CS5112: Algorithms and Data Structures for Applications

Lecture 11: Density estimation with nearest neighbors

Ramin Zabih

Some figures from Wikipedia/Google image search

Administrivia

- Reminder: HW comments and minor corrections on Slack
- HW3 coming soon
- **Anonymous** survey coming re: speed of course, etc.

Today

- NN for machine learning problems
- Density estimation to classify cats versus dogs
- Continuous versus discrete random variables

NN for machine learning

- Nearest neighbors is a fundamental ML technique
  - Used for classification, regression, etc.
- We will study (and implement!) NN algorithms
  - Exact algorithms on Tuesday next week
  - Approximate algorithms starting Thursday
- Today we will focus on understanding the use of NN

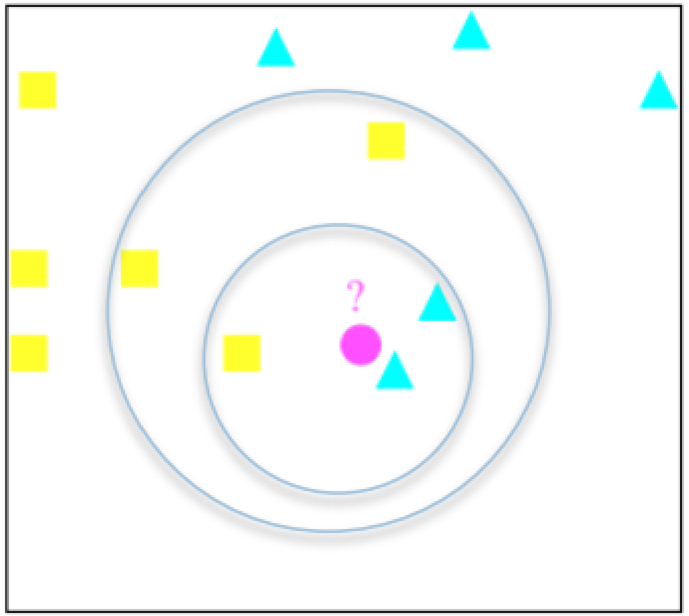
Classification and NN algorithms

- Suppose the height/weight of your query animal is very similar to the cats you have seen, and unlike the dogs you have seen, then it's probably a cat
- There's actually a lot going on in the sentence above:
  - "very similar"
  - "the cats you have seen"
  - "probably"
- You can classify directly from NN

NN and k-NN classification

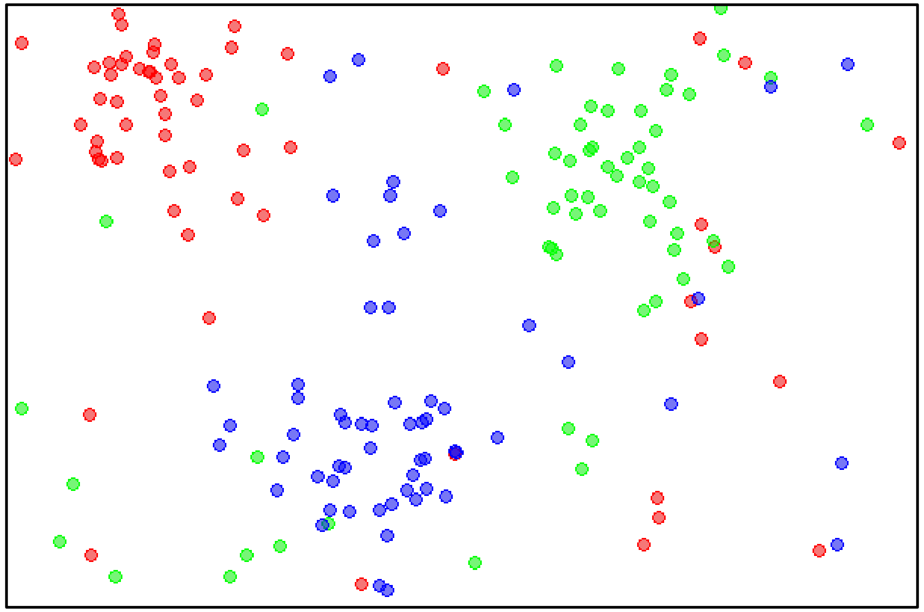
- Find the animal you've seen that's most similar to your query
  - NN classification
- What can go wrong?
- More robustly, look at the k most similar animals and take the mode (most common label)
  - k-NN classification
  - Choice of k?

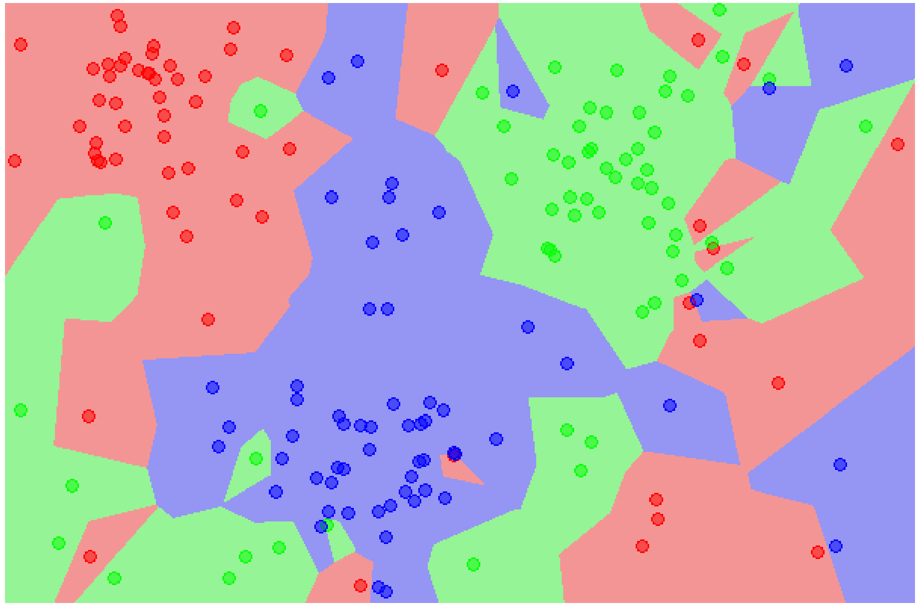
k-NN classifier small example



Slide credit: https://www.cs.rit.edu/~rlaz/PatternRecognition/, Richard Zanibbi

(k-)NN classifier example





CORNELL TECH

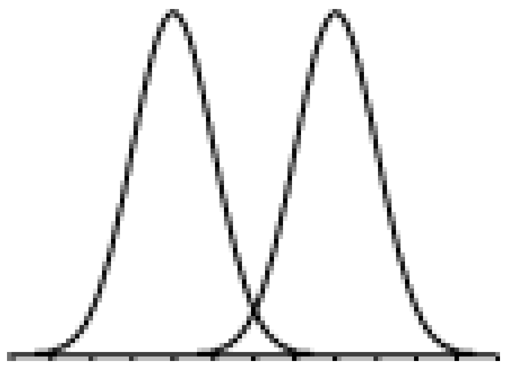
Classification and NN algorithms

- For many applications it's way more useful to have the density
  - Tells you a lot more about your data
- To classify we need to estimate the density
- Good way to do this is from nearest neighbors
  - Lots of other algorithms also but NN is very popular
- Basic intuition: most of the cats are where the cat density is high, and vice-versa
  - "When you hear hoofbeats, think of horses not zebras"

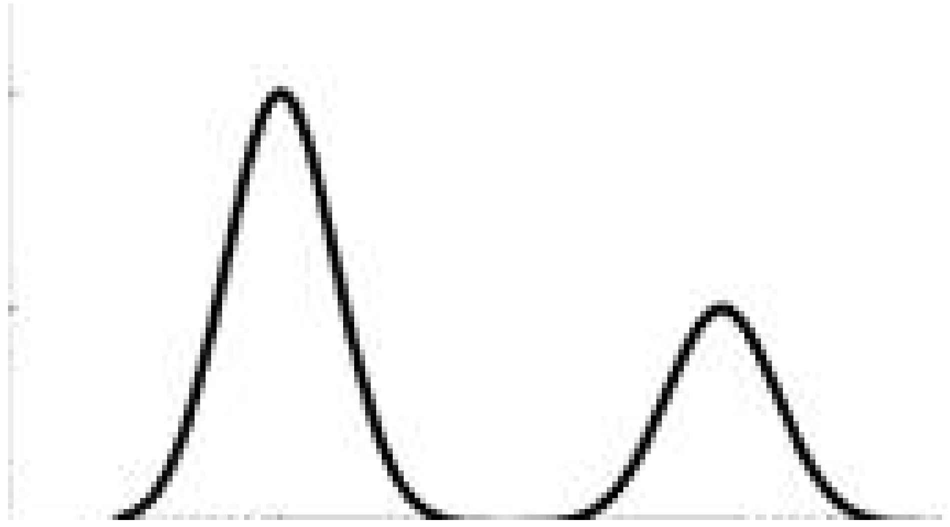
Cats versus dogs (simple version)

- Suppose we want to classify based on a single number
  - Such as weight
- Simple case: cats and dogs have their weights described by a Gaussian (normal) distribution
- Cats occur about as frequently as dogs in our data
- We just need to estimate the density for cats vs dogs
- This allows us to build our classifier

Cat vs dog classification from weight



"Simple" case



A not so simple case

NN Density estimation

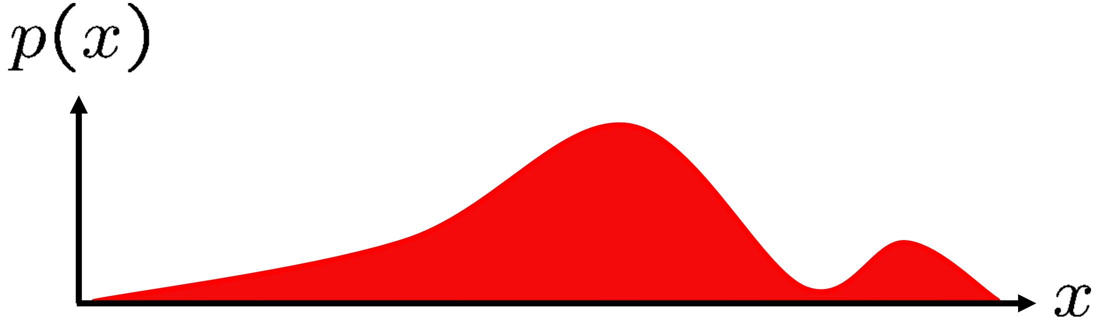
- Lots of practical questions boil down to density estimation
  - Even if you don't explicitly say you're doing it!
    - "How much do typical cats weigh?"
      - Google says: 7.9 – 9.9 lbs
- Your classes generally have some density in feature space
  - Hopefully they are compact and well-separated
- Given a new data point, which class does it belong to?
  - We just maximize $P(data|class)$, called the **likelihood**
    - Formalizes what we did on the previous slide

What is a density?

- Consider an arbitrary function p where

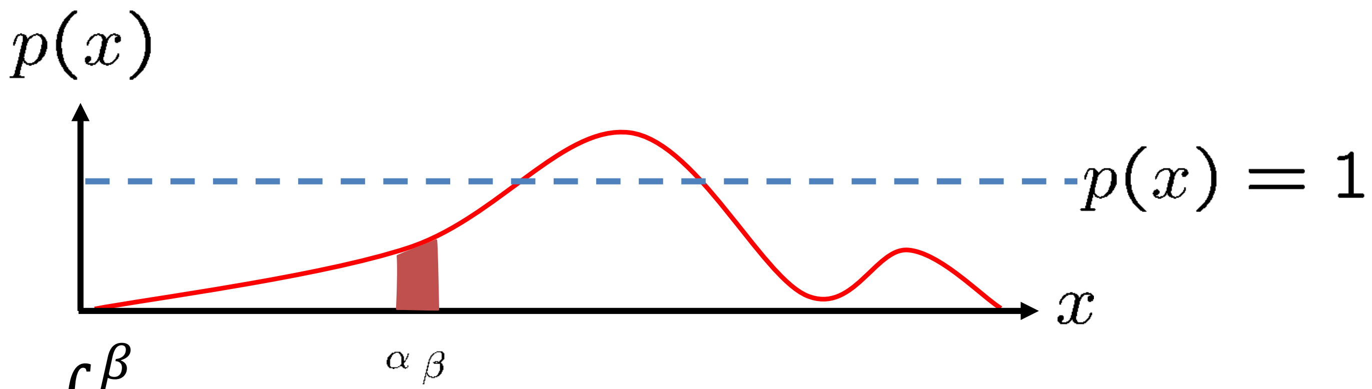
$$p(x) \geq 0$$

  – Can view it as a *probability density function*
    - The PDF for a real-valued random variable
    - If we weighed ∞ cats, what frequency of weights would we get?



A pitfall of interpreting densities

- The value of PDF at x is **not** the probability we would observe the weight x
  - Which is always zero (think about it!)
  - Instead, it gives the probability of getting a weight in a given interval



$$\int_{\alpha}^{\beta} p(x)dx = P[\alpha \leq weight \leq \beta]$$

Discrete case is easier

- Sometimes the values of the random variable are discrete
  - Instead of a PDF you have a probability mass function (PMF)
  - I.e., a histogram whose entries sum to 1
    - No bucket has a value greater than 1
- This is the true relative frequencies
  - i.e., what we would get in the limit as we weigh more and more cats

Sampling from a PDF

- Suppose we weigh a bunch of cats
  - This generates our *sample* (data set)
  - How does this relate to the true PDF?
- It simplifies life considerably to assume:
  - All cats have their weights from the same PDF (identical distributions)
  - No effect between weighing one cat and another (independence)

Welford's online mean algorithm

- Suppose we know that cats come from a Gaussian distribution but we have too many cats to store all their weights
- Can we estimate the mean (and variance) online?
- Online algorithms are very important for modern applications
- For the mean we have

$$\mu_n = \frac{1}{n}\sum_{i=1}^{n} x_i = \mu_{n-1} + \frac{1}{n}(x_n - \mu_{n-1})$$

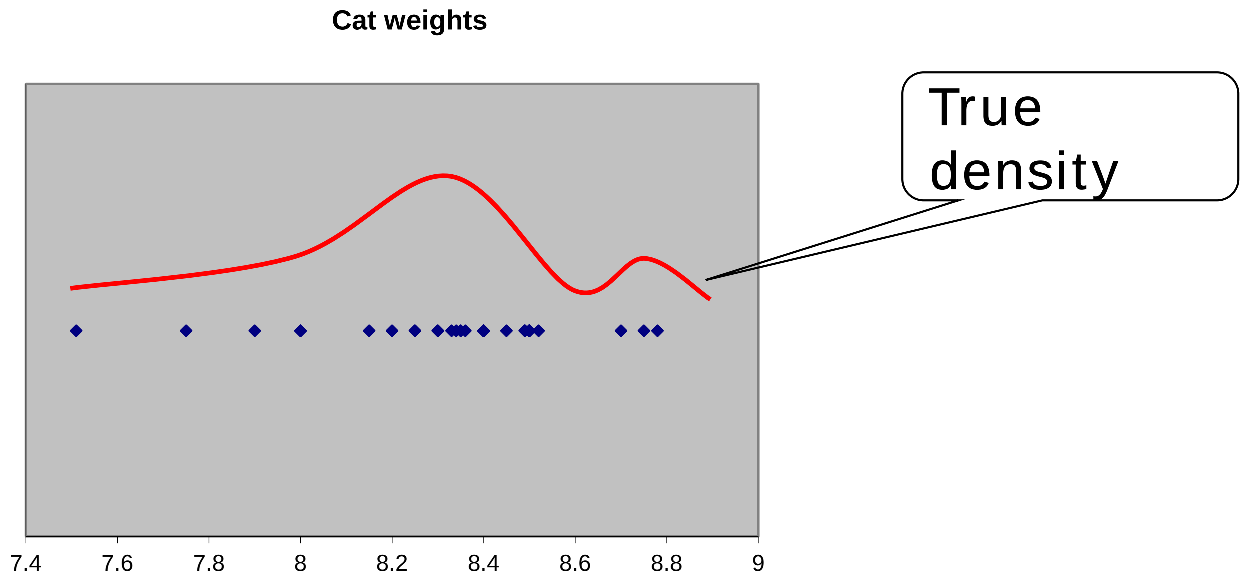
CORNELL TECH

Non-parametric approach

- We knew the underlying distribution
  - All we needed was to estimate the parameters
  - Obviously, this gives bad results when the true distribution isn't what we think it is
  - Non-Gaussian distributions are in general rare, and hard to handle
    - But they occur a **lot** in some areas
- Box's law: All models are wrong but some are useful

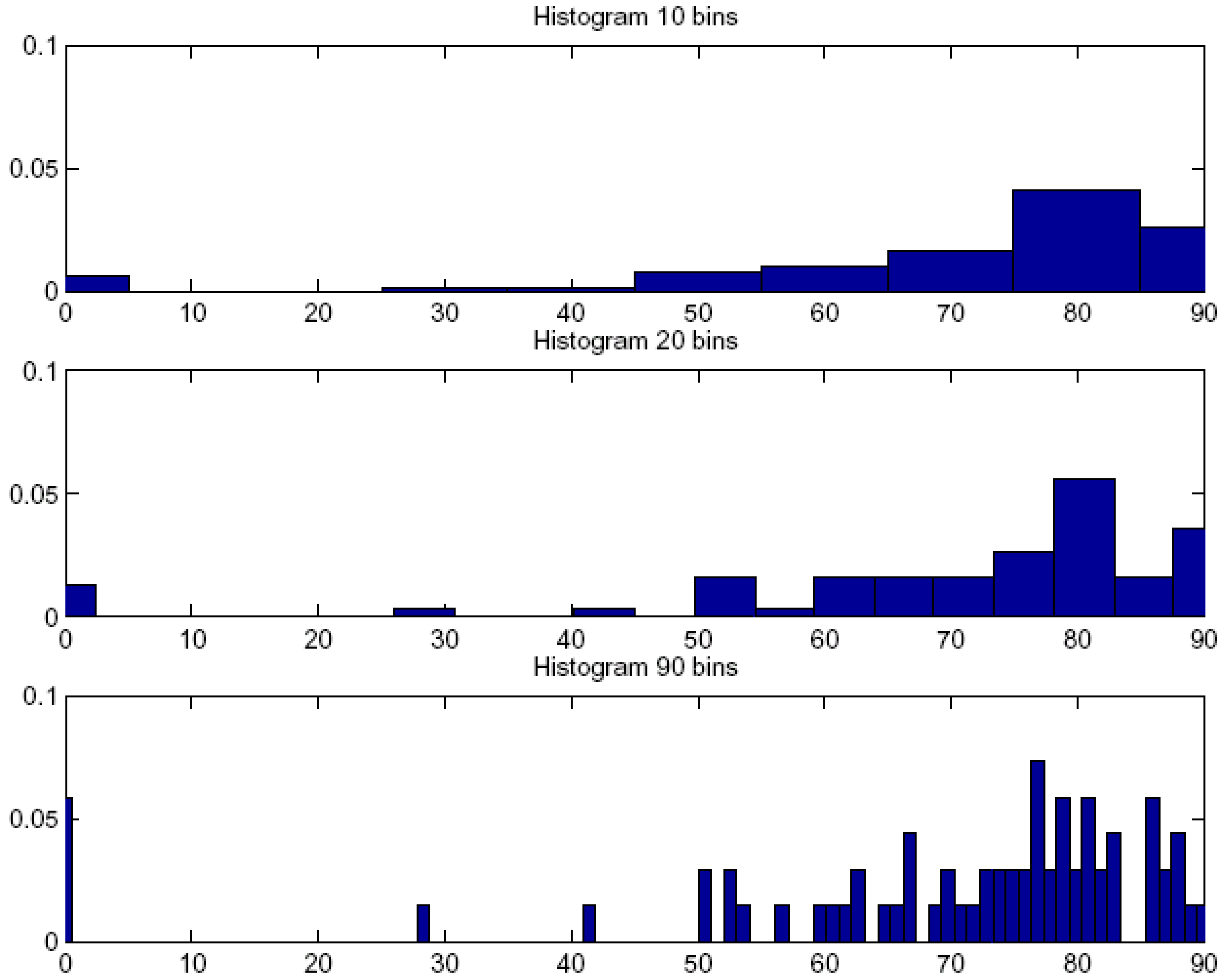
Is there a free lunch?

- Suppose we simply plot the data points
  - Assume 1-D for the moment (cat weights)



  - How to compute density from data?

Histogram representation



CORNELL TECH

Bin-size tradeoffs

- Fewer, larger bins give a smoother but less accurate answer
  - Tend to avoid "gaps"
    - i.e., places where the density is declared to be 0
- More, smaller bins have opposite property
- If you don't know anything in advance, there's no way to predict bin size
  - Also, note that this method isn't a great idea in high dimensions

Histogram-based estimates

- You can use a variety of fitting techniques to produce a curve from a histogram
  - Lines, polynomials, splines, etc.
  - Also called regression/function approximation
  - Normalize to make this a density
- If you know quite a bit about the underlying density you can compute a good bin size
  - But that's rarely realistic
  - And defeats the whole purpose of the non-parametric approach!

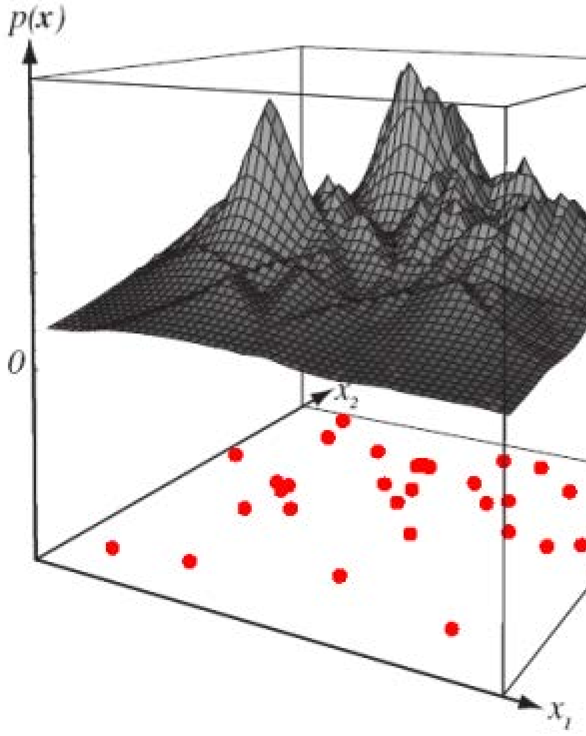
Nearest-neighbor estimate

- To estimate the density, count number of nearby data points
  - Like histogramming with sliding bins
  - Avoid bin-placement artifacts

$$\hat{p}(x) = \frac{\#\{\, x_i \mid \|x_i - x\| \leq \epsilon \,\}}{n}$$

  - Can fix epsilon and compute this quantity, or we can fix the quantity and compute epsilon

NN density estimation



Slide credit: https://www.cs.rit.edu/~rlaz/PatternRecognition/, Richard Zanibbi

Sliding sums

- Suppose we want to “smooth” a histogram, i.e. replace the values by the average over a window
  – How can we do this efficiently?