Logistics:
- Mid-term evaluation
- As we transition to in-person lectures and sections starting 1/31/2022, some OHs will be in-person and some will be on zoom.

ML

supervised ML		unsupervised ML
Data $\{(x_i, y_i)\}_{i=1}^n$		$\{x_i\}_{i=1}^n$
y_i cont.	y_i discrete	
Regression	Classification	
L1-L9	L10~L	

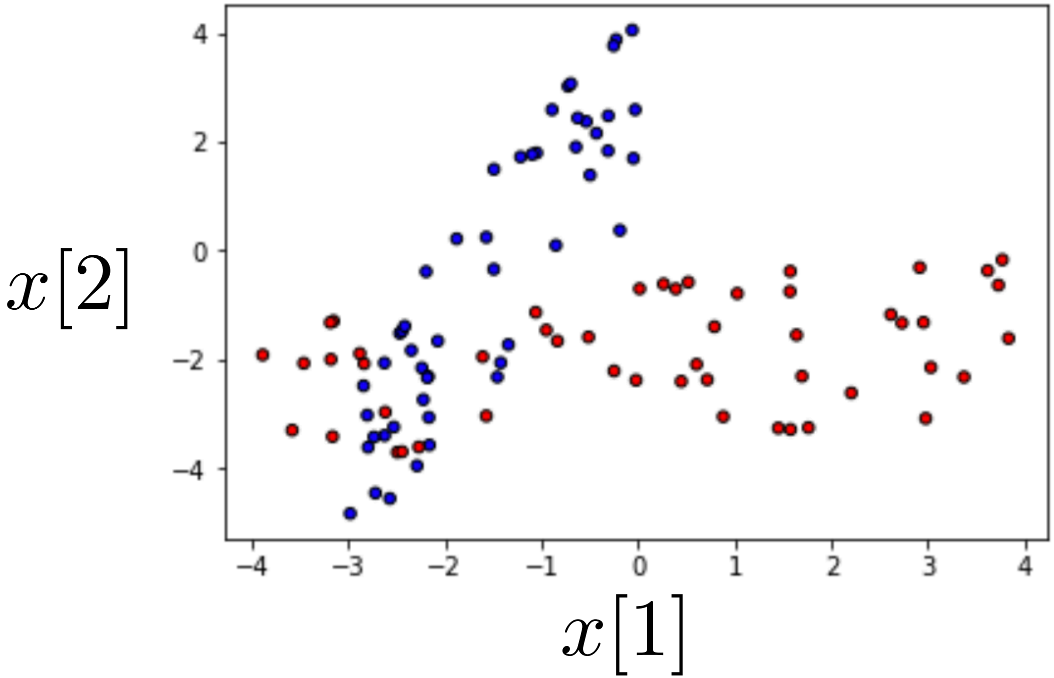
Lecture 11: Classification with logistic regression

- Regression: label is continuous valued
- Classification: label is discrete valued, e.g., {0,1}

  $\{-1,+1\}$

- Note that logistic regression is
  a classification algorithm not a regression algorithm

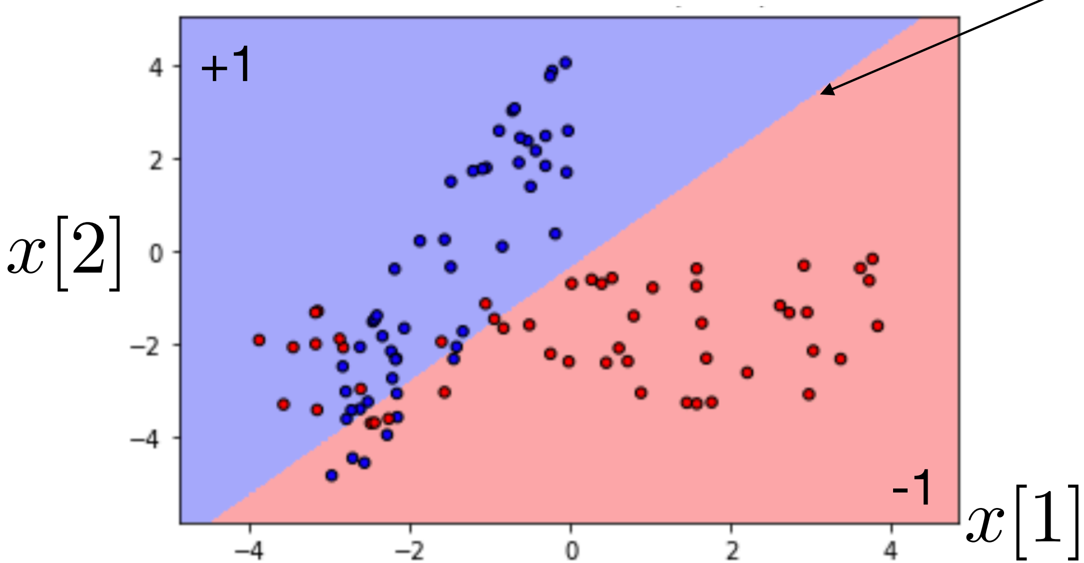
Training data for a binary classification problem



- in this example, each input is $x_i \in \mathbb{R}^2$
- Red points have label y_i=-1, blue points have label y_i=1
- We want a predictor that maps any $x \in \mathbb{R}^2$ to a prediction $\hat{y} \in \{-1, +1\}$

Example: linear classifier trained on 100 samples

simple decision boundary at $w^T x + b = 0$



- We fit a linear model: $w_0 + w_1 x[1] + w_2 x[2] = 0.8 - 1.1x[1] + 0.9x[2]$
- predict using $\hat{y} = \text{sign}(0.8 - 1.1x[1] + 0.9x[2])$
- decision boundary is the line (or hyperplane in higher dimensions) defined by

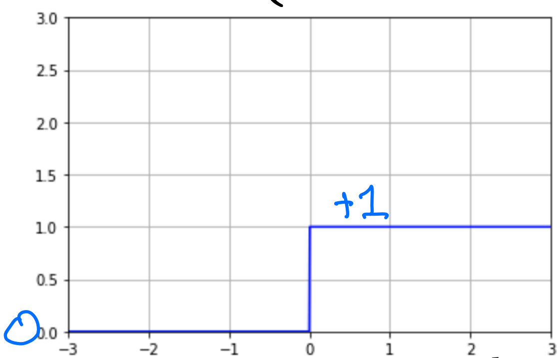
$$0.8 - 1.1x[1] + 0.9x[2] = 0$$

- note that a model $2w^T x + 2b$ has the same predictions as $w^T x + b$
- How do we find such a good linear classifier that fits the data?

Binary Classification with 0-1 loss

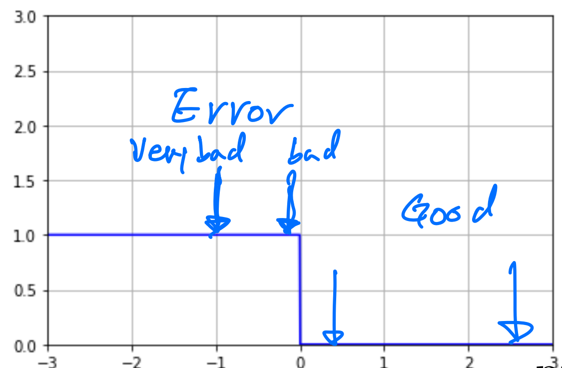
- **Learn** a linear model: $f : x \mapsto \hat{y} = b + x^T w$
  - x – input/features, $y \in \{-1, +1\}$ – label in target classes
  - Prediction: $\mathrm{sign}(\hat{y})$
- **Ideal loss function** $\ell(\hat{y}, y)$: $\min_{b,w} \; \underline{\underline{L(b,w)}} = \sum_{i=1}^{n} \ell(b + x_i^T w, y_i)$
  - **0-1 loss**, because we care about how many were classified correctly
  - What are weaknesses? gradient is zero (almost everywhere)

$$\ell(\hat{y}, -1) = \begin{cases} 0 & \hat{y} < 0 \\ +1 & \hat{y} \geq 0 \end{cases}$$



true y prediction $\hat{y}$

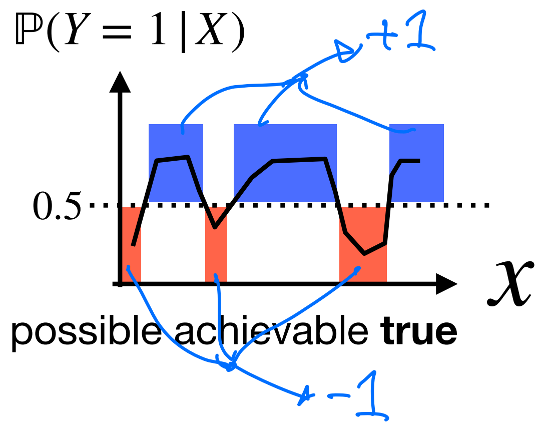
$$\ell(\hat{y}, +1) = \begin{cases} 0 & \hat{y} > 0 \\ +1 & \hat{y} \leq 0 \end{cases}$$



true y prediction $\hat{y}$

Binary Classification with 0-1 loss

- If we know the underlying distribution, $(x, y) \sim P_{X,Y}$ and if we do not restrict ourselves to **any function class**, then we could find the optimal predictor under **0-1 loss**, called **Bayes optimal classifier**
  - $f_{\text{Bayes}}(x) = \arg\max_{\hat{y} \in \{-1,1\}} \mathbb{P}_{Y|X}(Y = \hat{y} \,|\, X = x)$



- Claim: Bayes optimal classifier achieves the minimum possible achievable **true error for 0-1 loss**
- True error: $\mathbb{E}_{X,Y}[\ell(f(X), Y)] = \mathbb{P}\big(\,\text{sign}(f(X)) \neq Y\,\big)$
- Proof:
  We can write the true error of a classifier $f(\cdot)$ using chain rule as

$$\mathbb{E}_{XY}[\mathbb{I}(f(X)\neq Y)] = \mathbb{E}_X\Big[\,\mathbb{E}_{Y|X=x}[\mathbb{I}(f(x)\neq Y)\,|\,X=x]\,\Big] = \mathbb{E}_X\Big[\underbrace{\mathbb{P}(Y\neq f(x)\,|\,X=x)}_{\text{solved separately}}\Big]$$

  optimal classifier minimizes this true error, at every x

$$f_{\text{opt}}(x) = \arg\min_{\hat{y} \in \{-1,1\}} \mathbb{P}_{Y|X}(Y \neq \hat{y} \,|\, x)$$

- But, we do not know $P_{X,Y}$ and 0-1 loss cannot be optimized with gradient descent

Binary Classification with square loss

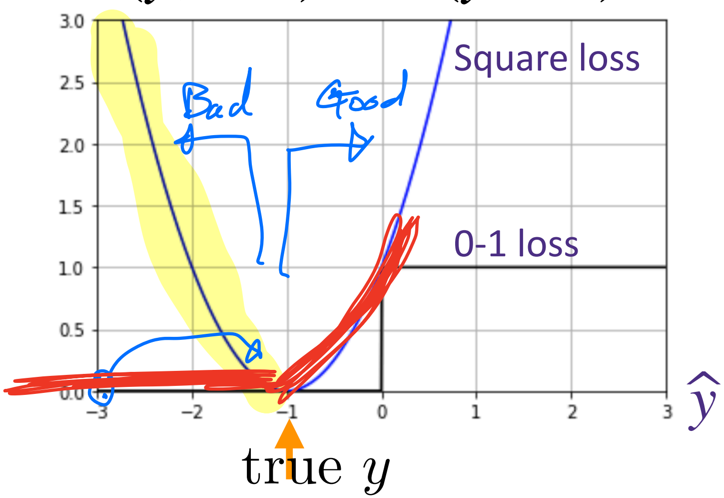
- **Learn** a linear model: $f : x \mapsto \hat{y} = b + x^T w$
  - x input/features, $y \in \{-1, +1\}$ label in target classes
  - Prediction: $\text{sign}(\hat{y})$
- **Square loss function** $\ell(b + x^T w, y) = (y - x^T w - b)^2$
  - This is the same as treating this as a linear regression problem

$$(\widehat{w}, \widehat{b}) = \arg\min_{b,w} \sum_{i=1}^{n} (y_i - (b + x_i^T w))^2$$

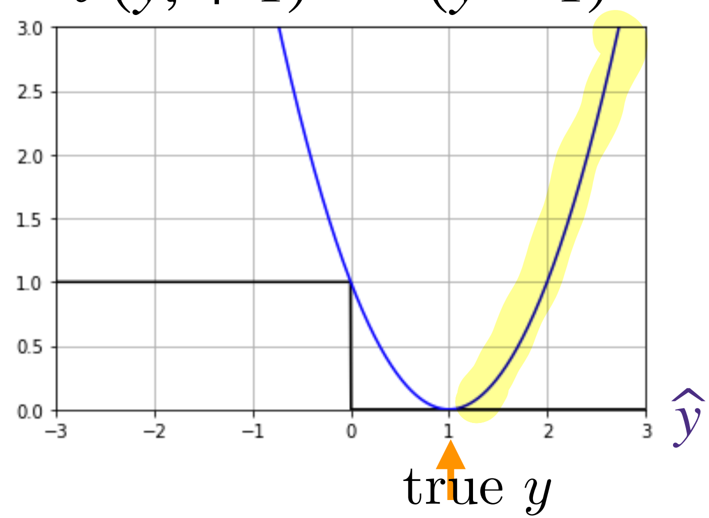
- What is the strengths and weaknesses?

+ closed form solution
- Penalyze unnecessarily overconfident pred.

$$\ell(\hat{y}, -1) = (\hat{y} + 1)^2$$

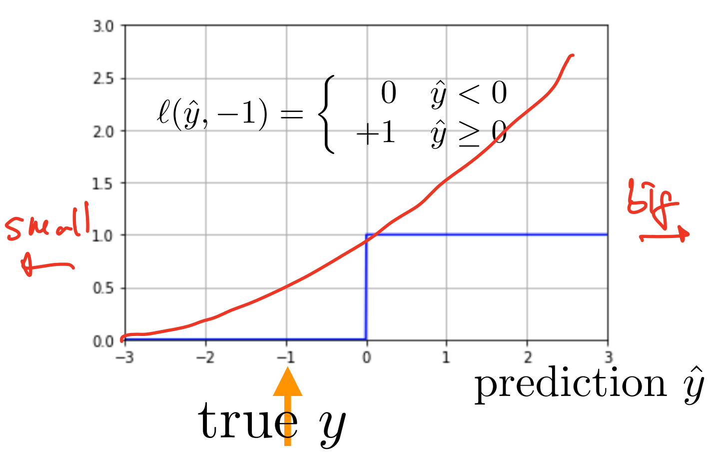


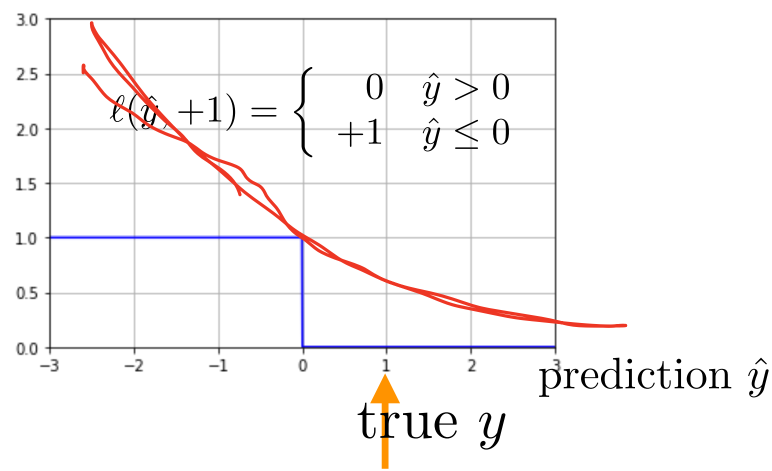
$$\ell(\hat{y}, +1) = (\hat{y} - 1)^2$$



Looking for a better loss function

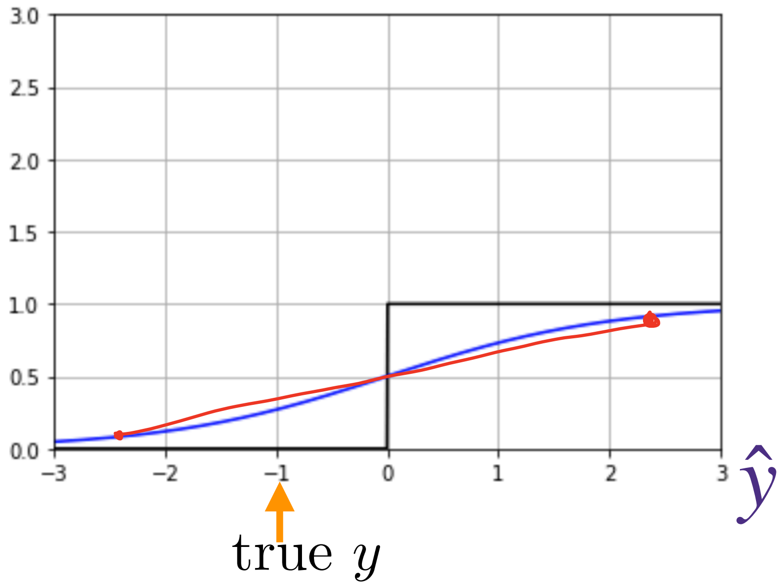
- we get better results using loss functions that
  - approximate, or captures the flavor of, the 0-1 loss
  - is more easily optimized (e.g. convex and/or non-zero derivatives)
- concretely, we want a **loss function**
  - with $\ell(\hat{y}, -1)$ small when $\hat{y} < 0$ and larger when $\hat{y} > 0$
  - with $\ell(\hat{y}, 1)$ small when $\hat{y} > 0$ and larger when $\hat{y} < 0$
  - Which has other nice characteristics, e.g., differentiable or convex

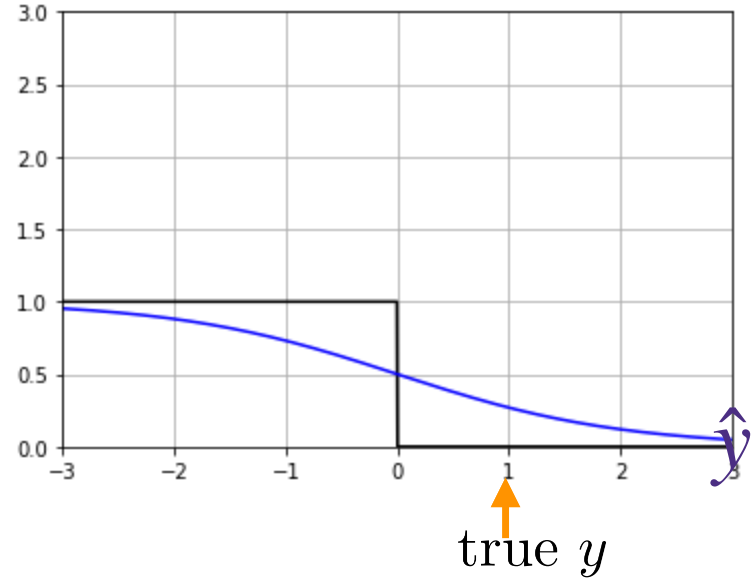




Sigmoid loss $\ell(\hat{y}, y) = \dfrac{1}{1 + e^{y\hat{y}}}$

$$\ell(\hat{y}, -1) = \frac{1}{1+e^{-\hat{y}}} \qquad \ell(\hat{y}, +1) = \frac{1}{1 + e^{\hat{y}}}$$





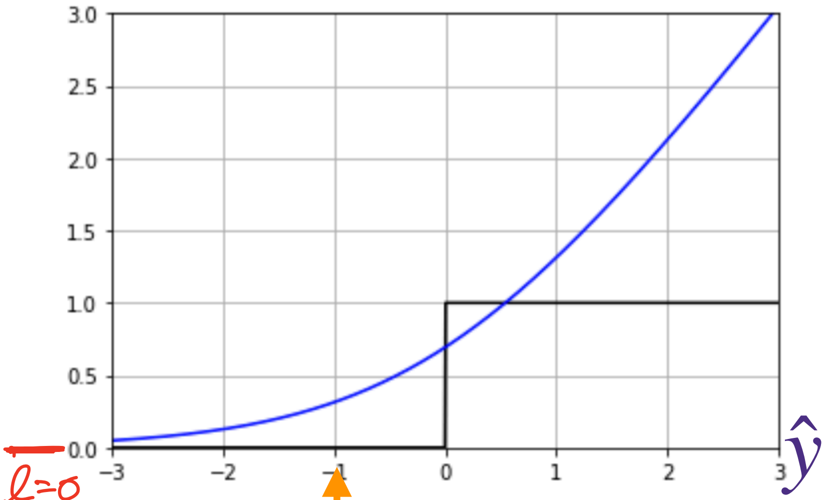
- differentiable approximation of 0-1 loss
- What is the weakness? Non-Convex $\longrightarrow$ finding global minimum is hard
- the two losses sum to one

$$\frac{1}{1 + e^{-\hat{y}}} + \frac{1}{1 + e^{\hat{y}}} = \frac{e^{\hat{y}}}{e^{\hat{y}} + 1} + \frac{1}{1 + e^{\hat{y}}} = 1$$

- softer (or smoothed) version of the 0-1 loss

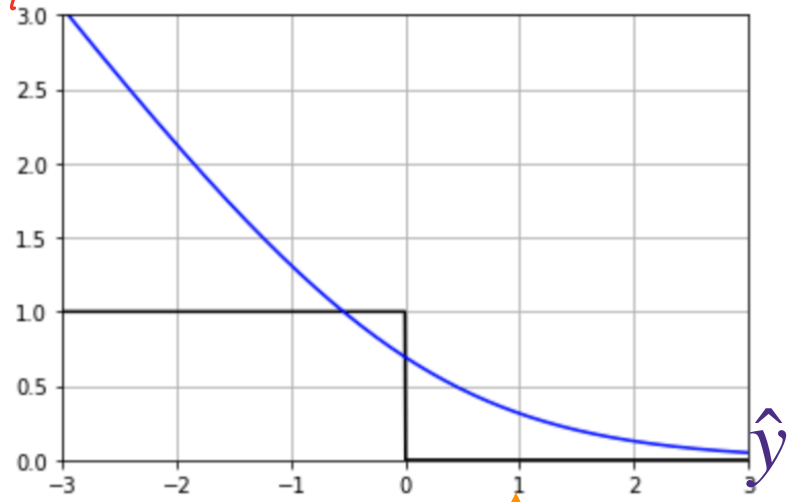
<u>Logistic loss</u> $\ell(\hat{y}, y) = \log(1 + e^{-y\hat{y}})$

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



true y

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



true y

- differentiable and convex in $\hat{y}$
- how do we show $\ell(\,\cdot\,, y)$ is convex?
- approximation of 0-1
- Most popular choice of a loss function for classification problems

logistic Regression

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

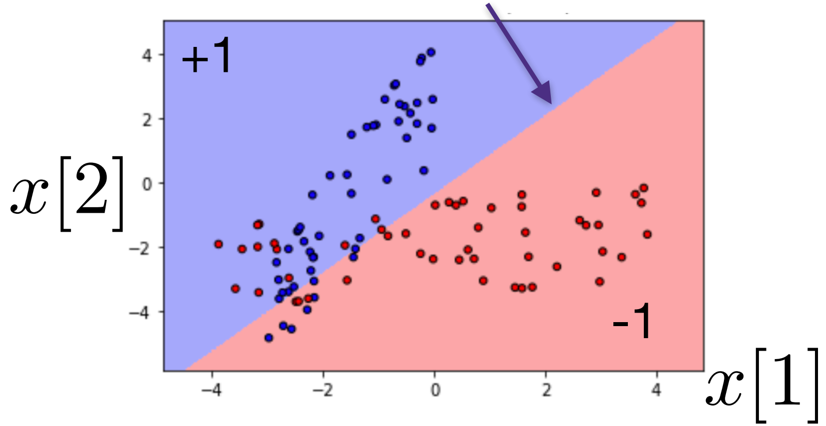
Logistic regression for binary classification

- Data $\mathcal{D} = \{(x_i \in \mathbb{R}^d, y_i \in \{-1, +1\})\}_{i=1}^n$
- Model: $\hat{y} = x^T w + b$
- Loss function: logistic loss $\ell(\hat{y}, y) = \log(1 + e^{-y\hat{y}})$
- Optimization: solve for

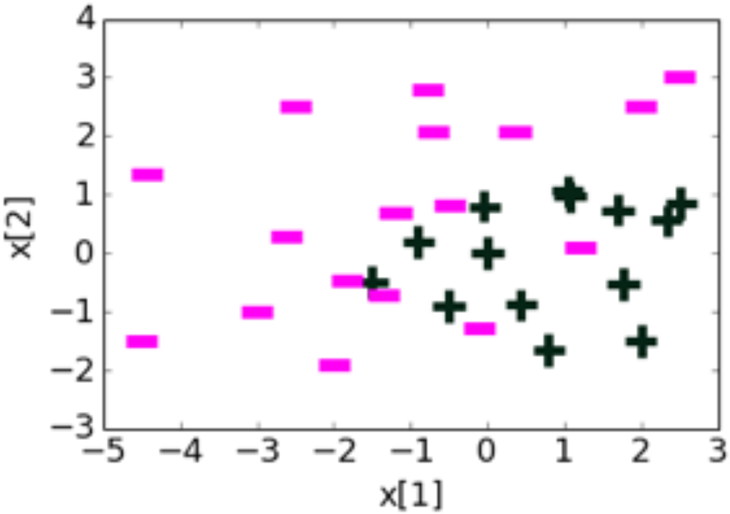
$$(\widehat{b}, \widehat{w}) = \arg\min_{b,w} \sum_{i=1}^{n} \log(1 + e^{-y_i(b + x_i^T w)})$$

- As this is a **smooth convex** optimization, it can be solved efficiently using gradient descent
- Prediction: $\text{sign}(b + x^T w)$

decision boundary at $w^T x + b = 0$



Example: adding more polynomial features

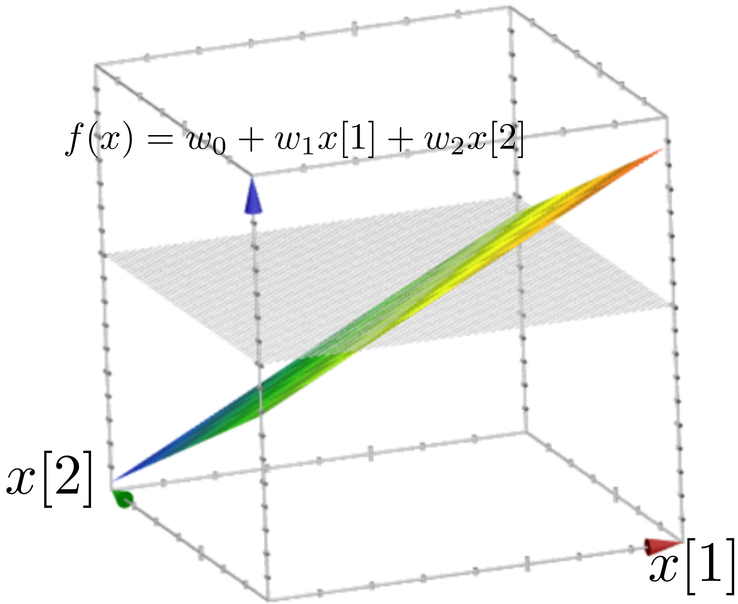


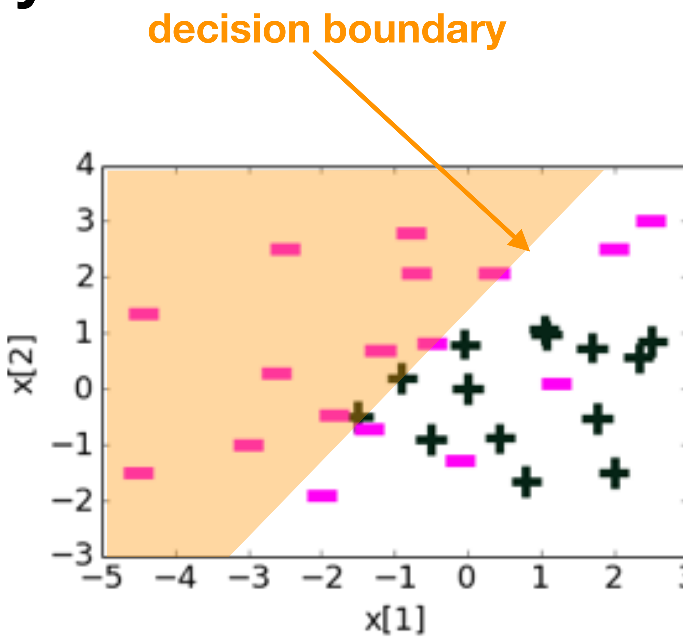
Polynomial features

$$\begin{bmatrix} h_0(x) = 1 \\ h_1(x) = x[1] \\ h_2(x) = x[2] \\ h_3(x) = x[1]^2 \\ h_4(x) = x[2]^2 \\ \vdots \end{bmatrix}$$

- data: ***x*** in 2-dimensions, ***y*** in {+1,-1}
- features: polynomials
- model: linear on polynomial features
- $$f(x) \;=\; w_0 h_0(x) + w_1 h_1(x) + w_2 h_2(x) + \cdots$$

Learned decision boundary





Feature	Value	Coefficient
$h_0(x)$	1	0.23
$h_1(x)$	x[1]	1.12
$h_2(x)$	x[2]	-1.07

- Simple **regression** models had **smooth** predictors
- Simple **classifier** models have **smooth** decision boundaries

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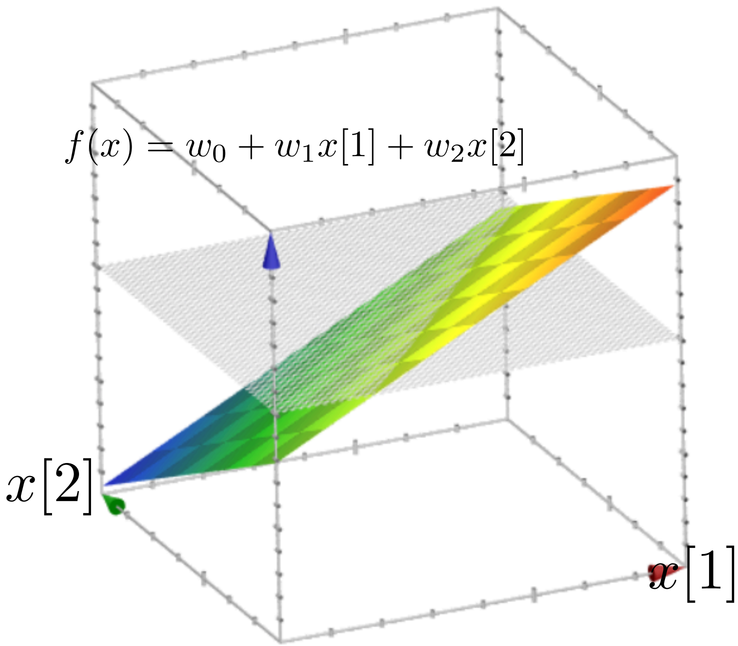

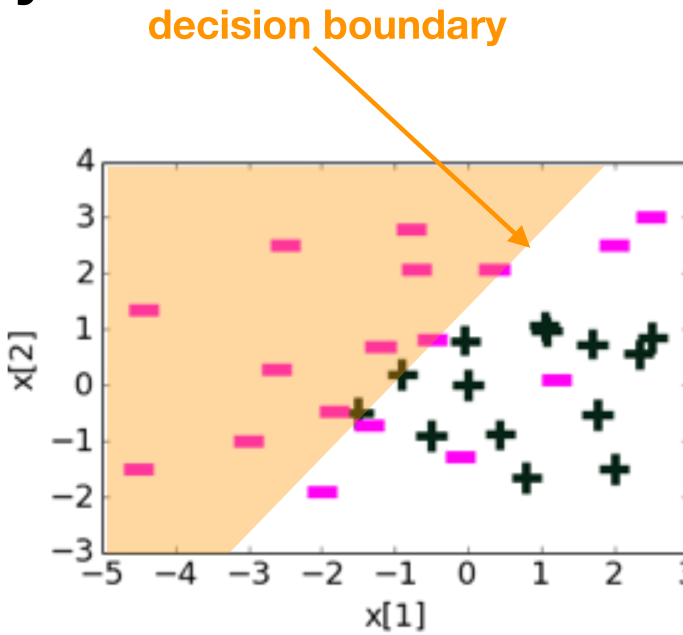

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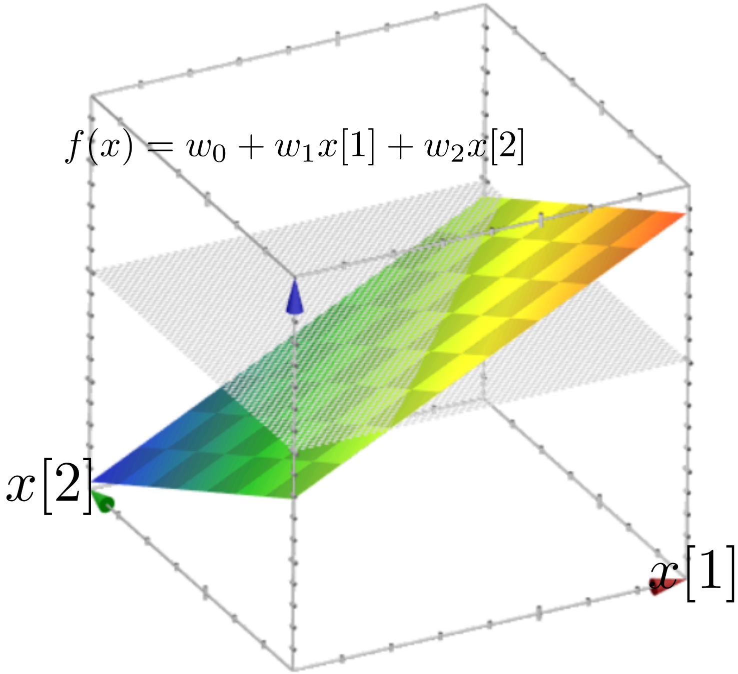

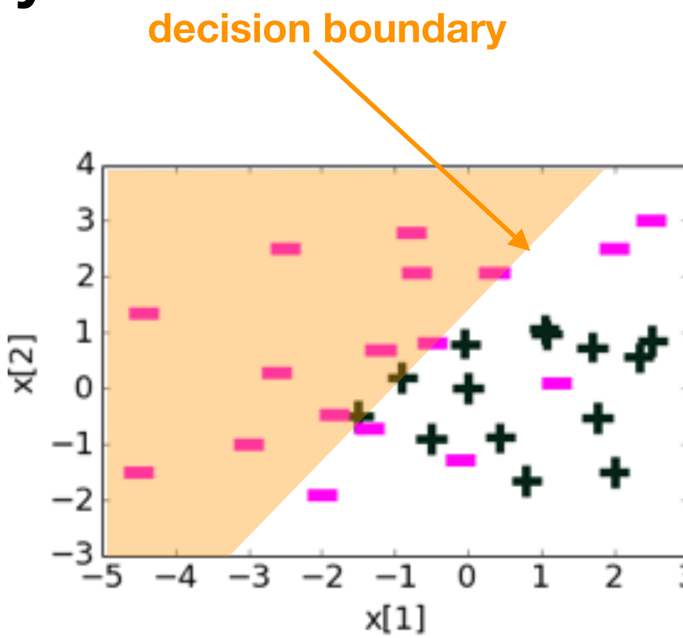

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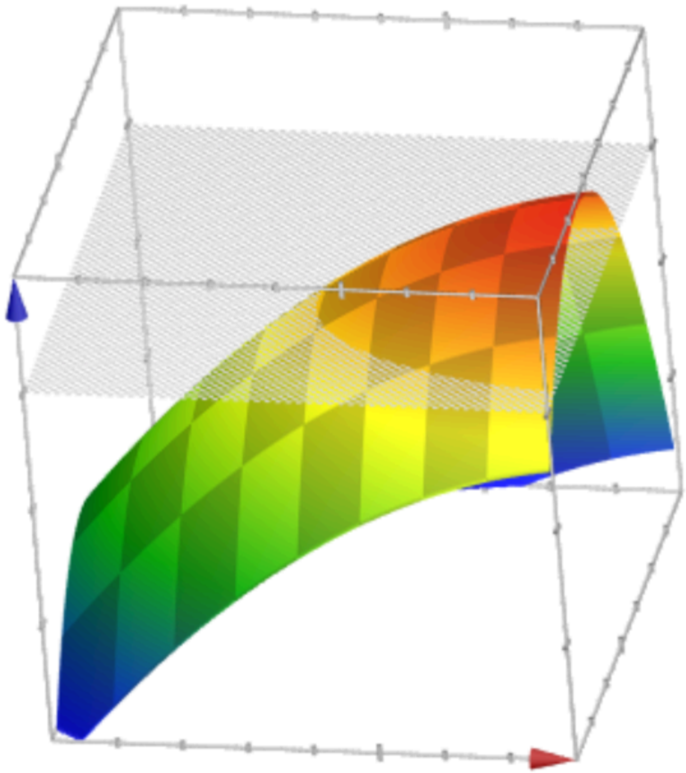
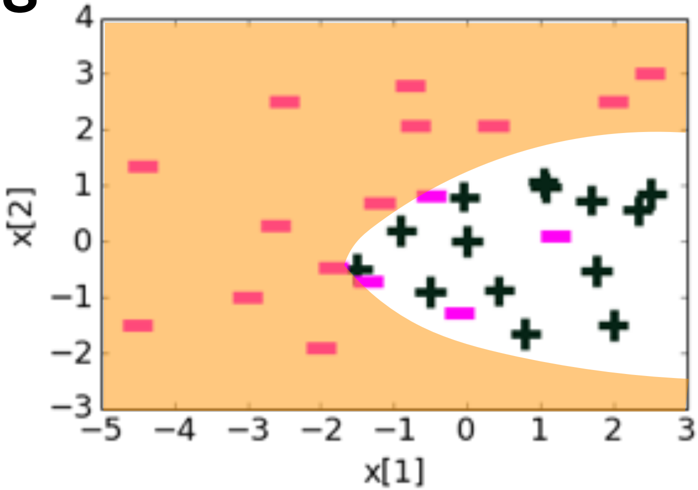
Adding quadratic features





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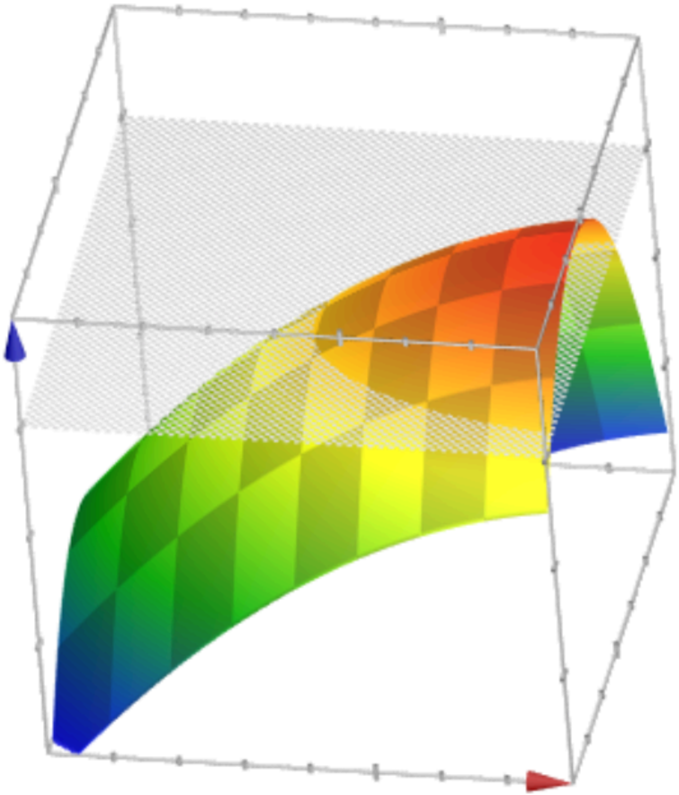
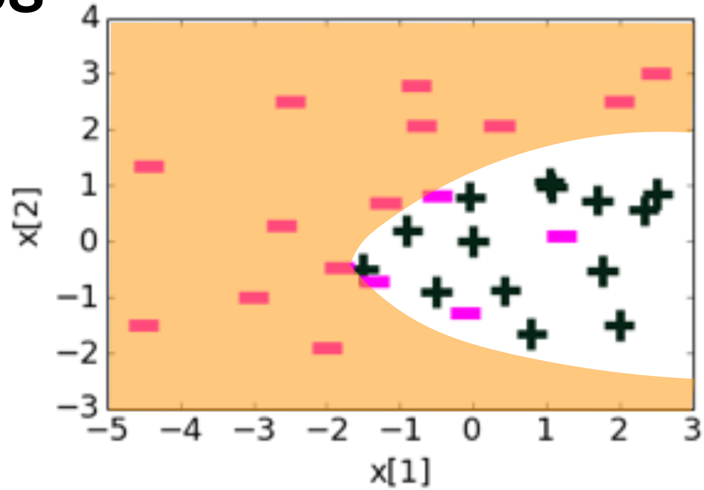
$h_0(x)$	1	1.68
$h_1(x)$	x[1]	1.39
$h_2(x)$	x[2]	-0.59
$h_3(x)$	$(x[1])^2$	-0.17
$h_4(x)$	$(x[2])^2$	-0.96
$h_5(x)$	x[1]x[2]	Omitted

- Adding more features gives more complex models
- Decision boundary becomes more complex

Adding quadratic features





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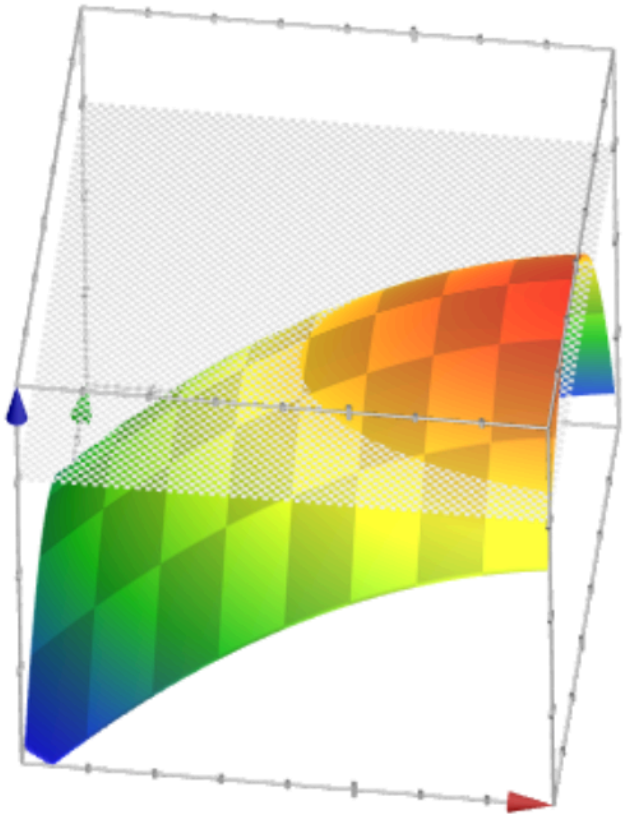

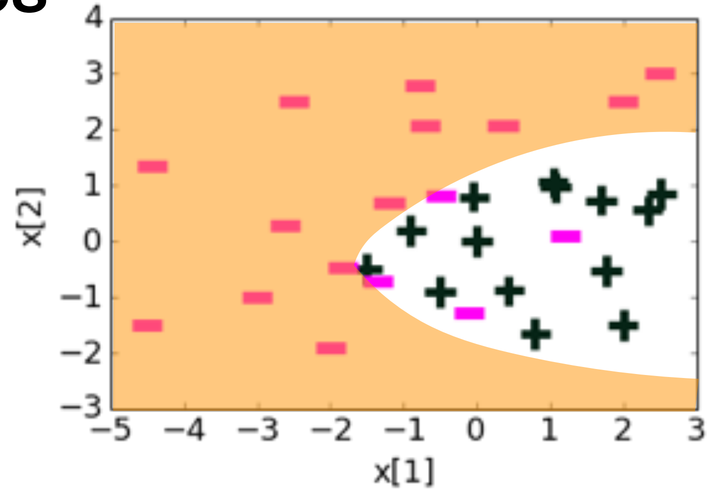

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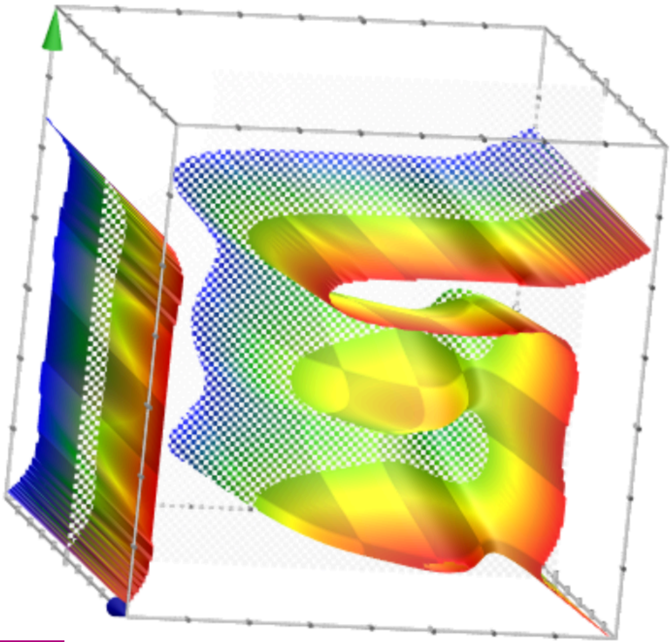
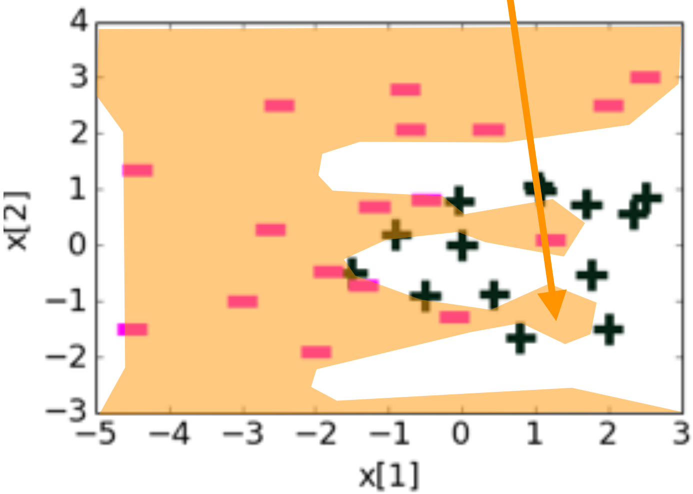
Adding higher degree polynomial features



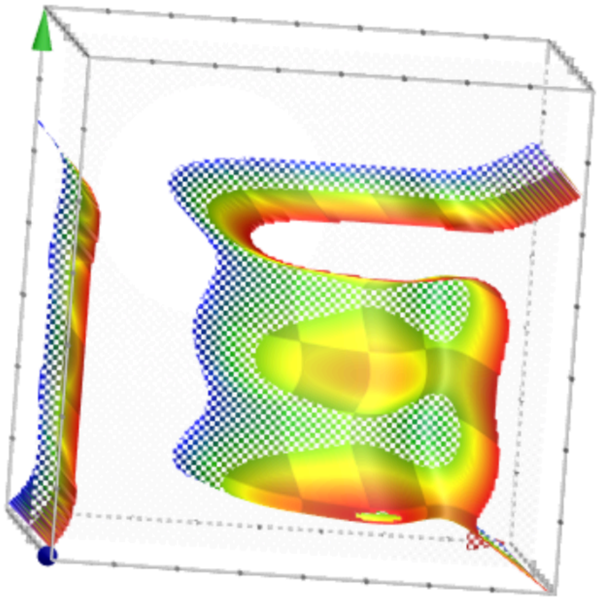
Overfitting leads to non-generalization



Feature	Value	Coefficient learned
$h_0(x)$	1	21.6
$h_1(x)$	x[1]	5.3
$h_2(x)$	x[2]	-42.7
$h_3(x)$	$(x[1])^2$	-15.9
$h_4(x)$	$(x[2])^2$	-48.6
$h_5(x)$	$(x[1])^3$	-11.0
$h_6(x)$	$(x[2])^3$	67.0
$h_7(x)$	$(x[1])^4$	1.5
$h_8(x)$	$(x[2])^4$	48.0
$h_9(x)$	$(x[1])^5$	4.4
$h_{10}(x)$	$(x[2])^5$	-14.2
$h_{11}(x)$	$(x[1])^6$	0.8
$h_{12}(x)$	$(x[2])^6$	-8.6

Coefficient values getting large

Adding higher degree polynomial features



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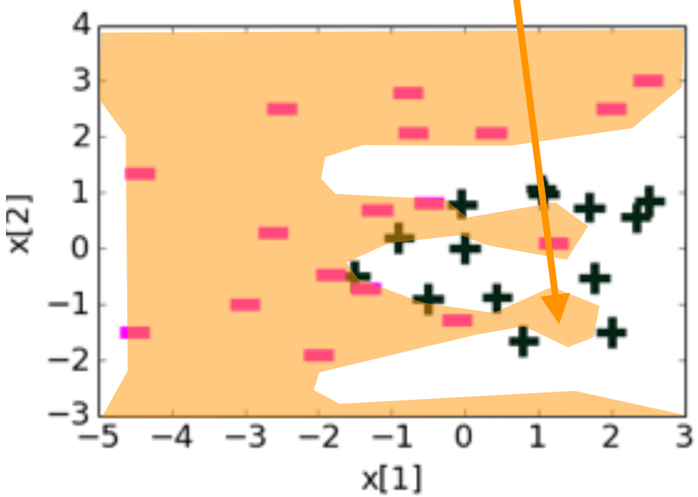

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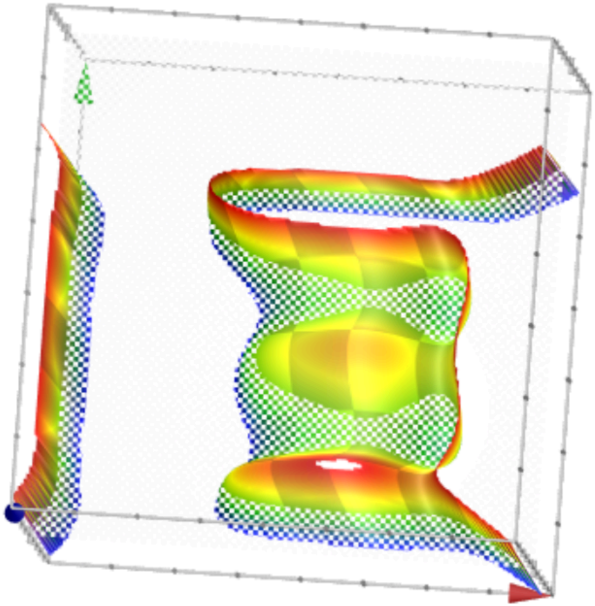

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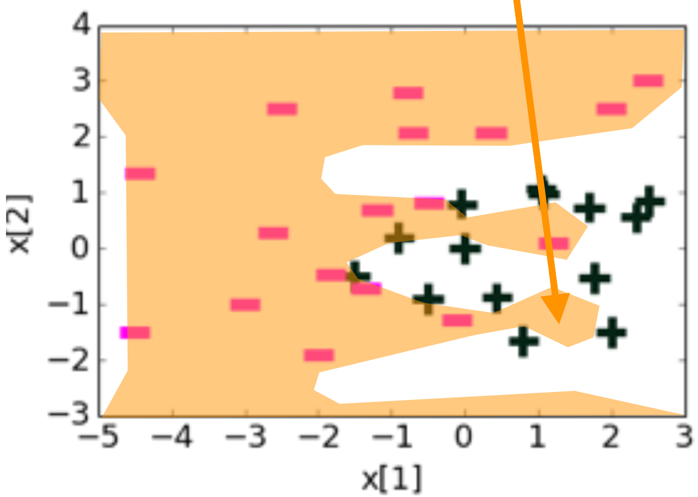

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$h_{12}(x)$	$(x[2])^6$	-8.6

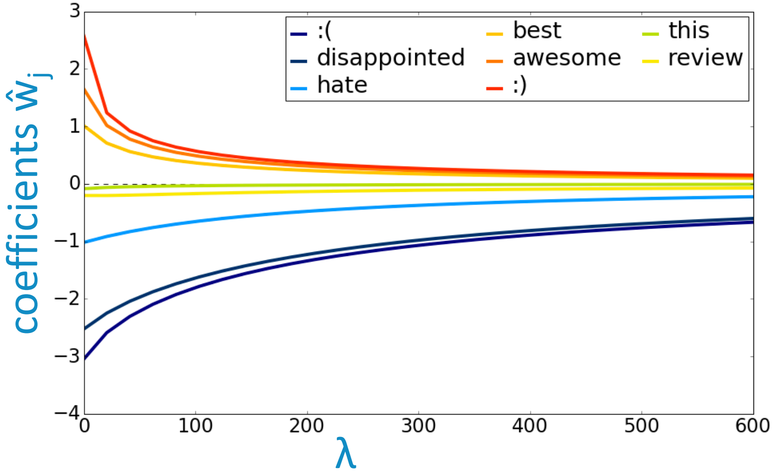
Coefficient values getting large

- Overfitting leads to very large values of

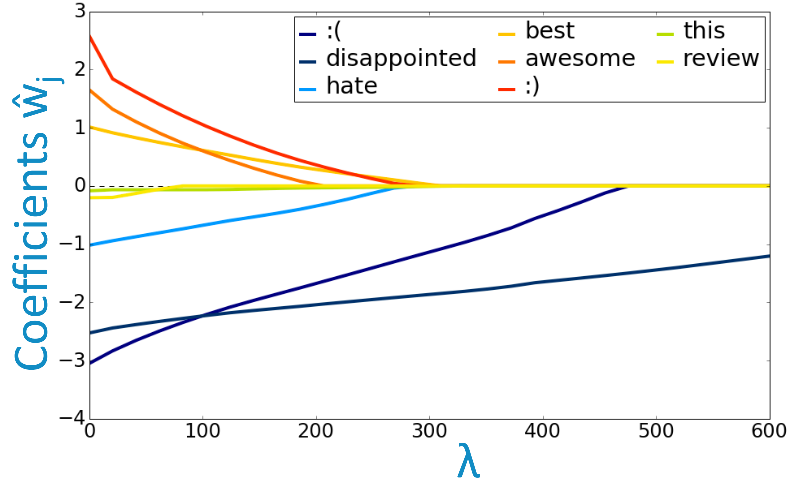
$$f(x) = w_0 h_0(x) + w_1 h_1(x) + w_2 h_2(x) + \cdots$$

Regularization path

ℓ_2 regularizer: $\|W\|_2^2 = |w_1|^2 + \cdots + |w_d|^2$



ℓ_1 regularizer: $\|w\|_1 = |w_1| + \cdots + |w_d|$



- Absolute regularizer (a.k.a ℓ_1 regularizer) gives sparse parameters, which is desired for interpretability, feature selection, and efficiency

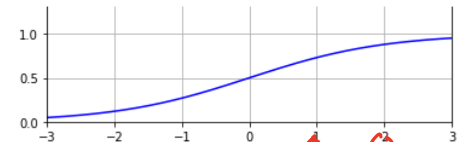
Probabilistic interpretation of logistic regression

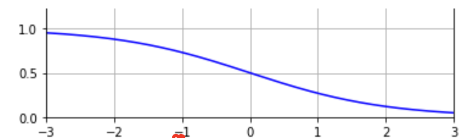
- just as Maximum Likelihood Estimator (MLE) under linear model and additive Gaussian noise model recovers **linear least squares**,
- we study a particular noise model that recovers **logistic regression** as MLE

No noise label : $y_i = \text{sign}(w_*^T x_i)$

- a probabilistic noise model for Binary labels:

$$\begin{cases} \mathbb{P}(y_i = +1 \,|\, x_i) = \dfrac{1}{1 + e^{-w_*^T x_i}} \\[2ex] \mathbb{P}(y_i = -1 \,|\, x_i) = \dfrac{1}{1 + e^{w_*^T x_i}} \end{cases}$$





$w_*^T x_i$

with a ground truth model parameter $w_* \in \mathbb{R}^d$

- this function $\sigma(z) = \dfrac{1}{1 + e^{-z}}$ is called a **logistic function** (not to be confused with logistic loss, which is different) or a **sigmoid function**
- if we know that the data came from such a model, but do not know the ground truth parameter $w \in \mathbb{R}^d$, we can apply MLE to find the best w
- this MLE recovers the logistic regression algorithm, exactly

Maximum Likelihood Estimator (MLE)

- if the data came from a probabilistic model model: $\Big(\underbrace{\frac{1}{1+e^{-w^Tx}}}_{\mathbb{P}(y_i=+1|x_i)}, \underbrace{\frac{1}{1+e^{w^Tx}}}_{\mathbb{P}(y_i=-1|x_i)}\Big)$

- log-likelihood of observing a data point (x_i, y_i) is

$$\text{log-likelihood} = \log\Big(\mathbb{P}(y_i|x_i)\Big) = \begin{cases} \log\left(\frac{1}{1+e^{-w^Tx_i}}\right) & \text{if } y_i = +1 \\ \log\left(\frac{1}{1+e^{w^Tx_i}}\right) & \text{if } y_i = -1 \end{cases}$$

- Maximum Likelihood Estimator is the one that maximizes the sum of all log-likelihoods on training data points

$$\hat{w}_{\text{MLE}} = \arg\max_{w} \ \mathbb{P}(\{y_1, \ldots, y_n\} \,|\, \{x_1, \ldots, x_n\})$$

$$= \arg\max_{w} \ \underbrace{\prod_{i=1}^{n} \mathbb{P}(y_i | x_i)}$$

(independence)

$$= \arg\max_{w} \ \sum_{i=1}^{n} \log \mathbb{P}(y_i | x_i)$$

$$\sum_{i: y_i=+1} \log\left(\frac{1}{1+e^{-w^Tx_i}}\right) + \sum_{i: y_i=-1} \log\left(\frac{1}{1+e^{w^Tx_i}}\right)$$

(substitution)

- notice that this is exactly the **logistic regression:**

$$\hat{w}_{\text{logistic}} = \arg\min_{w} \frac{1}{n}\Big(\sum_{i:y_i=-1} \log(1+e^{w^T x_i}) + \sum_{i:y_i=1} \log(1+e^{-w^T x_i}) \Big)$$

- once we have trained a model $\hat{w}_{\text{logistic}}$, we can make a hard prediction $\hat{y}$ of the label at an input example x

$$\hat{y} = \begin{cases} +1 & \text{if } \mathbb{P}(+1|x) \geq \mathbb{P}(-1|x) \\ -1 & \text{otherwise} \end{cases}$$

$$= \begin{cases} +1 & \text{if } \frac{1}{1+e^{-w^T x}} \geq \frac{1}{1+e^{w^T x}} \\ -1 & \text{otherwise} \end{cases}$$

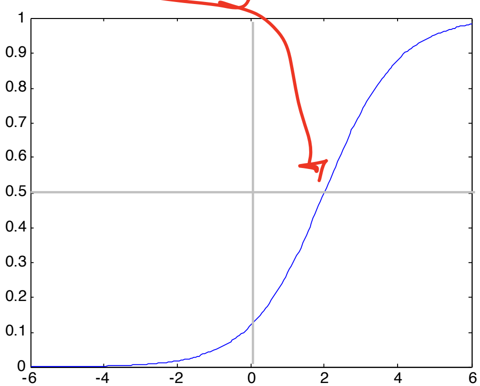
$$= \begin{cases} +1 & \text{if } 1 \leq e^{2w^T x} \\ -1 & \text{otherwise} \end{cases}$$

$$= \text{sign}(w^T x)$$

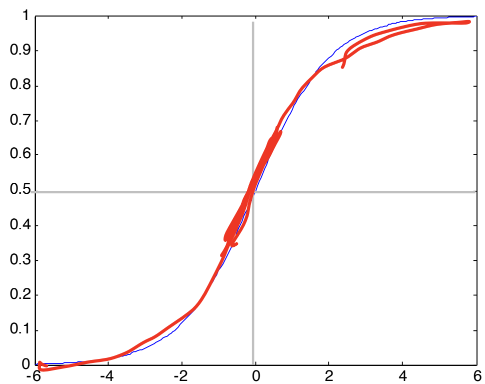
Understanding the sigmoid

$$g\left(w_0 + \sum_i w_i x_i\right) = \frac{1}{1 + e^{w_0 + \sum_i w_i x_i}}$$

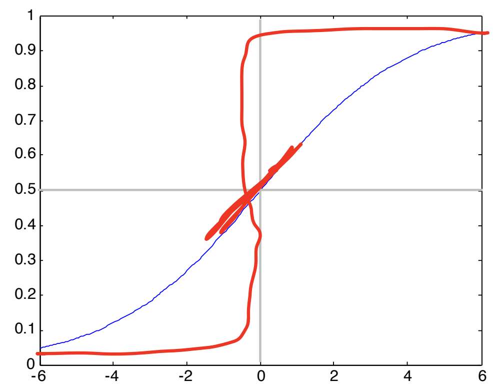
w_0=-2, w_1=-1



w_0=0, w_1=-1



w_0=0, w_1=-0.5

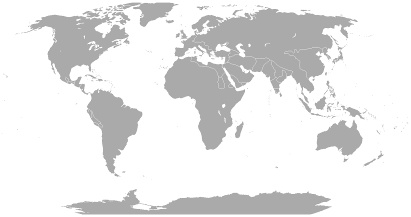


Multi-class regression

How do we encode categorical data *y*?

- so far, we considered Binary case where there are two categories
- encoding y is simple: {+1,-1}

- multi-class classification predicts categorial y
- taking values in $C = \{c_1, \ldots, c_k\}$
- c_j's are called **classes** or **labels**
- examples:



Country of birth
(Argentina, Brazil, USA,...)

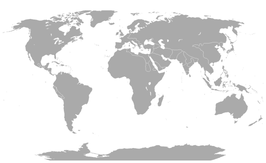
Zipcode
(10005, 98195,...)

All English words

- a **k-class classifier** predicts y given x

Embedding c_j's in real values

- for optimization we need to **embed** raw categorical c_j's into real valued vectors
- there are many ways to embed categorial data
    - True->1, False->-1
    - Yes->1, Maybe->0, No->-1
    - Yes->(1,0), Maybe->(0,0), No->(0,1)
    - Apple->(1,0,0), Orange->(0,1,0), Banana->(0,0,1)
    - Ordered sequence:
      (Horse 3, Horse 1, Horse 2) -> (3,1,2)
- we use **one-hot embedding** (a.k.a. **one-hot encoding**)
    - each class is a standard basis vector in $k-$dimension



Country of birth

(Argentina, Brazil, USA,...)

$\underbrace{\hphantom{xxxxxxxxxx}}_{\text{196 categories}}$

1-hot encoding

x	$h_1(x)$	$h_2(x)$	...	$h_{195}(x)$	$h_{196}(x)$
Brazil		1			
Zimbabwe					1

$\underbrace{\hphantom{xxxxxxxxxxxxxxxxxxxx}}_{\text{196 features}}$

Multi-class logistic regression

- data: categorical y in $\{c_1, \ldots, c_k\}$ with k categories

  we use one-hot encoding, s.t. $y = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$ implies that $y = c_1$

- model: linear vector-function makes a linear prediction $\hat{y} \in \mathbb{R}^k$

$$\hat{y}_i \; = \; f(x_i) \; = \; w^T x_i \quad \in \mathbb{R}^k$$

with model parameter matrix $w \in \mathbb{R}^{d \times k}$ and sample $x_i \in \mathbb{R}^d$

$$f(x_i) \; = \; \begin{bmatrix} f_1(x_i) \\ f_2(x_i) \\ \vdots \\ f_k(x_i) \end{bmatrix} \; = \; \underbrace{\begin{bmatrix} w_{1,0} & w_{1,1} & w_{1,2} & \cdots \\ w_{2,0} & w_{2,1} & w_{2,2} & \cdots \\ \vdots & & & \\ w_{k,0} & w_{k,1} & w_{k,2} & \cdots \end{bmatrix}}_{w^T} \underbrace{\begin{bmatrix} 1 \\ x_i[1] \\ \vdots \\ x_i[d] \end{bmatrix}}_{x_i} \; = \; \begin{bmatrix} w_{1,0} + w_{1,1}x_i[1] + w_{1,2}x_i[2] + \cdots \\ w_{2,0} + w_{2,1}x_i[1] + w_{2,2}x_i[2] + \cdots \\ \vdots \\ w_{k,0} + w_{k,1}x_i[1] + w_{k,2}x_i[2] + \cdots \end{bmatrix}$$

$$w = \begin{bmatrix} w[:,1] & w[:,2] & \cdots & w[:,k] \end{bmatrix}$$

- Logistic regression

2 classes

$$\mathbb{P}(y_i = -1 \mid x_i) = \frac{1}{1 + e^{w^T x_i}}$$

$$\mathbb{P}(y_i = +1 \mid x_i) = \frac{1}{1 + e^{-w^T x_i}} = \frac{e^{w^T x_i}}{1 + e^{w^T x_i}}$$

k classes

$$\mathbb{P}(y_i = c_1 \mid x_i) = \frac{e^{w[:,1]^T x_i}}{e^{w[:,1]^T x_i} + \cdots + e^{w[:,k]^T x_i}}$$

$$\vdots$$

$$\mathbb{P}(y_i = c_k \mid x_i) = \frac{e^{w[:,k]^T x_i}}{e^{w[:,1]^T x_i} + \cdots + e^{w[:,k]^T x_i}}$$

Without loss of generality setting w[:,1]=0 when $k = 2$ recovers the original binary class case

Maximum Likelihood Estimator

$$\text{maximize}_w \; \frac{1}{n} \sum_{i=1}^{n} \log(\mathbb{P}(y_i \mid x_i))$$

$$\text{maximize}_{w \in \mathbb{R}^d} \; \frac{1}{n} \sum_{i=1}^{n} \log\left(\frac{1}{1 + e^{-y_i w^T x_i}}\right)$$

$$\text{maximize}_{w \in \mathbb{R}^{d \times k}} \frac{1}{n} \sum_{i=1}^{n} \boxed{\sum_{j=1}^{k} \mathbf{I}\{y_i = c_j\} \log\left(\frac{e^{w[:,j]^T x_i}}{\sum_{j'=1}^{k} e^{w[:,j']^T x_i}}\right)}$$

$\mathbf{I}\{y_i = j\}$ is an indicator that is one only if $y_i = j$

Questions?