Supervised Learning:
K-Nearest Neighbors ~~and Decision Trees~~

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CS5350/6350: Machine Learning

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Modified by Longin Jan Latecki

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- **Goal:** predict the output $\mathbf{y}$ for an **unseen** test example $\mathbf{x}$
- **This lecture:** Two intuitive methods
  - K-Nearest-Neighbors
  - Decision Trees

K-Nearest Neighbor (K-NN)

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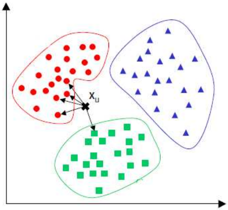
- Prediction Rule: Look at the K most similar training examples



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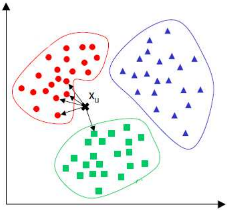

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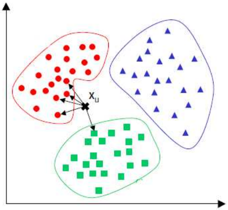

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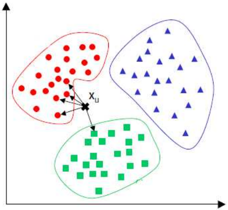

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- **Special Case:** 1-Nearest Neighbor

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- It simply uses the training data at the test time to make predictions

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- $\mathbf{x}_i^T \mathbf{x}_j = \sum_{m=1}^{D} x_{im} x_{jm}$ is called the **dot (or inner) product** of $\mathbf{x}_i$ and $\mathbf{x}_j$
    - Dot product measures the **similarity** between two vectors (orthogonal vectors have dot product=0, parallel vectors have high dot product)

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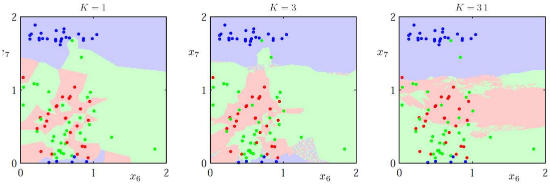
  - $\bar{x_m} = \frac{1}{N}\sum_{i=1}^{N} x_{im}$: empirical mean of m^{th} feature
  - $\sigma_m^2 = \frac{1}{N}\sum_{i=1}^{N}(x_{im} - \bar{x_m})^2$: empirical variance of m^{th} feature

K-NN: Some other distance measures

- Binary-valued features
  - Use Hamming distance: $d(x_i, x_j) = \sum_{m=1}^{D} \mathbb{I}(x_{im} \neq x_{jm})$
  - Hamming distance counts the number of features where the two examples disagree
- Mixed feature types (some real-valued and some binary-valued)?
  - Can use mixed distance measures
  - E.g., Euclidean for the real part, Hamming for the binary part
- Can also assign **weights** to features: $d(x_i, x_j) = \sum_{m=1}^{D} w_m d(x_{im}, x_{jm})$

Choice of K - Neighborhood Size



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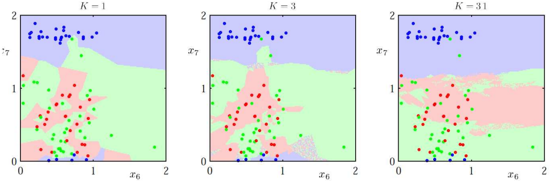

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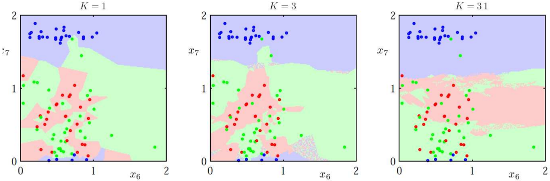

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- Choosing K
  - Often data dependent and heuristic based
  - Or using cross-validation (using some **held-out data**)
  - In general, a K too small or too big is bad!

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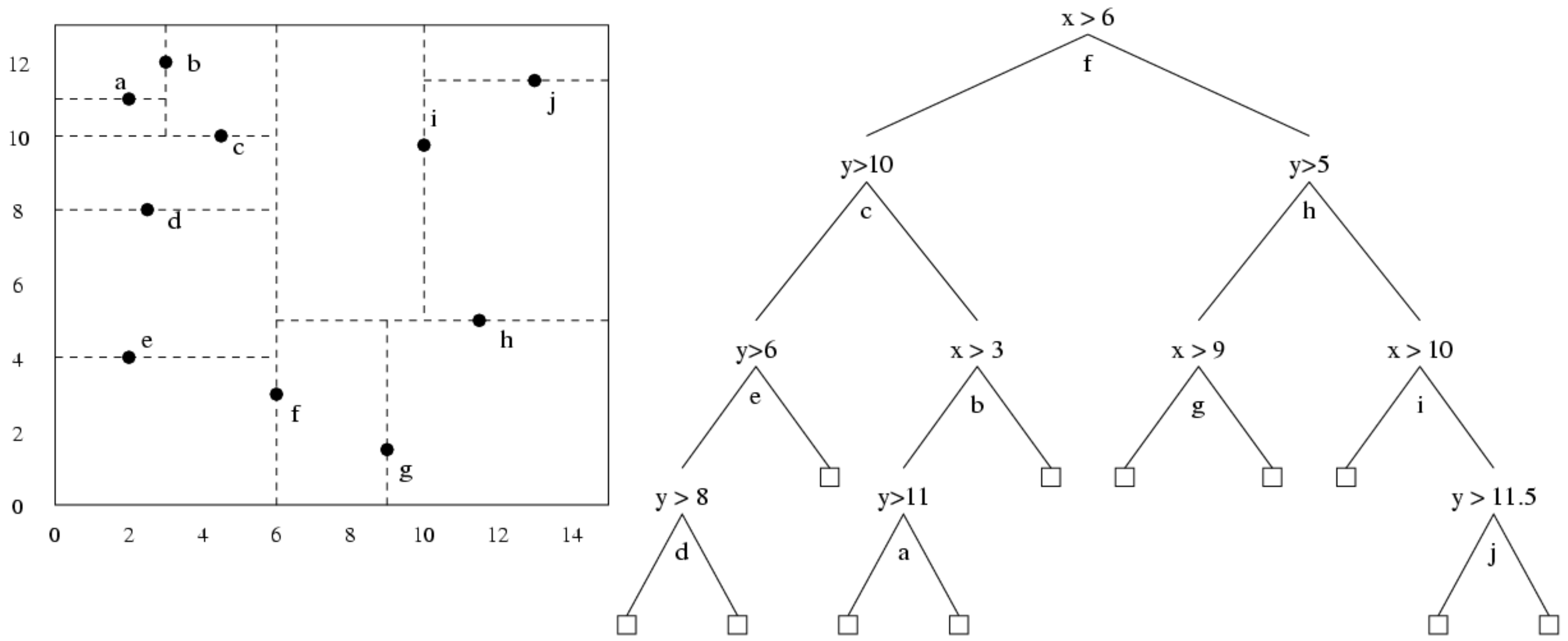
    - Distance computations with N training points (D features each)
  - Sensitive to noisy features
  - May perform badly in high dimensions (curse of dimensionality)
    - In high dimensions, distance notions can be counter-intuitive!

Not Covered (Further Readings)

- Computational speed-ups (don't want to spend $O(ND)$ time)
  - Improved data structures for fast nearest neighbor search
  - Even if *approximately* nearest neighbors, yet may be good enough
- Efficient Storage (don't want to store all the training data)
  - E.g., subsampling the training data to retain "prototypes"
  - Leads to computational speed-ups too!
- Metric Learning: Learning the "right" distance metric for a given dataset

kd-trees



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