# Probabilistic Machine Learning
## Lecture 26
## Making Decisions

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# The Toolbox

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## Framework:

$$\int p(x_1, x_2)\, dx_2 = p(x_1) \qquad p(x_1, x_2) = p(x_1 \mid x_2)p(x_2) \qquad p(x \mid y) = \frac{p(y \mid x)p(x)}{p(y)}$$

## Modelling:

- graphical models
- Gaussian distributions
- (deep) learnt representations
- Kernels
- Markov Chains
- Exponential Families / Conjugate Priors
- Factor Graphs & Message Passing

## Computation:

- Monte Carlo
- Linear algebra / Gaussian inference
- maximum likelihood / MAP
- Laplace approximations
- EM / variational approximations

# So you've got yourself a posterior …now what?

Taking a decision means *conditioning* on a variable you control

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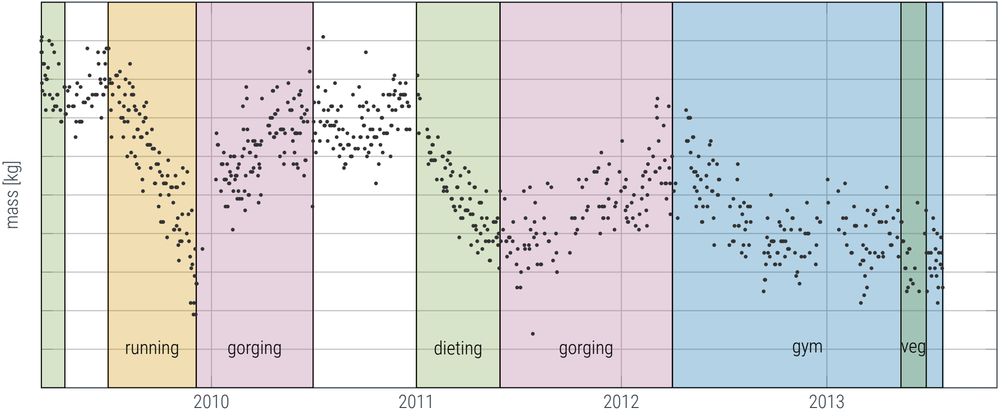



$p(w' \mid \text{run})$ $\qquad$ $p(w' \mid \text{diet})$

- probabilistic models can provide predictions $p(x \mid a)$ for a variable $x$ *conditional* on an action $a$
- given the choice, which value of $a$ do you prefer?

# Decision Theory

## The limit of probabilistic reasoning?

- probabilistic models can provide predictions $p(x \mid a)$ for a variable $x$ *conditional* on an action $a$
- given the choice, which value of $a$ do you prefer?

- assign a *loss* or *utility* $\ell(x)$
- choose $a$ such that it minimizes expected loss

$$a_* = \arg\min_a \int \ell(x) p(x \mid a) \, dx$$

# Expected Regret/utility

if you keep having to take the same decision, optimise the sum of its return

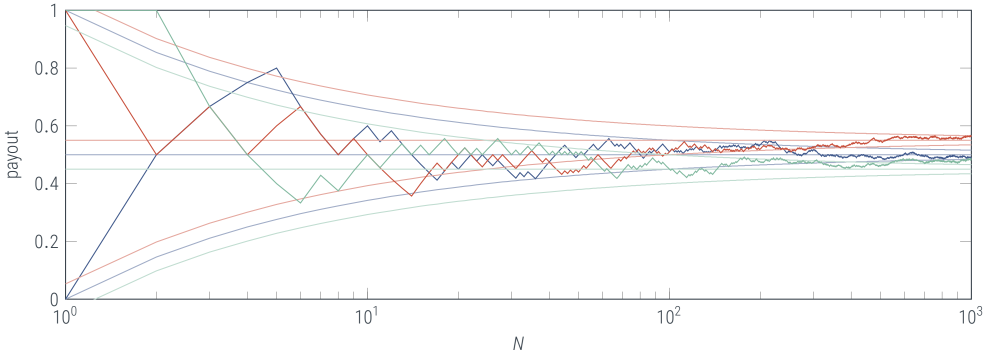
- consider *independent* draws $x_i$ with $x_i \sim p(x \mid a_i)$
- choose all $a_i = a_*$ to minimize the accumulated loss

$$L(n) = \mathbb{E}_p\left[\sum_i x_i\right]$$

- but what if you *don't know p*?

# Motivating (Historical) Example

## Experimental Design



Perhaps we shouldn't rule out an option yet if the posteriors over their expected return overlaps with that of our current guess for the best option?

- Assume $K$ choices.
- Taking choice $k \in [1, \dots, K]$ at time $i$ yields binary (Bernoulli) reward/loss $x_i$ with probability $\pi_k \in [0, 1]$, iid.
- conjugate priors $p(\pi_k) = \mathcal{B}(\pi, a, b) = B(a, b)^{-1} \pi^{a-1}(1 - \pi)^{b-1}$
- posteriors from $n_k$ trys of choice $k$ with $m_k$ successes: $p(\pi_k \mid n_k, m_k) = \mathcal{B}(\pi_k; a + m_k, b + (n_k - m_k))$
- for $a, b \rightarrow 0$, posterior has mean and variance

$$\bar{\pi}_k := \mathbb{E}_{p(\pi_k | n_k, m_k)}[\pi] = \frac{m_k}{n_k} \qquad \sigma_k^2 := \operatorname{var}_{p(\pi_k | n_k, m_k)}[\pi] = \frac{m_k(n_k - m_k)}{n_k^2(n_k + 1)} = \mathcal{O}(n_k^{-1})$$

Choose option $k$ that maximizes $\bar{\pi}_k + c\sqrt{\sigma_k^2}$ for some $c$. Which $c$?

Perhaps we shouldn't rule out an option yet if the posteriors over their expected return overlaps with that of our current guess for the best option?

Choose option $k$ that maximizes $\bar{\pi}_k + c\sqrt{\sigma_k^2}$ for some $c$. Which $c$?

- A large $c$ ensures uncertain options are preferred. If we make it too large, we will only *explore*.
- A small $c$ largely ignores uncertainty. We will only *exploit*.
- Idea: Let $c$ grow slowly over time, at rate less than $\mathcal{O}(n_k^{1/2})$. Then variance of chosen options will drop faster than $c$ grows, so their exploration will stop, unless their mean is good. But unexplored choices will eventually become dominant, thus always explored eventually.

# Not just for Bernoulli variables!

posterior contraction rates are universal

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### Theorem (Chernoff-Hoeffding)

*Let $X_1, \dots, X_n$ be random variables with common range $[0,1]$ and such that $\mathbb{E}[X_t \mid X_1, \dots, X_{t-1}] = \mu$. Let $S_n = X_1 + \dots + X_n$. Then for all $a \geq 0$,*

$$p(S_n - n\mu \leq -a) \leq e^{-2a^2/n} \qquad \text{and} \qquad p(S_n - n\mu \geq a) \leq e^{-2a^2/n}$$

# The Multi-Armed Bandit Setting

Discrete-Choice Experimental Design

[Auer, Cesa-Bianchi, Fischer, Machine Learning **47**(2002), 235–256]

Definitions:

- A $K$-**armed bandit** is a collection $X_{kn}$ of random variables, $1 \leq k \leq K$, $n \geq 1$ where $k$ is the arm of the bandit. Successive plays of $k$ yield rewards $X_{k1}, X_{k2}, \ldots$ which are **independent and identically distributed** according to an unknown $p$ with $\mathbb{E}_p(X_{ki}) = \mu_i$.
- A **policy** $A$ chooses the next machine to play at time $n$, based on past plays and rewards.
- Let $T_k(n)$ be number of times machine $k$ was played by $A$ during the first $n$ plays. The **regret** of $A$ is

$$R_A(n) = \mu^* \cdot n - \sum_j \mu_j \cdot \mathbb{E}_p[T_j(n)] \qquad \text{with } \mu^* := \max_{1 \leq k \leq K} \mu_k$$

# The Multi-Armed Bandit Setting



[Auer, Cesa-Bianchi, Fischer, Machine Learning **47**(2002), 235–256]

Algorithm: Let $\bar{x}_j$: empirical average of rewards from $j$, $n_j$: number of plays at $j$ in $n$ plays

```
procedure UCB(K)                                         // Upper Confidence Bound
    play each machine once
    while true do
        play j = arg max ( x̄_j + sqrt( 2 log n / n_j ) )
    end while
end procedure
```

$$j = \arg\max \left( \bar{x}_j + \sqrt{\frac{2 \log n}{n_j}} \right)$$

[Auer, Cesa-Bianchi, Fischer, Machine Learning **47**(2002), 235–256]

### Theorem (Auer, Cesa-Bianchi, Fischer)

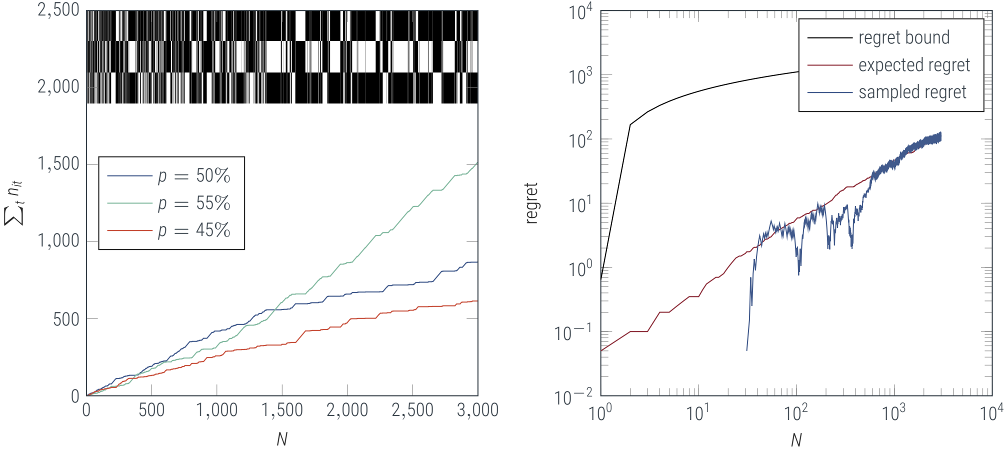
*Consider $K$ machines ($K > 1$) having **arbitrary** reward distributions $P_1, \dots, P_K$ with support in $[0, 1]$ and expected values $\mu_i = \mathbb{E}_P(X_i)$. Let $\Delta_i := \mu_* - \mu_i$. Then, the expected regret of UCB after any number $n$ of plays is at most*

$$\mathbb{E}_P[R_A(n)] \leq \left[ 8 \sum_{i:\mu_i \leq \mu^*} \left( \frac{\log n}{\Delta_i} \right) \right] + \left( 1 + \frac{\pi^2}{3} \right) \left( \sum_j \Delta_j \right)$$

Nb: The sums are over $K$, not $n$. So the regret is $\mathcal{O}(K \log n)$. UCB plays a sub-optimal arm at most logarithmically often.

# Visualization

$K = 3$, binary rewards



## Multi-Armed Bandit Algorithms

- apply to *independent, discrete* choice problems with stochastic pay-off
- algorithms based on upper confidence bounds incur regret bounded by $\mathcal{O}(\log n)$
- this even applies for the *adversarial* setting (Auer, Cesa-Bianchi, Freund, Schapire, 1995)

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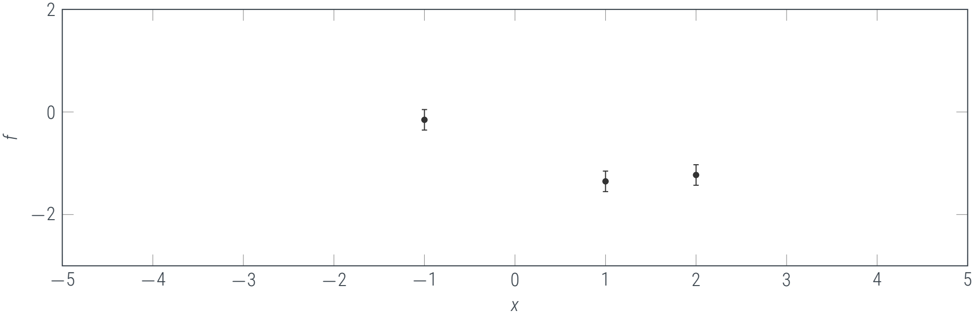
Unfortunately…

- No problem is ever discrete, finite and independent
- in a continuous problem, no “arm” can and should ever be played twice
- in many prototyping settings, early exploration is free

# Continuous-Armed Bandits

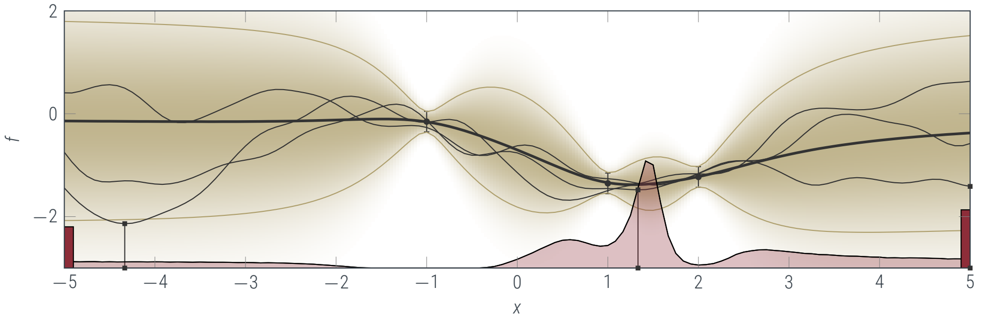
example application: parameter optimization




$$p(y \mid x) = \mathcal{N}(y; f_x, \sigma^2) \qquad x_* = \underset{x \in \mathbb{D}}{\arg\min} f(x) = ? \qquad R(T) := \sum_{t=1}^{T} f(x_t) - f(x_*)$$

# Continuous-Armed Bandits

example application: parameter optimization

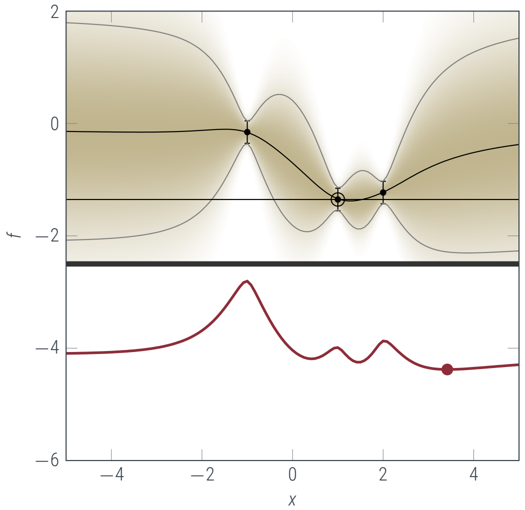



$$p(y \mid x) = \mathcal{N}(y; f_x, \sigma^2) \qquad p(f) = \mathcal{GP}(f; \mu, k) \quad \Rightarrow \quad p_{\min}(x_* = x) = \int_{\mathbb{R}} \int_{\mathbb{D}} \mathbb{I}(f(x) < f(\tilde{x}))\, d\tilde{x}\, dp(f \mid y)$$

# GP Upper Confidence Bound

Evaluate *optimistally*, where the function *may* be low

Srinivas, Krause, Kakade, Seeger, ICML 2009




- **utility** under $p(f \mid y) = \mathcal{GP}(f; \mu_{t-1}, \sigma^2_{t-1})$

$$u_i(x) = \mu_{i-1}(x) - \sqrt{\beta_t}\sigma_{t-1}(x)$$

- choose $x_t$ as $x_t = \arg\min_{x \in \mathbb{D}} u(x)$

**Theorem (Srinivas et al., 2009)**

*Let $\delta \in (0,1)$ and $\beta_t = 2\log(|\mathbb{D}|t^2\pi^2/6\delta)$.*
*Running GP-UCB with $\beta_t$ for **a sample** $f \sim GP(\mu, k)$,*

$$p\left(R_T \leq \sqrt{8T\beta_T\gamma_T/\log(1+\sigma^2)}\ \forall T \geq 1\right) \geq 1-\delta$$

*thus $\lim_{T \to \infty} R_T/T = 0$ ("no regret").*

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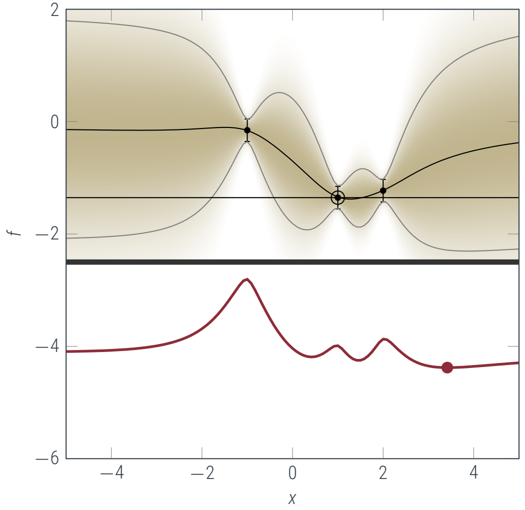


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**Theorem (Srinivas et al., 2009)**

*Assume that $f \in \mathcal{H}_k$ with $\|f\|_k^2 \leq B$, and the noise is zero-mean and $\sigma$-bounded almost surely. Let $\delta \in (0,1)$ and $\beta_t = 2B + 300\gamma_t \log^3(t/\delta)$. Running GP-UCB with $\beta_t$ and $p(f) = \mathcal{GP}(f; 0, k)$,*

$$p\left(R_T \leq \sqrt{8T\beta_T\gamma_T / \log(1+\sigma^2)}\ \forall T \geq 1\right) \geq 1-\delta$$

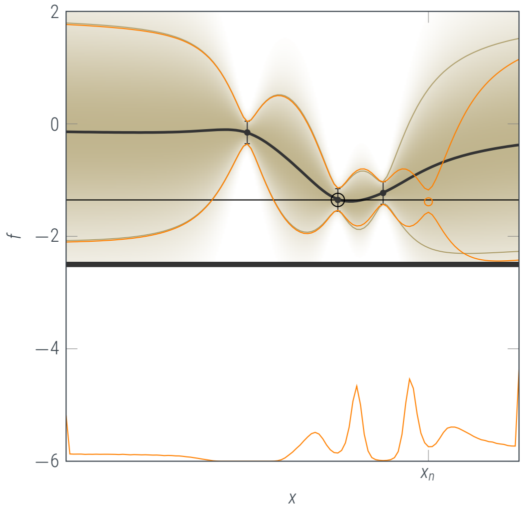
*thus $\lim_{T\to\infty} R_T/T = 0$ (“no regret”).*

What if you have budget for several experiments?

# Entropy Search

evaluate where you *expect to learn most about the minimum*

[Villemonteix et al., 2009; Hennig & Schuler, 2012]

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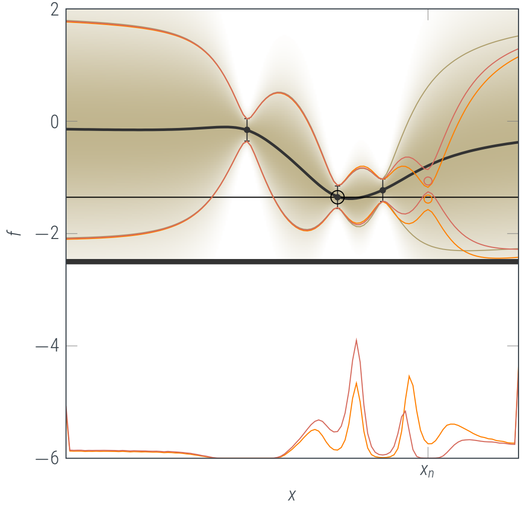
$$\begin{aligned}\bar{\mu}_a &= \mu_a + \kappa_{a*}\kappa_{**}^{-1}(y_* - \mu_*) \\ &= \mu_a + \underbrace{\kappa_{a*}\kappa_{**}^{-1/2}}_{=:L_{a*}} \cdot \underbrace{\kappa_{**}^{-1/2}(y_* - \mu_*)}_{u\sim\mathcal{N}(0,I)}\end{aligned}$$

$$\begin{aligned}\bar{\kappa}_{ab} &= \kappa_{ab} - \kappa_{a*}\kappa_{**}^{-1}\kappa_{*b} \\ &= \kappa_{ab} - L_{a*}L_{*b}\end{aligned}$$

- use this to predict $\hat{p}_{\min}(x)$ under $p(f \mid y, y_{t+1})$ (requires nontrivial numerics)

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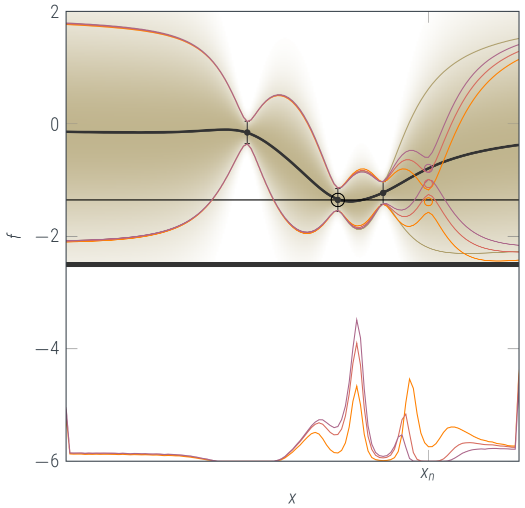


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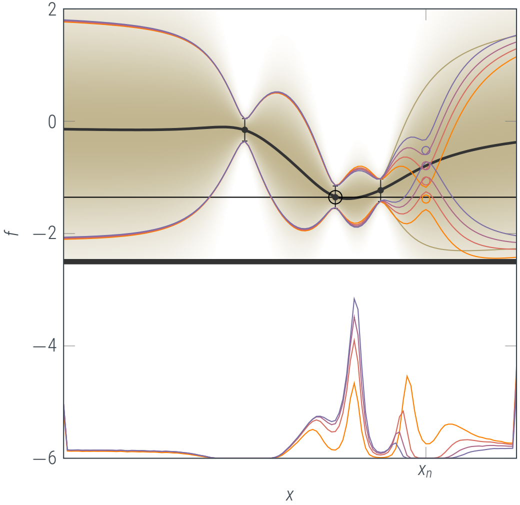


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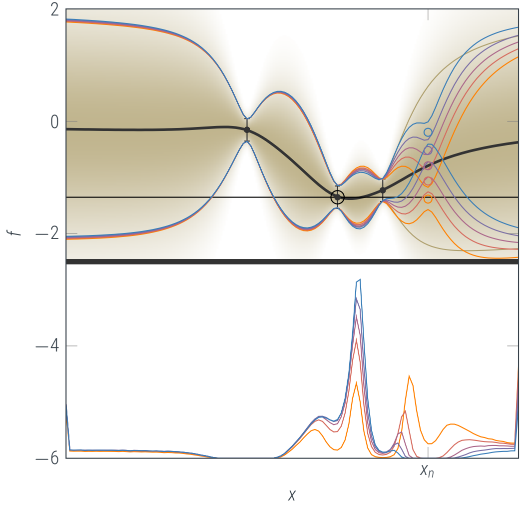


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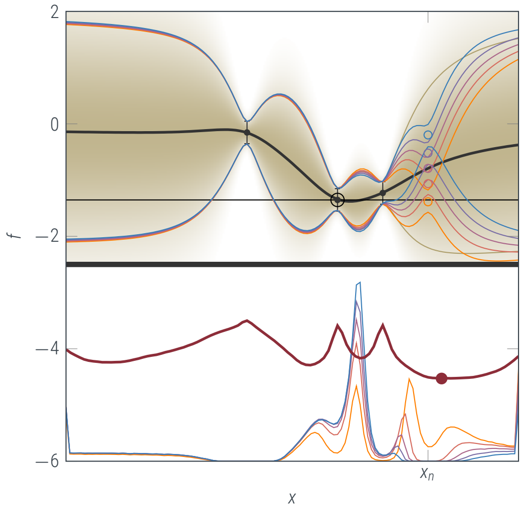


- don't evaluate where you think the minium lies!
- instead, evaluate where you **expect to learn most about the minimum!**

$$\mathbb{H}(p) := -\int p(x) \log \frac{p(x)}{b(x)}\, dx$$

with *base measure b*. Use utility

$$u(x) = \mathbb{H}_t(p_{\min}) - \mathbb{E}_{y_{t+1}}[\mathbb{H}_{t+1}(p_{\min})]$$

# Information vs. Regret

Entropy Search is qualitatively different from regret-based formulations

Settings in which information-based search is preferrable

- “prototyping-phase” followed by “product release”
- structured uncertainty with variable signal-to-noise ratio
- “multi-fidelity”: Several experimental channels of different cost and quality, e.g.
  - simulations vs. physical experiments
  - training a learning model for a variable time
  - using variable-size datasets

Regret-based optimization is easy to implement and works well on standard problems. But it is a strong simplification of reality, in which many pratical complications can not be phrased.

# Bayesian Optimization in Practice

recent (and not so recent) libraries

- https://amzn.github.io/emukit/
- https://github.com/HIPS/Spearmint
- https://github.com/hyperopt
- https://hpolib.readthedocs.io/en/development/
- https://github.com/automl
- https://sigopt.com/product/

## Summary — Experimental Design

- the **bandit setting** formalizes iid. sequential decision making under uncertainty
- bandit algorithms can achieve “no regret” performance, even without explicit probabilistic priors
- **Bayesian optimization** extends to continuous domain
- it lies right at the intersection of computational and physical learning
- requires significant computational resources to run *a numerical optimizer inside the loop*
- allows rich formulation of global, stochastic, continuous, structured, multi-channel design problems
- is currently the state of the art in the solution of challenging optimization problems