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 feature space
- increase its complexity

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Increase its complexity

By means of kernel methods:

- define a kernel function for a d-dimensional feature space:

$$k(\boldsymbol{x}, \boldsymbol{x}') = \phi(\boldsymbol{x})^T \phi(\boldsymbol{x}')$$

- such that, even if $d \to \infty$, it is still feasible to compute $k(\boldsymbol{x}, \boldsymbol{x}')$

Gaussian Process

GP Definition

- A Gaussian process is defined as a probability distribution over functions $\mathbf{y}(\mathbf{x})$ such that the set of values of $\mathbf{y}(\mathbf{x})$ evaluated at an arbitrary 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 $\mathbf{y}(\mathbf{x})$, so we take it to be zero
  - the covariance is given by the kernel function $\mathbb{E}[t(x_i)\, t(x_j)] = K(x_i, x_j)$
- With this formulation, Gaussian Process (GP) are kernel methods that can be applied to solve regression problems

Output Modeling

- Assume to have a target $t_n = y(\mathbf{x}_n) + \varepsilon_n$, where ε_n is a measurement noise which is not dependent on the specific point $\mathbf{x}_n$
- The joint distributions of the targets $\mathbf{t}$ of dimensions N is:

$$p(\mathbf{t}|\mathbf{y}) = \mathcal{N}(\mathbf{t}|\mathbf{y}, \sigma^2 I_N)$$

- since $p(\mathbf{y}) = \mathcal{N}(\mathbf{0}, K)$, we have:

$$p(\mathbf{t}) = \int p(\mathbf{t}|\mathbf{y})p(\mathbf{y})\, d\mathbf{y} = \mathcal{N}(\mathbf{t}|\mathbf{0}, C)$$

where $C(\mathbf{x}_n, \mathbf{x}_m) = K(\mathbf{x}_n, \mathbf{x}_m) + \delta_{nm}\sigma^2$ and δ_{nm} is the Dirac delta, i.e., $\delta_{nm} = 1 \iff n = m$

Making Predictions

We would like to predict the target t_{N+1} corresponding to a specific unseen input $\mathbf{x}_{N+1}$

From the definition we have:

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

where $C_{N+1} = \begin{pmatrix} C_N & \mathbf{k} \\ \mathbf{k}^\top & c \end{pmatrix}$, $\mathbf{k}$ is the vector of $K(\mathbf{x}_i, \mathbf{x}_{N+1})$, for each $i \in \{1, \dots, N\}$ and c is the covariance $C(\mathbf{x}_{N+1}, \mathbf{x}_{N+1})$

We need to compute: $p(t_{N+1}|\mathbf{t}_N, \mathbf{x}_1, \dots, \mathbf{x}_N)$

- Mean: $m(\mathbf{x}_{N+1}) = \mathbf{k}^\top C_N^{-1}\mathbf{t}$
- Variance: $\sigma^2(\mathbf{x}_{N+1}) = c - \mathbf{k}^\top C_N^{-1}\mathbf{k}$

GPs in Python

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

- Load the data and normalize them
- Select the value for the GP:
  - noise variance $\sigma^2 = Var[\varepsilon_n] = 0.2$
  - constant $\phi = 1$
  - lengthscale $l = 0.8$
- Initialize a GP regression model (`GaussianProcessRegressor`)
- Predict new values

Kernel:

$$\mathbf{K}_{ij} = \phi \exp\left\{-\frac{||x_i - x_j||_2}{2l^2}\right\}$$

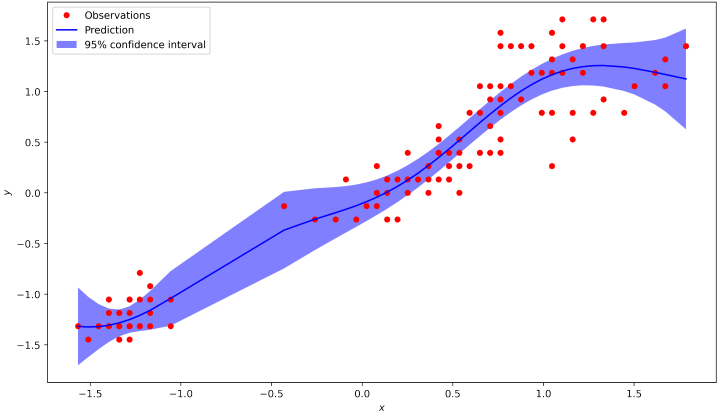
Hyperparameters

While GPs are a non-parametric methods, the parameters of the kernel has to be estimated or set:

- using a priori information on the problem we are analysing
- maximizing their loglikelihood 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)

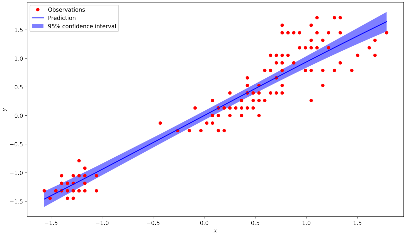
Results on the Iris Dataset

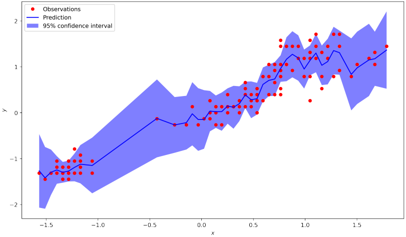


Parameters: $\phi = 3$, $l = 0.8$, and $\sigma^2 = 0.2$

Modify the Lengthscale

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





Controls the smoothness of the GP

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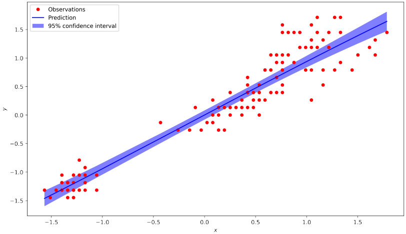
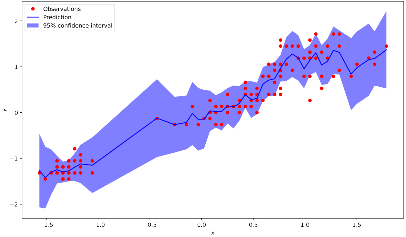
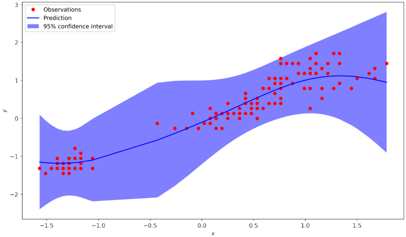


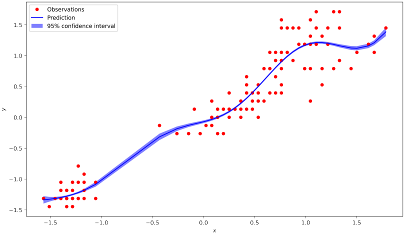


Controls the smoothness of the GP

Modify the Noise

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





Controls the point noise of the GP

Modify the Noise

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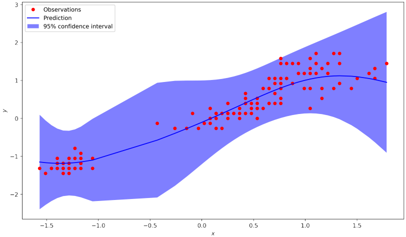

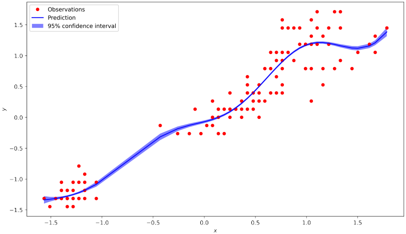

Controls the point noise of the GP

SVM

Support Vector Machines

- Flexible and theoretically supported method
- Initially only applied to classification, 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)

- Hypothesis space: $y_n = f(\mathbf{x}_n, \mathbf{w}) = sign\left(\mathbf{w}^T\mathbf{x}_n + b\right)$
- Loss measure: $||\mathbf{w}||^2 + C\sum_i \zeta_i$ s.t. $t_n(\mathbf{w}^T\mathbf{x}_n + b) \geq 1 - \zeta_i \ \forall n$
- Optimization method: 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_`)

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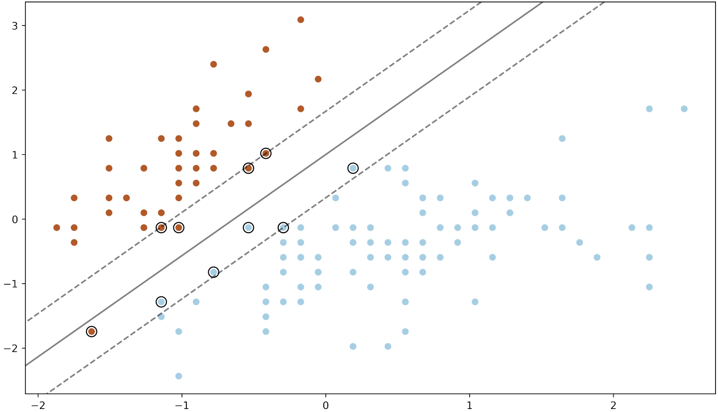

Adding a Kernel

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

- Hypothesis space: $y_n = f(\mathbf{x}_n, \mathbf{w}) = sign\left(\sum_n \alpha_i t_i K(\mathbf{x}_i, \mathbf{x}_n) + b\right)$
- 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

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