Bayesian optimisation

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ATLAS ML workshop

March 30, 2016

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 $f(x)$.

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;

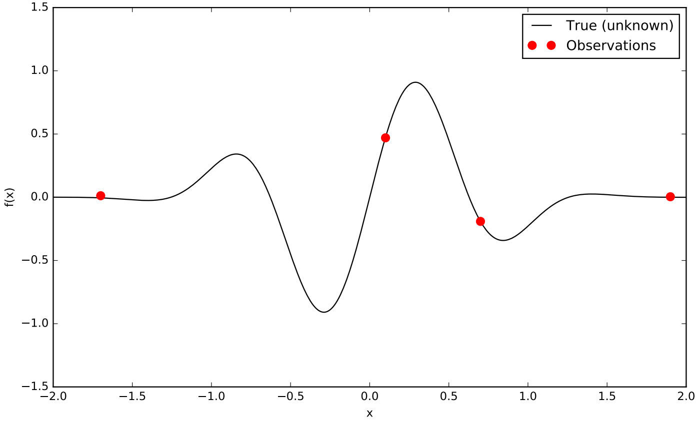
2. Compute the posterior predictive distribution;
   - Integrate out all possible true functions, using Gaussian process regression.

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

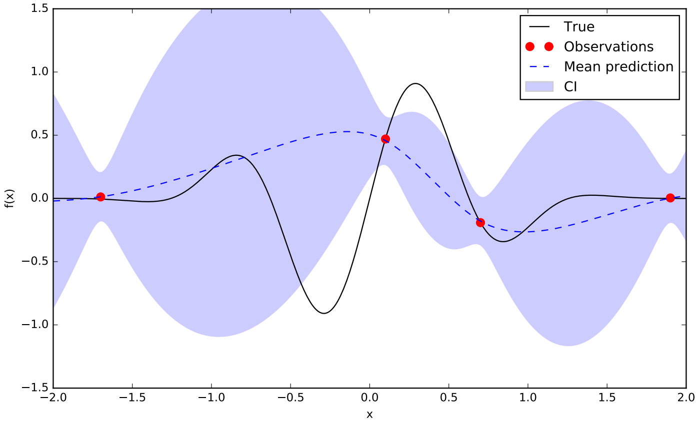
   $$x_{t+1} = \arg\max_x u(x)$$

   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

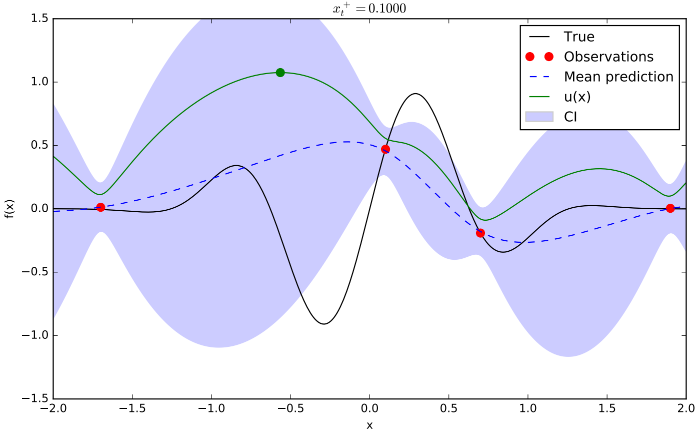
Acquisition functions $u(x)$ specify which sample x should be tried next:

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

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

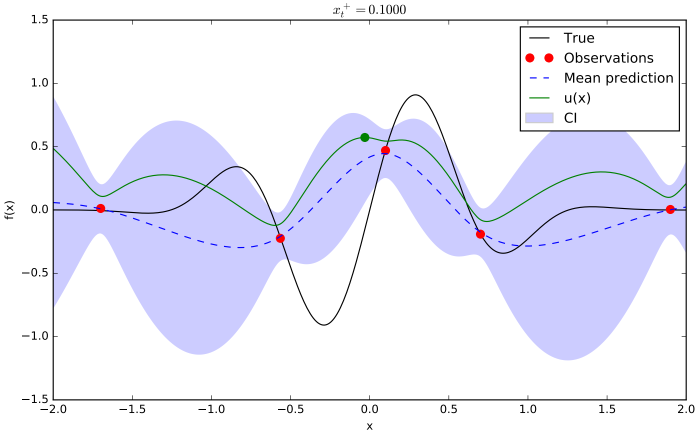
In most cases, acquisition functions provide knobs (e.g., κ) for controlling the exploration-exploitation trade-off.

Plugging everything together ($t = 0$)

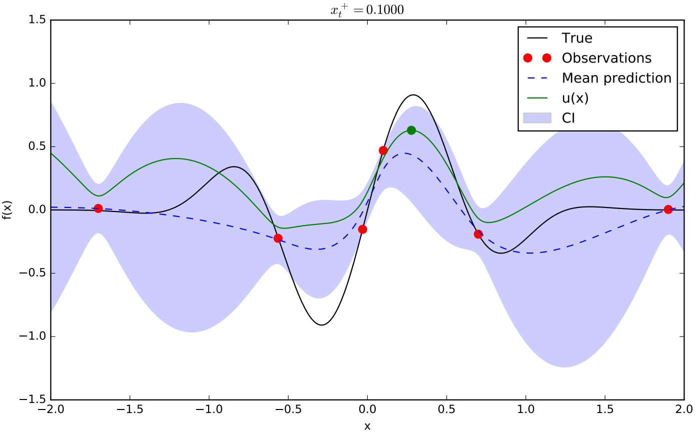


$$x_{t+1} = \arg\max_x \mathrm{u}(x)$$

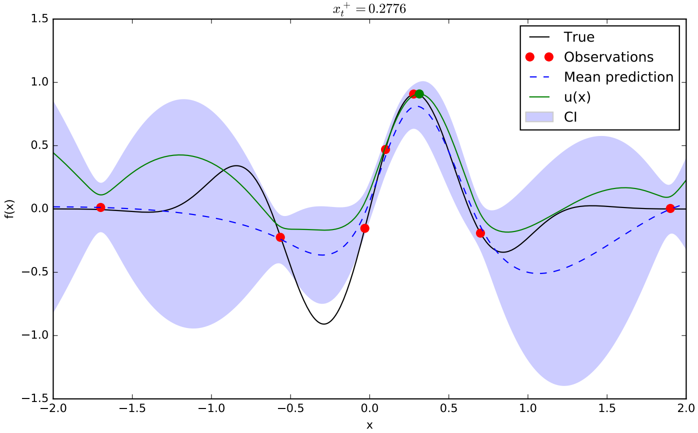
... and repeat until convergence ($t = 1$)



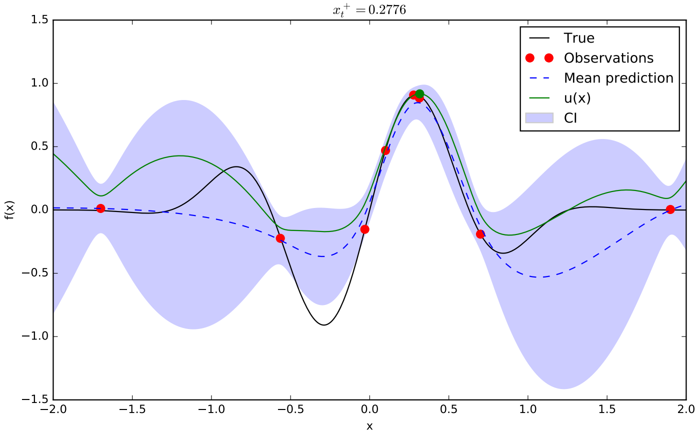
... and repeat until convergence ($t = 2$)



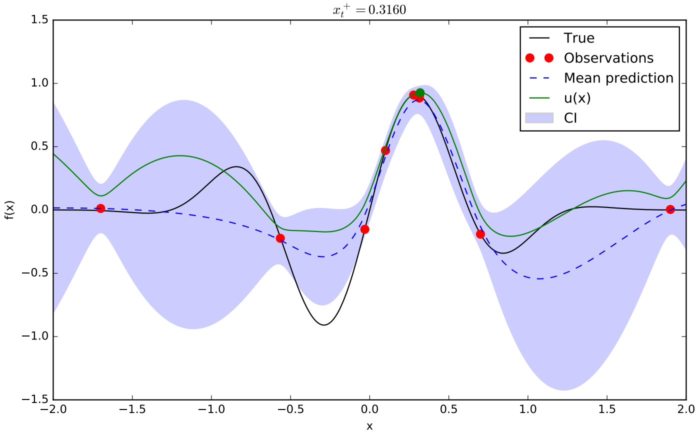
... and repeat until convergence ($t = 3$)



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



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



Applications in HEP?

Summary