Introduction to Machine Learning Lab 4: Kernel Regression

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1 Motivation

- Implement some typical kernel functions, and check their feasibility in different models. You may find that some kernels work better for some models while perform poorly for the other models:)
- Implement classic kernel methods like Nadaraya-Watson estimator and kernel ridge regression (KRR). Observe their differences and connections.
- Take KRR as a good example. Try to sharpen your hyperparameter fine-tuning feelings.

2 Tasks

Please read Lecture 5 carefully before doing this lab work.

1. Implement the following four kinds of kernel functions and use them to achieve the Nadaraya-Watson estimator shown in the lecture.

RBF:
$$K_h(\boldsymbol{x}, \boldsymbol{x}') = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{h}\right)$$
, Gate: $K_h(\boldsymbol{x}, \boldsymbol{x}') = \begin{cases} \frac{1}{h}, & \|\boldsymbol{x} - \boldsymbol{x}'\|_1 \le h \\ 0 & \text{Otherwise.} \end{cases}$

Triangle: $K_h(\boldsymbol{x}, \boldsymbol{x}') = \begin{cases} \frac{2}{h}(1 - \frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_1}{h}) & \|\boldsymbol{x} - \boldsymbol{x}'\|_1 \le h \\ 0 & \text{Otherwise} \end{cases}$, Linear: $K(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^T \boldsymbol{x}'$

where h is the hyperparameter. The NW estimator: $y_{new} = \sum_{n=1}^{N} \frac{K(\boldsymbol{x}_{new}, \boldsymbol{x}_n)}{\sum_{i=1}^{N} K(\boldsymbol{x}_{new}, \boldsymbol{x}_i)} y_n$.

2. Implement the closed-form solution of kernel ridge regression:

$$\min_{\boldsymbol{a}} \|\boldsymbol{y} - \boldsymbol{K}\boldsymbol{a}\|_{2}^{2} + \tau \boldsymbol{a}^{T} \boldsymbol{K} \boldsymbol{a}. \tag{2}$$

(Hint: Use as few computations as possible.)

3. **Struggle with KRR's SGD:** Implement a stochastic gradient descent (SGD) algorithm to solve (2). (Hint: Do your best to make it work, and think about whether it actually "works" or not.)