Lecture 17: Kernel Theory

With kernel ridge regression (KRR) and support vector regression (SVR) we learned three concepts:

1) Primal and dual formulations of a model

- Primal formulation expresses the model in terms of $\underline{\theta} \in \mathbb{R}^d$
- Dual formulation uses $\underline{\alpha} \in \mathbb{R}^N$ ($N \leftarrow$ size of training data set), and does not depend on the value of 'd'
- Both formulations are mathematically equivalent
  - Primal formulation is useful if $N > d$
  - Dual formulation is useful if $d > N$

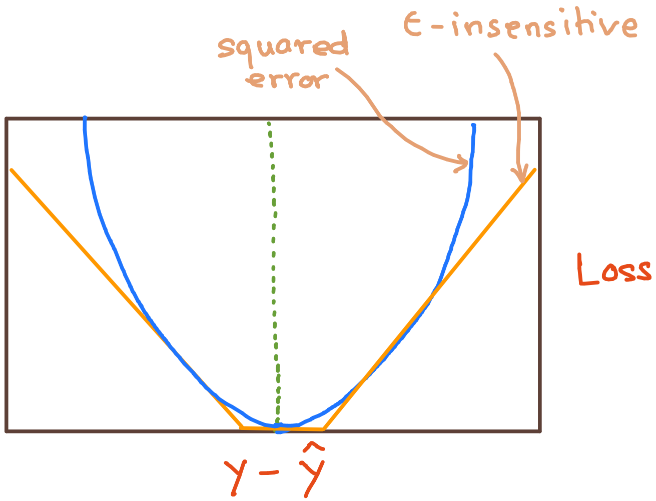
2) We introduced kernels $K(\underline{x}, \underline{x}')$ that allows us to let $d \to \infty$ without explicitly formulating an infinite vector of non-linear transformations $\underline{\phi}(\underline{x})$

- The dual formulation is particularly useful when using kernel methods, since the dimension of $\underline{\theta}$ in the primal formulation could be very large

3) We used different loss functions (and included L_2-regularization)

- KRR makes use of squared error loss
- SVR uses ϵ-insensitive loss

gives sparse $\underline{\alpha}$ in the dual formulation



Kernel theory

Lets look a bit more into kernels

- Kernel was defined as being any function that takes in two arguments and returns a scalar

- We also suggested that we will restrict ourselves to PSD kernels
  positive semi-definite

- Vanilla kNN $\longrightarrow$ kernel kNN (provides a variety of distance metrics)

  • Recall that vanilla kNN constructs prediction for $\underline{x}^*$ by taking the average or a majority vote among the k "nearest" neighbours

  • In its standard form, "nearest" was defined by the Euclidean distance

  • Euclidean distance between 2 points $\underline{x}$ and $\underline{x}'$: $\|\underline{x} - \underline{x}'\|_2$ (always +ve)

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- Since Euclidean distance is positive, we can consider squared Euclidean distance instead

$$\|\underline{x} - \underline{x}'\|_2^2 = (\underline{x} - \underline{x}')^T(\underline{x} - \underline{x}')$$

$$= \underline{x}^T\underline{x} + \underline{x}'^T\underline{x}' - 2\underline{x}^T\underline{x}'$$

For many kernels, these terms are mostly constants (e.g. RBF kernel)

Define a kernel $K(\underline{x}, \underline{x}') = \underline{x}^T\underline{x}'$

$$= K(\underline{x}, \underline{x}) + K(\underline{x}', \underline{x}') - \underbrace{2K(\underline{x}, \underline{x}')}$$

this term is more interesting

this term determines how close any two points are

$K(\underline{x}, \underline{x}')$ takes a large value if $\underline{x}$ and $\underline{x}'$ are close

- In kernel kNN, $K(\underline{x}, \underline{x}')$ can be replaced with any PSD kernel

- How can you use vanilla kNN where Euclidean distance has no natural meaning?

Example : Distance between words which reflect sentiment

Word	Sentiment
Tremendous	Positive
Horrific	Negative
Outrageous	Negative

- what could be the label for "horrendous"?

- One may think of converting the input space to numbers first and then use Euclidean distance

$x^* =$ Horrendous

$k = 1 \longrightarrow$ Positive

$k = 3 \longrightarrow$ Negative

- An easier way to compare is using, for ex, Levenstein distance (LD), which is the number of single-character edits needed to transform one word (string) into another

- One can construct a kernel as $K(\underline{x}, \underline{x}') = \exp\left(- \frac{(LD(x, x'))^2}{2\ell^2} \right)$

to implement kernel kNN (instead of vanilla kNN)

Lessons learned about kernels so far

- A kernel defines how close / similar any two points are
  - If $\kappa(\underline{x}^{(i)}, \underline{x}^*) > \kappa(\underline{x}^{(j)}, \underline{x}^*)$, then $\underline{x}^*$ is more similar to $\underline{x}^{(i)}$ than $\underline{x}^{(j)}$
  - It also implies that prediction $\hat{y}(\underline{x}^*)$ is most influenced by the training data points that are closest to $\underline{x}^*$
  - Therefore, a kernel plays an important role of determining the individual influence of each training data point when making a prediction

- No need to bother about the inner product $\underline{\phi}(\underline{x})^T \underline{\phi}(\underline{x}')$ once we have introduced the kernel $\kappa(\underline{x}, \underline{x}')$

Lessons learned about kernels so far

- Choice of a kernel corresponds to preference for certain types of functions
  - For example, the squared exponential (or RBF) kernel

$$K(\underline{x}, \underline{x}') = \exp\left(-\frac{\|\underline{x}-\underline{x}'\|_2^2}{2\ell^2}\right)$$

    implies a preference for smooth functions

  - In primal formulation, we choose features $\underline{\phi}(\underline{x})$ which will reflect the type of transformations we want to introduce. This choice is reflected to some extent in choosing kernels in the dual formulation

A machine learning engineer must choose a kernel wisely and should not simply resort to 'default' choices

What are valid choices of kernels?

- We already know that kernels are a way to represent non-linear feature transformation $\underline{\phi}(\underline{x})$

$$K(\underline{x}, \underline{x}') = \underline{\phi}(\underline{x})^T \underline{\phi}(\underline{x}')$$

- Question: Does an arbitrary kernel $K(\underline{x}, \underline{x}')$ always correspond to a feature transformation $\underline{\phi}(\underline{x})$?

  - The question is primarily of theoretical nature
  - Practically, it matters very less whether a kernel $K(\underline{x}, \underline{x}')$ admits a factorization $K(\underline{x}, \underline{x}') = \underline{\phi}(\underline{x})^T \underline{\phi}(\underline{x}')$ or not
  - Furthermore, the factorization has no direct correspondence to how well the kernel will perform in terms of E_{new}, which still has to be evaluated using cross-validation

Question: Does an arbitrary kernel $\kappa(\underline{x}, \underline{x}')$ always correspond to a feature transformation $\underline{\phi}(\underline{x})$?

Answer: Yes, if the kernel $\kappa(\underline{x}, \underline{x}')$ is PSD (positive semi-definite)
(no negative eigen-values)

Recall that a kernel is PSD if the Gram matrix $\underline{\underline{K}}(\underline{\underline{X}}, \underline{\underline{X}})$ is PSD for any $\underline{\underline{X}}$

- It holds that any kernel $\kappa(\underline{x}, \underline{x}')$ that is defined as an inner product between feature vectors $\underline{\phi}(\underline{x})$ is always PSD

$$\kappa(\underline{x}, \underline{x}') = \underline{\phi}(\underline{x})^T \underline{\phi}(\underline{x}')$$
$$= \langle \phi(\underline{x}), \phi(\underline{x}') \rangle$$

$\langle \cdot, \cdot \rangle \leftarrow$ inner product

Show $\underline{v}^T \underline{\underline{K}}(\underline{\underline{X}}, \underline{\underline{X}}) \underline{v} \geq 0$ for any vector v (do yourself)

Question: Does an arbitrary kernel $K(\underline{x}, \underline{x}')$ always correspond to a feature transformation $\underline{\phi}(\underline{x})$?

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$$\underbrace{\underline{\phi}(\underline{x})}_{\text{feature vector}} \xrightarrow{\text{inner product}} \underbrace{K(\underline{x}, \underline{x}')}_{\text{PSD}}$$

- The other direction also holds true, that is, for any PSD kernel $K(\underline{x}, \underline{x}')$ there always exist a feature vector $\underline{\phi}(\underline{x})$ such that $K(\underline{x}, \underline{x}')$ can be written as its inner product

$$\underbrace{\underline{\phi}(\underline{x})}_{\text{feature vector}} \longleftarrow \underbrace{K(\underline{x}, \underline{x}')}_{\text{if PSD}}$$

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- It can be shown that for any PSD kernel, it is possible to construct a function space, more specifically a Hilbert space, that is spanned by a feature vector $\underline{\phi}(\underline{x})$ s.t. $K(\underline{x}, \underline{x}') = \underline{\phi}(\underline{x})^T \underline{\phi}(\underline{x}')$

  - There are multiple ways to construct a Hilbert space space spanned by $\underline{\phi}(\underline{x})$. One of the ways is using the so-called reproducing kernel Hilbert space (RKHS) mapping

A brief introduction to Reproducing Kernel Hilbert Spaces (RKHS)

- Euclidean space is a space of vectors equipped with inner products between vectors

- Hilbert space is a generalization of Euclidean space to functions (which can be treated as infinite dimensional vectors). It allows inner product between functions

  space of functions with inner product

- A Hilbert space H is called the RKHS if there exists a kernel $K(\underline{x}, \underline{x}')$ with the reproducing property that

$$f(\underline{x}') = \langle f(\cdot), K(\cdot, \underline{x}') \rangle \quad \forall f \in H, \ \forall \underline{x}'$$

  - If we set $f(\cdot) = K(\cdot, \underline{x})$, then

$$\langle K(\cdot, \underline{x}), K(\cdot, \underline{x}') \rangle = K(\underline{x}, \underline{x}')$$

This reproducing property is the main building block of RKHS. This RKHS is spanned by the corresponding feature $\underline{\phi}(\underline{x})$ of kernel $K(\underline{x}, \underline{x}')$

Question: Does an arbitrary kernel $K(\underline{x},\underline{x}')$ always correspond to a feature transformation $\underline{\phi}(\underline{x})$?

Answer: Yes, if the kernel $K(\underline{x},\underline{x}')$ is PSD (positive semi-definite)
(no negative eigen-values)

$$\underbrace{\underline{\phi}(\underline{x})}_{\text{feature vector}} \xrightarrow{\text{inner product}} \underbrace{K(\underline{x},\underline{x}')}_{\text{PSD}}$$

$$\underbrace{\underline{\phi}(\underline{x})}_{\text{feature vector}} \longleftarrow \underbrace{K(\underline{x},\underline{x}')}_{\text{if PSD}}$$

(spans a RKHS)

- A given Hilbert space uniquely defines a kernel, but for a kernel there exists multiple Hilbert spaces which correspond to it

$$\underbrace{K(\underline{x},\underline{x}')}_{\text{if PSD}} \longrightarrow \underline{\phi}_1(\underline{x})$$

feature vector
(spans a RKHS)

$$\underbrace{K(\underline{x},\underline{x}')}_{\text{if PSD}} \longrightarrow \underline{\phi}_2(\underline{x})$$

feature vector

E.g. $K(\underline{x},\underline{x}') = \underline{x}^T\underline{x}'$

$\phi_1(\underline{x}) = x$
(one-dimensional)

$$\phi_2(\underline{x}) = \begin{bmatrix} x/\sqrt{2} \\ x/\sqrt{2} \end{bmatrix}$$

(two-dimensional)