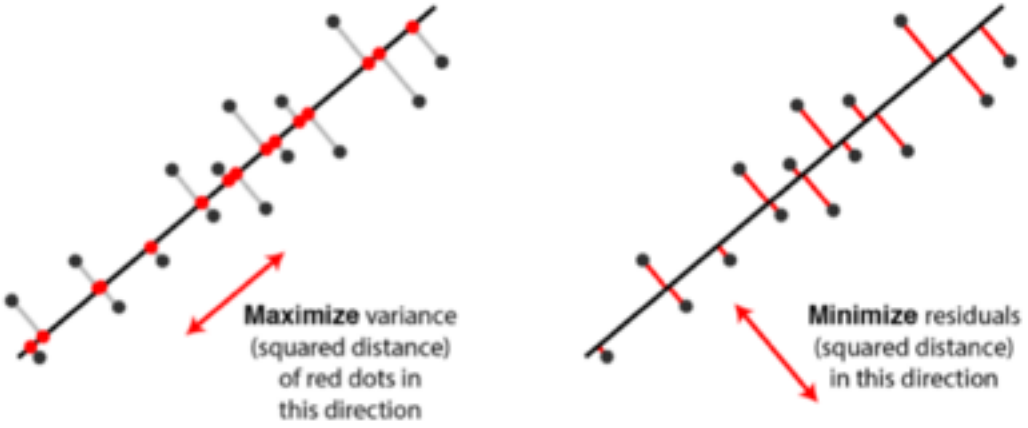
How can I interpret my ML system outputs?

Are my interpretations reasonable?

This course so far

How can one predict some value, find structure from data?



Two equivalent views of principal component analysis.

Let’s consider LASSO

We have come up with some sparse w for predicting y from x

How can we interpret the coefficients? Relative

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e.g. area in square feet and area in square meters

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Distribution shift: new hospital could have different equipment, demographics, staff training, location…

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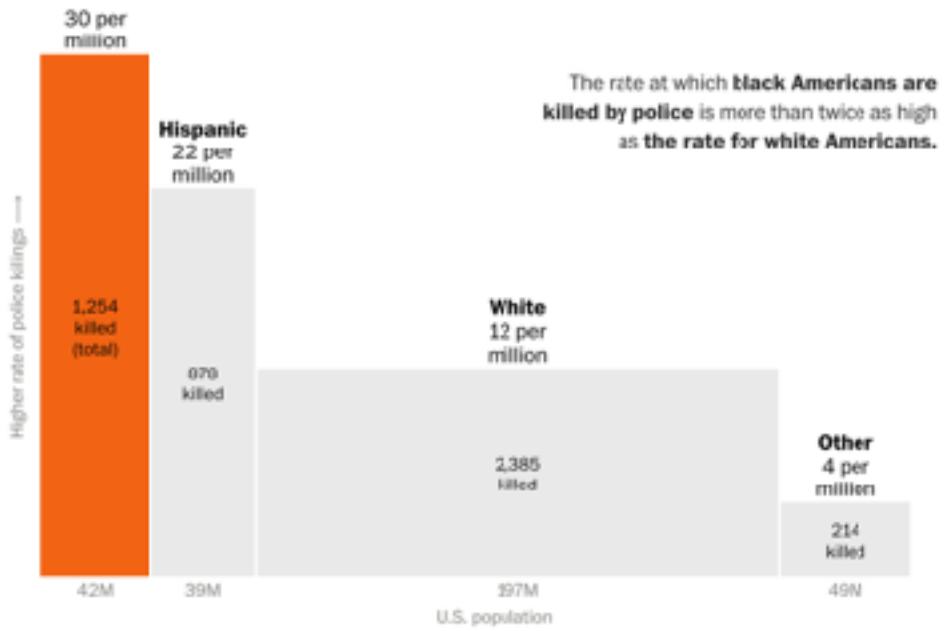
My particular hobby horse: the world is non-stationary!

Now, let’s talk about high-stakes decision making

Some sobering statistics

Many, many people are killed by police every year (10,429 in the past 9 years)

> half of which aren't reported to the FBI (reporting is voluntary)



Source: an excellent Washington Post interactive database

Design choices

Model Class

Features to collect

Loss function

Regularization

Optimization Method

Constraints

…

Design choices affect your model

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These will all affect what model you find, and how well and when that structure will generalize

… and that can have consequences "beyond" ML

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These will all affect what model you find, and how well and when that structure will generalize

Different models will have different kinds of errors, predictions, and failure modes

Consequence #1: Good predictions for whom?

The US Criminal Justice System

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This is a description of how things (largely) are and have been, not how they ought to be.

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Moreover, “reoffend” or “recidivate” are very, very, very far from precise terms in their use (in this lecture, and in industry).

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usually one which is violent.

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Concern: not all errors are equally costly.

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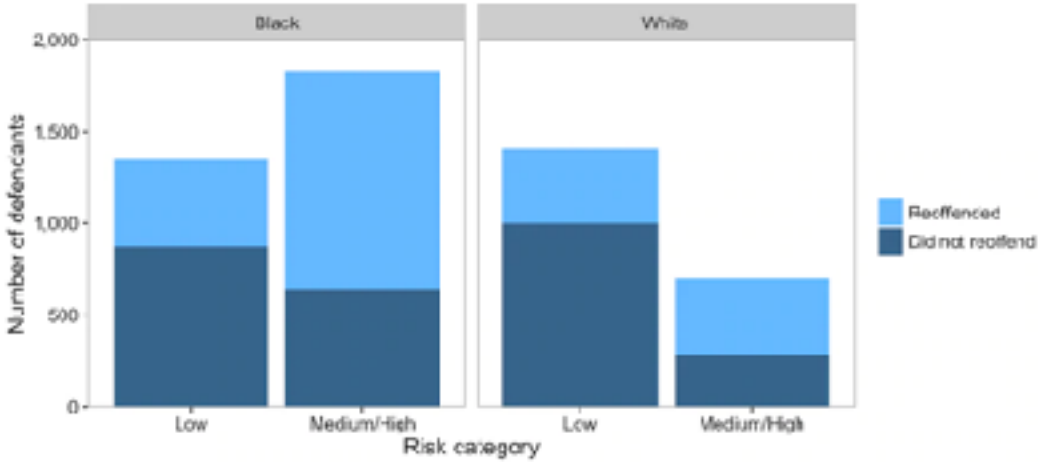

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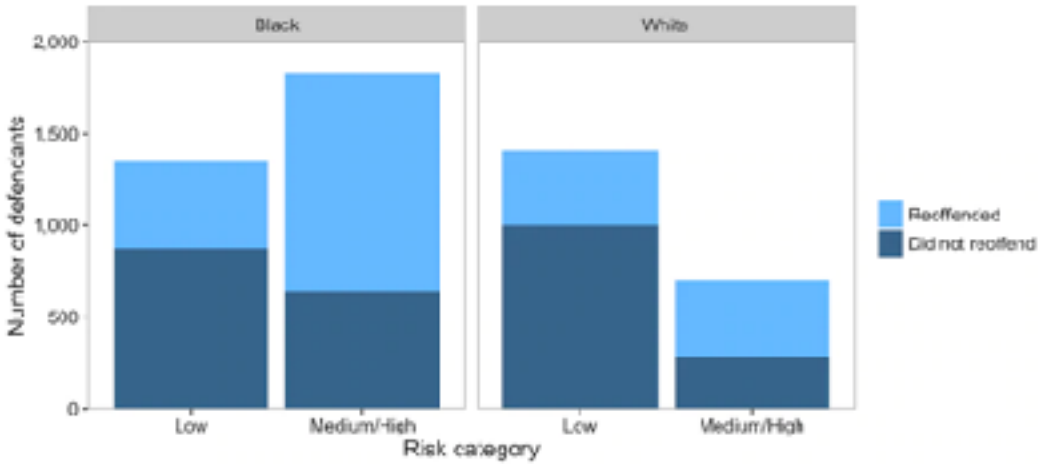

$$\mathbb{P}[\text{does not reoffend}|\text{predicted low risk, white}] < \mathbb{P}[\text{does not reoffend}|\text{predicted low risk, black}]$$

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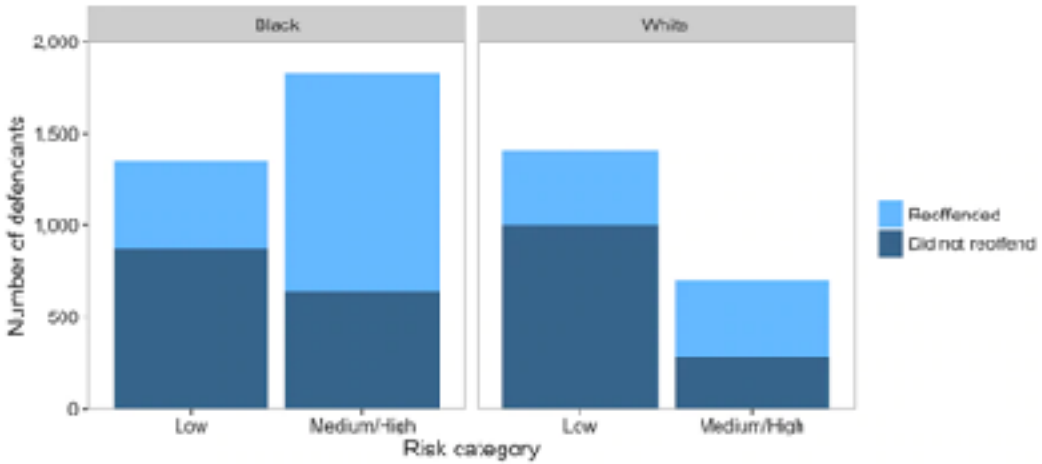

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False positive rate for black defendants higher than for white defendants.

Source: Washington Post

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Calibration of scores w.r.t. race

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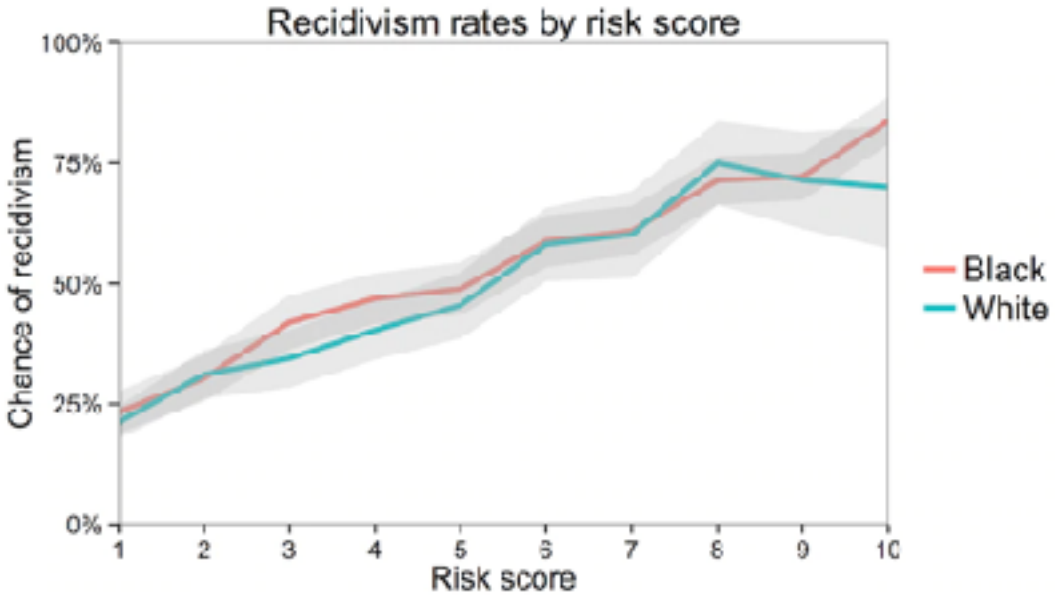

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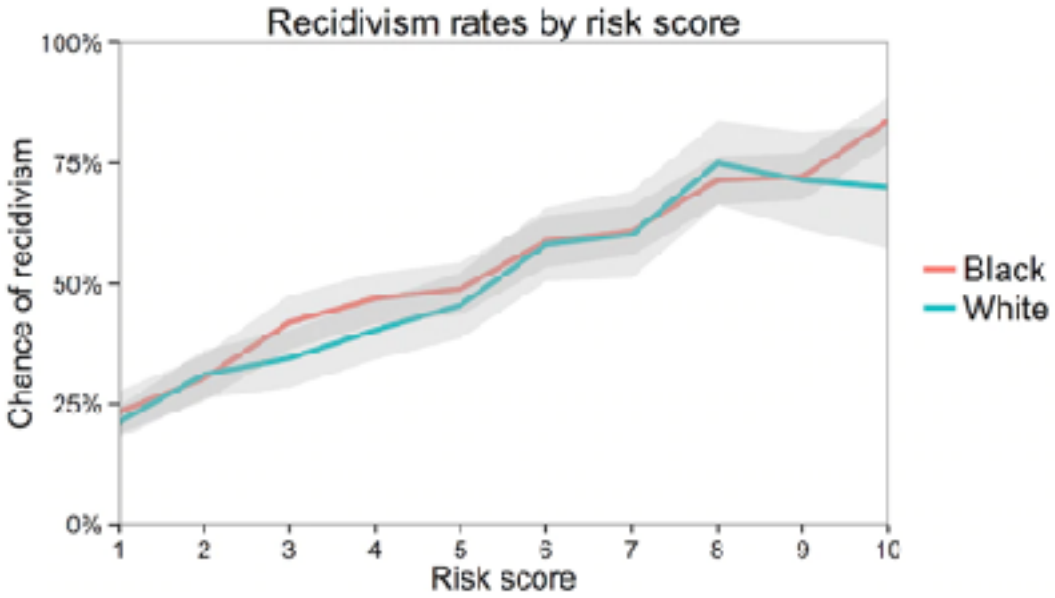

$$\mathbb{P}[\text{reoffend}|\text{prediction, white}] \approx \mathbb{P}[\text{reoffend}|\text{prediction, black}]$$

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Can any predictions be fair with respect to race?

$$\mathbb{P}[\text{does not reoffend}|\text{predicted low risk, white}] < \mathbb{P}[\text{does not reoffend}|\text{predicted low risk, black}]$$

while

$$\mathbb{P}[\text{reoffend}|\text{prediction, white}] \approx \mathbb{P}[\text{reoffend}|\text{prediction, black}]$$

How is this possible?

Is this avoidable?

Can any predictions be fair with respect to race?

False positives approximately equal and calibration are mutually exclusive, unless we have perfect predictions or the rate of what we are predicting is equal in every racial group.

… and this is true for more settings than just criminal justice.

Lending
Advertising
…

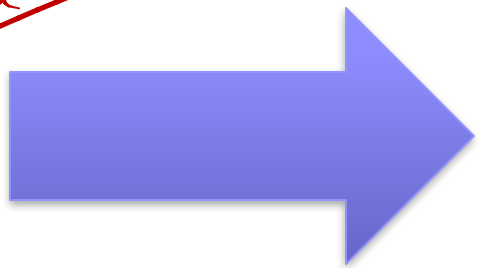
We are making a choice about how we allocate predictions.

Classification! Logistic "Regression" (linear classification), oh my…

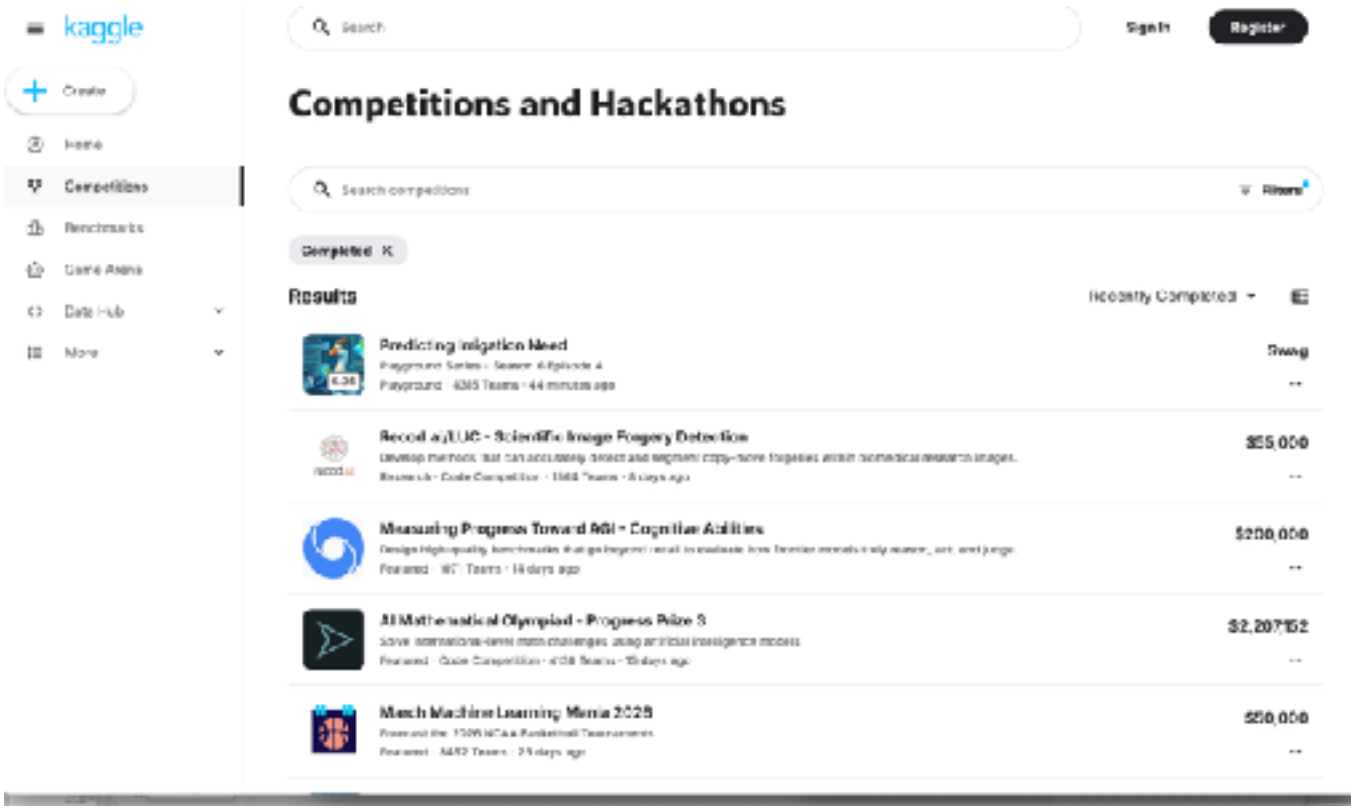
Thus far, regression:

predict a continuous value given some inputs

Weather prediction revisted



Recent Kaggle competitions



Classification

- Learn f: X -> Y
  - X - features
  - Y - target classes

- Loss Function
- Expected loss of f:

- Suppose you knew P(YIX) exactly, how should you classify?
  - Bayes-Optimal classifier:

Classification

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$$\ell(f(x), y) = \mathbf{1}\{f(x) \neq y\}$$

- Expected loss of f:

$$\mathbb{E}_{XY}[\mathbf{1}\{f(X) \neq Y\}] = \mathbb{E}_X[\mathbb{E}_{Y|X}[\mathbf{1}\{f(x) \neq Y\}|X = x]]$$

$$\mathbb{E}_{Y|X}[\mathbf{1}\{f(x) \neq Y\}|X = x] = \sum_i P(Y = i|X = x)\mathbf{1}\{f(x) \neq i\} = \sum_{i \neq f(x)} P(Y = i|X = x)$$

$$= 1 - P(Y = f(x)|X = x)$$

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  - Bayes-Optimal classifier:

$$f(x) = \arg\max_y \mathbb{P}(Y = y|X = x)$$

Binary Classification

- Learn f: X -> Y
  - X - features
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$$Y \in \{0, 1\}$$

- Loss Function

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Bayes Optimal Binary Classifier

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$$\{(x_i, y_i)\}_{i=1}^n$$

- What is a natural estimator for P(Y I X)?

Bayes Optimal Binary Classifier

- **Suppose we don't know P(YIX), but have n iid examples**

$$\{(x_i, y_i)\}_{i=1}^n \qquad Y \in \{0, 1\}$$

- **What is a natural estimator for P(Y I X)?**

$$\text{Fix some } \tilde{x} \in X$$

$$\text{Suppose } x_i = \tilde{x} \text{ for } m \leq n \text{ samples}$$

$$\text{What is a natural estimator for } \theta_* := \mathbb{P}(Y = 1 | X = \tilde{x})?$$

$$\text{If } k \text{ of the } m \text{ labels are equal to } Y = 1 \text{ then}$$

Bayes Optimal Binary Classifier

- **Suppose we don't know P(YIX), but have n iid examples**

$$\{(x_i, y_i)\}_{i=1}^n \qquad Y \in \{0, 1\}$$

- **What is a natural estimator for argmax_y P(Y = y I X)?**

$$\text{If } X = \{0,1\}^d, \text{ or is generally discrete}$$

$$\hat{f}(x) = \arg\max_{y \in \{0,1\}} \frac{\sum_{i=1}^n \mathbf{1}[\mathbf{x_i}=\mathbf{x},\mathbf{y_i}=\mathbf{y}]}{\sum_{i=1}^n \mathbf{1}[\mathbf{x_i}=\mathbf{x}]}$$

Issues?

Bayes Optimal Binary Classifier

- **What is a natural estimator for argmax_y P(Y = y I X)?**

If $X = \{0,1\}^d$, or is generally discrete $\quad Y \in \{0,1\}$

$$\hat{f}(x) = \arg\max_{y \in \{0,1\}} \frac{\sum_{i=1}^{n} \mathbf{1}[\mathbf{x_i}=\mathbf{x},\mathbf{y_i}=\mathbf{y}]}{\sum_{i=1}^{n} \mathbf{1}[\mathbf{x_i}=\mathbf{x}]}$$

Issues?

2^d possible inputs, for small d requires huge n

To make predictions for unseen inputs (xs),

need a **general** model for $\mathbb{P}(Y = 1|X = x)$

Process

Decide on a **model**

Find the function which fits the data best

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Decide on a model, Binary Classification

To make predictions for unseen inputs (xs),

need a **general** model for $\mathbb{P}(Y = 1|X = x)$

- **What about standard linear regression model?**

- **Need to map real values to [0,1]**
  - **We call such maps "link functions"**

Logistic Regression

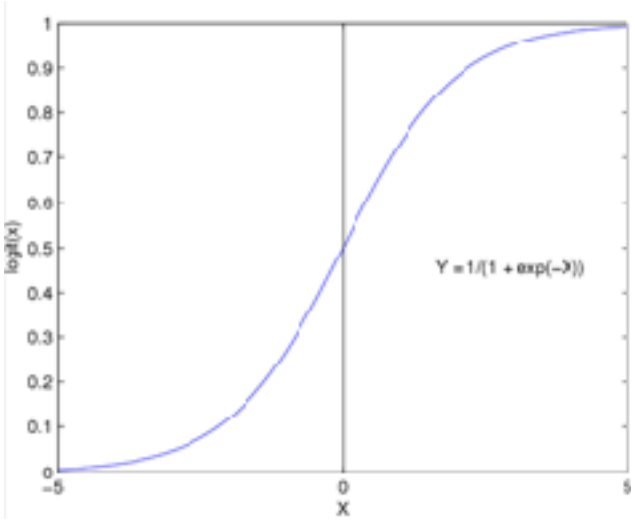
Actually classification, not regression :)

$$\text{Learn } \mathbb{P}(Y = 1|X = x) \text{ using } \sigma(w^T x), \text{ for link function } \sigma =$$

Logistic function(or Sigmoid): $\dfrac{1}{1 + exp(-z)}$

$$\mathbb{P}[Y = 1|X = x, w] = \sigma(w^T x) = \frac{1}{1 + \exp(-w^T x)}$$

$$\mathbb{P}[Y = 0|X = x, w] = 1 - \sigma(w^T x) = \frac{\exp(-w^T x)}{1 + \exp(-w^T x)} = \frac{1}{1 + \exp(w^T x)}$$

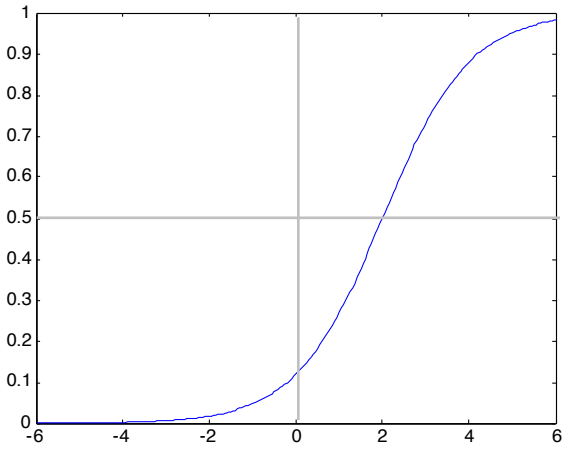


Features can be discrete or continuous!

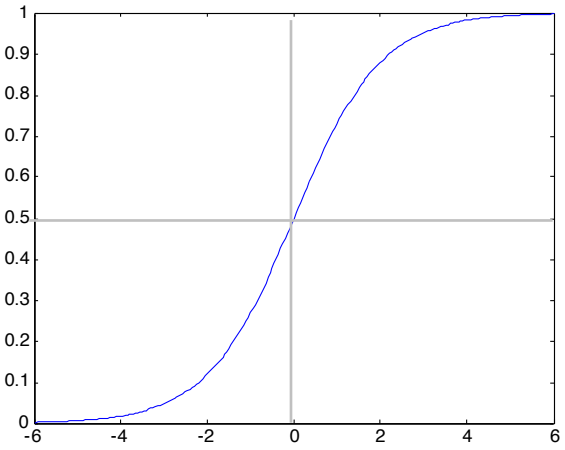
Understanding the sigmoid

$$\sigma(w_0 + \sum_k w_k x_k) = \frac{1}{1 + e^{w_0 + \sum_k w_k x_k}}$$

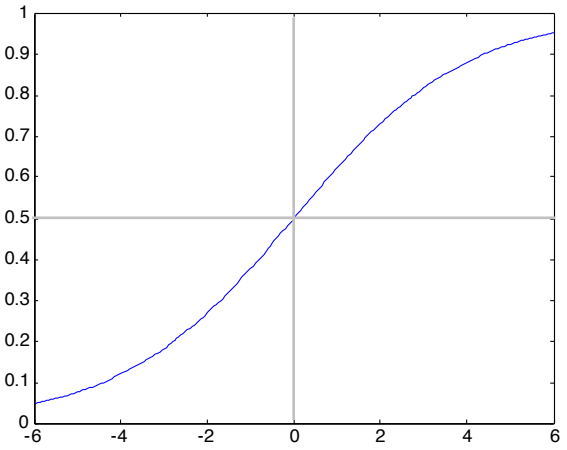
w_0=-2, w_1=-1



w_0=0, w_1=-1



w_0=0, w_1=-0.5



Sigmoid for binary classes

$$\mathbb{P}(Y=0|w,X) = \frac{1}{1+\exp(w_0+\sum_k w_k X_k)}$$

$$\mathbb{P}(Y=1|w,X) = 1-\mathbb{P}(Y=0|w,X) = \frac{\exp(w_0+\sum_k w_k X_k)}{1+\exp(w_0+\sum_k w_k X_k)}$$

$$\frac{\mathbb{P}(Y=1|w,X)}{\mathbb{P}(Y=0|w,X)} =$$

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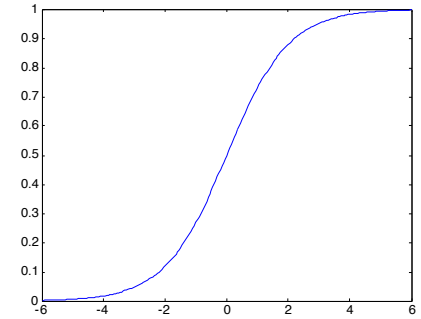
$$\frac{\mathbb{P}(Y=1|w,X)}{\mathbb{P}(Y=0|w,X)} = \exp(w_0+\sum_k w_k X_k)$$

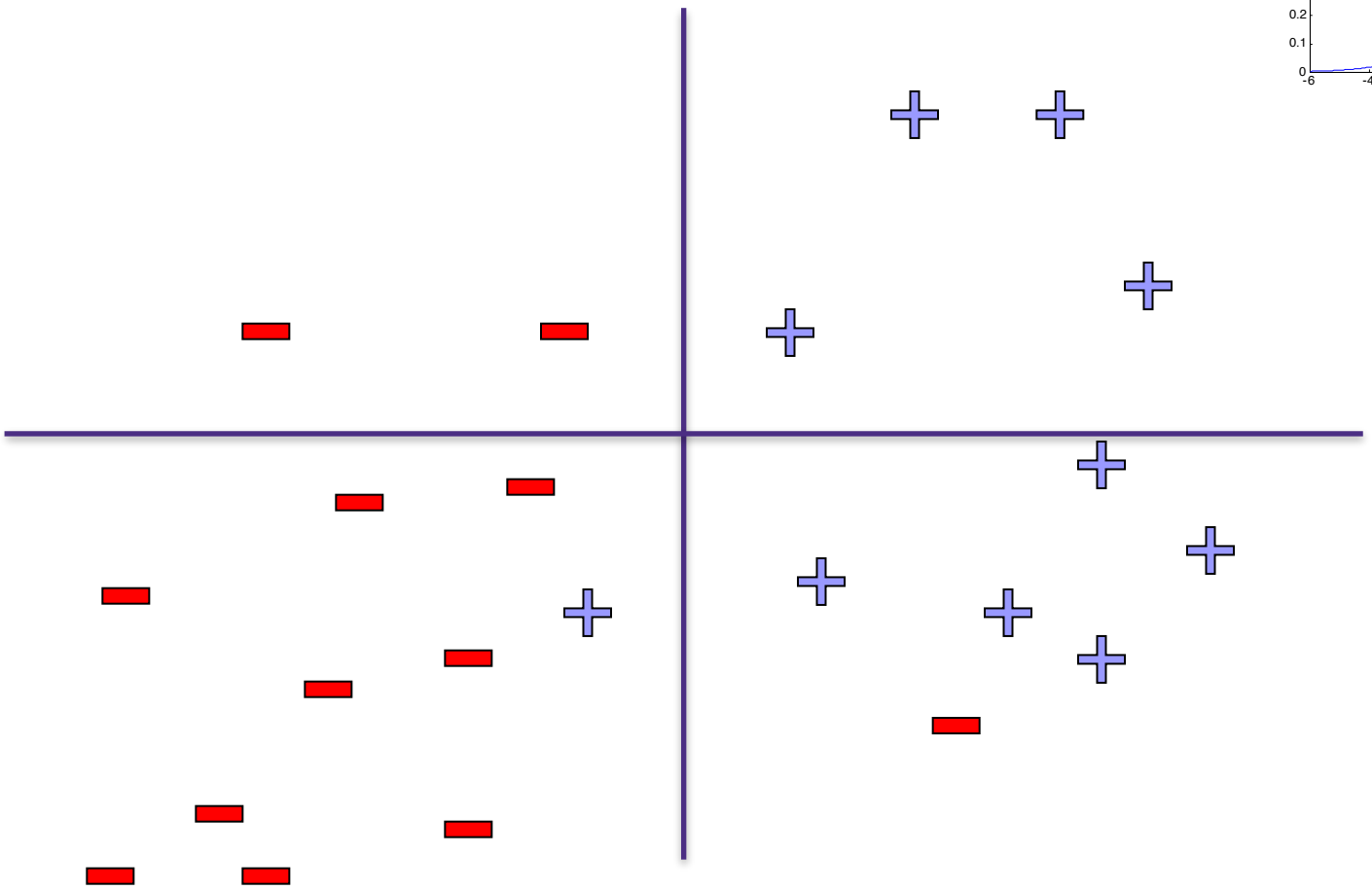
Linear Decision Rule!

$$\log\frac{\mathbb{P}(Y=1|w,X)}{\mathbb{P}(Y=0|w,X)} = w_0+\sum_k w_k X_k$$

Logistic Regression – a Linear classifier

$$\frac{1}{1 + exp(-z)}$$





$$\ln \frac{P(Y=0|X)}{P(Y=1|X)} = w_0 + \sum_i w_i X_i$$

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Use function to make prediction on new examples

Loss function: Conditional Likelihood

- **Have a bunch of iid data:** $\{(x_i, y_i)\}_{i=1}^{n} \quad x_i \in \mathbb{R}^d, \quad y_i \in \{-1, 1\}$

$$P(Y = -1|x, w) = \frac{1}{1 + \exp(w^T x)}$$

$$P(Y = 1|x, w) = \frac{\exp(w^T x)}{1 + \exp(w^T x)}$$

- **This is equivalent to:**

$$P(Y = y|x, w) = \frac{1}{1 + \exp(-y\, w^T x)}$$

- **So we can compute the maximum likelihood estimator:**

$$\widehat{w}_{MLE} = \arg\max_{w} \prod_{i=1}^{n} P(y_i|x_i, w)$$

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Logistic Loss: $\ell_i(w) = \log(1 + \exp(-y_i\, x_i^T w))$

Squared error Loss: $\ell_i(w) = (y_i - x_i^T w)^2$ (MLE for Gaussian noise)

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$$= \arg\min_w \sum_{i=1}^n \log(1 + \exp(-y_i\, x_i^T w)) = J(w)$$

What does $J(w)$ look like? Is it convex?

Loss function: Conditional Likelihood

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Good news: $J(\mathbf{w})$ is convex function of $\mathbf{w}$, no local optima problems

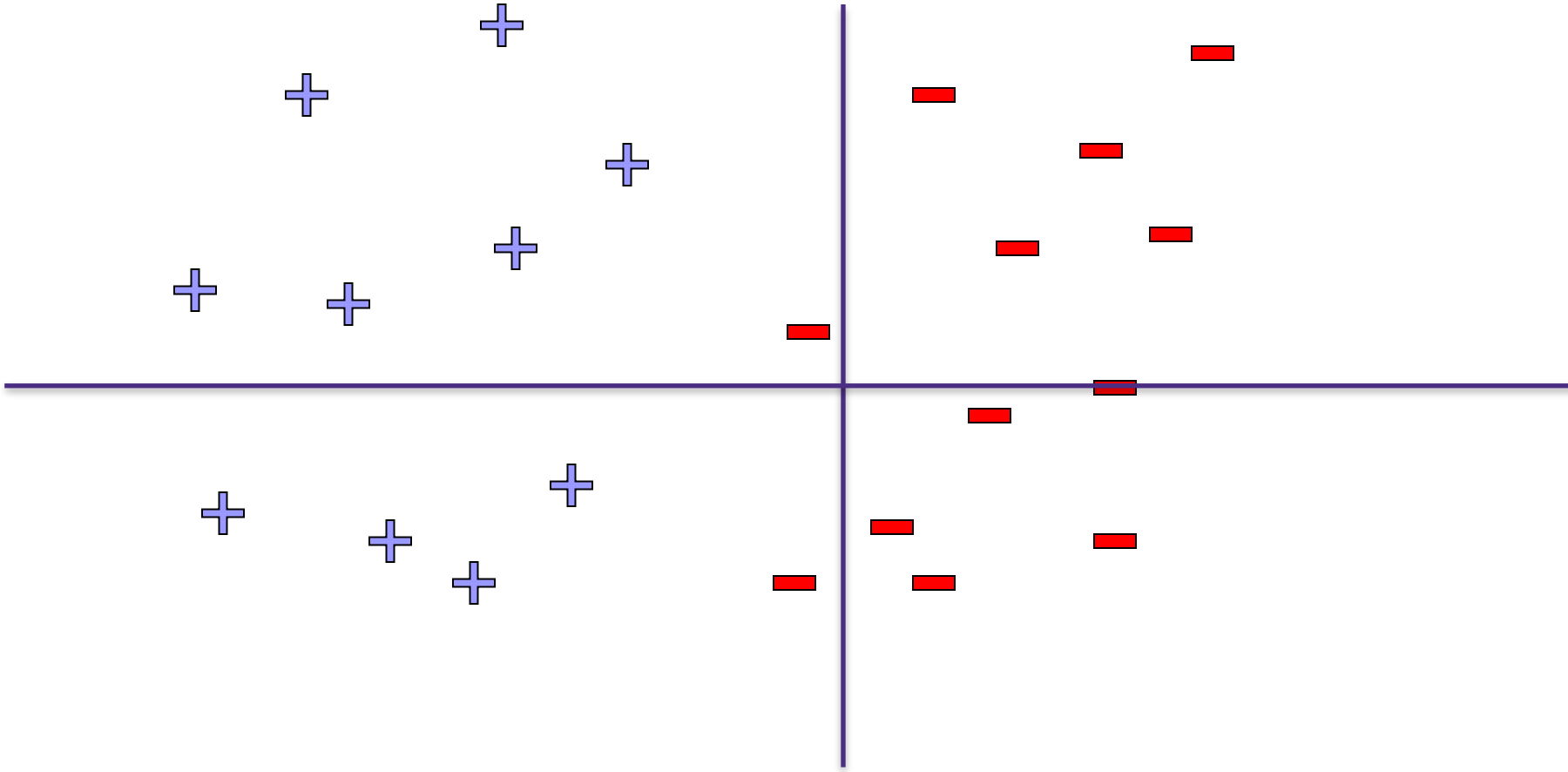
Bad news: no closed-form solution to maximize $J(\mathbf{w})$

Good news: convex functions easy to optimize

Linear Separability

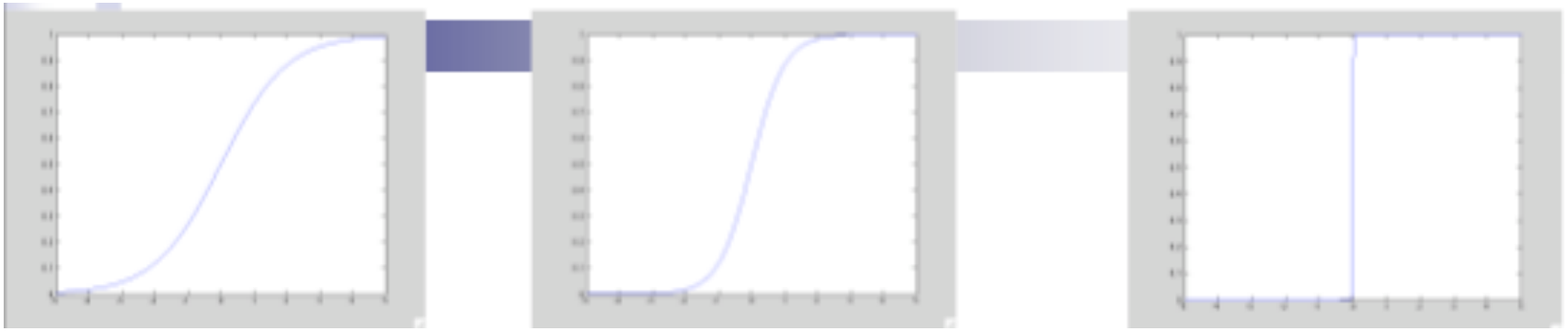
$$\arg\min_{w} \sum_{i=1}^{n} \log(1 + \exp(-y_i \, x_i^T w))$$

When is this loss small?



Large parameters → Overfitting

When data is linearly separable, weights ⇒ ∞



$$\frac{1}{1+e^{-x}} \qquad \frac{1}{1+e^{-2x}} \qquad \frac{1}{1+e^{-100x}}$$

Overfitting

Penalize high weights to prevent overfitting?

Regularized Conditional Log Likelihood

Add a penalty to avoid high weights/overfitting?:

$$\arg\min_{w,b} \sum_{i=1}^{n} \log\left(1 + \exp(-y_i\left(x_i^T w + b\right))\right) + \lambda||w||_2^2$$

Be sure to not regularize the offset b!

Multi-class classification

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- So far: binary $y \in \{-1, +1\}$

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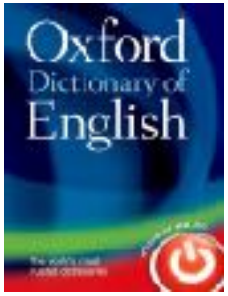

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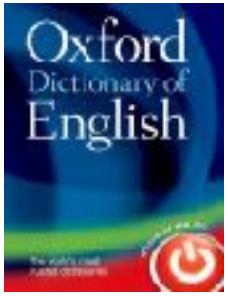

- A k-class classifier predicts y given x

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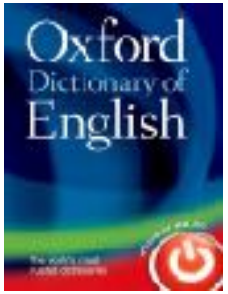

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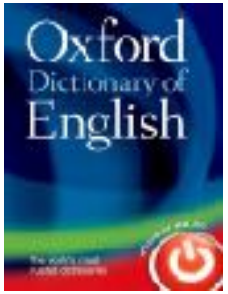

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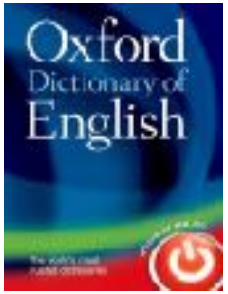

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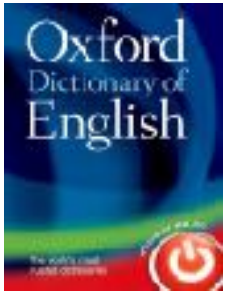

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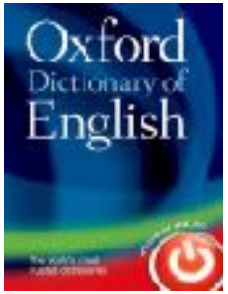

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One-HOT encoding labels + softmax

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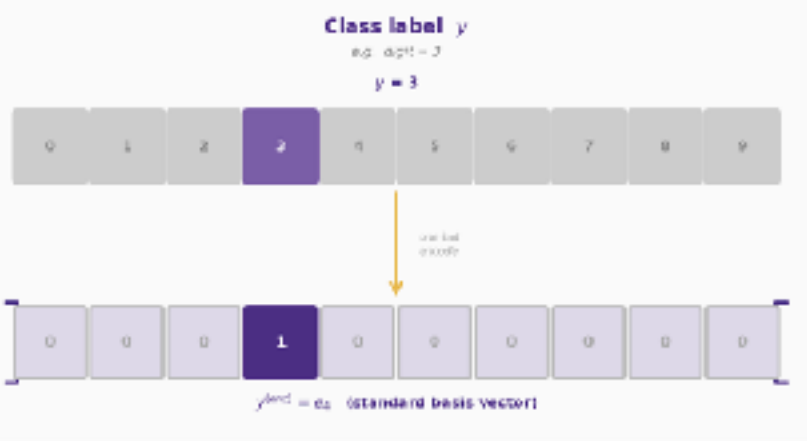

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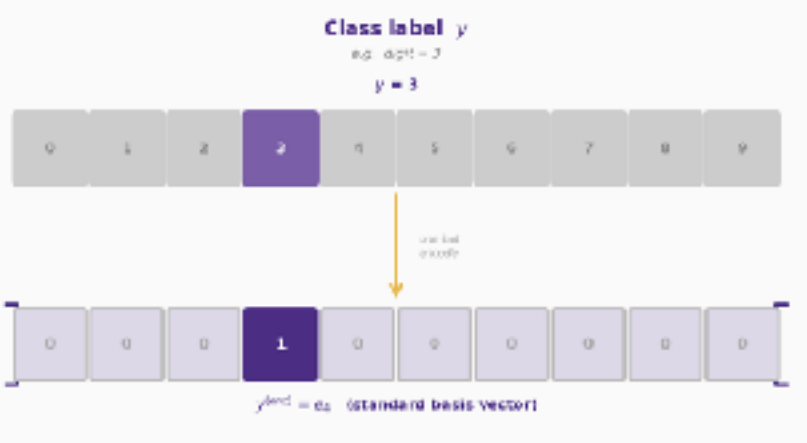

$\mathbb{P}[c_1 \,|\, x]$

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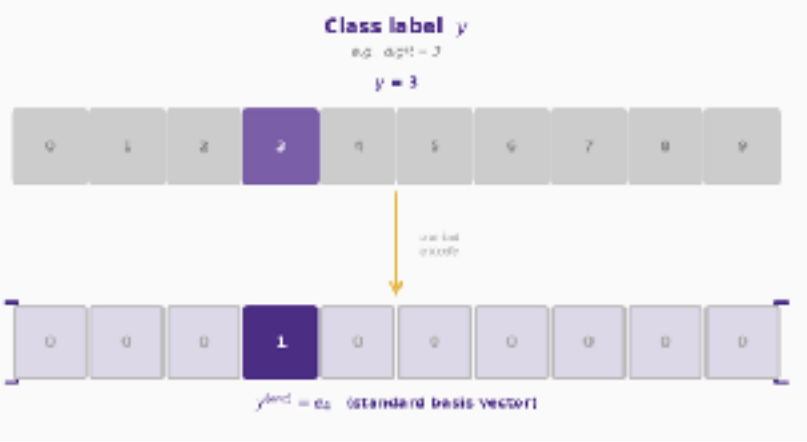

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One-HOT encoding labels + softmax

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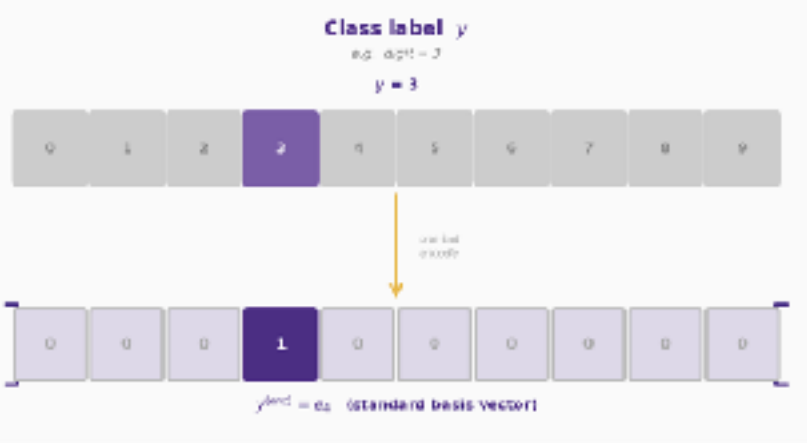

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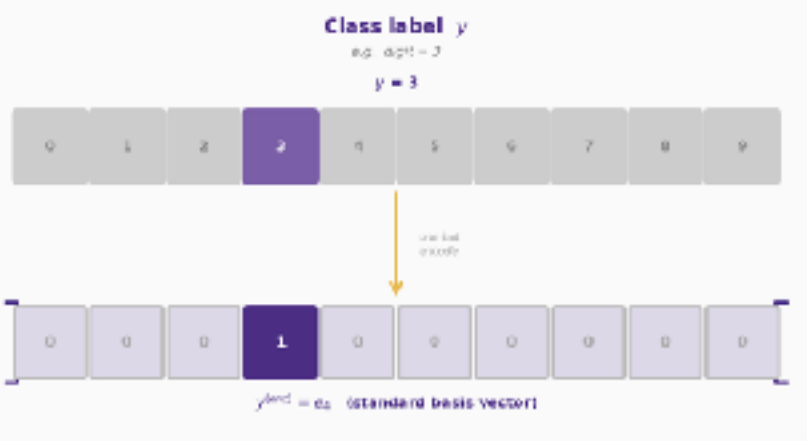

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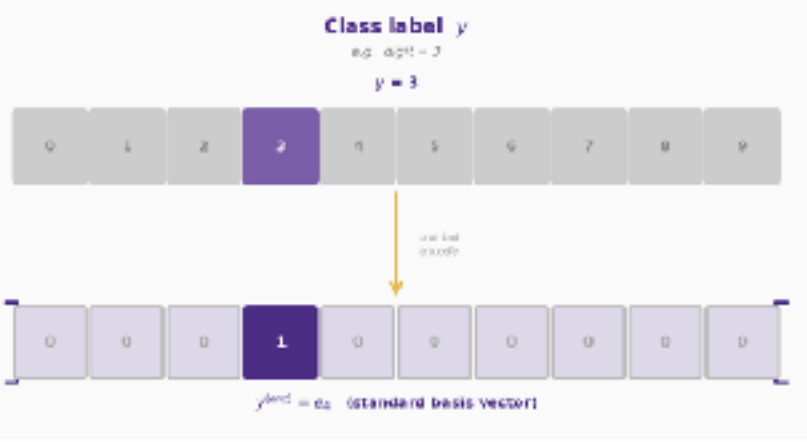

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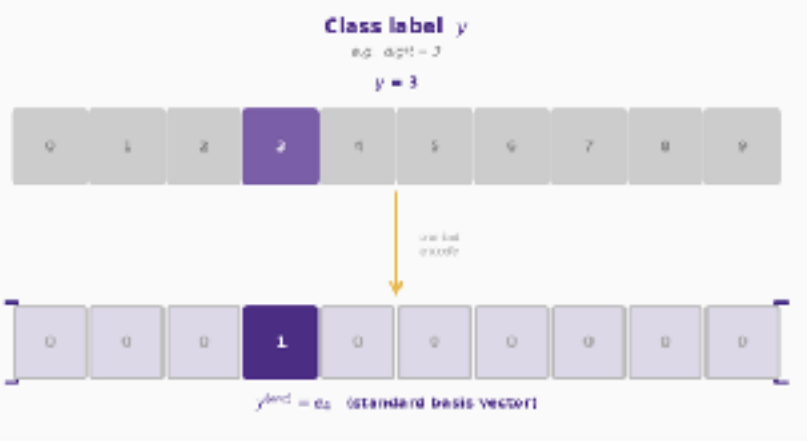

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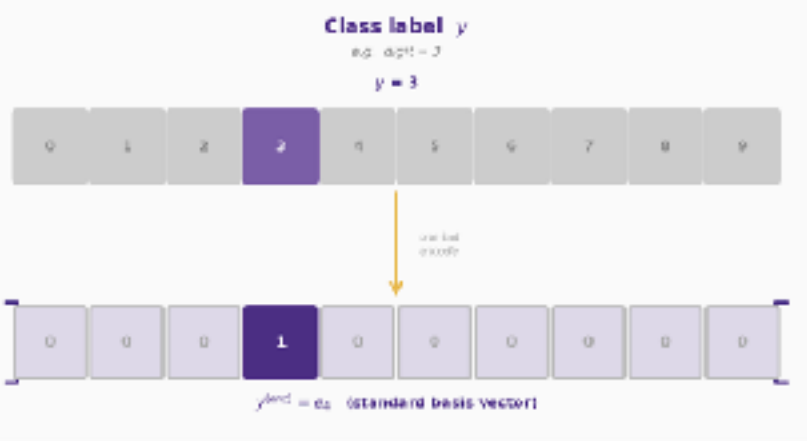

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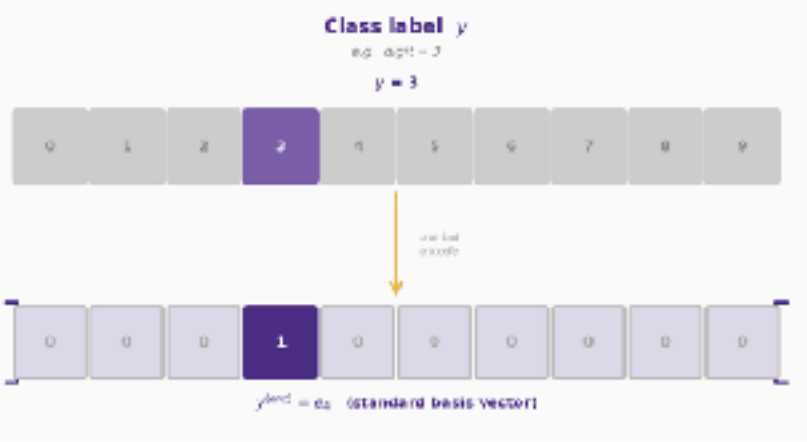

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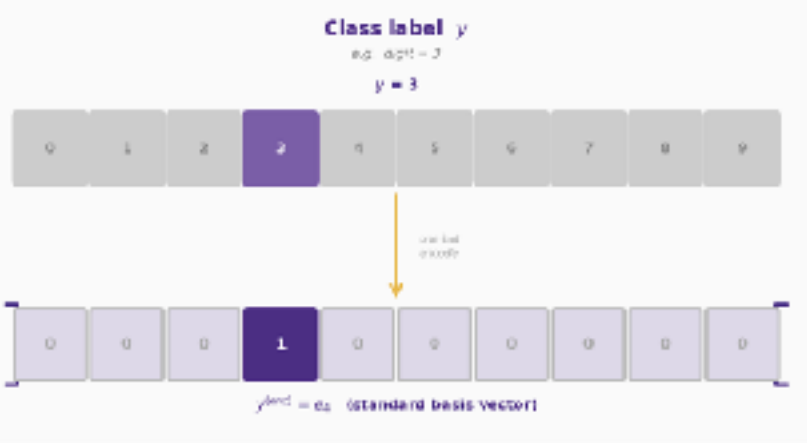

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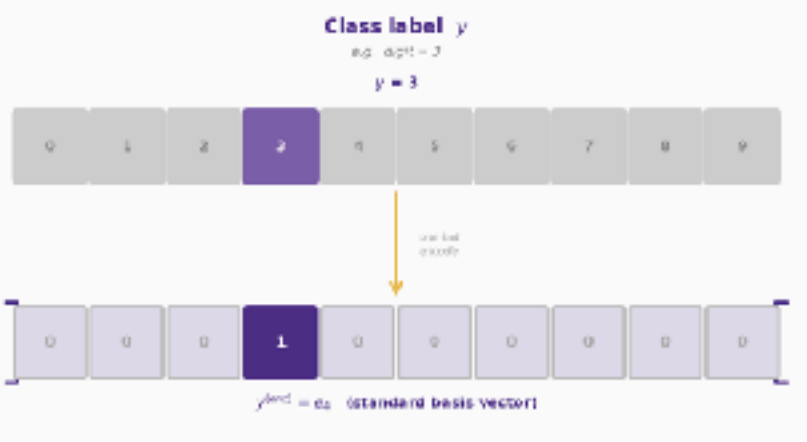

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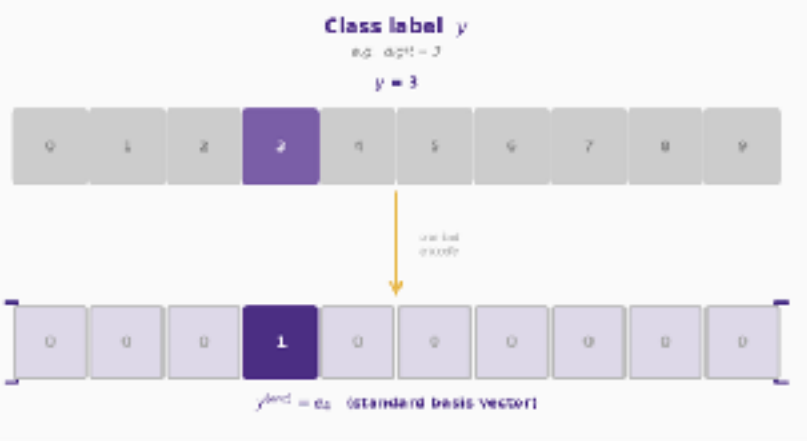

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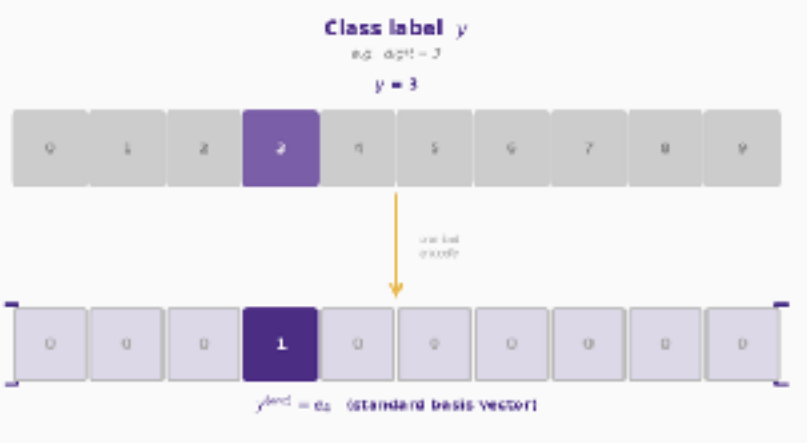

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Softmax classification

Softmax classification

2 classes

Conditional probabilities

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Binary cross entropy

Softmax classification

without loss of generality, set $k = 2,\ w_1 = 0$

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Is this a good idea?

You lose some precision, but it actually can be. Sometimes easier to optimize. Can win a kaggle competition this way. Look into "distributional RL"

The ML pipeline

1. Task
2. Data
3. Model family
4. Training loss
4. Optimize
5. Pick hyperparameters
6. Evaluate

Non-parametric methods Nearest Neighbours

Natasha Jaques

UNIVERSITY of WASHINGTON

Parametric vs non-parametric

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  # Today's class

This lecture: k nearest neighbors

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Simple

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- To classify a new point x:
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This lecture: k nearest neighbors

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What do we mean by nearest neighbors?

This lecture: k nearest neighbors

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What do we mean by nearest neighbors?
Smallest distance in feature space (with d features)

This lecture: k nearest neighbors

Simple

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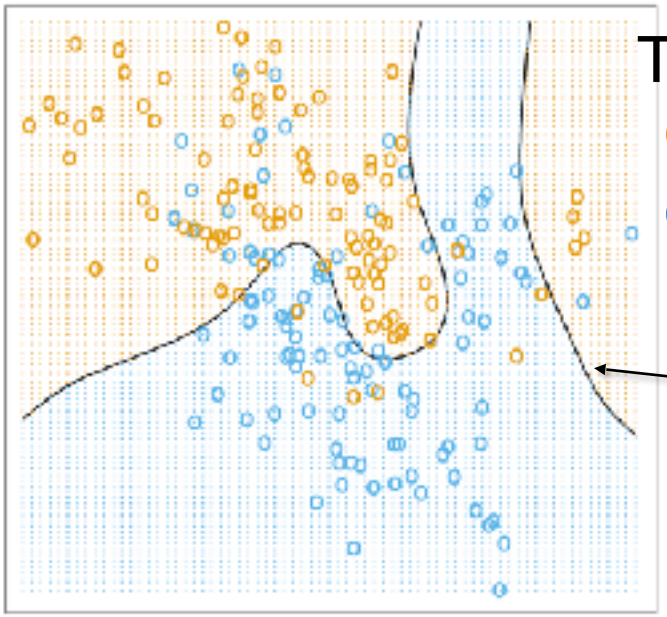
What do we mean by nearest neighbors?
Smallest distance in feature space (with d features)

- Design choices / hyperparameters:
  - Number of nearest neighbors k
  - Distance metric
  - Aggregation method

Example: Bayes classifier



Training data:

- True label: +1
- True label: -1

Optimal Bayes classifier:

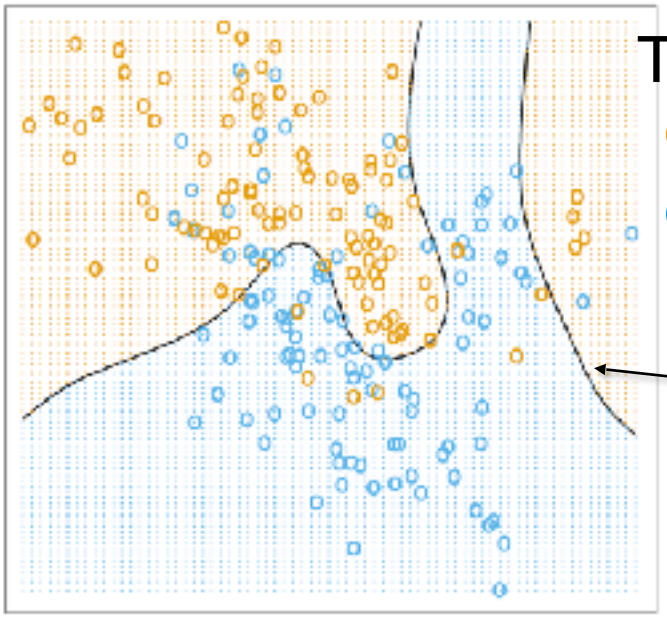
$$\mathbb{P}(Y = 1 | X = x) = \frac{1}{2}$$

Predicted label: +1

Predicted label: -1

Figures from Hastie et al.

Example: Bayes classifier



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Optimal Bayes classifier:

$$\mathbb{P}(Y = 1 | X = x) = \frac{1}{2}$$ # Ground truth

Predicted label: +1

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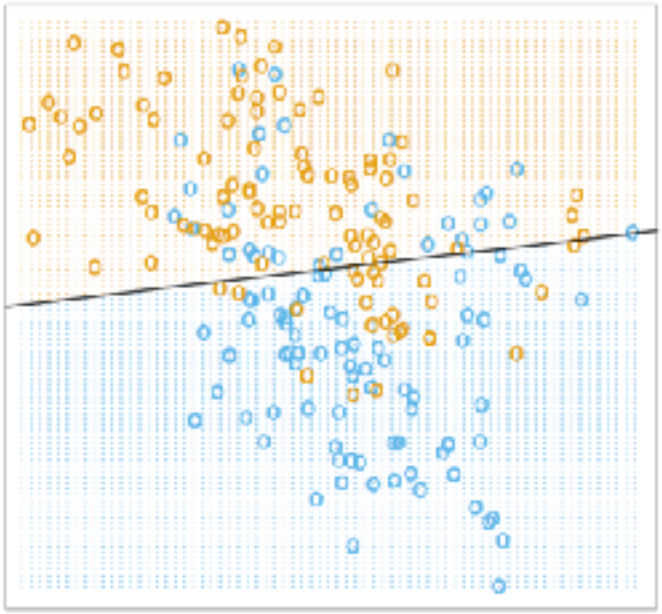
Figures from Hastie et al.

Linear decision boundary



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Learned linear decision bound

$$x^T w + b = 0$$

Predicted label: +1

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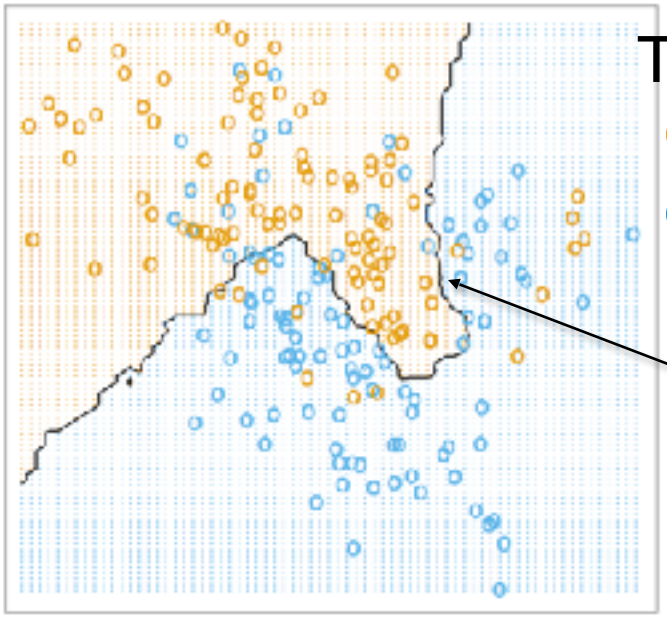
Figures from Hastie et al.

$k = 15$ nearest neighbors boundary



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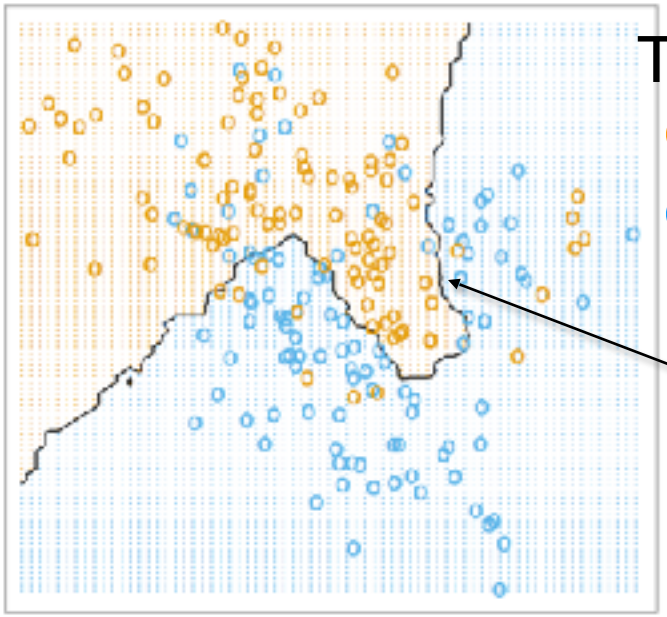
15 nearest neighbors decision boundary (majority vote)

Predicted label: +1

Predicted label: -1

Figures from Hastie et al.

$k = 15$ nearest neighbors boundary



Training data:

- True label: +1
- True label: -1

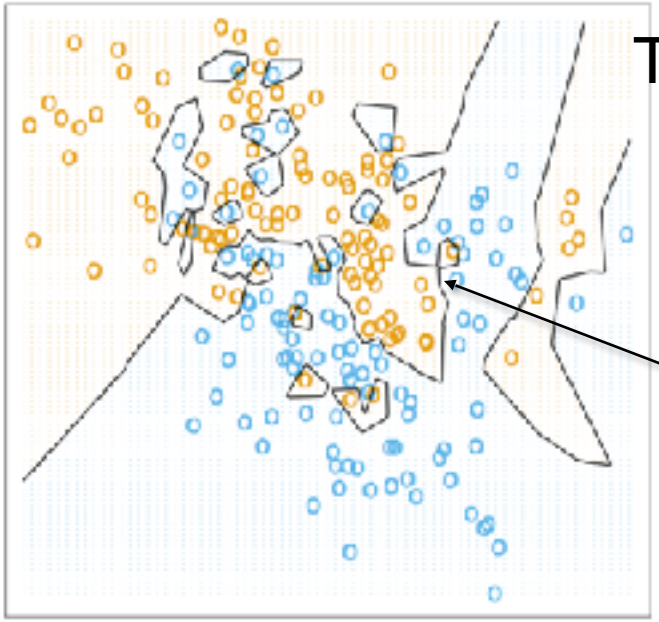
15 nearest neighbors decision boundary (majority vote)

- Predicted label: +1
- Predicted label: -1

Boundary depends on the training data points

Figures from Hastie et al.

$k = 1$ nearest neighbor boundary



Training data:

- True label: +1
- True label: -1

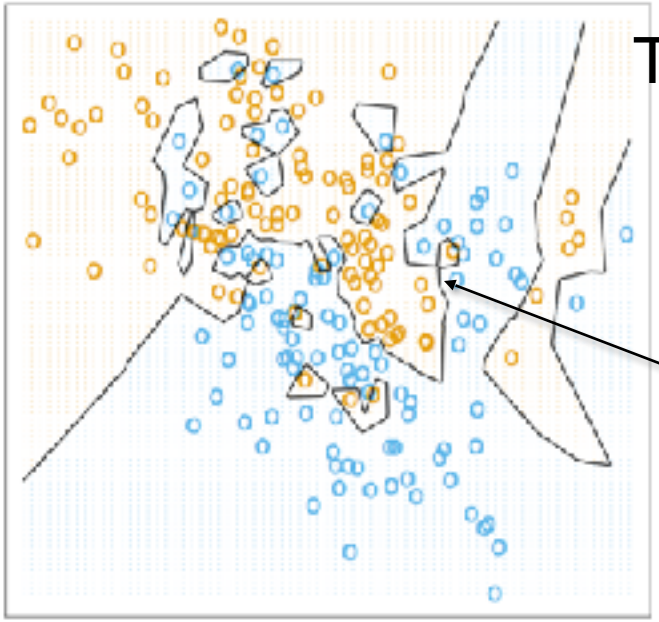
1 nearest neighbor decision boundary (majority vote)

Predicted label: -1

Predicted label: +1

Figures from Hastie et al.

$k = 1$ nearest neighbor boundary



Overfitting

Training data:

- True label: +1
- True label: -1

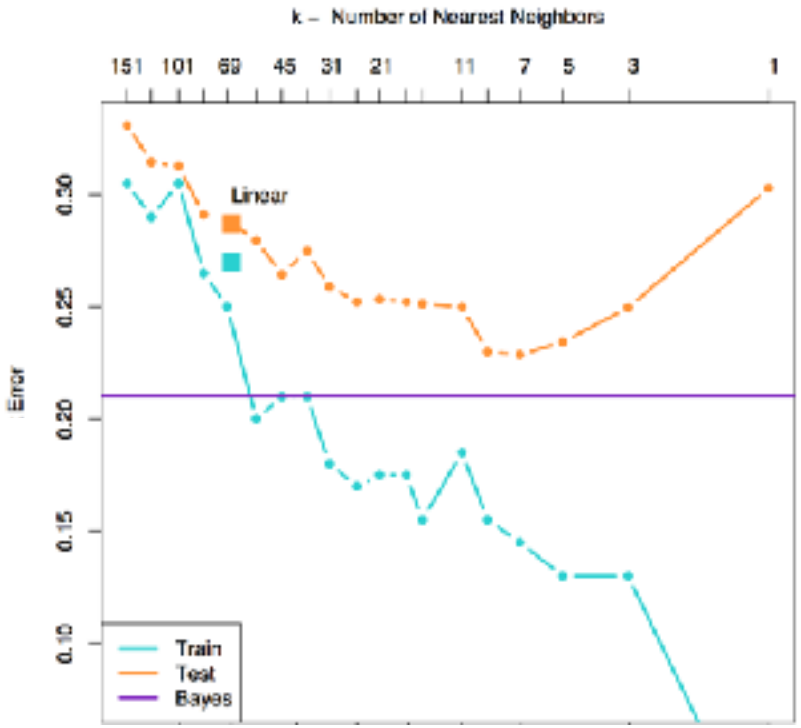
1 nearest neighbor decision boundary (majority vote)

Predicted label: -1

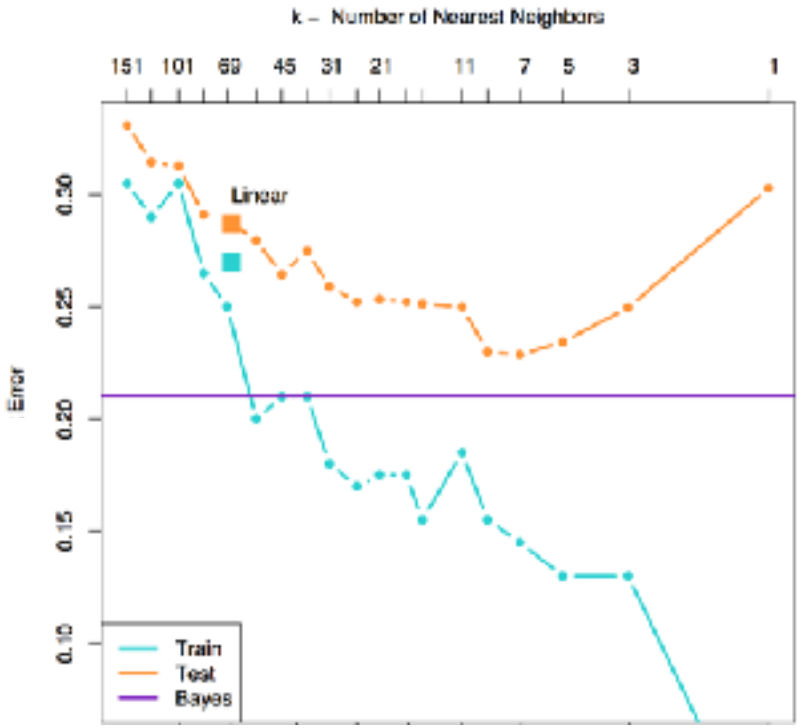
Predicted label: +1

Figures from Hastie et al.

k nearest neighbors error

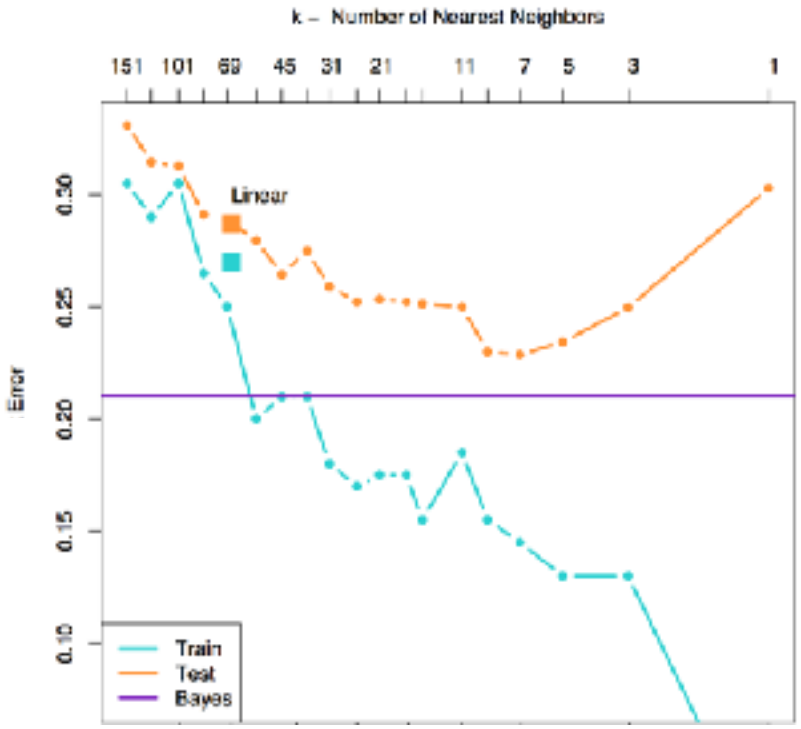


k nearest neighbors error



Overfitting

k nearest neighbors error



Underfitting

Overfitting

Parametric vs non-parametric

- A model is parametric if # parameters does not depend on # samples

- A model is non-parametric if # parameters increases with # samples

Parametric vs non-parametric

- A model is parametric if # parameters does not depend on # samples

  # After training, you can discard your data

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Parametric vs non-parametric

- A model is parametric if # parameters does not depend on # samples

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- A model is non-parametric if # parameters increases with # samples

  # Keep training data around for inference

Notable distance metrics & level sets

Notable distance metrics & level sets

ℓ_2 norm (Euclidean)

Notable distance metrics & level sets

ℓ_2 norm (Euclidean) $d(u, v) = \|u - v\|_2^2$

Notable distance metrics & level sets

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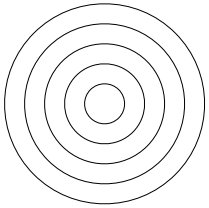

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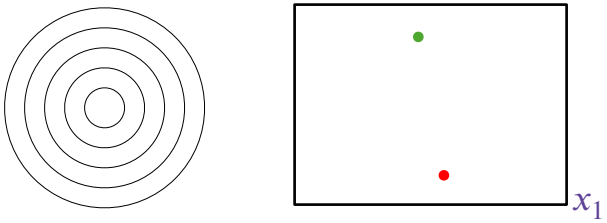

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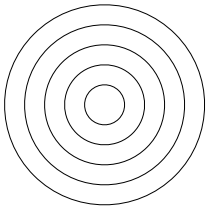

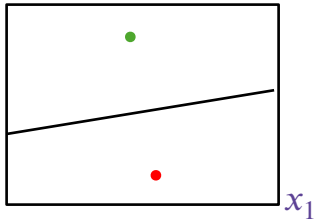

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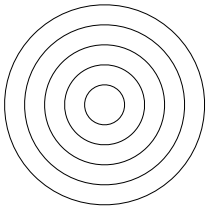

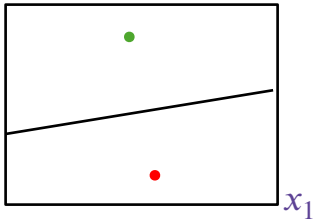

ℓ_1 norm (Manhattan, taxicab) $\|u - v\|_1 = \sum_{i=1}^{d} |u_i - v_i|$

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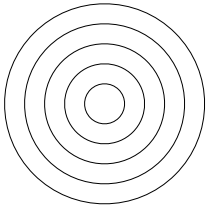

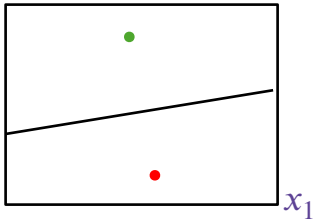

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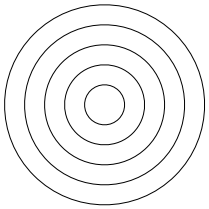

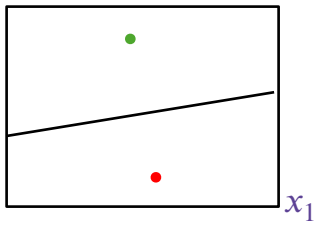

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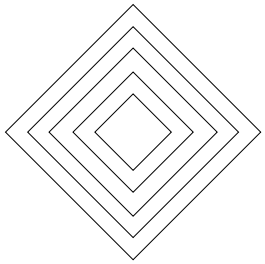

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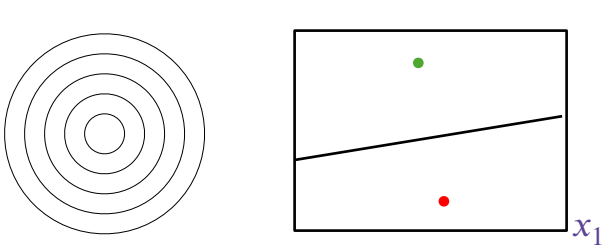

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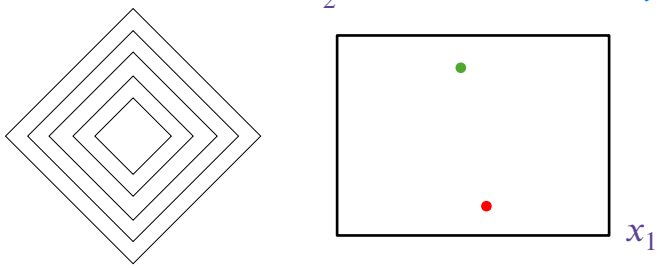

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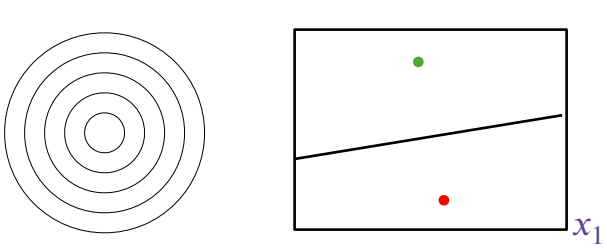

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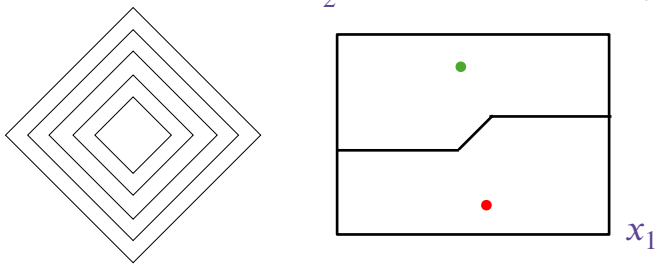

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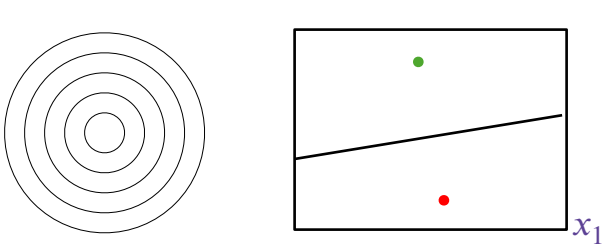

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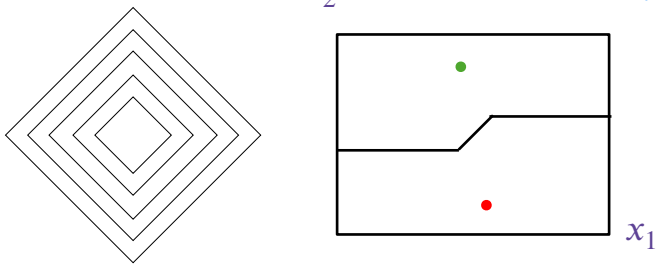

Mahalanobis norm

Notable distance metrics & level s

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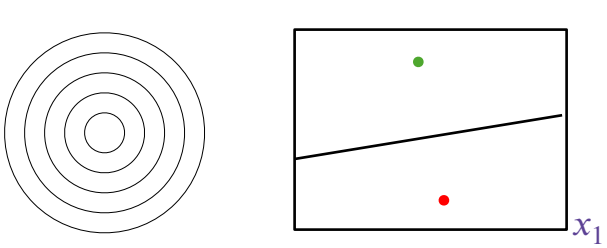

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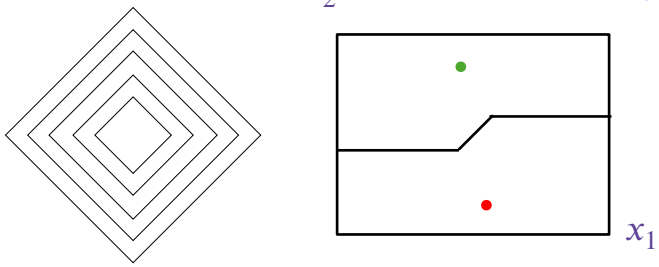

Mahalanobis norm $(u - v)^T M(u - v)$

Notable distance metrics & level s

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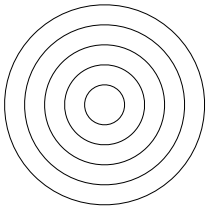

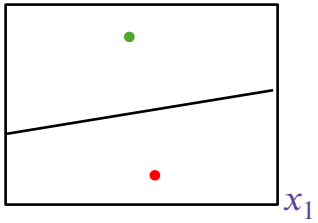

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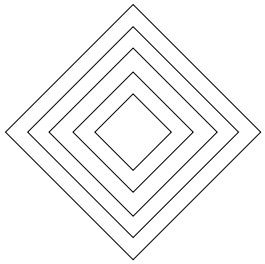

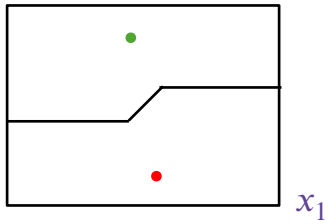

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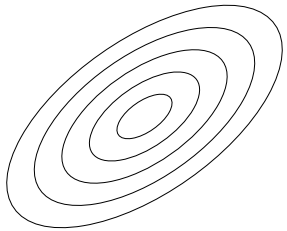

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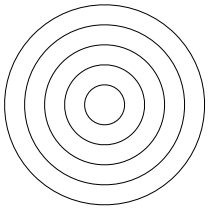

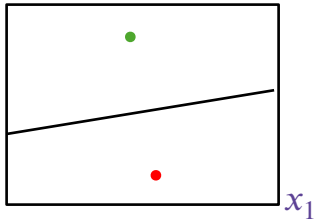

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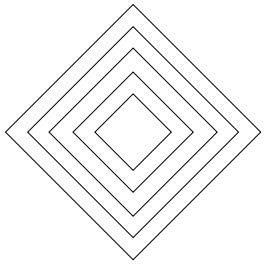

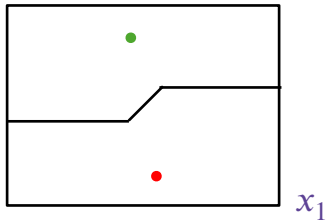

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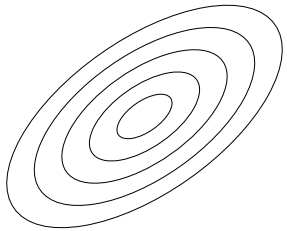

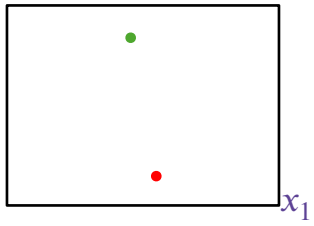

Notable distance metrics & level s

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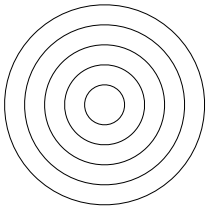

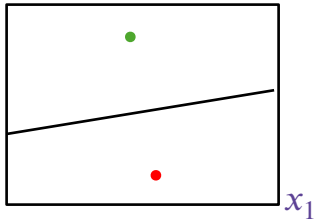

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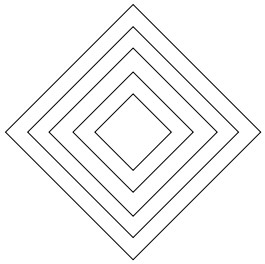

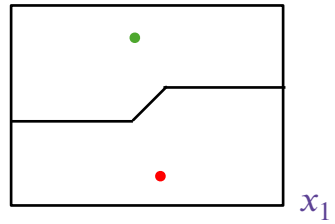

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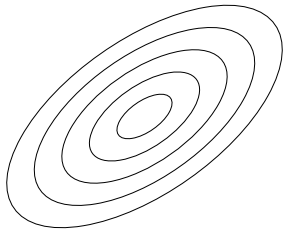

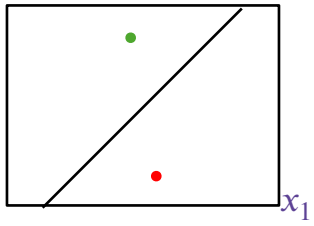

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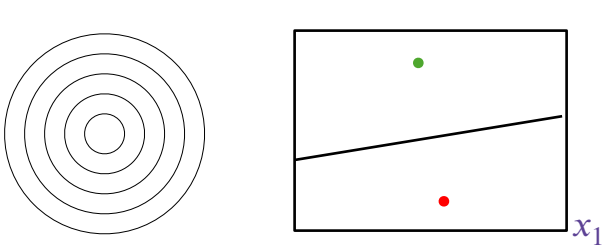

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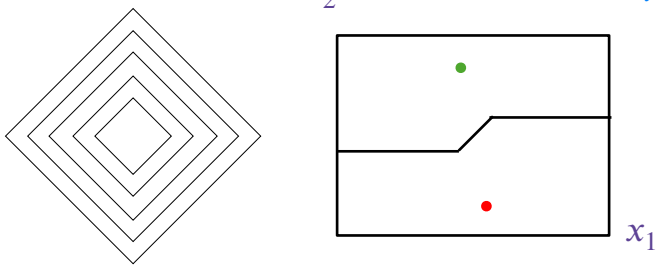

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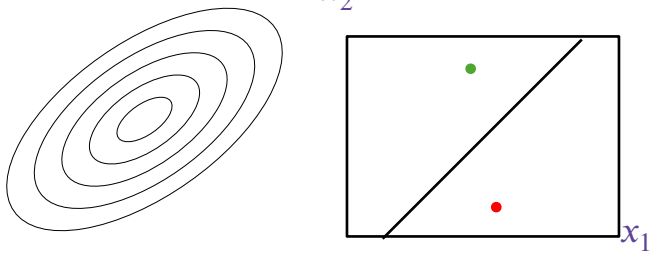

Weight different dimensions differently

Notable distance metrics & level s

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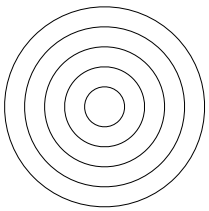

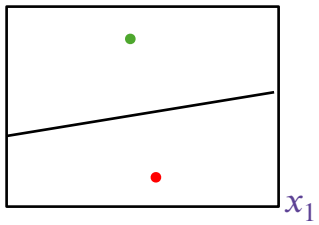

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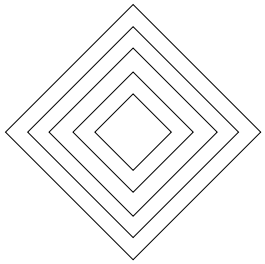

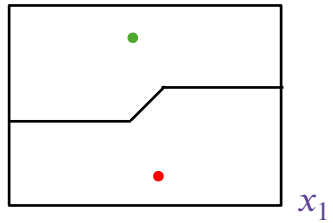

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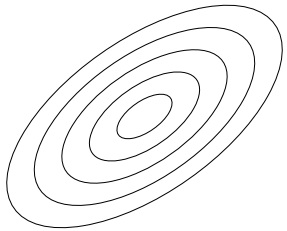
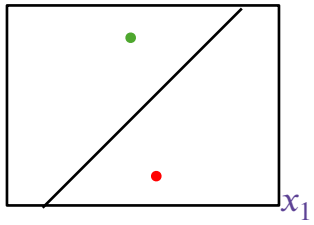


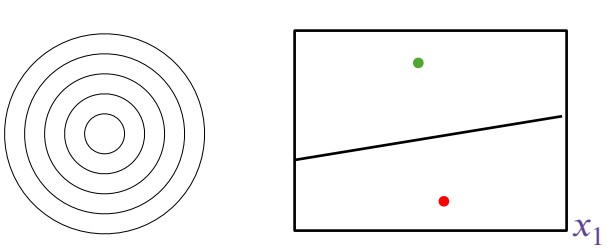


ℓ_∞ norm (max)

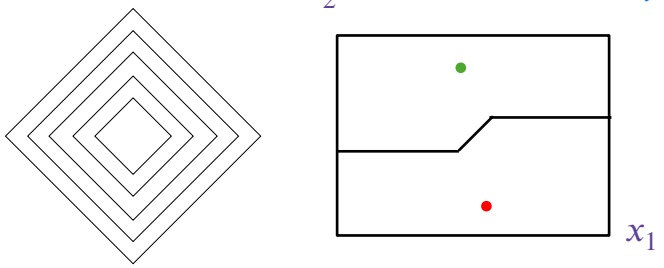
Weight different dimensions differently

Notable distance metrics & level s

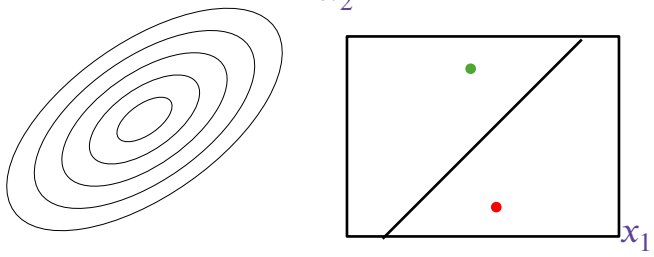
ℓ_2 norm (Euclidean) $d(u, v) = \|u - v\|_2^2$



ℓ_1 norm (Manhattan, taxicab) $\|u - v\|_1 = \sum_{i=1}^{d} |u_i - v_i|$



Mahalanobis norm $(u - v)^T M(u - v)$



ℓ_∞ norm (max) $\|u - v\|_\infty = \max_i |u_i - v_i|$

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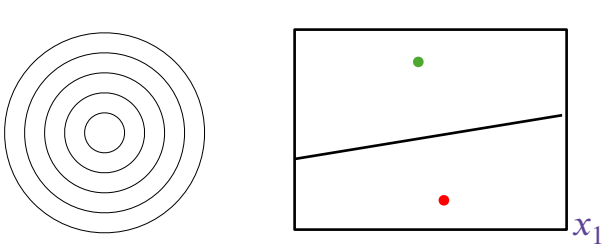

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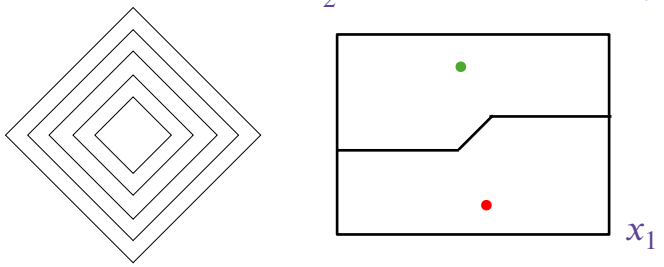

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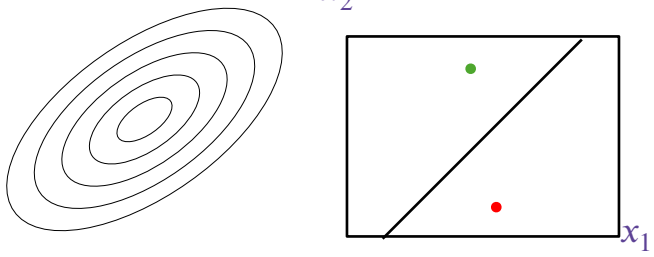

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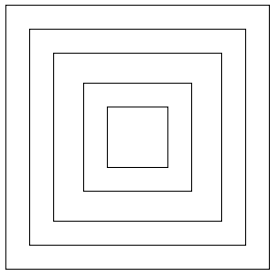

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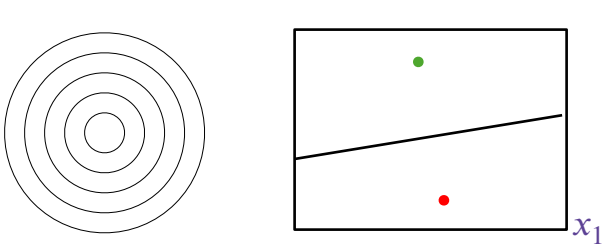

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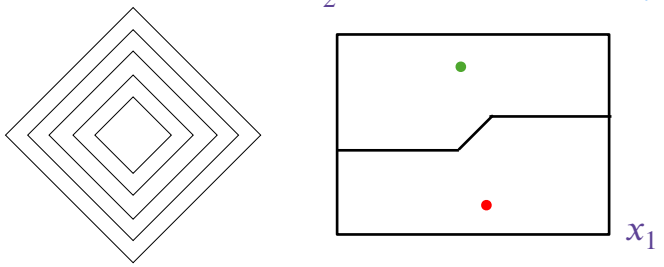

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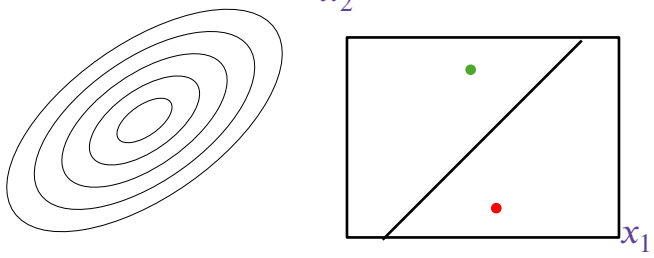

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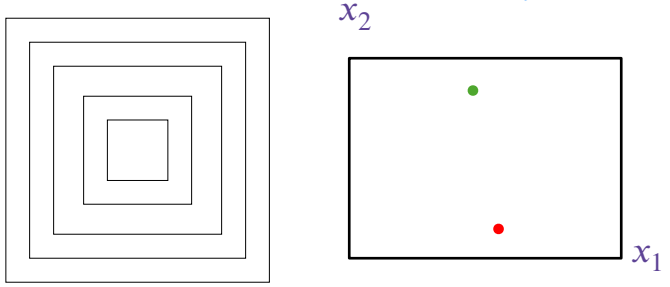

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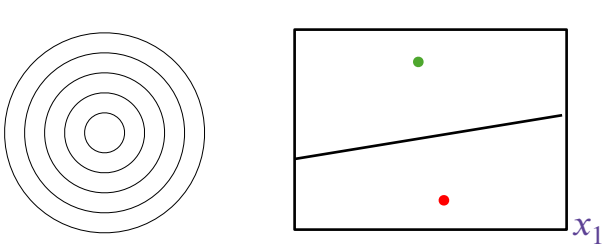

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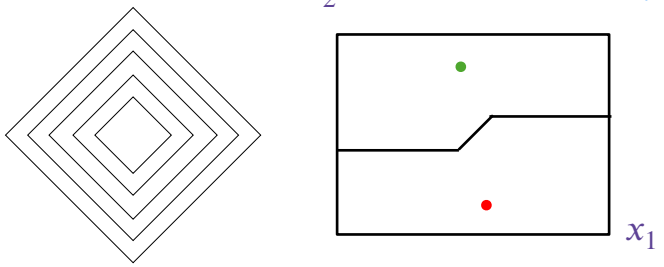

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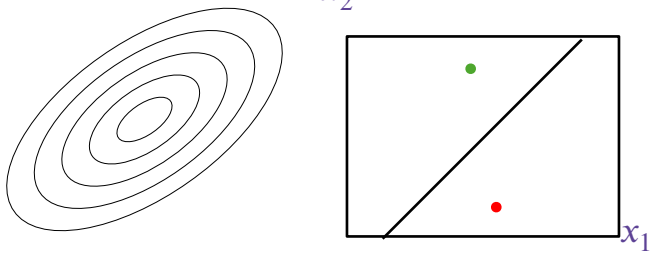

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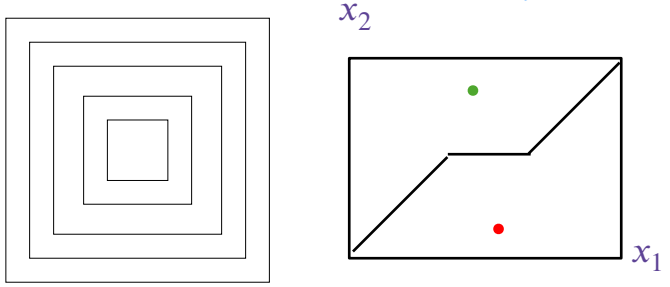

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Notable distance metrics & level s

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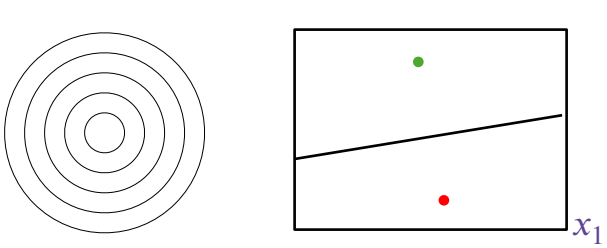

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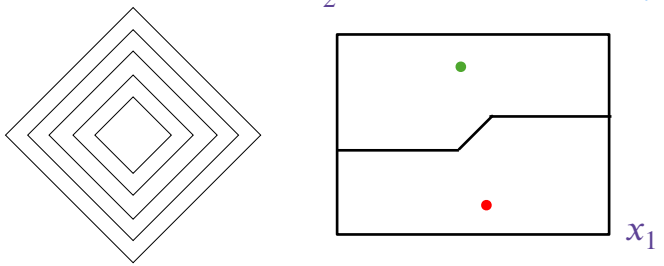

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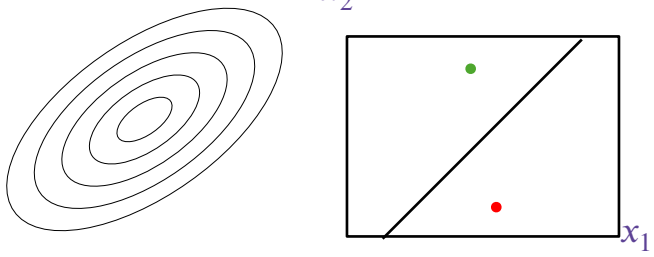

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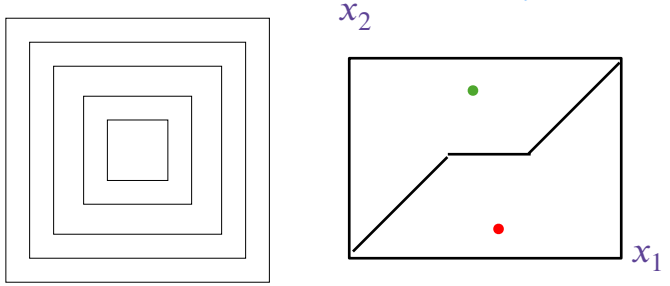
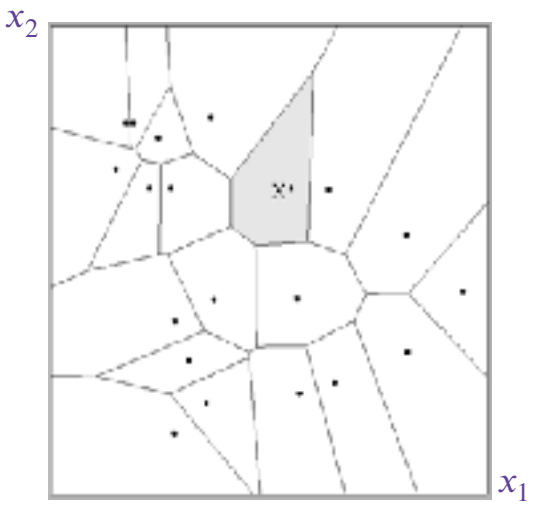


Weight different dimensions differently

Max distance between vectors

Example: distance metrics with $k = 1$ NN

$$d(x, x') = (x_1 - x_1')^2 + (x_2 - x_2')^2$$



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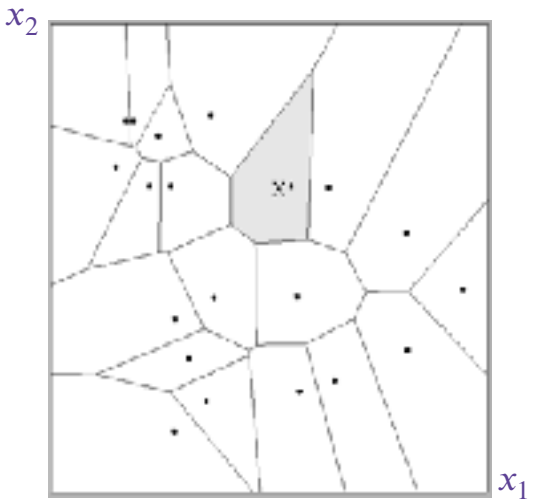
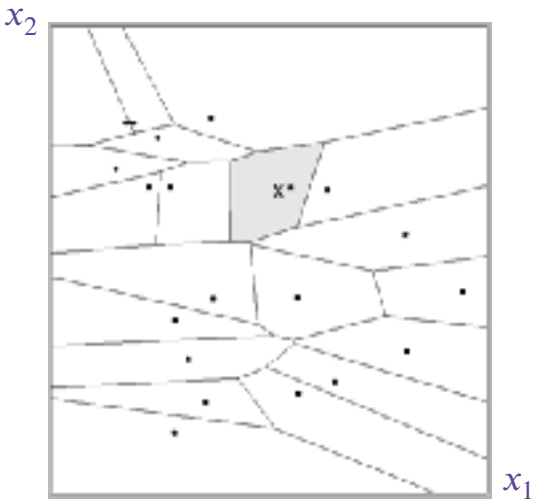


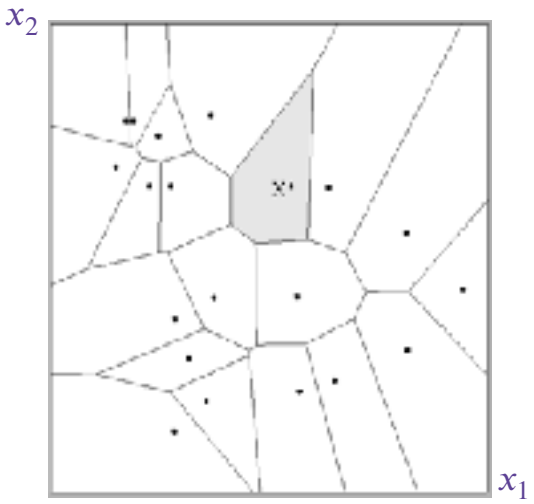
$$d(x, x') = (x_1 - x_1')^2 + 9(x_2 - x_2')^2$$



Example: distance metrics with $k = 1$ NN

L2

$$d(x, x') = (x_1 - x_1')^2 + (x_2 - x_2')^2$$



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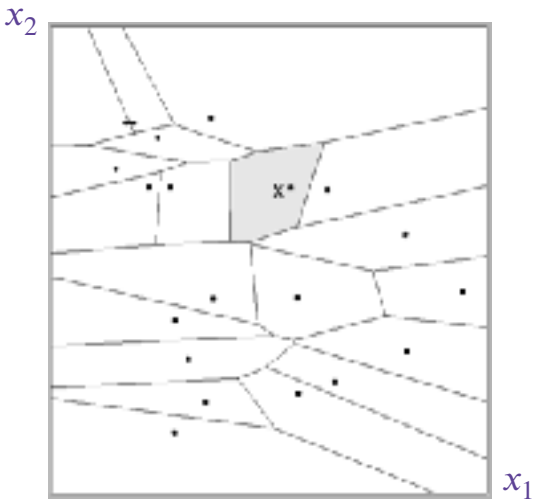

Example: distance metrics with $k = 1$ NN

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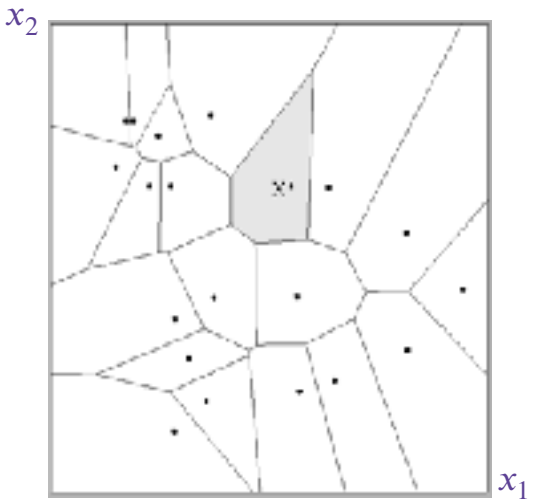

Mahalanobis

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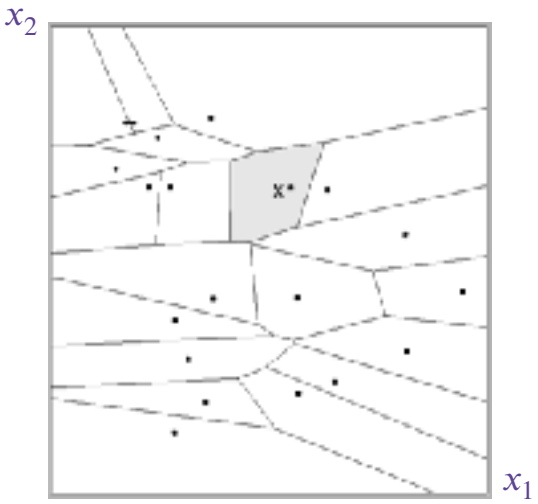

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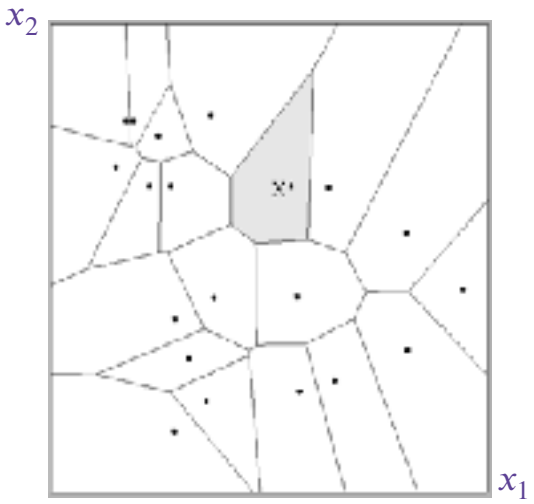

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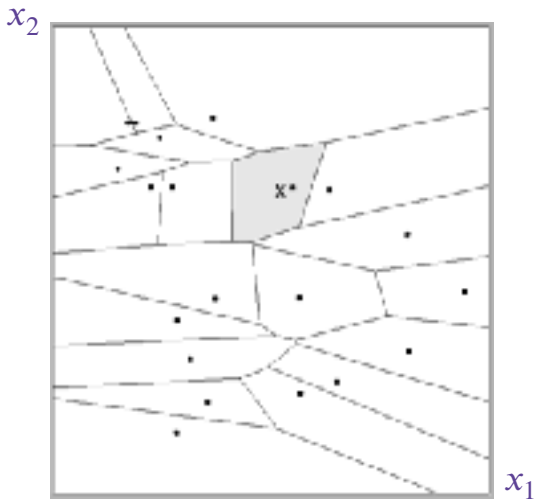
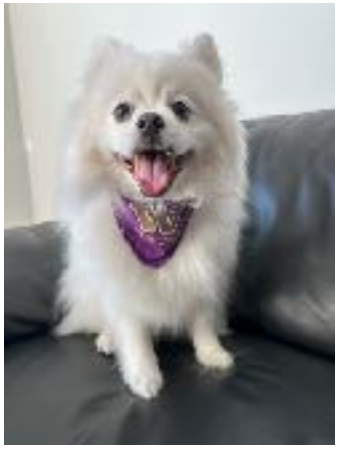


Know the geometry of your feature space

Learned distance metrics

Training data



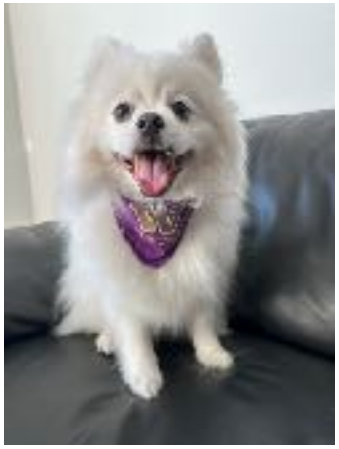
Dog

Cat

Test data

Learned distance metrics

Training data



Dog

Cat

Test data

Use a neural net to learn the distance function

kNN demo

- http://vision.stanford.edu/teaching/cs231n-demos/knn/

1-NN classification: Theoretical guarantees

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Assume: we have enough data and **our true function is smooth**

1-NN classification: Theoretical guarantees

$$D = \{(x^{(i)}, y^{(i)})\}_{i=1}^{n} \sim P$$

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1-NN classification: Theoretical guarantees

$$D = \{(x^{(i)}, y^{(i)})\}_{i=1}^{n} \sim P \qquad x^{(i)} \in \mathbb{R}^d$$

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1-NN classification: Theoretical guarantees

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Given test point x, let x_{NN} be the nearest neighbour in D

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Case 1: $y_{\text{NN}} = 1, y = 0$ w.p. $P(y = 1 \,|\, x_{\text{NN}}) P(y = 0 \,|\, x)$

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$P(y \,|\, x_{\text{NN}}) \to P(y \,|\, x)$

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By assumptions, distance between x and $x_{NN} \to 0$ as $n \to \infty$

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As $n \to \infty$,

$P(y \mid x_{NN}) \to P(y \mid x)$ # Why?

Error: $2P(y = 1 \mid x)P(y = 0 \mid x)$

By assumptions, distance between x and $x_{NN} \to 0$ as $n \to \infty$

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$P(y \mid x_{NN}) \to P(y \mid x)$ # Why?

Error: $2P(y = 1 \mid x)P(y = 0 \mid x)$

By assumptions, distance between x and $x_{NN} \to 0$ as $n \to \infty$

Define Bayes error:

$p^* = \min\{P(y = 1 \mid x), P(y = 0 \mid x)\}$

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As $n \to \infty$,

$P(y \,|\, x_{NN}) \to P(y \,|\, x)$ # Why?

By assumptions, distance between x and $x_{NN} \to 0$ as $n \to \infty$

Error: $2P(y = 1 \,|\, x)P(y = 0 \,|\, x)$

$= 2p^*(1 - p^*)$

Define Bayes error:

$p^* = \min\{P(y = 1 \,|\, x), P(y = 0 \,|\, x)\}$

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As $n \to \infty$,

$P(y \,|\, x_{NN}) \to P(y \,|\, x)$ # Why?

By assumptions, distance between x and $x_{NN} \to 0$ as $n \to \infty$

Error: $2P(y = 1 \,|\, x)P(y = 0 \,|\, x)$

$= 2p^*(1 - p^*) \quad \leq 2p^*$

Define Bayes error:

$p^* = \min\{P(y = 1 \,|\, x), P(y = 0 \,|\, x)\}$

1-NN classification: Theoretical guarantees

As $n \to \infty$, Error $= 2p^*(1 - p^*) \leq 2p^*$

Theorem[Cover, Hart, 1967] If P_X is supported everywhere in $\mathbb{R}^d$ and $P(Y = 1|X = x)$ is smooth everywhere, then as $n \to \infty$ the 1-NN classification rule has error at most twice the Bayes error rate.

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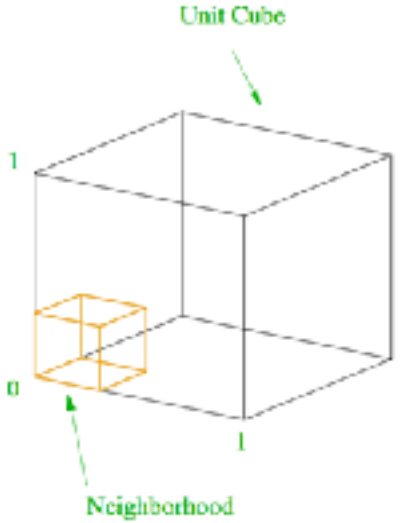
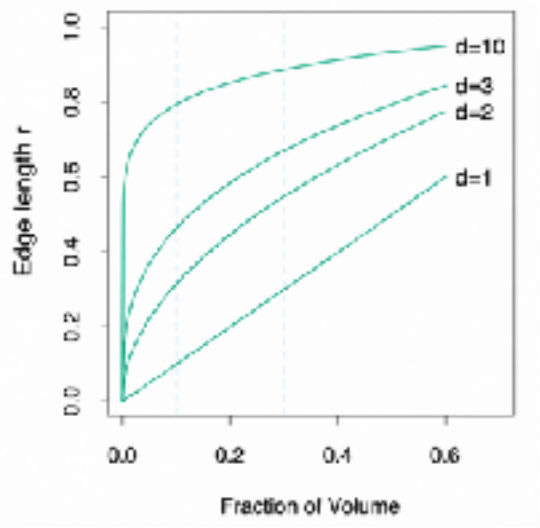
Curse of dimensionality, example 1





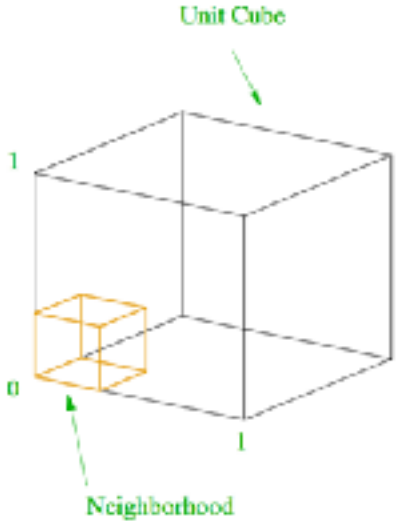
side length r

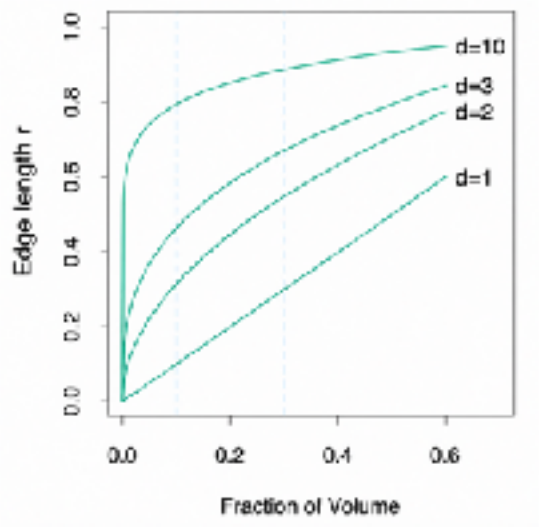
X is uniformly distributed over [0,1]^d. What is $P(X \in [0, r]^d)$?

How many samples do we need so that a nearest neighbor is within a cube of s length r?

Curse of dimensionality, example 1

If d = 1





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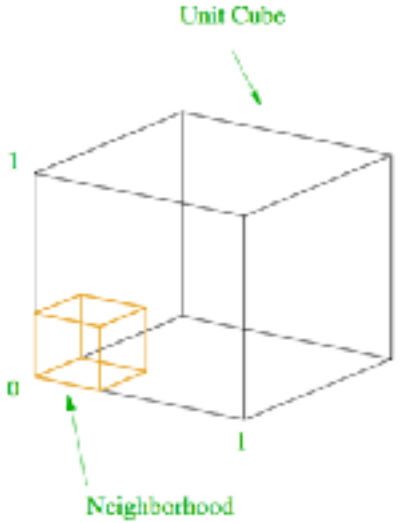

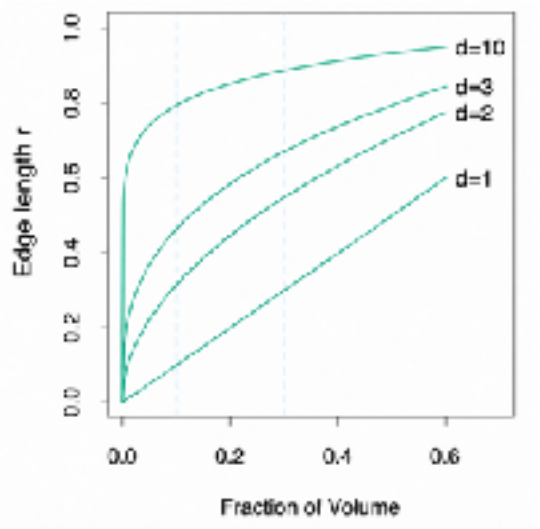

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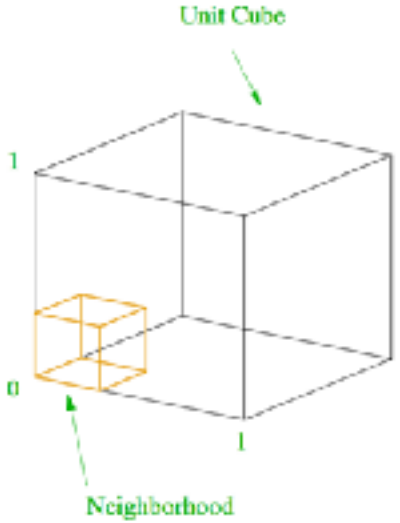

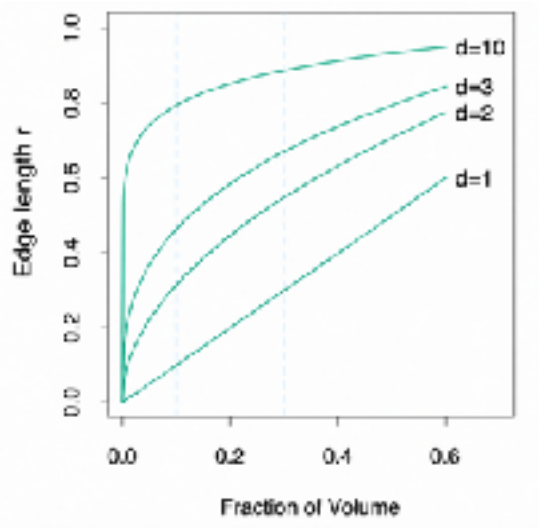

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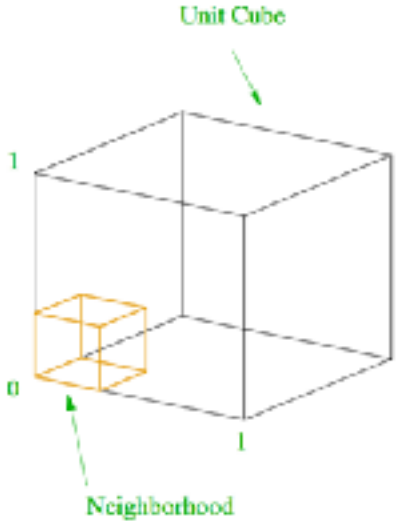

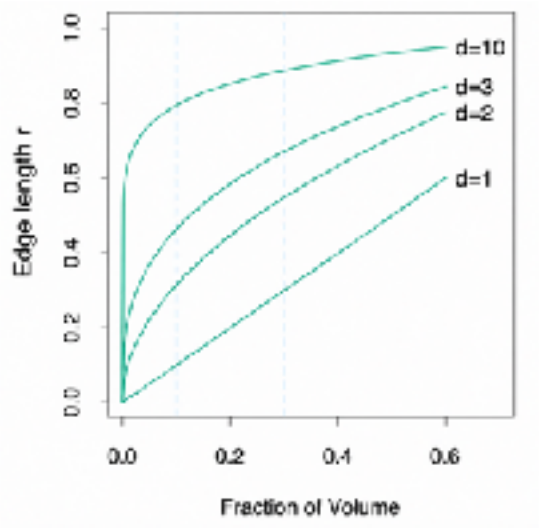

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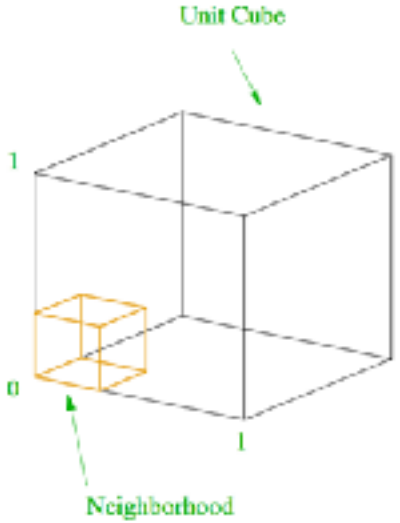

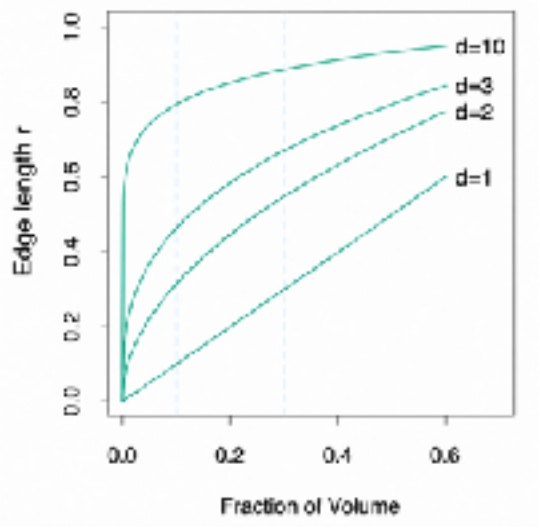

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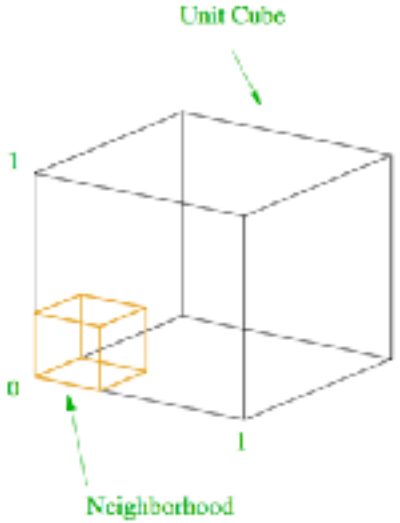

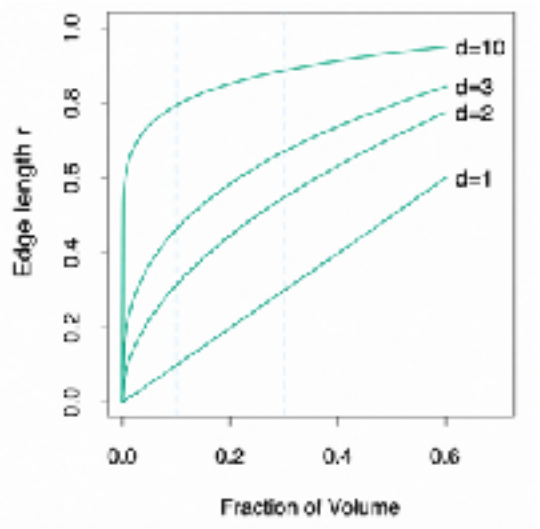

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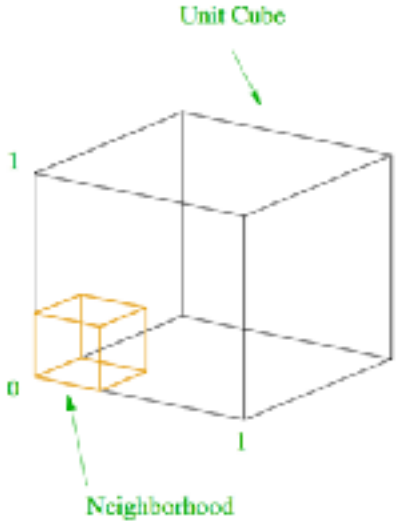

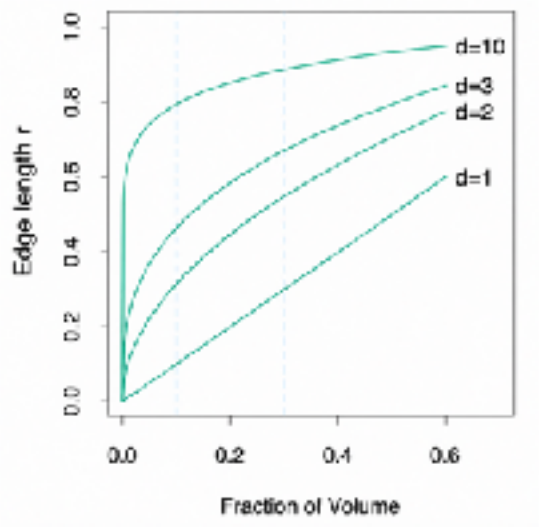

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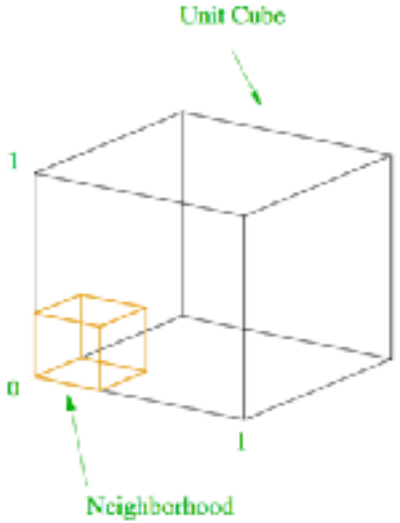
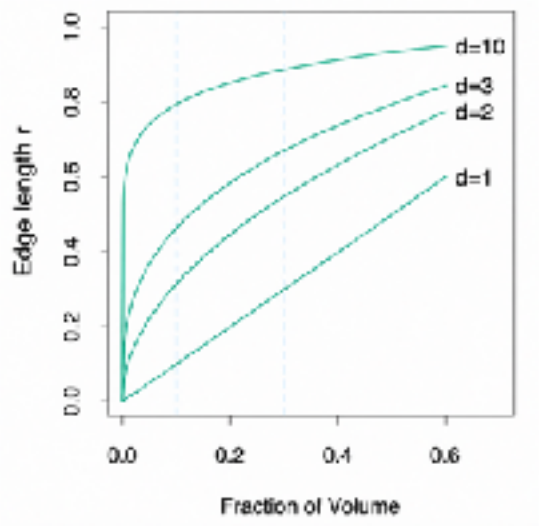
side length r

X is uniformly distributed over [0,1]^d. What is $P(X \in [0, r]^d) = \frac{1}{r^d}$ **?**

How many samples do we need so that a nearest neighbor is within a cube of length r**?**

Curse of dimensionality, example 1





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side length r

X is uniformly distributed over [0,1]^d. What is ?

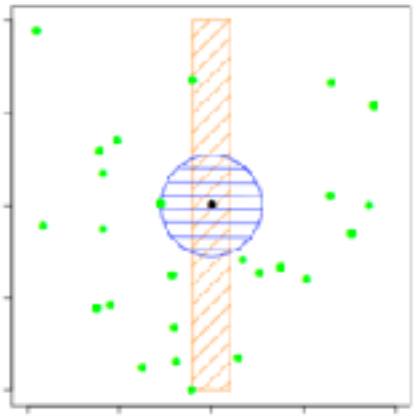
$$P(X \in [0, r]^d) = \frac{1}{r^d}$$

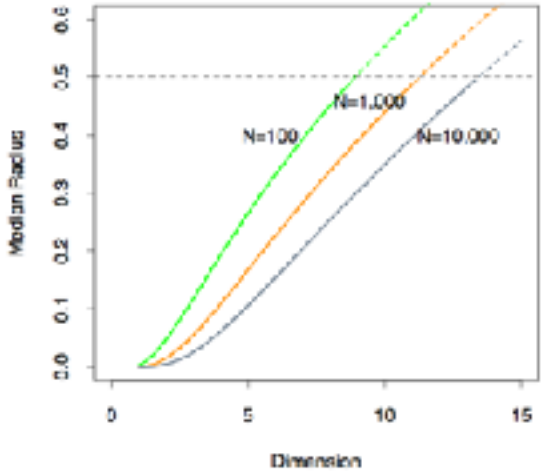
How many samples do we need so that a nearest neighbor is within a cube of length r?

Increases exponentially with dimension p!

Curse of dimensionality, example 2

$\{X_i\}_{i=1}^n$ are uniformly distributed over $[-.5, .5]^p$.





What is the median distance from a point at origin to its 1NN?

How many samples do we need so that a median Euclidean distance is within r?

Curse of dimensionality, example 2

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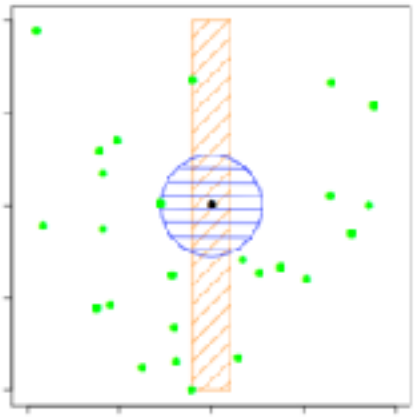

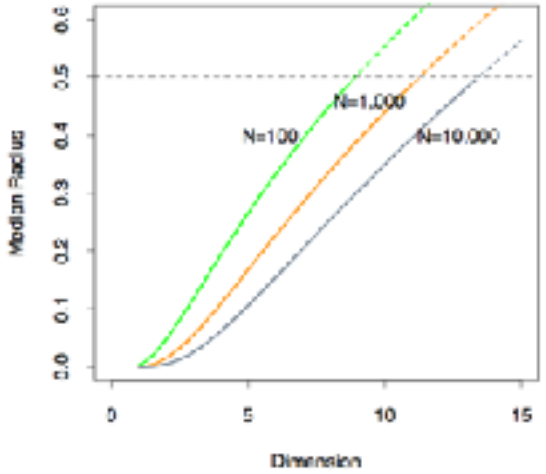

High dimensional space is hard to cover

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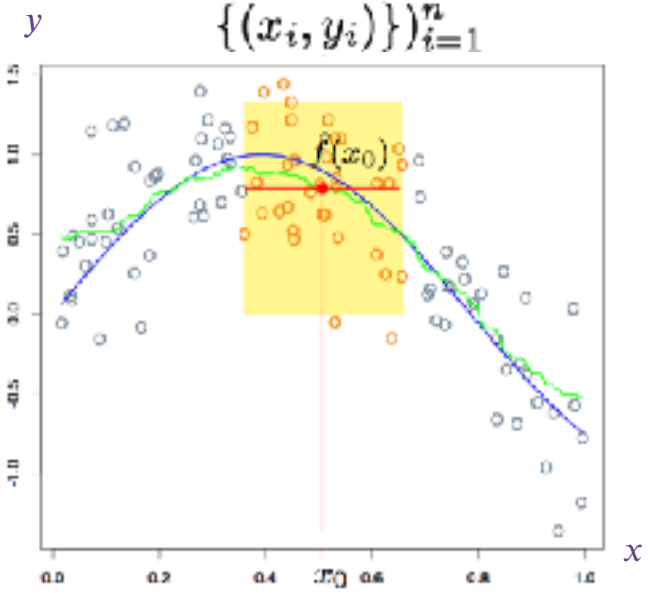
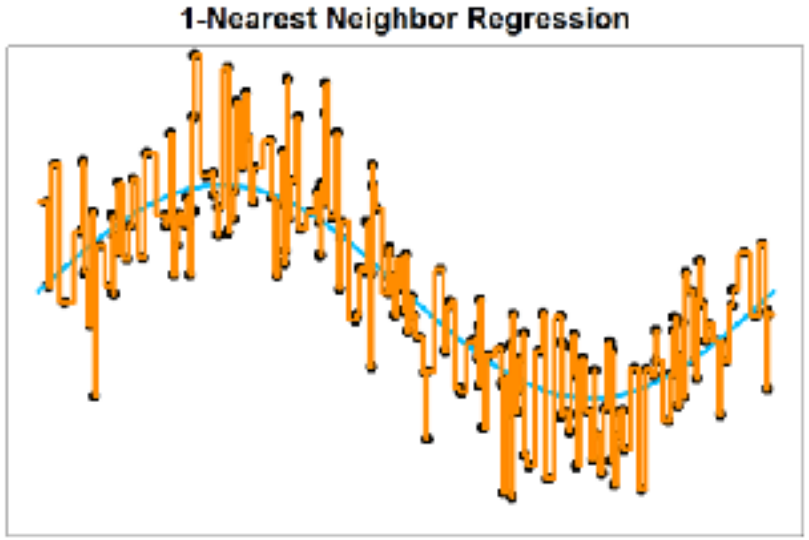
Slides are not updated beyond this point,
download the latest ones from the course website

Nearest neighbor regression

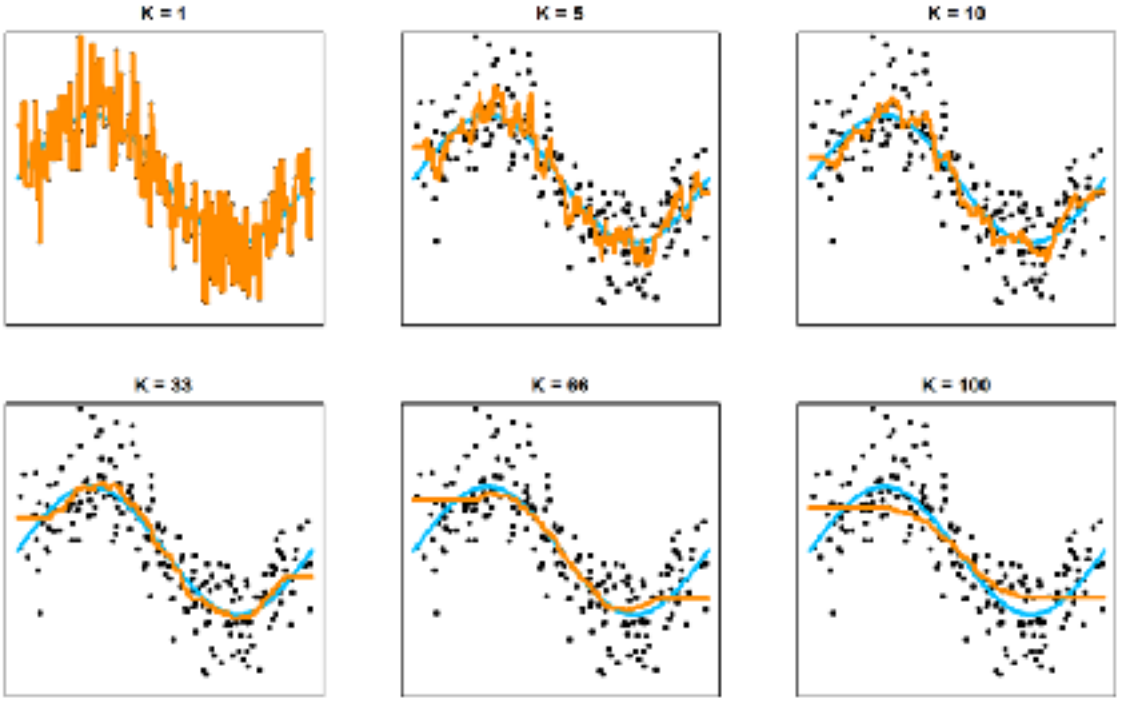


Overfitting



Figures from Ruoqing Zhu, Stat 542

Bias vs variance



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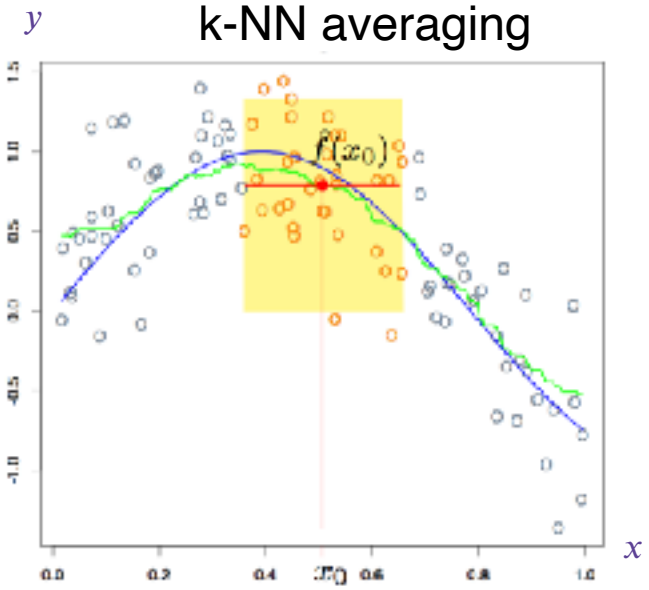
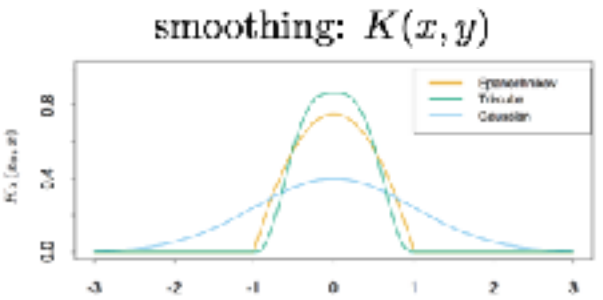
Smoothed nearest neighbor regression





$$\hat{f}(x) = \frac{\sum_{i=1}^{n} K\left(x, x^{(i)}\right) y^{(i)}}{\sum_{i=1}^{n} K\left(x, x^{(i)}\right)}$$

Smoothed nearest neighbor regression

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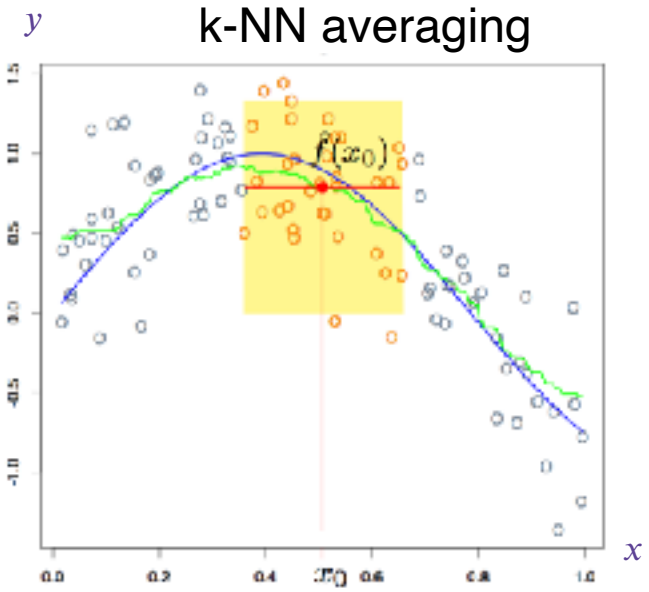
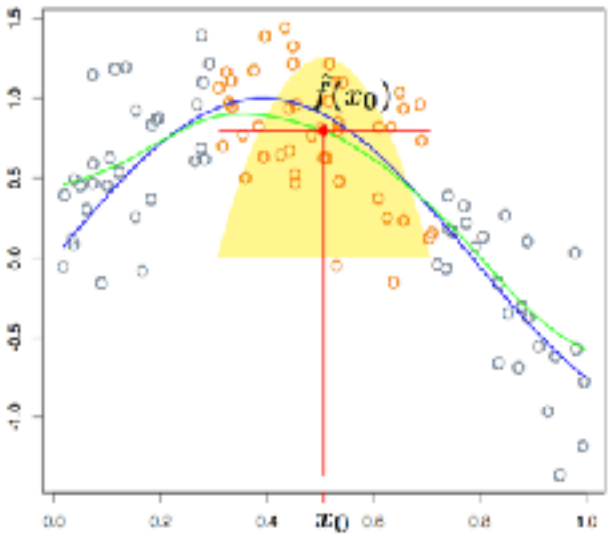
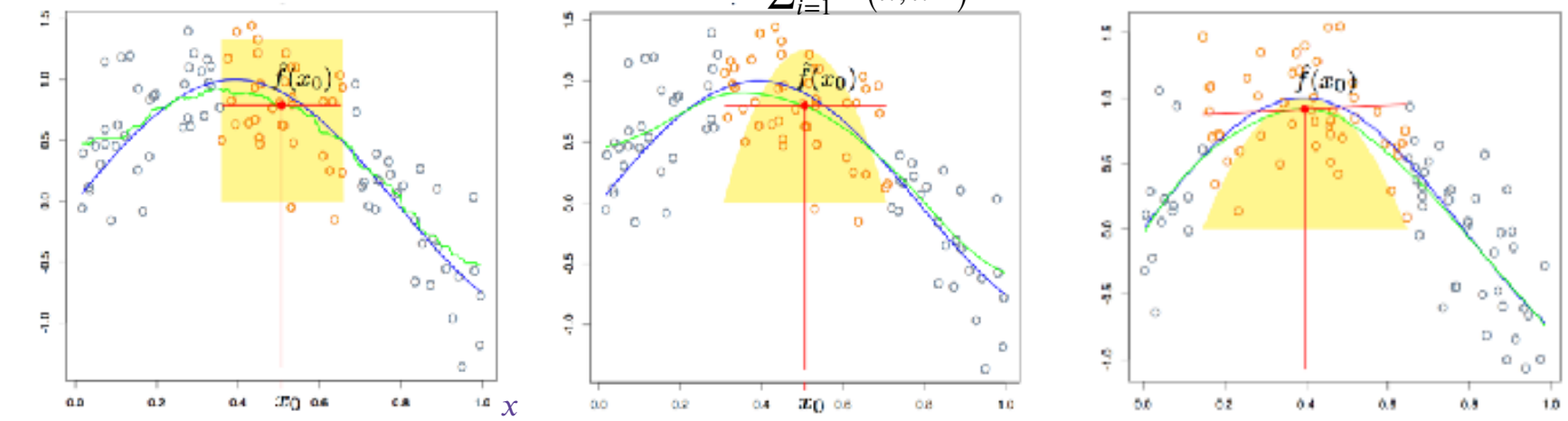




Locally linear regression

$$\hat{f}(x) = \frac{\sum_{i=1}^{n} K\left(x, x^{(i)}\right) y^{(i)}}{\sum_{i=1}^{n} K\left(x, x^{(i)}\right)}$$

k-NN averaging



Have we seen non-parametric methods before?

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- Kernel methods are non-parametric:

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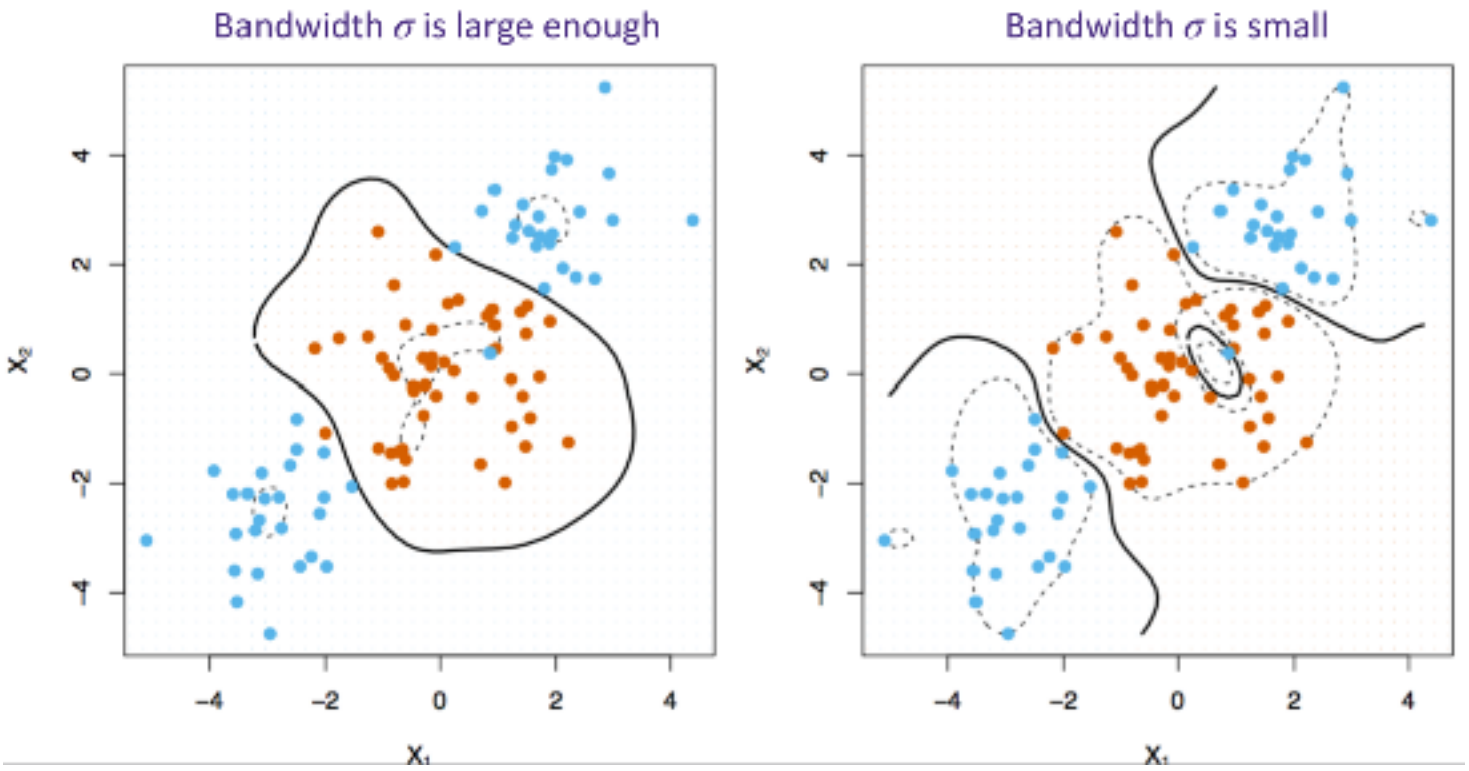
  # parameters goes up with # data

- Compare with (smoothed) nearest neighbors:

$$\hat{f}(x) = \frac{\sum_{i=1}^{n} K\left(x, x^{(i)}\right) y^{(i)}}{\sum_{i=1}^{n} K\left(x, x^{(i)}\right)}$$

The Radial Basis Function (RBF) kernel $\exp\left(-\frac{\left\|x^{(i)}-x\right\|_2^2}{2\sigma^2}\right)$



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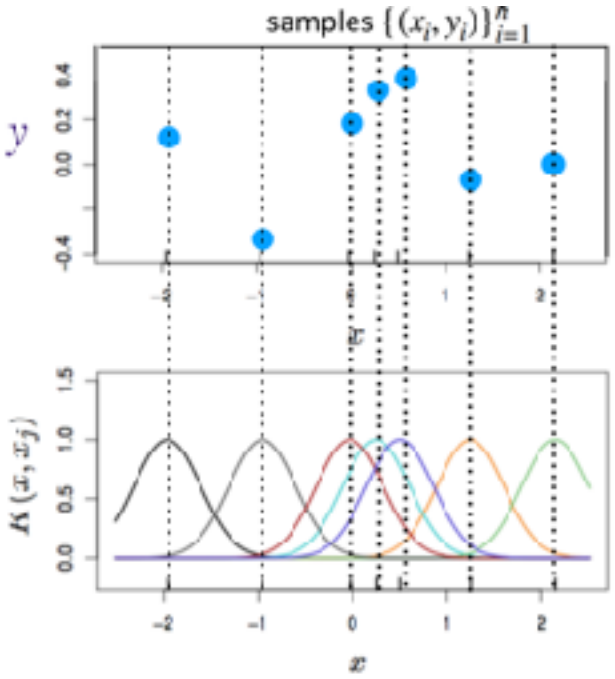

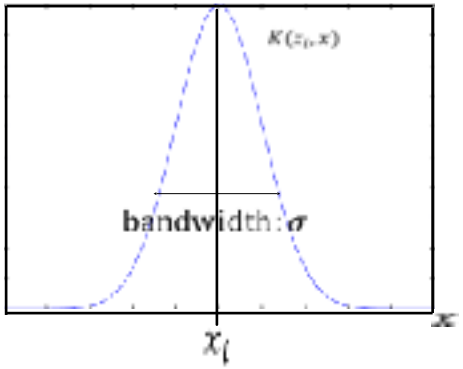

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- How many parameters?

Takeaways

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- You can use other forms of distance (not just Euclidean)
- Smoothing and local linear regression can improve performance (at the cost of higher variance)
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- Without a lot of data, neighborhoods aren’t “local” and methods suffer (curse of dimensionality)