Per-class algorithm selection for black-box optimisation

Koen van der Blom and Carola Doerr

Sorbonne Université

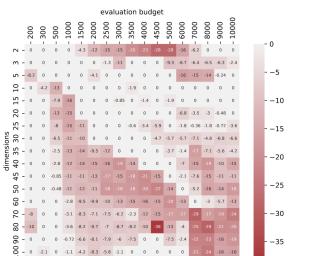
2023-11-28

Summary

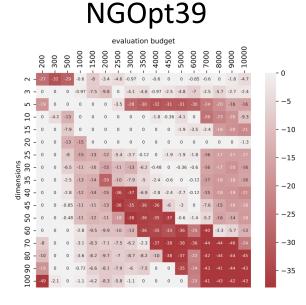
- Algorithm selection (AS) is great, e.g., for SAT \rightarrow Mostly per-instance
- Black-box optimisation \rightarrow No a priori instance-specific information
- Per-class AS \rightarrow Use problem properties for AS over sets of instances

Summary

- General data-driven AS framework
 - \rightarrow Outperform hand-made SOTA system by Meta (NGOpt)
- Extensions to grey-box problems possible, to use more information



Data-driven

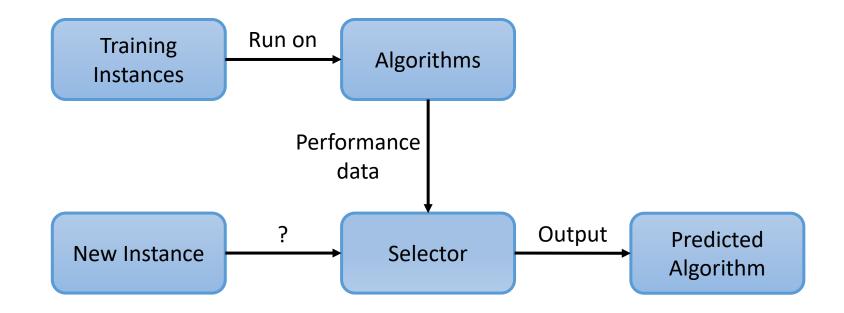


Koen van der Blom and Carola Doerr

This talk

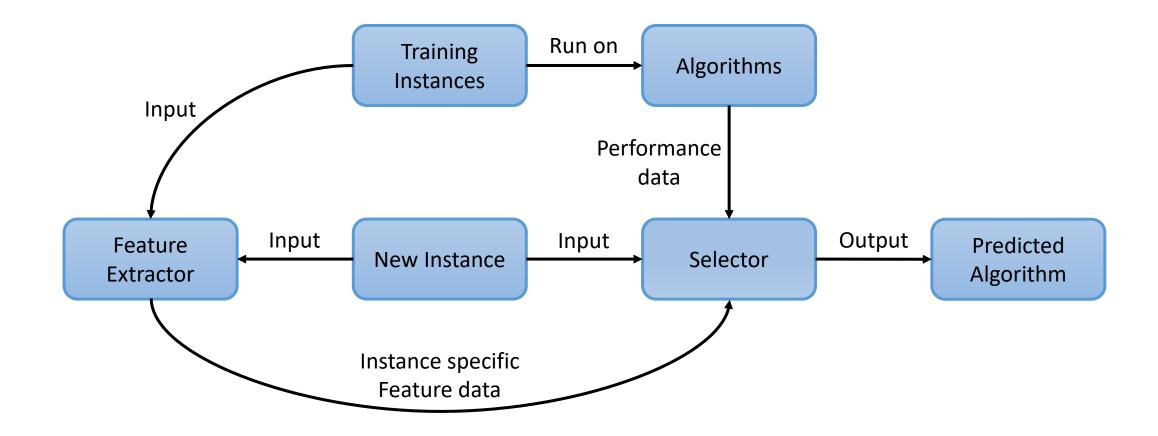
- Why we care about per-class algorithm selection
- How data-driven per-class algorithm selection works
- Comparison to hand-designed system
- Discussion of generality and extensibility

Algorithm selection [Rice, Adv. in Comp. 1976]



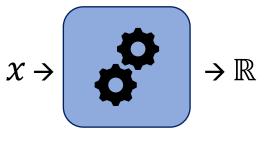
• No single algorithm is the best for every problem

Per-instance algorithm selection



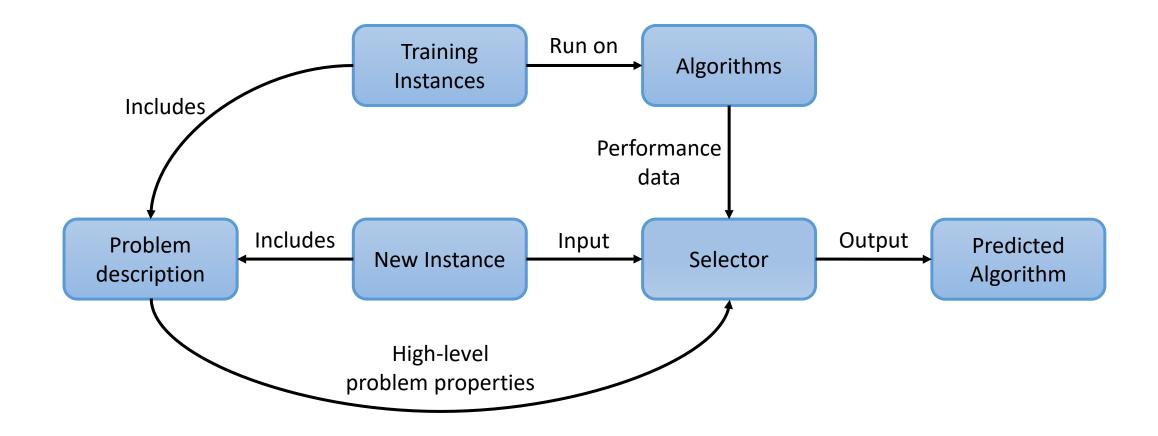
Black-box optimisation

• Optimise a problem with unknown internals



- Use sampling strategy to find the optimum
 - Evolutionary algorithms
 - Bayesian optimisation
 - ...
- No a priori instance specific \rightarrow Costs function evaluations to compute
 - Description
 - Features

Per-class algorithm selection



Properties vs. features

• Features

- Describe a problem instance
- Differ across instances
- Require function evaluations to determine

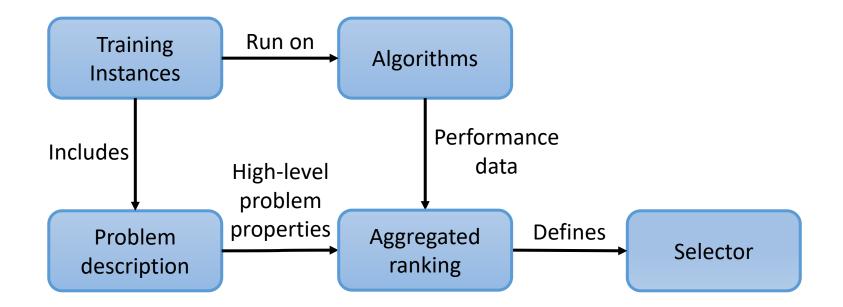
• Properties

- Describe the higher level problem class or domain
- Same across instances (in the same class/domain)
- Known a priori

Pros and cons to per-class algorithm selection

- No per-instance selection, but for larger groups
- Pro
 - Free Can make a decision before doing any evaluations
 - General Don't have to design features for each problem variant
- Con
 - Being less specific will usually mean lower performance

Data-driven selector – Basic idea



Considered problem properties

- Dimensions Number of decision variables
- Budget Number of function evaluations
- Properties we keep fixed
 - Variable type Continuous
 - No constraints
 - No noise

Comparison

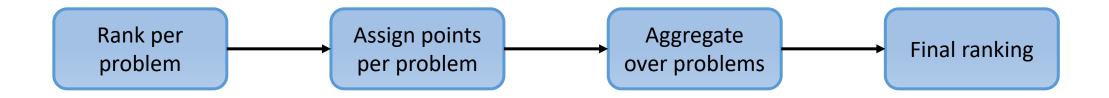
- NGOpt39 Vevergrad
 - Hand-designed competence map / selection wizard "what is good where" [Meunier et al., TEVC 2022]
- Data-driven selector
 - Choose from the algorithms included in NGOpt39 based on performance data
- Same algorithms + implementation, different selection method

Training

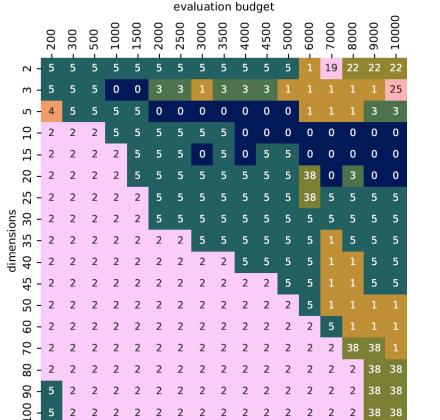
- Budgets: [1,...,<u>10000</u>]
- Dimensions: [1,...,100]
- Algorithms: All those used by NGOpt39 in this domain (34 total)
- Problems: 24 BBOB functions, instance 1, 25 repetitions each [Hansen et al. Tech. Rep. 2009]

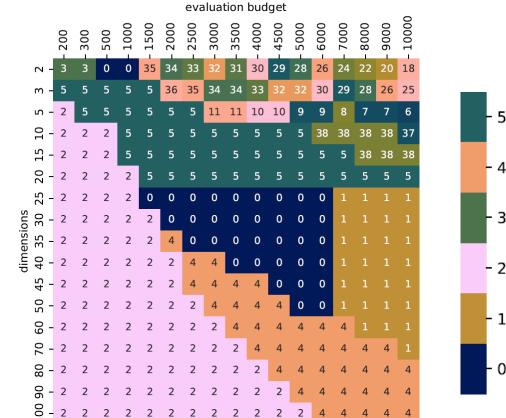
Ranking

- Per budget-dimension pair
 - Give an algorithm 1 point for each run in the top 25 per problem
 - Runs below the top 25 tied with the 25th best run are also awarded a point
 - Algorithm with most points is chosen for the budget-dimension pair



Data-driven vs. NGOpt39



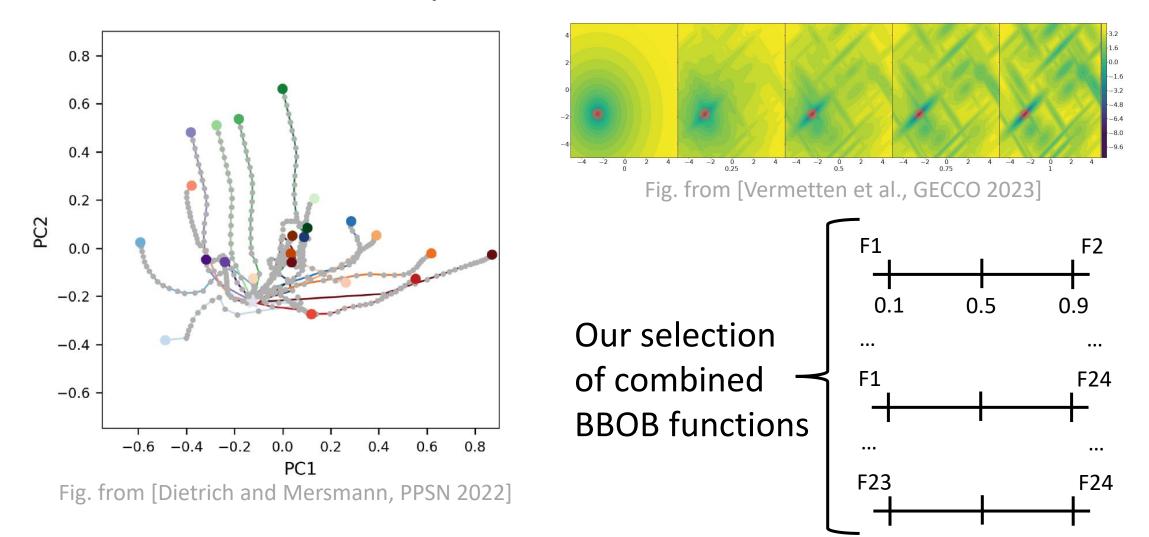




Testing

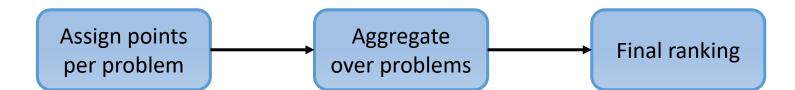
- Budgets: [200, 300, 500, 1000, ..., 5000, 6000, ..., 10000]
- Dimensions: [2, 3, 5, 10, ..., 50, 60, ..., 100]
- Algorithms:
 - 5 per budget-dimension pair
 - All those chosen by NGOpt39, or in the top 4 performers (excluding NGOpt39)
- Problems: 828 MA-BBOB functions, 1 repetition each

MA-BBOB – Many affine combinations

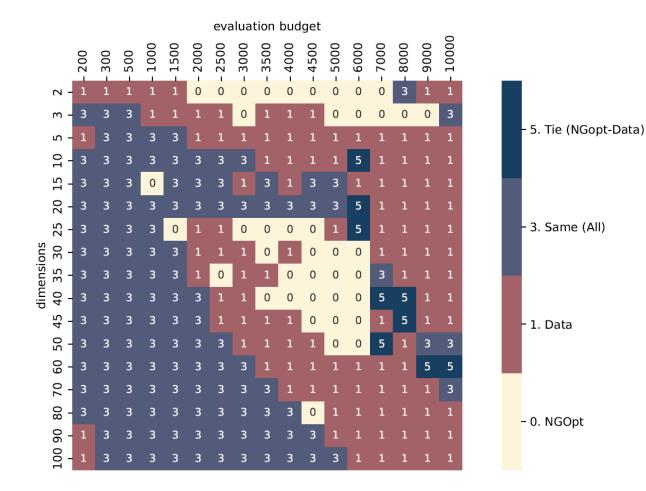


Test ranking

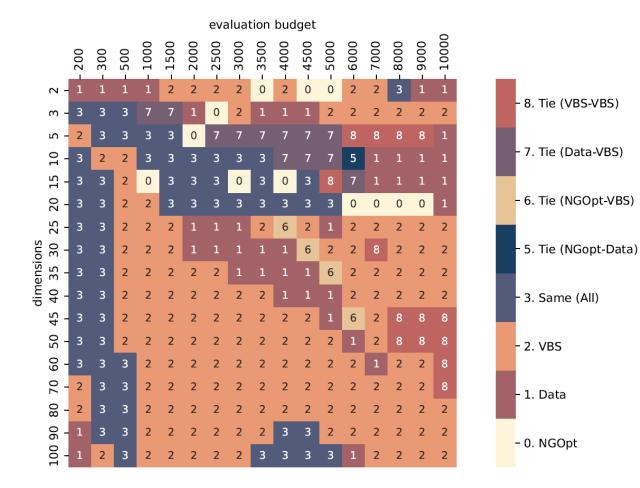
- One run per algorithm per problem
- Per budget-dimension pair
 - Give an algorithm 1 point for each problem where it is the best
 - Algorithms tied with the best algorithm on a problem also get a point
 - Algorithm with most points is chosen for the budget-dimension pair



Data-driven vs. NGOpt39 on MA-BBOB

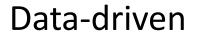


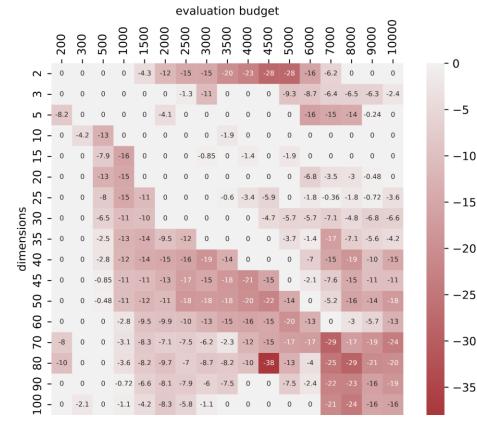
Wins compared to the VBS on MA-BBOB



Loss to the VBS on MA-BBOB (% of problems)

NGOpt39 evaluation budget 10000 1500 2500 3000 3500 4000 4500 5000 6000 7000 8000 0006 1000 2000 300 500 200 - 0 - -5 -4.2 0 -1.8 -0.36 -4.1 -9.3 -1.9 -3.5 -2.4 - -100 0 -1.3 -1.9 -1.8 -16 - -15 8 -11 -10 -6.5 0 -2.5 -13 -14 -10 -7.9 -5 -0.12 -17 18 -18 -16 -20 0 -2.8 -12 -14 -15 -36 -37 -6.9 -2.8 -2.4 -2.7 -0.12 -15 -0.85 -11 -11 -13 -38 -35 -36 -36 -6 -3 0 -7.6 -15 -25 -0.48 -11 -12 -11 -38 -36 -35 -37 -0.6 -1.4 -5.2 -16 -14 -40 -3.3 -5.7 -13 -2.8 -9.5 -9.9 -10 -13 70 - - 30 -3.1 -8.3 -7.1 -7.5 -6.2 -2.3 -44 -46 80 -8.7 -8.2 -10 -38 -37 -42 -44 -44 -45 -3.6 -8.2 -9.7 90 -35 -24 -43 -41 -44 -43 -7.5 0 0 -35 00 -2.1 0 -1.1 -4.2 -8.3 -5.8 -1.1 0 0 0 0

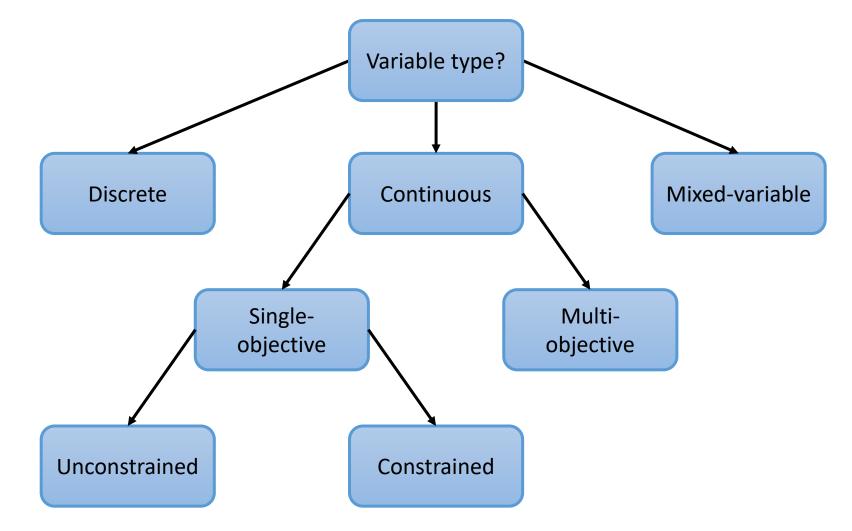




Moving forward

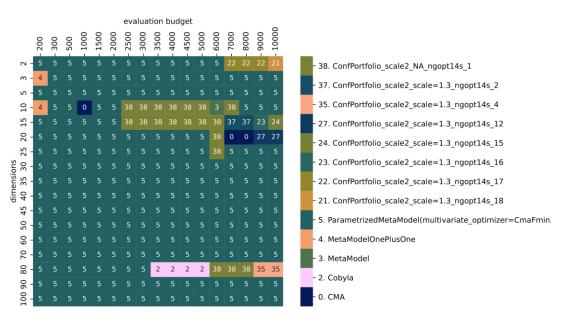
- Improve training instance set for generalisability
- Progressively add algorithms
- Evaluate different selection methods, e.g., for:
 - Worst case performance

Generalisation to other problem domains



Extension to grey-box setting

- Include user provided properties in the data-driven analysis
- Property needs to be known for the training data
- E.g., multimodal (F15-F24 in BBOB)



Take home

- Per-class algorithm selection for black-box optimisation works
- Data-driven system improves over hand-designed selectors
- General conceptual framework \rightarrow No features, no problem
 - Problems with constraints, multiple objectives, ... \rightarrow No problem!
- Extendable to grey-box setting
 - Have a multimodal problem?
 - \rightarrow Selection based on multimodal problems in the data

References

- [Dietrich and Mersmann 2022] Dietrich, K., Mersmann, O. (2022). Increasing the Diversity of Benchmark Function Sets Through Affine Recombination. In: Rudolph, G., Kononova, A.V., Aguirre, H., Kerschke, P., Ochoa, G., Tušar, T. (eds) Parallel Problem Solving from Nature – PPSN XVII. PPSN 2022. Lecture Notes in Computer Science, vol 13398. Springer, Cham. https://doi.org/10.1007/978-3-031-14714-2_41
- [Hansen et al. 2009] Real-parameter black-box optimization benchmark-ing 2009: Noiseless functions definitions. Technical Report RR-6829, Inria, France (2009).
- [Meunier et al. 2022] L. Meunier et al., "Black-Box Optimization Revisited: Improving Algorithm Selection Wizards Through Massive Benchmarking," in IEEE Transactions on Evolutionary Computation, vol. 26, no. 3, pp. 490-500, June 2022, doi: 10.1109/TEVC.2021.3108185.
- [Rice 1976] Rice, John R. "The algorithm selection problem." Advances in computers. Vol. 15. Elsevier, 1976. 65-118.
- [Vermetten et al. 2023] Diederick Vermetten, Furong Ye, and Carola Doerr. 2023. Using Affine Combinations
 of BBOB Problems for Performance Assessment. In Proceedings of the Genetic and Evolutionary
 Computation Conference (GECCO '23). Association for Computing Machinery, New York, NY, USA, 873–881.
 https://doi.org/10.1145/3583131.3590412