About this class

1. Introduce a basic class of learning methods, namely local methods.
2. Discuss the fundamental concept of bias-variance trade-off to understand parameter tuning (a.k.a. model selection)
Outline

Learning with Local Methods

From Bias-Variance to Cross-Validation
The problem

What is the price of one house given its area?
The problem

What is the price of one house given its area? Start from data...
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Let $S$ the houses example dataset ($n = 100$)

$$S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$$
The problem

What is the price of one house given its area? Start from data...

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Let $S$ the houses example dataset $(n = 100)$

$$S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$$

Given a new point $x^*$ we want to predict $y^*$ by means of $S$. 
Example

Let \( x^* \) a 300\( m^2 \) house.
Example

Let $x^*$ a $300 m^2$ house.

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MLCC 2015
Example

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What is its price?
Nearest Neighbors

**Nearest Neighbor**: $y^*$ is the same of the closest point to $x^*$ in $S$.

$$y^* = 311, 200$$
Nearest Neighbors

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Nearest Neighbors

- $S = \{(x_i, y_i)\}_{i=1}^{n}$ with $x_i \in \mathbb{R}^D, y_i \in \mathbb{R}$
- $x^*$ the new point $x^* \in \mathbb{R}^D$
- $y_{pred}$ the predicted output $y_{pred} = \hat{f}(x^*)$ where
  \[ f(x) = y_j \quad j = \arg\min_{i=1,...,n} ||x - x_i|| \]
Nearest Neighbors

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  \[
  f(x) = y_j \quad j = \arg\min_{i=1,\ldots,n} \|x - x_i\|
  \]

Computational cost $O(nD)$: we compute $n$ times the distance $\|x - x_i\|$ that costs $O(D)$
Nearest Neighbors

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Computational cost $O(nD)$: we compute $n$ times the distance $\|x - x_i\|$ that costs $O(D)$

In general let $d : \mathbb{R}^D \times \mathbb{R}^D$ a distance on the input space, then

\[ f(x) = y_j \quad j = \arg \min_{i=1,...,n} d(x, x_i) \]
Extensions

Nearest Neighbor takes $y^*$ is the same of the closest point to $x^*$ in $S$.

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Can we do better? (for example using more points)
K-Nearest Neighbors

**K-Nearest Neighbor:** $y^*$ is the mean of the values of the $K$ closest point to $x^*$ in $S$. If $K = 3$ we have

$$y^* = \frac{274,600 + 324,900 + 311,200}{3} = 303,600$$

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\( K \)-Nearest Neighbors

- \( S = \{(x_i, y_i)\}_{i=1}^n \) with \( x_i \in \mathbb{R}^D, y_i \in \mathbb{R} \)
- \( x^* \) the new point \( x^* \in \mathbb{R}^D \),
- Let \( K \) be an integer \( K << n \),
- \( j_1, \ldots, j_K \) defined as \( j_1 = \arg \min_{i \in \{1, \ldots, n\}} \|x - x_i\| \) and \( j_t = \arg \min_{i \in \{1, \ldots, n\} \setminus\{j_1, \ldots, j_{t-1}\}} \|x - x_i\| \) for \( t \in \{2, \ldots, K\} \),
- \( y_{pred} \) the predicted output \( y_{pred} = \hat{f}(x^*) \) where
K-Nearest Neighbors (cont.)

\[ f(x) = \frac{1}{K} \sum_{i=1}^{K} y_{j_i} \]
K-Nearest Neighbors (cont.)

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- **Computational cost** \( O(nD + n \log n) \): compute the \( n \) distances \( \|x - x_i\| \) for \( i = \{1, \ldots, n\} \) (each costs \( O(D) \)). Order them \( O(n \log n) \).
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- **General Metric** \( d \) \( f \) is the same, but \( j_1, \ldots, j_K \) are defined as \( j_1 = \arg \min_{i \in \{1, \ldots, n\}} d(x, x_i) \) and \( j_t = \arg \min_{i \in \{1, \ldots, n\} \setminus \{j_1, \ldots, j_{t-1}\}} d(x, x_i) \) for \( t \in \{2, \ldots, K\} \)
Parzen Windows

K-NN puts equal weights on the values of the selected points.

\[
\hat{f}(x) = \frac{\sum_{i=1}^{n} y_i k(x, x_i)}{\sum_{i=1}^{n} k(x, x_i)}
\]

where \( k \) is a similarity function

\[ k(x, x') \geq 0 \text{ for all } x, x' \in \mathbb{R}^D \]

\[ k(x, x') \to 1 \text{ when } \|x - x'\| \to 0 \]

\[ k(x, x') \to 0 \text{ when } \|x - x'\| \to \infty \]
Parzen Windows

K-NN puts equal weights on the values of the selected points. Can we generalize it?
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Closer points to $x^*$ should influence more its value
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PARZEN WINDOWS:

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Parzen Windows

Examples of $k$

- $k_1(x, x') = \text{sign} \left( 1 - \frac{\|x-x'\|}{\sigma} \right) +$ with a $\sigma > 0$
- $k_2(x, x') = \left( 1 - \frac{\|x-x'\|}{\sigma} \right) +$ with a $\sigma > 0$
- $k_3(x, x') = \left( 1 - \frac{\|x-x'\|^2}{\sigma^2} \right) +$ with a $\sigma > 0$
- $k_4(x, x') = e^{-\frac{\|x-x'\|^2}{2\sigma^2}}$ with a $\sigma > 0$
- $k_5(x, x') = e^{-\frac{\|x-x'\|}{\sigma}}$ with a $\sigma > 0$
K-Nearest neighbor depends on $K$.
When $K = 1$
K-Nearest neighbor depends on $K$. When $K = 2$
K-Nearest neighbor depends on $K$.
When $K = 3$
$K$-Nearest neighbor depends on $K$.
When $K = 4$
$K$-Nearest neighbor depends on $K$.
When $K = 5$
$K$-Nearest neighbor depends on $K$.
When $K = 9$
$K$-Nearest neighbor depends on $K$.
When $K = 15$
**K-NN example**

*K*-Nearest neighbor depends on *K*.

Changing *K* the result changes a lot! How to select *K*?
Outline

Learning with Local Methods

From Bias-Variance to Cross-Validation
Optimal choice for the Hyper-parameters

- $S = (x_i, y_i)_{i=1}^n$ training set. Name $Y = (y_1, \ldots, y_n)$ and $X = (x_1^T, \ldots, x_n^T)$.
- $K \in \mathbb{K}$ hyperparameter of the learning algorithm
- $\hat{f}_{S,K}$ learned function (depends on $S$ and $K$)
Optimal choice for the Hyper-parameters

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The expected loss \( \mathcal{E}_K \) is

\[
\mathcal{E}_K = \mathbb{E}_S \mathbb{E}_{x,y} (y - \hat{f}_{S,K}(x))^2
\]
Optimal choice for the Hyper-parameters

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The *expected loss* $\mathcal{E}_K$ is

$$\mathcal{E}_K = \mathbb{E}_S \mathbb{E}_{x,y} (y - \hat{f}_{S,K}(x))^2$$

*Optimal hyperparameter* $K^*$ *should minimize* $\mathcal{E}_K$
Optimal choice for the Hyper-parameters

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$$K^* = \arg \min_{K \in \mathbb{K}} \mathcal{E}_K$$
Optimal choice for the Hyper-parameters (cont.)

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Ideally! (In practice we don’t have access to the distribution)

- We can still try to understand the above minimization problem: does a solution exists? What does it depend on?
- Yet, ultimately, we need something we can compute!
Example: regression problem

Define the *pointwise expected loss*

\[ \mathcal{E}_K(x) = \mathbb{E}_S \mathbb{E}_{y|x}(y - \hat{f}_{S,K}(x))^2 \]
Example: regression problem

Define the *pointwise expected loss*

\[
E_K(x) = \mathbb{E}_S \mathbb{E}_{y|x} (y - \hat{f}_{S,K}(x))^2
\]

By definition \(E_K = \mathbb{E}_x E_K(x)\).
Define the *pointwise expected loss*

\[ \mathcal{E}_K(x) = \mathbb{E}_y \mathbb{E}_{y|x}(y - \hat{f}_{S,K}(x))^2 \]

By definition \( \mathcal{E}_K = \mathbb{E}_x \mathcal{E}_K(x) \).

Regression setting:

- Regression model \( y = f_*(x) + \delta \)
Example: regression problem

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Define the *pointwise expected loss*

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Now \( \mathcal{E}_K(x) = \mathbb{E}_S \mathbb{E}_{y|x} (y - \hat{f}_{S,K}(x))^2 = \mathbb{E}_S \mathbb{E}_{y|x} (f_*(x) + \delta - \hat{f}_{S,K}(x))^2 \)

that is

\[ \mathcal{E}_K(x) = \mathbb{E}_S (f_*(x) - \hat{f}_{S,K}(x))^2 + \sigma^2 \]

...
Define the *noisyless K-NN* (it is ideal!)

\[
\hat{f}_{S,K}(x) = \frac{1}{K} \sum_{l \in K_x} f_*(x_l)
\]
Define the *noisyless* $K$-NN (it is ideal!)

$$\hat{f}_{S,K}(x) = \frac{1}{K} \sum_{l \in K_x} f_{\ast}(x_l)$$

Note that $\hat{f}_{S,K}(x) = \mathbb{E}_{y | x} \hat{f}_{S,K}(x)$. 
Bias Variance trade-off for K-NN

Define the *noisyless K-NN* (it is ideal!)

\[
\tilde{f}_{S,K}(x) = \frac{1}{K} \sum_{l \in K_x} f_*(x_l)
\]

Note that \( \tilde{f}_{S,K}(x) = \mathbb{E}_{y|x} \hat{f}_{S,K}(x) \).

Consider

\[
\mathcal{E}_K(x) = (f_*(x) - \mathbb{E}_X \tilde{f}_{S,K}(x))^2 + \mathbb{E}_S (\tilde{f}_{S,K}(x) - \hat{f}_{S,K}(x))^2 + \sigma^2
\]

\[
\text{bias} \quad \text{variance}
\]

...
Bias Variance trade-off for K-NN

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Consider

\[
\mathcal{E}_K(x) = (f_*(x) - \mathbb{E}_X \tilde{f}_{S,K}(x))^2 + \frac{1}{K^2} \mathbb{E}_X \sum_{l \in K_x} \mathbb{E}_{y_l|x_l}(y_l - f_*(x_l))^2 + \sigma^2
\]

...
Bias Variance trade-off for K-NN

Define the noisyless K-NN (it is ideal!)

\[ \tilde{f}_{S,K}(x) = \frac{1}{K} \sum_{l \in K_x} f_*(x_l) \]

Note that \( \tilde{f}_{S,K}(x) = \mathbb{E}_{y|x} \hat{f}_{S,K}(x) \).

Consider

\[ \mathcal{E}_K(x) = \left( f_*(x) - \mathbb{E}_X \hat{f}_{S,K}(x) \right)^2 + \frac{\sigma^2}{K} \]

\( \mathcal{E}_K(x) \) is broken down into:

- Bias: \( \left( f_*(x) - \mathbb{E}_X \hat{f}_{S,K}(x) \right)^2 \)
- Variance: \( \frac{\sigma^2}{K} \)

...
Bias Variance trade-off
How to choose the hyper-parameters

Bias-Variance trade-off is theoretical, but shows that:
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- an optimal parameter exists and
How to choose the hyper-parameters

Bias-Variance trade-off is theoretical, but shows that:

- an optimal parameter exists and
- it depends on the noise and the unknown target function.
How to choose the hyper-parameters

Bias-Variance trade-off is theoretical, but shows that:
- an optimal parameter exists and
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How to choose $K$ in practice?
Bias-Variance trade-off is theoretical, but shows that:

- an optimal parameter exists and
- it depends on the noise and the unknown target function.

How to choose $K$ in practice?

- Idea: train on some data and validate the parameter on new unseen data as a proxy for the ideal case.
Hold-out Cross-validation

For each $K \in \mathbf{K}$
Hold-out Cross-validation

For each $K \in \mathbb{K}$

1. shuffle and split $S$ in $T$ (training) and $V$ (validation)
Hold-out Cross-validation

For each $K \in \mathcal{K}$

1. shuffle and split $S$ in $T$ (training) and $V$ (validation)
2. train the algorithm on $T$ and compute the empirical loss on $V$
   \[
   \hat{E}_K = \frac{1}{|V|} \sum_{x,y \in V} (y - \hat{f}_{T,K}(x))^2
   \]
Hold-out Cross-validation

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$$\hat{E}_K = \frac{1}{|V|} \sum_{x,y \in V} (y - \hat{f}_{T,K}(x))^2$$

3. Select $\hat{K}$ that minimize $\hat{E}_K$. 

The above procedure can be repeated to augment stability and $K$ selected to minimize error over trials.

There are other related parameter selection methods (k-fold cross validation, leave-one out...).
Hold-out Cross-validation

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2. train the algorithm on \( T \) and compute the empirical loss on \( V \)
   \[ \hat{\mathcal{E}}_K = \frac{1}{|V|} \sum_{x,y \in V} (y - \hat{f}_{T,K}(x))^2 \]
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Training and Validation Error behavior

Training vs. validation error
T = 50% S; n = 200

Training vs. validation error
T = 50% S; n = 200
K
Error
Validation error
Training error

^K = 8.
\( \hat{K} = 8. \)
Wrapping up

In this class we made our first encounter with learning algorithms (local methods) and the problem of tuning their parameters (via bias-variance trade-off and cross-validation) to avoid overfitting and achieve generalization.
Next Class

High Dimensions: Beyond local methods!