Lecture 3: Challenges in Machine Learning

DD2421

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How should we select/determine the right model f from data?

Basic idea for classification:

Given training data

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$$

of inputs $\mathbf{x}_i \in \mathbb{R}^d$ and their labels y_i.

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Compute the misclassification rate on D

$$err(f, D) = \frac{1}{N} \sum_{i=1}^{N} \text{Ind}\left(f(\mathbf{x}_i) \neq y_i\right)$$

Note: $\text{Ind}\,(x) = 1$ if $x =$ TRUE otherwise $\text{Ind}\,(x) = 0$

1. Overfitting
2. Cross-Validation
3. The Curse of Dimensionality
4. The Bias-Variance Trade-off
    - Concept of prediction errors
    - Decomposition of the MSE
    - Bias and variance

Overfitting

Visited in Lecture 2 using decision tree.

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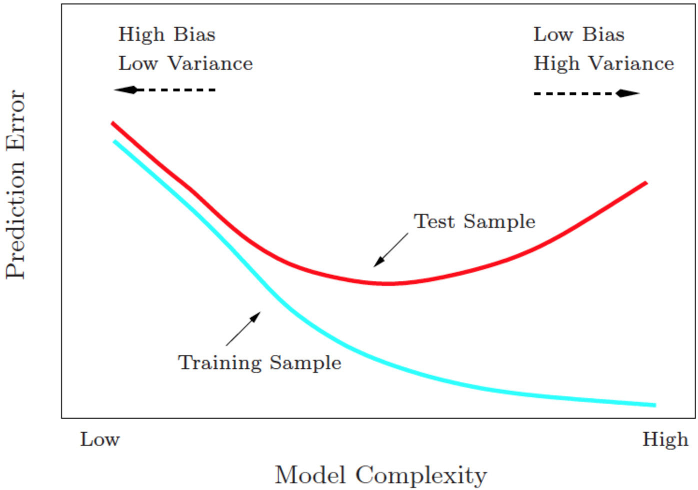
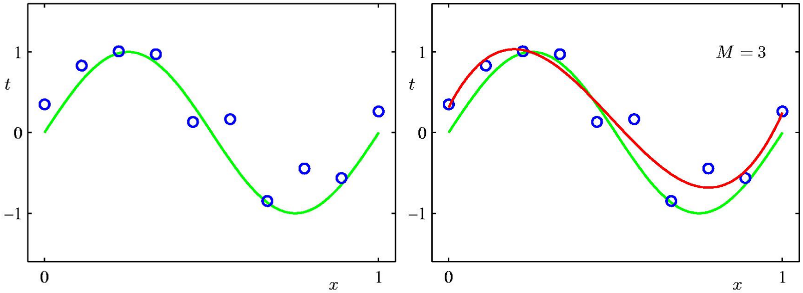
Overfitting

When the learned models are overly specialized for the training samples.



(T. Hastie et al, The Elements of Statistical Learning)

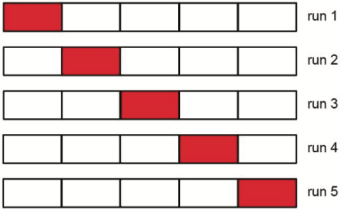
Example: Polynomial Curve Fitting (regression to sinusoidal)



$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

(C. Bishop, Pattern Recognition and Machine Learning)

K-fold cross validation (schematic for $K = 5$)



(K. Murphy, Machine Learning – A probabilistic perspective)

- *Training set* T: to fit the models
- *Validation set* V: to estimate prediction error for model selection (i.e. to determine *hyperparameters*)

If we are in a data-rich situation:

→ partition the data into three sets, *Training* set, *Validation* set, and *Test* set for assessment of the generalization error of the final chosen model.

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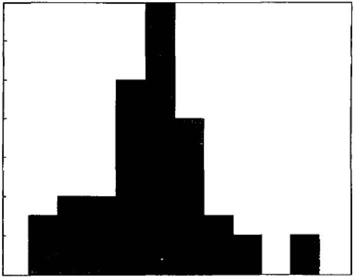
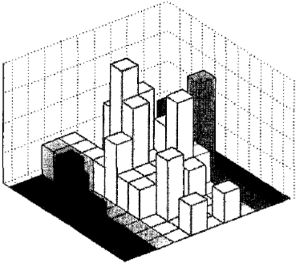
- Easy problems in low-dimensions are harder in high-dimensions
  – training more complex model with limited sample data
- In high-dimensions everything is far from everthing else
  – issues in Nearest Neighbours
- Any method that attempts to produce locally varying functions in small isotropic neighbourhoods will run into problems in high dimensions.

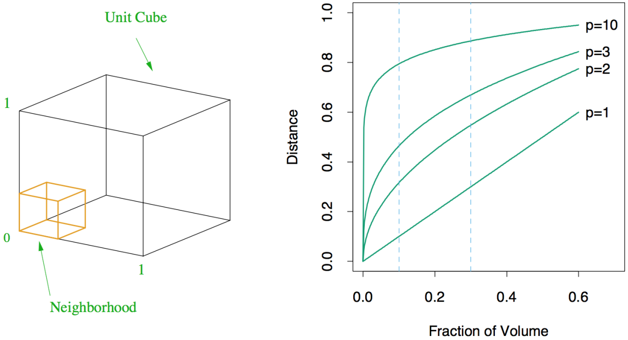
Example 1: Normal random numbers in 1-d and 2-d
(both plots for 100 inputs)





Too few data to represent the probability density function in 2-d.

Example 2: A subcubical neighbourhood for uniform data in a unit cube.



(T. Hastie et al, The Elements of Statistical Learning)

Graph: The side-length of the subcube needed to capture a fraction of the volume of the data (for different demensions p).

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Techniques for dimensionality reduction / feature selection exist.

The Bias-Variance Trade-off

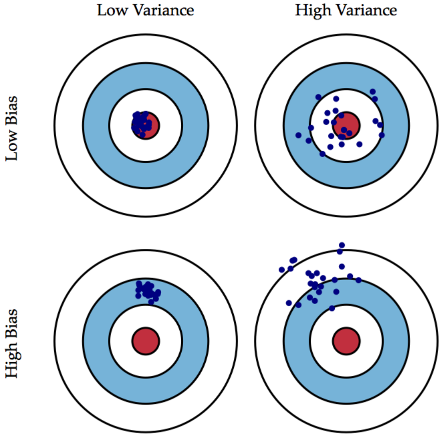
Concepts of prediction errors

Let us imagine we could repeat the modeling for many times – each time by gathering new set of training samples, $\mathcal{D}$.

The resulting models will have a range of predictions due to randomness in the underlying data set.

- Error due to **Bias**: the difference between the average (expected) prediction of our model and the correct value.
- Error due to **Variance**: the variability of a model prediction for a given data point between different realizations of the model.

Graphical illustration of bias and variance



(figure source: http://scott.fortmann-roe.com/docs/BiasVariance.html)

The bias-variance decomposition

Let us consider

$$\begin{aligned} f(\mathbf{x}) &: \quad \text{true function} \\ \hat{f}_{\mathcal{D}}(\mathbf{x}) &: \quad \text{prediction function (= model) estimated with } \mathcal{D} \end{aligned}$$

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and a conceptual tool:

$E_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(\mathbf{x})]$: average of models due to different sample sets
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The mean square error (MSE) for estimating $f(\mathbf{x})$

$$\begin{aligned} E_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(\mathbf{x}) - f(\mathbf{x}))^2] &= E_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(\mathbf{x}) - E[\hat{f}_{\mathcal{D}}(\mathbf{x})])^2] + (E[\hat{f}_{\mathcal{D}}(\mathbf{x})] - f(\mathbf{x}))^2 \\ &= \textbf{Variance} + (\textbf{Bias})^2 \end{aligned}$$

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To complete, we compute: $E_{\mathbf{x}}[E_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(\mathbf{x}) - f(\mathbf{x}))^2]]$

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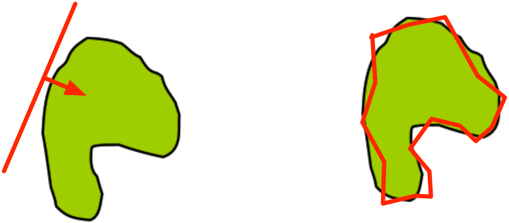
Taking $E_{\mathcal{D}}[\ \ldots\ ]$ for both sides, the cross term disappears (!) while the second term stays the same.

Characterization of a classifier: Bias

Bias of a classifier is the discrepancy between its averaged estimated and true function

$$E[\hat{f}_{\mathcal{D}}(\mathbf{x})] - f(\mathbf{x})$$



High-bias classifier **Low-bias classifier**

Low model complexity (small # of d.o.f.) $\Longrightarrow$ High-bias
High model complexity (large # of d.o.f.) $\Longrightarrow$ Low-bias

Characterization of a classifier: Variance

Variance of a classifier is the expected divergence of the estimated prediction function from its average value:

$$E_{\mathcal{D}}[(\hat{f}_{\mathcal{D}}(\mathbf{x}) - E[\hat{f}_{\mathcal{D}}(\mathbf{x})])^2]$$

This measures how dependent the classifier is on the random sampling made in the training set.

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Low model complexity (small # of d.o.f.) $\Longrightarrow$ Low-variance
High model complexity (large # of d.o.f.) $\Longrightarrow$ High-variance

High variance classifiers produce differing decision boundaries which are highly dependent on the training data.

Also called “flexible”.

Examples:

1. *decision trees*

The depth of the tree determines the variance. How?

2. *k Nearest-Neighbour*

k determines the variance. How?

Our intuition may tell:

- The presence of bias indicates something basically wrong with the model and algorithm...
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Not really!

Bias and variance are equally important as we are always dealing with a single realization of the data set.

Take home message: Match the model complexity to the data resources, not to the target complexity