k-Nearest Neighbors

Introduction to Non-Parametric Learners

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Galvanize

2016

Overview

Modeling

- Parametric vs. Non-parametric

k-Nearest Neighbors

- Intuition
- Training
- Prediction
- Choosing k

Curse of Dimensionality

- Completely Unintuitive

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Parametric Models

Models that can be described with a finite number of parameters.

- Linear Regression
- Logistic Regression
- Neural Networks

Non-parametric Models

Models whose parameters reside in an infinite-dimensioned parameter space.

- Decision Trees
- Support Vector Machines
- k-Nearest Neighbors

These models, variants of them, and their applications are what we're going to be learning about for the next two weeks.

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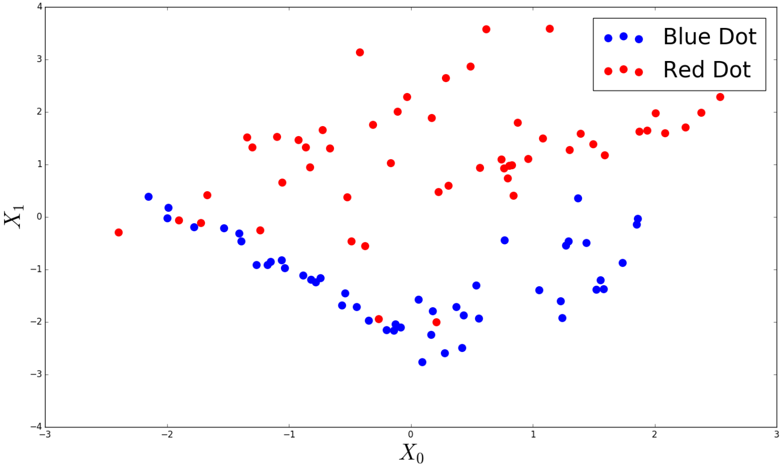
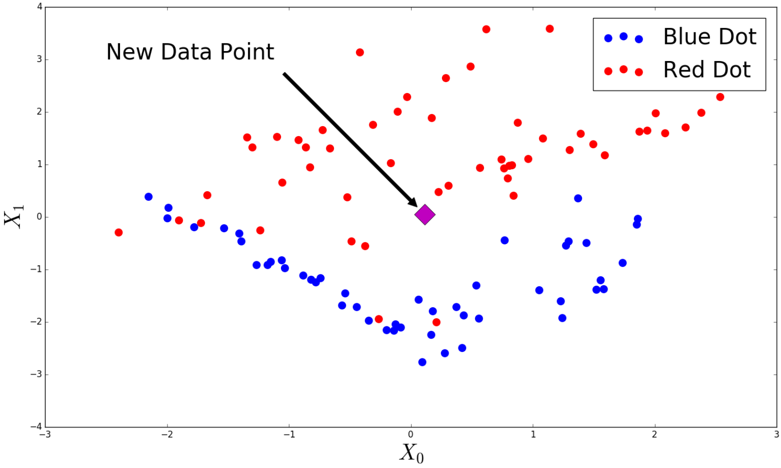
Intuition

- Consider trying to write your own supervised machine learning algorithm.
- It's expected receive data, X, and a corresponding targets, y, and with it be able to take it a new data point X_0 and output a prediction for its target.
- Let's stay simple for a moment and talk about ways that we could make such predictions.

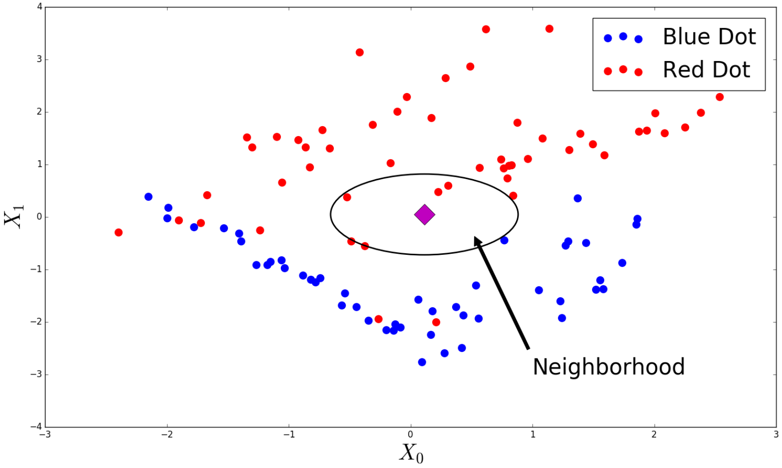
Example Data to Point At



New Data - How Do We Predict?



Check Out Some Close Points. They're Probably Similar!



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2. Look at the k points nearest the new point.
3. Predict the modal class amongst those k points for classification. For regression, choose the average (potentially weighted by distance) of the k points.

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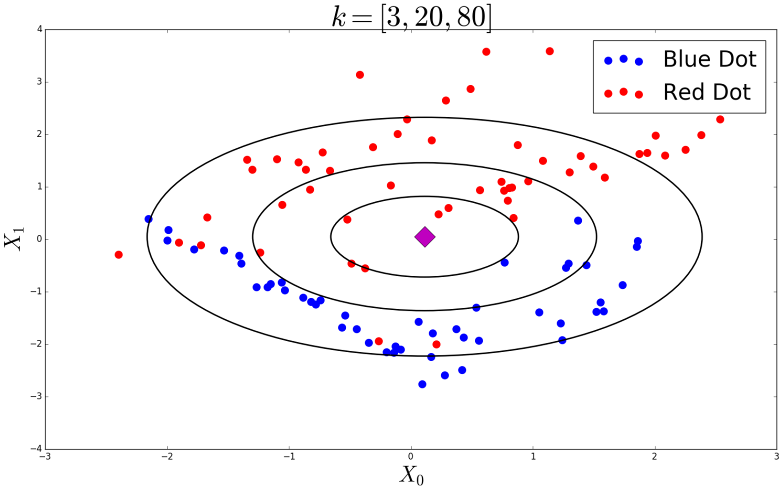
How to Choose k



Bias-Variance Trade-off?

Question

How does changing k alter the bias and variance in our kNN models?

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What happens when $k = n$?

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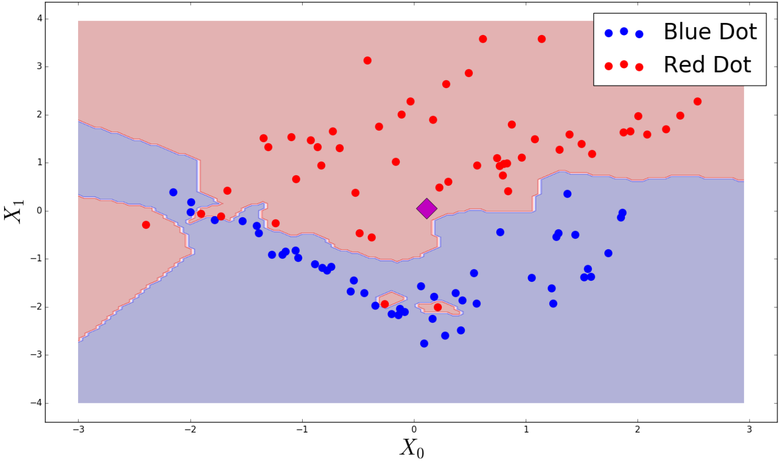
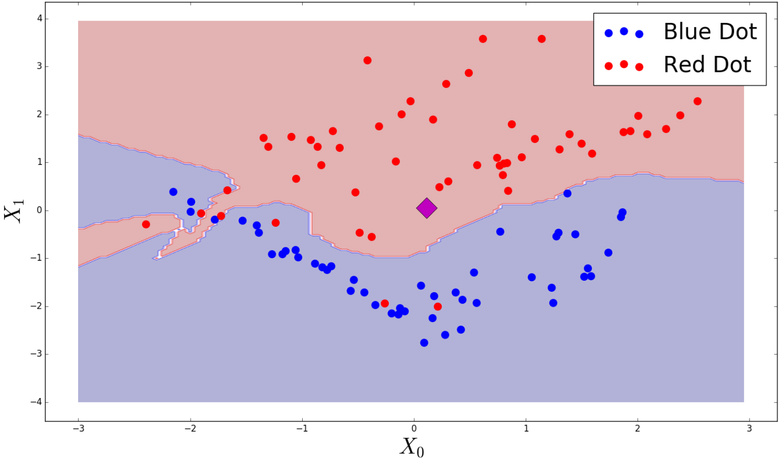
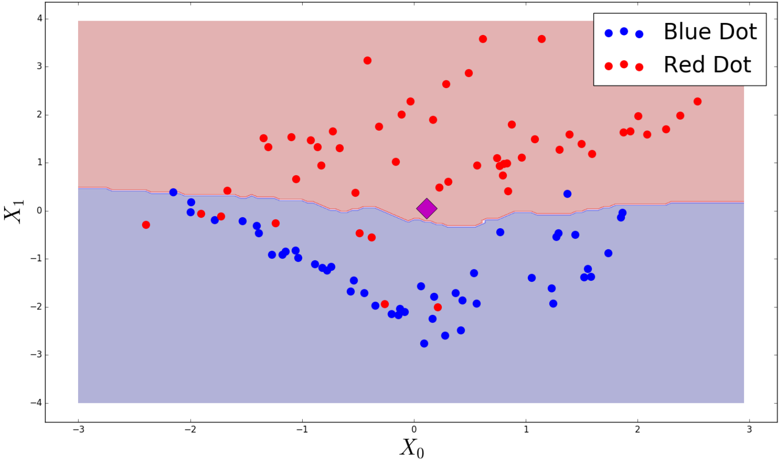
$k = 1$



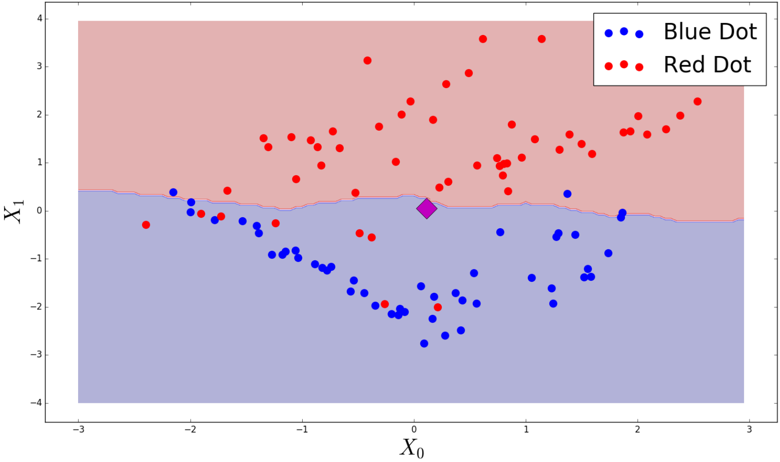
$k = 3$



$k = 20$



$k = 80$



Distance Metrics

So far we haven't been explicit about what distance metrics we're using. Some choices:

Euclidean $\sqrt{\sum_i (a_i - b_i)^2}$

Manhattan $\sum_i |a_i - b_i|$

Cosine $1 - \frac{a \cdot b}{||a||||b||}$

Pros

- Simple to use and intuitive.
- Extremely fast to train ;)
- Doesn't assume anything about the relationship between Xs and y.

Pros and Cons

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- Simple to use and intuitive.
- Extremely fast to train ;)
- Doesn't assume anything about the relationship between Xs and y.

Cons

- Slow to predict.
- Unreliable with high dimensional data.
- Doesn't work well with categorical features.

Advice

- A good place to start searching for k is $\sqrt{n}$.
- Make sure to normalize data before training.
- Not a widely used algorithm for the reasons we saw above, some potential uses:
  - Missing data imputation.
  - Anomaly detection.

Variants

- One variant is to weight the votes by $\frac{1}{d_i}$ so closer points get more weight.
- Use for regression, take (optionally, weighted) mean of continuous target rather than vote.
- Approximate nearest neighbors, overcomes performance issues.

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Our Intuition is Lacking

The intuition that we have developed as beings living in a spatially 3-dimensional world fails us when we try to reason about how far apart things are in high dimensions.

Hypercubes

Question

Consider a hypercube inside a unit-hypercube. How long would we need to make the side of the smaller hypercube to capture 10% of the volume of the unit-hypercube?

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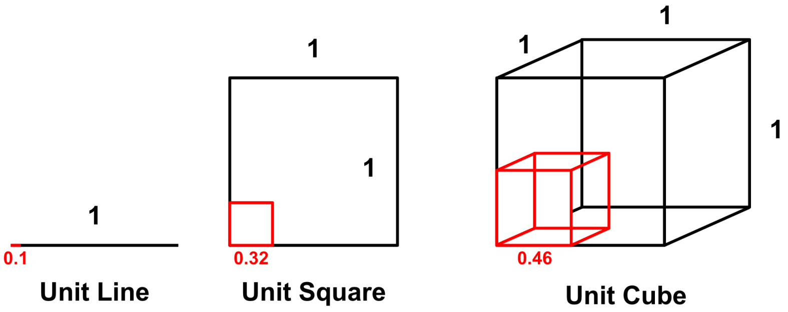
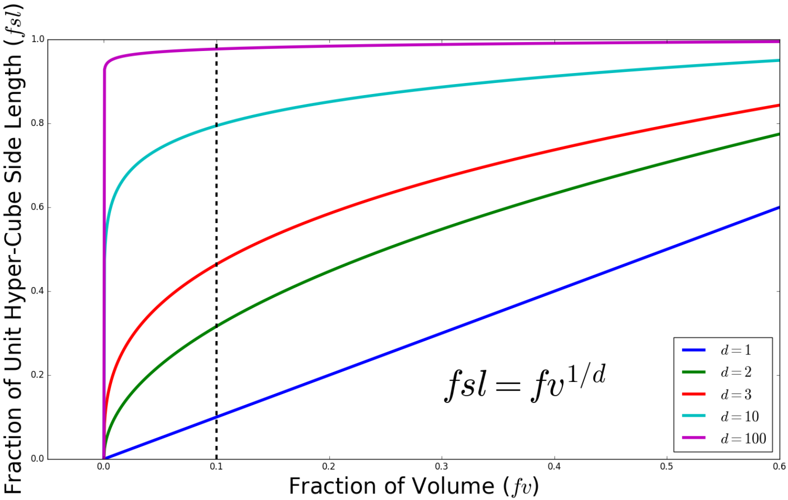


She's a Witch!



Fraction of Unit Hyper-Cube Side Length (fsl)
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
Fraction of Volume (fv)
$fsl = fv^{1/d}$
$d=1$
$d=2$
$d=3$
$d=10$
$d=100$