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Topic 3 continued
Linear Classification & Logistic Regression

PROF. LINDA SELLIE

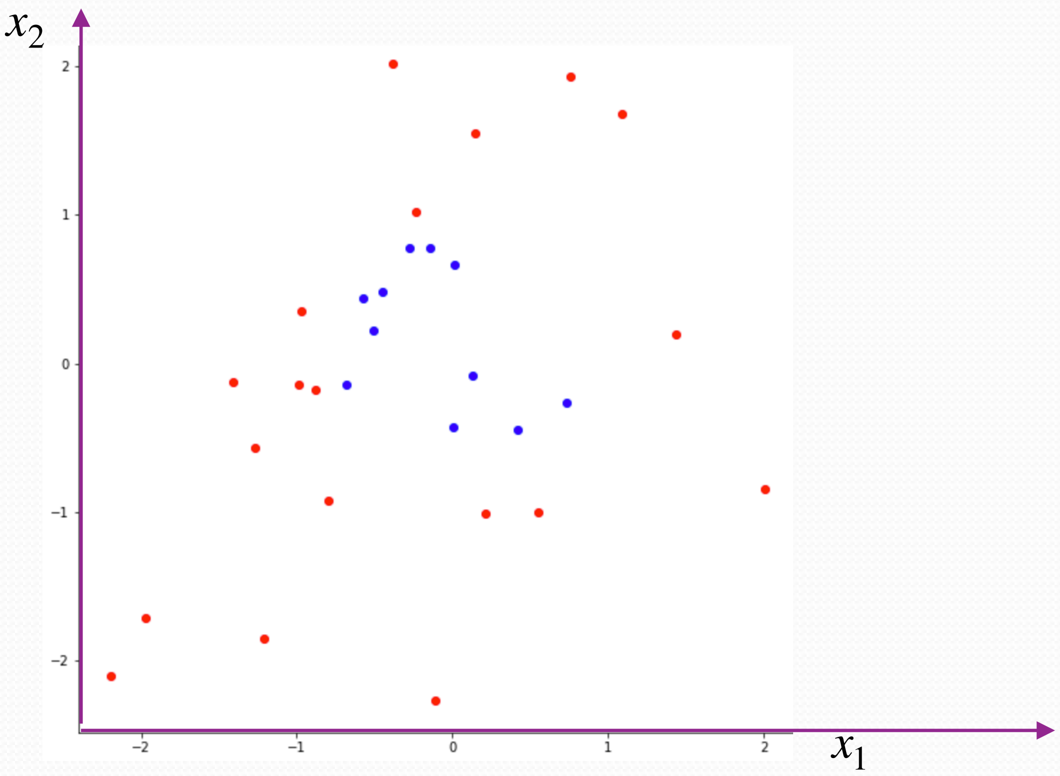
Some slides/approaches used are from Prof. Rangan
Many approaches used are from CMU 18-661

Outline

- Motivating example: How can we classify? — How can we use a hyperplane for a classification problem?
- Estimating probabilities — Can we predict not only which class an example belongs to - but a confidence score of that classification
- Maximum likelihood — How can we find the most likely hyperplane? Could we write a function to describe how likely a hyperplane was to have generated the dataset?
  - Iterative approach - gradient ascent — Maximizing the function
- Thinking about different types of error — Some errors are more costly than other errors. Can we modify our predictions to decrease one type of error (and perhaps increase another type of error?
  - Accuracy
  - Motivating example
- Transformation of the features — Extending our algorithm to nonlinear decision boundaries
- Preventing overfitting
- Multiple classes — What if we have more than two classes?

Non-linear Decision Boundary

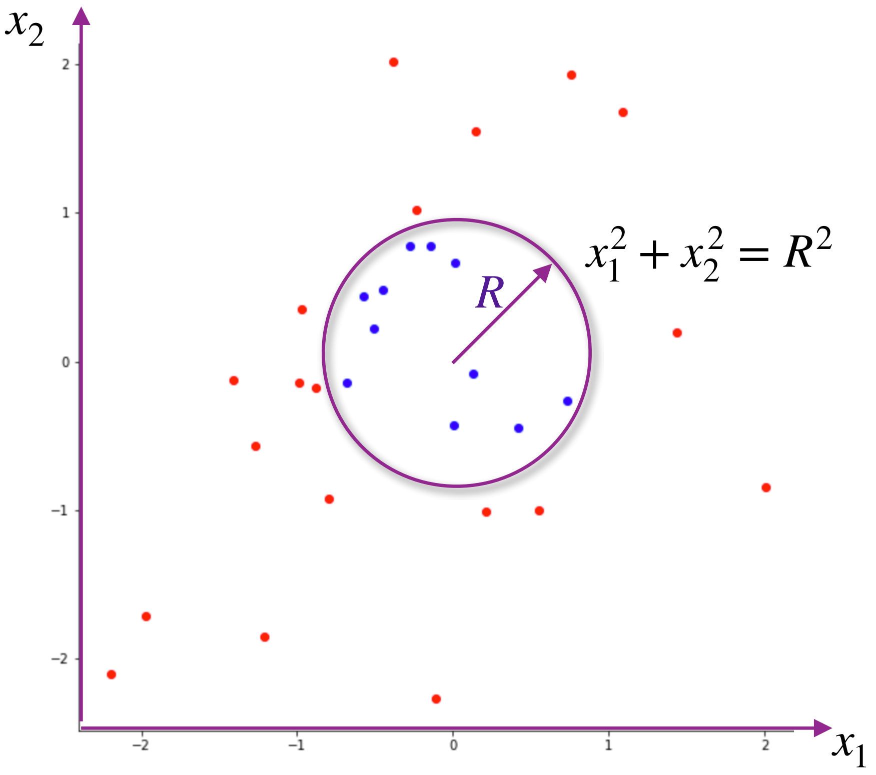
Could our logistic regression function do well on the dataset?

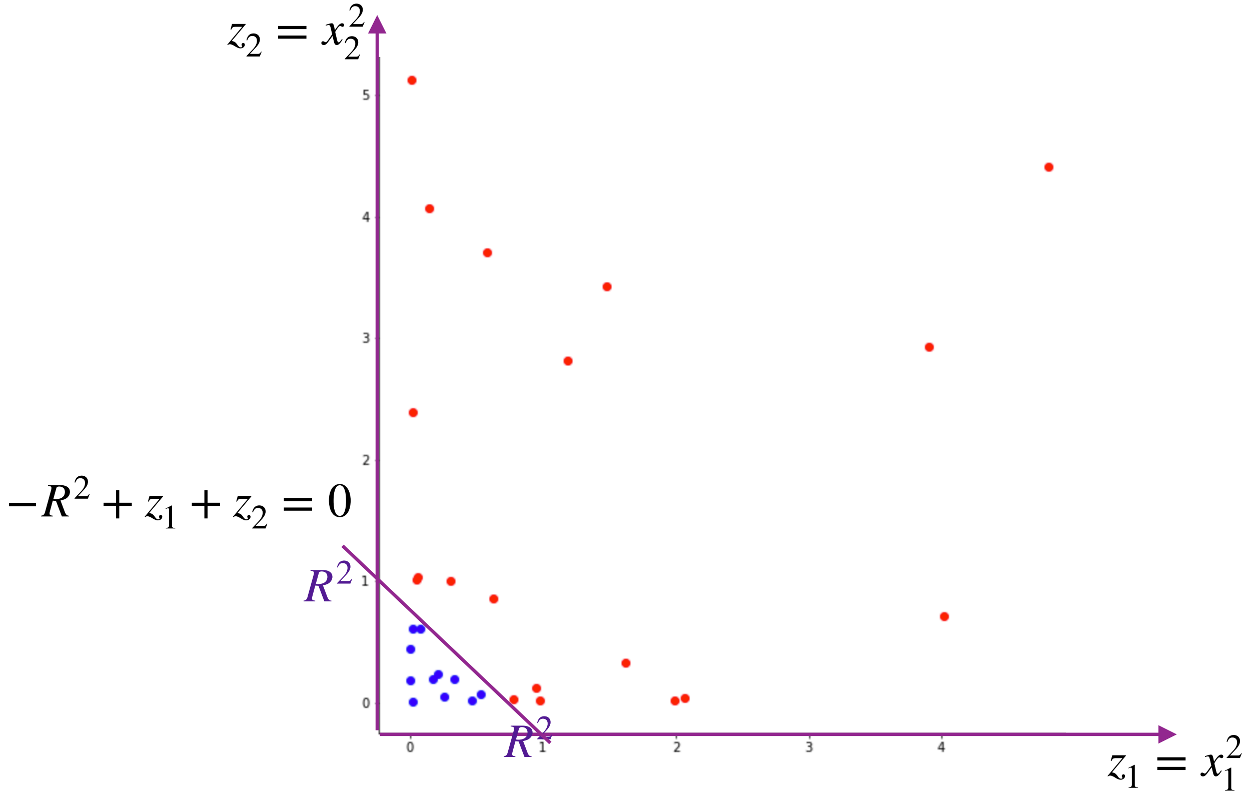


What do we do if our data had a more complex decision boundary?

Just as we did in linear regression, we can expand the model logistic model by transforming the features:

If we add features, can we separate the data?

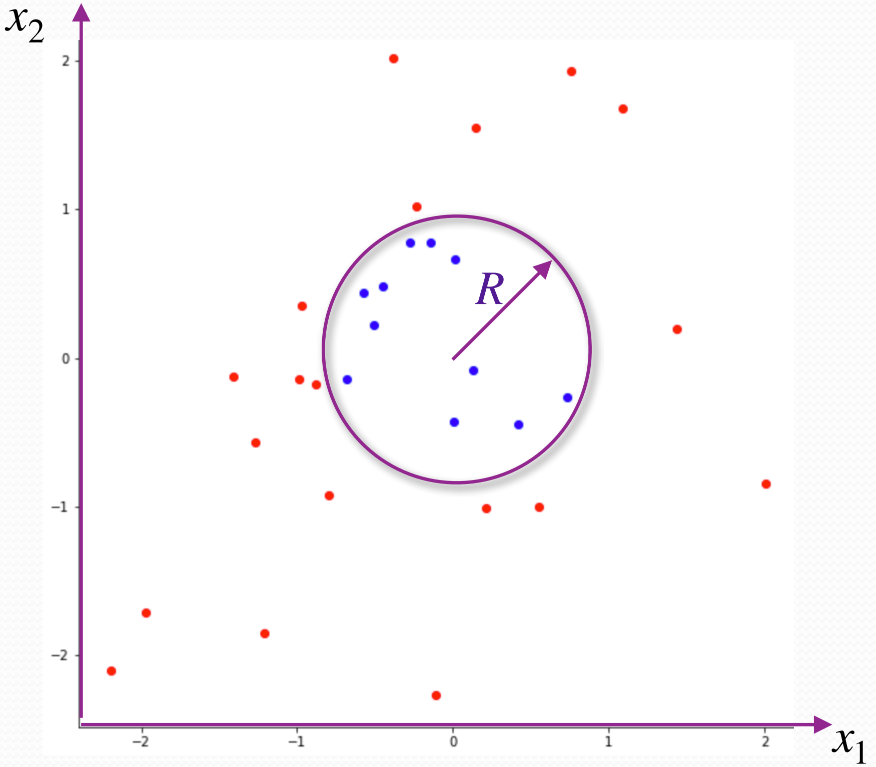


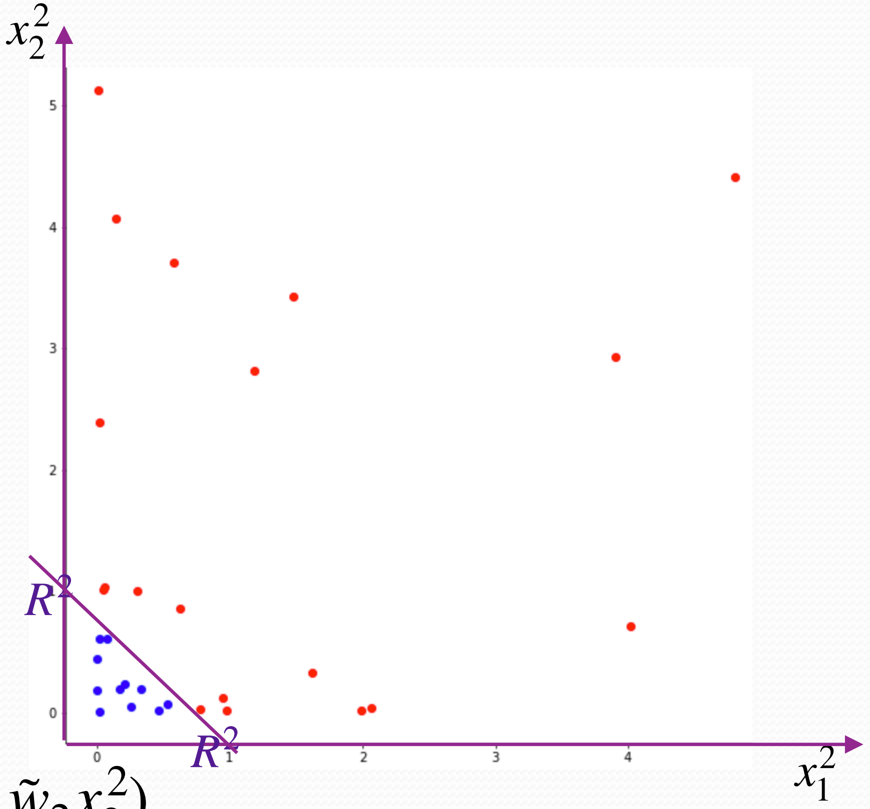


$$\mathbf{x} = \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix}$$

$$\Phi(\mathbf{x}) = \begin{bmatrix} 1 \\ (x_1)^2 \\ (x_2)^2 \end{bmatrix} = \begin{bmatrix} 1 \\ z_1 \\ z_2 \end{bmatrix} \qquad \tilde{\mathbf{w}} = \begin{bmatrix} -R^2 \\ 1 \\ 1 \end{bmatrix}$$

Prediction





$$pr(y = 1 \mid \mathbf{x}) = \sigma(\tilde{w}_0 + +\tilde{w}_2 x_1^2 + \tilde{w}_2 x_2^2)$$

If $pr(y = 1 \mid \mathbf{x}) = \sigma(-R^2 + x_1^2 + x_2^2) \leq 0$ .5 predict blue

If $pr(y = 1 \mid \mathbf{x}) = \sigma(-R^2 + x_1^2 + x_2^2)$ > 0.5 predict red

Pair share: what can we do to prevent overfitting?

$$\Phi_2(\mathbf{x}) = \Phi_2([1, x_1, x_2]^T) = [1, x_1, x_1^2, x_2, x_2^2, x_1 x_2]^T$$

$$\Phi_3(\mathbf{x}) = \Phi_3([1, x_1, x_2]^T) = \begin{bmatrix} 1 & x_1 & x_2 & x_1^2 & x_1 x_2 & x_2^2 & x_1^3 & x_1^2 x_2 & x_1 x_2^2 & x_2^3 \end{bmatrix}^T$$

$$\Phi_4(\mathbf{x}) = \Phi_4([1, x_1, x_2]^T) = \begin{bmatrix} 1 & x_1 & x_2 & x_1^2 & x_1 x_2 & x_2^2 & x_1^3 & x_1^2 x_2 & x_1 x_2^2 & x_2^3 & x_1^4 & x_1^3 x_2 & x_1^2 x_2^2 & x_1 x_2^3 & x_2^4 \end{bmatrix}^T$$

And so on

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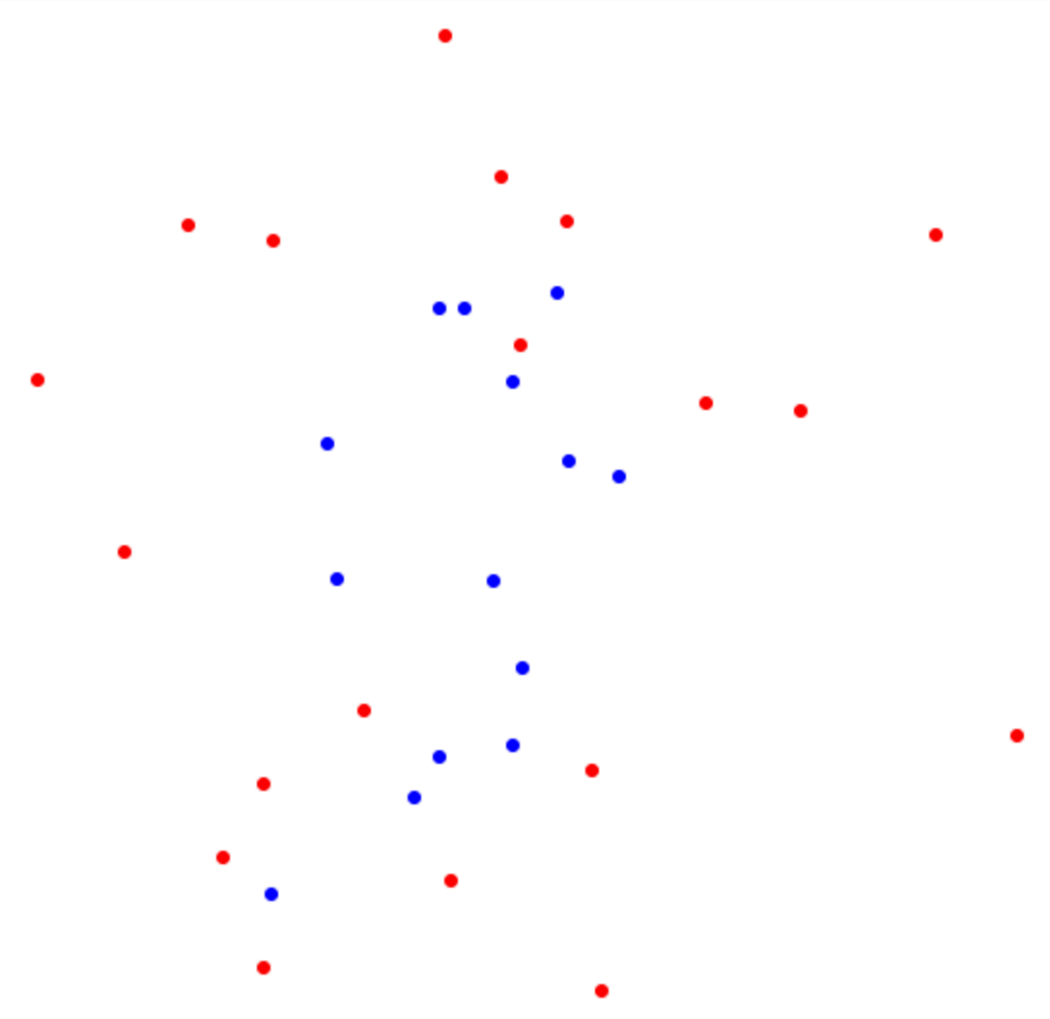

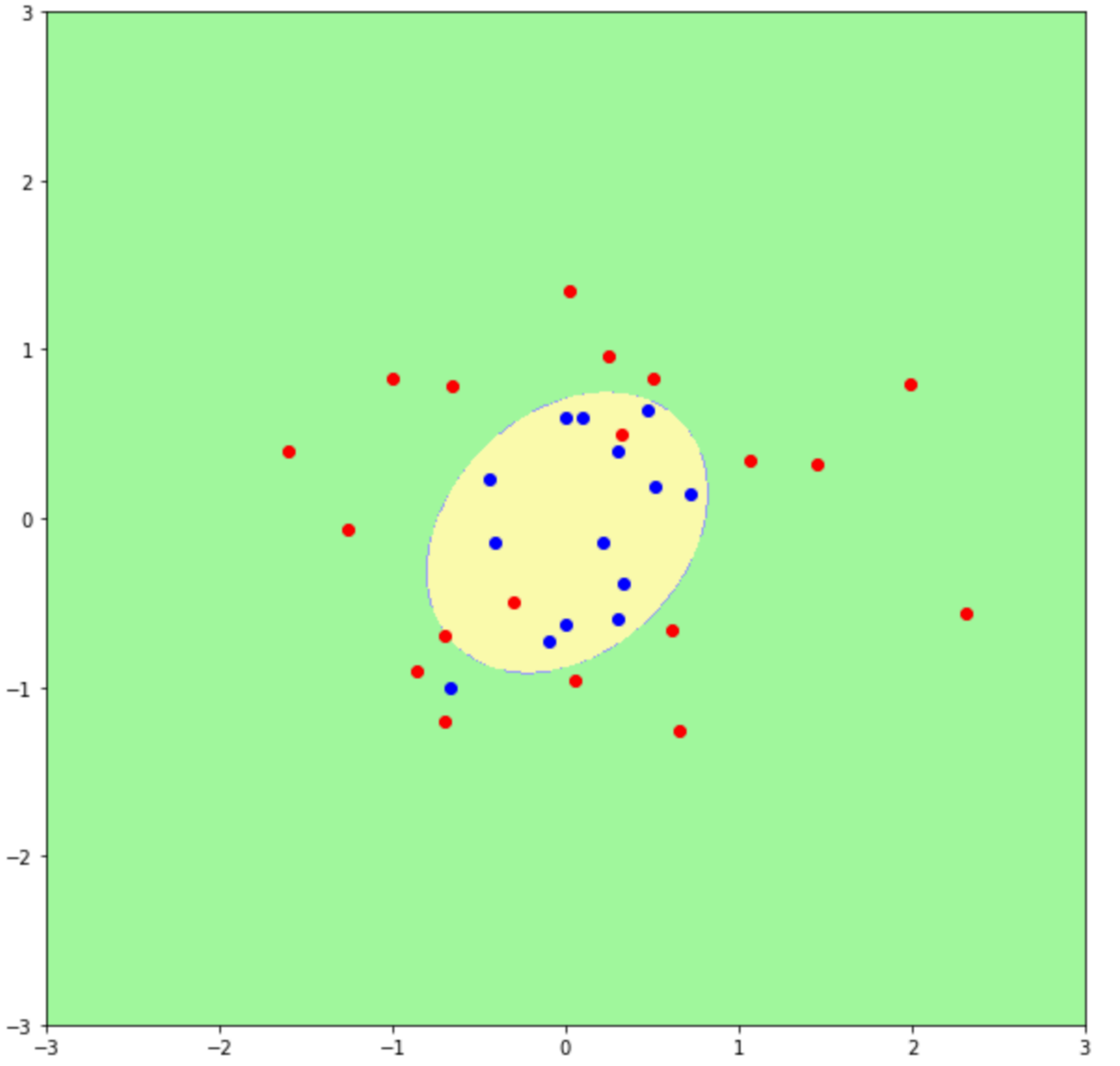
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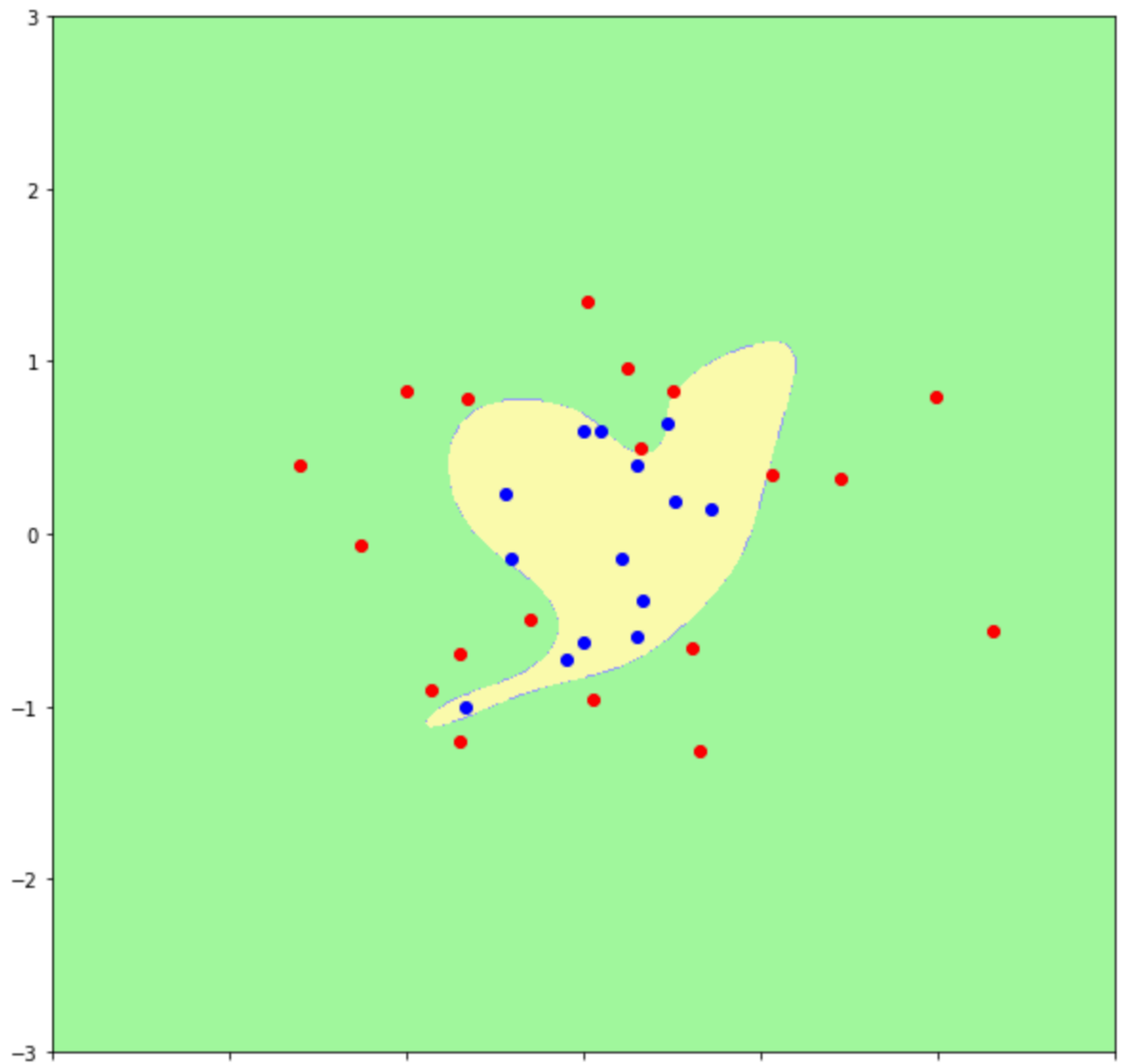
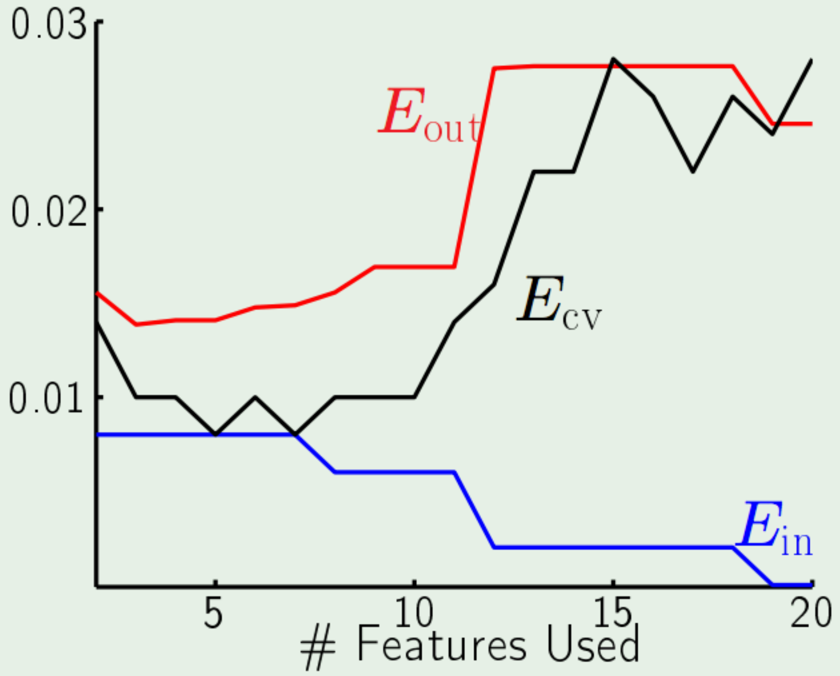


Too much flexibility in the model for quality and quantity of data → overfitting

What should we do to choose the right model?

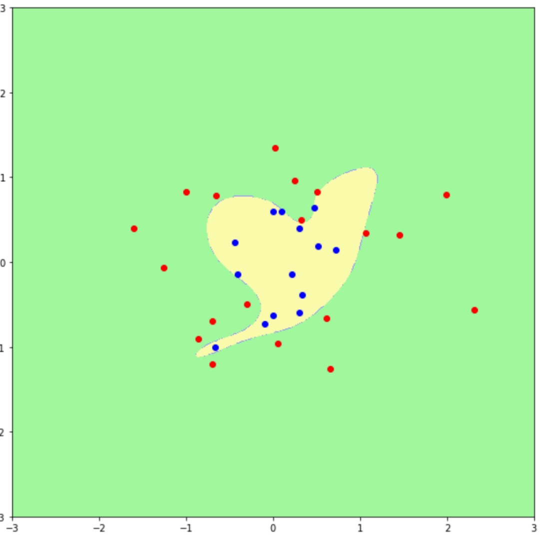
validation in action

Different errors



$$(1, x_1, x_2) \to (1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2, \ldots, x_1^5, x_1^4x_2, x_1^3x_2^2, x_1^2x_2^3, x_1x_2^4, x_2^5)$$

Slide modified from



How can we do constrained optimization?

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[-173.15294712]
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   -887.16725134  -637.23456062  -323.39361867  -441.59715309
    -87.41914152   -92.33185672   365.50986342   354.98813381
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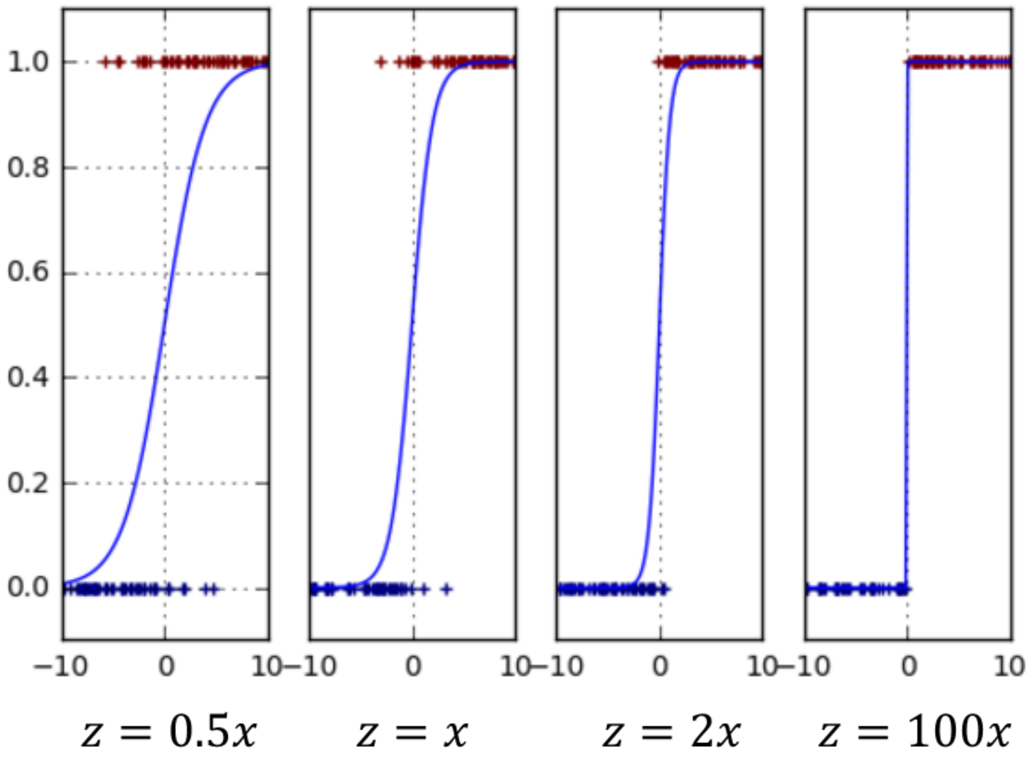
Logistic Model as a "Soft" Classifier



- Plot of

$$P(y = 1|x) = \frac{1}{1 + e^{-z}}, \qquad z = w_1 x$$

  - Markers are random samples
- Higher w_1: prob transition becomes sharper
  - Fewer samples occur across boundary
- As $w_1 \to \infty$ logistic becomes "hard" rule

$$P(y = 1|x) \approx \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

For linear regression:

- $E_{in}(\mathbf{w}) + \lambda(\|\mathbf{w}\|_2^2)$
- $E_{in}(\mathbf{w}) + \lambda(\|\mathbf{w}\|_1)$

Pair share:

How you would you add regularization to logistic regression? Use $\ell(w)$ to be the log likelihood function

Adding L2 regularization: $\underbrace{\frac{1}{N}\ell(\mathbf{w})}_{\text{Fit}} - \underbrace{\lambda(\|\mathbf{w}_{1:d}\|_2^2)}_{\text{Regularization term}}$

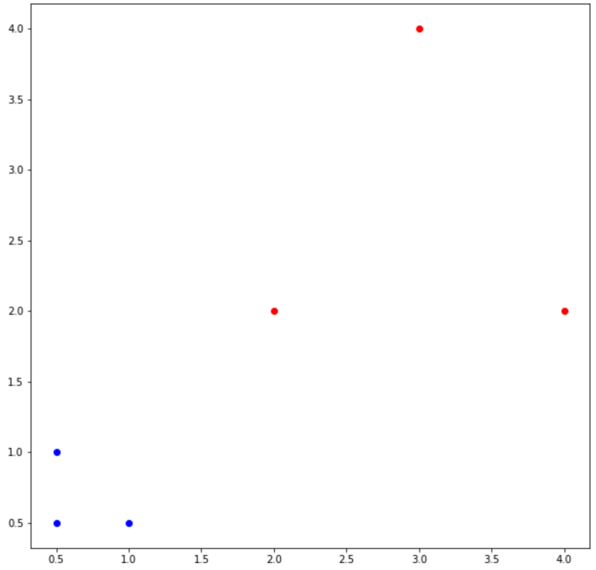
- The log likelihood function for logistic regression

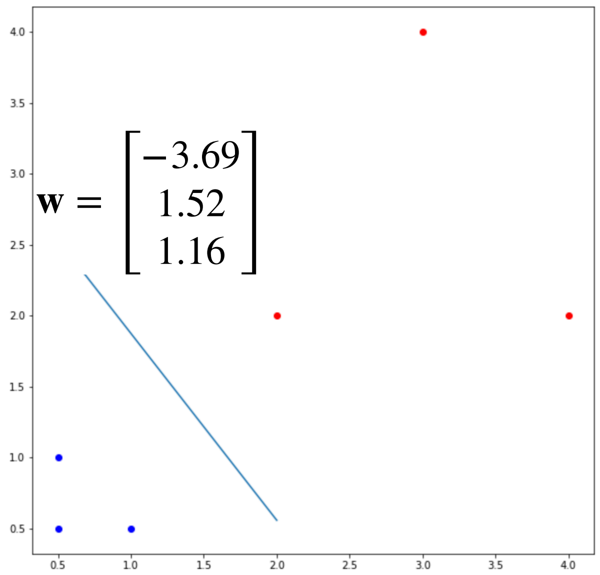
$$\ell_{\text{ridge}}(\mathbf{w}) = \frac{1}{N}\log L(\mathbf{w}) - \lambda(\|\mathbf{w}_{1:d}\|_2^2)$$

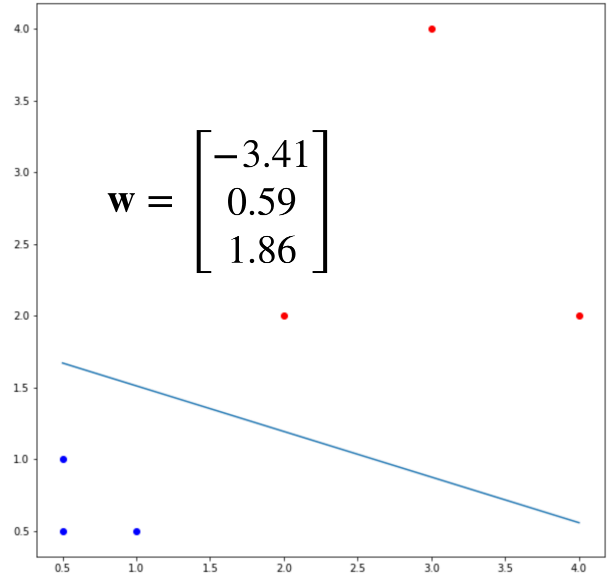
$$= \frac{1}{N}\sum_{i=1}^{N}\left(y^{(i)}\log\sigma(\mathbf{w}^T\mathbf{x}^{(i)}) + (1-y^{(i)})\log(1-\sigma(\mathbf{w}^T\mathbf{x}^{(i)}))\right) - \lambda(\|\mathbf{w}_{1:d}\|_2^2)$$

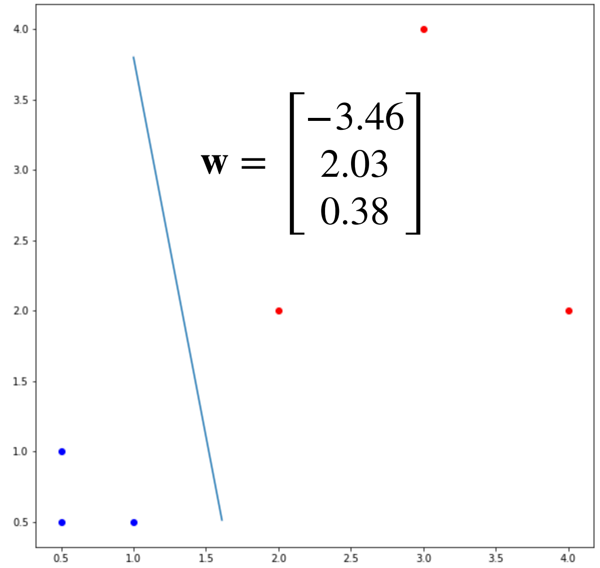
- Perform gradient ascent on this regularized function

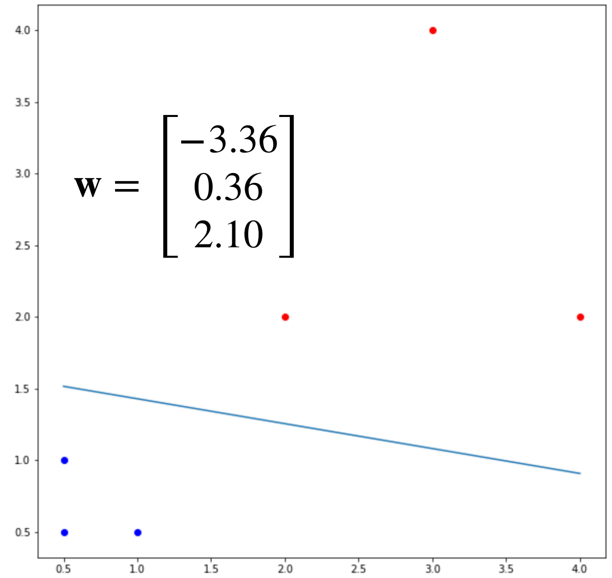
- Typically, we don't want to restrict the size of the intercept term

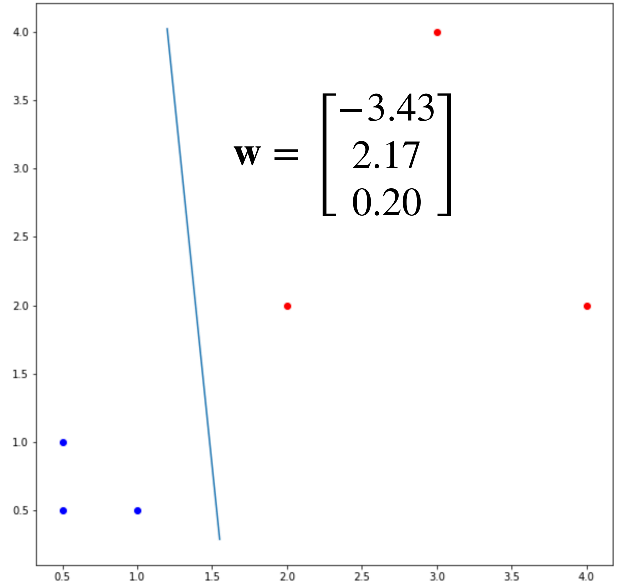












Pair share: What happens if I only regularize w_1?

Pair share: What happens if I only regularize w_2?

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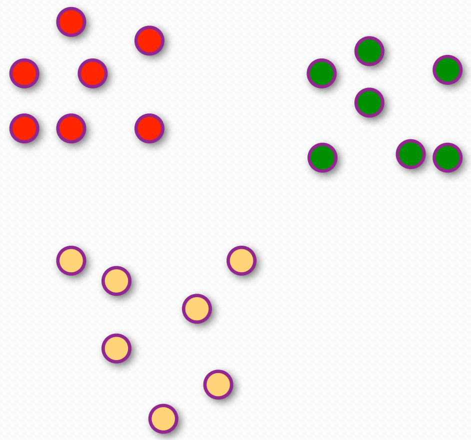
- Multi-class: every example belongs to **<u>one</u>** class.
- Multi-label: every example can belong to **<u>one or more</u>** classes

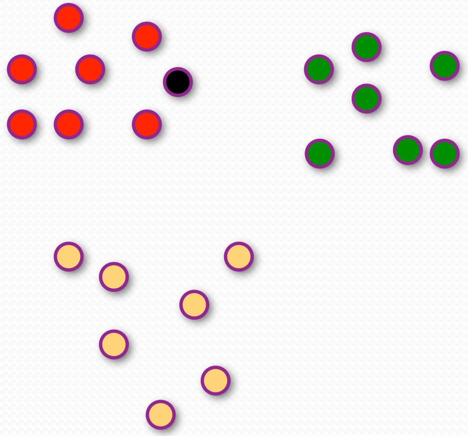
What if there is more than two classes?

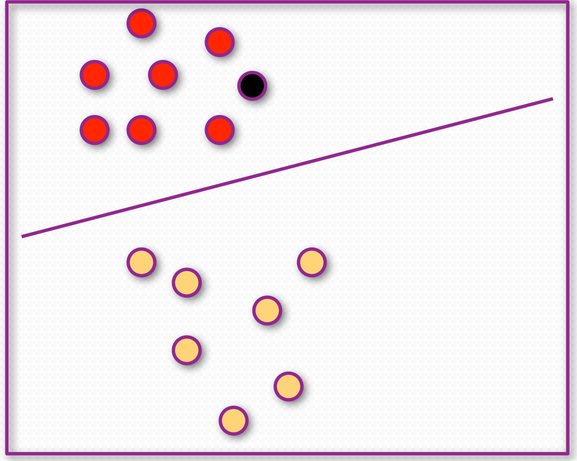
Multi-class classification

- Versicolor Iris vs Setosa Iris vs Veronica Iris
- 0 vs 1 vs 2 vs 3 … vs 9
- Dog vs Cat vs Mouse
- …



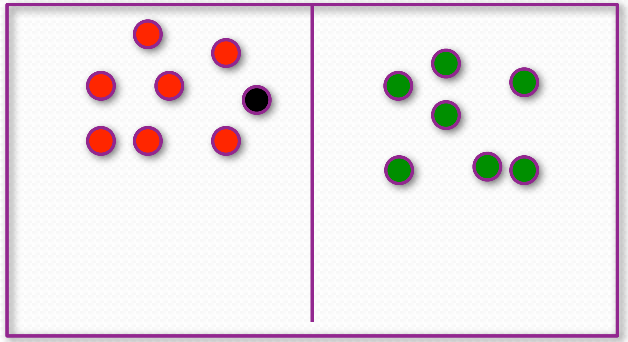
Turn multiple classes problem $C_1, C_2, \ldots, C_K$ into $\frac{K(K-1)}{2}$ binary classification problems





For each pair C_i, C_j of classes

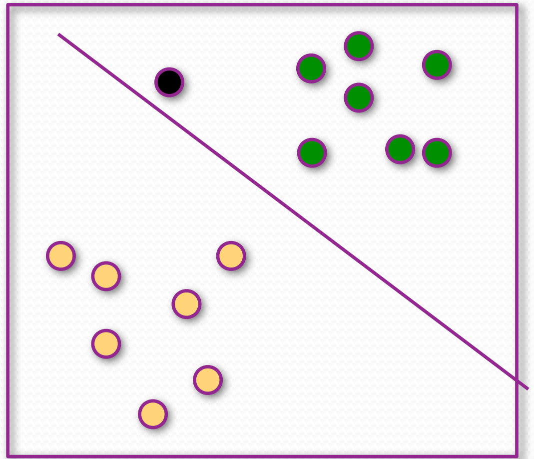
- Relabel training examples with label C_i into '1'
- Relabel training examples with label C_j into '0'
- Remove all other training examples



How do we predict given $\frac{K(K-1)}{2}$ binary classifiers? (i.e. K decision boundaries)

Step 1) Given a new example $\mathbf{x}$, predict the class that wins "majority of votes"

Step 2) If there is a tie, use confidence scores to resolve ties

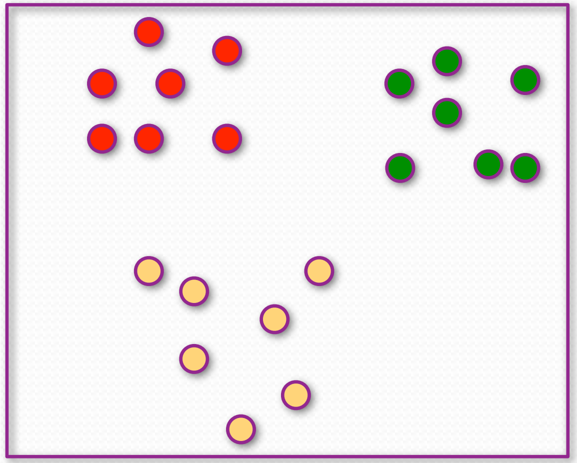


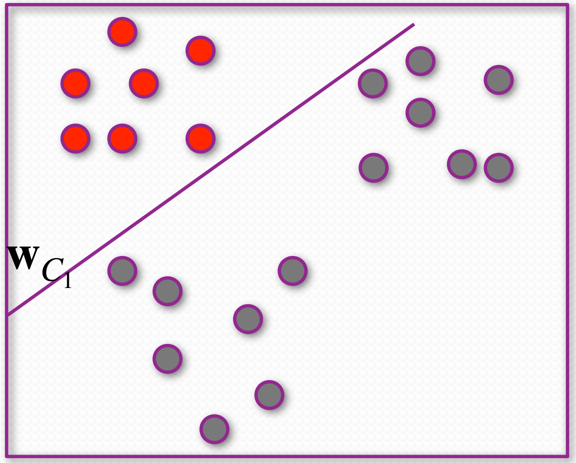
One-versus-Rest or One-Versus All Approach

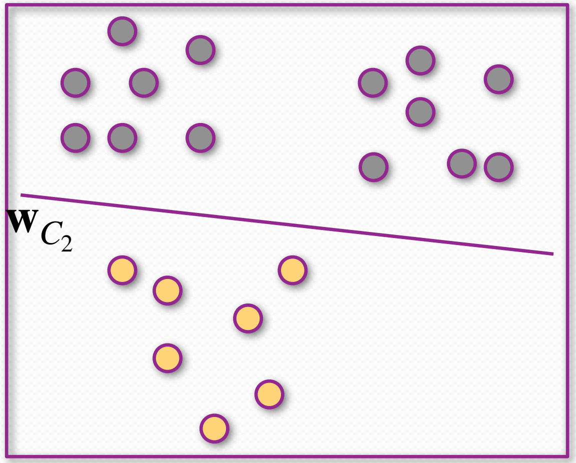
Turn multiple classes problem $C_1, C_2, \ldots, C_K$ into K binary classification problems

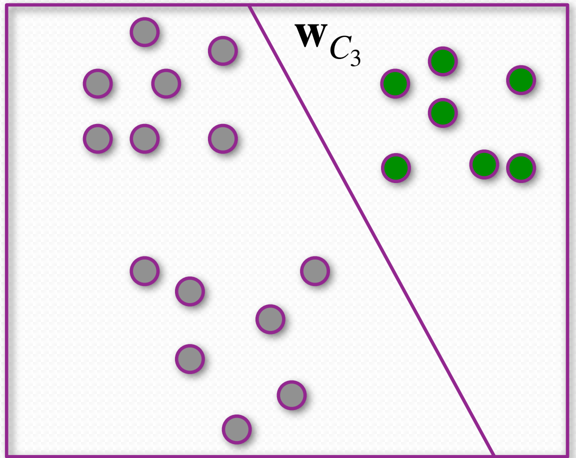
- Relabel training examples with label C_i into ‘1’
- Relabel all other training examples into ‘0’

Repeat K times using logistic regression to classify









How do we predict given K binary classifiers? (i.e. K decision boundaries)

Use confidence estimates $p(y = C_i \mid \mathbf{x})$ for $i = 1 \ldots K$

Predict C_i^* where

$$i = \arg \max_{i \in 1,\ldots,K} p(y = C_i \mid \mathbf{x}) = \sigma(\mathbf{w}_{C_i}^T \mathbf{x})$$

Works well in practice

Learning over local correctness - does not guarantee good global performance

One-versus-One Approach

K(K-1)/2 classifiers. Slow if K is large

Trained on a smaller subset of data which can result in variance

One-versus-Rest or One-Versus All Approach

K classifiers

In-balance in number of class 1 and class 0 training examples

For midterm 2, you will not be responsible for the material on the following slides

- Multi-class: every example belongs to **<u>one</u>** class.
- Multi-label: every example can belong to **<u>one or more</u>** classes

SOFTMAX- A GENERALIZED FORM OF LOGISTIC REGRESSION (*MULTI-CLASS*)

Called:
multiclass logistic regression, *softmax regression* and *multinomial regression*

Could our algorithm directly estimate the probability of label belonging to each of the K classes? (i.e. don't resort to a binary classification problem)

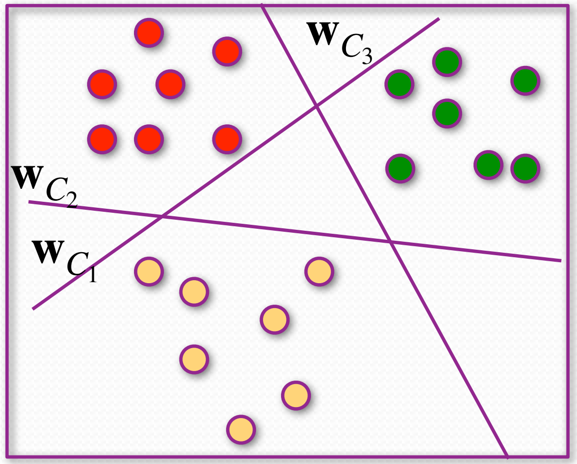
Computing $\mathbf{w}_1$, $\mathbf{w}_2$, $\mathbf{w}_3$, ..., $\mathbf{w}_K$ separately doesn't work since $\sum_{i=1}^{K} p(y = C_i \mid \mathbf{x}) = \sum_{i=1}^{K} \sigma(\mathbf{w}_i^T \mathbf{x}) \neq 1$

Idea: Learn the probabilities jointly (to keep the sum =1)

Intuition

$$\begin{bmatrix} \mathbf{w}_{C_1}^T \mathbf{x} \\ \mathbf{w}_{C_2}^T \mathbf{x} \\ \mathbf{w}_{C_3}^T \mathbf{x} \end{bmatrix}$$

One vs. rest decision boundary for each class.



To create prob distribution:

- Nonnegative
- Sum to one

Pair share: How could we turn these numbers into probabilities that sum to 1?

Intuition

- Setosa - C_1
- Versicolor -C_2
- Veronica - C_3

If $\mathbf{w}_{C_1}^T\mathbf{x} = -18$, $\mathbf{w}_{C_2}^T\mathbf{x} = 12$, and $\mathbf{w}_{C_3}^T\mathbf{x} = 6$

We predict **Versicolor**

We could turn these numbers to probabilities using softmax (well-formed conditional probabilities)

$$p(y = C_1 \mid \mathbf{x}) = \frac{e^{-18}}{e^{-18} + e^{12} + e^{6}} < 1$$

$$p(y = C_2 \mid \mathbf{x}) = \frac{e^{12}}{e^{-18} + e^{12} + e^{6}} < 1$$

$$p(y = C_3 \mid \mathbf{x}) = \frac{e^{6}}{e^{-18} + e^{12} + e^{6}} < 1$$

Normalization term makes the probabilities sum to 1

Keeps relative ordering!

One hot encoding

Not all approaches do a one hot encoding (1-of-K encoding) of the target

$$h(\mathbf{x}) = \begin{bmatrix} p(y = C_1 \mid \mathbf{x}) \\ p(y = C_2 \mid \mathbf{x}) \\ p(y = C_3 \mid \mathbf{x}) \end{bmatrix}$$

We will predict K different probabilities: $y^{(i)}$ becomes $\mathbf{y}^{(i)} = [y_1^{(i)}, y_2^{(i)}, \ldots, y_K^{(i)}]^T$

Using one hot encoding (1-of-K encoding).

$$y_j^{(i)} = \begin{cases} 1 & y^{(i)} = j \\ 0 & \text{otherwise} \end{cases}$$

If we have 3 classes:

class C_1 → $[1 \quad 0 \quad 0]^T$

class C_2 → $[0 \quad 1 \quad 0]^T$

class C_3 → $[0 \quad 0 \quad 1]^T$

Soft-max

W has dimension k x (d+1), we stacked the transpose of the coefficient vectors

$$W = \begin{bmatrix} -\mathbf{w}_1^T- \\ -\mathbf{w}_2^T- \\ -\mathbf{w}_3^T- \\ \cdots \\ -\mathbf{w}_K^T- \end{bmatrix}$$

$$\begin{bmatrix} -\mathbf{w}_1^T- \\ -\mathbf{w}_2^T- \\ -\mathbf{w}_3^T- \\ \cdots \\ -\mathbf{w}_K^T- \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \cdots \\ x_d \end{bmatrix} = \begin{bmatrix} \mathbf{w}_1^T\mathbf{x} \\ \mathbf{w}_2^T\mathbf{x} \\ \mathbf{w}_3^T\mathbf{x} \\ \cdots \\ \mathbf{w}_K^T\mathbf{x} \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \cdots \\ z_K \end{bmatrix}$$

score for each coefficient Vector

$$h(\mathbf{x}) = \begin{bmatrix} p(y=1 \mid \mathbf{x}) \\ p(y=2 \mid \mathbf{x}) \\ p(y=3 \mid \mathbf{x}) \\ \cdots \\ p(y=K \mid \mathbf{x}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{k} e^{\mathbf{w}_j^T\mathbf{x}}} \begin{bmatrix} e^{\mathbf{w}_1^T\mathbf{x}} \\ e^{\mathbf{w}_2^T\mathbf{x}} \\ \\ \\ e \end{bmatrix}$$

normalizing the score

Soft-max

W has dimension
k x (d+1), we stacked
the transpose of the
coefficient vectors

$$W = \begin{bmatrix} -\mathbf{w}_1^T- \\ -\mathbf{w}_2^T- \\ -\mathbf{w}_3^T- \\ \cdots \\ -\mathbf{w}_K^T- \end{bmatrix}$$

$$\begin{bmatrix} -\mathbf{w}_1^T- \\ -\mathbf{w}_2^T- \\ -\mathbf{w}_3^T- \\ \cdots \\ -\mathbf{w}_K^T- \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \cdots \\ x_d \end{bmatrix} = \begin{bmatrix} \mathbf{w}_1^T\mathbf{x} \\ \mathbf{w}_2^T\mathbf{x} \\ \mathbf{w}_3^T\mathbf{x} \\ \cdots \\ \mathbf{w}_K^T\mathbf{x} \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \cdots \\ z_K \end{bmatrix}$$

score for
each
coefficient
Vector

$$h(\mathbf{x}) = \begin{bmatrix} p(y=1 \mid \mathbf{x}) \\ p(y=2 \mid \mathbf{x}) \\ p(y=3 \mid \mathbf{x}) \\ \cdots \\ p(y=K \mid \mathbf{x}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{k} e^{\mathbf{w}_j^T\mathbf{x}}} \begin{bmatrix} e^{\mathbf{w}_1^T\mathbf{x}} \\ e^{\mathbf{w}_2^T\mathbf{x}} \\ \\ \\ e \end{bmatrix}$$

normalizing
the score

You will not responsible for the material on this slide for midterm 2

We will predict K different probabilities: $y^{(i)}$ becomes $\mathbf{y}^{(i)} = [y_1^{(i)}, y_2^{(i)}, \ldots, y_K^{(i)}]^T$

Using 1-of-K encoding (one hot encoding).

$$y_j^{(i)} = \begin{cases} 1 & y^{(i)} = j \\ 0 & \textbf{otherwise} \end{cases}$$

Approach is maximize Log likelihood

Only one of these is 1

Maximize $\log L = \sum_{i=1}^{N} \log p(y^{(i)} \mid \mathbf{x}^{(i)}) = \sum_{i=1}^{N} \log \prod_{k=1}^{K} p(C_k^{(i)} \mid \mathbf{x}^{(i)})^{y_k^{(i)}} = \sum_{i=1}^{N} \sum_{k=1}^{K} y_k^{(i)} \log p(C_k^{(i)} \mid \mathbf{x}^{(i)})$

$$= \sum_{i=1}^{N} \sum_{k=1}^{K} y_k^{(i)} \log \frac{e^{\mathbf{w}_k^T \mathbf{x}^{(i)}}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T \mathbf{x}^{(i)}}}$$

Negative Log likelihood for softmax is the cross entropy error

Concave thus parameters can be found using gradient ascent

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Using the indicator function $I\{\cdot\}$.
$I\{\text{true statement}\} = 1$
$I\{\text{false statement}\} = 0$

$$J(\mathbf{w}) = \sum_{i=1}^{N}\sum_{k=1}^{K} 1\{y^{(i)} = k\} \log p(y^{(i)} = k \mid \mathbf{x}^{(i)}; \mathbf{w})$$

$$J(\mathbf{w}) = \sum_{i=1}^{N}\sum_{k=1}^{K} 1\{y^{(i)} = k\} \log \frac{e^{\mathbf{w}_k^T\mathbf{x}^{(i)}}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}$$

$$J(\mathbf{w}) = \sum_{i=1}^{N}\sum_{k=1}^{K} 1\{y^{(i)} = k\} \left[\log e^{\mathbf{w}_k^T\mathbf{x}^{(i)}} - \log \sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}\right]$$

$$J(\mathbf{w}) = \sum_{i=1}^{N}\sum_{k=1}^{K} 1\{y^{(i)} = k\} \left[\mathbf{w}_k^T\mathbf{x}^{(i)} - \log \sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}\right]$$

A very complicated derivation creates

$$\nabla_{\mathbf{w}_k} J(\mathbf{w}) = \sum_{i=1}^{N} \mathbf{x}^{(i)} \left[1\{y^{(i)} = k\} - \frac{e^{\mathbf{w}_k^T\mathbf{x}^{(i)}}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}\right]$$

Randomly initialize w
For I = 1 to num_iters:
For each $\mathbf{w}_k$:
$\mathbf{w}_k = \mathbf{w}_k + \alpha \nabla_{\mathbf{w}_k} J(\mathbf{w})$

http://deeplearning.stanford.edu/tutorial/supervised/SoftmaxRegression/

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Here we are only updating the kth coefficient vector

Using the indicator function $I\{\cdot\}$.
$I\{\text{true statement}\} = 1$
$I\{\text{false statement}\} = 0$

$$\nabla_{\mathbf{w}_r} J(\mathbf{w}) = \sum_{i=1}^{N}\sum_{k=1}^{K} 1\{y^{(i)} = k\}\, \nabla_{\mathbf{w}_r}\left[\mathbf{w}_k^T\mathbf{x}^{(i)} - \log\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}\right]$$

$$\nabla_{\mathbf{w}_r} J(\mathbf{w}) = \sum_{i=1}^{N} 1\{y^{(i)} = r\}\, \nabla_{\mathbf{w}_r}\left[\mathbf{w}_r^T\mathbf{x}^{(i)} - \log\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}\right] + \sum_{i=1}^{N}\sum_{k=1,k\neq r}^{K} 1\{y^{(i)} = k\}\, \nabla_{\mathbf{w}_r}\left[\mathbf{w}_k^T\mathbf{x}^{(i)} - \log\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}\right]$$

$$\nabla_{\mathbf{w}_r} J(\mathbf{w}) = \sum_{i=1}^{N} 1\{y^{(i)} = r\}\left[\mathbf{x}^{(i)} - \nabla_{\mathbf{w}_r}\log\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}\right] + \sum_{i=1}^{N}\sum_{k=1,k\neq r}^{K} 1\{y^{(i)} = k\}\left[-\nabla_{\mathbf{w}_r}\log\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}\right]$$

Only one term in the sum has $\mathbf{w}_k$

$$\nabla_{\mathbf{w}_r} J(\mathbf{w}) = \sum_{i=1}^{N} 1\{y^{(i)} = r\}\left[\mathbf{x}^{(i)} - \frac{e^{\mathbf{w}_r^T\mathbf{x}^{(i)}}\mathbf{x}^{(i)}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}\right] + \sum_{i=1}^{N}\sum_{k=1,k\neq r}^{K} 1\{y^{(i)} = k\}\left[-\frac{e^{\mathbf{w}_r^T\mathbf{x}^{(i)}}\mathbf{x}^{(i)}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}\right]$$

$$\nabla_{\mathbf{w}_r} J(\mathbf{w}) = \sum_{i=1}^{N} 1\{y^{(i)} = r\}\mathbf{x}^{(i)}\left[1 - \frac{e^{\mathbf{w}_r^T\mathbf{x}^{(i)}}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}\right] + \sum_{i=1}^{N}\sum_{k=1,k\neq r}^{K} 1\{y^{(i)} = k\}\mathbf{x}^{(i)}\left[-\frac{e^{\mathbf{w}_r^T\mathbf{x}^{(i)}}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}\right]$$

1 or 0

$$\nabla_{\mathbf{w}_r} J(\mathbf{w}) = \sum_{i=1}^{N} \mathbf{x}^{(i)}\left[1\{y^{(i)} = r\} - \frac{e^{\mathbf{w}_r^T\mathbf{x}^{(i)}}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T\mathbf{x}^{(i)}}}\right]$$

How can we modify our existing model ?

Our existing model gave a probability of belonging to a class.

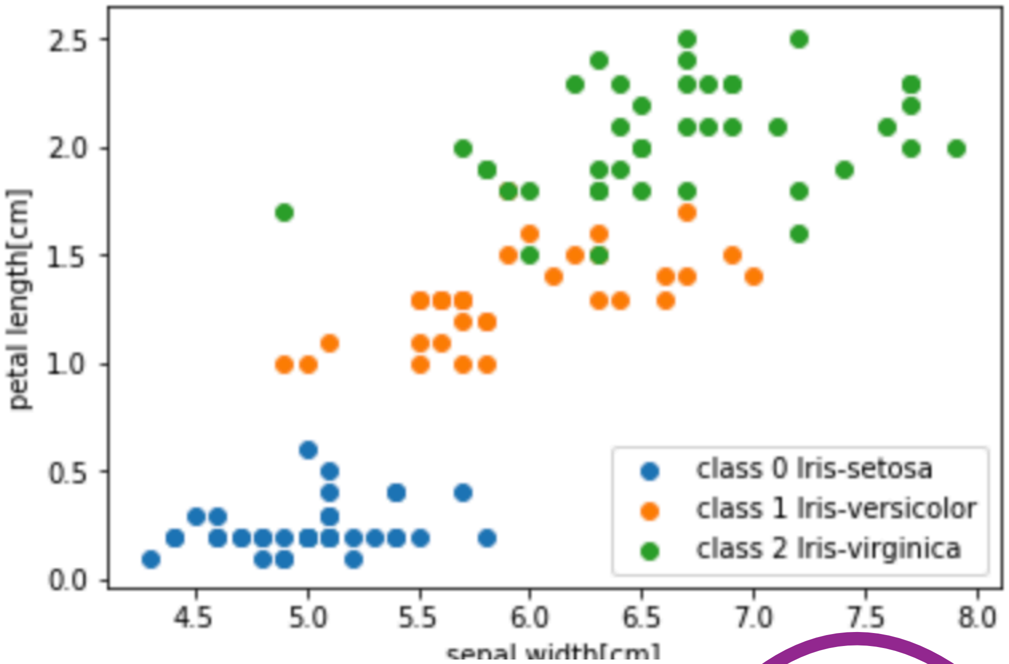
How can we provide an estimate of K classes? If K = 3 we can represent each class as follows:

$[1 \quad 0 \quad 0]^T$ $[0 \quad 1 \quad 0]^T$ $[0 \quad 0 \quad 1]^T$

class Setosa

class Versicolor

class Virginia



$$
X = \begin{bmatrix} 1 & 5.8 & 2.4 \\ 1 & 6 & 1 \\ 1 & 5.5 & 0.2 \\ 1 & 7.3 & 1.8 \\ 1 & 5 & 0.2 \\ 1 & 6.3 & 2.5 \\ 1 & 5 & 0.3 \\ 1 & 6.7 & 1.5 \\ 1 & 6.8 & 1.4 \\ 1 & 6.1 & 1.3 \end{bmatrix}
\qquad
y = \begin{bmatrix} 1 \\ 1 \\ 2 \\ 0 \\ 2 \\ 0 \\ 0 \\ 1 \\ 2 \\ 2 \end{bmatrix}
\rightarrow
\begin{bmatrix} [0,1,0] \\ [0,1,0] \\ [0,0,1] \\ [1,0,0] \\ [0,0,1] \\ [1,0,0] \\ [1,0,0] \\ [0,1,0] \\ [0,0,1] \\ [0,0,1] \end{bmatrix}
$$

Example

Suppose we are clarifying which iris out of 3 choices. If we have fit the model and thus have created **W**

$$[1 \quad 0 \quad 0]^T \qquad [0 \quad 1 \quad 0]^T \qquad [0 \quad 0 \quad 1]^T$$

class Setosa

class Versicolor

class Virginia

Code to create graphics adapted from Hands-On Machine Learning with Scikit-Learn & TensorFlow

$$(P(y = i \mid \mathbf{x})) = \left(\frac{e^{\mathbf{w}_i^T X_i}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T X_i}} \right)$$

W

41.09	-8.08	-18.02
2.09	1.16	3.79
-43.18	6.92	14.23

x

1
4
1.5

=

Z score

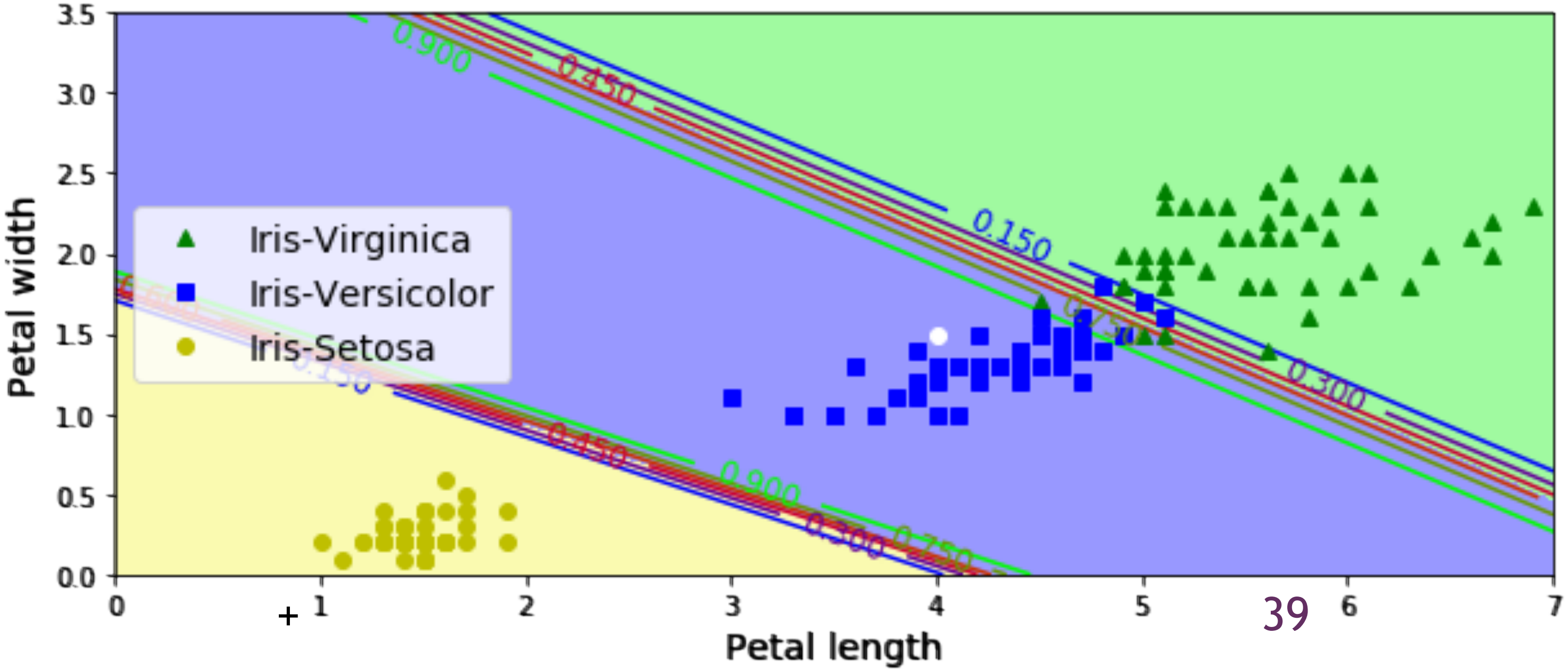
-18.28
12.43
5.84

e^{score}

1.15E-08
250404
346

normalize divide by 250750

4.60E-14
0.9986
0.00137



Example

Suppose we are clarifying which iris out of 3 choices. If we have fit the model and thus have created **W**

$$[1 \quad 0 \quad 0]^T \quad [0 \quad 1 \quad 0]^T \quad [0 \quad 0 \quad 1]^T$$

class Setosa

class Versicolor

class Virginia

$$(P(y=i \mid \mathbf{x})) = \left(\frac{e^{\mathbf{w}_i^T X_i}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T X_i}} \right)$$

W

41.09	-8.08	-18.02
2.09	1.16	3.79
-43.18	6.92	14.23

x

1
5.2
1.5

=

Z score

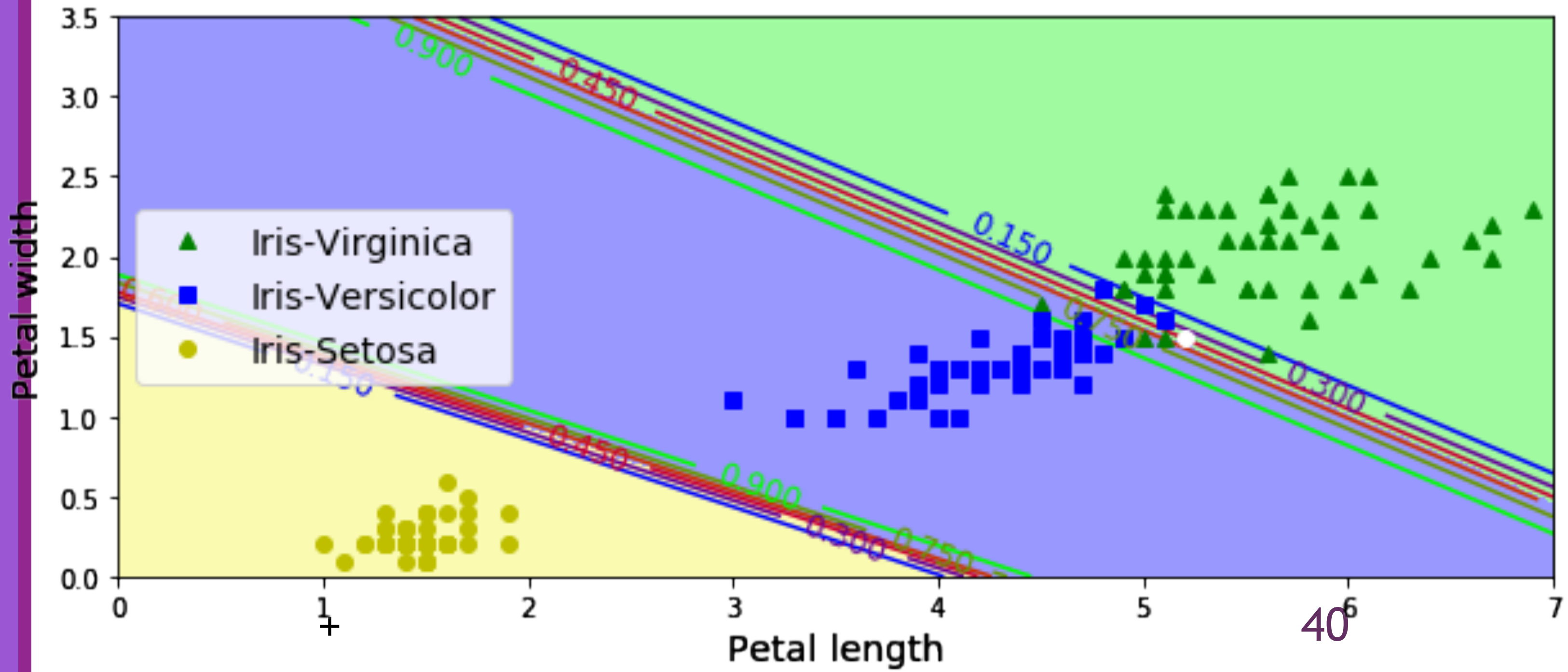
-27.98
13.83
14.15

e^{score}

7.06E-13
1013275.8
1397137.3

normalize divide by 2410413.2

2.93E-19
0.420
0.580



Example

Suppose we are clarifying which iris out of 3 choices. If we have fit the model and thus have created **W**

$$\left(P(y=i \mid \mathbf{x})\right) = \left(\frac{e^{\mathbf{w}_i^T X_i}}{\sum_{j=1}^{K} e^{\mathbf{w}_j^T X_i}}\right)$$

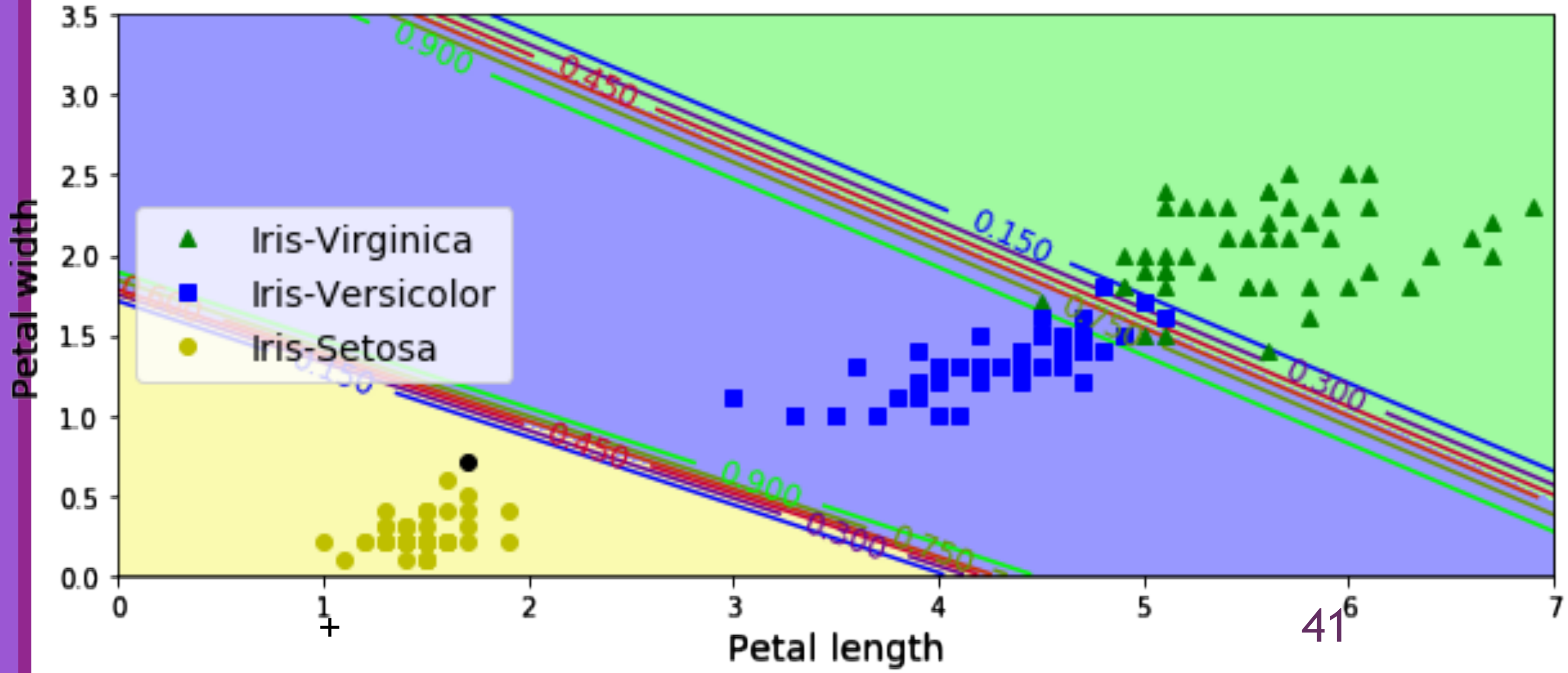
$$\underset{W}{\begin{bmatrix} 41.09 & -8.08 & -18.02 \\ 2.09 & 1.16 & 3.79 \\ -43.18 & 6.92 & 14.23 \end{bmatrix}} \underset{\mathbf{x}}{\begin{bmatrix} 1 \\ 1.7 \\ 0.7 \end{bmatrix}} = \underset{\text{Z score}}{\begin{bmatrix} 14.73 \\ 6.72 \\ -21.46 \end{bmatrix}} \rightarrow \underset{e^{\text{score}}}{\begin{bmatrix} 2501744.5 \\ 830.99 \\ 4.81E-10 \end{bmatrix}} \rightarrow \begin{bmatrix} 0.999679 \\ 0.000332 \\ 1.92E-16 \end{bmatrix}$$

normalize divide by 2502575.5

$[1 \quad 0 \quad 0]^T$ class Setosa

$[0 \quad 1 \quad 0]^T$ class Versicolor

$[0 \quad 0 \quad 1]^T$ class Virginia



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If K=2 Softmax ➜ Logistic Regression

We can subtract any fixed K dimensional vector from each of the K coefficient vectors w_j

$$p(y_i = j \mid \mathbf{x}; \mathbf{w}) = \frac{e_i^{(\mathbf{w}_j - \theta)^T \mathbf{x}}}{\sum_{i=1}^{K} e^{(\mathbf{w}_i - \theta)^T \mathbf{x}}}$$

$$p(y_i = j \mid \mathbf{x}; \mathbf{w}) = \frac{e_i^{(\mathbf{w}_j)^T \mathbf{x}} e_i^{(-\theta)^T \mathbf{x}}}{\sum_{i=1}^{K} e_i^{(\mathbf{w}_i)^T \mathbf{x}} e_i^{(-\theta)^T \mathbf{x}}}$$

$$p(y_i = j \mid \mathbf{x}; \mathbf{w}) = \frac{e_i^{(\mathbf{w}_j)^T \mathbf{x}}}{\sum_{i=1}^{K} e^{(\mathbf{w}_i)^T \mathbf{x}}}$$

For y ∈ {1,2}

$$h(\mathbf{x}) = \begin{bmatrix} p(y=1 \mid \mathbf{x}) \\ p(y=2 \mid \mathbf{x}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{2} e^{\mathbf{w}_j^T \mathbf{x}}} \begin{bmatrix} e^{\mathbf{w}_1^T \mathbf{x}} \\ e^{\mathbf{w}_2^T \mathbf{x}} \end{bmatrix}$$

$$= \frac{1}{e^{\vec{\mathbf{0}}^T \mathbf{x}} + e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}} \begin{bmatrix} e^{\vec{0}^T \mathbf{x}} \\ e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}} \end{bmatrix}$$

$$= \frac{1}{1 + e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}} \begin{bmatrix} 1 \\ e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}} \end{bmatrix}$$

$$= \begin{bmatrix} \dfrac{1}{1 + e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}} \\ \dfrac{e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}}{1 + e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{1 + e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}} \\ 1 - \dfrac{1}{1 + e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{1 + e^{(\mathbf{w}')^T \mathbf{x}}} \\ 1 - \dfrac{1}{1 + e^{(\mathbf{w}')^T \mathbf{x}}} \end{bmatrix}$$

You will not responsible for the material on this slide for midterm 2

If K=2 Softmax → Logistic Regression

For y ∈ {1,2}

$$h(\mathbf{x}) = \begin{bmatrix} p(y=1 \mid \mathbf{x}) \\ p(y=2 \mid \mathbf{x}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{2} e^{\mathbf{w}_j^T \mathbf{x}}} \begin{bmatrix} e^{\mathbf{w}_1^T \mathbf{x}} \\ e^{\mathbf{w}_2^T \mathbf{x}} \end{bmatrix}$$

$$\frac{1}{+ e^{(\mathbf{w_2} - \mathbf{w_1})^T \mathbf{x}}} \begin{bmatrix} e^{\vec{0}^T \mathbf{x}} \\ e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}} \end{bmatrix}$$

$$\frac{1}{+ e^{(\mathbf{w_2} - \mathbf{w_1})^T \mathbf{x}}} \begin{bmatrix} 1 \\ e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}} \end{bmatrix}$$

$$= \begin{bmatrix} \dfrac{1}{1 + e^{(\mathbf{w_2} - \mathbf{w_1})^T \mathbf{x}}} \\ \dfrac{e^{(\mathbf{w}_2 - \mathbf{w}_1)^T \mathbf{x}}}{1 + e^{(\mathbf{w_2} - \mathbf{w_1})^T \mathbf{x}}} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{1 + e^{(\mathbf{w_2} - \mathbf{w_1})^T \mathbf{x}}} \\ 1 - \dfrac{1}{1 + e^{(\mathbf{w_2} - \mathbf{w_1})^T \mathbf{x}}} \end{bmatrix} = \begin{bmatrix} \dfrac{1}{1 + e^{(\mathbf{w}')^T \mathbf{x}}} \\ 1 - \dfrac{1}{1 + e^{(\mathbf{w}')^T \mathbf{x}}} \end{bmatrix}$$

We can subtract any fixed K dimensional vector from each of the K coefficient vectors w_j

$$p(y_i = j \mid \mathbf{x}; \mathbf{w}) = \frac{e_i^{(\mathbf{w}_j - \theta)^T \mathbf{x}}}{\sum_{i=1}^{K} e^{(\mathbf{w}_i - \theta)^T \mathbf{x}}}$$

$$p(y_i = j \mid \mathbf{x}; \mathbf{w}) = \frac{e_i^{(\mathbf{w}_j)^T \mathbf{x}} e_i^{(-\theta)^T \mathbf{x}}}{\sum_{i=1}^{K} e_i^{(\mathbf{w}_i)^T \mathbf{x}} e_i^{(-\theta)^T \mathbf{x}}}$$

$$p(y_i = j \mid \mathbf{x}; \mathbf{w}) = \frac{e_i^{(\mathbf{w}_j)^T \mathbf{x}}}{\sum_{i=1}^{K} e^{(\mathbf{w}_i)^T \mathbf{x}}}$$

over-parameterized
there are multiple parameters that give the same answer

Using Sklearn's Logistic Regression

```
from sklearn.linear_model import LogisticRegression

clf = LogisticRegression(solver='sag',multi_class='multinomial')

clf.fit(X_train, y_train)

yhat_test = clf.predict(X_test)

score = clf.score(X_test, y_test)
```

make an instance of the model
Parameters set for this instance:
multi_class = 'multinomial'

Use the coefficient vector to predict

compute the accuracy

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

Using Sklearn’s Logistic Regression

```
from sklearn.linear_model import LogisticRegression

clf = LogisticRegression(solver=‘sag',multi_class='multinomial')

clf.fit(X_train, y_train)

yhat_test = clf.predict(X_test)

score = clf.score(X_test, y_test)
```

import the model
in Sklearn this will
implemented as a class

make an instance of the model
Parameters set for this instance:
multi_class = ‘multinomial'

Train the model. (i.e. run the
algorithm using X_train and y_train
to create the coefficient vector

Use the coefficient vector to predict

compute the accuracy

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

```python
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)#default is 1/4 test

scaler = StandardScaler()
X_train= scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)
```

```
X_train = [[ 7.   6. 10.   5.   3. 10.   9. 10.   2.]
           [ 8.   3.   8.   3.   4.   9.   8.   9.   8.]
           [ 8. 10. 10. 10.   6. 10. 10. 10.   1.]
           [ 1.   1.   1.   1.   2.   1.   1.   1.   1.]]
```

y_train = [1 1 1 0]

```
X_test = [[ 1.   1.   1.   1.   2.   5.   1.   1.   1.]
          [ 3.   1.   1.   1.   2.   1.   2.   1.   1.]
          [ 5.   5.   5.   2.   5. 10.   4.   3.   1.]
          [ 4.   7.   8.   3.   4. 10.   9.   1.   1.]]
```

```
y_test = [0 0 1 1]
```

```
[[ 0.92  0.94  2.31  0.77 -0.1   1.81  2.23  2.27  0.25]
 [ 1.28 -0.04  1.63  0.07  0.34  1.53  1.82  1.95  3.75]
 [ 1.28  2.25  2.31  2.53  1.23  1.81  2.63  2.27 -0.34]
 [-1.22 -0.7  -0.74 -0.64 -0.55 -0.68 -0.99 -0.62 -0.34]]
```

```
[[-1.22 -0.7  -0.74 -0.64 -0.55  0.43 -0.99 -0.62 -0.34]
 [-0.51 -0.7  -0.74 -0.64 -0.55 -0.68 -0.59 -0.62 -0.34]
 [ 0.21  0.61  0.62 -0.28  0.78  1.81  0.22  0.02 -0.34]
 [-0.15  1.27  1.63  0.07  0.34  1.81  2.23 -0.62 -0.34]]
```

Next, we create a logistic regression object. By default, the logistic regresssion object will use $L2$ regularization. Here we have selected not to have regularization by using *penalty*='*none*'. If regularization is used, the parameter `C` states the level of regularization. Higher values of `C` have `less` regularization. We can chose to set explicity the regularization, or have the optimal value determined for us.

Note that $\lambda = 1/C$.

```
logreg = linear_model.LogisticRegression(penalty='none')
```

Penalty choices: L1,L2, L1 and L2.
Default is L2

Then, we fit the model.

```
logreg.fit(X_train, y_train)
```

```
LogisticRegression(penalty='none')
```

	feature	slope
0	thick	1.194634
1	size_unif	0.260756
2	shape_unif	0.839409
3	marg	0.615559
4	cell_size	0.592045
5	bare	1.601667
6	chrom	0.843135
7	normal	0.740983
8	mit	0.340539

```
print(logreg.intercept_)
print(logreg.coef_)
```

```
yhat = logreg.predict(X_test)# the predict method will return 0 or 1
```

```
[0 0 1 1]
```

```
yhat_proba = logreg.predict_proba(X_test)
```

```
[[0.99 0.01]
 [1.   0.  ]
 [0.06 0.94]
 [0.01 0.99]]
```

score = clf.score(X_test, y_test)

"Return the mean accuracy"

```
0.947368
```

```
from sklearn.metrics import confusion_matrix
confusion_matrix(yhat, y_test)
```

"Confusion matrix whose i-th row and j-th column entry indicates the number of samples with true label being i-th class and predicted label being j-th class."

```
logreg = linear_model.LogisticRegression(solver='liblinear', penalty='l1', C=0.01)
```

```
logreg = linear_model.LogisticRegression( penalty='l2', C=0.08)
```

	feature	slope
0	thick	1.194634
1	size_unif	0.260756
2	shape_unif	0.839409
3	marg	0.615559
4	cell_size	0.592045
5	bare	1.601667
6	chrom	0.843135
7	normal	0.740983
8	mit	0.340539

```
[0 0 1 1]

[[0.99 0.01]
 [1.   0.  ]
 [0.06 0.94]
 [0.01 0.99]]
```

	feature	slope
0	thick	0.000000
1	size_unif	0.436027
2	shape_unif	0.191333
3	marg	0.000000
4	cell_size	0.000000
5	bare	0.484421
6	chrom	0.000000
7	normal	0.000000
8	mit	0.000000

```
[0 0 1 1]

[[0.56 0.44]
 [0.68 0.32]
 [0.22 0.78]
 [0.15 0.85]]
```

	feature	slope
0	thick	0.622906
1	size_unif	0.500051
2	shape_unif	0.560409
3	marg	0.431736
4	cell_size	0.453271
5	bare	0.892948
6	chrom	0.550934
7	normal	0.503239
8	mit	0.226096

```
[0 0 1 1]

[[0.97 0.03]
 [0.98 0.02]
 [0.17 0.83]
 [0.05 0.95]]
```