

732A99/TDDE01/732A68 Machine Learning

Lecture 3b Block 1: Support Vector Machines

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- Literature

- Lindholm, A., Wahlström, N., Lindsten, F. and Schön, T. B. *Machine Learning - A First Course for Engineers and Scientists*. Cambridge University Press, 2022. Chapter 8.3-8.5.

Support Vector Regression

- Kernel ridge regression = ridge regression in the feature space defined by the mapping $\phi(\cdot)$ rather than in the input space.

$$\hat{\theta} = \arg \min_{\theta} \frac{1}{n} \sum_{i=1}^n \left(\underbrace{\theta^T \phi(\mathbf{x}_i)}_{\hat{y}(\mathbf{x}_i)} - y_i \right)^2 + \lambda \|\theta\|_2^2 = (\Phi(\mathbf{X})^T \Phi(\mathbf{X}) + n\lambda \mathbf{I})^{-1} \Phi(\mathbf{X})^T \mathbf{y}, \quad (8.4a)$$

- Computing $\hat{\theta}$ can be problematic for some feature spaces, since they can be high or even infinite dimensional. However, $\hat{\theta}$ is just needed for prediction.

$$\hat{y}(\mathbf{x}_\star) = \underbrace{\hat{\theta}^T}_{1 \times d} \underbrace{\phi(\mathbf{x}_\star)}_{d \times 1} = \underbrace{\mathbf{y}^T}_{1 \times n} \underbrace{(\Phi(\mathbf{X})\Phi(\mathbf{X})^T + n\lambda \mathbf{I})^{-1}}_{n \times n} \underbrace{\Phi(\mathbf{X})\phi(\mathbf{x}_\star)}_{n \times 1}.$$

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- The formulation above in terms of θ is called the **primal formulation**. The formulation below in terms of α is called the **dual formulation**. Note that α is of dimension n (cf. θ which is of dimension d with $n \ll d$ typically).

$$\hat{\alpha} = \begin{bmatrix} \hat{\alpha}_1 \\ \hat{\alpha}_2 \\ \vdots \\ \hat{\alpha}_n \end{bmatrix} = \mathbf{y}^T (\mathbf{K}(\mathbf{X}, \mathbf{X}) + n\lambda \mathbf{I})^{-1}. \quad (8.14a)$$

$$\hat{y}(\mathbf{x}_{\star}) = \hat{\alpha}^T \mathbf{K}(\mathbf{X}, \mathbf{x}_{\star}). \quad (8.14b)$$

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- Clearly, $\hat{\theta} = \Phi(\mathbf{X})^T \hat{\alpha}$. This result is known as the **representer theorem**.

Support Vector Regression

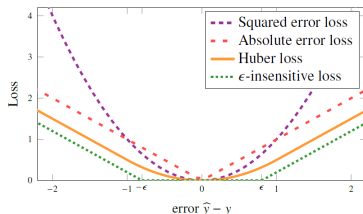


Figure 5.1: The loss functions for regression presented in the text, each as a function of the error $\hat{y} - y$.

- Replace the squared error loss function in kernel ridge regression with the ϵ -insensitive loss function, where ϵ is a user-defined hyperparameter.

$$L(y, \hat{y}) = \begin{cases} 0 & \text{if } |\hat{y} - y| < \epsilon, \\ |\hat{y} - y| - \epsilon & \text{otherwise,} \end{cases} \quad (5.9)$$

Support Vector Regression

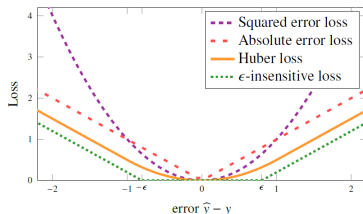


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- ▶ In the primal formulation, we predict as

$$\hat{y}(\mathbf{x}_\star) = \hat{\boldsymbol{\theta}}^\top \boldsymbol{\phi}(\mathbf{x}_\star), \quad (8.18a)$$

where $\hat{\boldsymbol{\theta}}$ is the solution to the optimization problem

$$\hat{\boldsymbol{\theta}} = \arg \min_{\boldsymbol{\theta}} \frac{1}{n} \sum_{i=1}^n \max\{0, |y_i - \underbrace{\boldsymbol{\theta}^\top \boldsymbol{\phi}(\mathbf{x}_i)}_{\hat{y}(\mathbf{x}_i)}| - \epsilon\} + \lambda \|\boldsymbol{\theta}\|_2^2. \quad (8.18b)$$

which has to be solved numerically (i.e., no closed-form solution exists).

Support Vector Regression

- In the dual formulation, we predict as

$$\widehat{y}(\mathbf{x}_\star) = \widehat{\boldsymbol{\alpha}}^\top \mathbf{K}(\mathbf{X}, \mathbf{x}_\star), \quad (8.19a)$$

where $\widehat{\boldsymbol{\alpha}}$ is the solution to the optimization problem

$$\widehat{\boldsymbol{\alpha}} = \arg \min_{\boldsymbol{\alpha}} \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{K}(\mathbf{X}, \mathbf{X}) \boldsymbol{\alpha} - \boldsymbol{\alpha}^\top \mathbf{y} + \epsilon \|\boldsymbol{\alpha}\|_1, \quad (8.19b)$$

$$\text{subject to } |\alpha_i| \leq \frac{1}{2n\lambda}. \quad (8.19c)$$

which has to be solved numerically. Luckily, the objective function is concave up and, thus, **it can be minimized efficiently**. Proving that the primal and dual optimization problems are equivalent is non-trivial.

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- It can be shown that $\widehat{\alpha}_i \neq 0$ only if $|\widehat{y}(\mathbf{x}_i) - y_i| \geq \epsilon$. The training data point $\{\mathbf{x}_i, y_i\}$ is called **support vector**. The prediction in Equation 8.19a depends only on the support vectors. This reduces the computation needed for prediction (cf. kernel ridge regression). This is the reason of using the ϵ -insensitive loss function.

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- **The larger ϵ is, the sparser $\widehat{\boldsymbol{\alpha}}$ is** and the fewer the computations needed for prediction. Does ϵ have a regularizing effect? That $\widehat{\boldsymbol{\alpha}}$ is sparse does not mean that $\widehat{\boldsymbol{\theta}}$ is sparse (recall the representer theorem, and that λ regularizes the primal formulation).

Support Vector Regression

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where $\hat{\alpha}$ is the solution to the optimization problem

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$$\text{subject to } |\alpha_i| \leq \frac{1}{2n\lambda}. \quad (8.19c)$$

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- ▶ Note that all the training data points are used during training (Equation 8.19b).
- ▶ Since many kernel functions (e.g., Gaussian kernel) do not include a constant offset term, an intercept $\hat{\alpha}_0$ is sometimes included in Equation 8.19a.

Support Vector Regression

Example 8.3: Support vector regression and kernel ridge regression

We consider yet again the car stopping distance problem from Example 2.2 in Figure 8.4. With the combined squared exponential and polynomial kernel from Example 8.2, $\lambda = 0.01$ and $\epsilon = 15$, we apply support vector regression to the data (red line). As a reference we also show the corresponding kernel ridge regression (blue line).

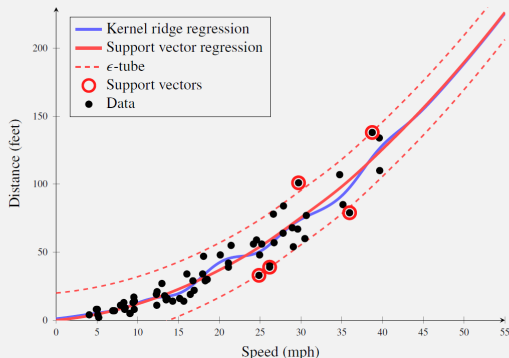


Fig.
8.4

In Figure 8.4 we have encircled (in red) all data points for which $\alpha_i \neq 0$, the so-called support vectors. We have also included the “ ϵ -tube” ($\hat{y}(\mathbf{x}) \pm \epsilon$; dotted lines), and we can confirm that all support vectors are located outside the “ ϵ -tube”. This is a direct effect of using the ϵ -insensitive loss, which explicitly encodes that the loss function for data points within ϵ from $\hat{y}(\mathbf{x})$ is exactly zero. If choosing a smaller ϵ , we would have more support vectors, and vice versa. Another consequence of the sparsity of α is that when computing a prediction (8.19a) with support vector regression, it is sufficient to do the computation using (in this case) only five data points. For kernel ridge regression, which does not have a sparse α , the prediction (8.14b) depends on all 62 data points.

Support Vector Classification

- Consider binary ($\{-1, +1\}$) classification with the classifier $\hat{y}(\mathbf{x}) = \text{sign}\{f(\mathbf{x})\}$, where $f(\mathbf{x})$ is to be learned. The **margin** of the classifier for the point $\{\mathbf{x}, y\}$ is $y \cdot f(\mathbf{x})$. Consider the hinge loss function:

$$L(y \cdot f(\mathbf{x})) = \begin{cases} 1 - y \cdot f(\mathbf{x}) & \text{for } y \cdot f(\mathbf{x}) \leq 1, \\ 0 & \text{otherwise.} \end{cases} \quad (5.17)$$

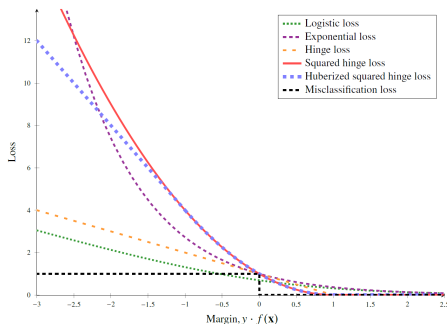


Figure 5.2: Comparison of some common loss functions for classification, plotted as a function of the margin.

Support Vector Classification

- In the primal formulation, we predict as

$$\widehat{y}(\mathbf{x}_\star) = \text{sign} \{ \boldsymbol{\theta}^\top \boldsymbol{\phi}(\mathbf{x}_\star) \} . \quad (8.32)$$

where $\widehat{\boldsymbol{\theta}}$ is the solution to the optimization problem

$$\widehat{\boldsymbol{\theta}} = \arg \min_{\boldsymbol{\theta}} \frac{1}{n} \sum_{i=1}^n \max \{ 0, 1 - y_i \boldsymbol{\theta}^\top \boldsymbol{\phi}(\mathbf{x}_i) \} + \lambda \|\boldsymbol{\theta}\|_2^2 . \quad (8.34)$$

which has to be solved numerically (i.e., no closed-form solution exists).

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which has to be solved numerically (i.e., no closed-form solution exists).

- In the dual formulation, we predict as

$$\hat{y}(\mathbf{x}_\star) = \text{sign} \left(\hat{\boldsymbol{\alpha}}^\top \mathbf{K}(\mathbf{X}, \mathbf{x}_\star) \right) \quad (8.35c)$$

where $\hat{\boldsymbol{\alpha}}$ is the solution to the optimization problem

$$\hat{\boldsymbol{\alpha}} = \arg \min_{\boldsymbol{\alpha}} \frac{1}{2} \boldsymbol{\alpha}^\top \mathbf{K}(\mathbf{X}, \mathbf{X}) \boldsymbol{\alpha} - \boldsymbol{\alpha}^\top \mathbf{y} \quad (8.35a)$$

$$\text{subject to } |\alpha_i| \leq \frac{1}{2n\lambda} \text{ and } 0 \leq \alpha_i y_i \quad (8.35b)$$

which has to be solved numerically. Luckily, the objective function is concave up and, thus, **it can be minimized efficiently**. Proving that the primal and dual optimization problems are equivalent is non-trivial.

Support Vector Classification

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- ▶ It can be shown that $\hat{\alpha}_i \neq 0$ only if the margin $y_i \cdot \hat{\boldsymbol{\alpha}}^\top \mathbf{K}(\mathbf{X}, \mathbf{x}_i) \leq 1$. The training data point $\{\mathbf{x}_i, y_i\}$ is called **support vector**. The prediction in Equation 8.35c depends only on the support vectors. This reduces the computation needed for prediction. This is the reason of using the hinge loss function.

Support Vector Classification

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Support Vector Classification

- It can be shown that **the support vectors are on the wrong side of the decision boundary or on the right side but too close to it**, exactly within

$$\frac{1}{\|\hat{\theta}\|_2} = \frac{1}{\|\Phi(\mathbf{X})^T \hat{\alpha}\|_2} \text{ from it in the feature space.}$$

Support Vector Classification

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- ▶ **The smaller λ** , the larger $\hat{\theta}$ and the smaller $\frac{1}{\|\hat{\theta}\|_2}$ and, thus, **the sparser $\hat{\alpha}$ is** and the fewer the computations needed for prediction. Does $1/\lambda$ have a regularizing effect? That $\hat{\alpha}$ is sparse does not mean that $\hat{\theta}$ is sparse (recall the representer theorem, and that λ regularizes the primal formulation).

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- ▶ Since many kernel functions (e.g., Gaussian kernel) do not include a constant offset term, an intercept $\hat{\alpha}_0$ is sometimes included in Equation 8.35c.

Support Vector Classification

Example 8.5: Support vector classification

We consider the binary classification problem with the data given in Figure 8.5 and apply support vector classification with the linear and the squared exponential kernel, respectively, in Figure 8.6. We mark the support vectors with yellow circles. For the linear kernel, the locations of the support vectors are either on the “wrong side” of the decision boundary or within $\frac{1}{\|\theta\|_2}$ from it, marked with dashed white lines. As we decrease λ we allow for larger θ and thereby a smaller band $\frac{1}{\|\theta\|_2}$ and consequently fewer support vectors.

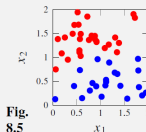


Fig. 8.5

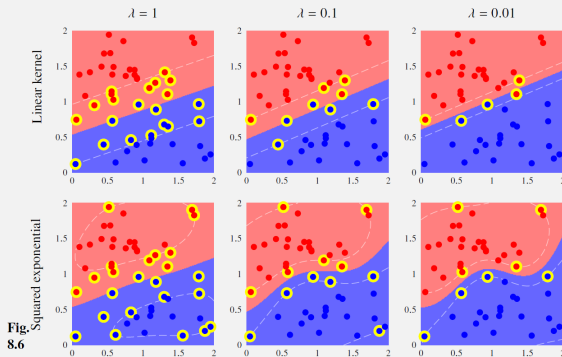


Fig. 8.6

When using the (indeed nonlinear) squared exponential kernel, the situation becomes somewhat harder to interpret. It still holds that the support vectors are either on the “wrong side” of the decision boundary or within $\frac{1}{\|\theta\|_2}$ from it, but the distance is measured in the infinite dimensional $\phi(\mathbf{x})$ -space. Mapping this back to the original input space we observe this heavily nonlinear behavior. The meaning of the dashed white lines are the same as above. This also serves as a good illustration of the power in using kernels.

Summary

- Support Vector Regression
- Support Vector Classification