

k-Nearest Neighbors (kNN)

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Original Slides: Ryan Henning

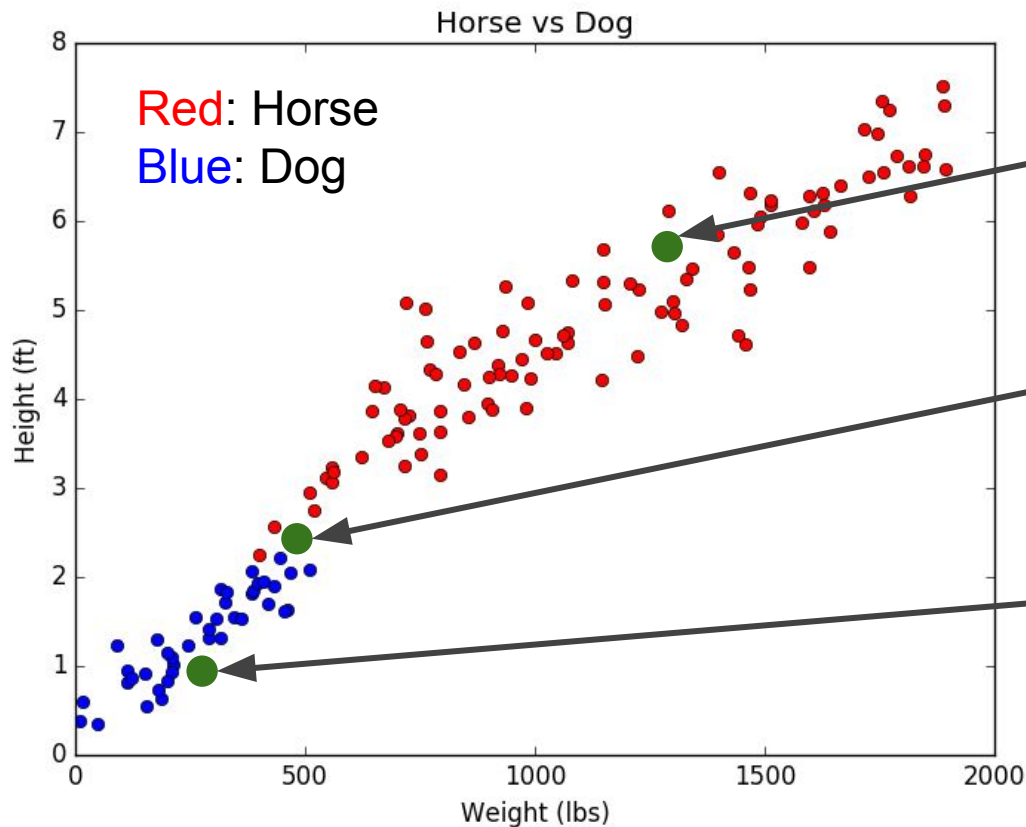


- k-Nearest Neighbors
- The Curse of Dimensionality
- Parametric vs Nonparametric Models

Morning Objectives: kNN

- Describe the k-Nearest-Neighbors algorithm
- State common distance metrics used for kNN
- Describe the effect of varying k
- Explain the importance of scaling for kNN
- Describe the curse of dimensionality
- Implement the kNN algorithm in Python

Is it a big dog or a small horse?



New datapoint:
Is it a horse or a dog?

New datapoint:
Is it a horse or a dog?

New datapoint:
Is it a horse or a dog?

The k-Nearest Neighbors algorithm:

Training algorithm:

1. Store all the data... that's all.

Prediction algorithm (predict the class of a new point x'):

1. Calculate the distance from x' to all points in your dataset.
2. Sort the points in your dataset by increasing distance from x' .
3. Predict the probability of each target class using the k closest points.

What is k ?



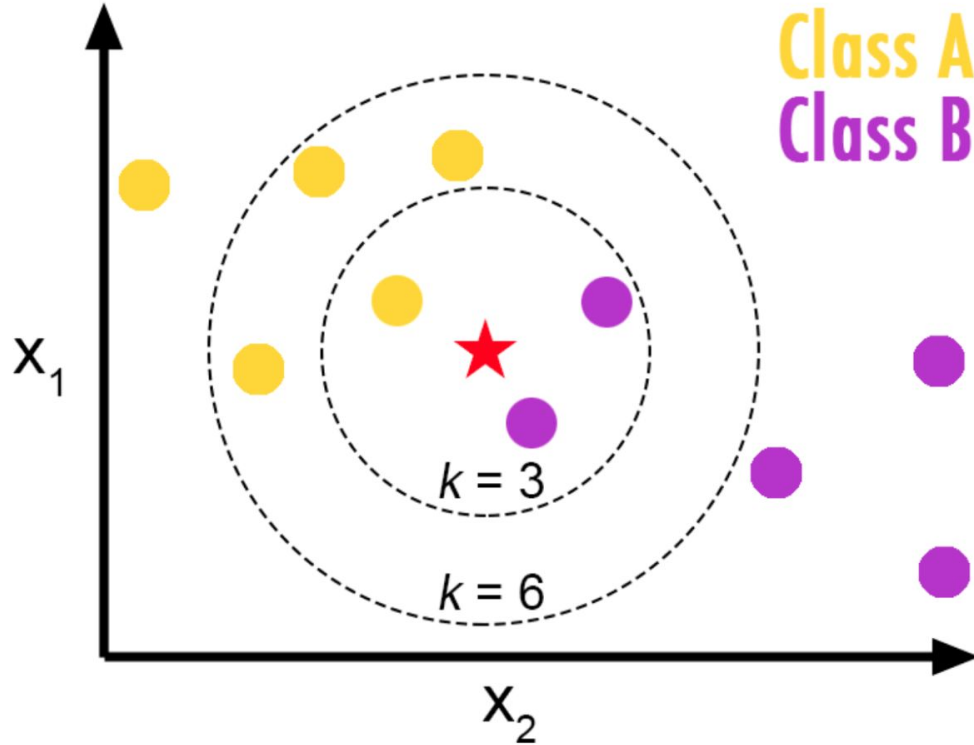
Distance Metrics

Euclidean Distance (L2):
$$\sum_i (a_i - b_i)^2$$

Manhattan Distance (L1):
$$\sum_i |a_i - b_i|$$

Cosine Distance = 1 - Cosine Similarity:
$$1 - \frac{a \cdot b}{||a|| ||b||}$$

kNN: you pick k

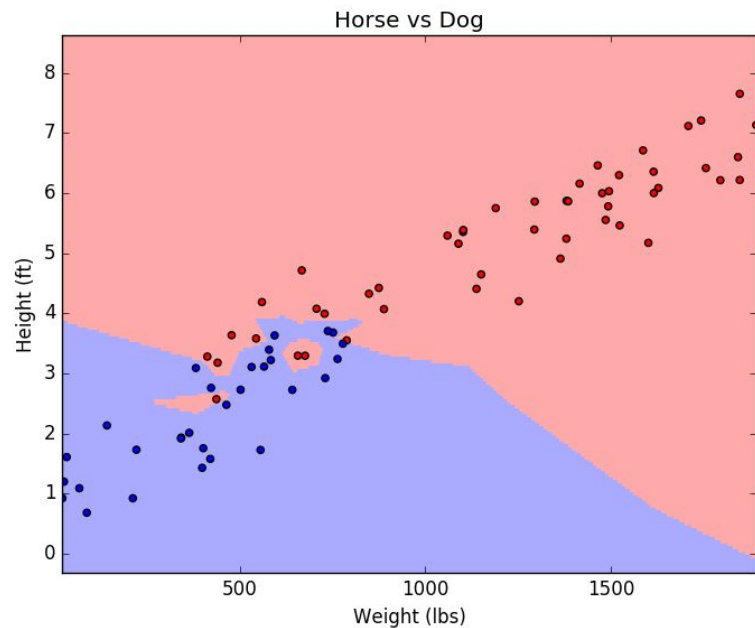


What is the prediction for ★
when $k=3$?

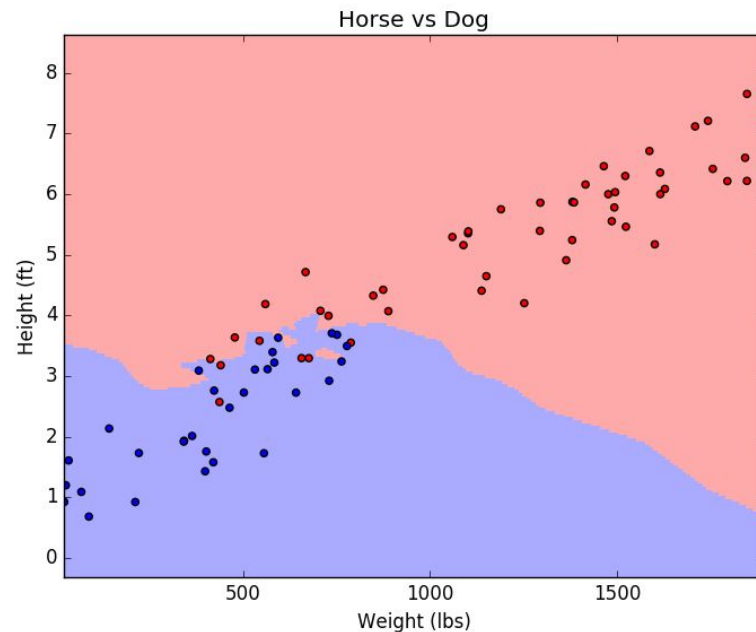
What is the prediction for ★
when $k=6$?

The only hyperparameter... k ... the number of nearest neighbors to consider

$k=1$

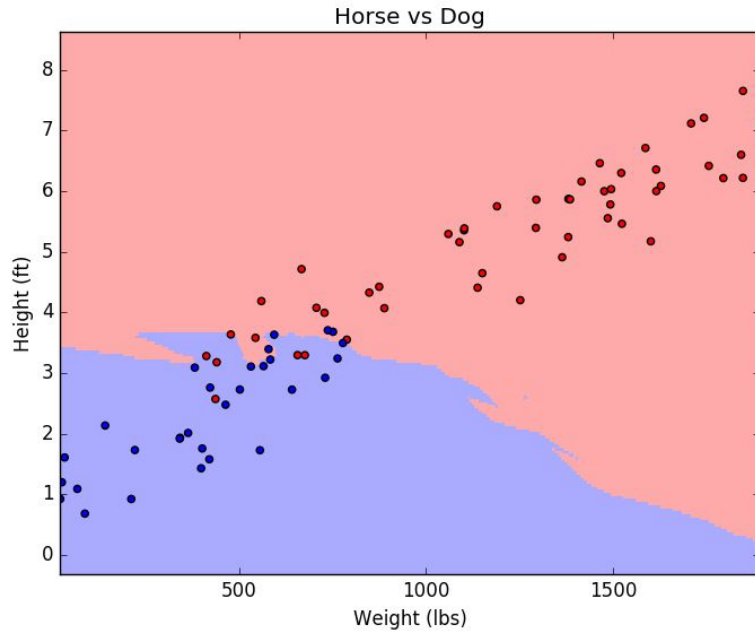


$k=5$

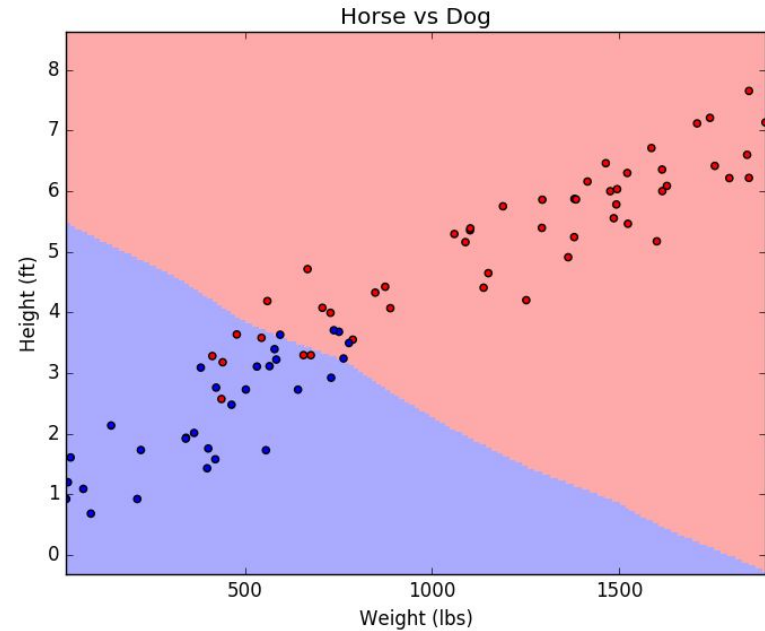


The only hyperparameter... k ... the number of nearest neighbors to consider

k=10

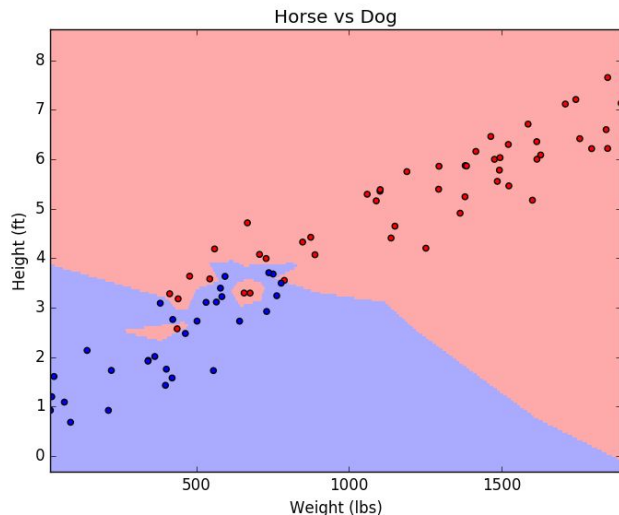


k=50



Which model seems overfit?

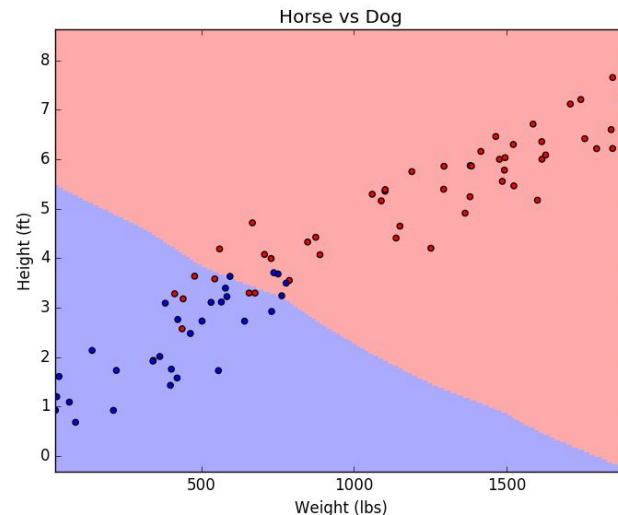
k=1



As a
general
rule, start
with:

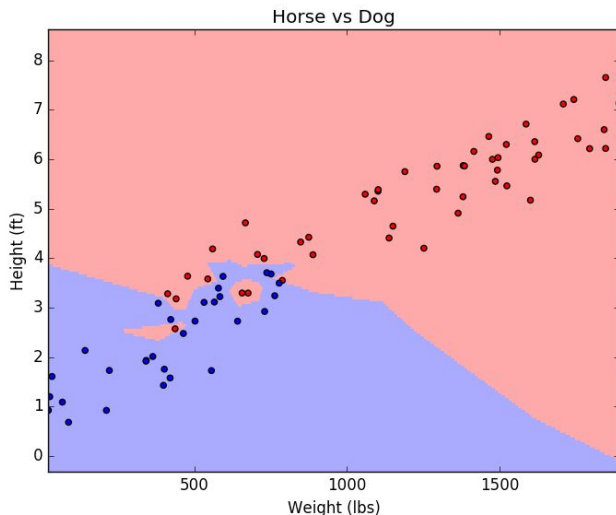
$$k = \sqrt{n}$$

k=50

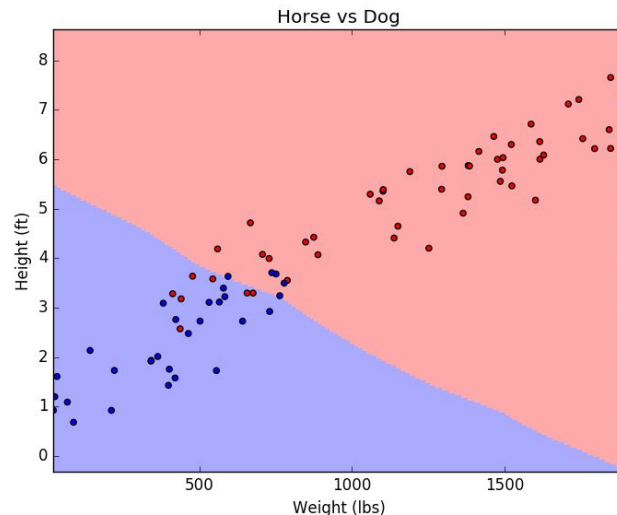


What happens to model variance when k increases?

$k=1$



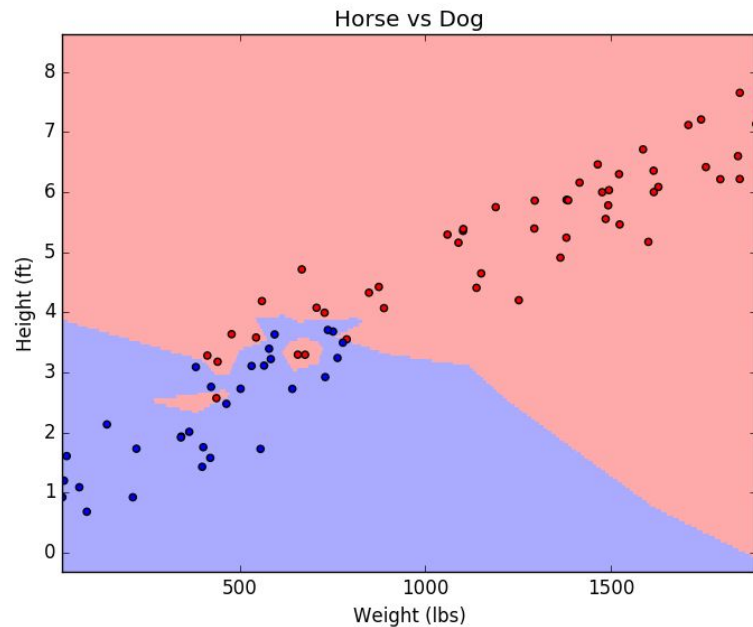
$k=50$



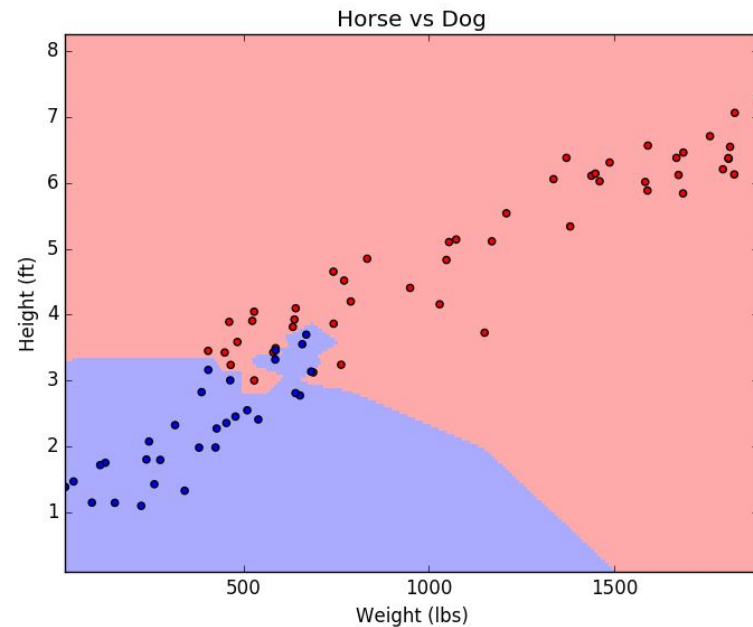
See the high variance?

Each dataset is randomly generated from the same population.

$k=1$

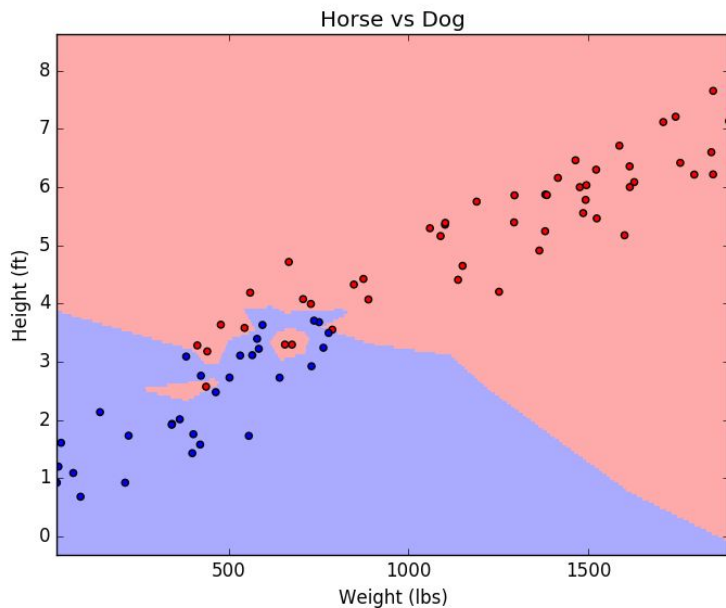


$k=1$

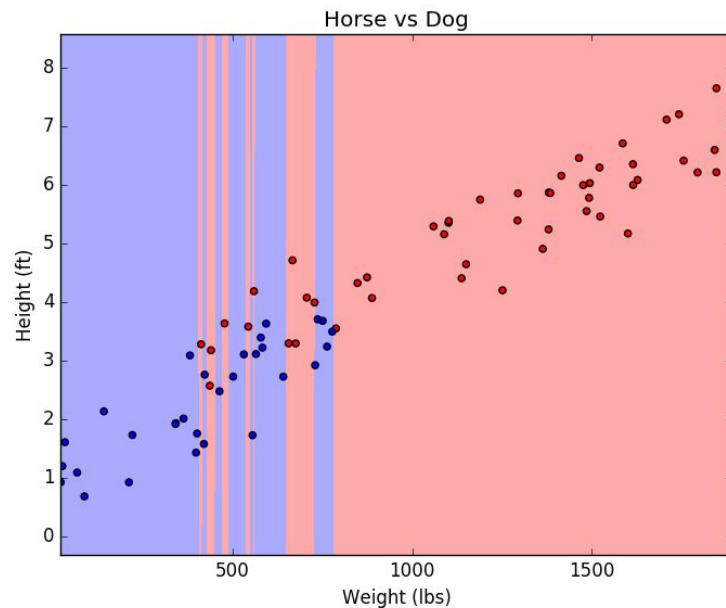


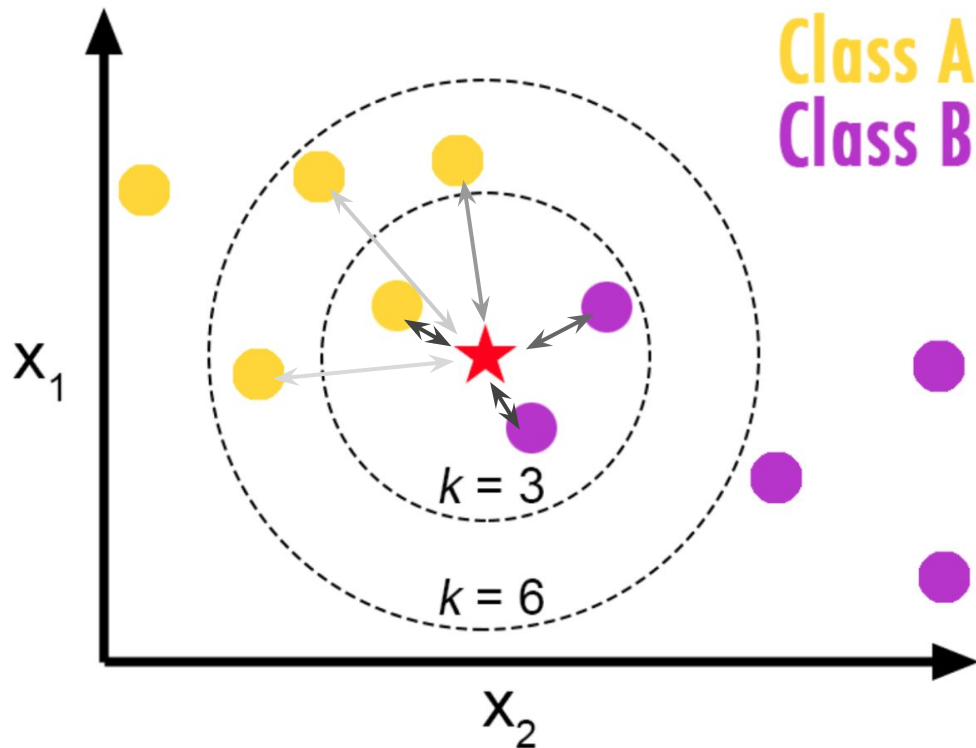
Be careful with the scale of your features!

k=1, scaled features



k=1, original-scale features





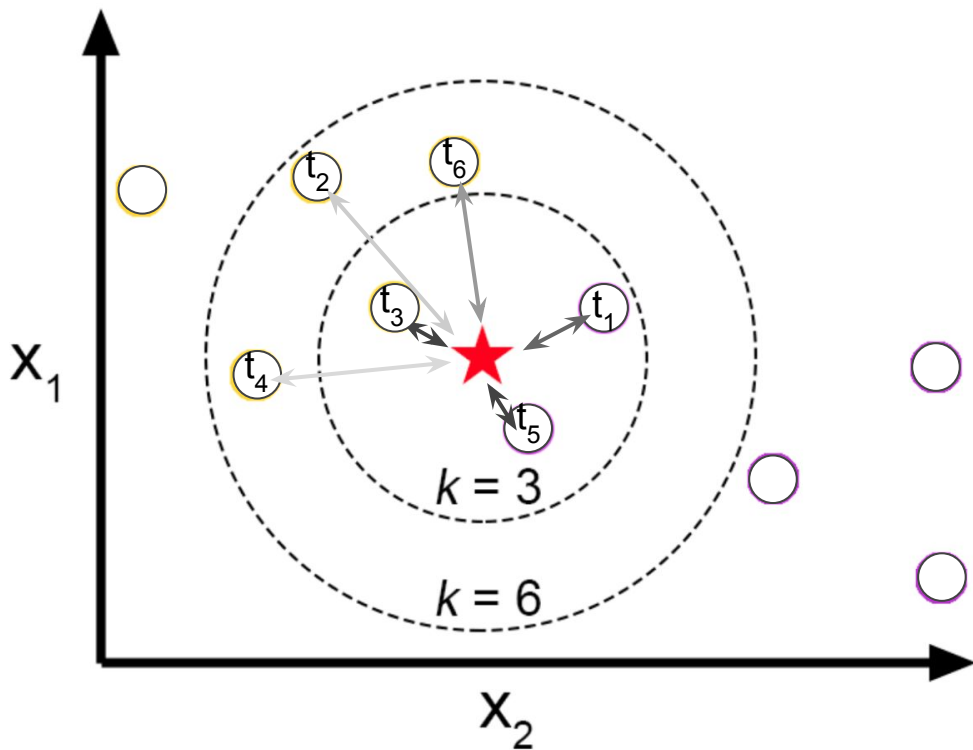
Let the k nearest points have distances:

$$d_1, d_2, \dots, d_k$$

The i^{th} point votes with a weight of:

$$\frac{1}{d_i}$$

small distances are weighted more!



Let the k nearest points have distances:

$$d_1, d_2, \dots, d_k$$

Let the k nearest points have targets:

$$t_1, t_2, \dots, t_k$$

How can we do regression with kNN?

Predict the mean value of the k neighbors, or predict a weighted average.

kNN in high dimensions...

kNN is problematic when used with high dimensional (d) spaces...
... but it works pretty well (in *general*) for $d < 5$

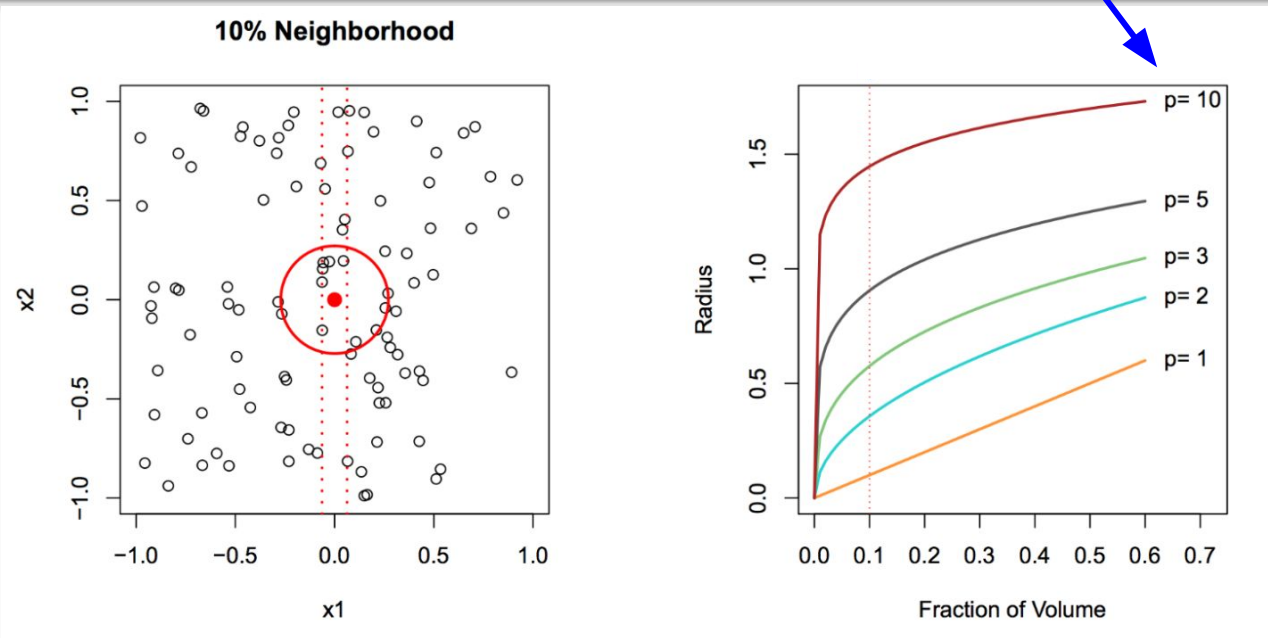
The nearest neighbors can be very **“far away”** in high dimensions...

Say you want to use a neighborhood of 10% (i.e. $k = 0.1 * n$)

Let's see how this looks as we increase the dimensionality... (next slide)

The Curse of Dimensionality

p = dimensionality



When $p=1$, we are only considering x_1 . When $p=2$, we are considering x_1 and x_2 .

Notice the required radius in 2D is much larger than the required radius in 1D.

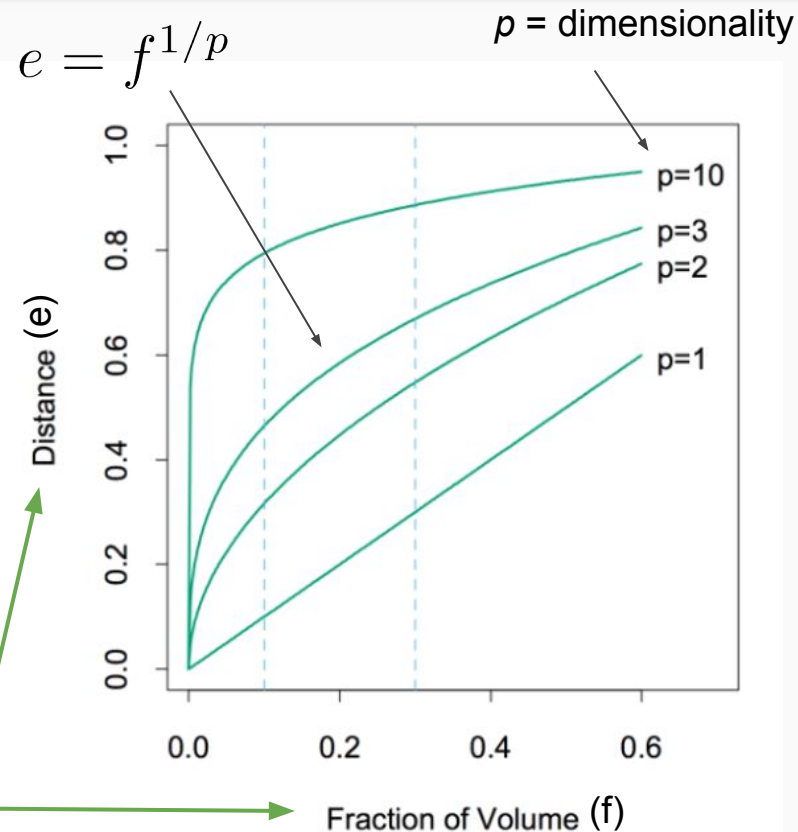
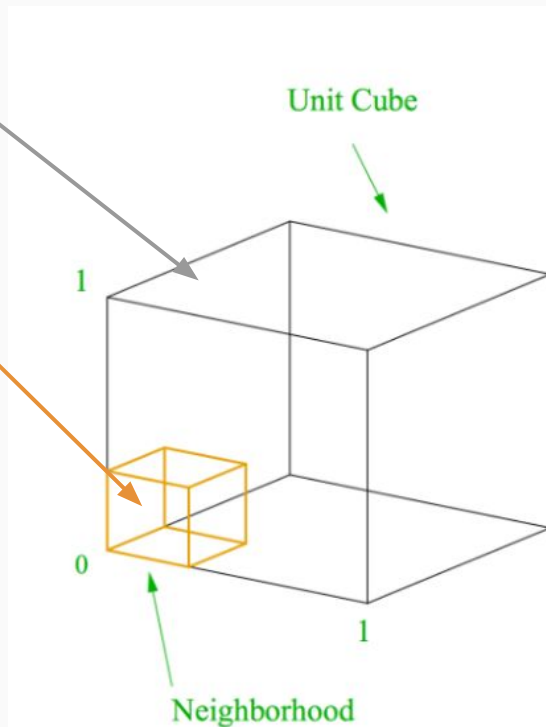
As we increase the dimensionality, we lose the concept of locality.

The Curse of Dimensionality (another perspective)

Say we have a unit (hyper)cube.

We want to create another (hyper)cube inside the outer cube so that we fill X% of the outer cube.

How long must the edges of the inner cube be?



Say you have a dataset with 100 samples, each with only one predictor.

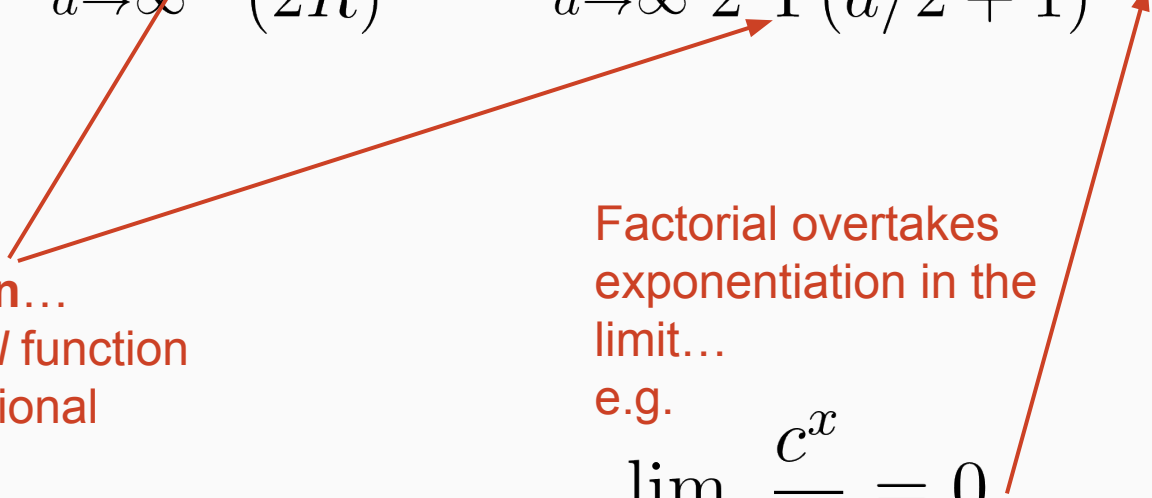
But, one predictor doesn't tell you enough, so you collect a new dataset, and this time you measure 10 predictors for each sample.

How many samples do you need in your new (10 predictor) dataset to achieve the same “sample density” as you originally had (in the one-predictor dataset)?

Just 100^{10} , that not that many... just

100,000,000,000,000,000,000,000,000,000

Don't freak out...

$$\lim_{d \rightarrow \infty} \frac{V_{\text{sphere}}(R, d)}{V_{\text{cube}}(R, d)} = \lim_{d \rightarrow \infty} \frac{\frac{\pi^{d/2} R^d}{\Gamma(d/2 + 1)}}{(2R)^d} = \lim_{d \rightarrow \infty} \frac{\pi^{d/2}}{2^d \Gamma(d/2 + 1)} = 0$$


Euler's gamma function...

basically, it's the *factorial* function that can operate on fractional numbers

Factorial overtakes exponentiation in the limit...

e.g.

$$\lim_{x \rightarrow \infty} \frac{c^x}{x!} = 0$$

What does this mean?

The Curse of Dimensionality... takeaways

- kNN (or any method that relies on distance metrics) will suffer in high dimensions.
 - Nearest neighbors are “far” away in high dimensions (even for $d=10$).
- A 10% neighborhood in a high dimensional unit hypercube requires a hypersphere with large radius.
 - Hyperspheres are weird in high dimensions...
 - “They are super-pointy!” (Ryan’s interpretation)
- High dimensional data tends to be sparse; it’s easy to overfit sparse data.
 - It takes A LOT OF DATA to make up for increased dimensionality.

Parametric vs Non-parametric Models

Parametric models have a fixed number of learned parameters.

- Logistic regression is parametric.
- kNN is non-parametric.

Parametric models are more structured. The added structure often combats the curse of dimensionality... as long as the structure is derived from reasonable assumptions.

Alternate perspective: Parametric models are not distance based, so the curse doesn't apply!

Summary: kNN

Pros:

- super-simple
- training is trivial (store the data)
- works with any number of classes
- easy to add more data
- few hyperparameters:
 - k
 - *distance metric*

Cons:

- high prediction cost (especially for large datasets)
- high-dims = bad
 - we'll learn dimensionality reduction methods in two weeks!
- categorical features don't work well...

Review Objectives: kNN

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AM Exercise: Implement the kNN algorithm in Python