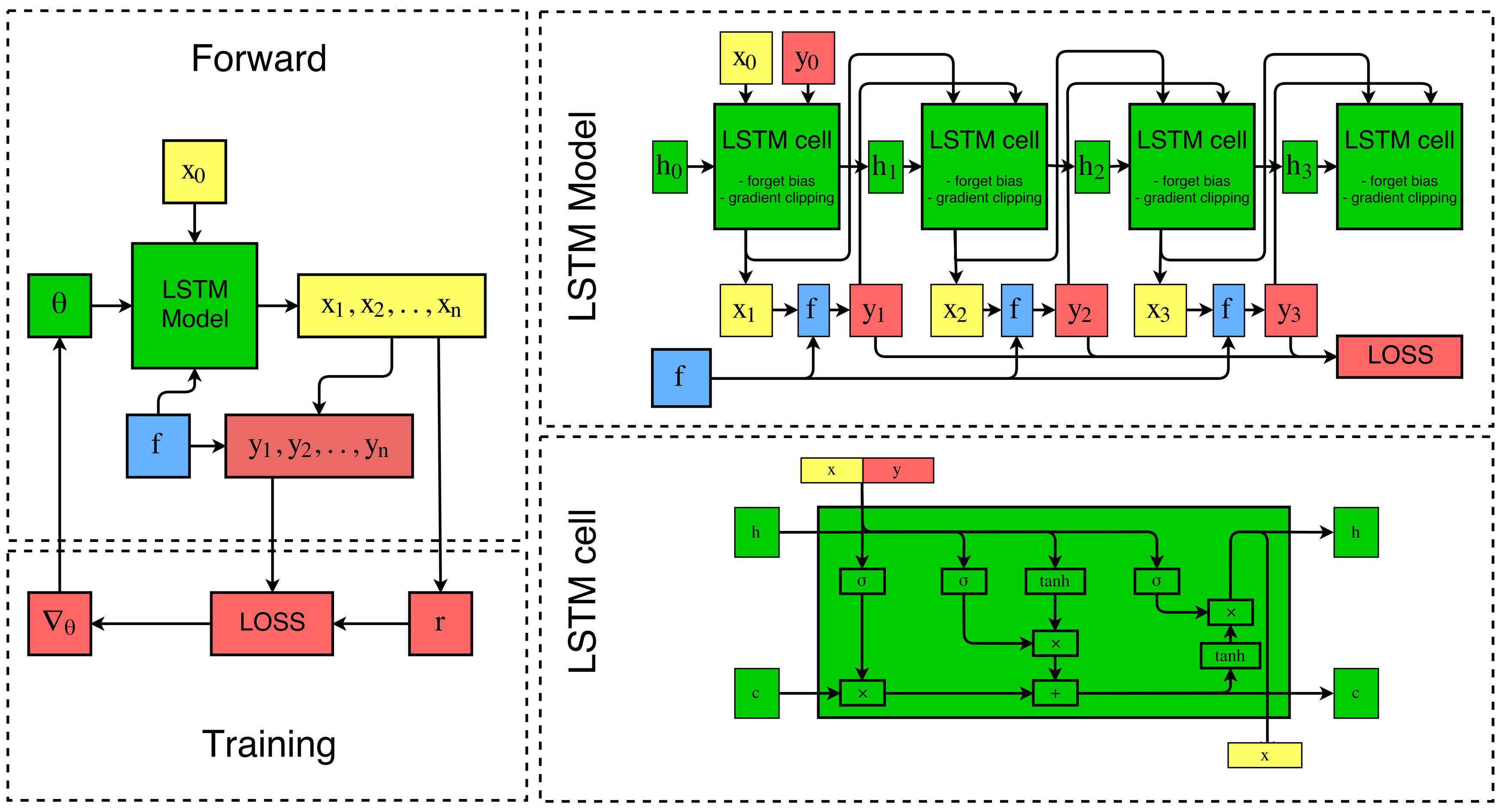
Abstract

We extend on the work of Chen et al., who introduce a new, learning-based, approach to global Black-Box optimization [1]. They train a LSTM model [2], on functions sampled from a Gaussian process, to output an optimal sequence of sample points, i.e. a sequence of points that minimize those training functions.

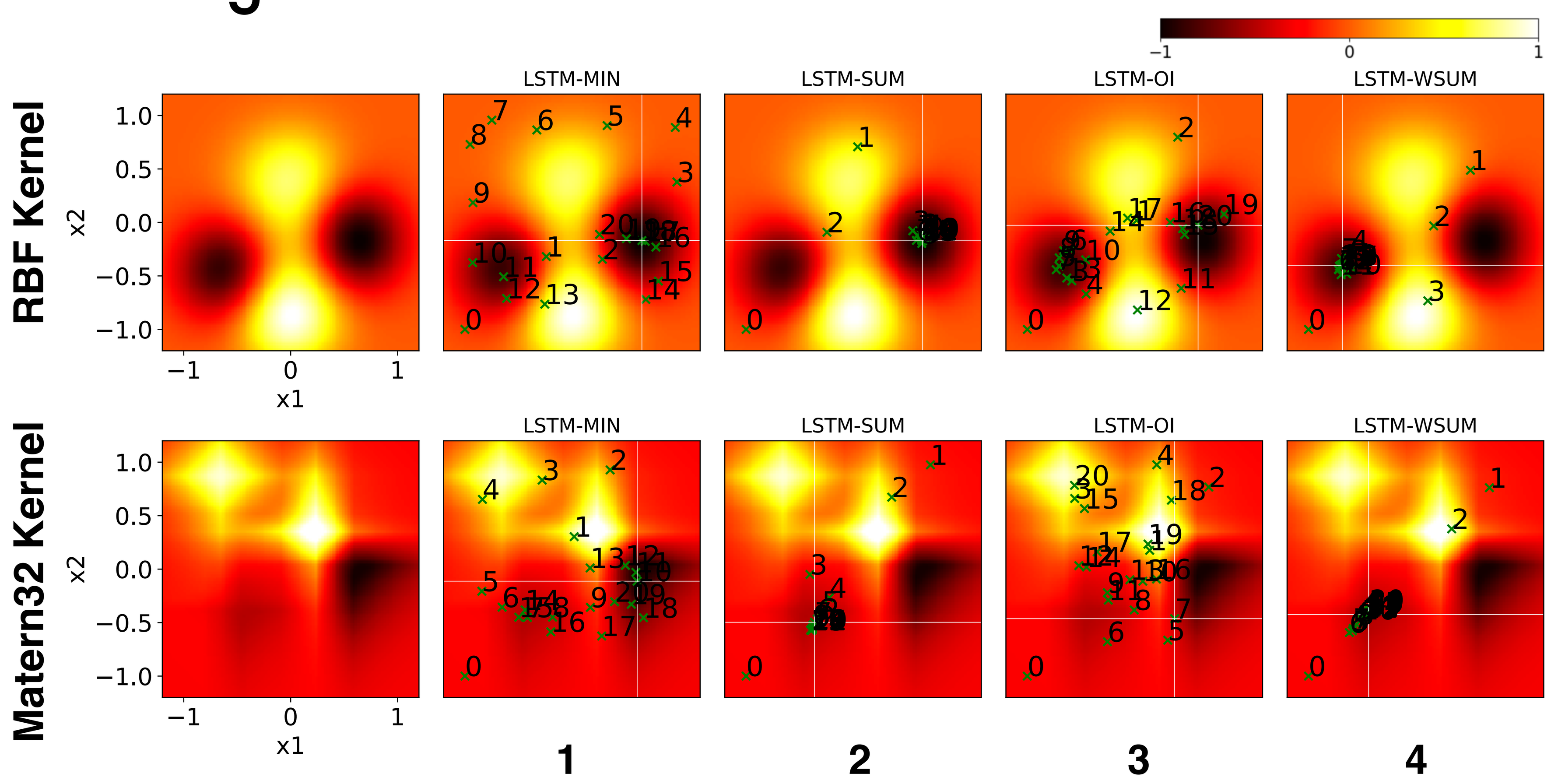
We verify the claims made by the authors, confirming that such a trained model is able to generalize to a wide variety of synthetic Black-Box functions, as well as to the real world problem of airfoil optimization.

We show that the method performs comparable to state-of-the-art Black-Box optimization algorithms, while outperforming them by a wide margin w.r.t. computation time. We thoroughly investigate the effects of different loss functions and training distributions on the methods performance and examine ways to improve it in the presence of prior knowledge.

Model



Training data and loss functions

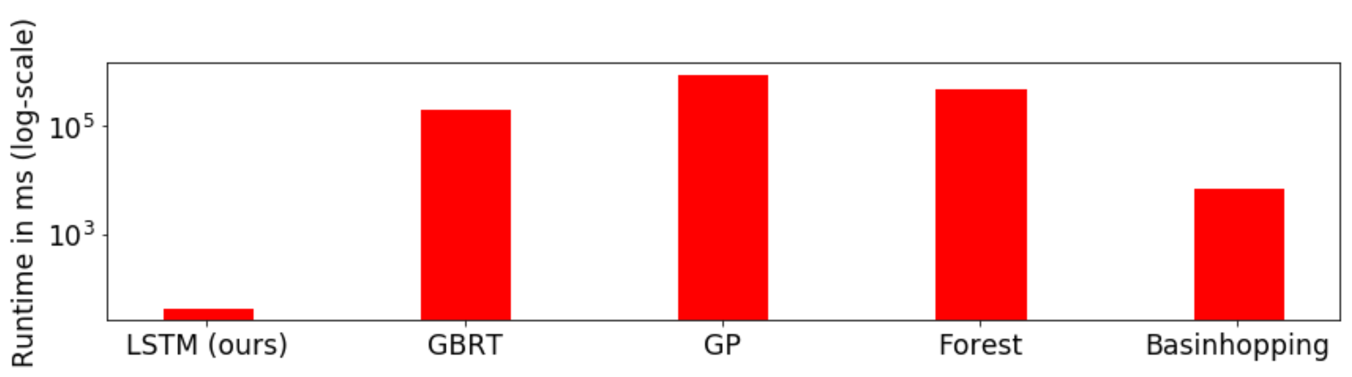


$$\mathbf{1}: \; L_{\mathbf{MIN}}(\theta) = \min_{k=1,..,n} f(x_k) \qquad \mathbf{2}: \; L_{\mathbf{SUM}}(\theta) = \sum_{k=1}^{n} f(x_k)$$

$$\mathbf{3}: \; L_{\mathbf{OI}}(\theta) = \sum_{k=1}^{n} \max(0, f(x_k) - \min_{i<k} f(x_i)) \qquad \mathbf{4}: \; L_{\mathbf{WSUM}}(\theta) = \sum_{k=1}^{n} \frac{1}{2^{n-k}} f(x_k)$$

- Sampling behavior for different loss functions

Computation time

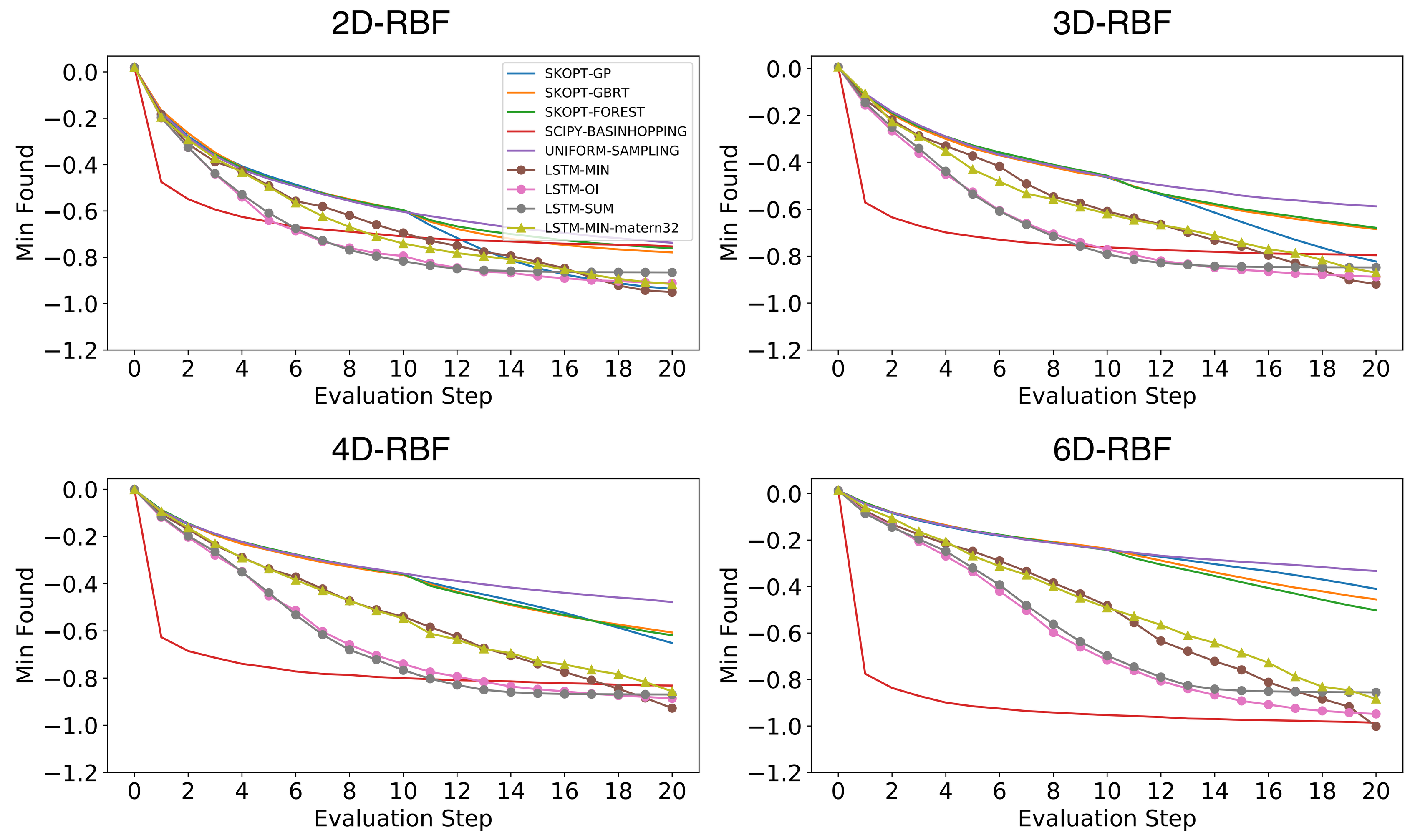


- Time taken in milliseconds by our approach and other optimization algorithms to propose 20 sampling points for 100 different 2D objective functions (Computed on a Intel® Core™ M-5Y10 CPU, 4 cores @ 0.8 GHz, 8GB Memory)

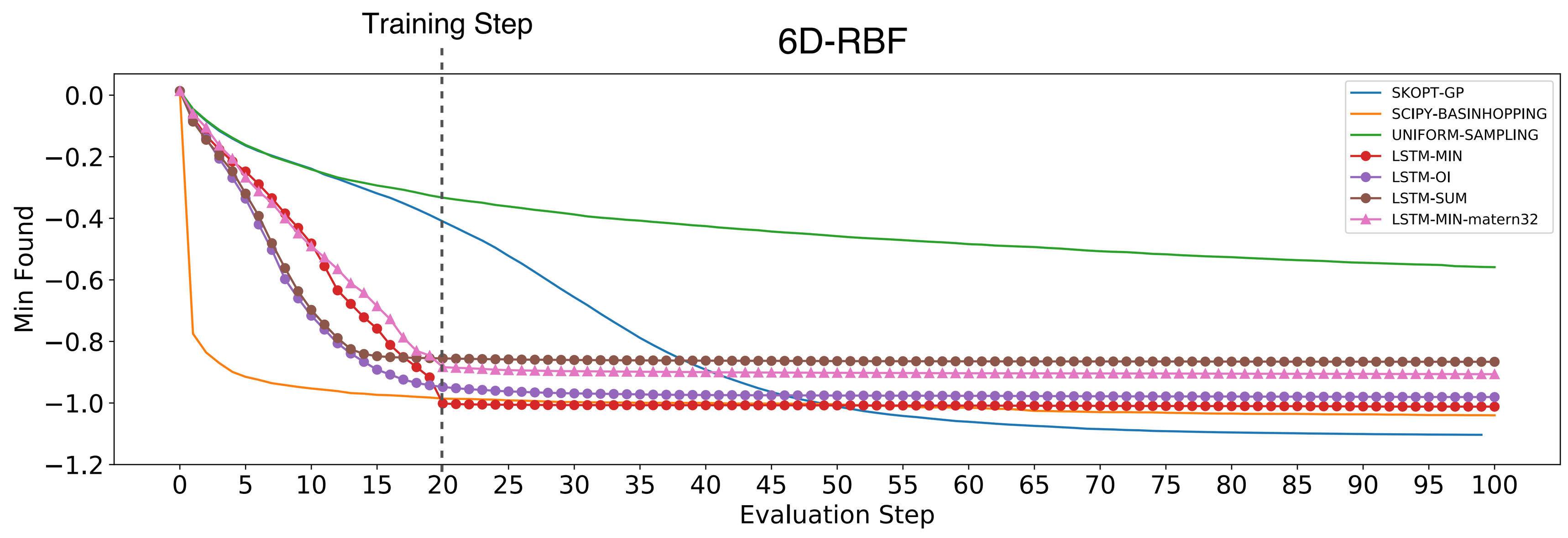
References

[1] Chen, Yutian, et al. "Learning to Learn without Gradient Descent by Gradient Descent."
[2] Hochreiter, Sepp, and Jürgen Schmidhuber. "Long short-term memory." Neural computation 9.8 (1997): 1735-1780.
[3] Wales, D J, and Doye J P K, Global Optimization by Basin-Hopping and the Lowest Energy Structures of Lennard-Jones Clusters Containing up to 110 Atoms. Journal of Physical Chemistry A, 1997, 101, 5111.
[4] SKOPT, http://scikit-optimize.github.io

Results on Test Functions

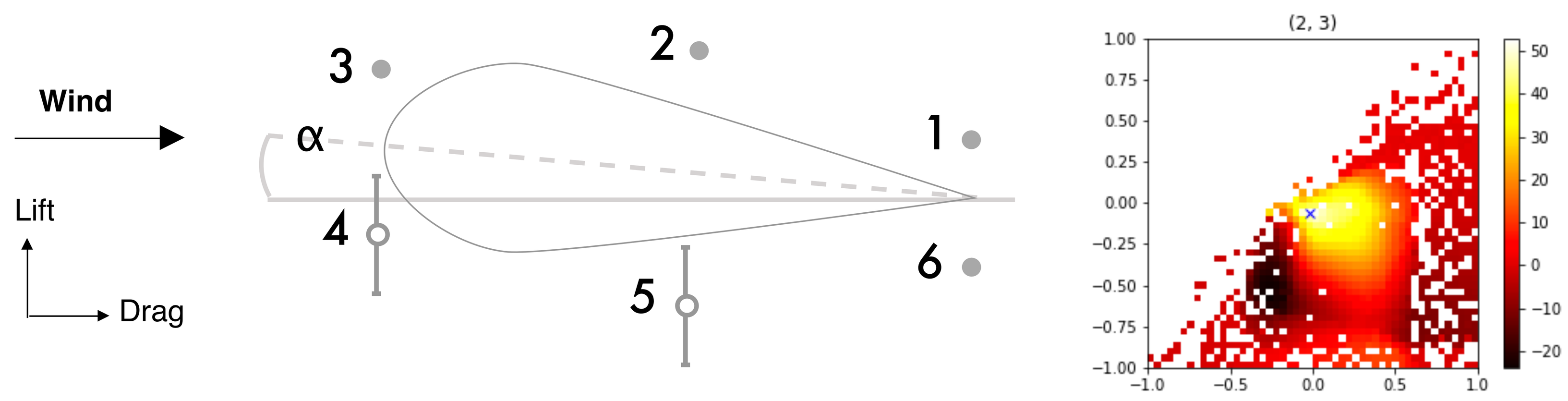


- Performance of our method and other commonly used Black-Box optimizers [3],[4] on functions sampled from a Gaussian process prior (average taken over 2000 test functions). Noting that, Basinhopping method evaluates the objective functions potentially more than once per step

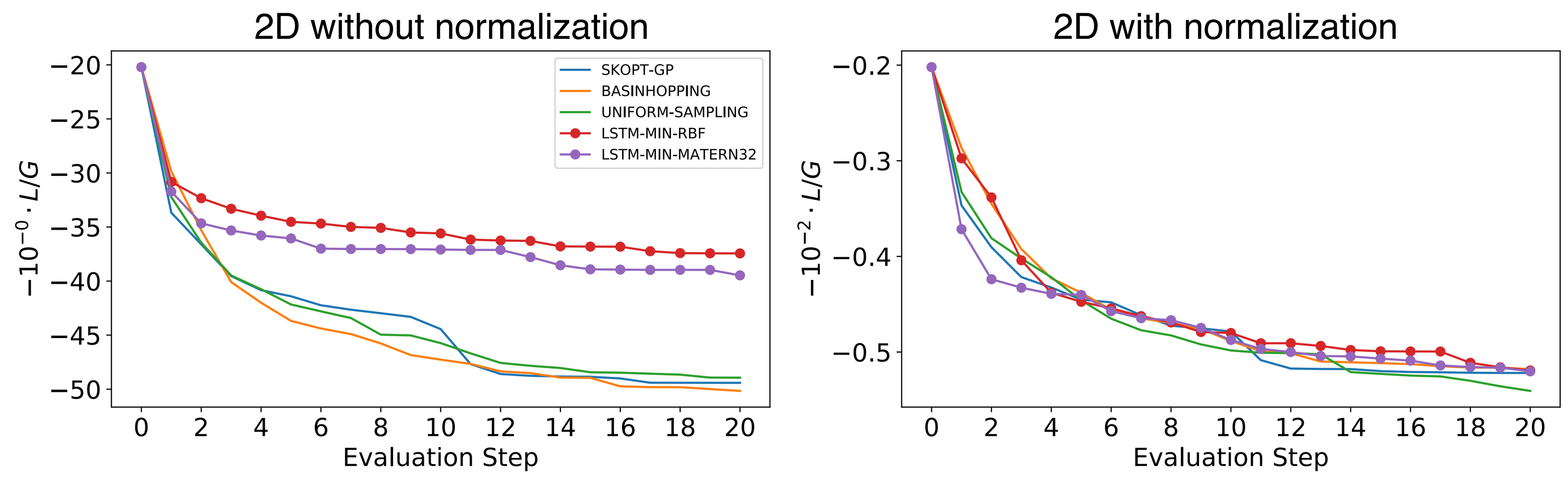


- Performance of our method over 100 evaluation steps, when trained only on sequences of 20 steps.

Airfoil Optimization



Goal : $\max \frac{L}{G} \approx \min -\frac{L}{G}$



- Results on an airfoil shape optimization problem. Average over 100 different combinations of angle of attack and pairs of control points.

Conclusions

- The model learns by itself to trade-off exploration and exploitation during sampling; we can adapt this behavior by the choice of loss function.
- The model performs well in high dimensions; inference time scales only linearly with the dimension.
- It is possible to incorporate prior knowledge into the method by the choice of a suitable training function distribution; this can lead to improved performance.
- Our approach requires the objective function to be somewhat normalized; this however is no restriction if rough upper and lower bounds to the function values are known.
- The method doesn't work "out-of-the-box"; Training is time consuming.

Acknowledgement