Bayesian Machine Learning - Lecture 4

Guido Sanguinetti

Institute for Adaptive and Neural Computation
School of Informatics
University of Edinburgh
gsanguin@inf.ed.ac.uk

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Today's lecture

More types of learning

- We have considered extensively the supervised learning scenario, where data are input/ output pairs
- Often, the reason why we are interesting in predictions is that outputs are difficult/ expensive to collect
- Frequently, many *unlabelled* data instances are available
- *Semi-supervised learning* aims to improve predictions by somehow exploiting the empirical distribution of the inputs
- *Active learning* aims to devise query strategies for selecting informative labels
- **CAVEAT**: neither has any theoretical guarantees of working. But in practice they often do.

Active learning scenarios

- Assumption 1: there is an inexpensive mechanism to generate input points
- Assumption 2: there is an expensive mechanism to discover the label of arbitrary input points (*an Oracle*)
- Scenario 1: any input point is accessible (membership query synthesis)
- Scenario 2: input points come streaming, you need to choose whether to label or discard (stream-based selective sampling)
- Scenario 3: an empirical distribution of possible inputs is provided, from which we can easily sample (pool based sampling)

Illustrative diagram

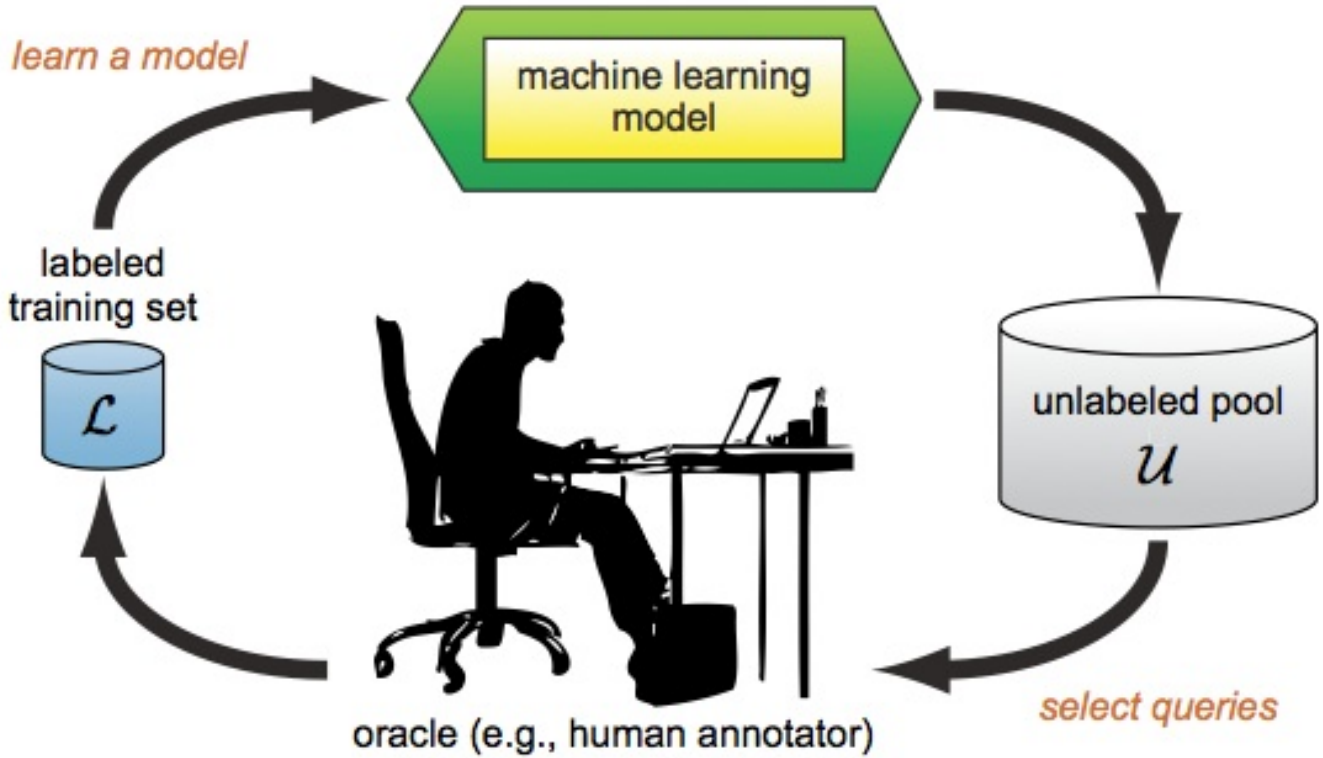


Figure taken from B. Settles, Active Learning Literature Survey, available at `burrsettles.com/pub/settles.activelearning.pdf`

Querying by uncertainty

- We'll focus on a classification pool based scenario for ease
- We assume we have a probabilistic model, i.e. something which provides us with a class probability for all input points (based on the observed labels)
- An obvious criterion for selecting a query is to focus on where you know least
- *Uncertainty sampling* selects as next query the input point for which the highest class probability is lowest
- *Entropy sampling* selects as next query the input point for which the entropy of the predictive distribution is highest
- The two are related (but not equivalent if more than two classes)

Querying by committee

- We assume that we have an ensemble of (probabilitstic) models
- The next query point is chosen as the one on which models disagree most
- Closely related to model selection
- The criteria for disagreement vary
- *Vote entropy* maximises the entropy of a vote distribution (drawbacks?)
- *KL selection* maximises the KL-divergence between models and an average model

Expected model change

- Another idea is to select the point that will lead to the largest change in model parameters
- Theoretically, one should loop through all points and all possible outcomes; clearly impossible
- For models trained by gradient-based methods, one can evaluate the expectation of the likelihood gradient and choose the point with largest gradient

Bayesian Optimisation and Active Learning

- Active learning proposes a dynamic world-view where learning takes place in cycles, intelligently selecting instances to query
- Bayesian Optimisation uses similar ideas to tackle optimisation
- It replaces a hard optimisation problem with an iterative approach where an easier problem is solved at every iteration
- Closely related to Reinforcement Learning (which I will not discuss in this course)

Reasons why optimisation is hard

- Optimisation is the task of finding a global optimum of a function
- Optimisation can be hard because the function has multiple local optima, or because the function argument is very high dimensional
- Optimisation can be hard also because the function is difficult to evaluate
- Example 1: global weather models map parameters and initial conditions to predicted temperature at a spot. This function needs to be computed on a supercomputer
- Example 2: hydro-solubility of a protein depends on its ammino-acid sequence. This function (of a discrete variable) is computed by engineering new proteins!
- Bayesian Optimisation can help in this case

BO key idea and terminology

- At every step of the algorithm, we have a few function evaluations and want to select a point where to evaluate the function next
- **KEY IDEA**: treat the function as a random variable, use the existing function evaluations to compute a *posterior* distribution over the functions, and use this distribution to select the new point
- The posterior mean is called the *surrogate function*
- The surrogate is used to create an *acquisition function* which is maximised to find the next evaluation
- The measure of success is the *cumulative regret*

$$R_T = \frac{1}{T}\sum_{t=1}^{T}(f(x_t) - f(x^*))^2$$

- Let's see an example

Exploration-exploitation

- It will come as no surprise that GPs can be used in Bayesian optimisation to construct a surrogate function
- Directly optimising the surrogate however is a bad idea (why?)
- One needs a strategy to trade-off *exploitation* (looking around areas which you know to be promising) and *exploration* (checking out areas which you don't know much about)

The GP-UCB rule

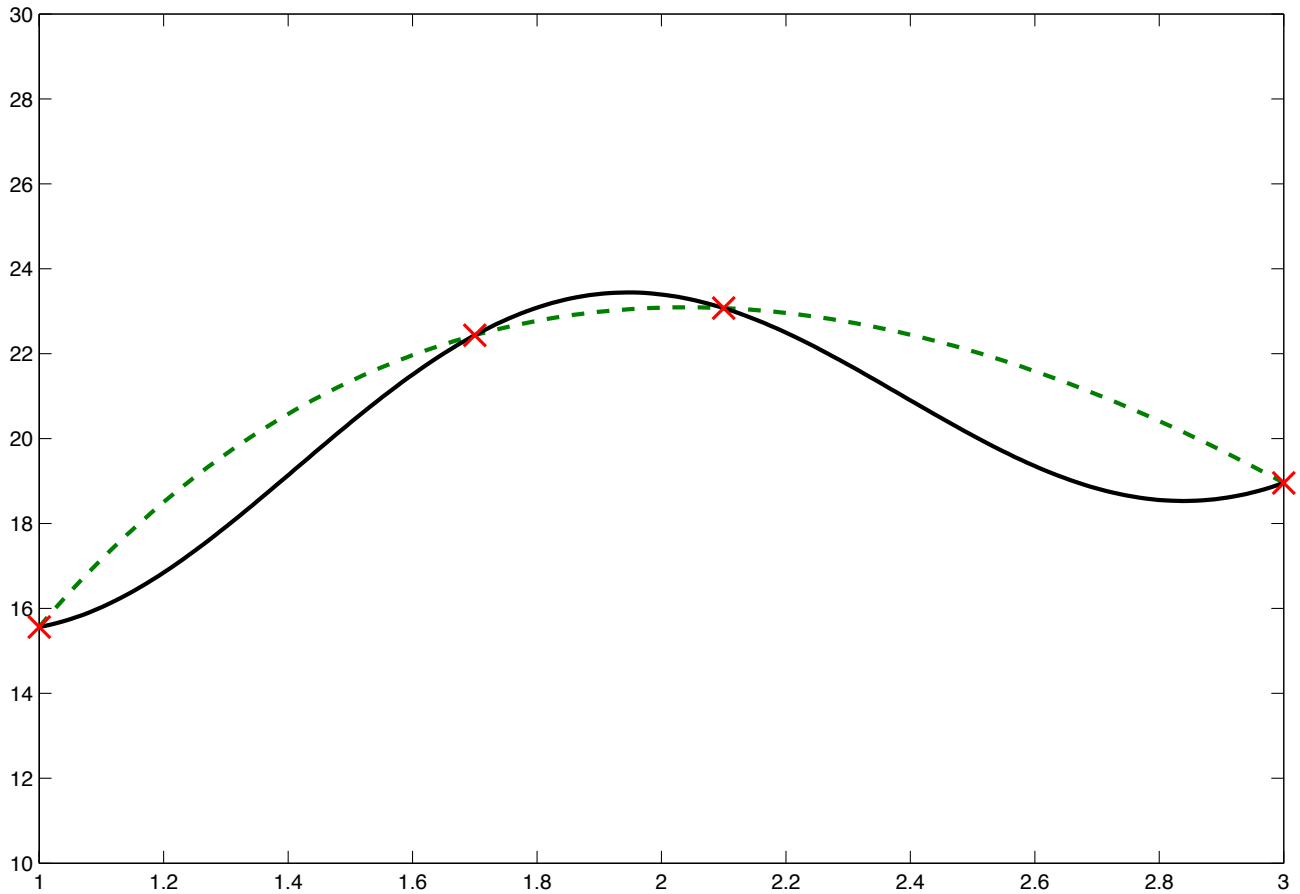
- GPs also provide uncertainty quantification (in fact, they provide full distributions on outputs at any point)
- One can trade-off exploration and exploitation by selecting regions where the function could conceivably be high, rather than regions where we expect it to be high
- The Gaussian Process Upper Confidence Bound (GP-UCB) algorithm maximises the following acquisition function to select its next point

$$F(x) = E[f(x)] + \beta_t \sqrt{var(f(x))}$$

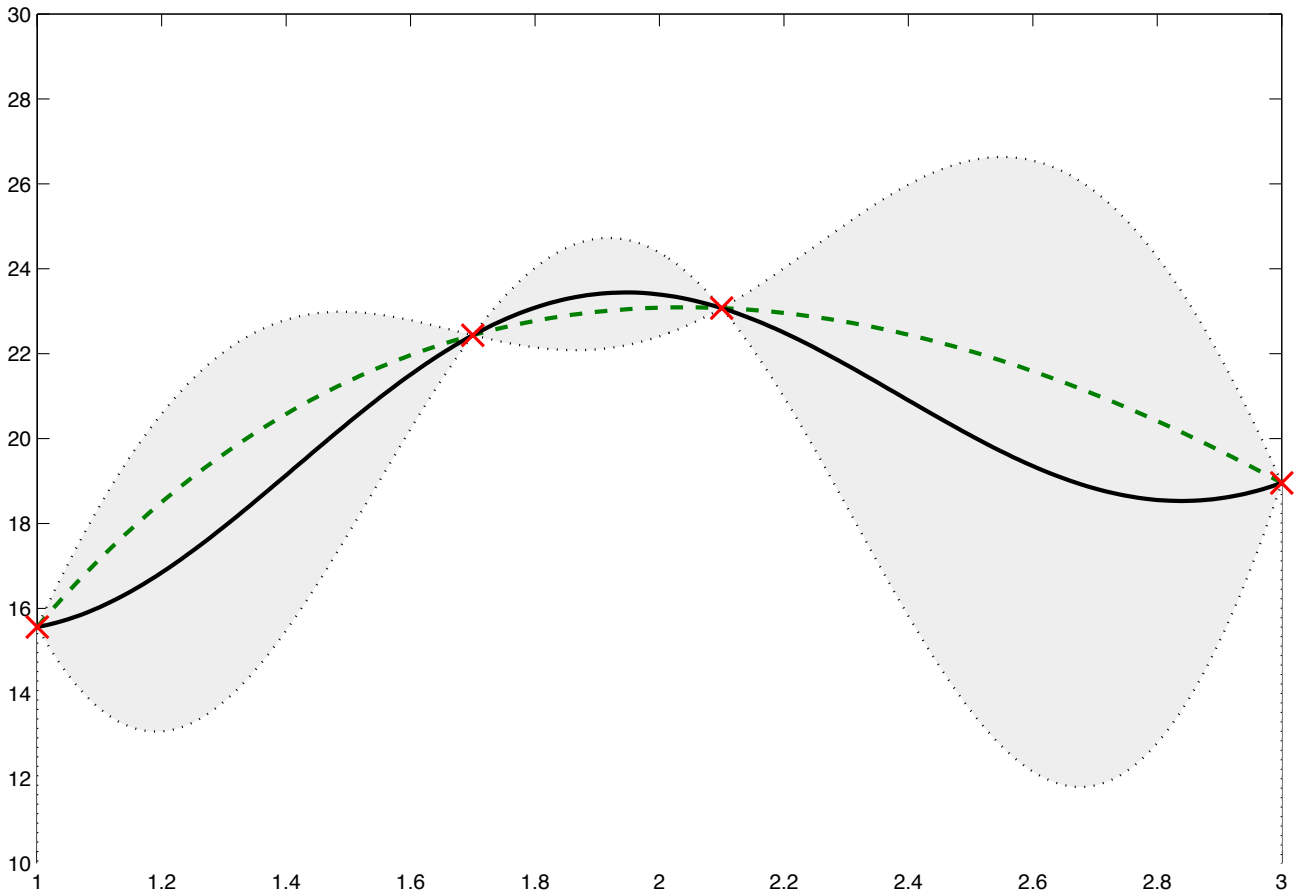
which is an upper quantile of the single point marginals

- Surprisingly, Srinivas et al proved that this algorithm is globally convergent in probability, i.e. given δ, ϵ with probability $1 - \epsilon$ the regret will become smaller than δ

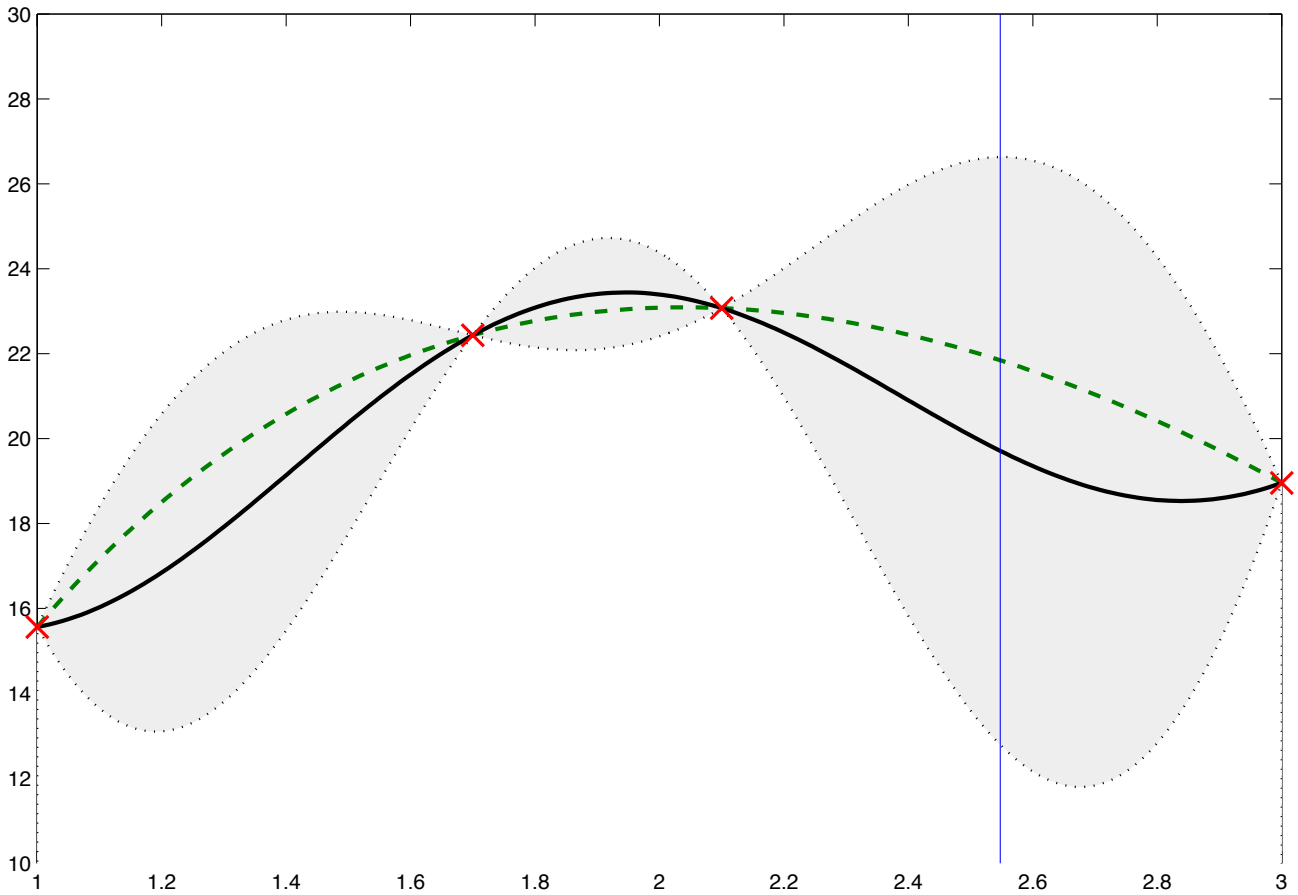
The GP-UCB algorithm - example



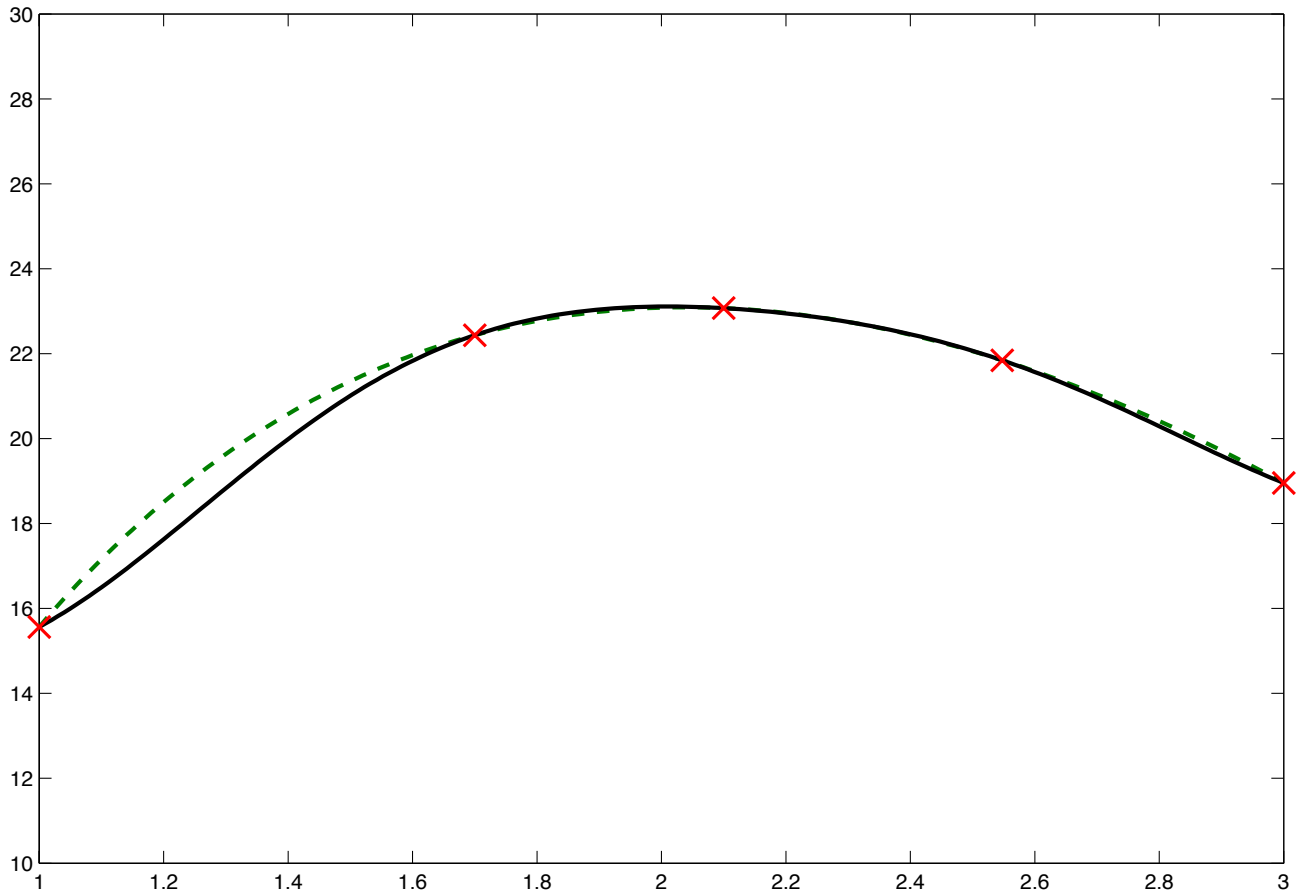
The GP-UCB algorithm - example



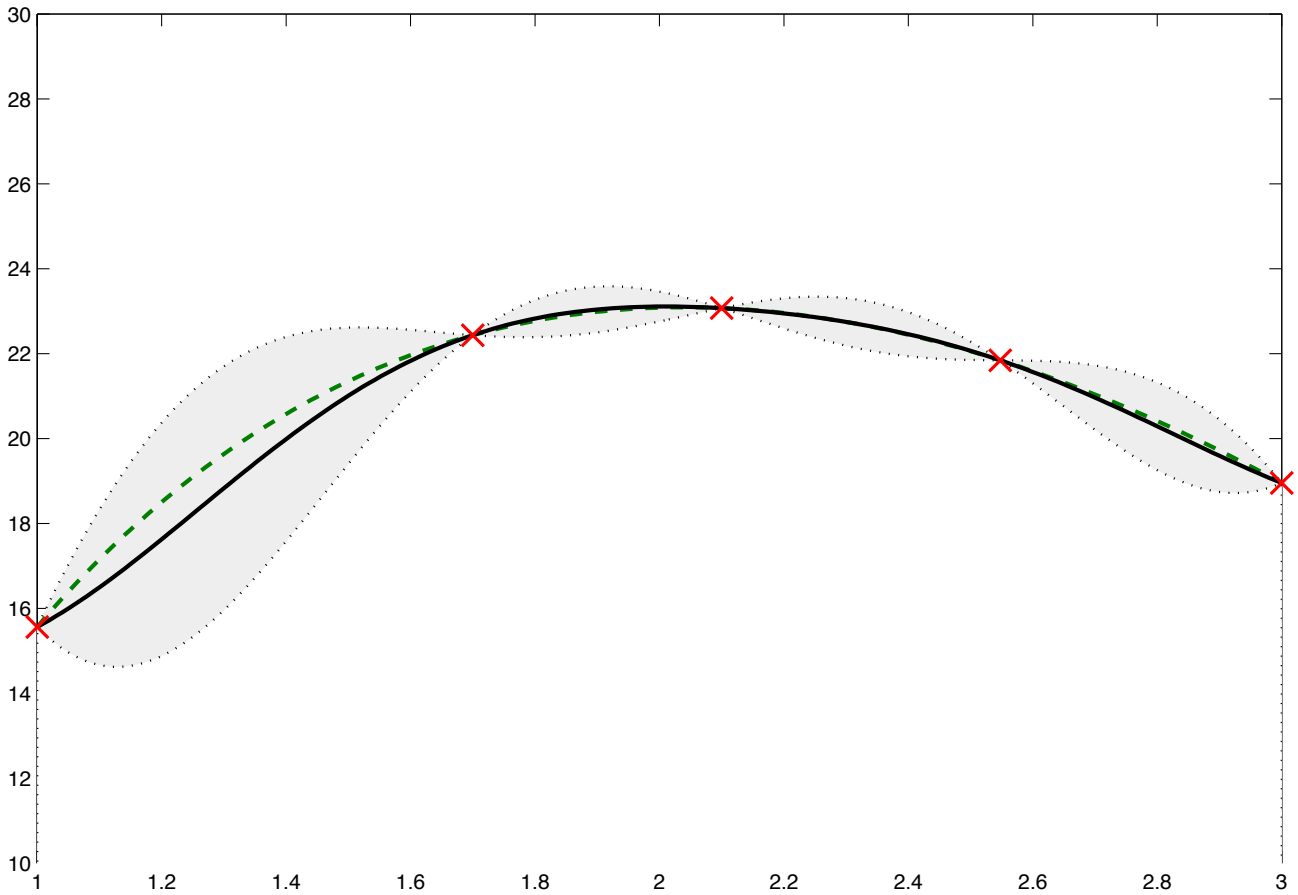
The GP-UCB algorithm - example



The GP-UCB algorithm - example



The GP-UCB algorithm - example



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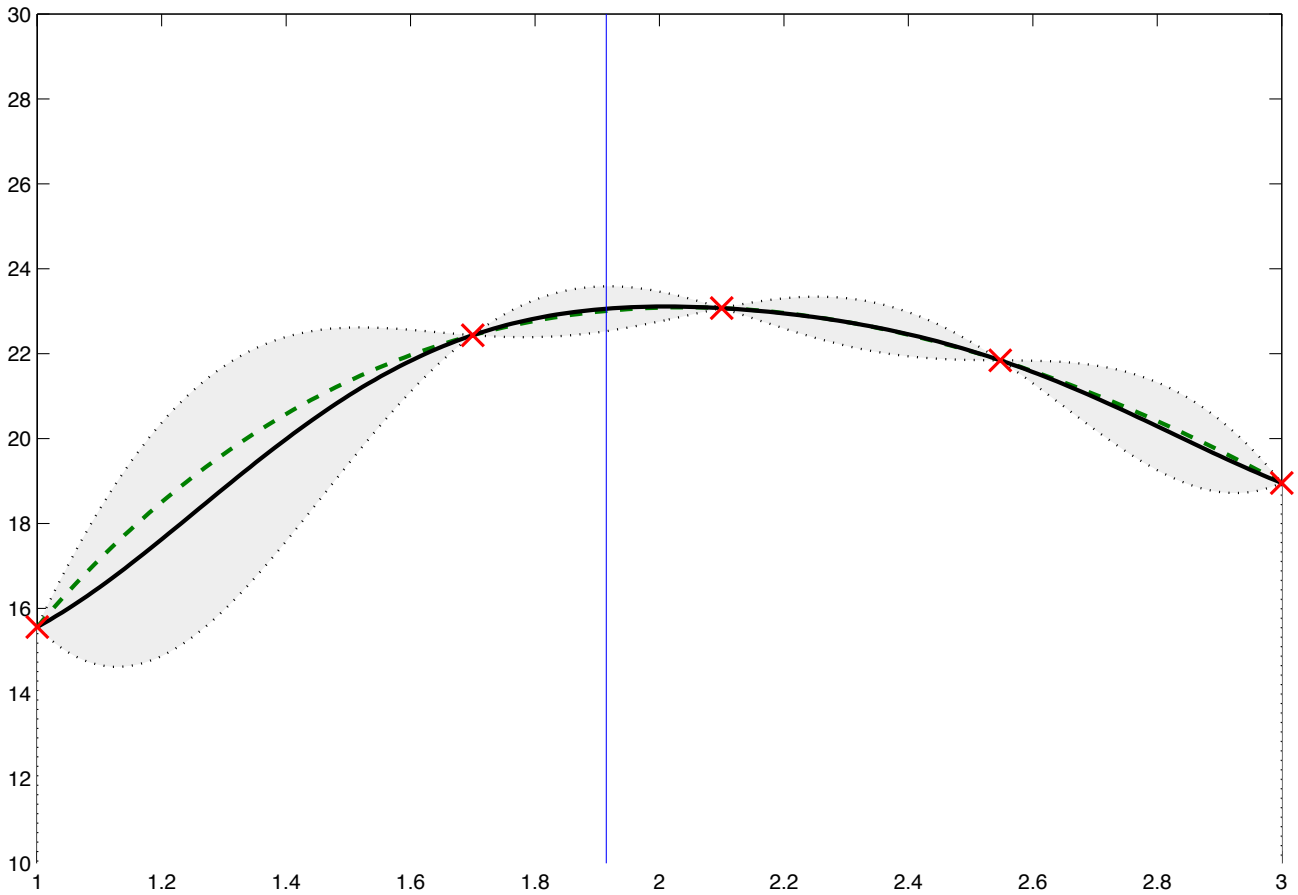

Why it works

- Srinivas et al (IEEE Trans Inf Th 2012) linked the expectation of the cumulative regret to a *submodular function*
- Submodular functions obey a diminishing returns rule $\rightarrow$ greedy optimisation provably works for submodular functions
- The upper quantile β_t term must be increased according to a specific schedule for the guarantees to work

Limitations of GP-UCB

- The cubic scaling of GP regression limits the dimensionality of the space, in my experience anything above 10 is fancyful
- Optimising the acquisition function is still an NP-hard problem! In fact, the acquisition function can be nastier (more multimodal) than the original function
- Convergence is not very fast ($O(\sqrt{T})$) $\rightarrow$ in cases where the true function is *really* expensive to optimise this could be too much

Tomorrow's lab

- Implementation of GP regression-based techniques on a toy example
- Sample functions from a GP with RBF covariance with $\alpha^2 = 4$ and $\lambda^2 = 4$ evaluated on the grid 0.1:0.1:10
- Evaluate the function $f(x) = \exp[-(x-2)^2] + 2\exp[-\frac{(x-6)^2}{3}$ at the points 1:1:9, adding i.i.d Gaussian noise with variance 0.04, to get observations **y**
- Use GP regression with the previous kernel to compute the posterior function values on the grid 0.1:0.1:10
- Use GP-UCB with fixed $\beta = 2$ to optimise the function