Machine Learning

Kernel Methods

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Definition of Different Models

What to do in the case the model you are considering is not performing well even by tuning properly the parameters (cross-validation)?

We have two opposite options:

- simplify the model
- **increase its complexity**

In the second hypothesis, one might see the problem in a more complex space:

- use handcrafted features
- look at the problem in the **kernel** space

Constructing Kernels

Constructing Kernels

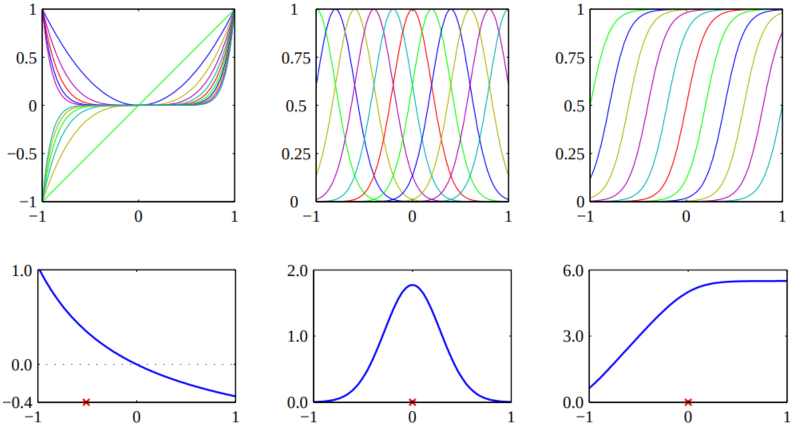
- To exploit kernel substitution need **valid** kernel functions
- First method
  - **Choose a feature space** mapping $\boldsymbol{\phi}(\mathbf{x})$ and use it to find corresponding kernel

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^T \boldsymbol{\phi}(\mathbf{x}') = \sum_{i=1}^{M} \phi_i(\mathbf{x})\phi_i(\mathbf{x}')$$

    - where $\boldsymbol{\phi}(\mathbf{x})$ are basis functions such as polynomial
    - for each i we choose $\phi_i(x) = x^i$ in the one-dimensional case

Construction of Kernel Functions from Basis Functions

One-dimensional input space



Testing whether a function is a valid kernel

- Second method
    - Without having to construct the function $\phi(\mathbf{x})$ explicitly
- **Necessary and sufficient** condition for a function $k(\mathbf{x}, \mathbf{x}')$ to be a kernel is
    - Gram matrix $\mathbf{K}$, whose elements are given by $k(\mathbf{x}_n, \mathbf{x}_m)$ is positive semi-definite for all possible choices of the set $\{\mathbf{x}_n\}$
        - Positive semi-definite is **not** the same thing as a matrix whose elements are non-negative
        - It means $\mathbf{y}^\top \mathbf{K} \mathbf{y} \geq 0$ for non-zero vectors $\mathbf{y}$ with real entries, i.e., $\sum_n \sum_m K_{n,m} y_n y_m \geq 0$ for any real numbers $\mathbf{y}$

Theorem

Mercer's theorem ***Any*** *continuous, symmetric, positive semi-definite kernel function $k(x, x')$ can be expressed as a* ***dot product*** *in a high-dimensional space*

- **New kernels** can be constructed from simpler kernels as **building blocks**

Techniques for Constructing Kernels

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$ the following new kernels will be valid

1. $k(\mathbf{x}, \mathbf{x}') = ck_1(\mathbf{x}, \mathbf{x}')$
2. $k(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}')$, where $f(\cdot)$ is any function
3. $k(\mathbf{x}, \mathbf{x}') = q(k_1(\mathbf{x}, \mathbf{x}'))$, where $q(\cdot)$ is a polynomial with non-negative coefficients
4. $k(\mathbf{x}, \mathbf{x}') = exp(k_1(\mathbf{x}, \mathbf{x}'))$
5. $k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}')$
6. $k(\mathbf{x}, \mathbf{x}') = k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}')$
7. $k(\mathbf{x}, \mathbf{x}') = k_3(\boldsymbol{\phi}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}'))$, where $\boldsymbol{\phi}(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$
8. $k(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T A\mathbf{x}'$, where A is a symmetric positive semidefinite matrix
9. $k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b)$, where x_a and x_b are variables with $\mathbf{x} = (x_a, x_b)$
10. $k(\mathbf{x}, \mathbf{x}') = k_a(\mathbf{x}_a, \mathbf{x}'_a)k_b(\mathbf{x}_b, \mathbf{x}'_b)$

Gaussian Processes

GP Definition

- A Gaussian process is defined as a probability distribution over functions $y(\mathbf{x}_i)$
    - values of $y(\mathbf{x}_i)$ evaluated at any set of points $\mathbf{x}_1, \dots, \mathbf{x}_N$ jointly have a Gaussian distribution
- This distribution is completely specified by the mean and the covariance:
    - usually, we do not have any prior information about the mean of $y(\mathbf{x})$, so we take it to be zero
    - the covariance is given by the **kernel** function

$$\mathbb{C}\mathrm{ov}[y(\mathbf{x}_i), y(\mathbf{x}_j)|\mathbf{x}_i, \mathbf{x}_j] = \mathbb{E}[y(\mathbf{x}_i)\, y(\mathbf{x}_j)|\mathbf{x}_i, \mathbf{x}_j] = K(\mathbf{x}_i, \mathbf{x}_j)$$

- With this formulation, **Gaussian Process** (GP) are kernel methods that can be applied to solve regression problems

Output Modeling

- The **target** is $t = y(\mathbf{x}) + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ is a noise independent on the point $\mathbf{x}$
- The conditional distribution of the targets $\mathbf{t}_N = (t_1, \dots, t_N)^\top$ of size N is:

$$p(\mathbf{t}_N | \mathbf{y}_N) = \mathcal{N}(\mathbf{t}_N | \mathbf{y}_N, \sigma^2 \mathbf{I}_N) \qquad \text{where } \mathbf{y}_N = (y(\mathbf{x}_1), \dots, y(\mathbf{x}_N))^\top$$

- The **prior** is $p(\mathbf{y}_N) = \mathcal{N}(\mathbf{0}, \mathbf{K}_N)$, where:

$$\mathbf{K}_N = \begin{pmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & \dots & K(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ K(\mathbf{x}_N, \mathbf{x}_1) & \dots & K(\mathbf{x}_N, \mathbf{x}_N) \end{pmatrix}$$

- Thus, the marginal distribution of the target is:

$$p(\mathbf{t}_N) = \int p(\mathbf{t}_N | \mathbf{y}_N) p(\mathbf{y}) \, \mathrm{d}\mathbf{y}_N = \mathcal{N}(\mathbf{t}_N | \mathbf{0}, \mathbf{C}_N) \qquad \text{where } \mathbf{C}_N = \mathbf{K}_N + \sigma^2 \mathbf{I}_N$$

Making Predictions

- We want to **predict** the target t_{N+1} corresponding to a specific unseen input $\mathbf{x}_{N+1}$
- From the definition we have:

$$p(\mathbf{t}_{N+1}) = \mathcal{N}(\mathbf{t}_{N+1}|\mathbf{0}, \mathbf{C}_{N+1}),$$

where:

$$\mathbf{C}_{N+1} = \begin{pmatrix} \mathbf{C}_N & \mathbf{k} \\ \mathbf{k}^\top & c \end{pmatrix}$$

$$\mathbf{k} = (K(\mathbf{x}_1, \mathbf{x}_{N+1}), \dots, K(\mathbf{x}_N, \mathbf{x}_{N+1}))^\top \qquad c = K(\mathbf{x}_{N+1}, \mathbf{x}_{N+1}) + \sigma^2$$

- We need to compute $p(t_{N+1}|\mathbf{t}_N, \mathbf{x}_1, \dots, \mathbf{x}_N) = \mathcal{N}(m(\mathbf{x}_{N+1}), \sigma^2(\mathbf{x}_{N+1}))$ where
  - Mean: $m(\mathbf{x}_{N+1}) = \mathbf{k}^\top \mathbf{C}_N^{-1} \mathbf{t}$
  - Variance: $\sigma^2(\mathbf{x}_{N+1}) = c - \mathbf{k}^\top \mathbf{C}_N^{-1} \mathbf{k}$

GPs in Python

Model the relationship between petal length and width as a GP:

- Load the data and normalize them
- Select the values of:
  - noise variance $\sigma^2 = \mathbb{V}\mathrm{ar}[\varepsilon] = 0.2$
  - constant $k = 1$
  - lengthscale $l = 0.8$

$$K(\mathbf{x}_i, \mathbf{x}_j) = k \exp\left\{ -\frac{\|\mathbf{x}_i - \mathbf{x}_j\|_2^2}{2l^2} \right\}$$

- Initialize a GP regression model (`GaussianProcessRegressor`)
- Predict new values

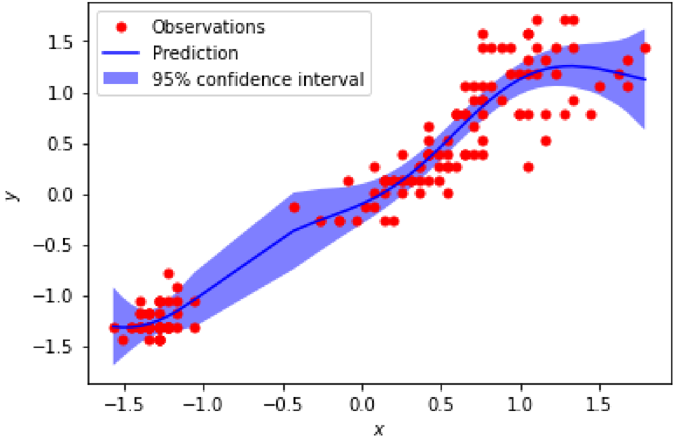
Hyperparameters

While GPs are a **non-parametric** methods, σ^2 and the parameters of the kernel (e.g., l and k) has to be estimated or set:

- using **a priori** information on the problem we are analyzing
- maximizing their **log-likelihood** on an independent dataset
- possibly improved as new data are collected

Caveat: most of the time you will see that they are estimated using the same data used for the prediction. This is clearly not a good ML practice (equivalent to overfitting)

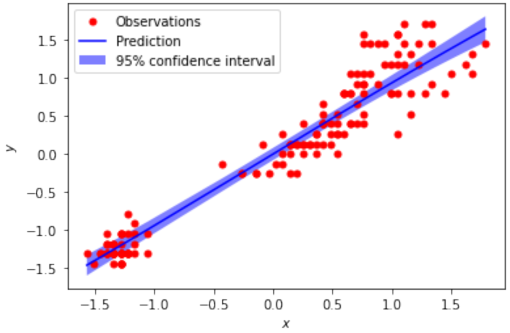
Results on the Iris Dataset

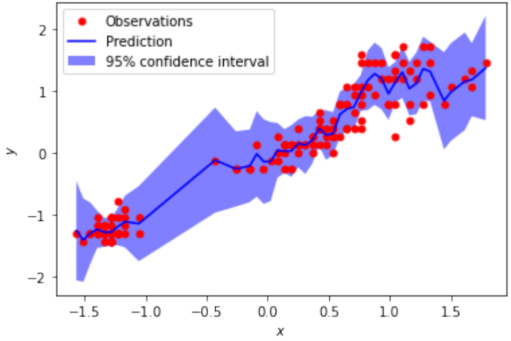


Parameters: $k = 3$, $l = 0.8$, and $\sigma^2 = 0.2$

Modify the Lengthscale

- Left: $k = 3$, $l = 8$, and $\sigma^2 = 0.2$
- Right: $k = 3$, $l = 0.08$, and $\sigma^2 = 0.2$

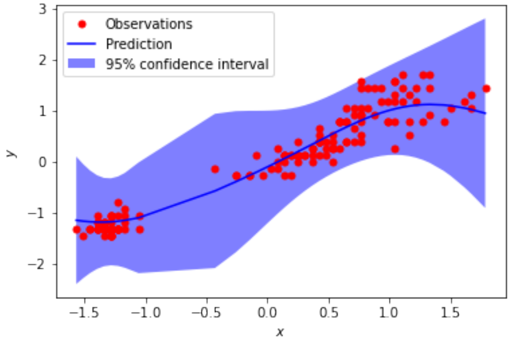


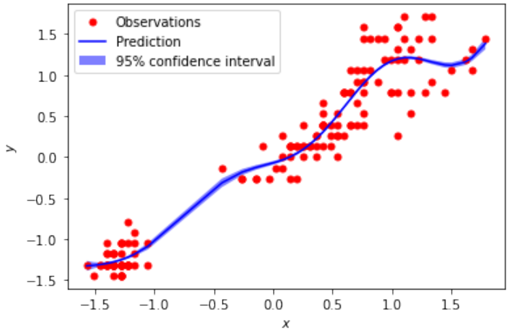


Controls the smoothness of the GP

Modify the Noise

- Left: $k = 3$, $l = 0.8$, and $\sigma^2 = 10$
- Right: $k = 3$, $l = 0.8$, and $\sigma^2 = 0.002$





Controls the target noise of the GP

Support Vector Machines

Support Vector Machines (SVM)

- Flexible and **theoretically supported** method
- Initially applied to classification only, over the years it has been extended to deal with regression, clustering and anomaly detection problems
- Idea: find the **hyperplane maximizing the margins** (distance between the boundary and the points)

Support Vector Machines (SVM)

- Hypothesis space: $y(\mathbf{x}) = f(\mathbf{x}; \mathbf{w}) = \text{sign}(\mathbf{w}^\top \mathbf{x} + b)$
- Loss function computed over $\mathcal{D} = \{(\mathbf{x}_n, t_n)\}_{n=1}^N$ with $t_n \in \{-1, 1\}$:

$$\begin{aligned} \underset{\mathbf{w},\zeta_1,\dots\zeta_N}{\text{minimize}} \quad & \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{n=1}^{N} \zeta_i \\ \text{s.t.} \quad & t_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 - \zeta_i \qquad \forall n \in \{1, \dots, N\} \\ & \zeta_i \geq 0 \qquad \forall n \in \{1, \dots, N\} \end{aligned}$$

where $C > 0$ is a hyperparameter

- Optimization method: sequential quadratic optimization

Linear SVM in Python

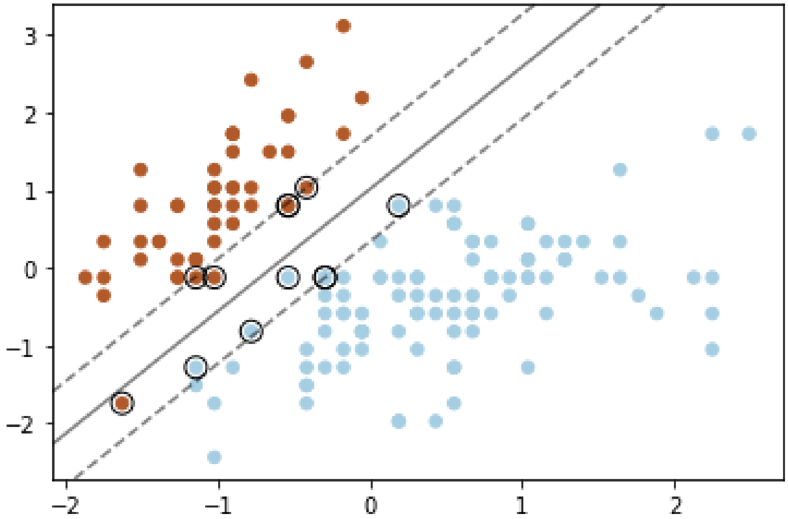
To train a linear classification SVM:

- Define an SVM: `SVM_model.svm.SVC(kernel='linear')`
- Train the SVM: `SVM_model.fit(input, target)`

We are interested to determine:

- Boundary $\mathbf{w}^T \mathbf{x}_n + b = 0$
- Margins $\mathbf{w}^T \mathbf{x}_n + b = \pm 1$
- Support vectors (`SVM_model.support_vectors_`)

Results on the Iris Dataset



Adding a Kernel

The use of kernels in the SVM is almost native (non-parametric method):

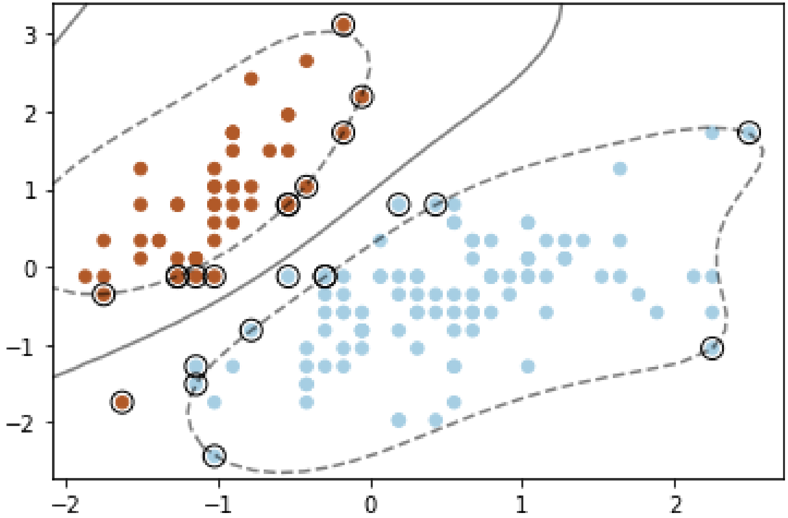
- Hypothesis space: $y(\mathbf{x}) = f(\mathbf{x}; \mathbf{w}) = \text{sign}\left(\sum_{n=1}^{N} \alpha_n t_n K(\mathbf{x}_n, \mathbf{x}) + b\right)$
- Loss measure: loss function in the dual formulation
- Optimization method: quadratic optimization

In `Python`:

- Define an SVM: `SVM_model.svm.SVC()`
- Train the SVM: `SVM_model.fit(input, target)`

We do not have an explicit formula for the boundary and the margins anymore

Results on the Iris Dataset


3
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