Bayesian optimisation

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Problem statement

$$x^* = \arg\max_x f(x)$$

Constraints:

- f is a black box for which no closed form is known;
  - gradients $\frac{df}{dx}$ are not available.
- f is expensive to evaluate;
- uncertainty on observations y_i of f (i.e., $y_i = f(x_i) + \epsilon_i$).

Goal: find x^* while minimizing the number of evaluations $f(x)$.

Disclaimer

If you do not have these constraints, there is certainly a better optimisation algorithm than Bayesian optimisation.

(e.g., L-BFGS-B, Powell's method (as in Minuit), etc)

Bayesian optimisation

for $t = 1 : T$,

1. Given observations (x_i, y_i) for $i = 1 : t$, build a probabilistic model for the objective f;

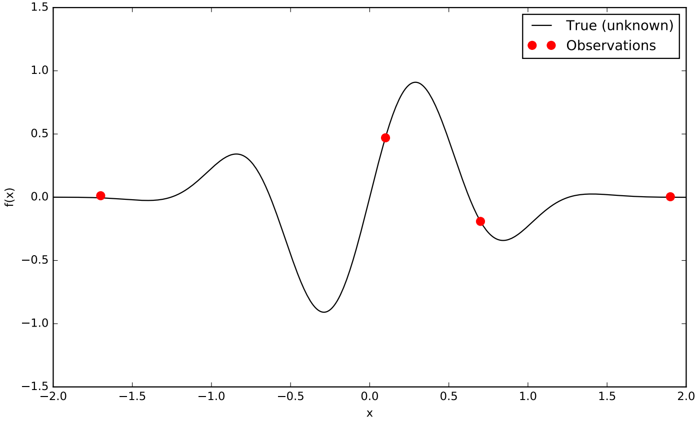
2. Compute the posterior predictive distribution;
   - Integrate out all possible true functions, using Gaussian process regression.

3. Optimise a cheap utility function u based on the posterior for sampling the next point.

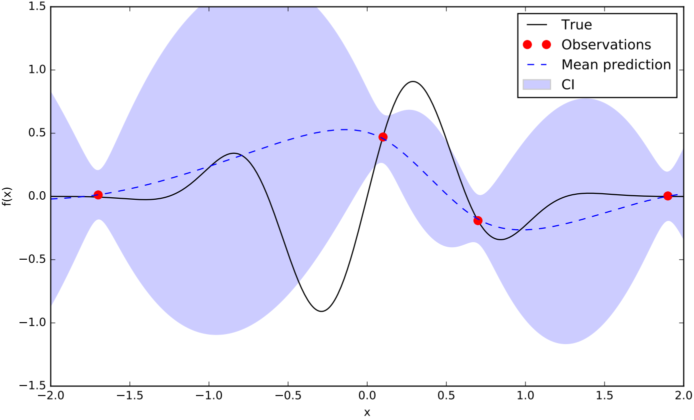
   $$x_{t+1} = \arg\max_x u(x)$$

   Exploit uncertainty to balance exploration against exploitation.
4. Sample the next observation y_{t+1} at x_{t+1}.

Where shall we sample next?



Build a probabilistic model for the objective function



This gives a posterior distribution over functions that could have generated the observed data.

Acquisition functions

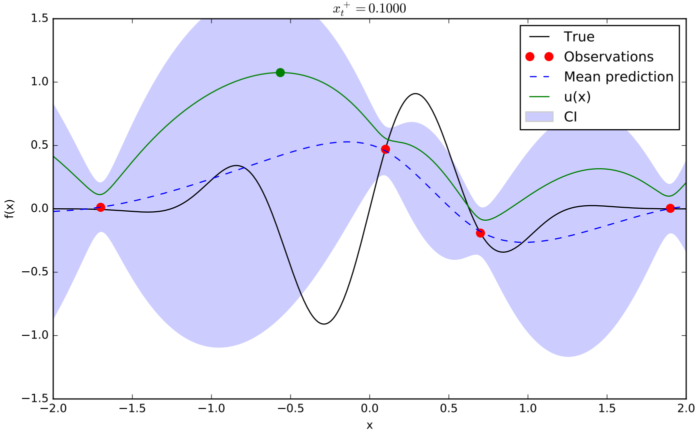
Acquisition functions $\mathrm{u}(x)$ specify which sample x should be tried next:

- Upper confidence bound $\mathrm{UCB}(x) = \mu_{GP}(x) + \kappa\sigma_{GP}(x)$;
- Probability of improvement $\mathrm{PI}(x) = P(f(x) \geq f(x_t^+) + \kappa)$;
- Expected improvement $\mathrm{EI}(x) = \mathbb{E}[f(x) - f(x_t^+)]$;
- ... and many others.

where x_t^+ is the best point observed so far.

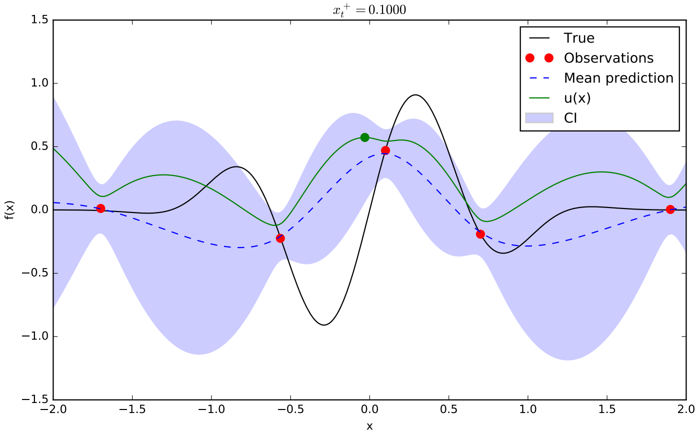
In most cases, acquisition functions provide knobs (e.g., κ) for controlling the exploration-exploitation trade-off.

Plugging everything together ($t = 0$)

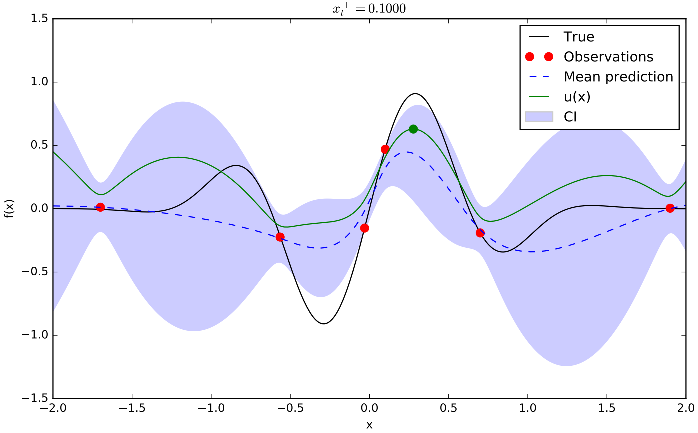


$$x_{t+1} = \arg\max_x \mathrm{UCB}(x)$$

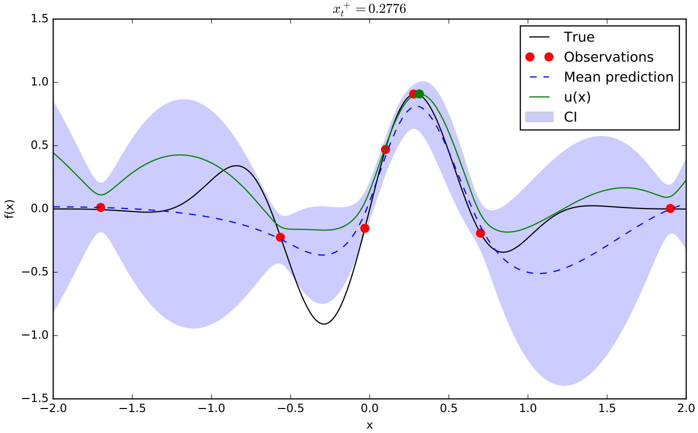
… and repeat until convergence ($t = 1$)



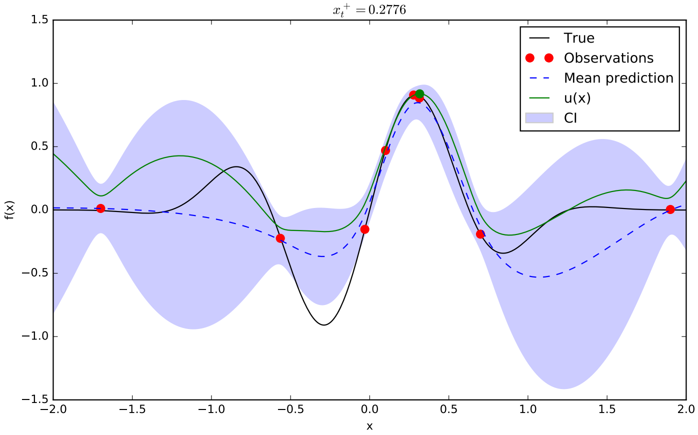
... and repeat until convergence ($t = 2$)



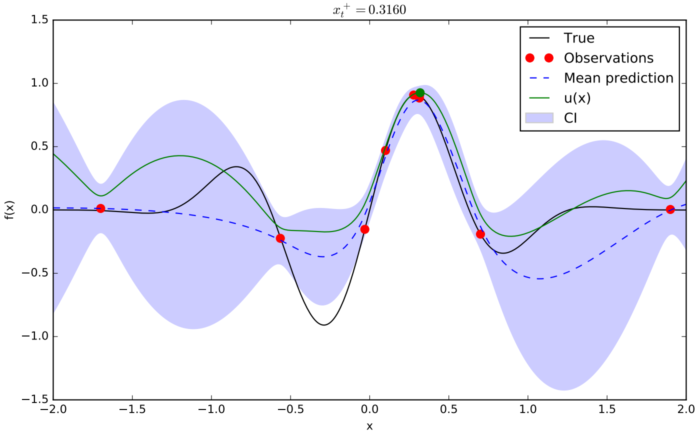
... and repeat until convergence ($t = 3$)



… and repeat until convergence ($t = 4$)



... and repeat until convergence ($t = 5$)



Limitations

- Bayesian optimisation has parameters itself!
  - Choice of the kernel
  - Parameter wrapping
  - Initialization scheme

- Gaussian processes usually do not scale well to many observations and to high-dimensional data.
  - Sequential model-based optimization provides a direct and effective alternative (i.e., replace GPs by a tree-based model).

Applications

- Bayesian optimization has been used in many scientific fields, including robotics, machine learning or life sciences.

- Use cases for high energy physics?
  - Optimisation of simulation parameters in event generators;
  - Optimisation of compiler flags to maximize execution speed;
  - Optimisation of hyper-parameters in machine learning for HEP;
  - ... ideas?

Software

Summary