Basic Kernel Methods

Machine Learning

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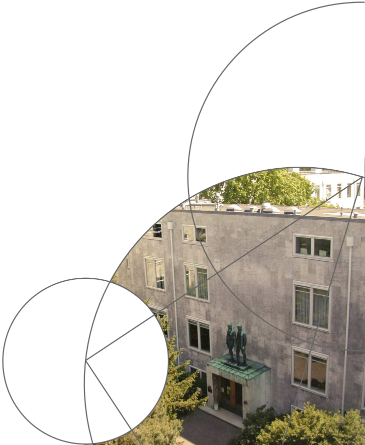

Outline

1. Kernel Perceptron

2. Kernel Nearest Neighbor

3. Representer Theorem

4. Regularization Networks

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Perceptron learning algorithm

Algorithm 1: Kernel perceptron

Input: data $\{(x_1, y_1), \dots\} \subseteq (\mathcal{X} \times \{-1, 1\})^N$, kernel k

Output: hypothesis $h(x) = \operatorname{sgn}\left(\sum_{i=1}^N \alpha_i y_i k(x_i, x)\right)$

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$\boldsymbol{\alpha} \leftarrow \mathbf{0}$
repeat
    for $i = 1, \dots, N$ do
        if $y_i \sum_{j=1}^N \alpha_j y_j k(x_j, x_i) \leq 0$ then
            $\alpha_i \leftarrow \alpha_i + 1$
until no mistake made within for loop
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κ-nearest neighbor (κ-NN)

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Algorithm 2: $\kappa$-nearest neighbor
Input: kernel $k$, $\kappa \in \mathbb{N}^+$, data
       $\{(x_1, y_1), \dots\} \subseteq (\mathcal{X} \times \{-1, 1\})^N$, new input $x$ to be
       classified
Output: predicted label $y$ of $x$
$S = \{(x_1, y_1), \dots\}$
$S_\kappa = \emptyset$
while $|S_\kappa| < \kappa$ do
    $S' \leftarrow \left\{ \operatorname{argmin}_{(x_i, y_i) \in S} \sqrt{k(x, x) - 2k(x, x_j) + k(x_j, x_j)} \right\}$
    $S_\kappa \leftarrow S_\kappa \cup S'$
    $S \leftarrow S \setminus S'$
Result: $y = \operatorname{sgn}\left( \frac{1}{|S_\kappa|} \sum_{(x_i, y_i) \in S_\kappa} y_i \right)$
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Representer theorem

Let $\Omega : [0, \infty[\to \mathbb{R}$ be a strictly monotonic increasing function, $\mathcal{H}$ a RKHS with kernel k on $\mathcal{X}$ and L a loss function. Given $S = \{(x_1, y_1), \dots, (x_N, y_N)\} \subset (\mathcal{X} \times \mathbb{R})^N$, each minimizer $f \in \mathcal{H}^b$ of the regularized empirical risk

$$\sum_{i=1}^{N} L(y_i, f(x_i)) + \Omega(\|f\|_k^2)$$

admits a representation of the form

$$f(x) = \sum_{i=1}^{N} \alpha_i k(x_i, x) + b$$

with $\alpha_1, \dots, \alpha_N, b \in \mathbb{R}$.

Proof of representer theorem

Projecting candidate solution onto span of training patterns

$$f(x) = f_{\|}(x) + f_{\perp}(x) + b = \sum_{i=1}^{N} \alpha_i k(x_i, x) + f_{\perp}(x) + b$$

$$\forall j \in \{1, \dots, N\} : f(x_j) = \langle f(\cdot), k(x_j, \cdot) \rangle + b$$

$$= \sum_{i=1}^{N} \alpha_i k(x_i, x_j) + \langle f_{\perp}(\cdot), k(x_j, \cdot) \rangle + b = \sum_{i=1}^{N} \alpha_i k(x_i, x_j) + b$$

$$\Omega \left(\left\| \sum_{i=1}^{N} \alpha_i k(x_i, .) \right\|_k^2 + \|f_{\perp}\|_k^2 \right) \geq \Omega \left(\left\| \sum_{i=1}^{N} \alpha_i k(x_i, .) \right\|_k^2 \right)$$

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Regularization networks I

The squared loss function gives an empirical risk

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - f(x_i))^2 \ \ .$$

Applying regularization leads to regularized riks

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - f(x_i))^2 + \gamma\|f\|^2$$

for $f \in \mathcal{H}$; we know there is a solution of the form

$$f(x) = \sum_{i=1}^{N}\alpha_i k(x_i, x) \ \ .$$

Regularization networks II

We have $\partial f(x)/\partial \alpha_i = k(x_i, x)$. Setting functional derivative of regularized loss to zero yields for all $i = 1, \dots, N$:

$$\frac{2}{N}\sum_{j=1}^{N}(y_j - f(x_j))k(x_i, x_j) - 2\gamma\langle f, k(x_i, \cdot)\rangle = 0$$

$$\sum_{j=1}^{N}(y_j - f(x_j))k(x_i, x_j) - N\gamma f(x_i) = 0$$

$$\sum_{j=1}^{N}\left[y_j - \sum_{m=1}^{N}\alpha_m k(x_m, x_j)\right]k(x_i, x_j) - N\gamma\sum_{l=1}^{N}\alpha_l k(x_l, x_i) = 0$$

$$\sum_{j=1}^{N}\left[y_j - \sum_{m=1}^{N}\alpha_m k(x_m, x_j) - N\gamma\alpha_j\right]k(x_i, x_j) = 0$$

Regularization networks III

$$\sum_{j=1}^{N}\left[y_j-\sum_{m=1}^{N}\alpha_m k(x_m,x_j)-N\gamma\alpha_j\right]k(x_i,x_j)=0$$

for all i is fulfilled if for all j

$$y_j-\sum_{m=1}^{N}\alpha_m k(x_m,x_j)-N\gamma\alpha_j=0$$

(which is necessary if k is strictly positive definite)

In matrix form we have

$$\boldsymbol{y}-(N\gamma\boldsymbol{I}+\boldsymbol{K})\boldsymbol{\alpha}=\mathbf{0}$$

→ Algorithm “almost magical for its simplicity and effectiveness” (Poggio & Smale, 2003)

Regularization networks IV

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Algorithm 3: Regularization network
Input: kernel $k$, regularization parameter $\gamma \in \mathbb{R}^+$, data
       $\{(x_1, y_1), \dots\} \subseteq (\mathcal{X} \times \mathbb{R})^N$
Output: hypothesis $h(x) = \sum_{i=1}^{N} \alpha_i k(x_i, x)$
$\boldsymbol{y} = (y_1, \dots, y_N)^\mathsf{T}$
$\boldsymbol{I} = \mathrm{diag}(1, \dots, 1) \in \mathbb{R}^{N \times N}$
$\boldsymbol{K} \in \mathbb{R}^{N \times N}, [\boldsymbol{K}]_{ij} = k(x_i, x_j)$
$\boldsymbol{\alpha} \leftarrow (N\gamma\boldsymbol{I} + \boldsymbol{K})^{-1}\boldsymbol{y}$
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Summary

- Kernel trick leads to many simple, but effective algorithms
- Regularization networks algorithm is key learning method
- Minimizer of the regularized loss lies in the span of the kernels centered on the training points

References:

B. Schölkopf and A. J. Smola, Learning with Kernels, MIT Press, 2002.

T. Poggio and S. Smale, The mathematics of learning: Dealing with data. Notices of the American Mathematical Society, 50(5):537–544, 2003