

Bounce

Reliable High-Dimensional Bayesian Optimization for Combinatorial and Mixed Spaces

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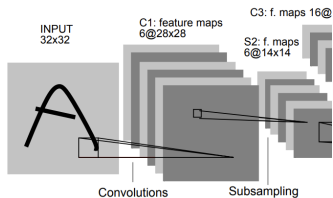
Applications



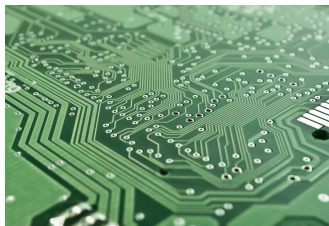
Chemical Engineering¹



Drug Discovery¹



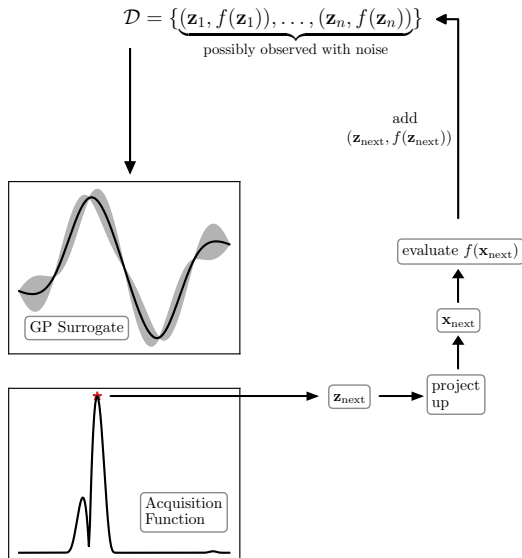
Neural Architecture Search²



Hardware Design¹

¹Pixabay , ²LeCun et al., 1998

Subspace Bayesian-Optimization for High Dimensions

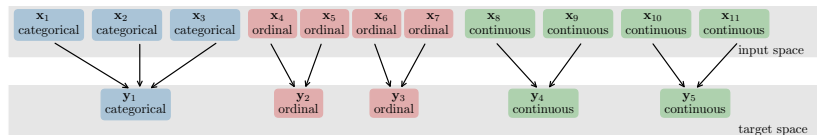


The surrogate model is defined in a low-dimensional subspace of the input space.

When evaluating the next candidate, we map it to the original input space.

Binning procedure

All variables in a bin are of the same type.



Binning procedure

We allow the binning of categorical variables of different cardinalities to reduce the problem's dimensionality.

	z^1	z^2	z^3
$x_1 = 1$	1	0	0
$x_1 = 2$	0	1	0
$x_1 = 3$	0	0	1

Binning procedure for categorical variables

Binning procedure

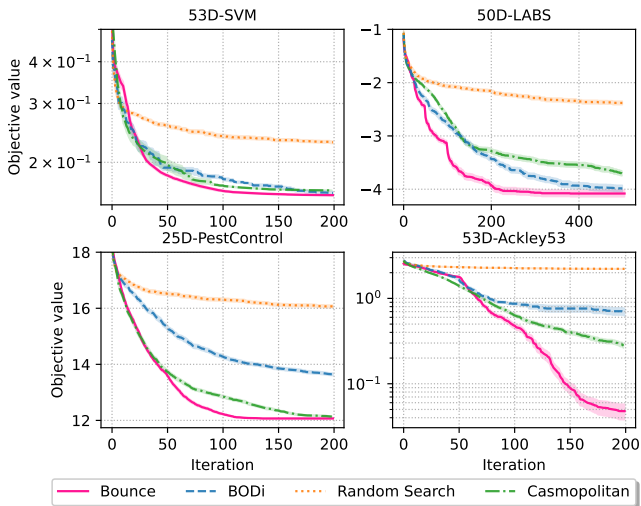
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	z^1	z^2	z^3		z^1	z^2	z^3
$x_1 = 1$	1	0	0	$x_2 = 1$	1	0	0
$x_1 = 2$	0	1	0	$x_2 = 2$	0	1	0
$x_1 = 3$	0	0	1		0	0	1

Binning procedure for categorical variables

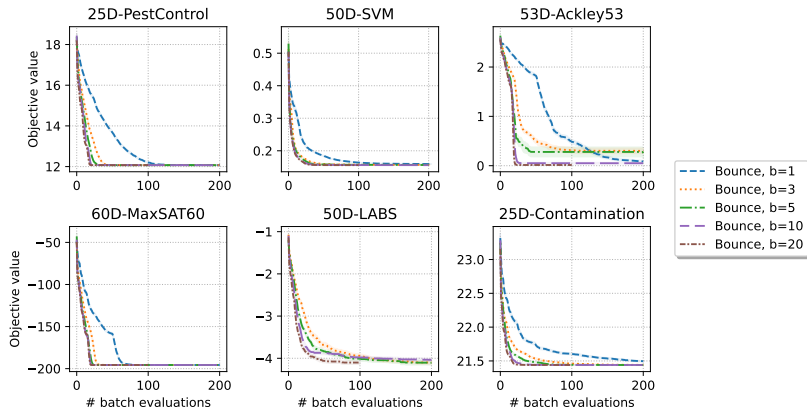
Results

We evaluate Bounce on a diverse set of problems and show state-of-the-art performance.



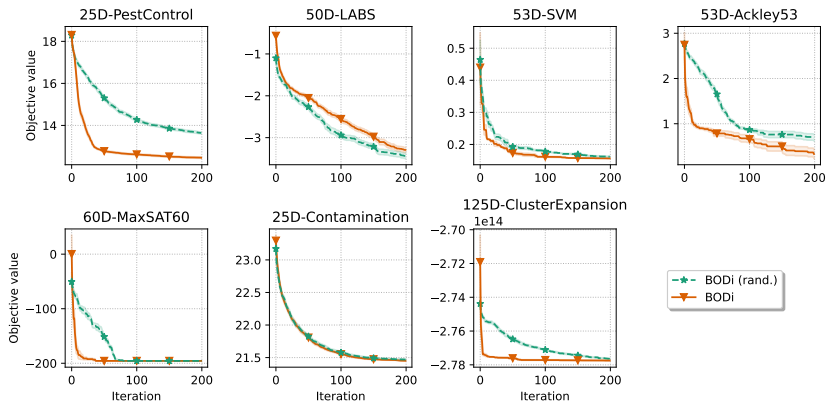
Batching

Bounce can leverage parallel function evaluations to speed up optimization.



Susceptibility of other methods to the location of the optimizer

We analyze why BODi and COMBO are susceptible to the location of the optimizer. Bounce is robust to the location of the optimizer.



Summary

Bounce ...

- ▶ is a reliable BO algorithm for continuous, combinatorial, and mixed spaces.
- ▶ is robust to the location of the optimizer.
- ▶ leverages parallel function evaluations to speed up optimization.
- ▶ achieves state-of-the-art performance on a diverse set of problems.
- ▶ is open-source and available at github.com/LeoIV/bounce.

