

Day 3: Classification, logistic regression

Introduction to Machine Learning Summer School
June 18, 2018 - June 29, 2018, Chicago

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20 June 2018

Topics so far

- Supervised learning, linear regression
- Yesterday
 - Overfitting,
 - Ridge and lasso Regression
 - Gradient descent
- Today
 - Bias variance trade-off
 - Classification
 - Logistic regression
 - Regularization for logistic regression
 - Classification metrics

Bias-variance tradeoff

Empirical vs population loss

- **Population distribution** Let $(x, y) \sim \mathcal{D}$ e.g, $\Pr(x) = \text{uniform}(0,1)$
y = $w^* \cdot x + \epsilon$ where $\epsilon = \mathcal{N}(0,0.1)$
 $\Rightarrow \Pr(y|x) = \mathcal{N}(w^* \cdot x, 0.1)$
 $\Pr(x, y) = \Pr(x) \Pr(y|x)$
- We have
 - Loss function $\ell(\hat{y}, y)$
 - Hypothesis class \mathcal{H}
 - Training data $S = \{(x^{(i)}, y^{(i)}): i = 1, 2, \dots, N\} \sim_{\text{iid}} \mathcal{D}^N$
 - Think of S as random variable
- What we really want $f \in \mathcal{H}$ to minimize **population loss**

$$L_{\mathcal{D}}(f) \triangleq \mathbf{E}_{\mathcal{D}}[\ell(f(x), y)] = \int_{(x,y)} \ell(f(x), y) \Pr(x, y)$$

- ERM minimizes **empirical loss**

$$L_S(f) \triangleq \widehat{\mathbf{E}}_S[\ell(f(x), y)] = \frac{1}{N} \sum_{i=1}^N \ell(f(x^{(i)}), y^{(i)})$$

Empirical vs population loss

$$L(f) \triangleq \mathbf{E}_{\mathcal{D}}[\ell(f(x), y)] = \int_{(x,y)} \ell(f(x), y) \Pr(x, y)$$

$$L_S(f) \triangleq \hat{\mathbf{E}}_S[\ell(f(x), y)] = \frac{1}{N} \sum_{i=1}^N \ell(f(x^{(i)}), y^{(i)})$$

- \hat{f}_S from some model **overfits** to S if there is $f^* \in \mathcal{H}$ with
 $\hat{\mathbf{E}}_S[\ell(\hat{f}_S(x), y)] \leq \hat{\mathbf{E}}_S[\ell(f^*(x), y)]$ but $\mathbf{E}_{\mathcal{D}}[\ell(\hat{f}_S(x), y)] \gg \mathbf{E}_{\mathcal{D}}[\ell(f^*(x), y)]$
- If f is independent of S_{train} then both $L_{S_{train}}(f)$ and $L_{S_{test}}(f)$ are good approximations of $L_{\mathcal{D}}(f)$
- But generally, \hat{f} depends on S_{train} . Why?
 - $L_{S_{train}}(\hat{f}_{S_{train}})$ is no more a good approximation of $L_{\mathcal{D}}(f)$
 - $L_{S_{test}}(\hat{f}_{S_{train}})$ is still a good approximation of $L_{\mathcal{D}}(f)$ since $\hat{f}_{S_{train}}$ is independent of S_{test}

Optimum Unrestricted Predictor

- Consider population squared loss

$$\operatorname*{argmin}_{f \in \mathcal{H}} L(f) \triangleq \mathbf{E}_{\mathcal{D}}[\ell(f(x), y)] = \mathbf{E}_{(x,y)}[(f(x) - y)^2]$$

- Say \mathcal{H} is unrestricted – any function $f: x \rightarrow y$ is allowed

Bias variance decomposition

- Best unrestricted predictor $f^{**}(x) = \mathbf{E}_y[y|x]$
- $L(f_S) = \mathbf{E}_x[(f_S(x) - f^{**}(x))^2] + \mathbf{E}_{x,y}[(f^{**}(x) - y)^2]$

- $\mathbf{E}_S L(f_S) = \mathbf{E}_S \mathbf{E}_x \left[(f_S(x) - f^{**}(x))^2 \right] + \text{noise}$

$$\begin{aligned} \mathbf{E}_S \mathbf{E}_x \left[(f_S(x) - f^{**}(x))^2 \right] &= \mathbf{E}_x \left[\mathbf{E}_S \left[(f_S(x) - f^{**}(x))^2 | x \right] \right] \\ &= \mathbf{E}_x \mathbf{E}_S \left[(f_S(x) - \mathbf{E}_S[f_S(x)] + \mathbf{E}_S[f_S(x)] - f^{**}(x))^2 | x \right] \\ &= \mathbf{E}_x \mathbf{E}_S [(f_S(x) - \mathbf{E}_S[f_S(x)])^2 | x] + \mathbf{E}_x \left[(\mathbf{E}_S[f_S(x)] - f^{**}(x))^2 \right] \\ &\quad + 2 \mathbf{E}_x \left[\mathbf{E}_S [(\mathbf{E}_S[f_S(x)] - f^{**}(x))(f_S(x) - \mathbf{E}_S[f_S(x)])] | x \right] \\ &= \mathbf{E}_{S,x} [(f_S(x) - \mathbf{E}_S[f_S(x)])^2] + \mathbf{E}_x \left[(\mathbf{E}_S[f_S(x)] - f^{**}(x))^2 \right] \end{aligned}$$

$$\begin{aligned} \mathbf{E}_S L(f_S) &= \mathbf{E}_{S,x} [(f_S(x) - \mathbf{E}_S[f_S(x)])^2] \\ &\quad + \mathbf{E}_x \left[(\mathbf{E}_S[f_S(x)] - f^{**}(x))^2 \right] \\ &\quad + \mathbf{E}_{x,y} [(f^{**}(x) - y)^2] \end{aligned}$$

= variance
+ bias²
+ noise

Bias-variance tradeoff

$$\begin{aligned}\mathbf{E}_S L(f_S) &= \mathbf{E}_{S,x} [(f_S(x) - \mathbf{E}_S[f_S(x)])^2] \\ &+ \mathbf{E}_x \left[(\mathbf{E}_S [f_S(x)] - f^{**}(x))^2 \right] \\ &+ \mathbf{E}_{x,y} [(f^{**}(x) - y)^2]\end{aligned}$$

= variance
+ bias²
+ noise

- $f_S \in \mathcal{H}$
- noise is irreducible
- variance can be reduced by
 - get more data
 - make f_S less sensitive to S
 - less number of candidates in \mathcal{H} to choose from → less variance
 - reducing the “complexity” of model class \mathcal{H} decreases variance
- bias² $\geq \min_{f \in \text{conv}(\mathcal{H})} \mathbf{E}_x \left[(f(x) - f^{**}(x))^2 \right]$
 - expanding model class \mathcal{H} decreases bias

Model complexity

- reducing the complexity of model class \mathcal{H} decreases variance
- **expanding model class \mathcal{H} decreases bias**
- Complexity \approx number of choices in \mathcal{H}
 - For any loss L , for all $f \in \mathcal{H}$ with probability greater than $1 - \delta$

$$L(f) \leq L_S(f) + \sqrt{\frac{\log|\mathcal{H}| + \log \frac{1}{\delta}}{N}}$$

- many other variants for infinite cardinality classes
- often bounds are loose
- Complexity \approx number of degrees of freedom
 - e.g., number of parameters to estimate
 - more data \rightarrow can fit more complex models
- Is $\mathcal{H}_1 = \{x \rightarrow w_0 + w_1 \cdot x - w_2 \cdot x\}$ more complex than $\mathcal{H}_2 = \{x \rightarrow w_0 + w_1 \cdot x\}$?
 - What we need is how many different “behaviors” we can get on same S

Summary

- Overfitting
 - What is overfitting?
 - How to detect overfitting?
 - Avoiding overfitting using model selection
- Bias – variance tradeoff

Classification

- Supervised learning: estimate a mapping f from input $x \in \mathcal{X}$ to output $y \in \mathcal{Y}$
 - **Regression** $\mathcal{Y} = \mathbb{R}$ or other continuous variables
 - **Classification** \mathcal{Y} takes discrete set of values
 - Examples:
 - $\mathcal{Y} = \{\text{spam, nospam}\}$,
 - digits (not values) $\mathcal{Y} = \{0,1,2,\dots,9\}$
- Many successful applications of ML in vision, speech, NLP, healthcare

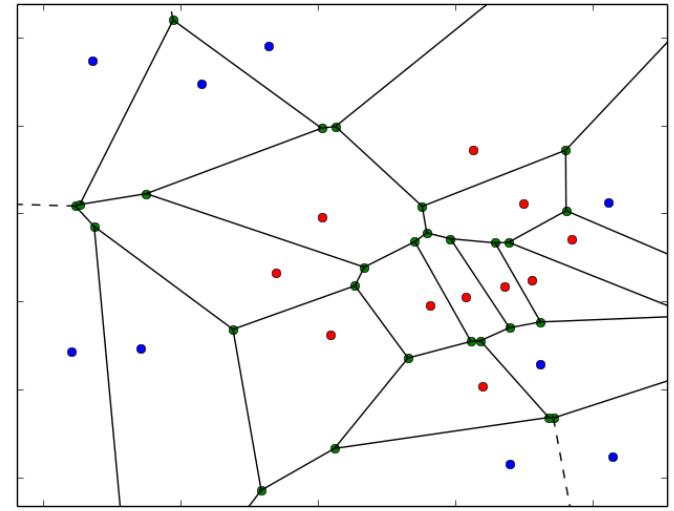
Classification vs Regression

- Label-values do not have meaning
 - $\mathcal{Y} = \{\text{spam, nospam}\}$ or $\mathcal{Y} = \{0,1\}$ or $\mathcal{Y} = \{-1,1\}$
- Ordering of labels does not matter (for most parts)
 - $f(x) = "0"$ when $y = "1"$ is as bad as $f(x) = "9"$ when $y = "1"$
- Often $f(x)$ does not return labels y
 - e.g. in binary classification with $\mathcal{Y} = \{-1,1\}$ we often estimate $f: \mathcal{X} \rightarrow \mathbb{R}$ and then post process to get $\hat{y}(f(x)) = \mathbf{1}[f(x) \geq 0]$
 - mainly for computational reasons
 - remember, we need to solve $\min_{f \in \mathcal{H}} \sum_i \ell(f(x^{(i)}), y^{(i)})$
 - discrete values → combinatorial problems → hard to solve
 - more generally $\mathcal{H} \subset \{f: \mathcal{X} \rightarrow \mathbb{R}\}$ and loss $\ell: \mathbb{R} \times \mathcal{Y} \rightarrow \mathbb{R}$
 - compare to regression, where typically $\mathcal{H} \subset \{f: \mathcal{X} \rightarrow \mathcal{Y}\}$ and loss $\ell: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$

Non-parametric classifiers

Nearest Neighbor (NN) Classifier

- Training data $S = \{(x^{(i)}, y^{(i)}): i = 1, 2, \dots, N\}$
- Want to predict label of new point x
- **Nearest Neighbor Rule**
 - Find the closest training point: $i^* = \arg \min_i \rho(x, x^{(i)})$
 - Predict label of x as $\hat{y}(x) = y^{(i^*)}$
- **Computation**
 - Training time: Do nothing
 - Test time: search the training set for a NN



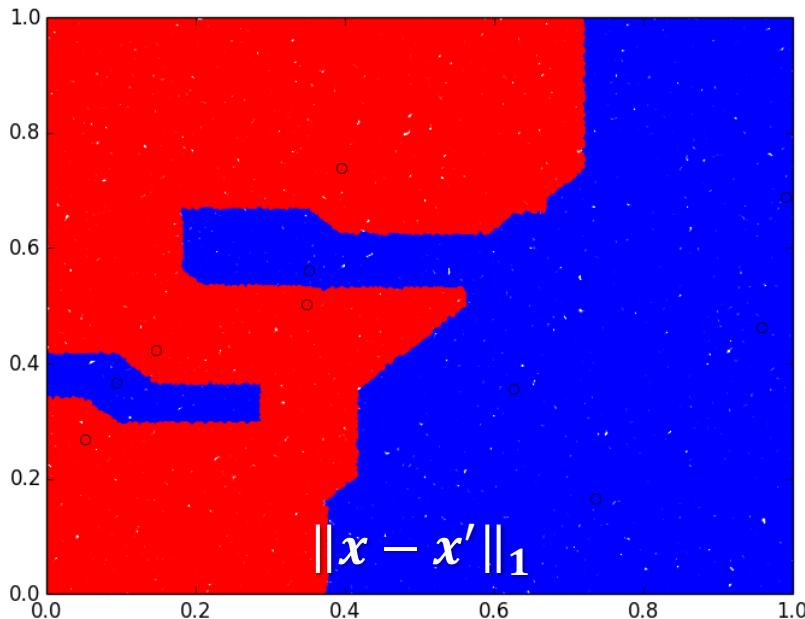
Nearest Neighbor (NN) Classifier

- Where is the main model?

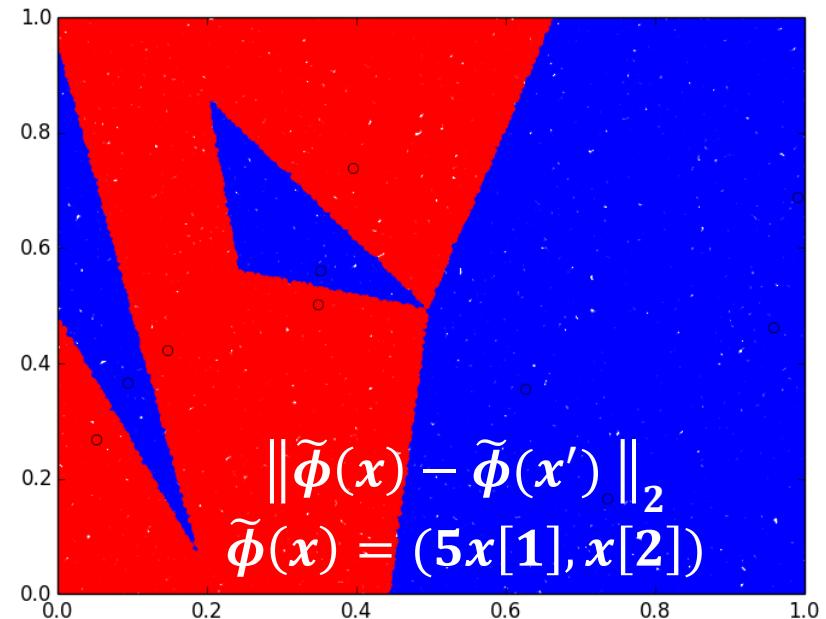
- $i^* = \arg \min_i \rho(x, x^{(i)})$

- What is the right “distance” between images? Between sound waves? Between sentences?

- Often $\rho(x, x') = \|\phi(x) - \phi(x')\|_2$ or other norms $\|x - x'\|_1$



$$\|x - x'\|_1$$



$$\begin{aligned} & \|\tilde{\phi}(x) - \tilde{\phi}(x')\|_2 \\ & \tilde{\phi}(x) = [5x[1], x[2]] \end{aligned}$$

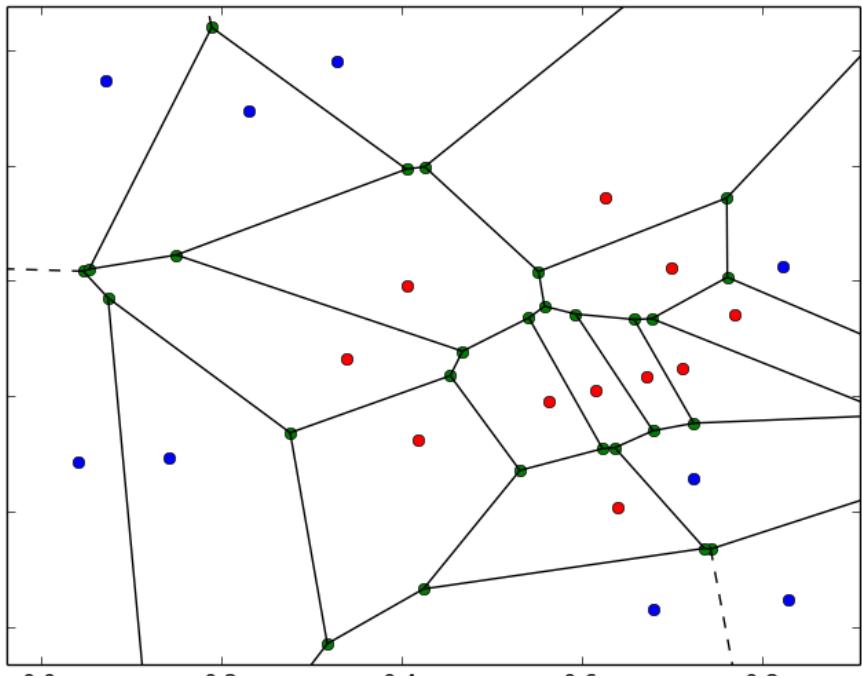
k-Nearest Neighbor (kNN) classifier

- Training data $S = \{(x^{(i)}, y^{(i)}): i = 1, 2, \dots, N\}$
- Want to predict label of new point x
- **k-Nearest Neighbor Rule**
 - Find the k closest training point: $i_1^*, i_2^*, \dots, i_k^*$
 - Predict label of x as
$$\hat{y}(x) = \text{majority}(y^{(i_1^*)}, y^{(i_2^*)}, \dots, y^{(i_k^*)})$$
- Computation
 - Training time: Do nothing
 - Test time: search the training set for k NNs

k -Nearest Neighbor

- **Advantages**
 - no training
 - universal approximator – non-parametric
- **Disadvantages**
 - not scalable
 - test time memory requirement
 - test time computation
 - easily overfits with small data

Training vs test error



1-NN

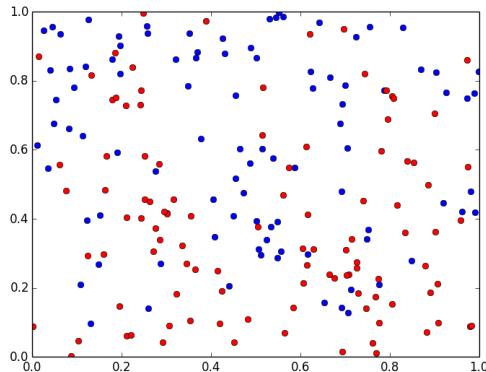
- Training error?
 - 0
- Test error?
 - Depends on $\Pr(x, y)$

k-NN

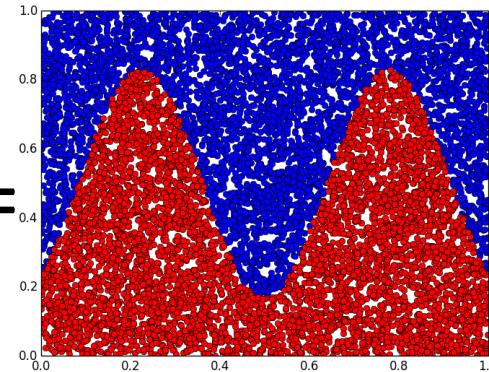
- Training error: can be greater than 0
- Test error: again depends on $\Pr(x, y)$

k -Nearest Neighbor: Data Fit / Complexity Tradeoff

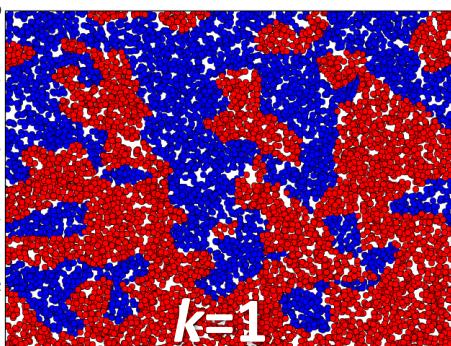
$S =$



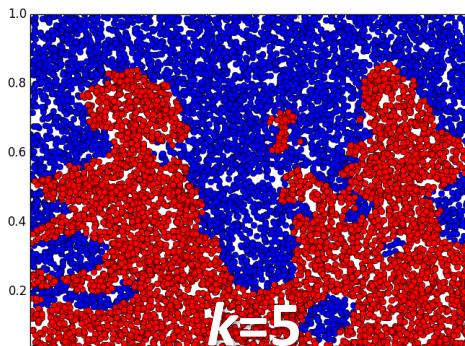
$h^* =$



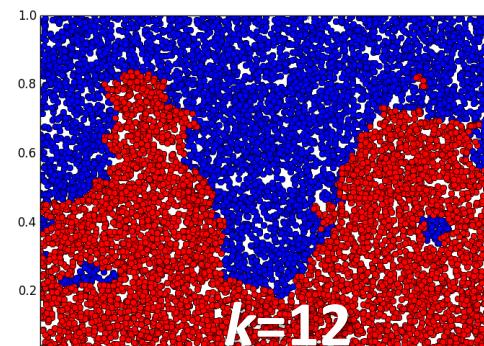
$k=1$



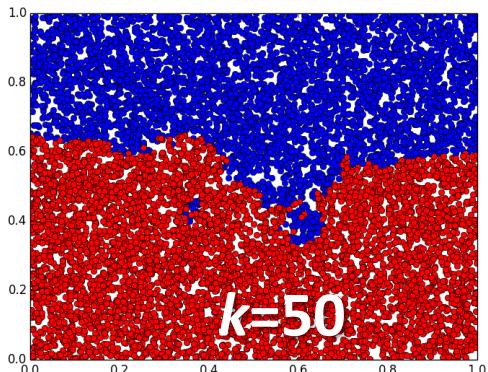
$k=5$



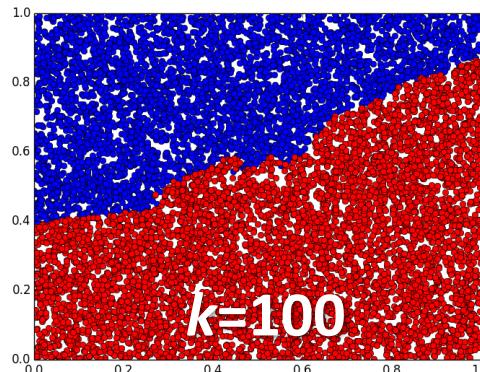
$k=12$



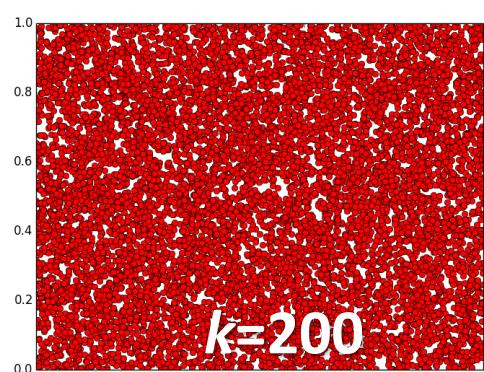
$k=50$



$k=100$

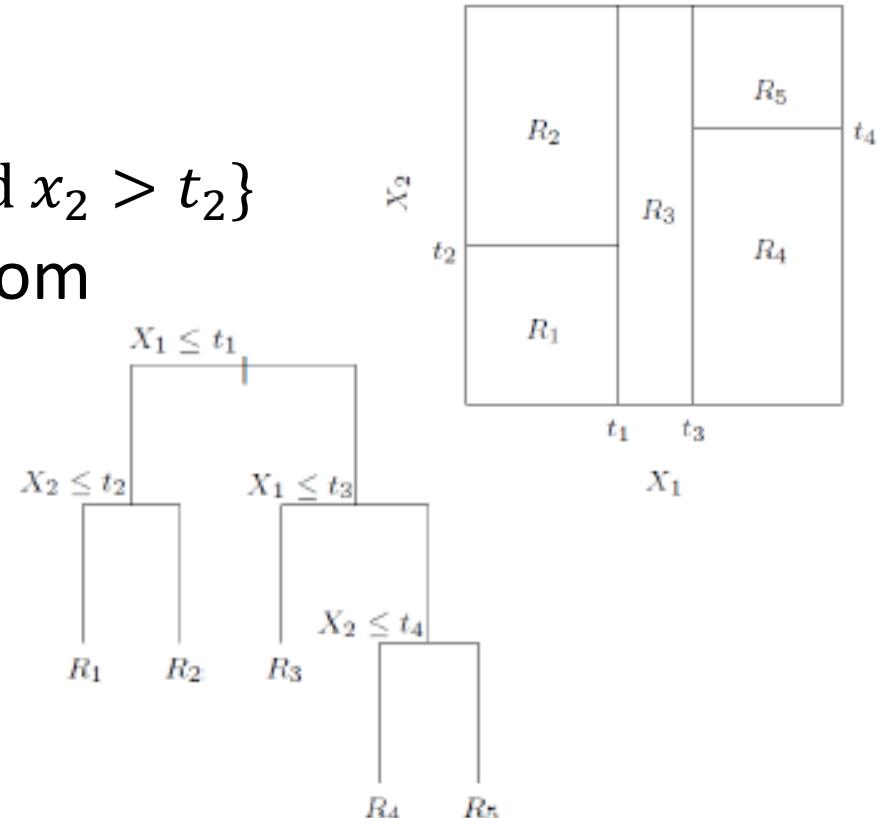


$k=200$



Space partition

- kNN partitioning of \mathcal{X} (or \mathbb{R}^d) into regions of +1 and -1
- What about discrete valued features x ?
- Even for continuous x , can we get more structured partitions?
 - easy to describe
 - e.g., $R_2 = \{x: x_1 < t_1 \text{ and } x_2 > t_2\}$
 - reduces degrees of freedom
- Any non-overlapping partition using only (hyper) rectangles
→ representable by a tree



Decision trees

- Focus on binary trees (trees with at most two children at each node)
- How to create trees?
- What is a “good” tree?
 - Measure of “purity” at each leaf node where each leaf node corresponding to a region R_i

$$\text{purity(tree)} = \sum_{R_i} |\# \text{ blue at } R_i - \# \text{ red at } R_i|$$

There are various metrics of (im)purity that are used in practice, but the rough idea is the same

Decision trees

- How to create trees?
- Training data $S = \{(x^{(i)}, y^{(i)}): i = 1, 2, \dots, N\}$, where $y^{(i)} \in \{\text{blue}, \text{red}\}$
- At each point,

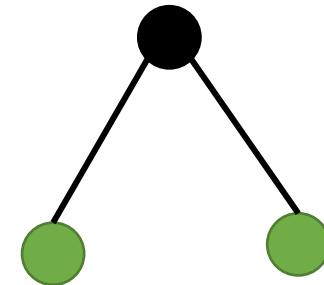
$$\text{purity}(tree) = \sum_{\text{leaf}} |\# \text{ blue at leaf} - \# \text{ red at leaf}|$$

- Start with all data at root
 - only one *leaf* = *root*. What is $\text{purity}(tree)$?



Decision trees

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 - only one *leaf* = *root*. What is $\text{purity}(tree)$?
- Create a split based on a rule that **increases** the amount of “**purity**” of tree.
 - How complex can the rules be?

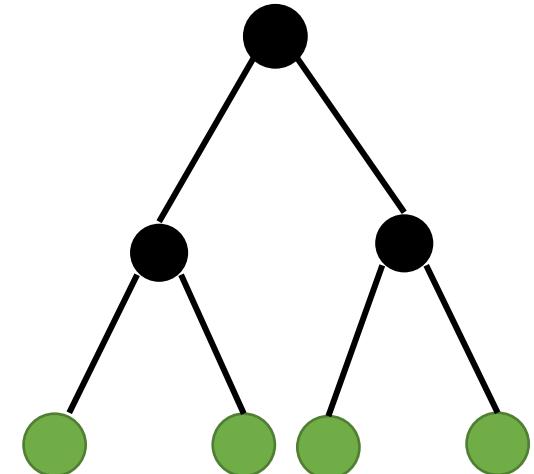


Decision trees

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- Training data $S = \{(x^{(i)}, y^{(i)}): i = 1, 2, \dots, N\}$, where $y^{(i)} \in \{\text{blue}, \text{red}\}$
- At each point,

$$\text{purity}(tree) = \sum_{\text{leaf}} |\# \text{ blue at leaf} - \# \text{ red at leaf}|$$

- Start with all data at root
 - only one *leaf* = *root*. What is $\text{purity}(tree)$?



- Create a split based on a rule that **increases** the amount of “**purity**” of tree.
 - How complex can the rules be?
- Repeat

When to stop?
what is the complexity of a DT?

- Limit the number of leaf nodes

Decision trees

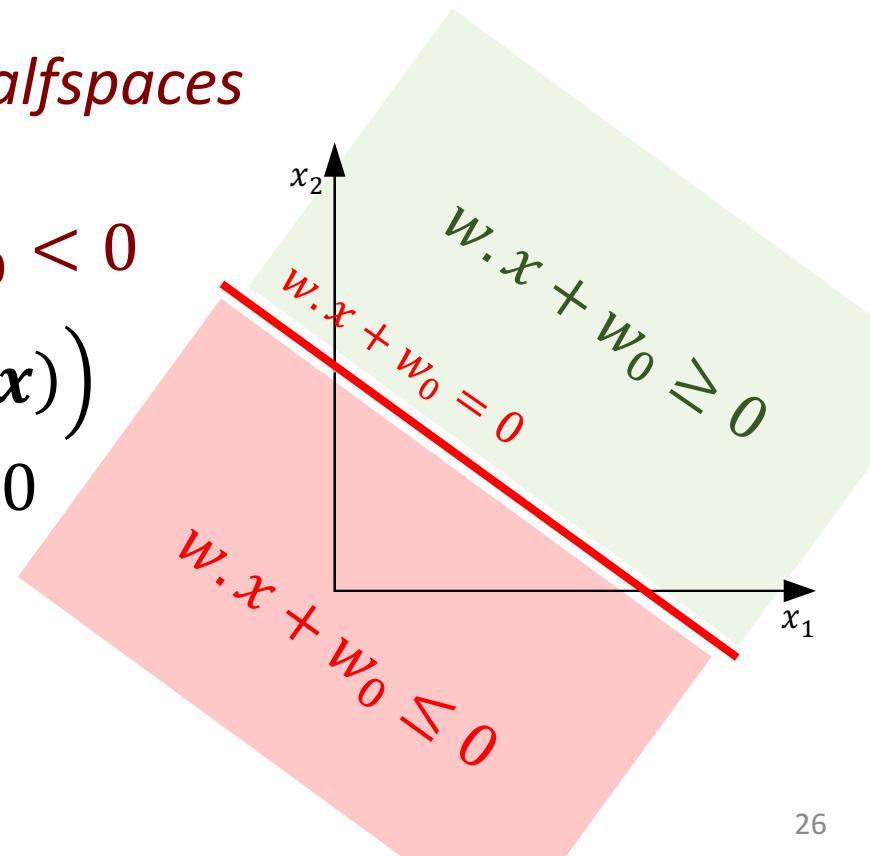
- Advantages
 - interpretable
 - easy to deal with non-numeric features
 - natural extensions to multi-class, multi-label
- Disadvantages
 - not scalable
 - hard decisions – non-smooth decisions
 - often overfits in spite of regularization
- Check CART package in scikit-learn

Parametric classifiers

- What is the equivalent of linear regression?
 - something easy to train
 - something easy to use at test time
- $f(\mathbf{x}) = f_{\mathbf{w}}(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + w_0$
- $\mathcal{H} = \{f_{\mathbf{w}} = \mathbf{x} \rightarrow \mathbf{w} \cdot \mathbf{x} + w_0 : \mathbf{w} \in \mathbb{R}^d, w_0 \in \mathbb{R}\}$
- but $f(\mathbf{x}) \notin \{-1, 1\}$! how do we get labels?
 - reasonable choice
 $\hat{y}(\mathbf{x}) = 1$ if $f_{\widehat{\mathbf{w}}}(\mathbf{x}) \geq 0$ and $\hat{y}(\mathbf{x}) = -1$ otherwise
 - linear classifier: $\hat{y}(\mathbf{x}) = \text{sign}(\widehat{\mathbf{w}} \cdot \mathbf{x} + \widehat{w}_0)$

Parametric classifiers

- $\mathcal{H} = \{f_{\mathbf{w}} = \mathbf{x} \rightarrow \mathbf{w} \cdot \mathbf{x} + w_0 : \mathbf{w} \in \mathbb{R}^d, w_0 \in \mathbb{R}\}$
- $\hat{y}(\mathbf{x}) = \text{sign}(\hat{\mathbf{w}} \cdot \mathbf{x} + \hat{w}_0)$
- $\hat{\mathbf{w}} \cdot \mathbf{x} + \hat{w}_0 = 0$ (linear) decision boundary or separating *hyperplane*
 - that separates \mathbb{R}^d into two *halfspaces* (*regions*)
 $\hat{\mathbf{w}} \cdot \mathbf{x} + \hat{w}_0 > 0$ and $\hat{\mathbf{w}} \cdot \mathbf{x} + \hat{w}_0 < 0$
- more generally, $\hat{y}(\mathbf{x}) = \text{sign}(\hat{f}(\mathbf{x}))$
→ decision boundary is $\hat{f}(\mathbf{x}) = 0$



Linear classifier

Classification vs Regression

- Label-values do not have meaning
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 - e.g. in binary classification with $\mathcal{Y} = \{-1,1\}$ we often estimate $f: \mathcal{X} \rightarrow \mathbb{R}$ and then post process to get $\hat{y}(f(x)) = \mathbf{1}[f(x) \geq 0]$
 - mainly for computational reasons
 - remember, we need to solve $\min_{f \in \mathcal{H}} \sum_i \ell(f(x^{(i)}), y^{(i)})$
 - discrete values → combinatorial problems → hard to solve
 - more generally $\mathcal{H} \subset \{f: \mathcal{X} \rightarrow \mathbb{R}\}$ and loss $\ell: \mathbb{R} \times \mathcal{Y} \rightarrow \mathbb{R}$
 - compare to regression, where typically $\mathcal{H} \subset \{f: \mathcal{X} \rightarrow \mathcal{Y}\}$ and loss $\ell: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$

Classification vs Regression

- Label-values do not have meaning
 - $\mathcal{Y} = \{s_1, s_2, \dots, s_n\}$

- Ordering of labels
 - $f(x) = \text{rank}(x)$

- Often $f(x)$ is continuous
 - e.g. in linear regression: $f: \mathcal{X} \rightarrow \mathbb{R}$

- mainly two types
 - regression
 - classification

- mainly two types
 - regression
 - classification

What if we ignore above
and solve classification
using regression?

- discrete values → combinatorial problems → hard to solve
 - more generally $\mathcal{H} \subset \{f: \mathcal{X} \rightarrow \mathbb{R}\}$ and loss $\ell: \mathbb{R} \times \mathcal{Y} \rightarrow \mathbb{R}$
 - compare to regression, where typically $\mathcal{H} \subset \{f: \mathcal{X} \rightarrow \mathcal{Y}\}$ and loss $\ell: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$

if $y = "1"$

estimate

$(x) \geq 0]$

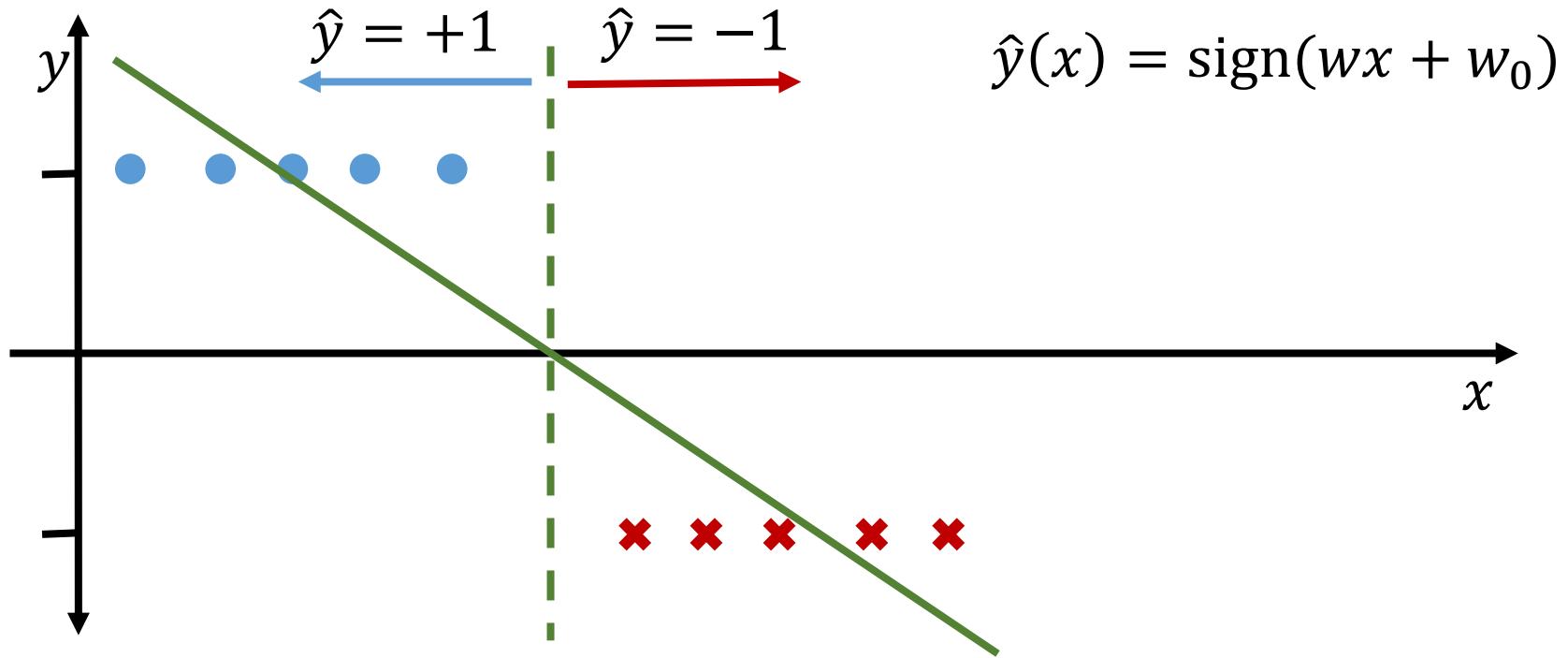
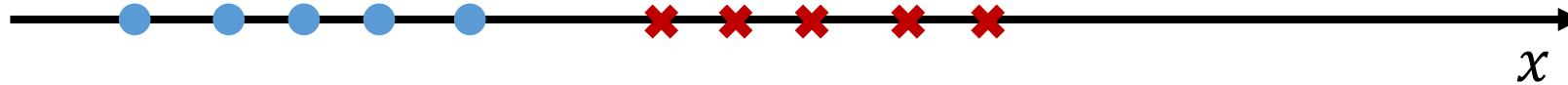
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Classification as regression

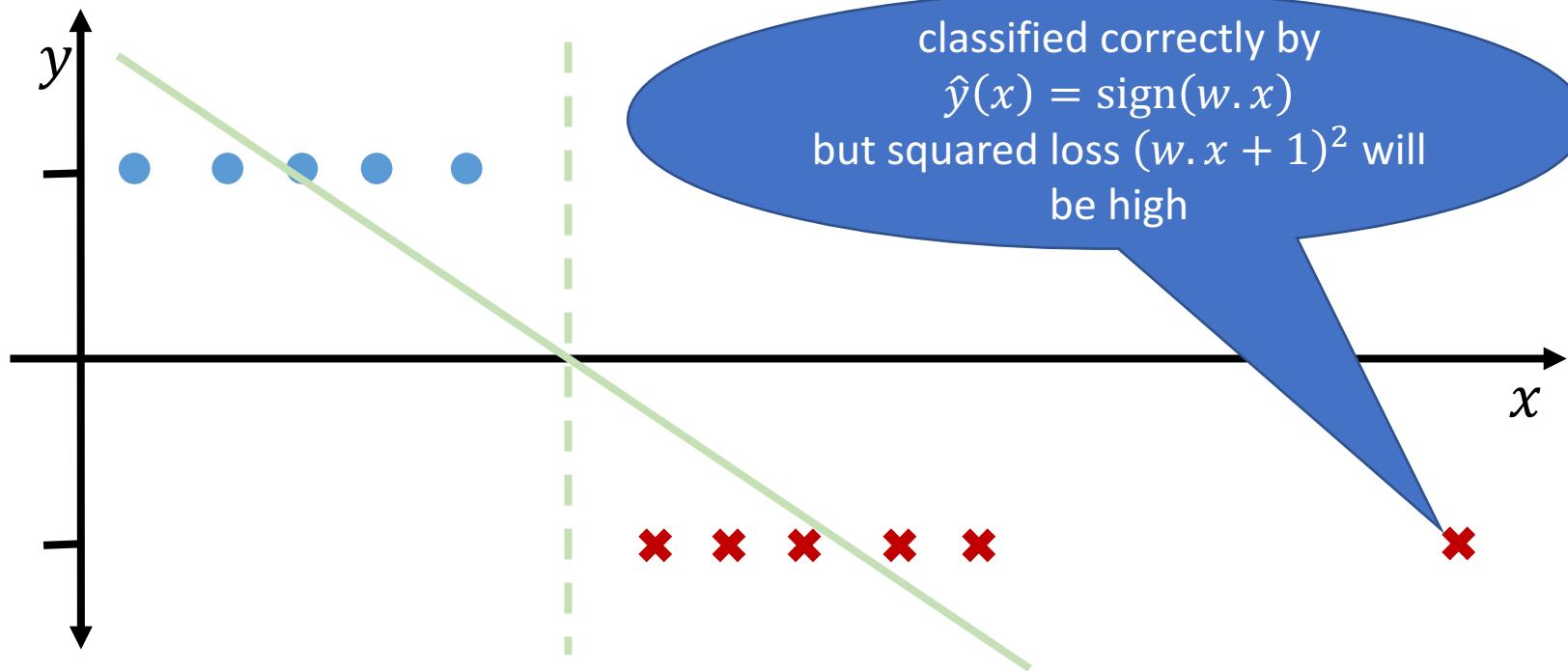
- Binary classification $\mathcal{Y} = \{-1, 1\}$ and $\mathcal{X} \in \mathbb{R}^d$
- Treat it as regression with squared loss, say linear regression
 - Training data $S = \{(\mathbf{x}^{(i)}, y^{(i)}): i = 1, 2, \dots, N\}$
 - ERM

$$\hat{\mathbf{w}}, \hat{w}_0 = \operatorname{argmin}_{\mathbf{w}, w_0} \sum_i (\mathbf{w} \cdot \mathbf{x}^{(i)} + w_0 - y^{(i)})^2$$

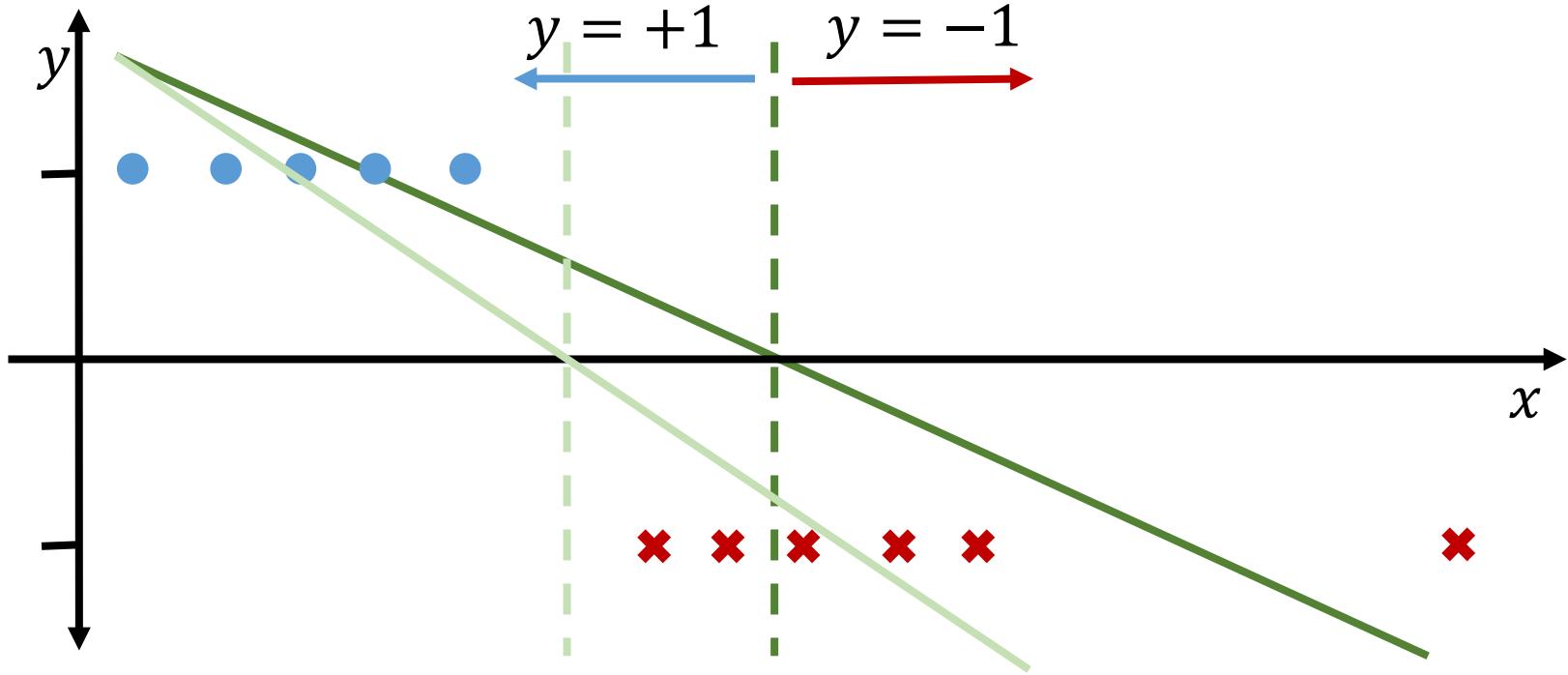
Classification as regression



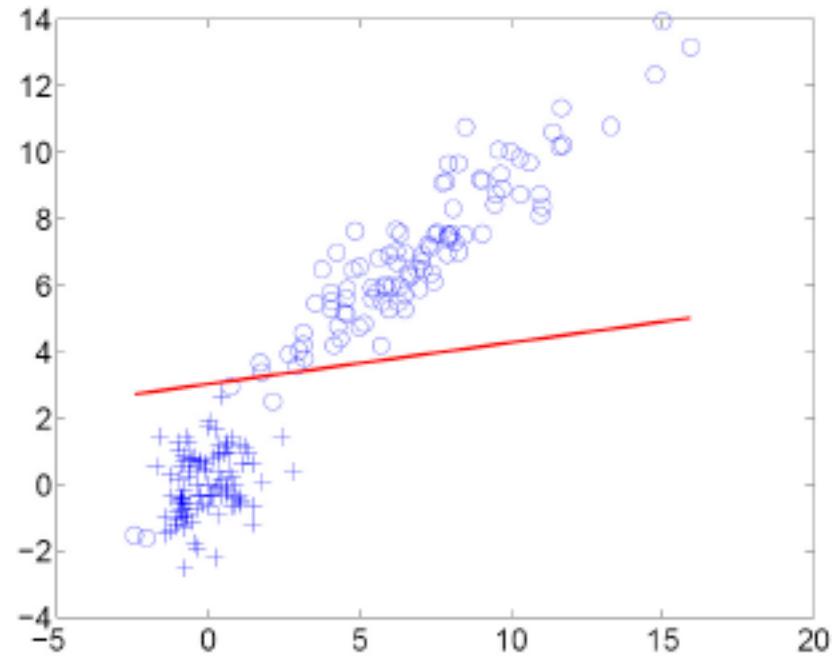
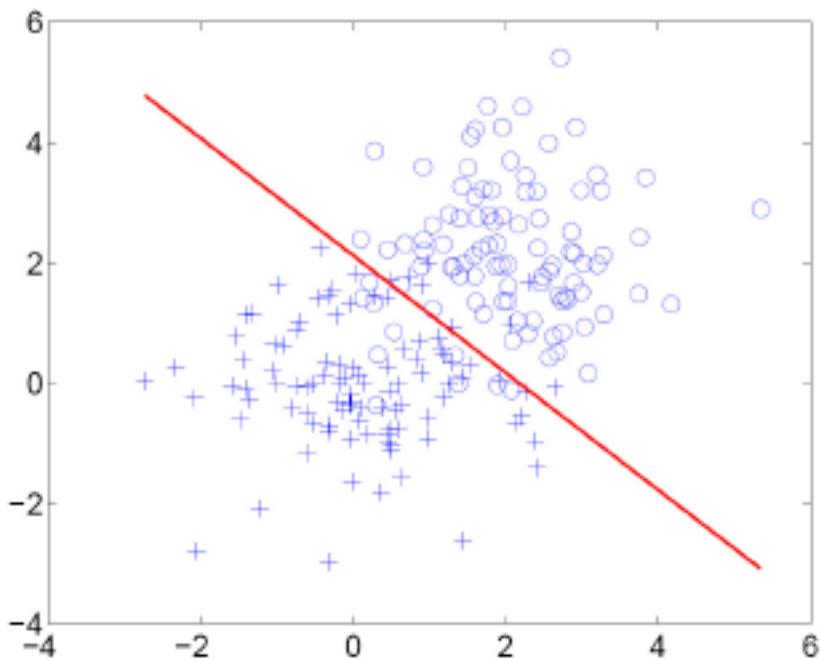
Classification as regression



Classification as regression



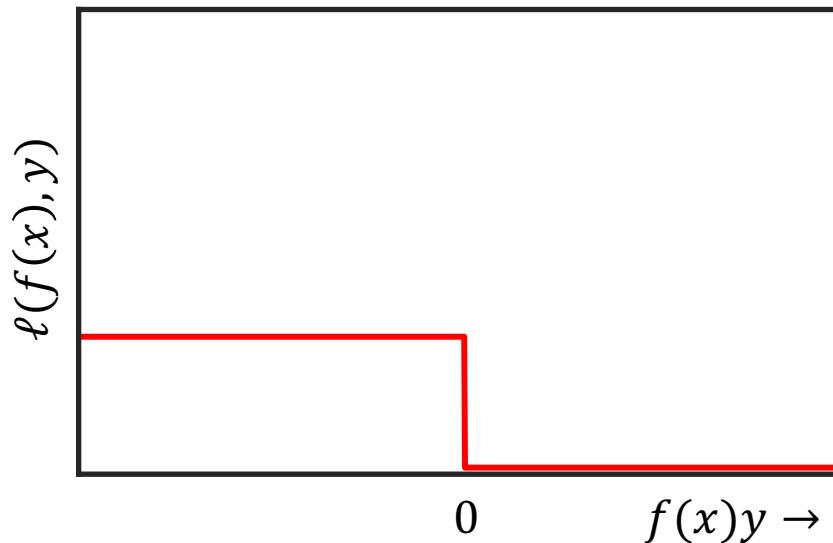
Classification as regression



Surrogate Losses

- The correct loss to use is 0-1 loss **after** thresholding

$$\begin{aligned}\ell^{01}(f(x), y) &= \mathbf{1}[\text{sign}(f(x)) \neq y] \\ &= \mathbf{1}[\text{sign}(f(x)y) < 0]\end{aligned}$$

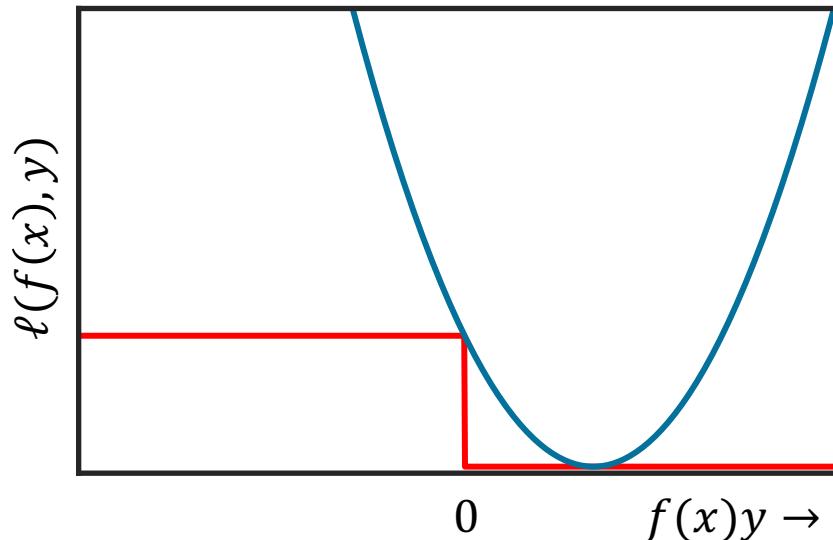


Surrogate Losses

- The correct loss to use is 0-1 loss *after* thresholding

$$\begin{aligned}\ell^{01}(f(x), y) &= \mathbf{1}[\text{sign}(f(x)) \neq y] \\ &= \mathbf{1}[\text{sign}(f(x)y) < 0]\end{aligned}$$

- Linear regression uses $\ell^{LS}(f(x), y) = (f(x) - y)^2$



- Why not do ERM over $\ell^{01}(f(x), y)$ directly?
 - non-continuous, non-convex

Surrogate Losses

- Hard to optimize over ℓ^{01} , find another loss $\ell(\hat{y}, y)$
 - Convex (for any fixed y) → easier to minimize
 - An upper bound of ℓ^{01} → small $\ell \Rightarrow$ small ℓ^{01}
- Satisfied by squared loss

→ but has “large” loss even when $\ell^{01}(\hat{y}, y) = 0$

- Two more surrogate losses in this course

- Logistic loss

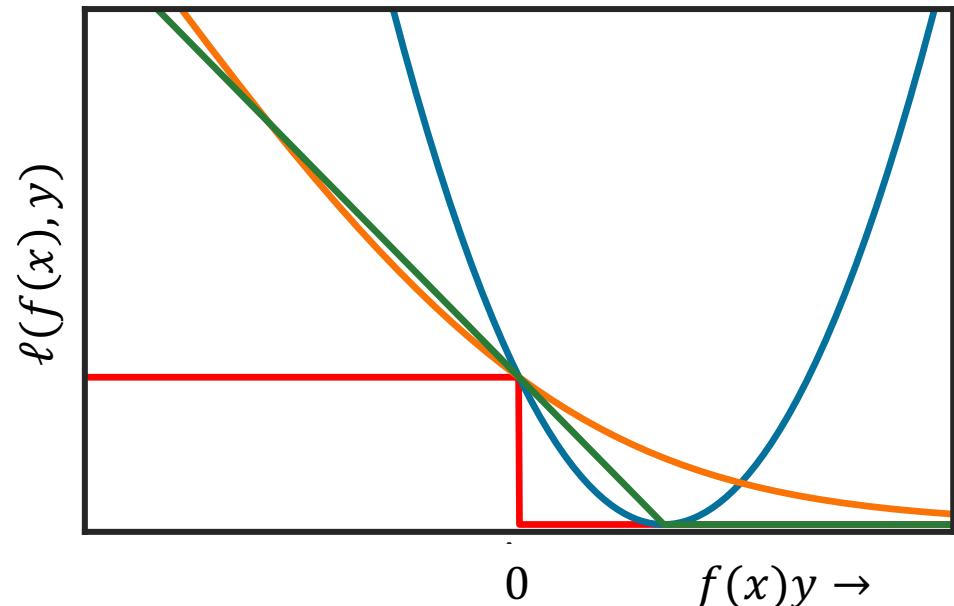
$$\ell^{\log}(\hat{y}, y) = \log(1 + \exp(-\hat{y}y))$$

(TODAY)

- Hinge loss

$$\ell^{hinge}(\hat{y}, y) = \max(0, 1 - \hat{y}y)$$

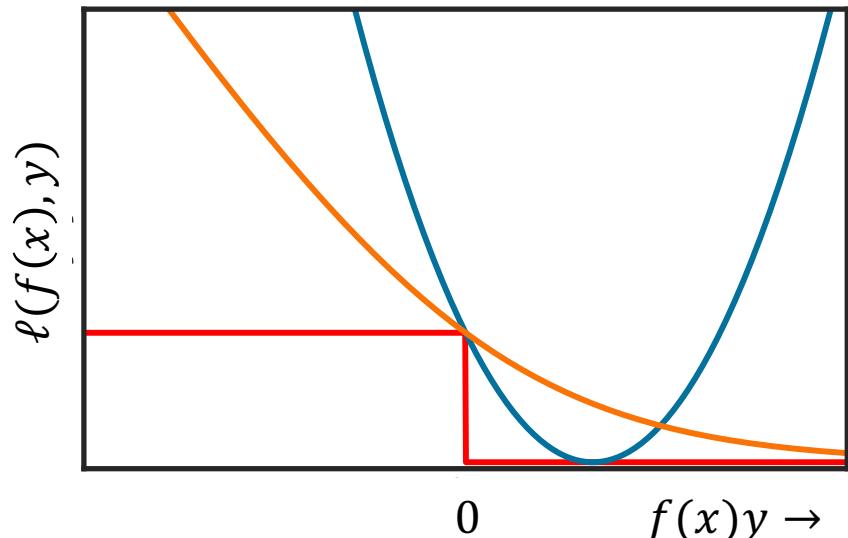
(TOMORROW)



Logistic Regression

Logistic regression: ERM on surrogate loss

Logistic loss
 $\ell(f(x), y) = \log(1 + \exp(-f(x)y))$



- $S = \{(\mathbf{x}^{(i)}, y^{(i)}): i = 1, 2, \dots, N\}, \quad \mathcal{X} = \mathbb{R}^d, \quad \mathcal{Y} = \{-1, 1\}$
- Linear model $f(\mathbf{x}) = f_{\mathbf{w}}(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + w_0$
- Minimize training loss

$$\hat{\mathbf{w}}, \hat{w}_0 = \operatorname{argmin}_{\mathbf{w}, w_0} \sum_i \log(1 + \exp(-(\mathbf{w} \cdot \mathbf{x}^{(i)} + w_0)y^{(i)}))$$

- Output classifier $\hat{y}(\mathbf{x}) = \operatorname{sign}(\mathbf{w} \cdot \mathbf{x} + w_0)$

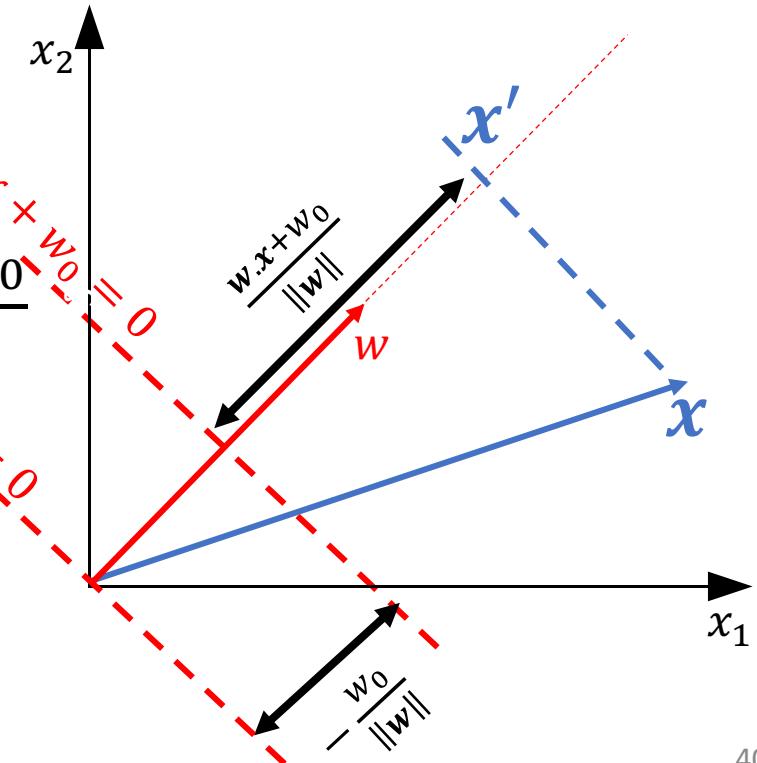
Logistic regression

$$\hat{\mathbf{w}}, \hat{w}_0 = \underset{\mathbf{w}, w_0}{\operatorname{argmin}} \sum_i \log \left(1 + \exp(-(\mathbf{w} \cdot \mathbf{x}^{(i)} + w_0) y^{(i)}) \right)$$

- Learns a linear decision boundary
 - $\{\mathbf{x}: \mathbf{w} \cdot \mathbf{x} + w_0 = 0\}$ is a hyperplane in \mathbb{R}^d - decision boundary
 - $\{\mathbf{x}: \mathbf{w} \cdot \mathbf{x} + w_0 = 0\}$ divides \mathbb{R}^d into two halfspace (regions)
 - $\{\mathbf{x}: \mathbf{w} \cdot \mathbf{x} + w_0 \geq 0\}$ will get label +1 and
 $\{\mathbf{x}: \mathbf{w} \cdot \mathbf{x} + w_0 < 0\}$ will get label -1

- Maps \mathbf{x} to a 1D coordinate

$$x' = \frac{\mathbf{w} \cdot \mathbf{x} + w_0}{\|\mathbf{w}\|}$$



Logistic Regression

$$\hat{\mathbf{w}}, \hat{w}_0 = \operatorname{argmin}_{\mathbf{w}, w_0} \sum_i \log(1 + \exp(-(\mathbf{w} \cdot \mathbf{x} + w_0)y))$$

- Convex optimization problem
- Can solve using gradient descent
- Can also add usual regularization: ℓ_2, ℓ_1
 - More details in the next session