Surrogate-assisted optimisation

Prof. Juergen Branke

About myself

- Professor of Operational Research
- Warwick Business School, UK
- EA researcher for 27 years
- Main research areas
  - Optimisation under uncertainty
  - Multi-objective optimisation
  - Simulation-based optimisation
- Area/Associate Editor of IEEE Trans Evol. Comp., Evol Comp. Journal, Journal of Heuristics, Journal of Multi-Criteria Decision Analysis

Surrogate assisted optimisation

Motivation - How long can you wait?

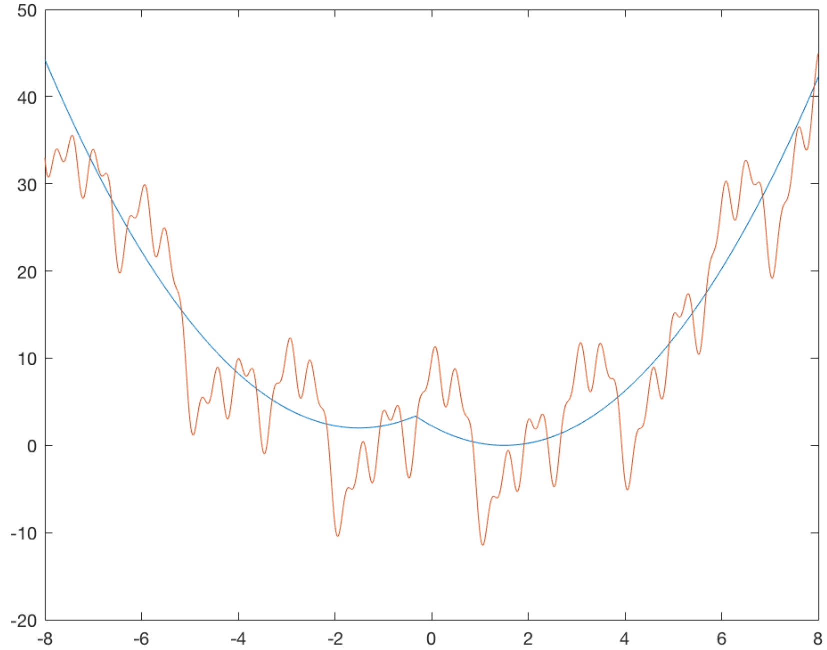
- EAs typically require thousands of function evaluations
- Let us assume we need 100,000 evaluations
- If every evaluation takes 1 minute…
- … this is 70 days runtime!

Motivation (2)

- Evaluating a single solution can be computationally very expensive
- Evaluating a solution can be costly
- Evaluating a solution can be dangerous
- Evaluating a solution may require user interaction

→ Number of fitness evaluations is limited

Surrogate models



- “Substitute”
- Often also called “Metamodel”
- Much cheaper, but not necessarily as accurate
- Replace some of the expensive function evaluations by surrogate-model based evaluations

Where does the surrogate model come from?

Simplified:

- More coarse grained simulation
- Smaller simulation
- Abort simulation early

Learned:

- From data systematically sampled from search space
- From data collected during the run

Surrogate assisted optimisation – design questions

- Type of model
  - Linear/quadratic regression, Gaussian Process, Artificial Neural Network, Ensemble, etc.
- Training data
  - Global vs. local models
- Which individuals to evaluate based on metamodel, which on full model

How to choose a surrogate model

- Model flexibility: how rugged is the underlying landscape?
- Do we need a local or a global model?
- Is the full evaluation deterministic or stochastic?
- Computational complexity: How long does it take to train? To evaluate?
- Does it provide an error estimate?

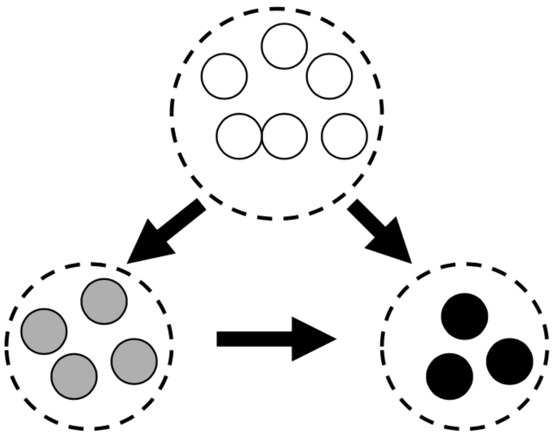
Basic model management strategies

Which individuals to evaluate with full model?

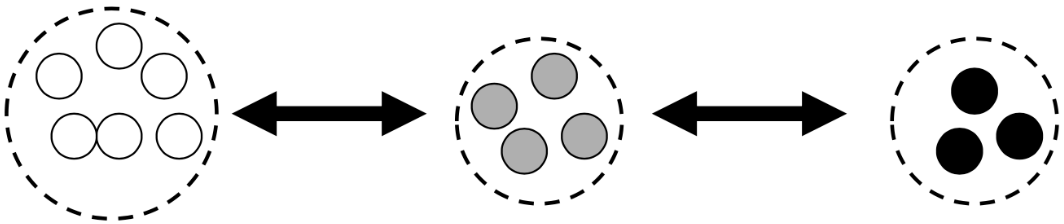
- Population based
- Generation based
- Individual based
- Trust-region method in local search

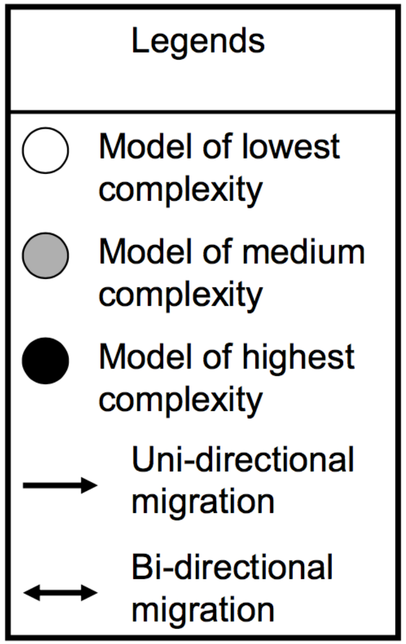
Population-based model management

- Injection island model (Eby et al, 1998)

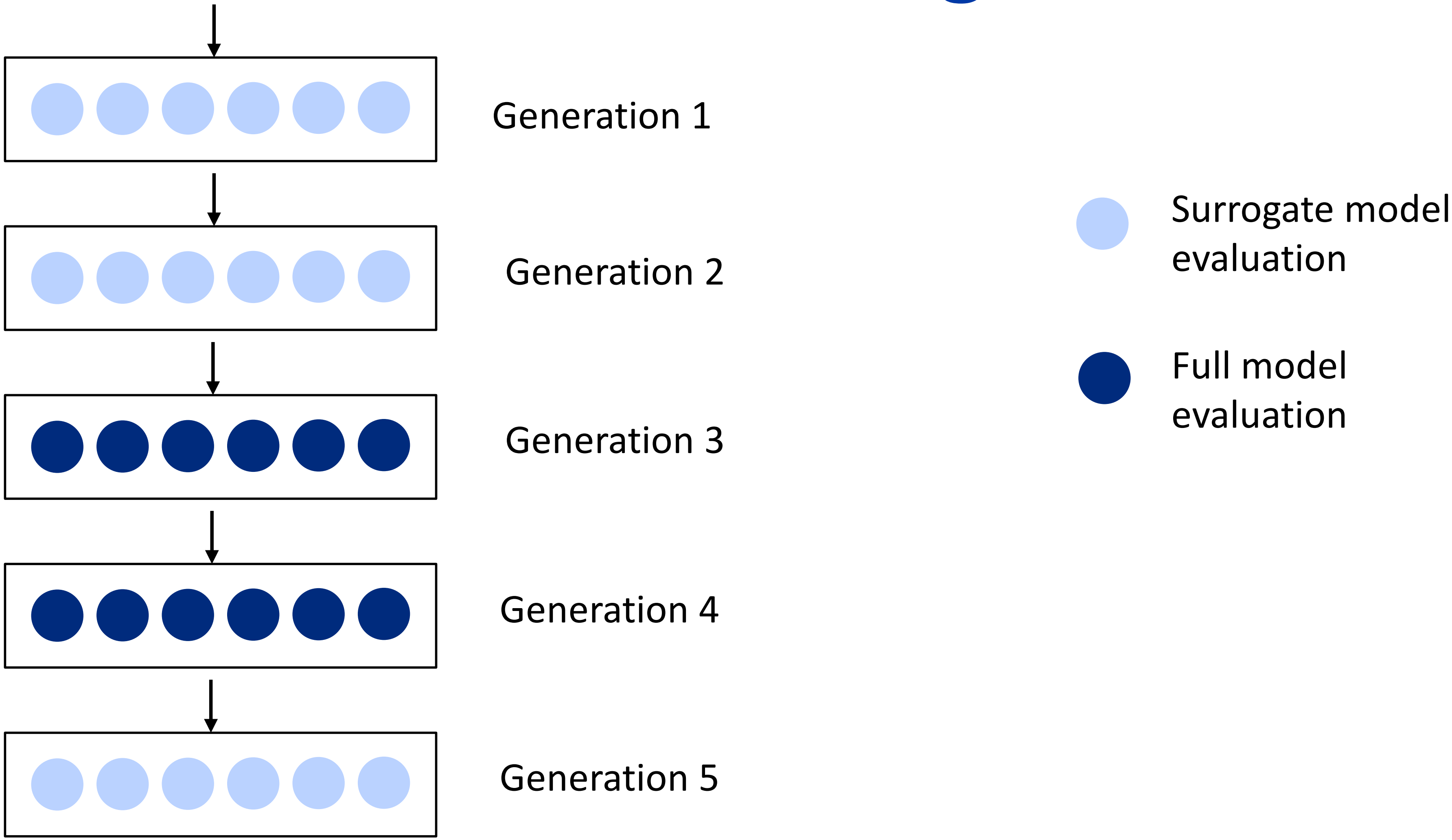


- Hierarchical model (Sefrioui and Periaux, 2000)

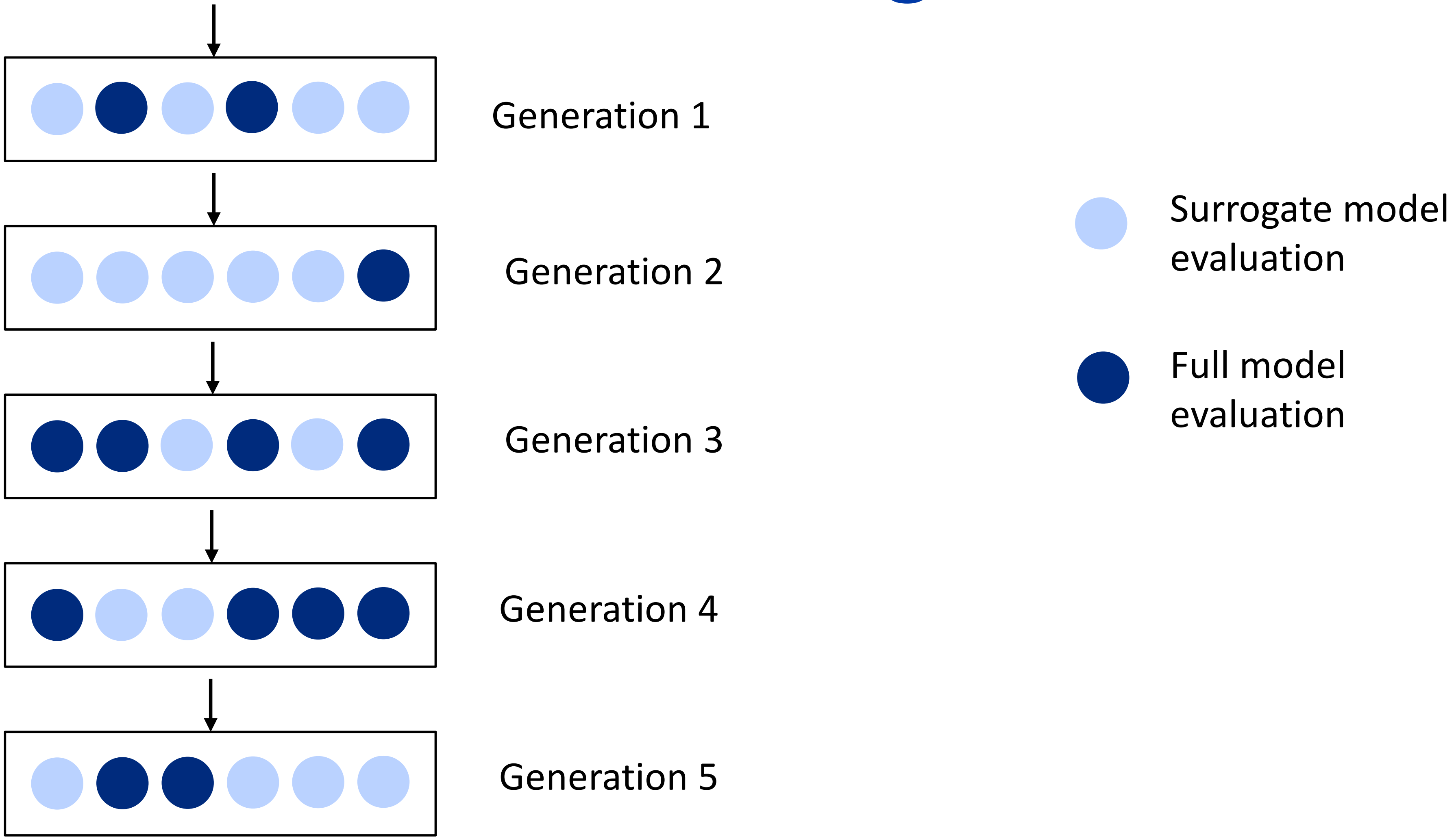




Generation-based management



Individual-based management



Which solutions to evaluate?

- Promising solutions?
- Representative solutions?
- Solutions where surrogate model is uncertain?
- Solutions that improve accuracy of surrogate model?
- Fixed or flexible budget?

Learning vs. optimisation

From an optimisation point of view, we want to

- Fully evaluate the best solutions
- Fully evaluate where we are most uncertain
- Ensure the selection works accurately

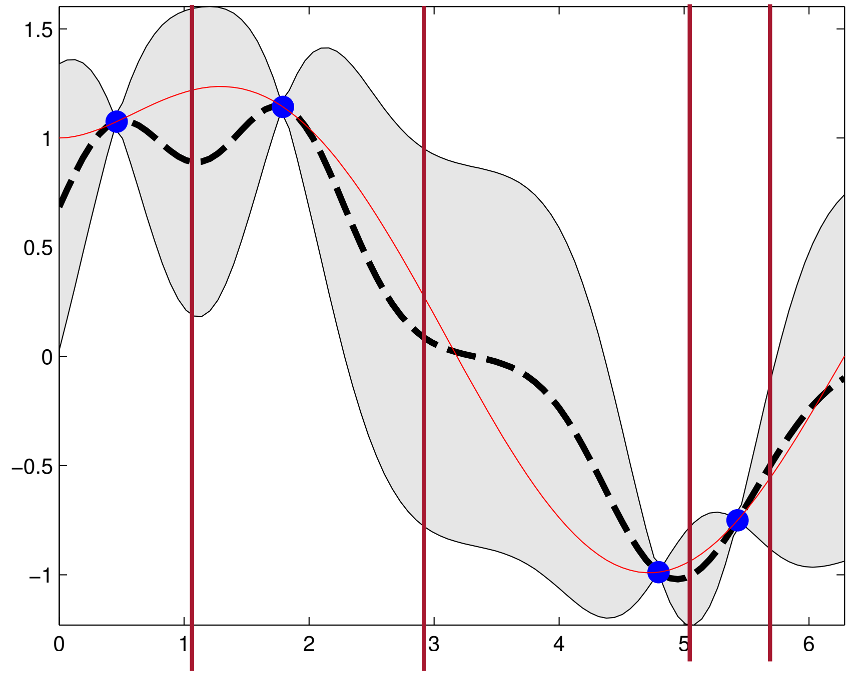
From a modelling point of view, we want to

- Evaluate where we can most improve model accuracy
- Evaluate where we are most uncertain

- EAs evaluate many solutions in promising areas, so these areas can be modelled accurately
- Model does not need to accurately predict fitness, only accurately predict ranking

Estimating uncertainty

- Uncertainty can be estimated by
  - Ensemble
  - Distance to fully evaluated solutions
  - Gaussian Process models

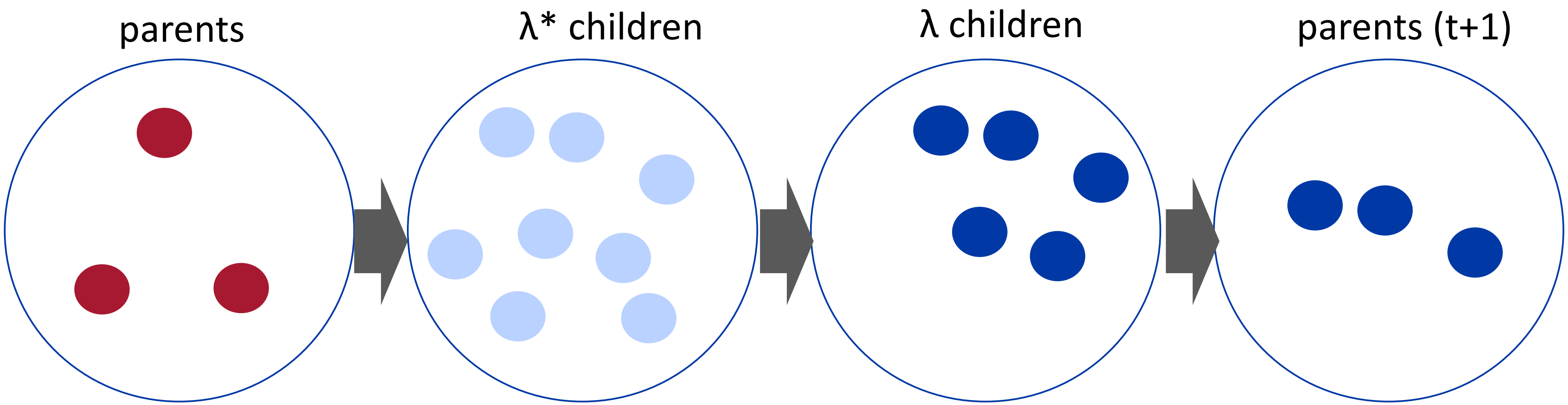


Most typical uses of metamodels

- Pre-selection
- Locally optimise each solution / Trust region method

Pre-selection

- Generate an abundance of children
- Pre-select λ children based on metamodel
- Fully evaluate pre-selected children

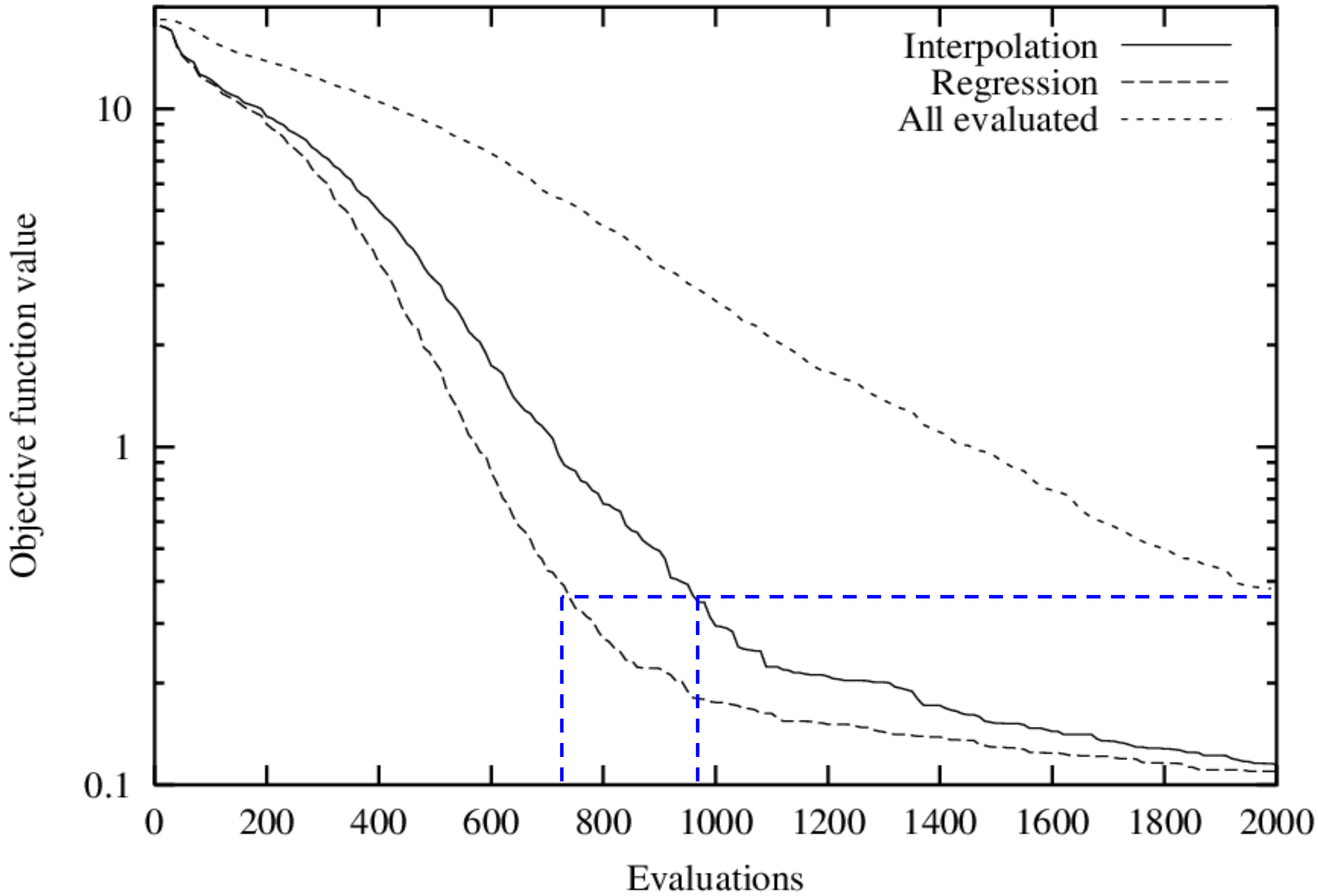


Trust region method

For each individual

- Repeat at most k times, or until no better solution found
  - Build local surrogate model
  - Perform local search on surrogate model within Trust region
  - Evaluate best found solution
  - Replace individual with best found solution if better
  - Adapt Trust region

Benefit [Branke&Schmidt 2004]

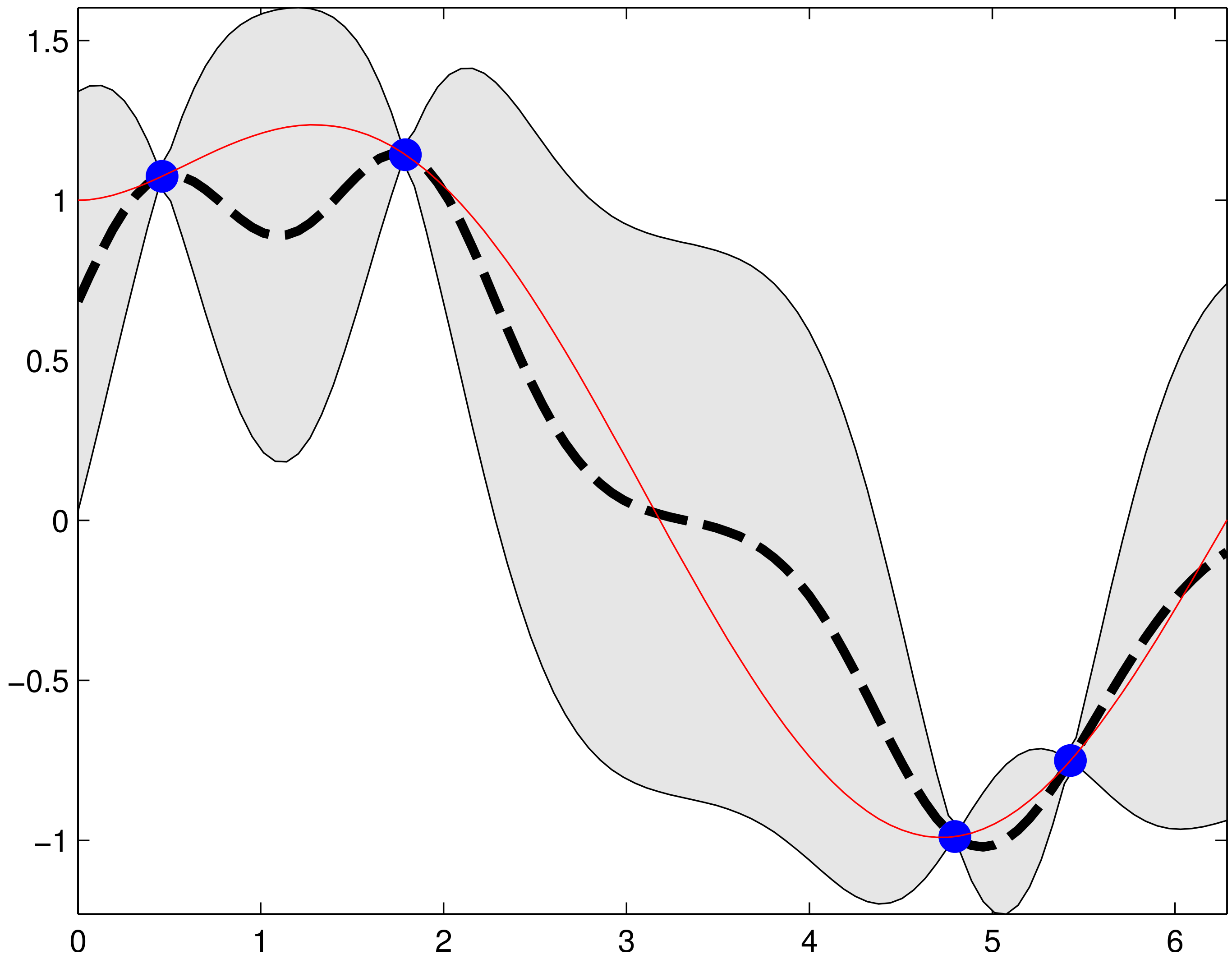


Efficient Global Optimisation (EGO)

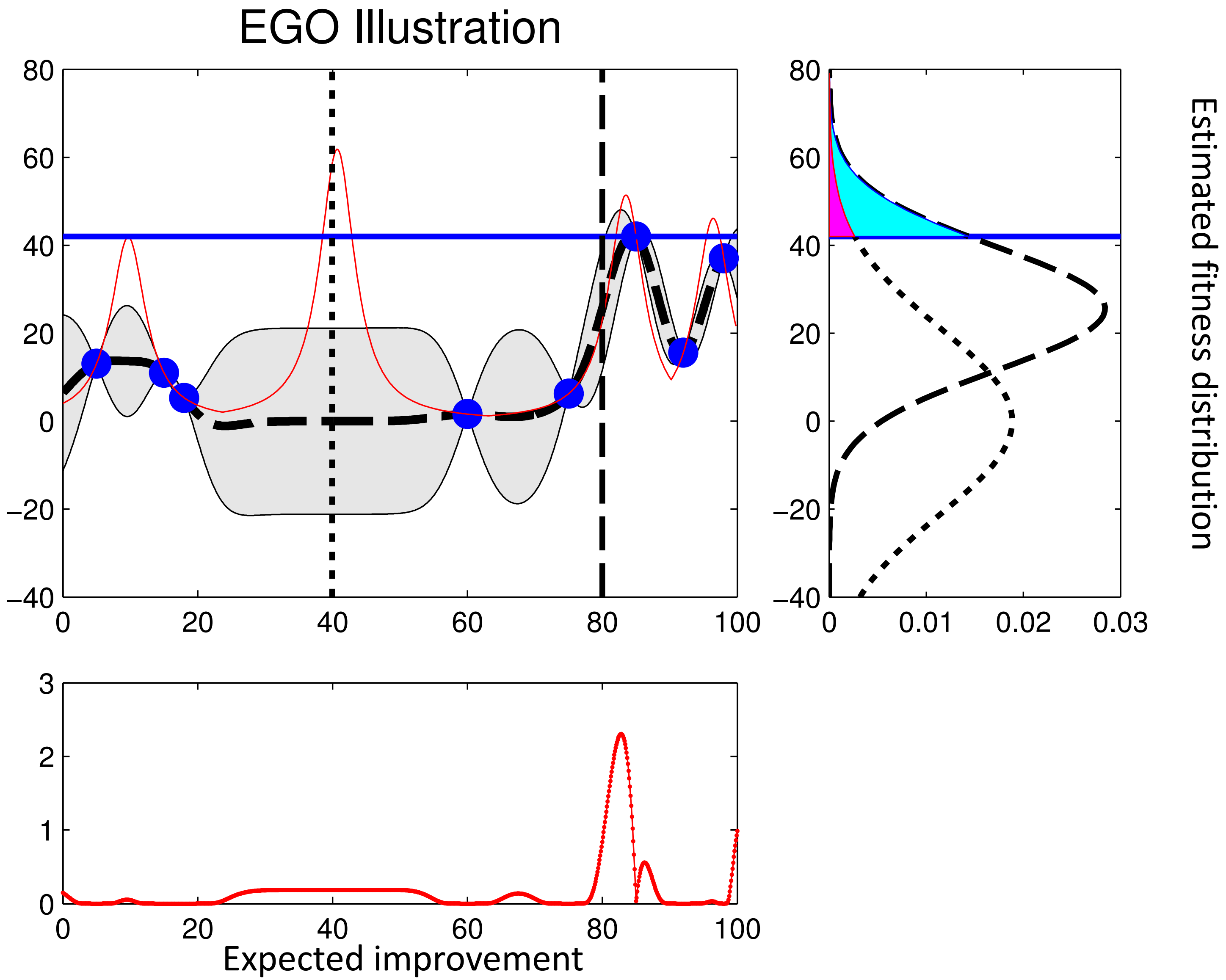
[Jones, Schonlau, Welch 1998]

- Collect some data
- Fit a Gaussian Process (GP) to data
- Response model provides information about
  - expected value
  - uncertainty
- Use response model to determine next data point (replacing crossover and mutation!)
- Expected improvement makes explicit trade-off between exploration and exploitation

Example: GP in 1 dimension



Max expected improvement principle



EGO algorithm

Take initial n_0 samples

Build GP model

WHILE stopping criterion not met DO

    Estimate hyperparameters using maximum likelihood estimation

    Take additional sample at position with maximum EI

    Update GP model

Return best found solution

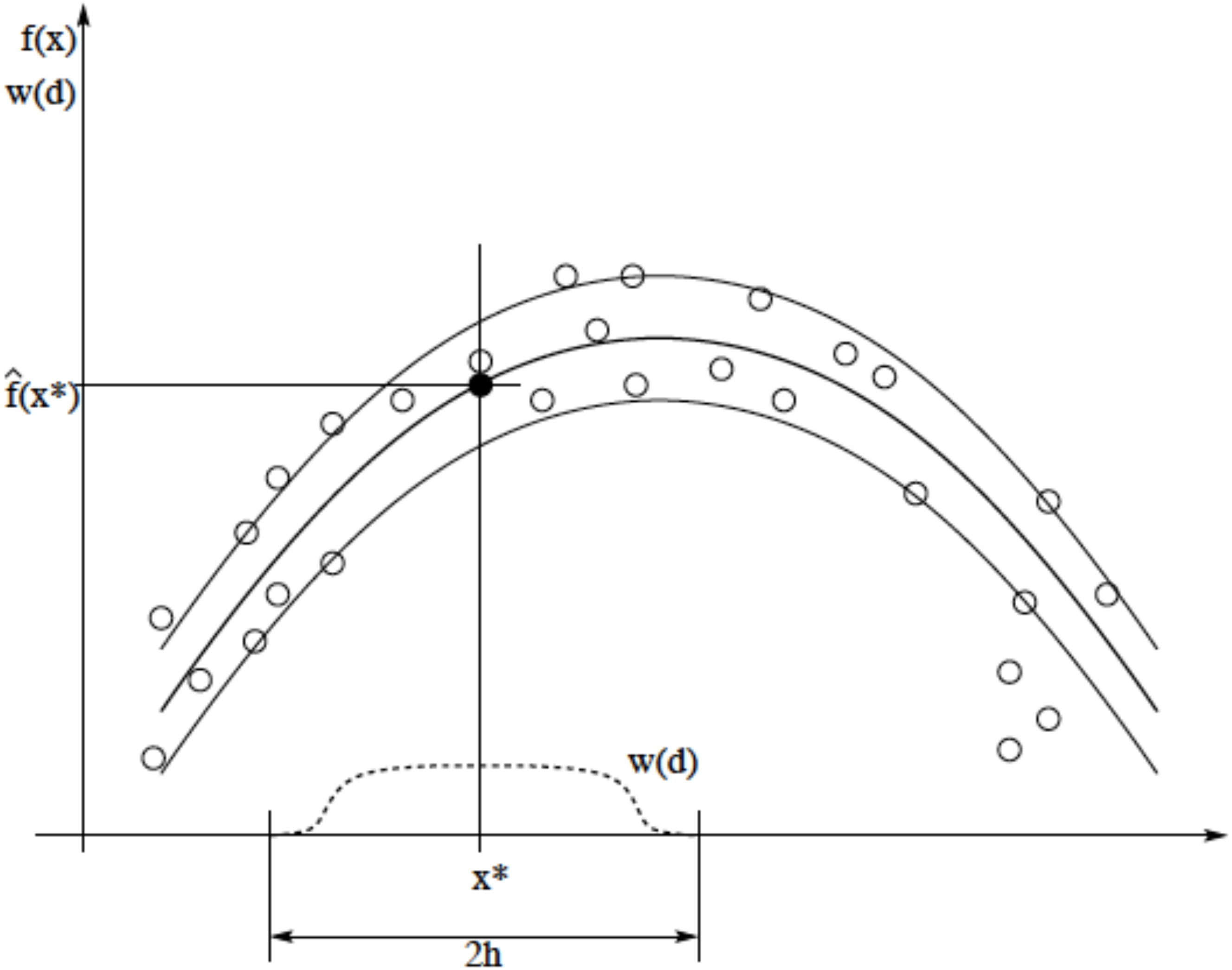
Surrogate for Genetic Programming

- GP typically uses a tree representation
- Surrogate models require distance metric
- Different trees can encode the same solution
  - Permutations
  - Equal meaning
  - Bloat
- Not clear how to define distance between trees

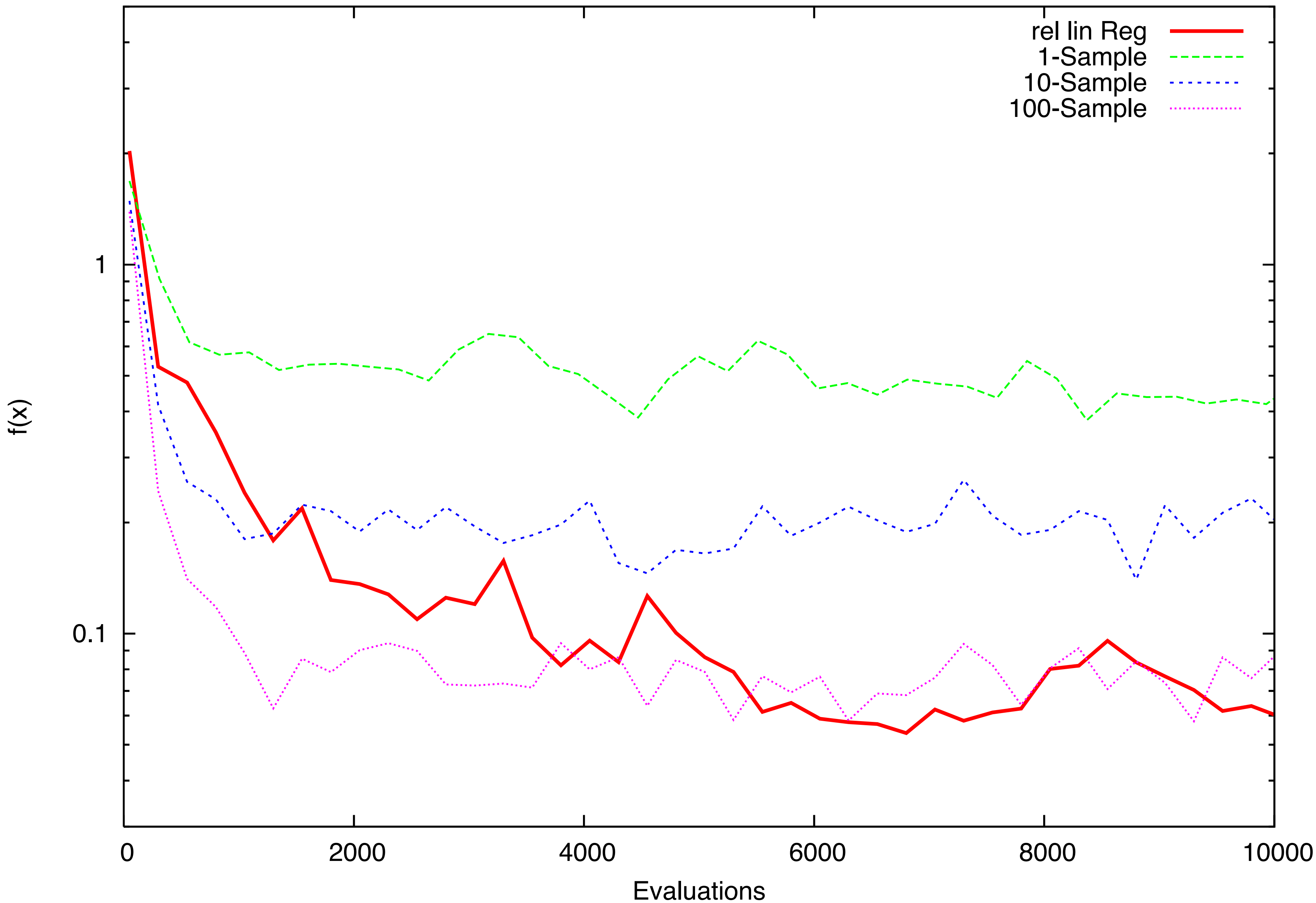
Idea: Phenotypic distance [Hildebrandt & Branke 2015]

- Distance not between genotypes (trees) but between behaviour
- Problem specific
- Example: Dispatching rules for scheduling
  - How do they rank a set of jobs?

Surrogates and noise – average over space [Branke & Schmidt 2001]



Benefit


rel lin Reg
1-Sample
10-Sample
100-Sample
1
0.1
f(x)
0
2000
4000
6000
8000
10000
Evaluations

Conclusion

- Surrogate models are a powerful way to reduce the computation time
- Various ways to decide which individuals should be evaluated with the full model
  - Pre-selection
  - Trust-region local search
- Efficient Global Optimisation
- Surrogates for GP
- Surrogates with noise

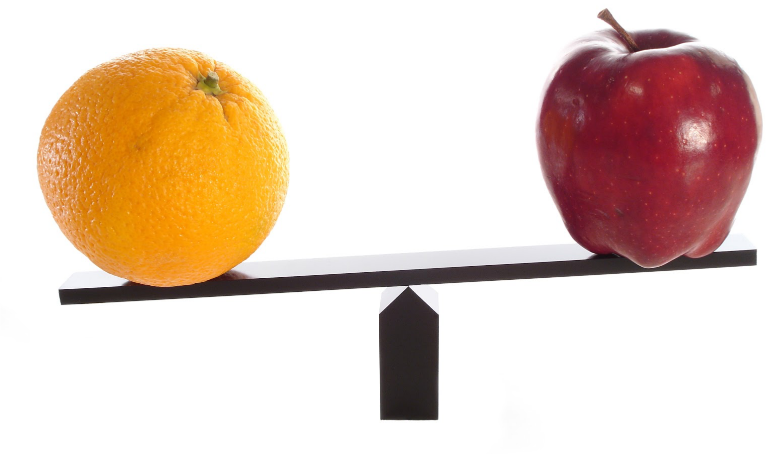
More research needed

- Theory
- Combinatorial optimisation
- Interactive evolution
- Multi-fidelity optimisation
- Constraint handling
- High dimensional problems
- Multi-objective problems


QUESTIONS

Assignment 1 –
Statistical tests used at GECCO

- EAs are stochastic algorithms
- A single run is never sufficient to compare EAs
- Statistical tests are needed to make comparisons with confidence



Assignment 1 – Statistical tests used at GECCO

1. Go through the papers at GECCO, compile some summary statistics regarding what statistical tests are used
2. Talk to some of the presenters and ask why they have or have not used a particular test
3. Compile a recommendation which test should be used depending on the experiments performed

Assignment 2 - Statistical test in practice

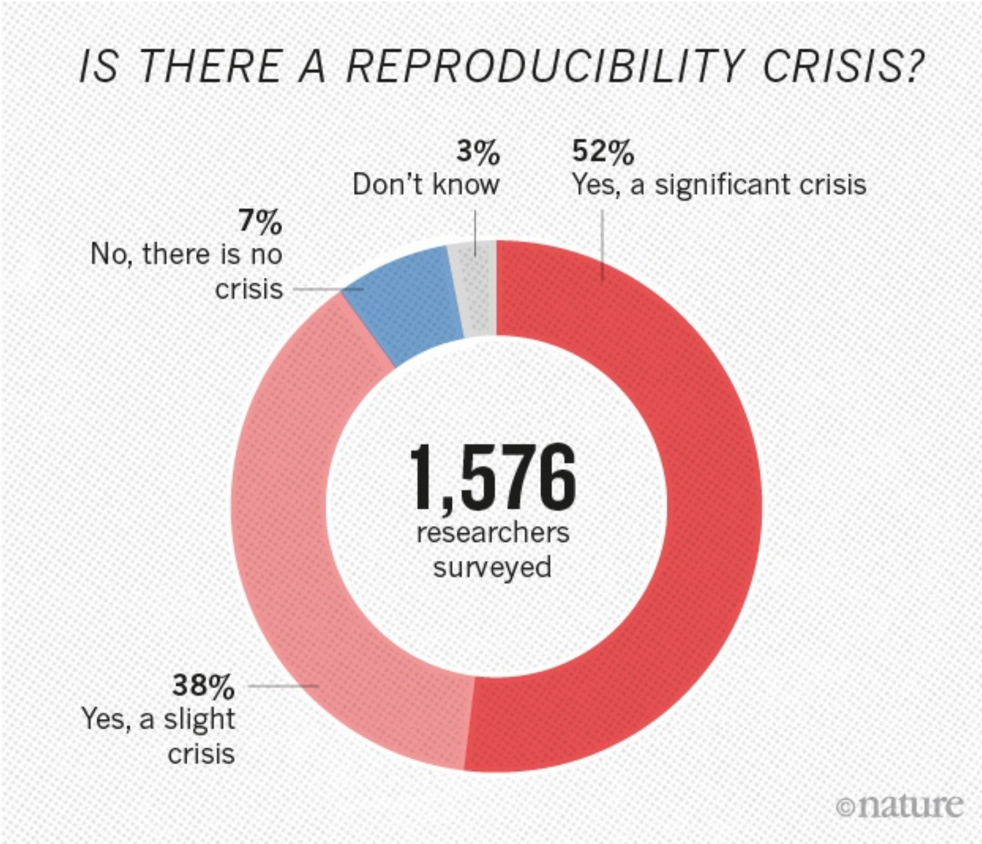
1. Take two standard EAs implemented in any package, or even a single algorithm, but with two different parameter settings. Compare them on an optimisation problem of your choice

Assignment 2 - Statistical test in practice

2. Answer the following questions:
    - How does the number of replications influence the results?
    - How does the runtime (number of evaluations) influence your conclusions?
    - What do your results say about the relative performance on some other optimisation problem? On the same optimisation problem but a larger number of dimensions?
3. Compile a recommendation on how to compare algorithms

Assignment 3
Reproducing scientific results

- "A scientific result is not truly established until it is independently confirmed"
- Many published results are not reproducible

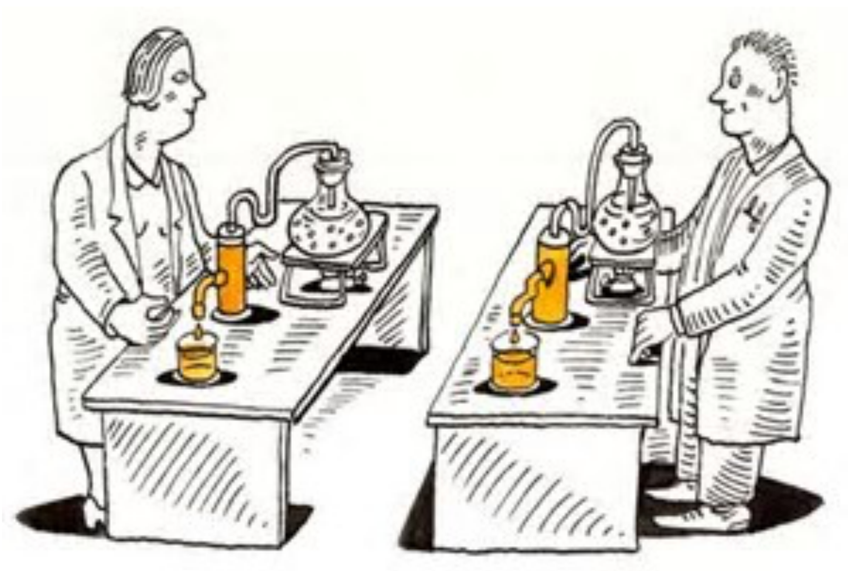


Assignment 3
Reproducing scientific results

1. Choose any paper presented at GECCO, and try to replicate its results
2. Keep a detailed record of all the challenges you faced
   - Description ambiguous
   - Algorithm details missing
   - No access to data
   - Different hardware
   - ...

Assignment 3
Reproducing scientific results

3. Make some recommendations for reproducible science in evolutionary computation



Expected deliverable

- Short written report, summarizing the main observations and conclusions
- 10 min presentation to be held in front of the panel

I’m looking forward to working with you!