Nearest neighbor methods

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Introduction to Machine Learning
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Outline

- Objects (or observations): $LS = \{o_1, \ldots, o_N\}$
- Attribute vector: $\boldsymbol{a}^i = (a_1(o_i), \ldots, a_n(o_i))^T$, $\forall i = 1, \ldots, N.$
- Outputs: $y^i = y(o_i)$ or $c^i = c(o_i)$, $\forall i = 1, \ldots, N.$
- LS Table

o	$a_1(o)$	$a_2(o)$	$\ldots$	$a_n(o)$	$y(o)$
1	a_1^1	a_2^1	$\ldots$	a_n^1	y^1
2	a_1^2	a_2^2	$\ldots$	a_n^2	y^2
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
N	a_1^N	a_2^N	$\ldots$	a_n^N	y^N

Nearest neighbor methods

Intuition: similar objects should have similar output values.

- NB: all inputs are numerical scalars
- Define distance measure in the input space:

$$d_a(o, o') = (\boldsymbol{a}(o) - \boldsymbol{a}(o'))^T(\boldsymbol{a}(o) - \boldsymbol{a}(o')) = \sum_{i=1}^{n}(a_i(o) - a_i(o'))^2$$

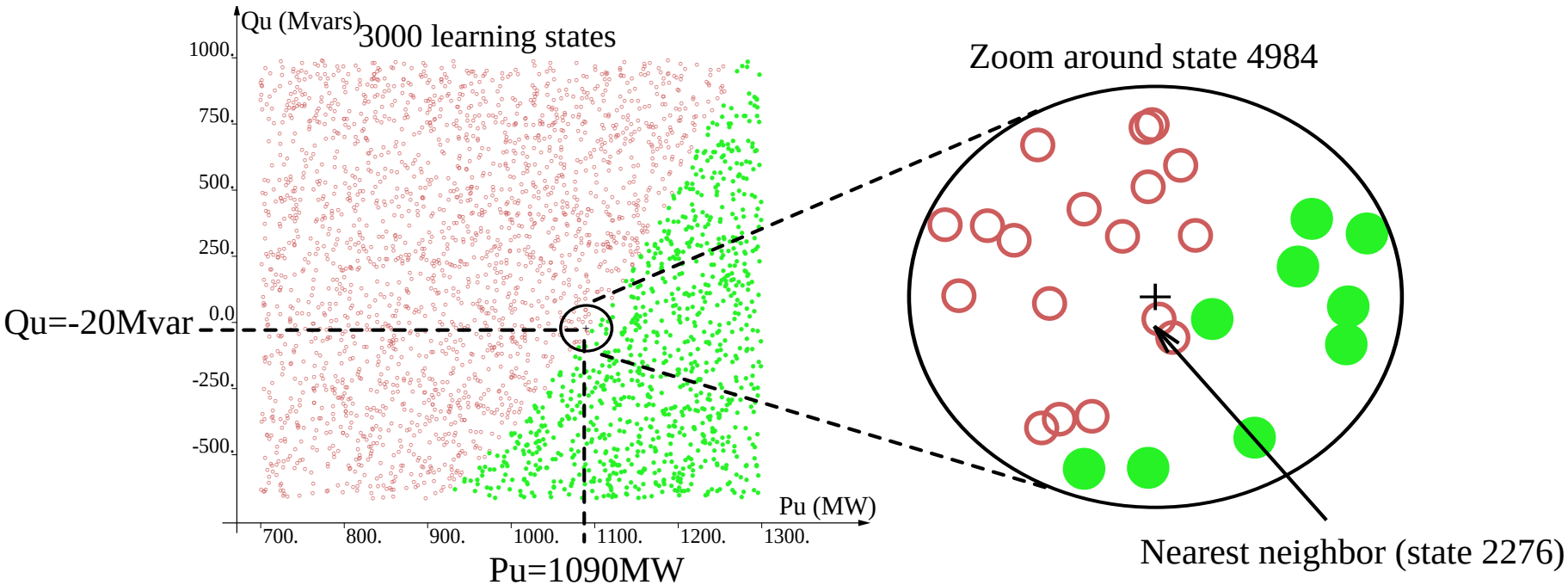
- Nearest neighbor:

$$NN_a(o, LS) = \arg\min_{o' \in LS} d_a(o, o')$$

- Extrapolate output from nearest neighbor:

$$\hat{y}_{NN}(o) = y(NN_a(o, LS))$$

Nearest neighbor methods: illustration



Properties of the NN method

Computational

- Training: storage of the LS ($n \times N$)
- Testing: N distance computations $\Rightarrow N \times n$ computations

Accuracy

- Asymptotically ($N \to \infty$): suboptimal (except if problem is deterministic)
- Strong dependence on choice of attributes $\Rightarrow$ weighting of attributes

$$d_a^w(o, o') = \sum_{i=1}^{n} w_i (a_i(o) - a_i(o'))^2$$

or attribute selection...

Refinements of the NN method

1. The k-NN method:
   - Instead of using only the nearest neighbor, one uses the k (a number to be determined) nearest neighbors:

$$kNN_a(o, LS) = First(k, Sort(LS, d_a(o, \cdot)))$$

   - Extrapolate from k nearest neighbors, e.g. for regression

$$\hat{y}_{kNN}(o) = k^{-1} \sum_{o' \in kNN_a(o,LS)} y(o')$$

     and majority class for classification.
   - k allows to control overfitting (like pruning of trees).
   - Asymptotically ($N \to \infty$): $k(N) \to \infty$ and $\frac{k(N)}{N} \to 0 \Rightarrow$ optimal method (minimum error)

Refinements of the NN method

2. Condensing and editing of the LS:

   - Condensing: remove 'useless' objects LS
   - Editing: remove 'outliers' from LS
   - Apply first editing then condensing (see notes)

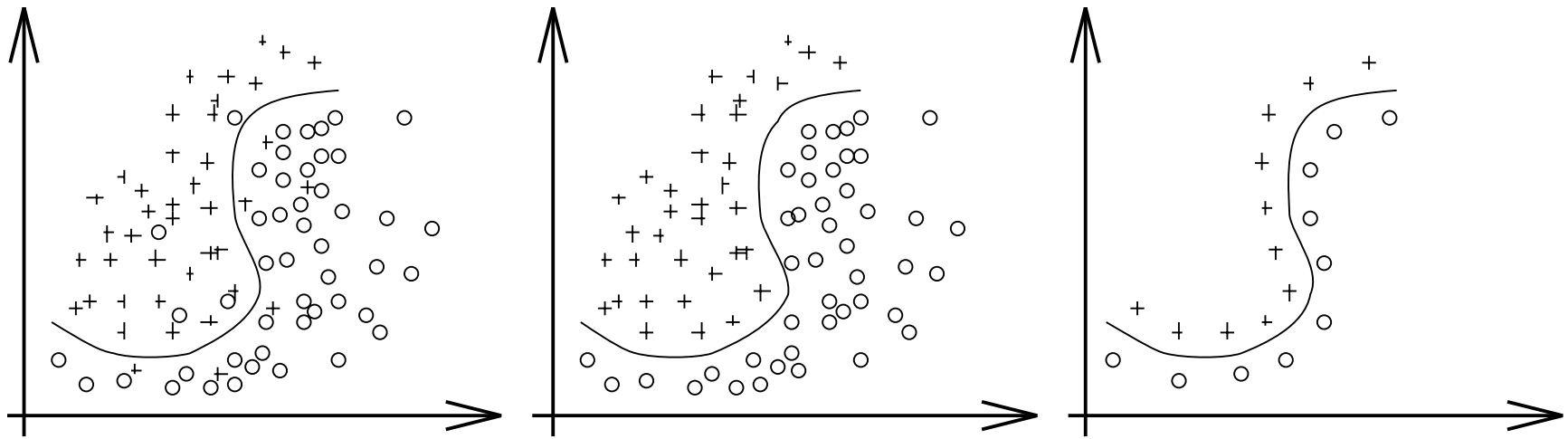
3. Automatic tuning of the weight vector w...

4. Parzen windows and/or kernel methods:

$$\hat{y}_K(o) = \sum_{o' \in LS} y(o') K(o, o')$$

   where $K(o, o')$ is a measure of similarity

Nearest neighbor, editing and condensing



Relation between tree-based and kernel-based methods

Kernel defined by a regression tree:

- Let $\mathcal{L}_i, i = 1, \ldots, |\mathcal{T}|$ denote the leaves of $\mathcal{T}$.
- Let N_i denote the number of objects in the sub-LS of $\mathcal{L}_i$.
- Let $K_{\mathcal{T}}(o, o')$ be equal to N_i^{-1} if o and o' reach same leaf $\mathcal{L}_i$, and 0 otherwise.
- Then the approximation of the regression tree may be written as

$$\hat{y}_{\mathcal{T}}(o) = \sum_{o' \in LS} y(o') K_{\mathcal{T}}(o, o').$$

Scalar product representation of tree kernels

Kernel defined by a regression tree:

- Let $\mathcal{L}_i, i = 1, \ldots, |\mathcal{T}|$ denote the leaves of $\mathcal{T}$.
- Let N_i denote the number of objects in the sub-LS of $\mathcal{L}_i$.
- For each leaf, define a function attribute $a_{\mathcal{L}_i}(o)$ by $a_{\mathcal{L}_i}(o) = N_i^{-1/2}$ if o reaches $\mathcal{L}_i$, and zero otherwise.
- Let $\boldsymbol{a}_{\mathcal{T}}(o) = (a_{\mathcal{L}_1}(o), \ldots, a_{\mathcal{L}_{|\mathcal{T}|}}(o))^T$
- Then we have that

$$K_{\mathcal{T}}(o, o') = \boldsymbol{a}_{\mathcal{T}}^T(o)\boldsymbol{a}_{\mathcal{T}}(o')$$

- and

$$\hat{y}_{\mathcal{T}}(o) = \sum_{o' \in LS} y(o')\boldsymbol{a}_{\mathcal{T}}^T(o)\boldsymbol{a}_{\mathcal{T}}(o').$$

Relation between kernel-based and linear methods

Let us consider a two-class classification problem, and define $y(o) = 1$ if $c(o) = c_1$ and $y(o) = -1$ if $c(o) = c_2$.
Let us construct a simple classifier:

- Center of class 1: $\boldsymbol{c}_+ = N_+^{-1} \sum_{o' \in LS_+} \boldsymbol{a}(o')$
- Center of class 2: $\boldsymbol{c}_- = N_-^{-1} \sum_{o' \in LS_-} \boldsymbol{a}(o')$
- Classifier: $\hat{y}(o) = 1$ if $d(\boldsymbol{c}_+, \boldsymbol{a}(o)) < d(\boldsymbol{c}_-, \boldsymbol{a}(o))$.
- Define $\boldsymbol{c} = \frac{\boldsymbol{c}_+ + \boldsymbol{c}_-}{2}$ and $\Delta\boldsymbol{c} = \boldsymbol{c}_+ - \boldsymbol{c}_-$
- With these notations we have $\hat{y}(o) = sgn((\boldsymbol{a}(o) - \boldsymbol{c})^T \Delta\boldsymbol{c})$
- In other words:

$$\hat{y}(o) = sgn\left(N_+^{-1} \sum_{o' \in LS_+} \boldsymbol{a}^T(o')\boldsymbol{a}(o) - N_-^{-1} \sum_{o' \in LS_-} \boldsymbol{a}^T(o')\boldsymbol{a}(o) + \boldsymbol{b} \right)$$

where $b = \frac{1}{2}(||\boldsymbol{c}_-||^2 - ||\boldsymbol{c}_+||^2)$

Further reading

Reference book (Hastie *et al.*, 2009):

- Section 2.3
- Section 13.3

Frequently asked questions

- How to choose a value for k ?
- Asymptotic ($N \to \infty$) properties of 1-NN vs k-NN
  - Under which conditions is 1-NN asymptotically consistent?
  - Explain why: $k(N) \to \infty$ and $\frac{k(N)}{N} \to 0 \Rightarrow$ optimal method (minimum error)
- Discuss computational complexity and interpretability