CMSC 478
Lecture 4

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Supervised Learning: Logistic Regression

Some slides are slightly adapted from Chris Re, Stanford ML

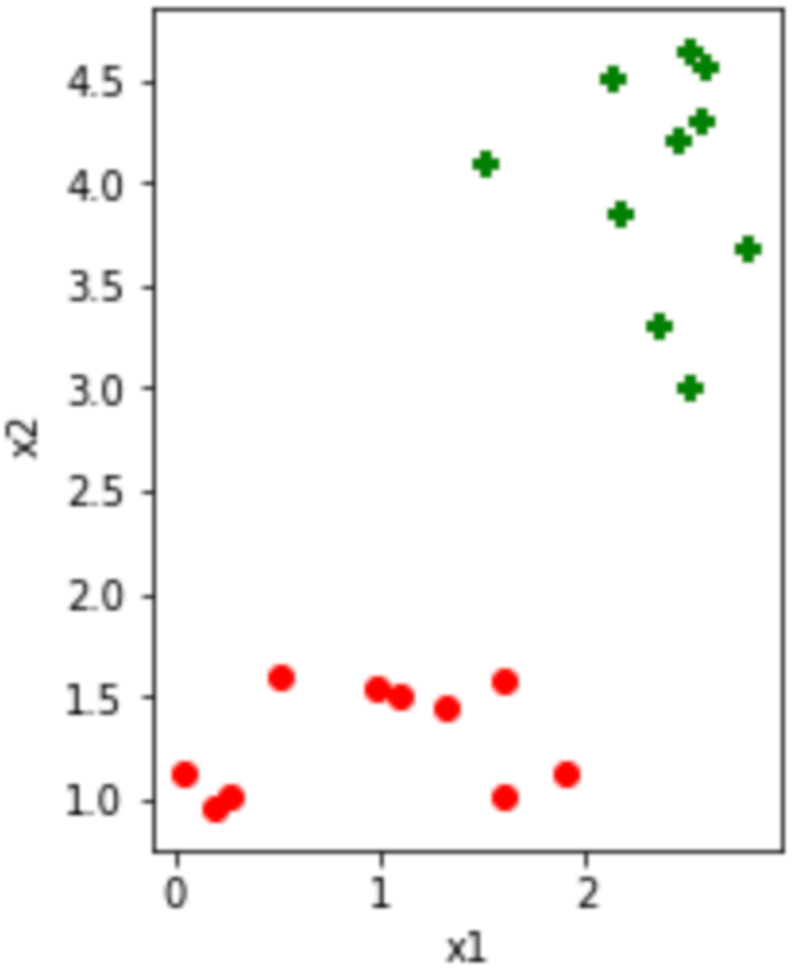
Optimization Method Summary

Method	Compute per Step	Number of Steps to convergence
SGD	$\theta(d)$	$\approx \epsilon^{-2}$
Minibatch SGD		
GD	$\theta(nd)$	$\approx \epsilon^{-1}$
Newton	$\Omega(nd^2)$	$\approx \log(1/\epsilon)$

- In classical stats, d is small (< 100), n is often small, and *exact parameters matter*
- In modern ML, d is huge (billions, trillions), n is huge (trillions), and parameters used *only* for prediction
  - These are approximate number of computing steps
  - Convergence happens when loss settles to within an error range around the final value.
  - Newton would be very fast, where SGD needs a lot of step, but individual steps are fast, makes up for it
- As a result, (minibatch) SGD is the *workhorse* of ML.

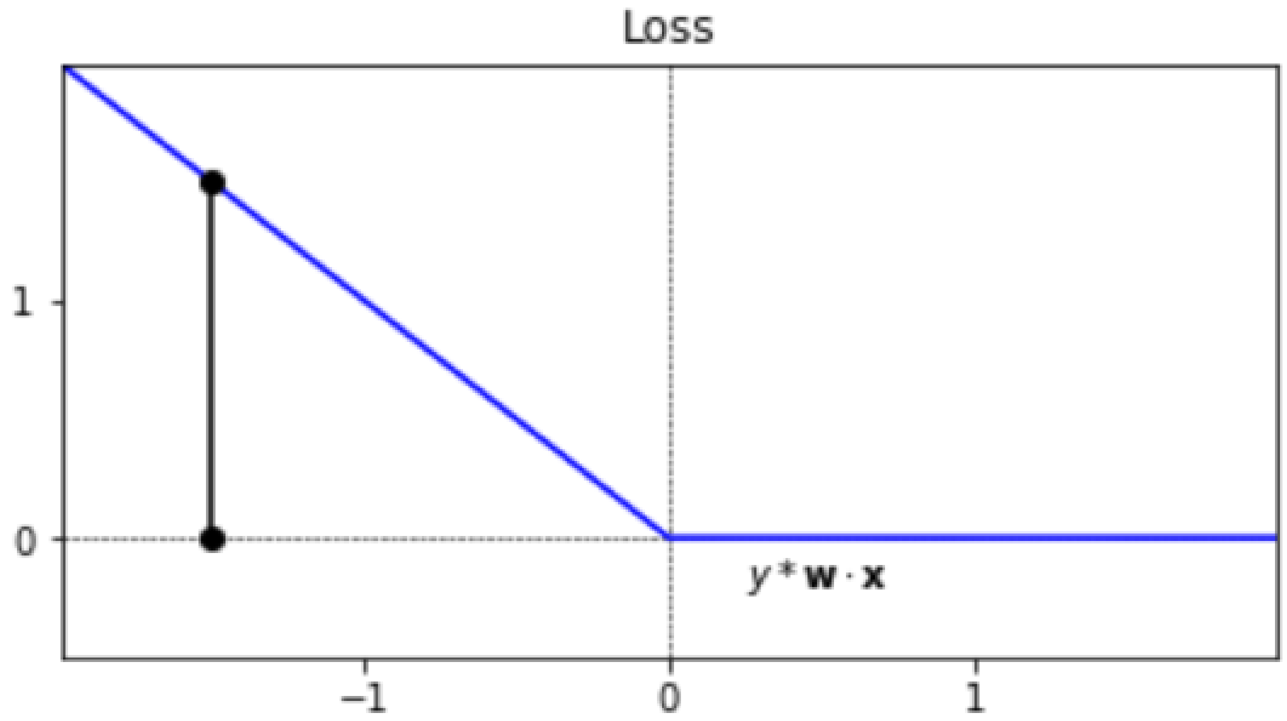
Linear Classification

	x1	x2	y
0	0.048589	1.120275	-1
1	0.200023	0.956716	-1
2	1.595538	1.023582	-1
3	1.315929	1.452371	-1
4	1.087080	1.513219	-1
5	0.512235	1.594651	-1
6	0.265039	1.008506	-1
7	1.606480	1.571889	-1
8	0.977585	1.550227	-1
9	1.908708	1.121259	-1
10	2.503476	3.002576	1



Perceptron Loss

$$L_P(y, \mathbf{w}\cdot\mathbf{x}) = \begin{cases} 0 & \text{if } y * \mathbf{w}\cdot\mathbf{x} > 0 \\ -y * \mathbf{w}\cdot\mathbf{x} & \text{otherwise} \end{cases}$$

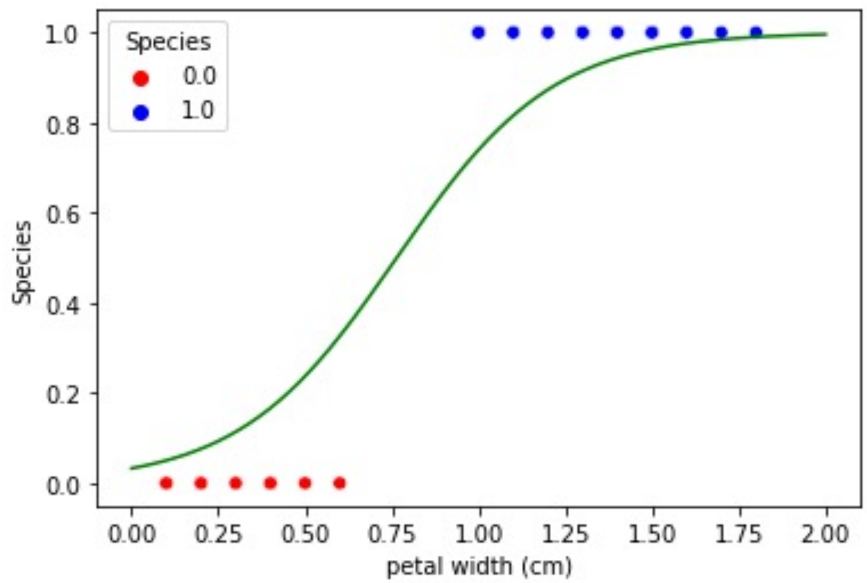


```python
def perceptron(df, label = 'y', epochs = 100, bias = True):

    if bias:
        df = df.copy()
        df.insert(0, '_x0_', 1)

    w = np.zeros(len(df.columns) - 1)
    features = [column for column in df.columns if column != label]

    for _ in range(epochs):
        errors = 0
        for _, row in df.iterrows():
            x = row[features]
            y = row[label]
            if y * np.dot(w, x) <= 0:
                w = w + y * x
                errors += 1
            yield w.copy()
        if errors == 0:
            break
```



Graph of Iris Dataset with logistic regression

Logistic Regression: Link Functions

Given a training set $\{(x^{(i)}, y^{(i)})$ for $i = 1, \ldots, n\}$ let $y^{(i)} \in \{0, 1\}$.
Want $h_\theta(x) \in [0, 1]$. Let's pick a smooth function:

$$h_\theta(x) = g(\theta^T x)$$

Here, g is a link function. There are *many*...

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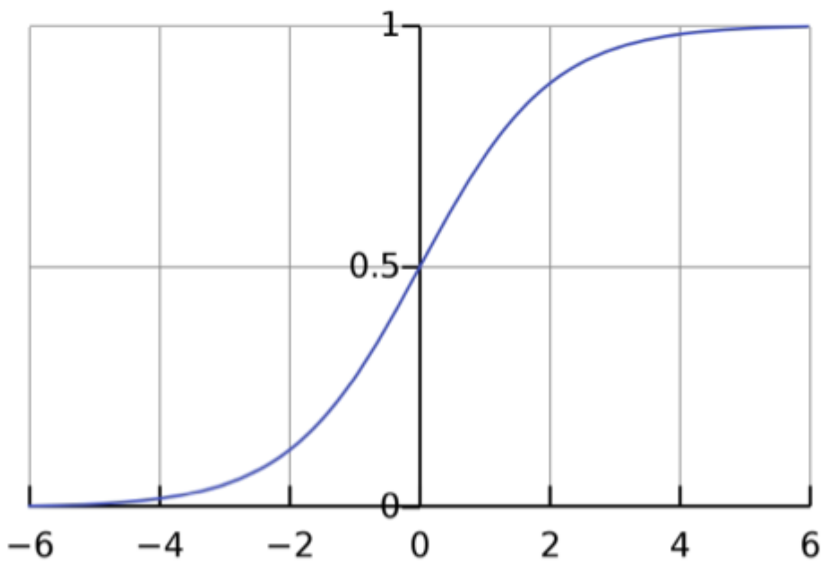
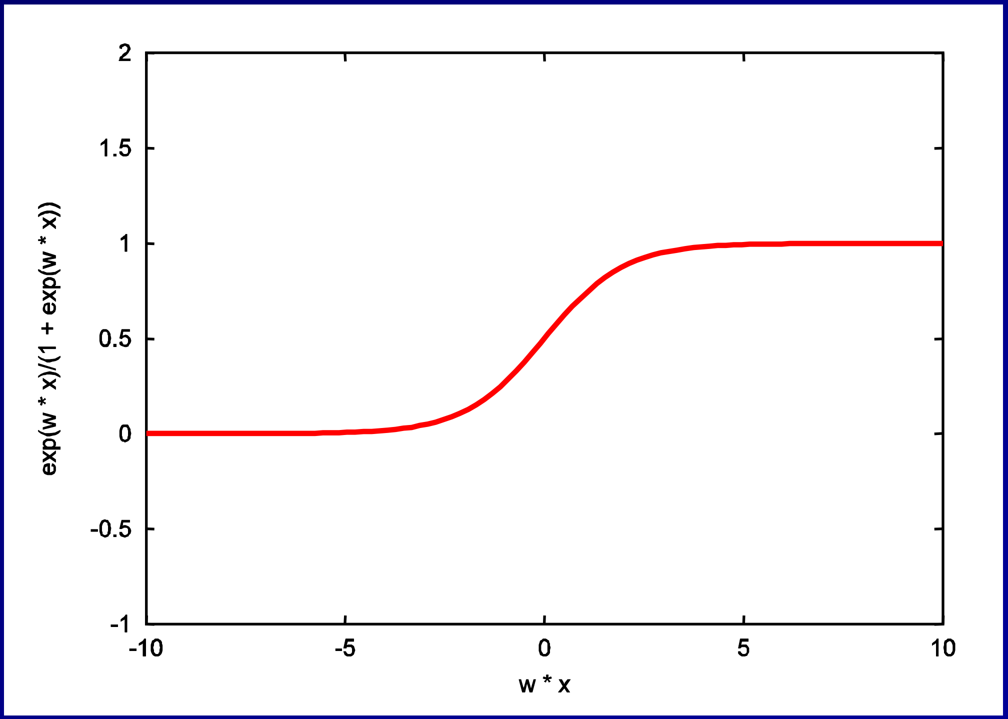
$$g(z) = \frac{1}{1 + e^{-z}}.$$



Why the exp function?

- One reason: A linear function has a range from [$-\infty$, ∞] and we need to force it to be positive and sum to 1 in order to be a probability:



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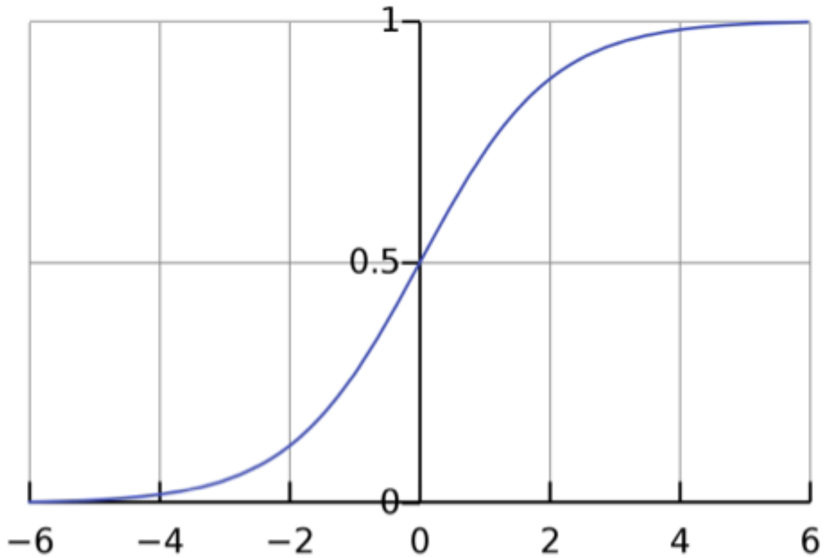
SIGMOID



How do we interpret $h_\theta(x)$?

$$P(y = 1 \mid x; \theta) = h_\theta(x)$$
$$P(y = 0 \mid x; \theta) = 1 - h_\theta(x)$$

Logistic Regression: Link Functions

Let's write the Likelihood function. Recall:

$$P(y = 1 \mid x; \theta) = h_\theta(x)$$
$$P(y = 0 \mid x; \theta) = 1 - h_\theta(x)$$

Then,

$$L(\theta) = P(y \mid X; \theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta)$$

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Conditional Distribution P(y | X)

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How do we go to something similar to a cost function from P (y I X; θ) ?

- Maximum Likelihood Estimation (MLE)

Logistic Regression: Link Functions

Let's write the Likelihood function. Recall:

$$
\begin{aligned}
P(y = 1 \mid x; \theta) =& h_\theta(x) \\
P(y = 0 \mid x; \theta) =& 1 - h_\theta(x)
\end{aligned}
$$

Then,

$$
\begin{aligned}
L(\theta) =& P(y \mid X; \theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta) \\
=& \prod_{i=1}^{n} h_\theta(x^{(i)})^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}} \quad \text{exponents encode ``if-then''}
\end{aligned}
$$

Logistic Regression: Link Functions

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Then,

$$L(\theta) = P(y \mid X; \theta) = \prod_{i=1}^{n} p(y^{(i)} \mid x^{(i)}; \theta)$$
$$= \prod_{i=1}^{n} h_\theta(x^{(i)})^{y^{(i)}} (1 - h_\theta(x^{(i)}))^{1-y^{(i)}} \quad \text{exponents encode ``if-then''}$$

Taking logs to compute the log likelihood $\ell(\theta)$ we have:

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

Now to solve it...

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(x^{(i)}))$$

We maximize for θ but we already saw how to do this! Just compute derivative, run (S)GD and you're done with it!

Takeaway: This is *another* example of the max likelihood method: we setup the likelihood, take logs, and compute derivatives.

Time Permitting: There is magic in the derivative. . .

Even more, the batch update can be written in a *remarkably familiar* form:

$$\theta^{(t+1)} = \theta^{(t)} + \sum_{j \in B} (y^{(j)} - h_\theta(x^{(j)}))x^{(j)}.$$

We sketch why (you can check!) We drop superscripts to simplify notation and examine a single data point:

$$\begin{aligned}
&y \log h_\theta(x) + (1-y)\log(1-h_\theta(x)) \\
=& -y\log(1+e^{-\theta^T x}) + (1-y)(-\theta^T x) - (1-y)\log(1+e^{-\theta^T x}) \\
=& -\log(1+e^{-\theta^T x}) - (1-y)(\theta^T x)
\end{aligned}$$

We used $1 - h_\theta(x) = \frac{e^{-\theta^T x}}{1-e^{-\theta^T x}}$. We now compute the derivative of this expression wrt θ and get:

$$\frac{e^{-\theta^T x}}{1+e^{-\theta^T x}}x - (1-y)x = (y - h_\theta(x))x$$

Batch Gradient Ascent for Logistic Regression

Given: training examples $(\mathbf{x}_i, y_i)$, $i = 1 \ldots N$

Let $\mathbf{w} = (0, 0, 0, 0, \ldots, 0)$ be the initial weight vector.

Repeat until convergence

  Let $\mathbf{g} = (0, 0, \ldots, 0)$ be the gradient vector.

  For $i = 1$ **to** N **do**

    $p_i = 1/(1 + \exp[-\mathbf{w} \cdot \mathbf{x}_i])$

    $\text{error}_i = y_i - p_i$

    For $j = 1$ **to** n **do**

      $g_j = g_j + \text{error}_i \cdot x_{ij}$

  $\mathbf{w} := \mathbf{w} + \eta \mathbf{g}$ step in direction of increasing gradient

- An online gradient ascent algorithm can be constructed, of course
- Most statistical packages use a second-order (Newton-Raphson) algorithm for faster convergence. Each iteration of the second-order method can be viewed as a weighted least squares computation, so the algorithm is known as Iteratively-Reweighted Least Squares (IRLS)

Perceptron Learning Algorithm

- Modify link function to output either 0 or 1.
- Make g to be a threshold function
- Then use same $h_\theta(x) = g(\theta^T x)$ using this g
- Follow the same update rule for θ

$$g(z) = \begin{cases} 1 & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases}$$

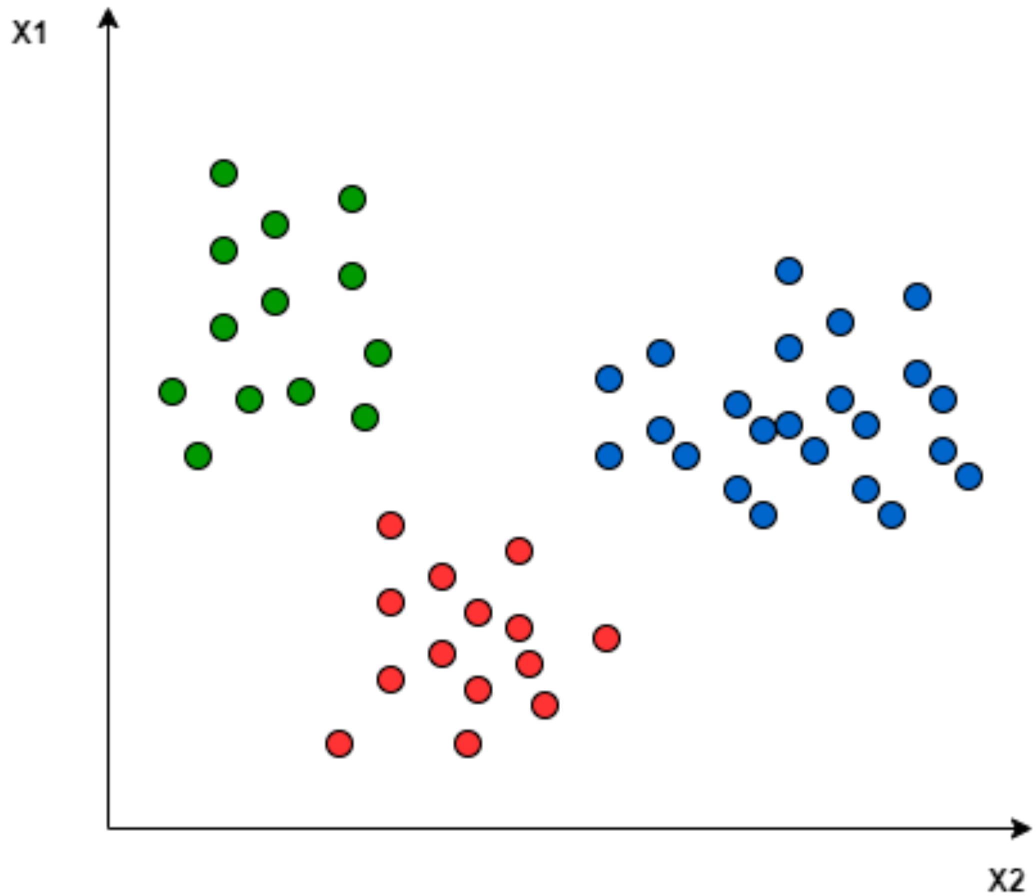
Logistic Regression Implements a Linear Discriminant Function

- In the 2-class 0/1 loss function case, we should predict $\hat{y} = 1$ if

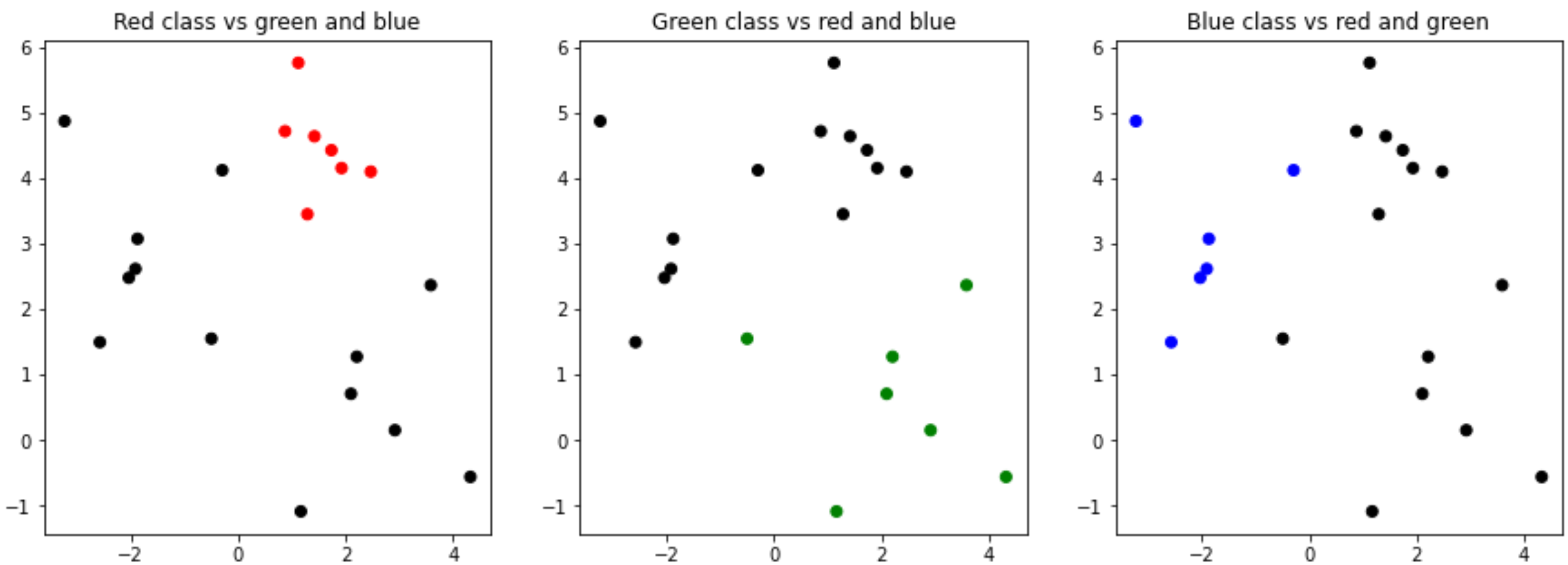
$$
\begin{aligned}
E_{y|\mathbf{x}}[L(0,y)] &> E_{y|\mathbf{x}}[L(1,y)] \\
\sum_y P(y|\mathbf{x})L(0,y) &> \sum_y P(y|\mathbf{x})L(1,y) \\
P(y=0|\mathbf{x})L(0,0) + P(y=1|\mathbf{x})L(0,1) &> P(y=0|\mathbf{x})L(1,0) + P(y=1|\mathbf{x})L(1,1) \\
P(y=1|\mathbf{x}) &> P(y=0|\mathbf{x}) \\
\frac{P(y=1|\mathbf{x})}{P(y=0|\mathbf{x})} &> 1 \qquad \text{if } P(y=0|X) \neq 0 \\
\log \frac{P(y=1|\mathbf{x})}{P(y=0|\mathbf{x})} &> 0 \\
\mathbf{w} \cdot \mathbf{x} &> 0
\end{aligned}
$$

- A similar derivation can be done for arbitrary L(0,1) and L(1,0).

Extending LR to K>2 classes



1 vs All



Red class vs green and blue
Green class vs red and blue
Blue class vs red and green
6
5
4
3
2
1
0
−1
−2
0
2
4

A Quick and Dirty Intro to Multiclass Classification.
This technique is *the daily workhorse of modern AI/ML*

Multiclass

Suppose we want to choose among k discrete values, e.g., $\{\text{'Cat'}, \text{'Dog'}, \text{'Car'}, \text{'Bus'}\}$ so $k = 4$.

We encode with **one-hot** vectors i.e. $y \in \{0,1\}^k$ and $\sum_{j=1}^{k} y_j = 1$.

$$\underset{\text{'Cat'}}{\begin{pmatrix}1\\0\\0\\0\end{pmatrix}} \quad \underset{\text{'Dog'}}{\begin{pmatrix}0\\1\\0\\0\end{pmatrix}} \quad \underset{\text{'Car'}}{\begin{pmatrix}0\\0\\1\\0\end{pmatrix}} \quad \underset{\text{'Bus'}}{\begin{pmatrix}0\\0\\0\\1\end{pmatrix}}$$

A prediction here is actually a *distribution* over the k classes. This leads to the SoftMax function described below (derivation in the notes!). That is our hypothesis is a vector of k values:

$$P(y = j | x; \bar{\theta}) = \frac{\exp(\theta_j^T x)}{\sum_{i=1}^{k} \exp(\theta_i^T x)}.$$

Here each θ_j has the *same dimension* as x, i.e., $x, \theta_j \in R^{d+1}$ for $j = 1, \ldots, k$.

Extending Logistic Regression to K > 2 classes

- Choose class K to be the "reference class" and represent each of the other classes as a logistic function of the odds of class *k* versus class K:

$$
\begin{aligned}
\log \frac{P(y=1|\mathbf{x})}{P(y=K|\mathbf{x})} &= \mathbf{w}_1 \cdot \mathbf{x} \\
\log \frac{P(y=2|\mathbf{x})}{P(y=K|\mathbf{x})} &= \mathbf{w}_2 \cdot \mathbf{x} \\
&\vdots \\
\log \frac{P(y=K-1|\mathbf{x})}{P(y=K|\mathbf{x})} &= \mathbf{w}_{K-1} \cdot \mathbf{x}
\end{aligned}
$$

- Gradient ascent can be applied to simultaneously train all of these weight vectors $\mathbf{w}_k$

Summary of Introduction to Classification

- We used the principle of maximum likelihood (and a probabilistic model) to extend to classification.

Deriving a Learning Algorithm

- Since we are fitting a conditional probability distribution, we no longer seek to minimize the loss on the training data. Instead, we seek to find the probability distribution *h* that is most likely given the training data
- Let S be the training sample. Our goal is to find *h* to maximize P(*h* | S):

$$\begin{aligned}
\operatorname*{argmax}_h P(h|S) &= \operatorname*{argmax}_h \frac{P(S|h)P(h)}{P(S)} && \text{by Bayes' Rule} \\
&= \operatorname*{argmax}_h P(S|h)P(h) && \text{because } P(S) \text{ doesn't depend on } h \\
&= \operatorname*{argmax}_h P(S|h) && \text{if we assume } P(h) = \text{uniform} \\
&= \operatorname*{argmax}_h \log P(S|h) && \text{because log is monotonic}
\end{aligned}$$

The distribution P(S|*h*) is called the likelihood function. The log likelihood is frequently used as the objective function for learning. It is often written as $\ell(\mathbf{w})$.

The *h* that maximizes the likelihood on the training data is called the maximum likelihood estimator (MLE)

Summary of Introduction to Classification

- We used the principle of maximum likelihood (and a probabilistic model) to extend to classification.
- We developed logistic regression from this principle.
  - Logistic regression is *widely* used today.

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- We used the principle of maximum likelihood (and a probabilistic model) to extend to classification.
- We developed logistic regression from this principle.
  - Logistic regression is *widely* used today.
- We noticed a familiar pattern: take derivatives of the likelihood, and the derivatives had this (hopefully) intuitive *"misprediction form"*

Computing the Likelihood

- In our framework, we assume that each training example ($\mathbf{x}_i$,y_i) is drawn from the same (but unknown) probability distribution P($\mathbf{x}$,y). This means that the log likelihood of S is the sum of the log likelihoods of the individual training examples:

$$\begin{aligned} \log P(S|h) &= \log \prod_i P(\mathbf{x}_i, y_i|h) \\ &= \sum_i \log P(\mathbf{x}_i, y_i|h) \end{aligned}$$

Computing the Likelihood (2)

- Recall that *any* joint distribution P(a,b) can be factored as P(a|b) P(b). Hence, we can write

$$\begin{aligned}\operatorname*{argmax}_h \log P(S|h) &= \operatorname*{argmax}_h \sum_i \log P(\mathbf{x}_i, y_i|h) \\ &= \operatorname*{argmax}_h \sum_i \log P(y_i|\mathbf{x}_i, h) P(\mathbf{x}_i|h)\end{aligned}$$

- In our case, P(**x** | *h*) = P(**x**), because it does not depend on *h*, so

$$\begin{aligned}\operatorname*{argmax}_h \log P(S|h) &= \operatorname*{argmax}_h \sum_i \log P(y_i|\mathbf{x}_i, h) P(\mathbf{x}_i|h) \\ &= \operatorname*{argmax}_h \sum_i \log P(y_i|\mathbf{x}_i, h)\end{aligned}$$

Log Likelihood for Conditional Probability Estimators

- We can express the log likelihood in a compact form known as the cross entropy.
- Consider an example ($\mathbf{x}_i, y_i$)
  - If $y_i = 0$, the log likelihood is $\log [1 - p_1(\mathbf{x}; \mathbf{w})]$
  - if $y_i = 1$, the log likelihood is $\log [p_1(\mathbf{x}; \mathbf{w})]$
- These cases are mutually exclusive, so we can combine them to obtain:

  $\ell(y_i; \mathbf{x}_i,\mathbf{w}) = \log P(y_i \mid \mathbf{x}_i,\mathbf{w}) = (1 - y_i) \log[1 - p_1(\mathbf{x}_i;\mathbf{w})] + y_i \log p_1(\mathbf{x}_i;\mathbf{w})$
- The goal of our learning algorithm will be to find **w** to maximize

  $J(\mathbf{w}) = \sum_i \ell(y_i; \mathbf{x}_i,\mathbf{w})$

Fitting Logistic Regression by Gradient Ascent

$$
\begin{aligned}
\frac{\partial J(\mathbf{w})}{\partial w_j} &= \sum_i \frac{\partial}{\partial w_j} \ell(y_i; \mathbf{x}_i, \mathbf{w}) \\
\frac{\partial}{\partial w_j} \ell(y_i; \mathbf{x}_i, \mathbf{w}) &= \frac{\partial}{\partial w_j} \left((1 - y_i) \log[1 - p_1(\mathbf{x}_i; \mathbf{w})] + y_1 \log p_1(\mathbf{x}_i; \mathbf{w}) \right) \\
&= (1 - y_i) \frac{1}{1 - p_1(\mathbf{x}_i; \mathbf{w})} \left(- \frac{\partial p_1(\mathbf{x}_i; \mathbf{w})}{\partial w_j} \right) + y_i \frac{1}{p_1(\mathbf{x}_i; \mathbf{w})} \left(\frac{\partial p_1(\mathbf{x}_i; \mathbf{w})}{\partial w_j} \right) \\
&= \left[\frac{y_i}{p_1(\mathbf{x}_i; \mathbf{w})} - \frac{(1 - y_i)}{1 - p_1(\mathbf{x}_i; \mathbf{w})} \right] \left(\frac{\partial p_1(\mathbf{x}_i; \mathbf{w})}{\partial w_j} \right) \\
&= \left[\frac{y_i (1 - p_1(\mathbf{x}_i; \mathbf{w})) - (1 - y_i) p_1(\mathbf{x}_i; \mathbf{w})}{p_1(\mathbf{x}_i; \mathbf{w})(1 - p_1(\mathbf{x}_i; \mathbf{w}))} \right] \left(\frac{\partial p_1(\mathbf{x}_i; \mathbf{w})}{\partial w_j} \right) \\
&= \left[\frac{y_i - p_1(\mathbf{x}_i; \mathbf{w})}{p_1(\mathbf{x}_i; \mathbf{w})(1 - p_1(\mathbf{x}_i; \mathbf{w}))} \right] \left(\frac{\partial p_1(\mathbf{x}_i; \mathbf{w})}{\partial w_j} \right)
\end{aligned}
$$

Gradient Computation (continued)

- Note that p_1 can also be written as

$$p_1(\mathbf{x}_i;\mathbf{w}) = \frac{1}{(1+\exp[-\mathbf{w}\cdot\mathbf{x}_i])}.$$

- From this, we obtain:

$$\begin{aligned}
\frac{\partial p_1(\mathbf{x}_i;\mathbf{w})}{\partial w_j} &= -\frac{1}{(1+\exp[-\mathbf{w}\cdot\mathbf{x}_i])^2}\frac{\partial}{\partial w_j}(1+\exp[-\mathbf{w}\cdot\mathbf{x}_i]) \\
&= -\frac{1}{(1+\exp[-\mathbf{w}\cdot\mathbf{x}_i])^2}\exp[-\mathbf{w}\cdot\mathbf{x}_i]\frac{\partial}{\partial w_j}(-\mathbf{w}\cdot\mathbf{x}_i) \\
&= -\frac{1}{(1+\exp[-\mathbf{w}\cdot\mathbf{x}_i])^2}\exp[-\mathbf{w}\cdot\mathbf{x}_i](-x_{ij}) \\
&= p_1(\mathbf{x}_i;\mathbf{w})(1-p_1(\mathbf{x}_i;\mathbf{w}))x_{ij}
\end{aligned}$$

Completing the Gradient Computation

- The gradient of the log likelihood of a single point is therefore

$$
\begin{aligned}
\frac{\partial}{\partial w_j}\ell(y_i;\mathbf{x}_i,\mathbf{w}) &= \left[\frac{y_i - p_1(\mathbf{x}_i;\mathbf{w})}{p_1(\mathbf{x}_i;\mathbf{w})(1-p_1(\mathbf{x}_i;\mathbf{w}))}\right]\left(\frac{\partial p_1(\mathbf{x}_i;\mathbf{w})}{\partial w_j}\right) \\
&= \left[\frac{y_i - p_1(\mathbf{x}_i;\mathbf{w})}{p_1(\mathbf{x}_i;\mathbf{w})(1-p_1(\mathbf{x}_i;\mathbf{w}))}\right] p_1(\mathbf{x}_i;\mathbf{w})(1-p_1(\mathbf{x}_i;\mathbf{w}))x_{ij} \\
&= (y_i - p_1(\mathbf{x}_i;\mathbf{w}))x_{ij}
\end{aligned}
$$

- The overall gradient is

$$
\frac{\partial J(\mathbf{w})}{\partial w_j} = \sum_i (y_i - p_1(\mathbf{x}_i;\mathbf{w}))x_{ij}
$$

Classification Lecture Summary

- We saw the differences between classification and regression.
- We learned about a principle for probabilistic interpretation for linear regression and classification: **Maximum Likelihood**.
  - We used this to derive logistic regression.
  - The Maximum Likelihood principle will be used again next lecture (and in the future)