Machine Learning

Non-parametric Regression: k-NN Method and its variants. Bias-Variance trade-off for k-NN Regression. Mean (Absolute) Test Error.

Aleksandr Petiushko

ML Research

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SOFIA UNIVERSITY

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1. Non-parametric Regression

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2. k-NN Regression: Mean (Absolute) Test Error

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Non-parametric Regression

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Assumption

Close objects correspond to close answers

Non-parametric Regression

The simplest model

We approximate the desired dependence by a constant in some neighborhood

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Nadaraya-Watson kernel regression[1]

If there are several objects from the training sample in the vicinity of the point, then it is reasonable to use the weighted average as a prediction of the algorithm

$$a(x) = \frac{\sum\limits_i y_i \omega_i(x)}{\sum\limits_i \omega_i(x)},$$

where $\omega_i(x) = K_h(x, x_i)$, a function K_h is called a **kernel** with smoothing window width h.

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k-NN Regression prediction

Let us have for every x_0 k nearest neighbors $(x_1, \dots, x_k)$ with the ground truth labels $(y_1, \dots, y_k)$. Then the Nadaraya-Watson kernel regression formula will transform into the following:

$$a(x_0) = \frac{1}{k} \sum_{i=1}^{k} y_i$$

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Note: It means we are just averaging the labels of k nearest neighbors.

Examples of more complicated Kernels

- $K_h(x, x_i) = K(\frac{||x-x_i||}{h})$

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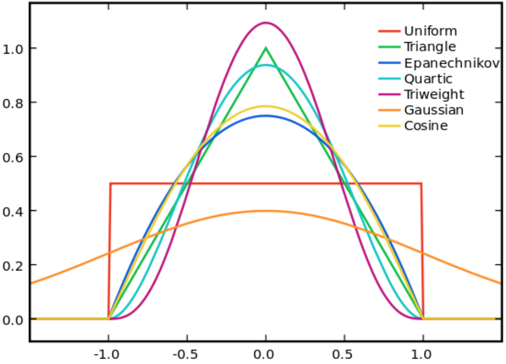

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k-NN Regression: Mean Test Error

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Note: It means we are just averaging the absolute error for every point-wise prediction across the test set.

Reminder: bias-variance tradeoff

Definitions

Let $y = y(x) = f(x) + \varepsilon$ be the target dependence, where $f(x)$ is the deterministic function, $\varepsilon \sim N(0, \sigma^2)$ and $a(x)$ is the machine learning algorithm.

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$$E(y - a)^2 = \sigma^2 + variance(a) + bias^2(f, a)$$

Bias and Variance of k-NN Regression

Bias

$$bias^2(f,a) = (E(f(x_0) - a(x_0)))^2 = \left(f(x_0) - \frac{1}{k}\sum_{i=1}^{k} f(x_i)\right)^2$$

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Variance

$$Variance(a) = D\left(\frac{1}{k} \sum_{i=1}^{k} y(x_i) \right) = \frac{1}{k^2} D\left(\sum_{i=1}^{k} y(x_i) \right) =$$

$$= \frac{1}{k^2} D\left(\sum_{i=1}^{k} (f(x_i) + \varepsilon_i) \right) = \frac{1}{k^2} D\left(\sum_{i=1}^{k} f(x_i) \right) + \frac{1}{k^2} D\left(\sum_{i=1}^{k} \varepsilon_i \right) =$$

$$= 0 + \frac{1}{k^2} k\sigma^2 = \frac{\sigma^2}{k}$$

Bias-Variance tradeoff of k-NN Regression

$$Error(x_0) = E(a(x_0) - f(x_0))^2 = \left(f(x_0) - \frac{1}{k}\sum_{i=1}^{k} f(x_i) \right)^2 + \frac{\sigma^2}{k} + \sigma^2$$

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Note: Under "reasonable assumptions" the bias of the 1-NN estimator vanishes entirely as the size of the training set approaches infinity

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- To compute the k-NN Regression Prediction we are averaging the nearest neighbors labels,
- To compute the k-NN Regression Mean (Absolute) Test Error we are averaging the absolute error for every point-wise prediction across the test set.

Thank you!