

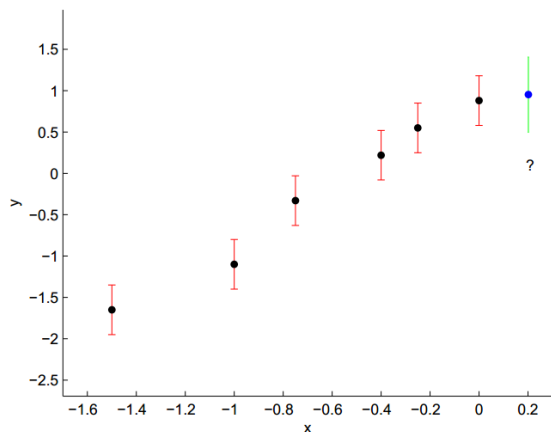
Gaussian Process Active Learning

Gaussian Process Regression

n observations: $\mathbf{y} = \{y_1, \dots, y_n\}$

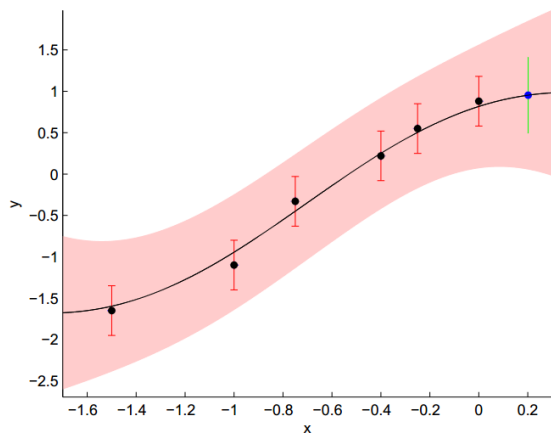
covariance:

$$K = \begin{bmatrix} k(x_1, x_1) & k(x_1, x_2) & \cdots & k(x_1, x_n) \\ k(x_2, x_1) & k(x_2, x_2) & \cdots & k(x_2, x_n) \\ \vdots & \vdots & \ddots & \vdots \\ k(x_n, x_1) & k(x_n, x_2) & \cdots & k(x_n, x_n) \end{bmatrix}$$



For $\mathbf{x}^*$, $K_* = [k(x_*, x_1) \quad k(x_*, x_2) \quad \cdots \quad k(x_*, x_n)]$ $K_{**} = k(x_*, x_*)$

How to get y_* ?



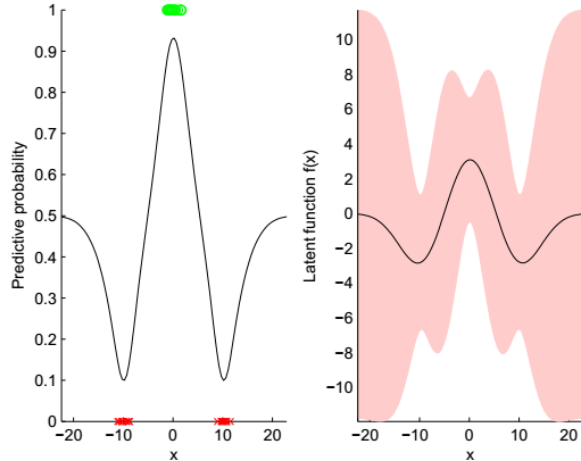
假设：数据服从均值为0 的联合高斯分布。

$$\begin{bmatrix} \mathbf{y} \\ y_* \end{bmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} K & K_*^T \\ K_* & K_{**} \end{bmatrix}\right)$$



$$y_* | \mathbf{y} \sim \mathcal{N}(K_* K^{-1} \mathbf{y}, K_{**} - K_* K^{-1} K_*^T)$$

Gaussian Process Classification



1. Finding the probability $p(f_*|\mathbf{f})$ is similar to GPR, i.e.

$$p(f_*|\mathbf{f}) = \mathcal{N}(K_*K^{-1}\hat{\mathbf{f}}, K_{**} - K_*(K')^{-1}K_*^T)$$

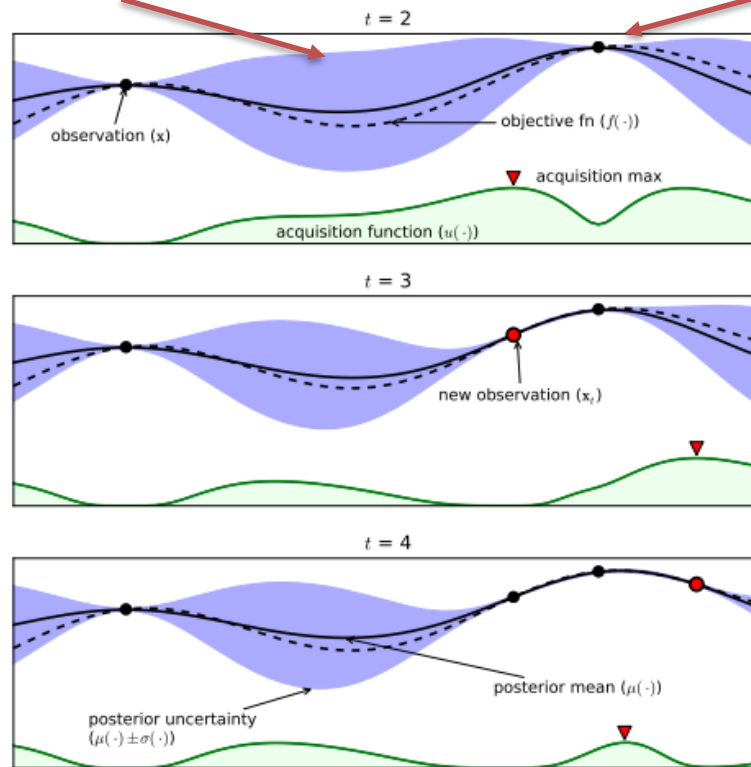
2. Squash f_* to find the probability of class membership.

$$\pi(f) = \text{prob}(y = 1|f)$$

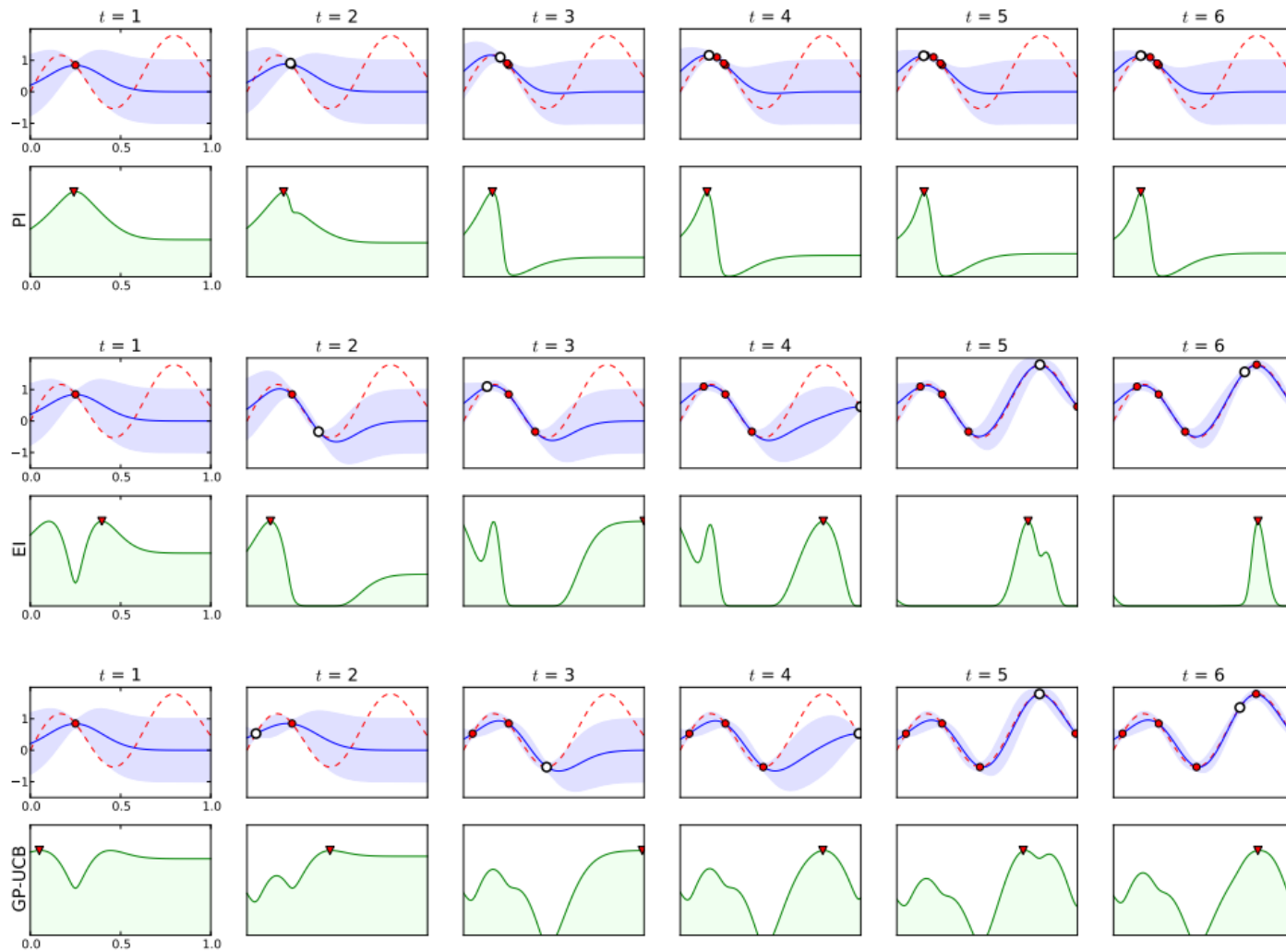
Bayesian Optimization

Exploration

Exploitation



Acquisition Function



Active Learning for GP

$$Q_{\mu_*}(\mathcal{U}) = \operatorname{argmin}_{\hat{\mathbf{x}}^{(i)} \in \mathcal{U}} |\mu_*(\hat{\mathbf{x}}^{(i)})| \quad \text{Exploitation}$$

$$Q_{\sigma_*^2}(\mathcal{U}) = \operatorname{argmax}_{\hat{\mathbf{x}}^{(i)} \in \mathcal{U}} \sigma_*^2(\hat{\mathbf{x}}^{(i)}) \quad \text{Exploration}$$

$$Q_{\text{unc}}(\mathcal{U}) = \operatorname{argmin}_{\hat{\mathbf{x}}^{(i)} \in \mathcal{U}} \frac{|\mu_*(\hat{\mathbf{x}}^{(i)})|}{\sqrt{\sigma_*^2(\hat{\mathbf{x}}^{(i)})}} \quad \text{Trade-off}$$

PU Learning

- 有限的正类样本
- 负类种类多样
- 查询到负类的处理方式
- 模型的更新

The **distribution of the three groups** of examples **changes** over a period of time as more and more examples get labeled

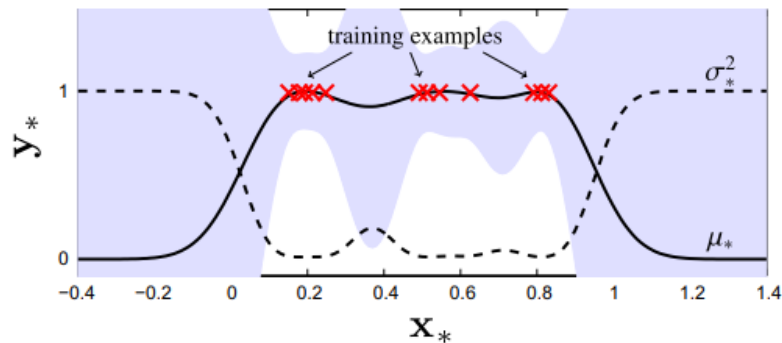
Discard negative:

- Label instances which are located near the surface of the SVDD sphere
- Identify instances in the unlabeled pool that fit the target class best, and label these instances first
- First pick the instances which the initial model considers to match the learned class the *least*

Keep negative:

- 转化为二分类的监督学习或半监督学习

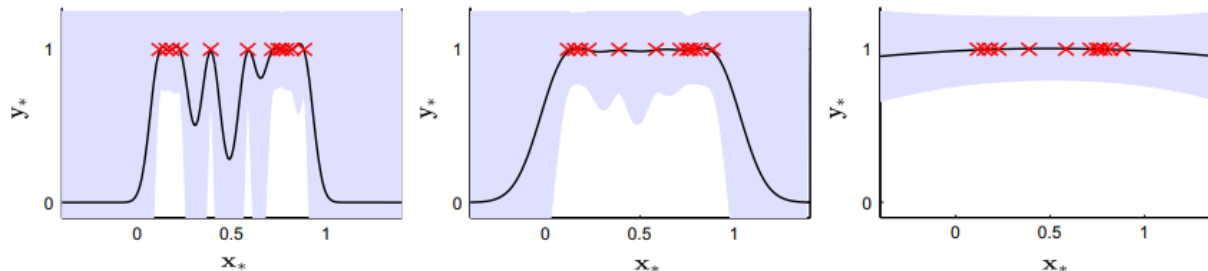
GP in One-Class Classification



$$\mu_* = \mathbf{k}_*^T (\mathbf{K} + \sigma_n^2 \mathbf{I})^{-1} \mathbf{1}$$

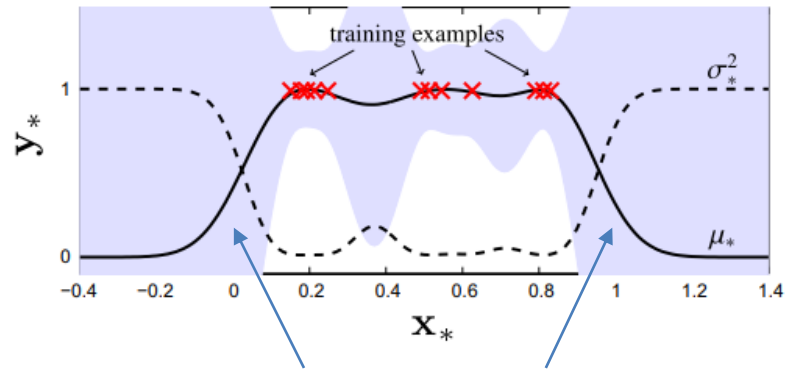
The mean decreases with distance from the training data.

problem



[Kemmler et.al, Pattern Recognition, 2013]

GPAL for PU



- Query Strategy: trade-off
- Model Update: 如何利用未标记数据