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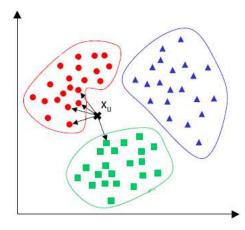
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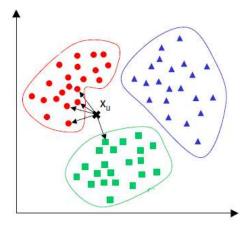
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- Goal: predict the output y for an unseen test example x
- This lecture: Two intuitive methods
 - K-Nearest-Neighbors
 - Decision Trees

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- Given training data $\mathcal{D} = \{(\mathbf{x}_1, \mathbf{y}_1), \dots, (\mathbf{x}_N, \mathbf{y}_N)\}$ and a test point
- Prediction Rule: Look at the K most similar training examples



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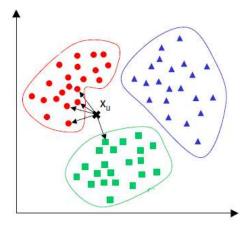
- For classification: assign the majority class label (majority voting)
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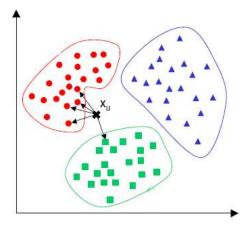
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- Special Case: 1-Nearest Neighbor

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K-Nearest Neighbors Algorithm

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Note: *K*-Nearest Neighbors is called a *non-parametric* method

 Unlike other supervised learning algorithms, K-Nearest Neighbors doesn't learn an explicit mapping f from the training data

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- Unlike other supervised learning algorithms, K-Nearest Neighbors doesn't learn an explicit mapping f from the training data
- It simply uses the training data at the test time to make predictions

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August 25, 2011

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$$d(\mathbf{x}_{i},\mathbf{x}_{j}) = \sqrt{\sum_{m=1}^{D} (x_{im} - x_{jm})^{2}} = \sqrt{||\mathbf{x}_{i}||^{2} + ||\mathbf{x}_{j}||^{2} - 2\mathbf{x}_{i}^{T}\mathbf{x}_{j}}$$

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- Generalization of the distance between points in 2 dimensions
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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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- Note: Features should be on the same scale
- Example: if one feature has its values in millimeters and another has in centimeters, we would need to normalize

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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

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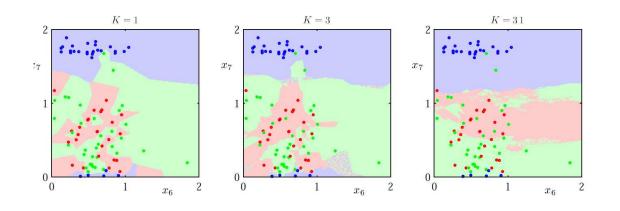
K-NN: Some other distance measures

- 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: $d(x_i, x_j) = \sum_{m=1}^{D} w_m d(x_{im}, x_{jm})$

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Choice of K - Neighborhood Size



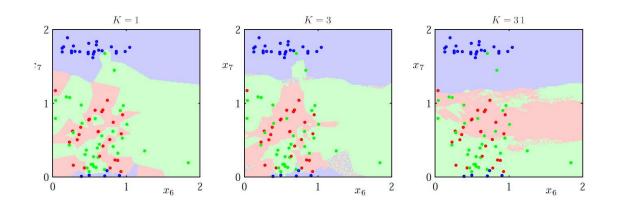
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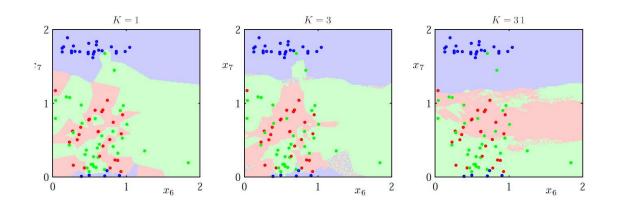


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Choice of K - Neighborhood Size



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- Large K
 - Creates fewer larger regions
 - Usually leads to smoother decision boundaries (caution: too smooth decision boundary can underfit)
- 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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• What's nice

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• Simple and intuitive; easily implementable

• What's nice

- Simple and intuitive; easily implementable
- Asymptotically consistent (a theoretical property)
 - With infinite training data and large enough *K*, *K*-NN approaches the best possible classifier (Bayes optimal)

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- Simple and intuitive; easily implementable
- Asymptotically consistent (a theoretical property)
 - With infinite training data and large enough K, K-NN approaches the best possible classifier (Bayes optimal)

What's not so nice...

- Store all the training data in memory even at test time
 - Can be memory intensive for large training datasets
 - An example of non-parametric, or **memory/instance-based** methods
 - Different from parametric, model-based learning models

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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!

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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

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