Bayesian Machine Learning

A PyMCentric Introduction

Quan Nguyen

Modeling success rate

Question: What is the success rate of a binary event?

$$\theta = ?$$

Making inference: the prior distribution

$$\theta \in [0, 1]$$

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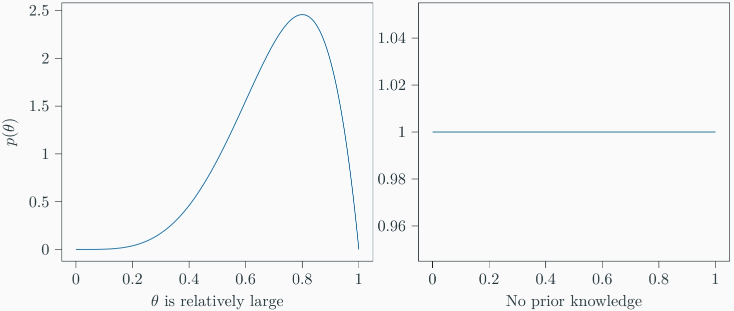

Making inference: the likelihood

$\mathcal{D} = \{1, 0, 1, \ldots, 1\}$: k ones and $n - k$ zeros

$$p(\text{first one} \mid \theta) = \theta$$

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$$\ldots$$

$$p(\mathcal{D} \mid \theta) = \theta^k (1 - \theta)^{n-k}$$

Making inference: Bayes' theorem

$$p(\theta \mid \mathcal{D}) = \frac{p(\mathcal{D} \mid \theta)p(\theta)}{p(\mathcal{D})} = \frac{p(\mathcal{D} \mid \theta)p(\theta)}{\int p(\mathcal{D} \mid \theta)p(\theta)d\theta}$$

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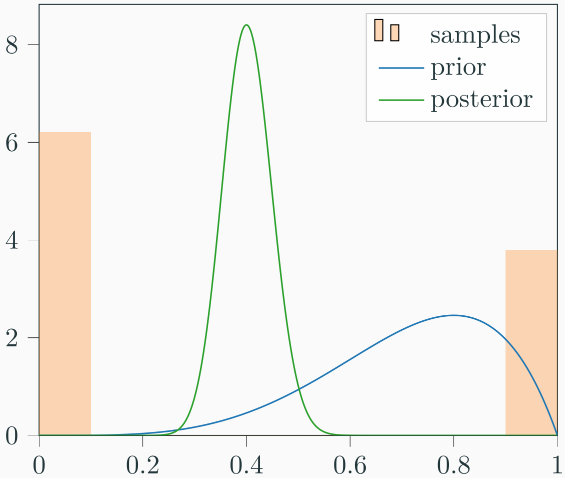
Most of the time, the denominator cannot be computed exactly, but approximated using samples.

Making inference: the posterior distribution



Modeling a latent function

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Gaussian Processes (GPs): normal distribution prior for every function value.

- Mean function $\mu(x)$: central tendency of our function belief
- Covariance function $K(x, x')$: controls the smoothness of function belief
- Can be updated using Bayes' theorem

$$\mu_{\mathcal{D}}(x) = \mu(x) + K(x, \mathbf{x})(\mathbf{\Sigma} + \mathbf{N})^{-1}(\mathbf{y} - \boldsymbol{\mu})$$
$$K_{\mathcal{D}}(x, x') = K(x, x') - K(x, \mathbf{x})(\mathbf{\Sigma} + \mathbf{N})^{-1}K(\mathbf{x}, x')$$

GP inferences: the prior

```
ℓ = 1
η = 3

with pm.Model() as model:
    cov_func = η**2 * pm.gp.cov.Matern52(ℓ, 1)
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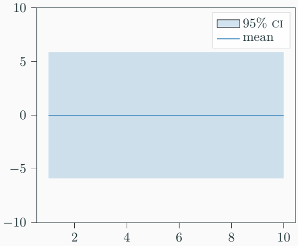

Figure 1: GP prior

GP inferences: the posterior

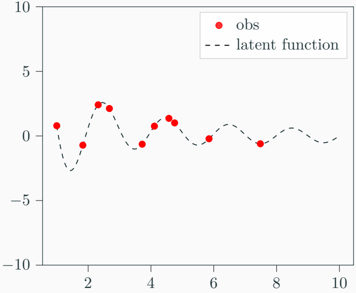

Figure 2: Observations from the latent function

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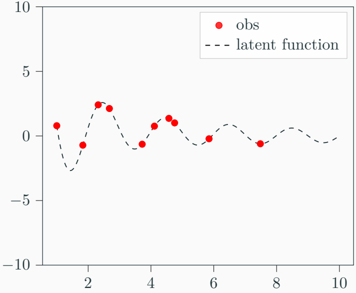

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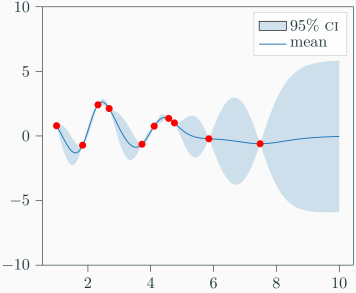

Figure 3: GP posterior conditioned on observations

GP hyper-parameters

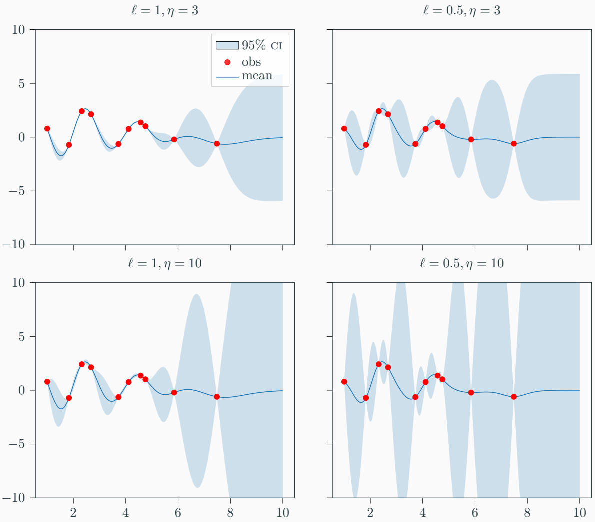

Figure 4: Effect of hyper-parameters on the posterior GP

GPs in PyMC3

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with pm.Model() as model:
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    η = pm.HalfCauchy('η', beta=3)

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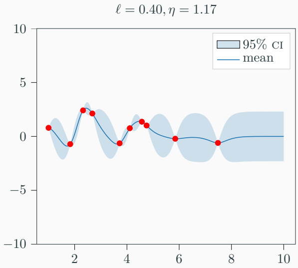

Figure 5: GP posterior via MAP

Linear regression

$$y = \mathbf{w}^T \mathbf{x} + \varepsilon$$

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Optimal $\mathbf{w}$ via *least squares*:

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Bayesian linear regression:

$$p(\mathbf{w} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \boldsymbol{\Sigma})$$
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$p(y \mid \mathbf{x}, \mathcal{D})$ can be computed.

Linear regression: an example

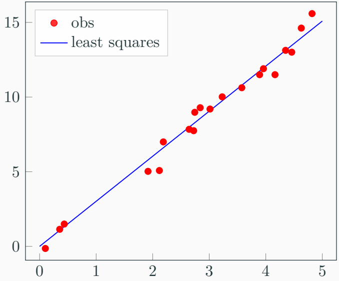
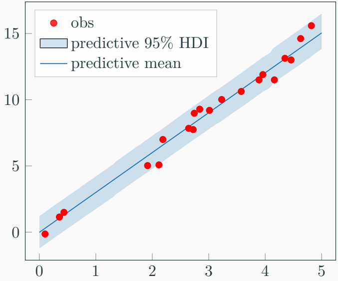


Figure 1: Least-squares solution



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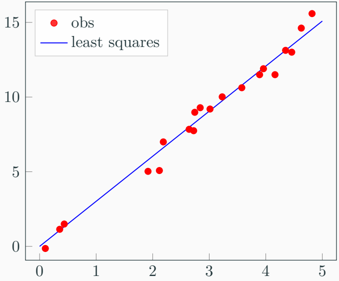

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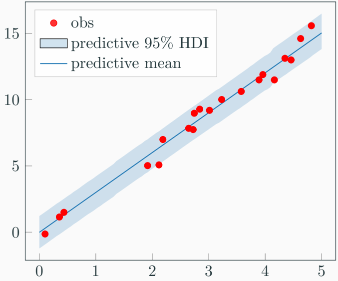

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Bayesian neural networks: Thomas Wiecki - Probablistic Programming Data Science with PyMC3

Bayesian decision theory

Two main components:

- Bayesian beliefs about unknown quantities
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$$u(\text{decision}, \text{outcome}) = v \in \mathbb{R},$$
$$d^* = \arg\max \mathbb{E}_{\text{outcome}} \left[u(\text{decision}) \right]$$

Bayesian-optimal The Price is Right

Setup:

- Compete against an opponent to guess product price p as $g \in \mathbb{R}$.
- Opponent's guess: $\bar{p}$.
- If a guess is above p then the player gets nothing.
- If a guess is not above p, then the player with the closer guess wins the product.
- Our belief about p: $\mathcal{N}(p; \mu, \sigma^2)$.
- What is the optimal decision d^*?

Deriving the optimal decision

General process: compute the utility of each action given the values of the unknown quantities and marginalize over those values according to our belief.

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Expected utility of a decision g

$$\mathbb{E}\left[u(g)\right] = \int u(g \mid p)p(p)dp; \quad g^* = \arg\max_g \mathbb{E}\left[u(g))\right]$$

Visualizing the optimal decision

Example: $p \sim \mathcal{N}(100, 10^2)$; $\overline{p} = 75$.

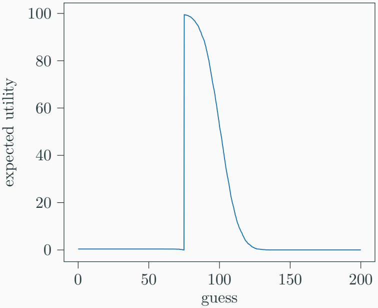

Figure 1: Expected utility as a function of our guess

The multi-armed bandit problem

Problem setup:

- k slot machines, each returns a coin with probability θ_i
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Modeling the return rates: placing a prior on each θ_i and update accordingly.

The Bayesian optimal policy

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- $\mathbb{E}\left[\text{future reward} \mid \text{current outcome}\right]$ is generally intractable.
- Need policies that *approximates* the optimal policy.
- Goal: have an $\mathcal{O}(\log t)$ upper-bound on the expected *regret*.

The Upper-Confidence Bound policy

At iteration $t = 1, 2, \dots, N$, for each arm i with the corresponding posterior belief $p(\theta_i)$, compute with constant c:

$$q_i(t) = Q_i \left(1 - \frac{1}{t \, (\log N)^c} \right),$$

where Q_i is the corresponding quantile function of $p(\theta_i)$.

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Justification: $q_i(t)$ is high if either (1) $\mathbb{E}[\theta_i]$ is high or (2) there is significant uncertainty in $p(\theta_i)$.

$\rightarrow$ Exploration vs. exploitation

The Thompson Sampling policy

At iteration $t = 1, 2, \ldots, N$, for each arm i with the corresponding posterior belief $p(\theta_i)$, draw a sample as an approximation of the true rate:

$$\overline{\theta_i} \sim p(\theta_i).$$

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Thompson Sampling: Sid Ravinutala - Thompson Sampling and COVID testing

Bayesian optimization

Problem setup:

- Access to potentially noisy output of a black-box function $y = f(\cdot) + \varepsilon$ but not its gradients
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Modeling the objective function: Gaussian processes.

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Expected Improvement:

$$\mathbb{E}\left[y - \overline{y} \mid y > \overline{y}, x, \mathcal{D}\right] = \int_{\overline{y}}^{\infty} (y - \overline{y}) p(y \mid x, \mathcal{D}) dy.$$

Distribution of the true maximizer

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PyMC-powered Bayesian optimization: pyGPGO.

Other Bayesian decision-making problems

Active learning: interactively asking for new data points to minimize cost and maximize predictive performance.[1]

[1] Settles, Burr. Active learning literature survey. University of Wisconsin-Madison Department of Computer Sciences, 2009.

[2] Garnett, Roman, et al. "Bayesian optimal active search and surveying." arXiv preprint arXiv:1206.6406 (2012).

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Active search: interactively asking for new data points to discover a rare class of data points while minimizing cost.[2]

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