Data Driven Approaches in (Multi-objective) Bayesian Optimisation - An Introductory Course

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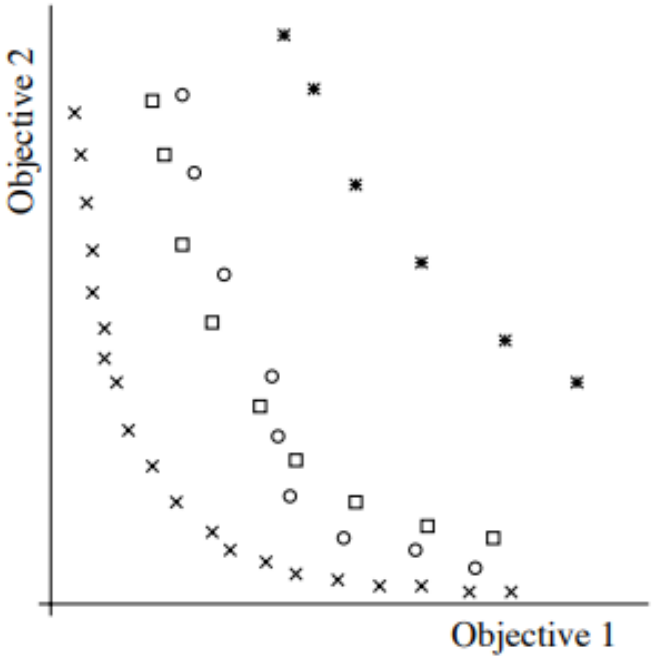
Quality Indicators

- Many multi-objective optimisation algorithms exist
- How to check the convergence of an algorithm
- How to quantify: Algorithm 'A' is better than Algorithm 'B'

Quality Indicators



× True Pareto Front
□ Estimated Pareto optimal individuals, algorithm A
✱ Estimated Pareto optimal individuals, algorithm B
○ Estimated Pareto optimal individuals, algorithm C

- Illustration of the Pareto front, and three estimates of it.
- The estimate of algorithm A is clearly more accurate than algorithm B, as is algorithm C compared to algorithm B, but the comparison of algorithm A and algorithm C is not as easy to quantify.
- How might we measure the *quality* of an estimated Pareto front?

Quality Indicators

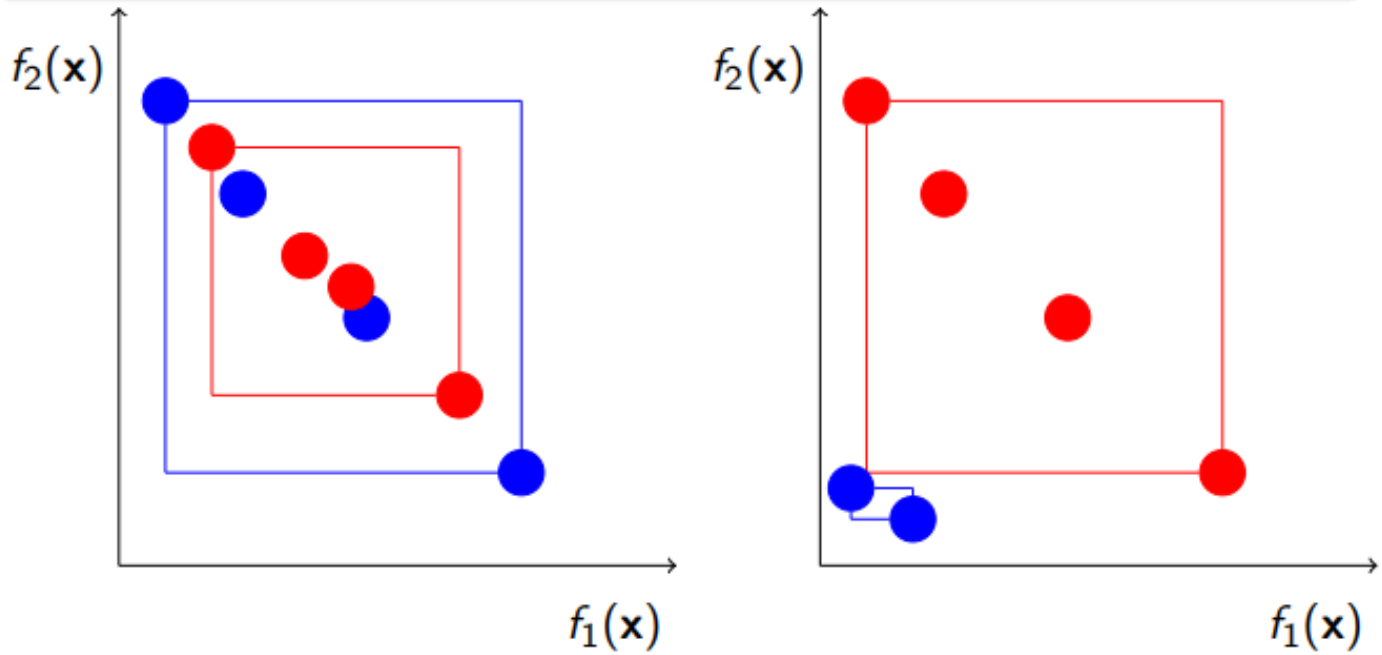
- There exist over 100 indicators[1]
- Not all indicators serve the same purpose
- Currently, there is no perfect quality indicator, i.e. one that is **simultaneously**
  1. easy to compute
  2. easy to interpret and parameterless
  3. independent of the shape of the Pareto front
  4. possesses desirable properties such as Pareto compliance

[1] Miqing Li and Xin Yao. 2019. Quality Evaluation of Solution Sets in Multiobjective Optimisation: A Survey. ACM Comput. Surv. 52, 2, Article 26 (March 2020), 38 pages. https://doi.org/10.1145/3300148

Quality Indicators

Spread

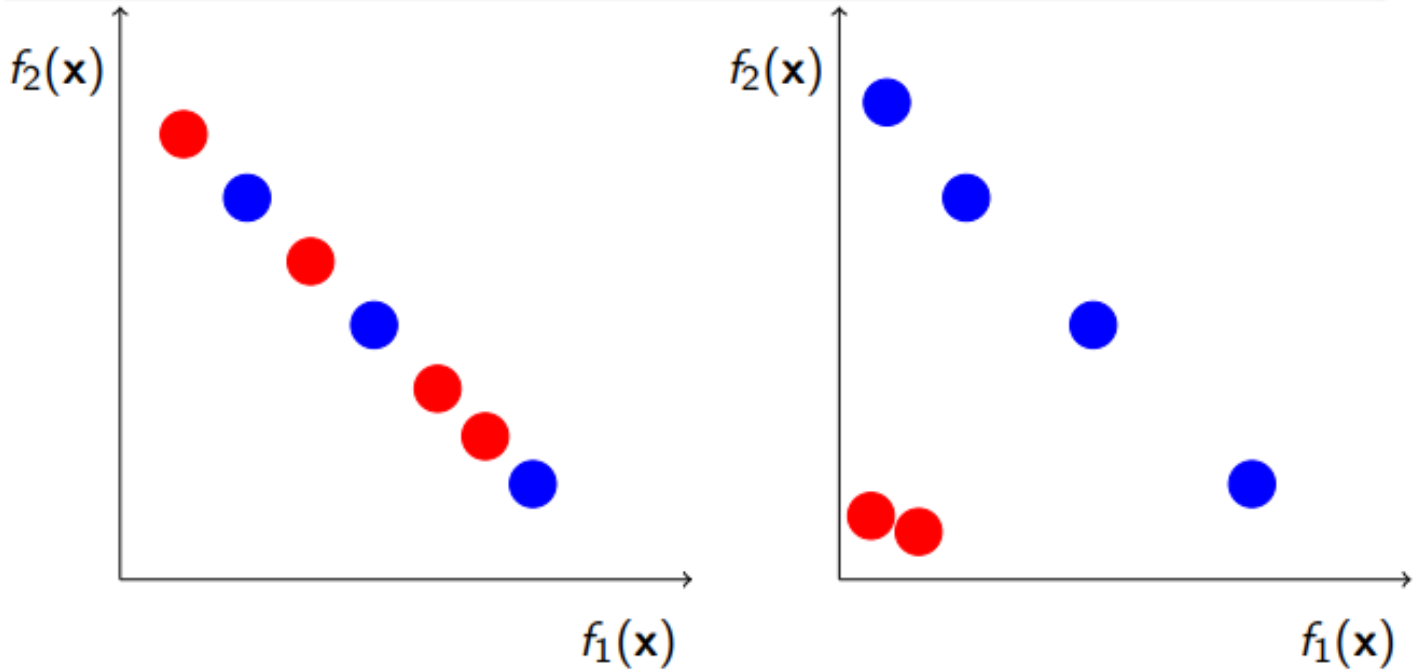
Length of the diagonal of the hyper-rectangle that is created by the extreme function values of the non-dominated set



Quality Indicators

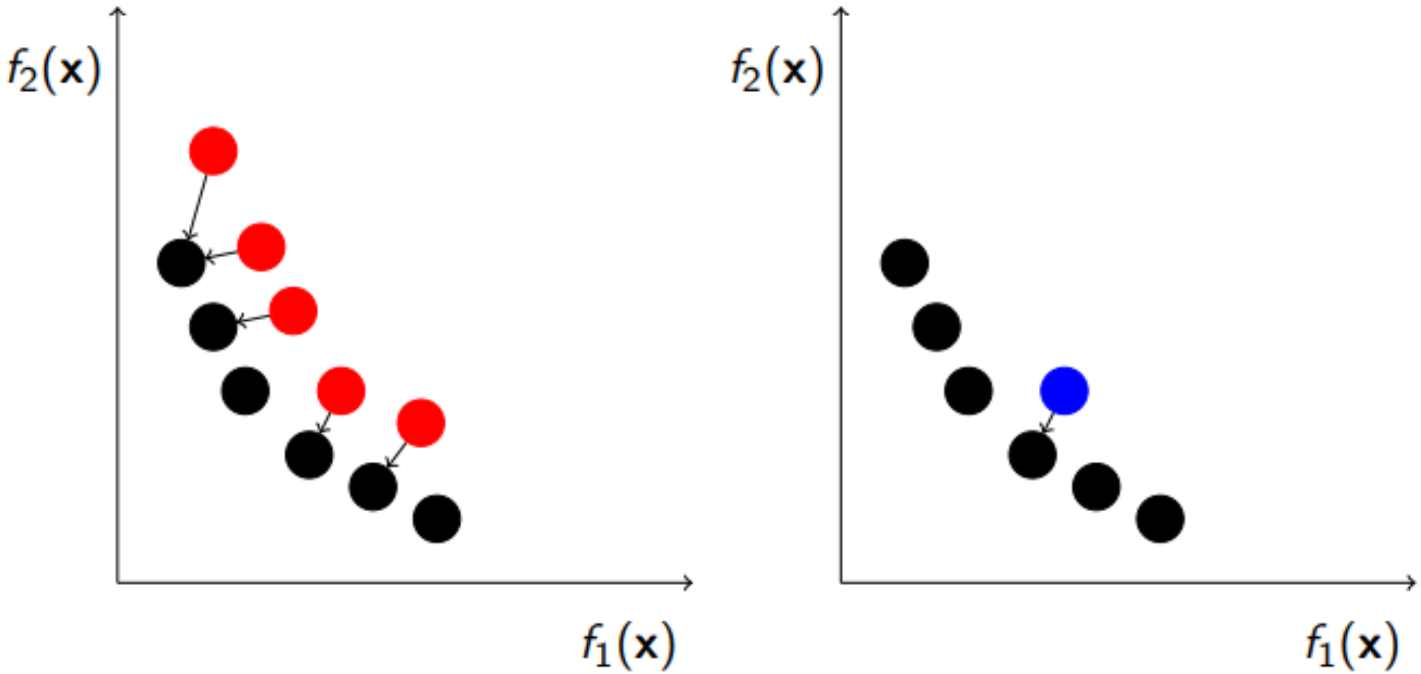
Cardinality

Cardinality of the non-dominated set, i.e. $|A|$ versus $|B|$



Quality Indicators

Generational Distance (GD)

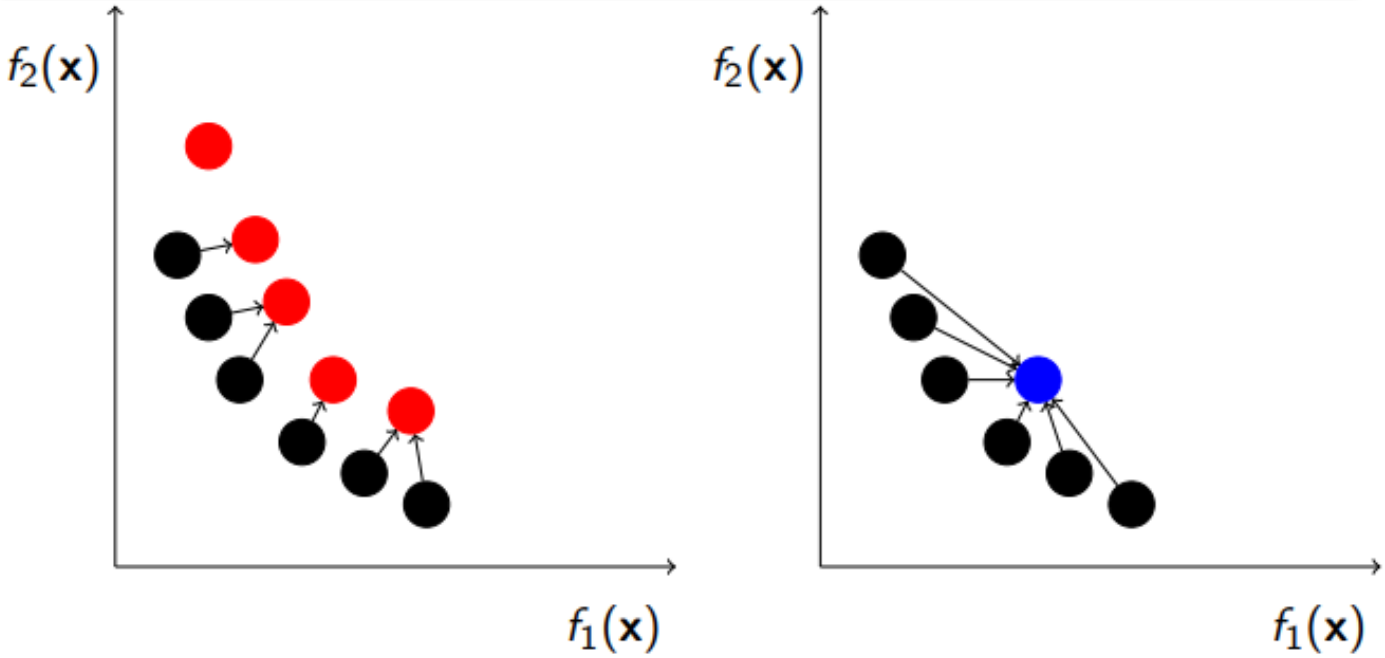


$$GD = \frac{\sqrt{\sum_{i=1}^{|A|} d(\mathbf{f}(A_i), \mathcal{F}_{samp})}}{|A|}$$

Quality Indicators

Inverted Generational Distance (IGD)

$$IGD = \frac{\sqrt{\sum_{i=1}^{|\mathcal{F}_{samp}|} d(\mathcal{F}_{samp,i}, \mathbf{f}(A))}}{|\mathcal{F}_{samp}|}$$



Quality Indicators

Pareto Compliance

A property that we would really like in a quality measure, or indicator, it that it **does not contradict Pareto set-dominance**.

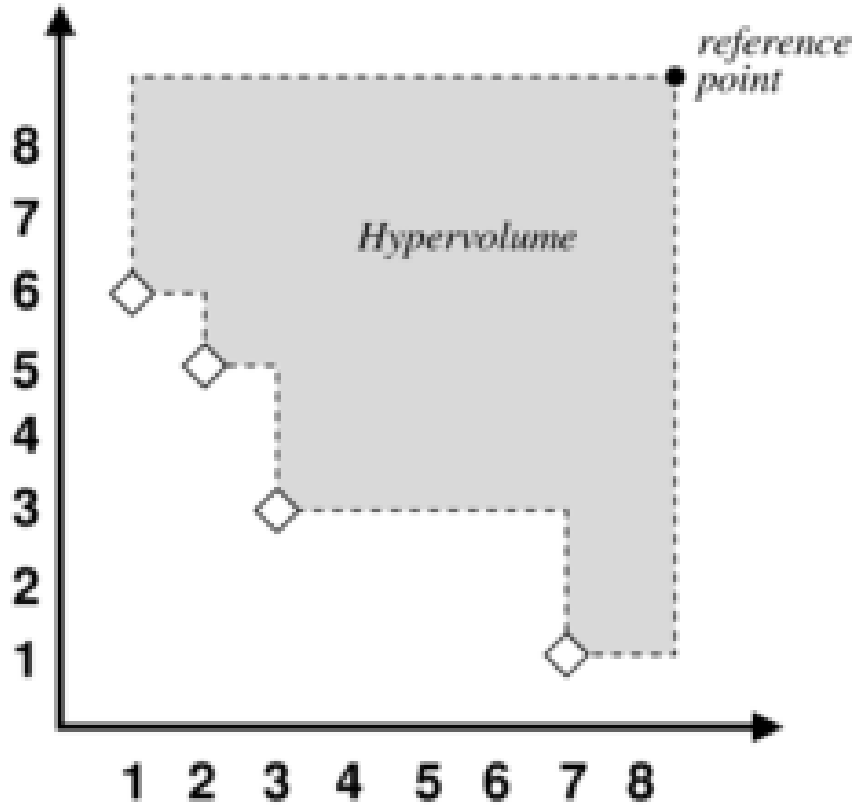
Weak compliance $\rightarrow$ if $A \lhd B$, $I(A)$ better or equal to $I(B)$ **in all cases**

(Strict) compliance $\rightarrow$ if $A \lhd B$, $I(A)$ better to $I(B)$ **in all cases**

Unfortunately, IGD **is not Pareto compliant** (neither strictly or weakly)

Quality Indicators

Hypervolume (S-metric, Lebesgue measure) - strictly Pareto compliant



Comparing Optimisers

- There are a large number of different ways of implementing multi-objective algorithms
- Given there are many different multi-objective optimisers, how do we select which algorithms are better than others on particular problems?
- Different optimisers will have different properties, e.g. computational complexity, scalability (in terms of objectives and/or solution parameters), convergence, spread and performance on quality indicators.

Often you will not be able to compare on all of these properties, and will therefore select some subset which is most appropriate.

Sources of variation in Optimisers

1. Different optimisers (different operators).
2. Different parametrisations (meta-parameters) of the algorithms.
3. Stochastic nature of the algorithms.
4. Starting points of the algorithms.
5. Errors in implementation.
6. Noise in the evaluations/parameters.

Summary

- Lots of quality measures/indicators in the literature for multi-objective optimisation (over 100!)
- Most of them have issues/drawbacks