Blackbox Optimization using LSTMs

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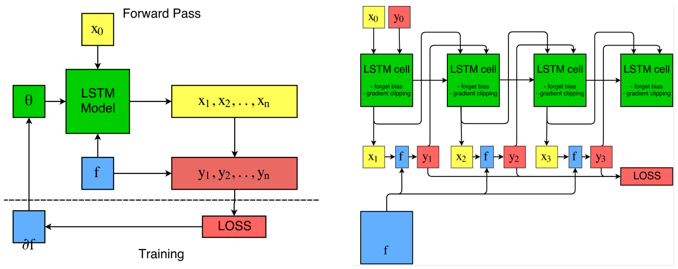
Summary

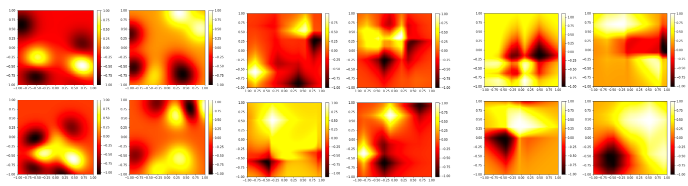
We present a new, learning-based, approach to global Black Box optimization. We train a LSTM to output a sequence of sample points that seek to minimize a given objective function.

Our experiments show that the learned model is able to generalize to a variety of synthetic Black-Box functions, as well as to the real world problem of airfoil optimization. Moreover, our model performs comparable to state-of-the-art Black-Box optimization algorithms w.r.t. the minimum function value found and even outperforms them w.r.t. computation time.

Model



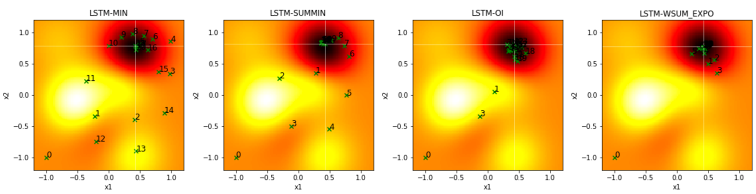
Training Data



RBF Matern32 Airfoil Prior

GP functions on different kernels

Comparison of Loss Functions



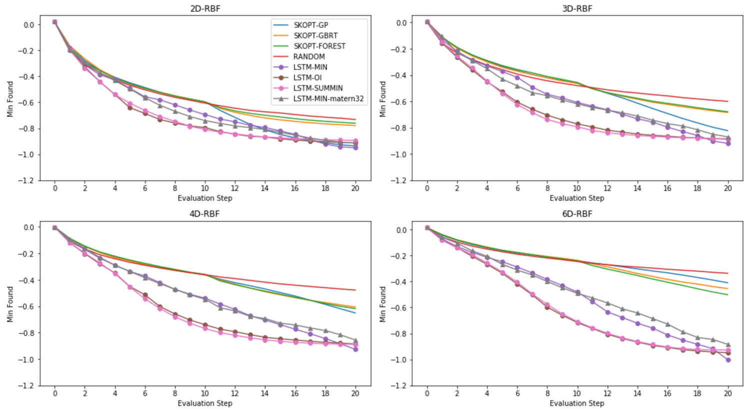
$$L_{\mathrm{SUM}}(\theta) = \sum_{k=1}^{n} f(x_k), \quad L_{\mathrm{OI}}(\theta) = \sum_{k=1}^{n} \max(0, f(x_k) - \min_{i<k} f(x_i))$$

$$L_{\mathrm{MIN}}(\theta) = \min_{k=1,\ldots,n} f(x_k), \quad L_{\mathrm{WSUM}}(\theta) = \sum_{k=1}^{n} w_k f(x_k)$$

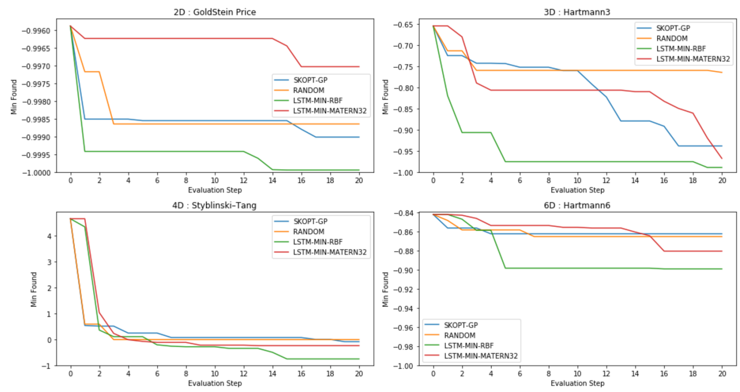
References

[1] Andrychowicz, Marcin, et al. "Learning to learn by gradient descent by gradient descent." Advances in Neural Information Processing Systems. 2016.
[2] Mockus, Jonas. "The Bayesian approach to global optimization." System Modeling and Optimization (1982): 473-481.
[3] Hochreiter, Sepp, and Jürgen Schmidhuber. "Long short-term memory." Neural computation 9.8 (1997): 1735-1780.

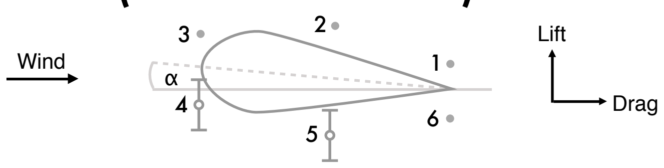
Results on Test Functions



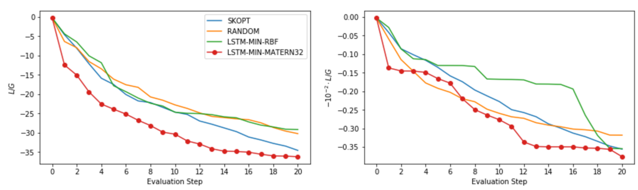
Results on Benchmask Functions



Results (on Airfoil data)



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



Conclusions

- Our model learns by itself to trade-off exploration and exploitation during sampling; we can guide its behavior by the choice of the loss function we use during training
- Our model performs well also in high dimensions, and inference time scales only linearly with the dimension
- Our approach requires the objective function to be somewhat normalized; this however is no restriction if rough upper and lower bounds

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$$y_{\{ 2 <= i < 6 \}} = [-1,1]$$
$$\alpha = [-5,5]$$