Lecture 9: Nonparametric Methods (KNN, Decision Trees, Random Forests)

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Reading materials & Reference

Reading materials:

- Chapter 16, 18, Probabilistic Machine Learning: an introduction.
- Chapter 8, The Elements of Statistical Learning (Hastie, Tibshirani, Friedman).
- EPFL, CS-433 Machine Learning, Lecture on k-NN.

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Motivation: Why Nonparametric Methods?

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This leads us to nonparametric methods,
which make minimal assumptions about the data distribution.

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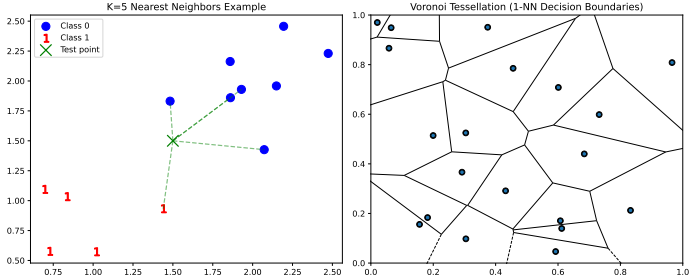

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Key choices:

- The number of neighbors K.
- The distance metric $d(\cdot, \cdot)$ (e.g., Euclidean, Manhattan). Features must be normalized!

KNN: Visual Example

- **K=5 Example**:
  - Test point (X) with 5 nearest neighbors
  - Class probability: $p(y = 1|x, \mathcal{D}) = \frac{3}{5}$
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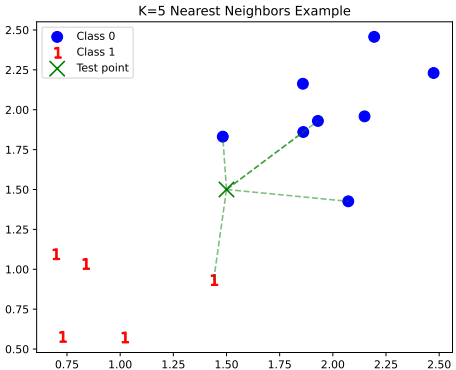

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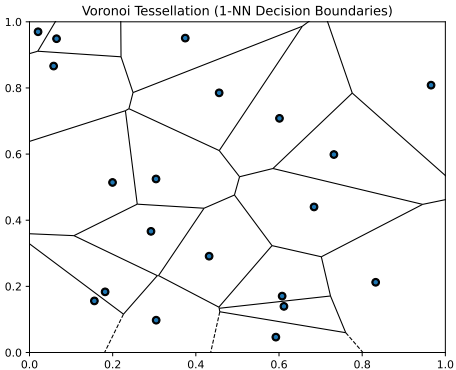
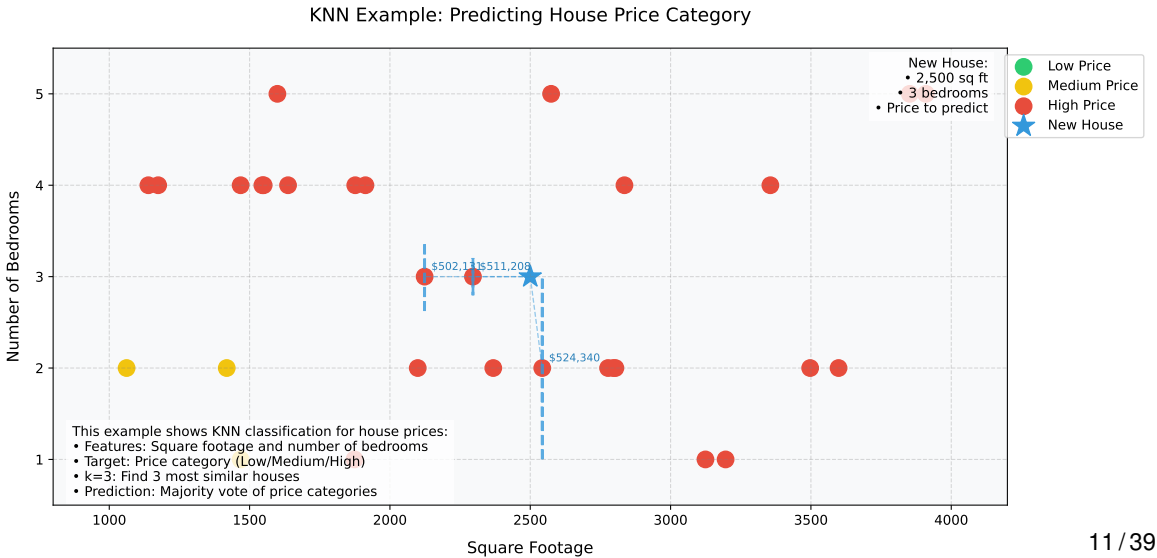
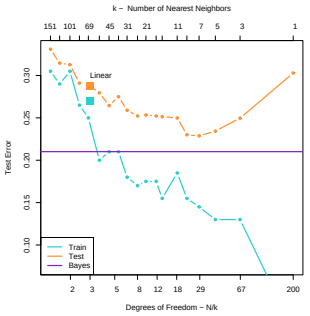


KNN: Prediction house price categories



KNN: Choosing K (Bias-Variance Tradeoff)



Small K (e.g., $K = 1$)

- **Low Bias:** Very flexible, complex decision boundary.
- **High Variance:** Very sensitive to noise, prone to overfitting.
- Model is **complex**.

Large K (e.g., $K = N$)

- **High Bias:** Over-smoothed boundary (predicts the majority class).
- **Low Variance:** Very stable, not sensitive to noise.
- Model is **simple**.

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- To capture just $\alpha = 1\%$ of the data (which is uniformly distributed in a $[0, 1]^d$ hypercube), we need a smaller hypercube of side length $r = \alpha^{1/d}$.
  - $d = 1 : r = 0.01^{1/1} = 0.01$ (a tiny slice)
  - $d = 10 : r = 0.01^{1/10} \approx 0.63$ (63% of each axis)
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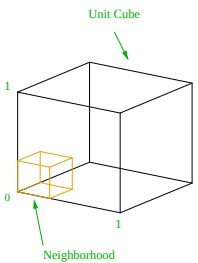

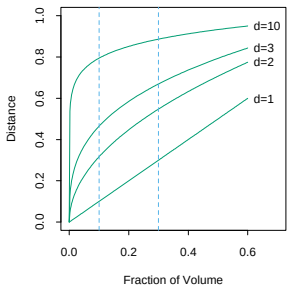

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The core assumption of KNN (that "similar" points are "nearby")
breaks down in high dimensions.

Deeper Dive: Proof for Curse of Dimensionality (Claim 2)

Goal: Find the hypercube side length r such that the probability of finding *at least one* of N data points inside is 50%.

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  - The error of this optimal classifier is the Bayes Risk, $\mathcal{L}(f_*)$:

$$\mathcal{L}(f_*) = \mathbb{E}_x[\min\{\eta(x), 1 - \eta(x)\}]$$

    This is the absolute minimum, irreducible error for the problem.

Proof of Bayes Classifier

Let $\eta(x) = \mathbb{P}\{Y = 1 | X = x\}$ be the true, unknown conditional probability of class 1.

$$\begin{aligned}
\eta(x) \geq 1/2 &\iff \mathbb{P}(Y = 1 | X = x) \geq 1/2 \\
&\iff \mathbb{P}(Y = 1 | X = x) \geq \mathbb{P}(Y = 0 | X = x) \\
&\iff 1 \in \underset{y \in \{0,1\}}{\operatorname{argmax}} \mathbb{P}(Y = y | X = x)
\end{aligned}$$

Thus $\mathbf{1}_{\eta(x) \geq 1/2} = \operatorname{argmax}_{y \in \{0,1\}} \mathbb{P}(Y = y | X = x) = f_*(x)$

Proof of Bayes Risk Formula

Let $\eta(x) = \mathbb{P}\{Y = 1|X = x\}$ be the true, unknown conditional probability of class 1.

$$
\begin{aligned}
\mathcal{L}(f_*) &= \mathbb{E}_{(X,Y)\sim\mathcal{D}}[\mathbf{1}_{f_*(X)\neq Y}] \\
&= \mathbb{E}_{X\sim\mathcal{D}_X}[\mathbb{E}_{Y\sim\mathcal{D}_{Y|X}}[\mathbf{1}_{f_*(X)\neq Y}|X]] \\
&= \mathbb{E}_{X\sim\mathcal{D}_X}[\mathbb{E}_{Y\sim\mathcal{D}_{Y|X}}[\mathbf{1}_{f_*(X)\neq Y}|X]\mathbf{1}_{\eta(X)\geq 1/2} + \mathbb{E}_{Y\sim\mathcal{D}_{Y|X}}[\mathbf{1}_{f_*(X)\neq Y}|X]\mathbf{1}_{\eta(X)<1/2}] \\
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\end{aligned}
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Deeper Dive: Generalization bound for 1-NN (The Bound)

- **Key Assumption:** We need to assume that the problem is "learnable". We assume the probability function $\eta(x)$ is Lipschitz continuous:

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(In words: if two points x and x' are close, their probabilities $\eta(x)$ and $\eta(x')$ must also be close.)

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- The 1-NN error is bounded by:
  - (Twice the optimal Bayes risk) + (A "geometric term" that depends on the average distance to the nearest neighbor).

Deeper Dive: 1-NN Analysis (Interpretation)

What does the bound $\mathbb{E}[\mathcal{L}] \leq 2\mathcal{L}(f_*) +$ (geometric term) tell us?

- **Limit 1: As $N \to \infty$ (fixed d)**
  - The average distance to the nearest neighbor $\to 0$.
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$$\mathbb{E}_{S_{train}}[\mathcal{L}(f_{S_{train}})] \leq 2\mathcal{L}(f_*)$$

  - **Takeaway:** With infinite data, the 1-NN error is at most *twice the optimal (Bayes) error*. It's good, but not "consistent" (it doesn't converge *to* $\mathcal{L}(f_*)$).

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- **Limit 2: As $d \to \infty$ (fixed N)**
  - The geometric term $\approx 4c\sqrt{d}N^{-1/(d+1)}$.
  - To keep this error term constant, N must grow *exponentially* with d.
  - **Takeaway:** This is the mathematical proof of the Curse of Dimensionality. For a fixed number of samples N, the error explodes as dimension d increases.

Recap of kNN

- k-NN: a local averaging method for regression and classification
  - use a notion of distance to define *neighborhoods* (= k nearest neighbors)
  - the prediction is a function of these neighborhoods
    - e.g., majority selection for classification, weighted sum for regression
- Bias-variance: small/large k leads to low/high bias and high/low variance
- Curse of dimensionality: as $d \to \infty$, it is harder to define local neighborhoods
- For $N \to \infty$, 1-NN is competitive with Bayes classifier
- N needs to scale exponentially in d to achieve the same error

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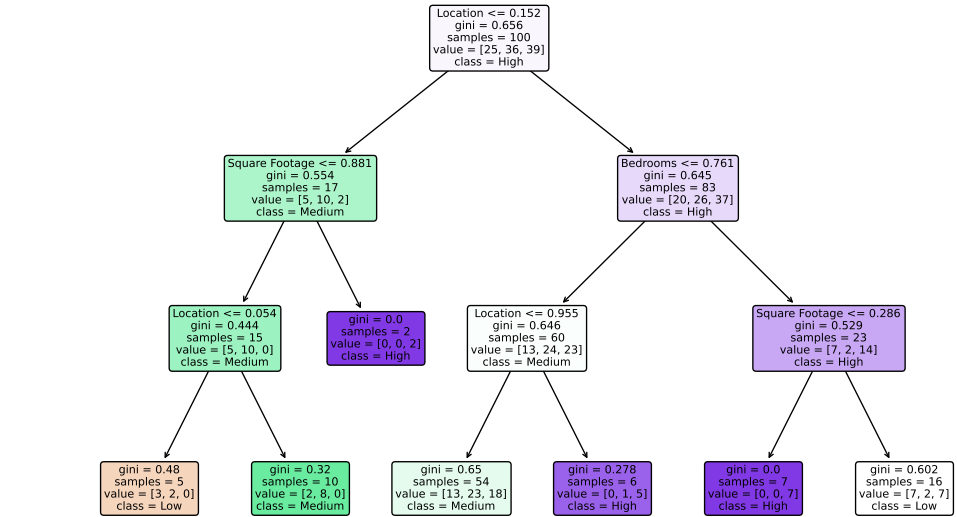
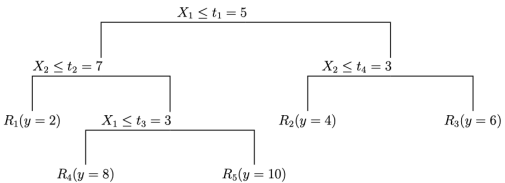
- This is a white-box model: the decision logic is highly interpretable.

Decision Trees



Decision Trees: Regression Tree



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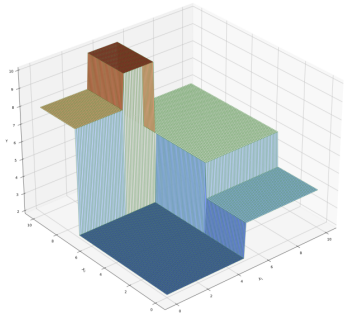

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- **Algorithm**:
  1. If stopping criteria met:
     - Create leaf node with majority class
     - Return
  2. For each feature $f \in \mathcal{F}$:
     - Find best split point t minimizing impurity
     - Calculate information gain: $\text{IG}(f, t) = I(D) - \sum_{s \in \{L,R\}} \frac{|D_s|}{|D|} I(D_s)$
  3. Choose (f^*, t^*) with maximum information gain
  4. Split $\mathcal{D}$ into $\mathcal{D}_L$ and $\mathcal{D}_R$
  5. Recursively grow left and right subtrees

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- We measure purity (or impurity) and choose the split that **maximizes** the Information Gain:

$$\text{IG}(f, t) = \text{Impurity}(\mathcal{D}) - \left(\frac{|\mathcal{D}_L|}{|\mathcal{D}|} \text{Impurity}(\mathcal{D}_L) + \frac{|\mathcal{D}_R|}{|\mathcal{D}|} \text{Impurity}(\mathcal{D}_R) \right)$$

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For Regression

- Mean Squared Error (MSE)
  - Measures variance of the target variable y.
  - MSE $= \frac{1}{N} \sum_{i=1}^{N} (y_i - \bar{y})^2$
  - Goal is to minimize variance in the leaves.

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- **Customer Churn Prediction**:
  - Features: Usage patterns, payment history, customer service interactions
  - Example: Telecom company predicting customer retention
    - Monthly bill amount?
    - Number of service calls?
    - Contract length?

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- This works because averaging *de-correlated* models reduces variance.

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This **further de-correlates** the trees,
which significantly reduces variance and makes the model more robust.

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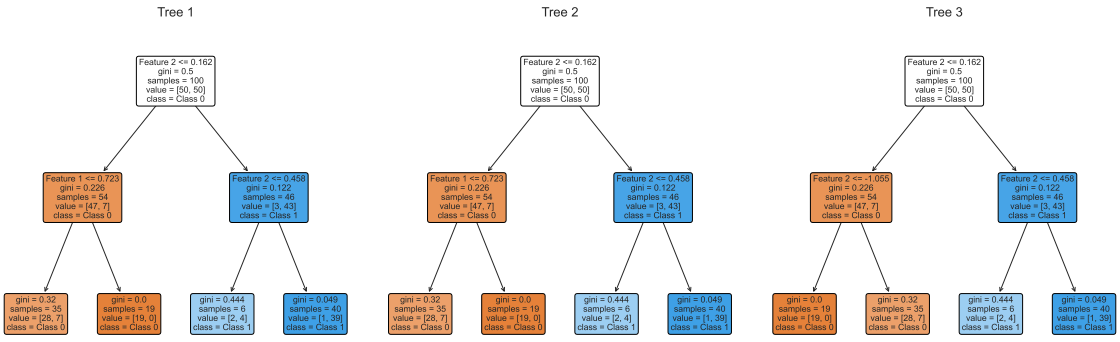

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- **Benefit:** This gives an unbiased estimate of the test error *for free*, without needing a separate validation set or cross-validation.

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Comparison of Nonparametric Methods

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