CS 886
Applied Machine Learning
K-Nearest Neighbours

Dan Lizotte

University of Waterloo

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Instance-based learning

- Non-parametric learning
- k-nearest neighbour
- Efficient implementations
- Variations

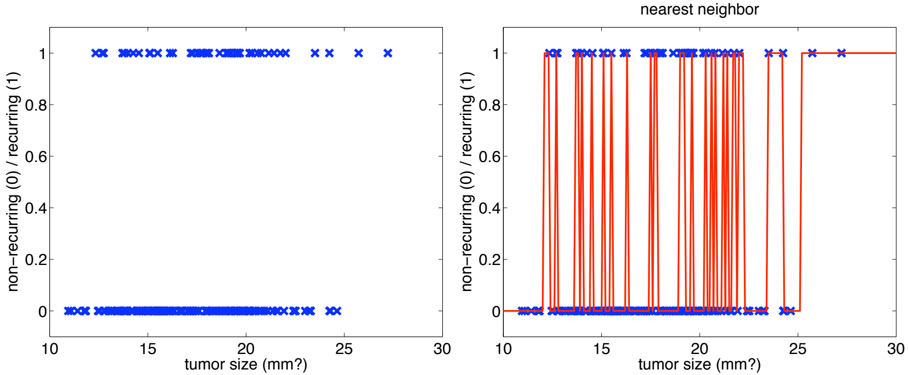
Parametric supervised learning

- So far, we have assumed that we have a data set D of labeled examples
- From this, we learn a *parameter vector* of a *fixed size* such that some error measure based on the training data is minimized
- These methods are called *parametric*, and their main goal is to summarize the data using the parameters
- Parametric methods are typically global, i.e. have one set of parameters for the entire data space
- But what if we just remembered the data?
- When new instances arrive, we will compare them with what we know, and determine the answer

Non-parametric (memory-based) learning methods

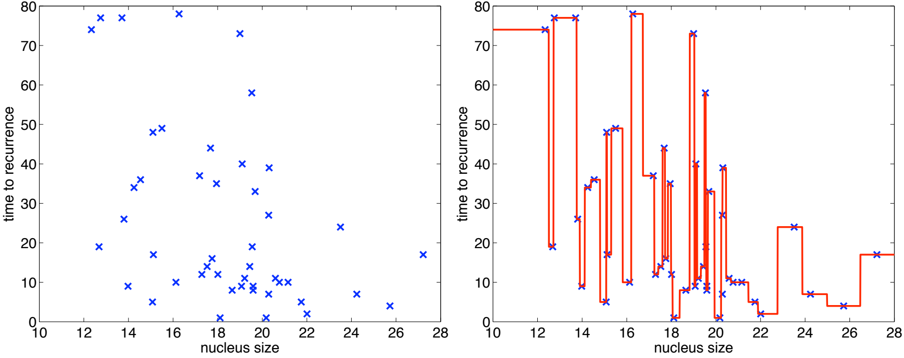
- Key idea: just store all training examples $\langle \mathbf{x}_{\mathrm{i}}, y_i \rangle$
- When a query is made, compute the value of the new instance based on the values of the *closest (most similar) points*
- Requirements:
  - A distance function
  - How many closest points (neighbors) to look at?
  - How do we compute the value of the new point based on the existing values?

Simple idea: Connect the dots!



Wisconsin data set, classification

Simple idea: Connect the dots!



Wisconsin data set, regression

One-nearest neighbor

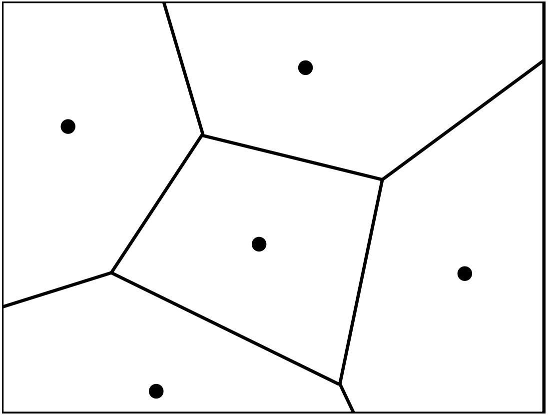
- Given: Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, distance metric d on $\mathcal{X}$.
- Training: Nothing to do! (just store data)
- Prediction: for $\mathbf{x} \in \mathcal{X}$
  - Find nearest training sample to $\mathbf{x}$.

$$i^* \in \arg\min_i d(\mathbf{x}_i, \mathbf{x})$$

  - Predict $y = y_{i^*}$.

What does the approximator look like?

- Nearest-neighbor does not explicitly compute decision boundaries
- But the effective decision boundaries are a subset of the *Voronoi diagram* for the training data



Each line segment is equidistant between two points of opposite classes.

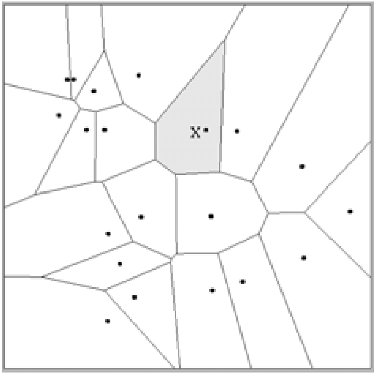
What kind of distance metric?

- Euclidian distance
- Maximum/minimum difference along any axis
- Weighted Euclidian distance (with weights based on domain knowledge)

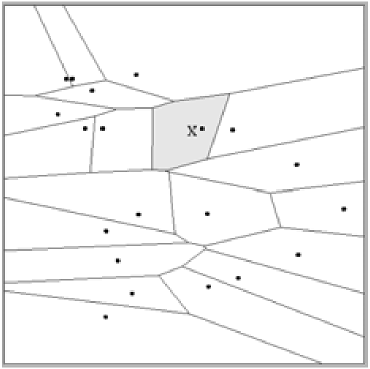
$$d(\mathbf{x}, \mathbf{x}') = \sum_{j=1}^{n} u_j (\mathbf{x}_j - \mathbf{x}'_j)^2$$

- An arbitrary distance or similarity function d, specific for the application at hand (works best, if you have one)

Distance metric is really important!



features weighted equally



vertical matters more

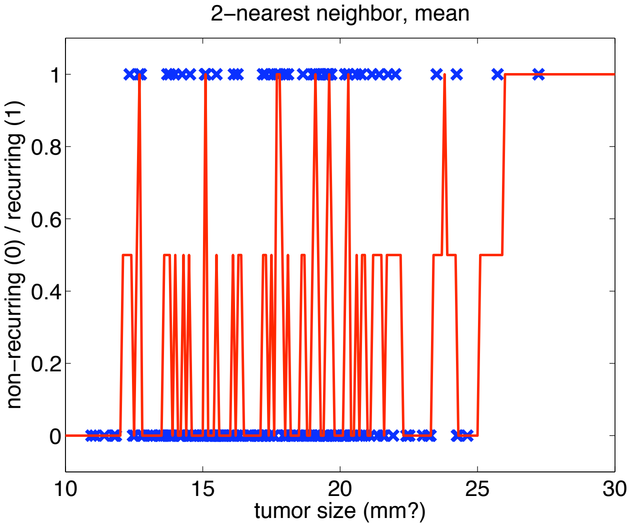
Distance metric tricks

- You may need to do preprocessing:
  - *Scale* the input dimensions (or normalize them)
  - Determine weights for features based on cross-validation (or information-theoretic methods)
- Distance metric is often domain-specific
  - E.g. string edit distance in bioinformatics
  - E.g. trajectory distance in time series models for walking data
- Distance metric can be learned sometimes (more on this later)

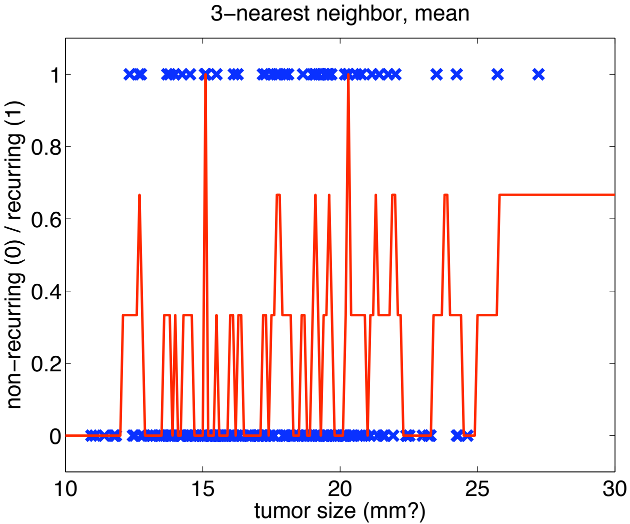
k-nearest neighbor

- Given: Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$, distance metric d on $\mathcal{X}$.
- Learning: Nothing to do!
- Prediction: for $\mathbf{x} \in \mathcal{X}$
  - Find the k nearest training samples to $\mathbf{x}$.
    Let their indices be $i_1, i_2, \ldots, i_k$.
  - Predict
    - $y =$ mean/median of $\{y_{i_1}, y_{i_2}, \ldots, y_{i_k}\}$ for regression
    - $y =$ majority of $\{y_{i_1}, y_{i_2}, \ldots, y_{i_k}\}$ for classification, or empirical probability of each class

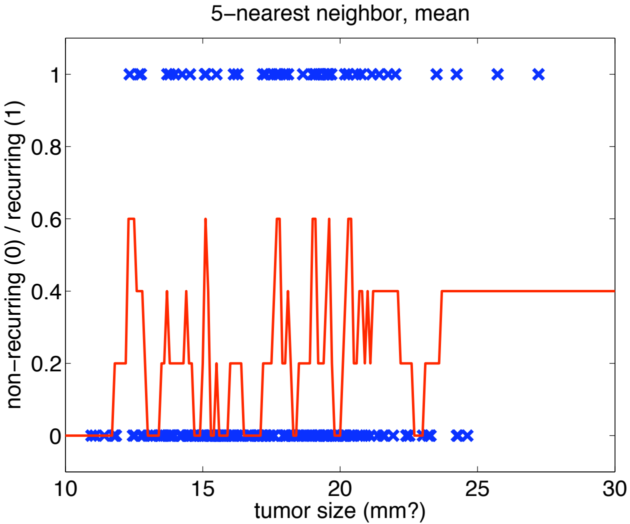
Classification, 2-nearest neighbor, empirical distribution



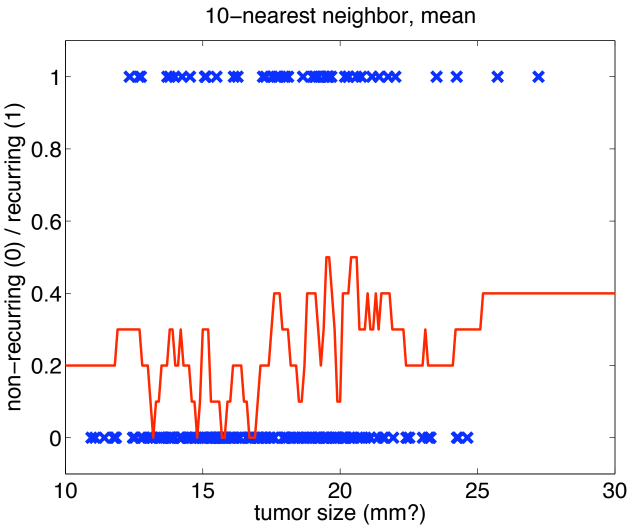
Classification, 3-nearest neighbor



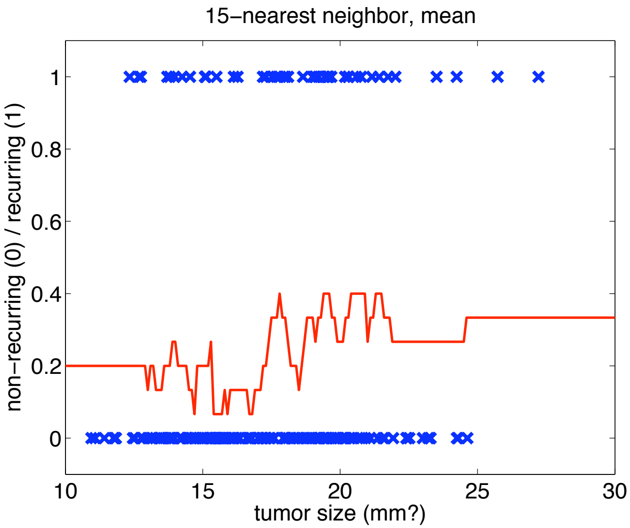
Classification, 5-nearest neighbor



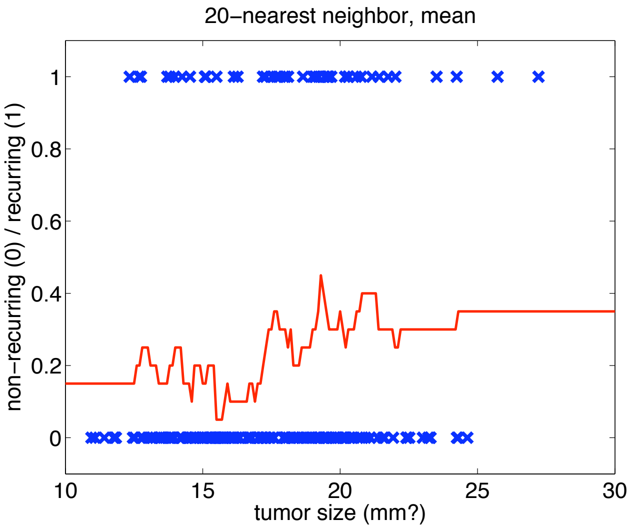
Classification, 10-nearest neighbor



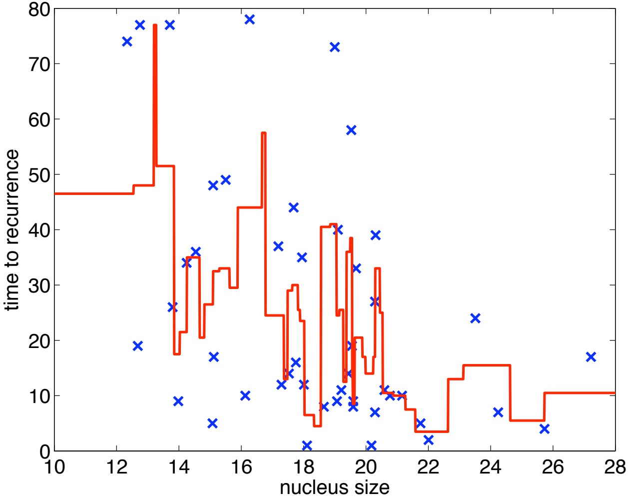
Classification, 15-nearest neighbor



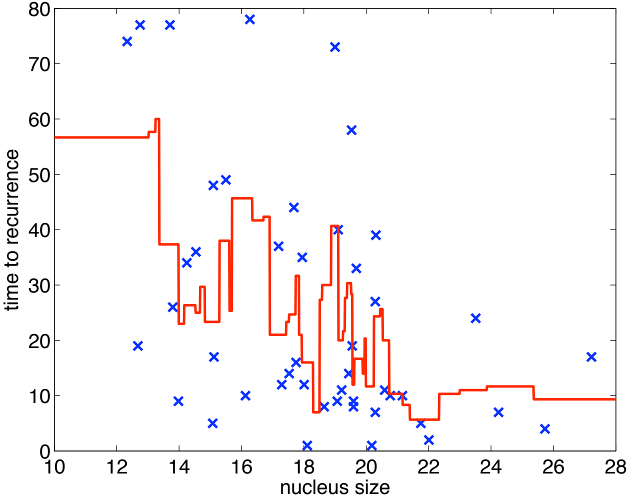
Classification, 20-nearest neighbor



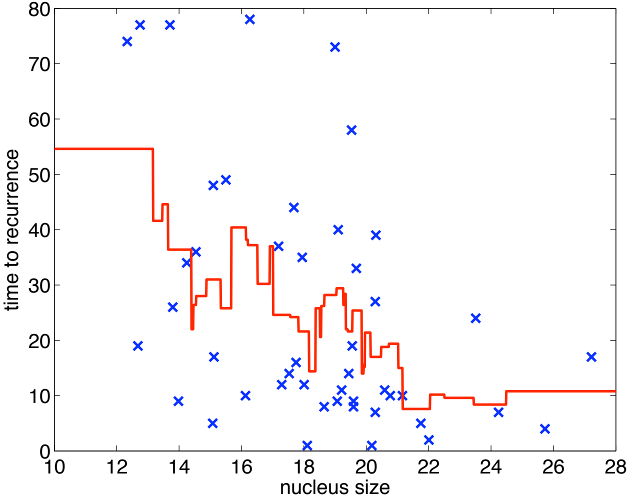
Regression, 2-nearest neighbor, mean prediction



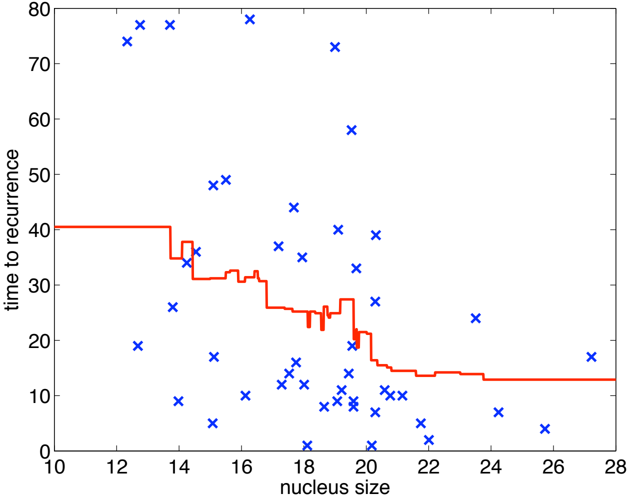
Regression, 3-nearest neighbor



Regression, 5-nearest neighbor



Regression, 10-nearest neighbor



Bias-variance trade-off

- If k is low, very non-linear functions can be approximated, but we also capture the noise in the data
  Bias is low, variance is high
- If k is high, the output is much smoother, less sensitive to data variation
  High bias, low variance
- A validation set can be used to pick the best k

Distance-weighted (kernel-based) nearest neighbor

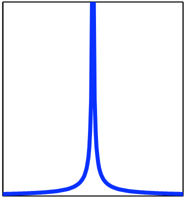
- Inputs: Training data $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, distance metric d on $\mathcal{X}$, weighting function $w : \mathbb{R} \mapsto \mathbb{R}$.
- Learning: Nothing to do!
- Prediction: On input $\mathbf{x}$,
  - For each i compute $w_i = w(d(\mathbf{x}_i, \mathbf{x}))$.
  - Predict weighted majority or mean. For example,

$$y = \frac{\sum_i w_i y_i}{\sum_i w_i}$$

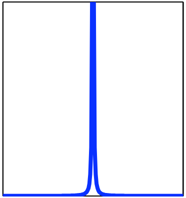
- How to weight distances?

Some weighting functions

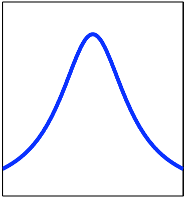
$$\frac{1}{d(\mathbf{x}_i, \mathbf{x})}$$



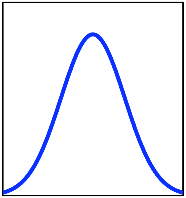
$$\frac{1}{d(\mathbf{x}_i, \mathbf{x})^2}$$



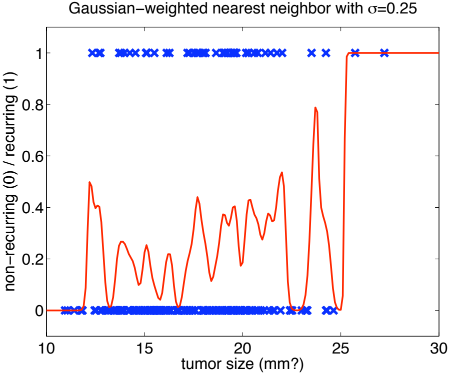
$$\frac{1}{c + d(\mathbf{x}_i, \mathbf{x})^2}$$



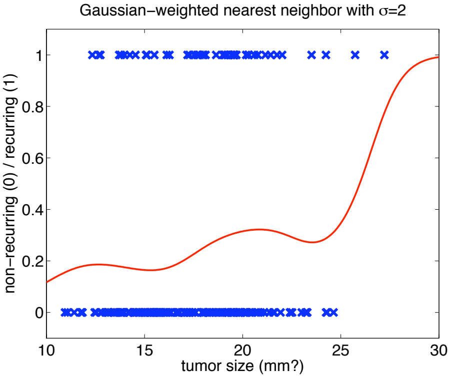
$$e^{-\frac{d(\mathrm{x}_i, \mathrm{x})^2}{\sigma^2}}$$



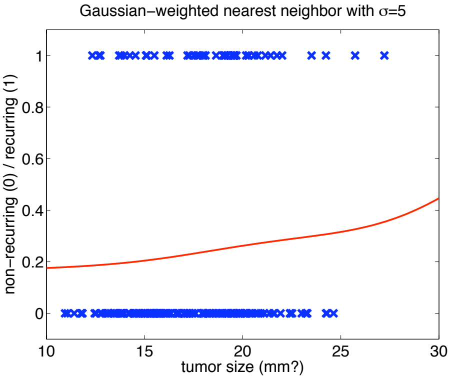
Example: Gaussian weighting, small σ



Gaussian weighting, medium σ



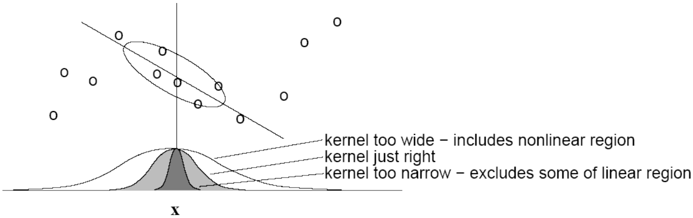
Gaussian weighting, large σ



All examples get to vote! Curve is smoother, but perhaps too smooth.

Locally-weighted linear regression

- Weighted linear regression: different weights in the error function for different points (see homework 1)
- Locally weighted linear regression: weights *depend on the distance to the query point*
- Uses a linear fit rather than just an average



Lazy and eager learning

- *Lazy*: wait for query before generalizing
  E.g. Nearest Neighbor
- *Eager*: generalize before seeing query
  E.g. Backpropagation, Linear regression,

Does it matter?

Pros and cons of lazy and eager learning

- Eager learners must create global approximation
- Lazy learners can create many local approximations
- An eager learner does the work off-line, summarizes lots of data with few parameters
- A lazy learner has to do lots of work sifting through the data at query time
- Typically lazy learners take longer time to answer queries and require more space

When to consider instance-based learning

- Instances map to points in $\mathbb{R}^p$
- Not too many features per instance (maybe < 20)
- Advantages:
  - Training is very fast
  - Easy to learn complex functions over few variables
  - Can give back confidence intervals in addition to the prediction
  - Variable resolution (depends on the density of data points)
  - Does not lose any information
  - Often wins if you have enough data
- Disadvantages:
  - Slow at query time
  - Query answering complexity depends on the number of instances
  - *Easily fooled by irrelevant features* (for most distance metrics)