Classification: Linear Models

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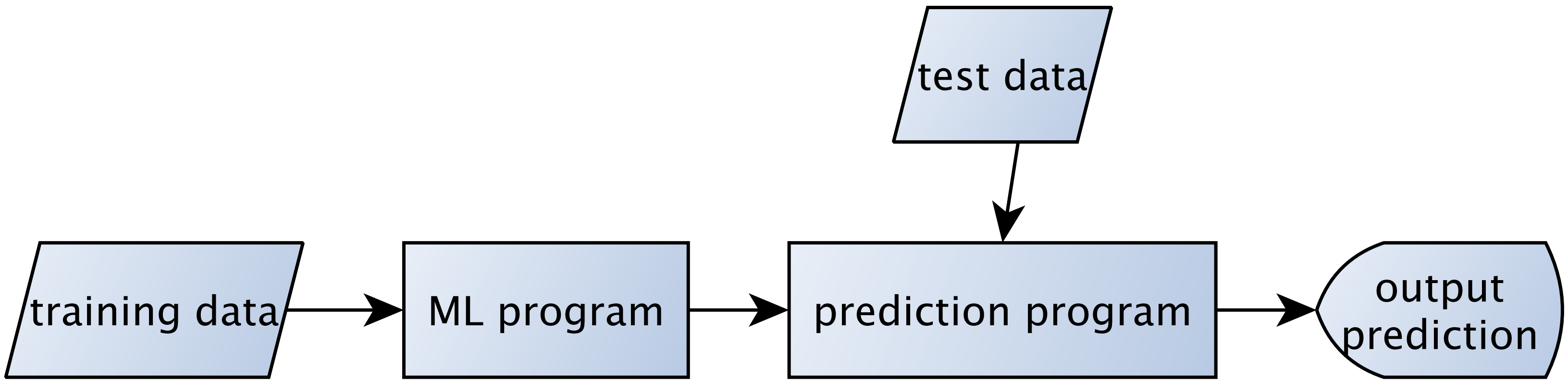
Deep Learning 980

Classification Problems

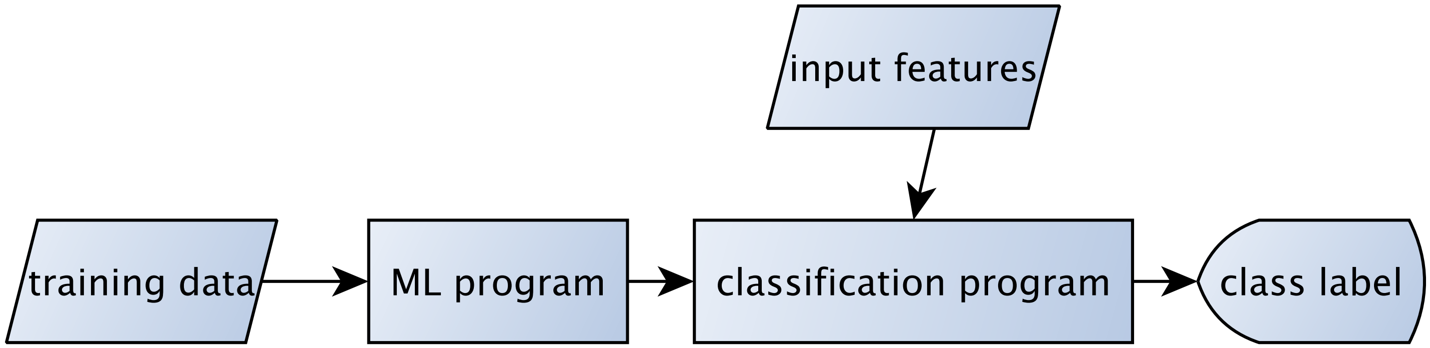
Machine Learning as Program Synthesis

- We can think of a machine learning system as a program that produces a program



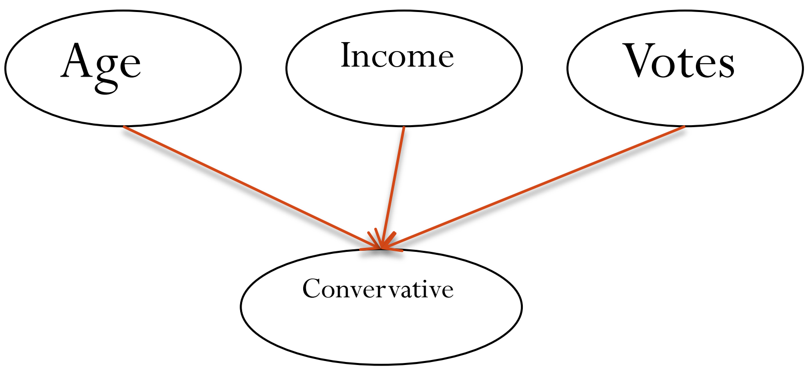
Classifying Examples

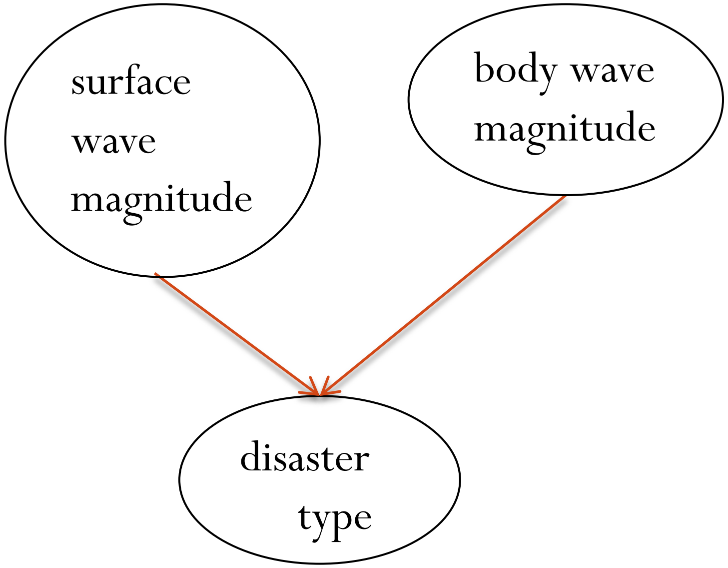
- Many predictive problems in machine learning seek to build a program with the following I/O specs.
- Input: A list/tuple/vector of **features** $x_1,..,x_m$
- Output: A discrete class label.
  - If there are only two possible classes/labels, we have a **binary** classification problem.



Examples

- Will the person vote conservative, given age, income, previous votes?
- Is the patient at risk of diabetes given body mass, age, blood test measurements?
- Predict Earthquake vs. nuclear explosion given body wave magnitude and surface wave magnitude.

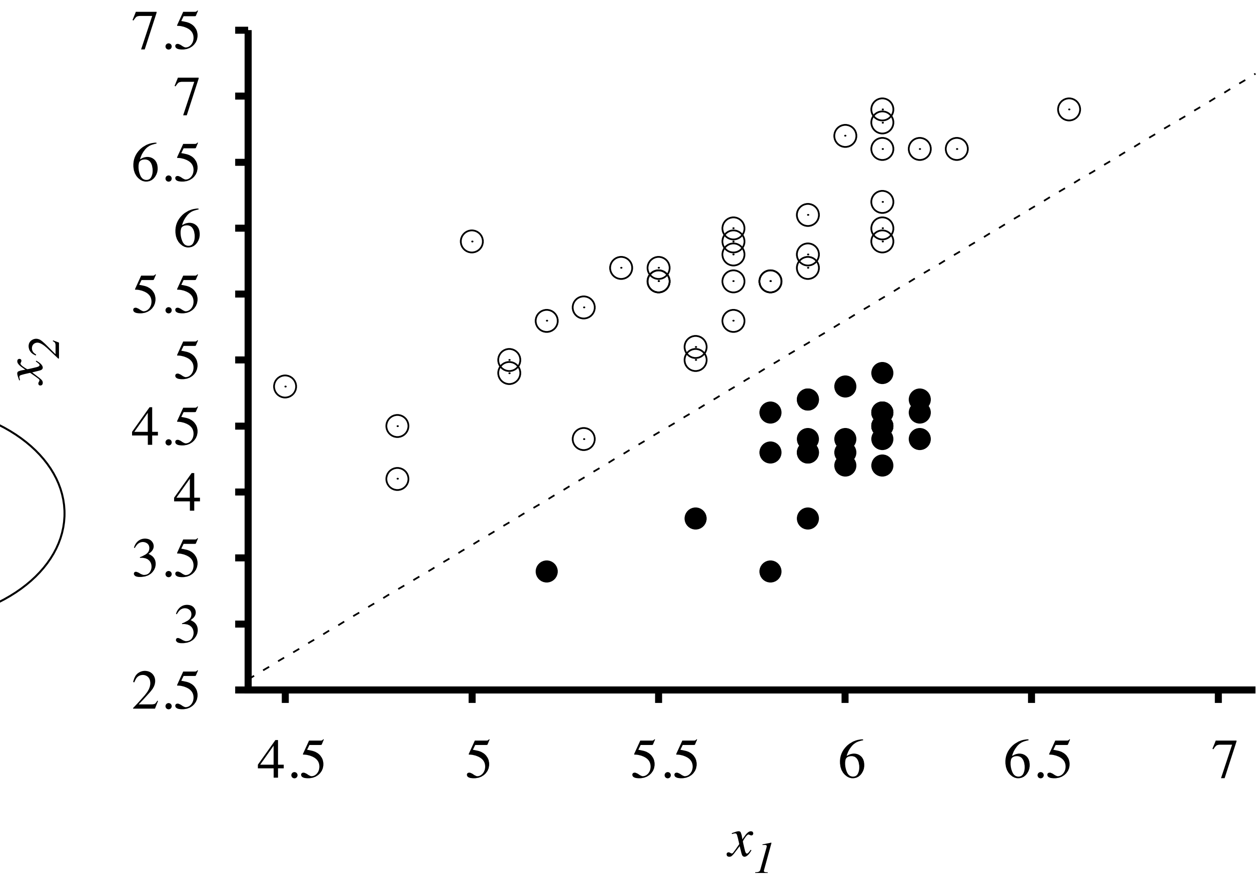




Learning to Classify

- For classification, there are many datasets of the form
  $(\text{input}_1,\text{output}_1),\ldots,(\text{input}_n,\text{output}_n)$
  - Mathematical notation: $(\boldsymbol{x}_1,y_1),\ldots,(\boldsymbol{x}_n,y_n)$.
    - If y is discrete → <u>classification</u> problem
    - If y is continuous → <u>regression</u> problem
  - Supervised Learning: the data tell us the right answer
  - The basis of most neural net methods

Example Data



x1 = surface wave magnitude

x2 = body wave magnitude

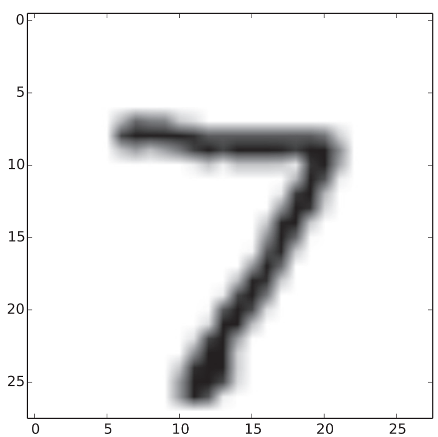
white = earthquake

black = nuclear explosion

Russell and Norvig Figure 18.15

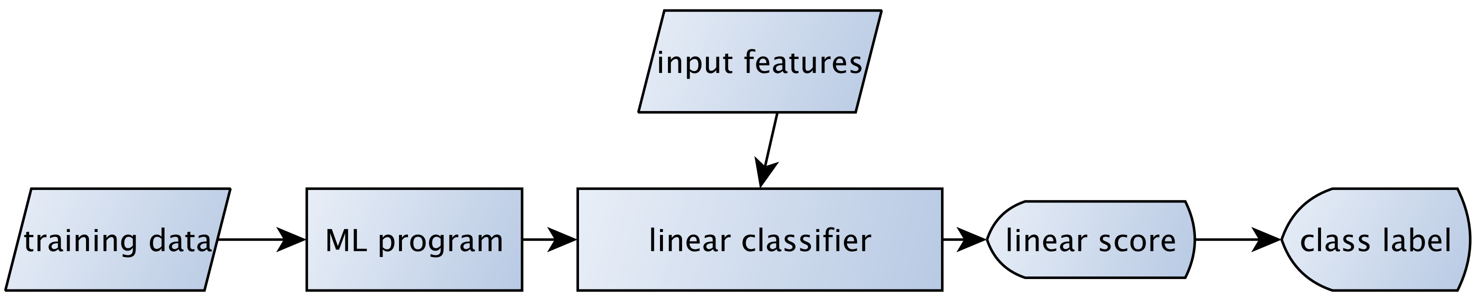
Example: Classifying Digits

- Classify image as “7” vs. “not 7”.
- Represent input image as vector **x** with 28x28 =784 numbers.
- Discussion: is this representation a good idea?



	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	185	159	151	60	36	0	0	0	0	0	0	0	0	0
8	254	254	254	254	241	198	198	198	198	198	198	198	198	170
9	114	72	114	163	227	254	225	254	254	254	250	229	254	254
10	0	0	0	0	17	66	14	67	67	67	59	21	236	254
11	0	0	0	0	0	0	0	0	0	0	0	83	253	209
12	0	0	0	0	0	0	0	0	0	0	22	233	255	83
13	0	0	0	0	0	0	0	0	0	0	129	254	238	44
14	0	0	0	0	0	0	0	0	0	59	249	254	62	0
15	0	0	0	0	0	0	0	0	0	133	254	187	5	0
16	0	0	0	0	0	0	0	0	9	205	248	58	0	0
17	0	0	0	0	0	0	0	0	126	254	182	0	0	0
18	0	0	0	0	0	0	0	75	251	240	57	0	0	0
19	0	0	0	0	0	0	19	221	254	166	0	0	0	0
20	0	0	0	0	0	3	203	254	219	35	0	0	0	0
21	0	0	0	0	0	38	254	254	77	0	0	0	0	0
22	0	0	0	0	31	224	254	115	1	0	0	0	0	0
23	0	0	0	0	133	254	254	52	0	0	0	0	0	0
24	0	0	0	61	242	254	254	52	0	0	0	0	0	0
25	0	0	0	121	254	254	219	40	0	0	0	0	0	0
26	0	0	0	121	254	207	18	0	0	0	0	0	0	0
27	0	0	0	0	0	0	0	0	0	0	0	0	0	0

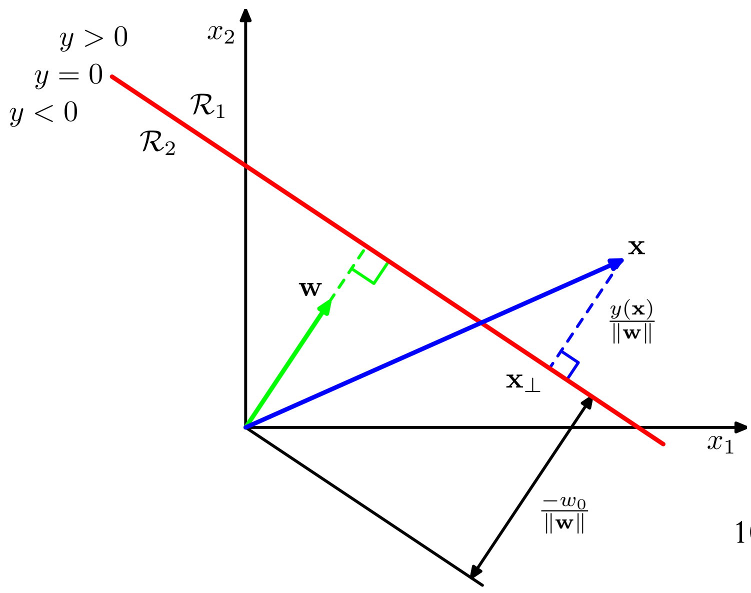
Linear Classification Models



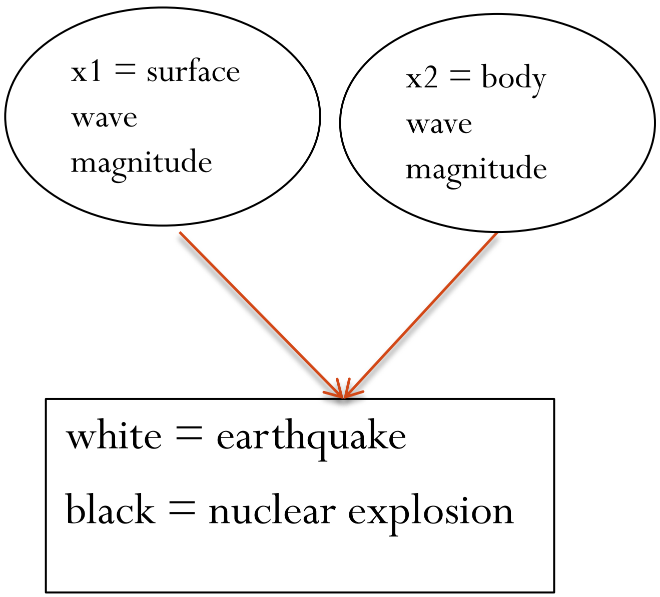
Linear Classification Models

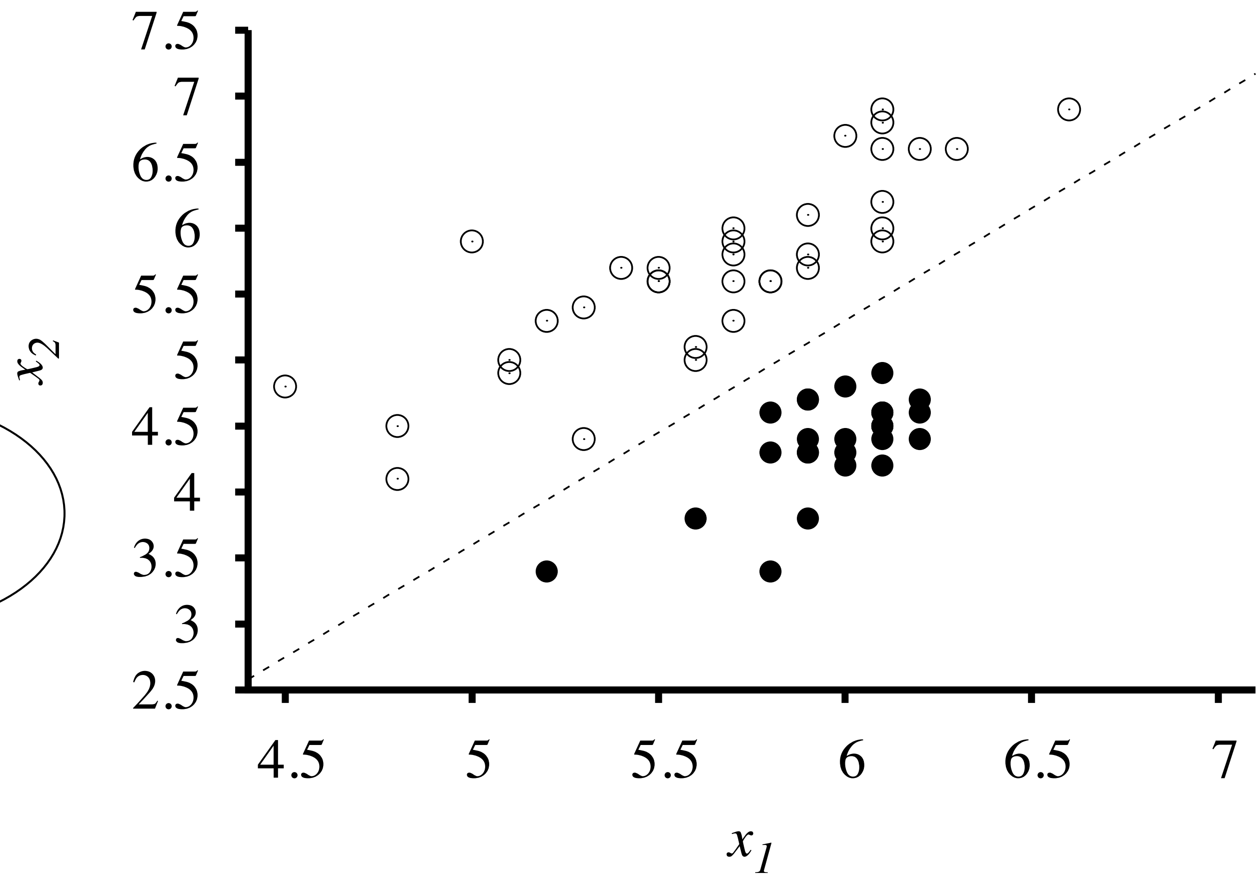
- General Idea:

1. Simple linear model y(**x**) = **w** · **x**
   - **w** is a list of weight parameters to be learned
2. Classify as positive if *y(x)* crosses a threshold, typically 0.
   - The **decision boundary** *y(x)=0* defines a line for 2 input features, a hyperplane for > 2.



Example: Linear Separation

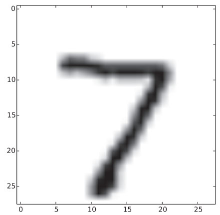




Russell and Norvig Figure 18.15

Example: Classifying Digits

- Classify input vector as "7" vs. "not 7".
- Represent input image as vector **x** with 28x28 =784 numbers.
- Target t = 1 for "positive", -1 for "negative".
- Prediction function y:R^{784} ➔R.
- Classify **x** as positive if y(**x**) >0, negative o.w.
- Discussion: how can we handle multiple classes, e.g. digits from 1..10?



The Bias Weight

- Usually a linear includes a bias term (aka intercept, baseline) b.
  - E.g. $y(x_1,x_2) = \mathrm{b} + w_1 x_1 + w_2 x_2$
- Equivalently: add an imaginary constant 1 input $x_0 = 1$ and set $b = w_0$
  - E.g. $\mathrm{y}(x_0 = 1, x_1, x_2) = \mathbf{w} \cdot \mathbf{x} = w_0 x_0 + w_1 x_1 + w_2 x_2 = w_0 1 + w_1 x_1 + w_2 x_2$

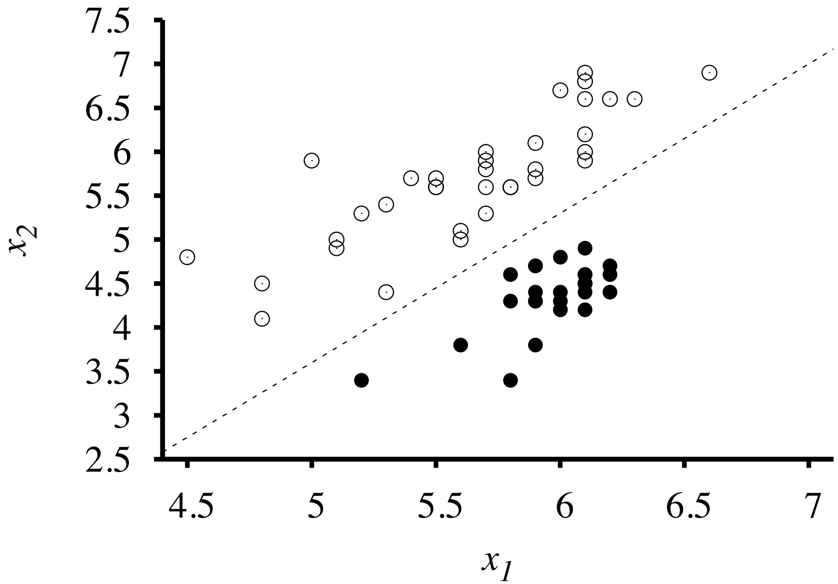
Strengths of Linear Classifiers

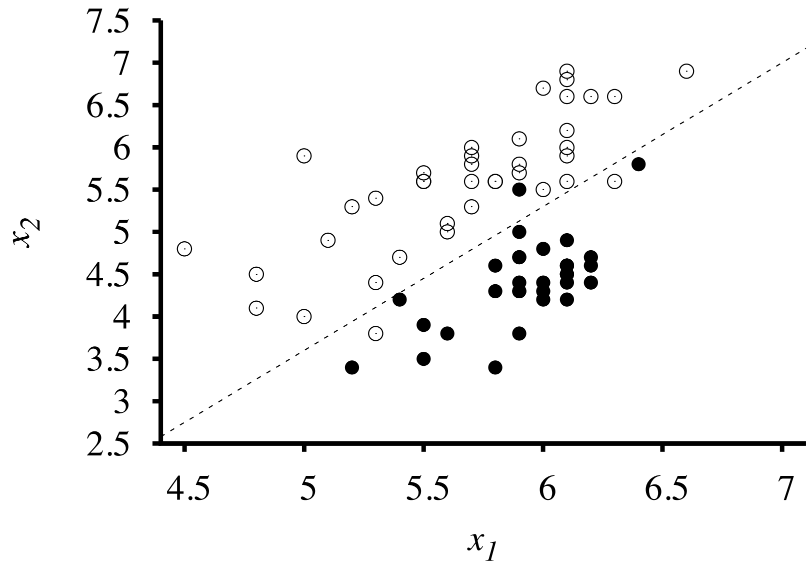
- Efficient to learn
- Interpretable
  - in many applications, the "effects" are most important – which features receive the biggest weight.
- Can *quantify predictive uncertainty*
  - derive confidence bounds on accuracy of predictions.
- In machine learning, interpretability and quantifying uncertainty often go together, but trade off against accuracy.
- Science manages to combine all three.

Convexity and Linear Separability

- A set of points C is convex if for any two points **x,y** in C, fraction $0 \leq \alpha \leq 1$ we have $\alpha\mathbf{x}+(1-\alpha)\mathbf{y}$ is also in C.
- If two classes are linearly separable, they are convex.
- Separating Hyperplane Theorem: There exists a linear separator for two disjoint sets (classes) if and only if each each set (class) is convex.
- Illustration

Linear Separability and Convexity



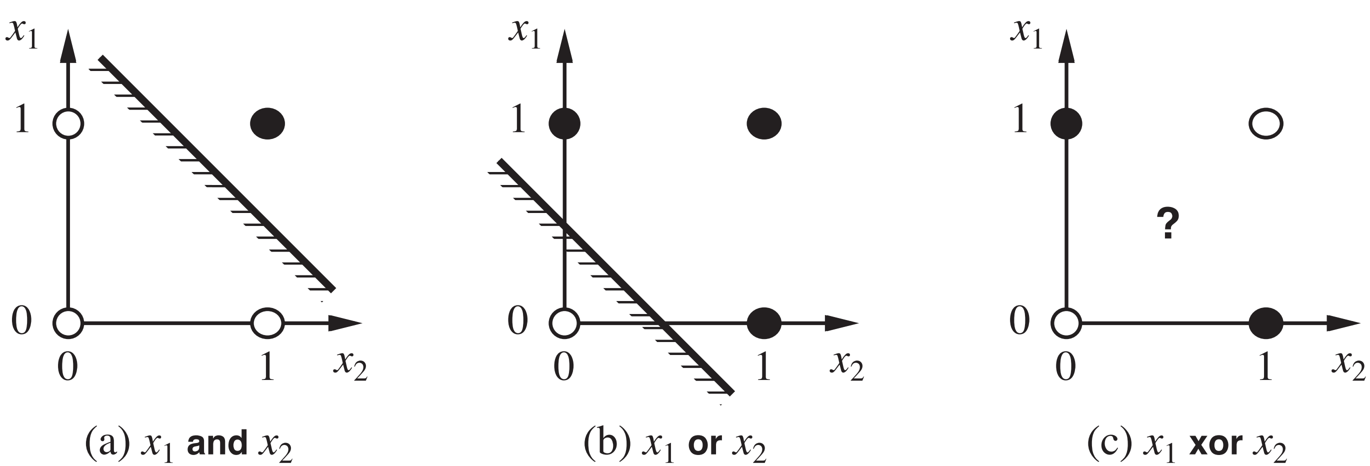


Data with outliers removed:
convex, separable

Original data:
non-convex, non-separable

Nonseparability

- Linear discriminants can solve problems only if the classes can be separated by a line (hyperplane).
- Canonical example of non-separable problem is X-OR.



Responses to Nonseparability

Classes cannot be separated by a linear discriminant

separate classes not completely
but "well"

Fisher discriminant (not covered)
logistic regression

add unobserved features

neural network
support vector machine

Gradient Descent Learning

Learning a Linear Classifier

- Most learning for continuous data follows a decision-theoretic (Bayesian) approach to learning.

1. For a given data set D, define an **error function** E(**w**,D) that measures how well the weights **w** fit the data D.
2. Find **w** that minimize the error for a given input data set D.
3. In neural net learning, the basic minimization algorithm is **gradient descent**.

Gradient Descent: Choosing a direction

- Intuition: think about trying to find street number 1000 on a block. You stop and see that you are at number 100. Which direction should you go, left or right?
- You initially check every 50 houses or so where you are. What happens when you get closer to the goal 1000?
- The fly and the window: the fly sees that the wall is darker, so the light gradient goes down: bad direction.
- See here for illustration (around 38 sec)

Gradient Descent Scheme

1. Initialize weight vectors somehow.
   - Typically randomly, more on this later.
2. Update $$w_{i+1} := w_i - \eta \frac{\partial E}{\partial w_i}$$
3. Until some convergence criterion is true

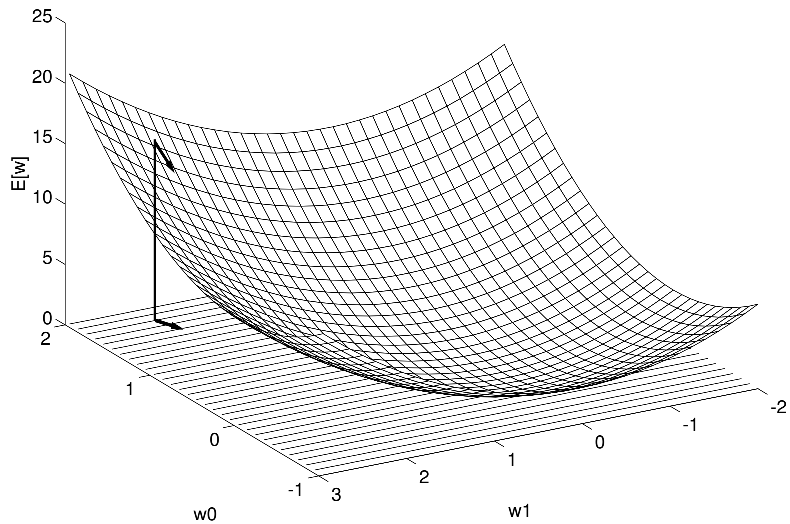
- Complexity comment: assuming gradients are easy to compute, *every update step is linear in the number of weights.*

➢ *Learning time depends on number of steps required until convergence*

Gradient Descent in One Dimension

- Update Rule
  $\mathbf{x := x - \ f'(x)}$ where η is a step size
  Example:
- Try to find y that minimizes f(y) = y^2.
- Your current location is y = -3.
- What is f'(y)?
- Answer: the derivative function is $2y$.
- Evaluated at the location -3, the derivative is ∇= -6.
- To minimize, we move in the opposite direction -∇.
- Letting the step size η= 1, your new location is
  -3 – (-6) = -3+6=3

Gradient Descent In Multiple Dimensions



Gradient

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right]$$

Training rule:

$$\Delta \vec{w} = -\eta \nabla E[\vec{w}]$$

i.e.,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i}$$

Gradient Descent: Example.

- Try to find x,y that minimize
  $f(x,y) = 3x + y^2$.
- Your current location is $x = 10$, $y = -3$.
- What is $\frac{\partial f}{\partial x}$ $\frac{\partial f}{\partial y}$
- Answer: the gradient vector is *(3, 2y)*.
- Evaluated at the location (10,-3), the gradient is $\nabla = (3, -6)$.
- To minimize, we move in the opposite direction $-\nabla$.
- Letting the step size $\eta = 1$, your new location is
  (10,-3) - (3,-6) = (7, 3).

Gradient Descent: Exercise

- Try to find x,y that minimize
  $f(x,y) = 3x + y^2$.
- Your current location is $x = 7$, $y = 3$.
- The gradient vector is $(3, 2y)$.
- Letting the step size $\eta = 1$, what is your new location?
- Demos
  - Visualization
  - Excel Demo
  - UBC neural net tool

Perceptron Learning

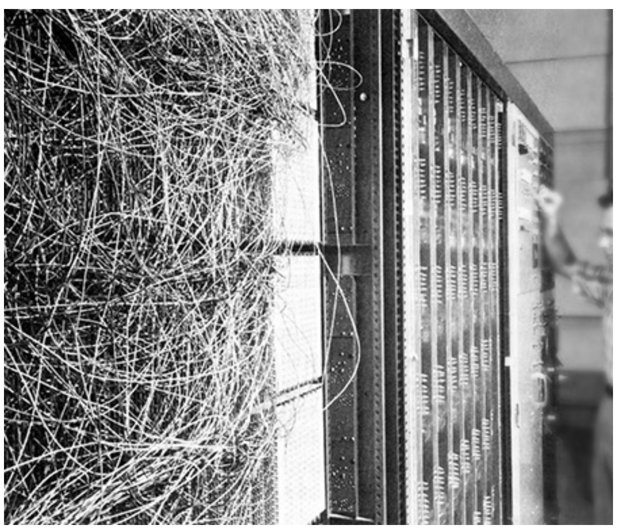
Defining an Error Function

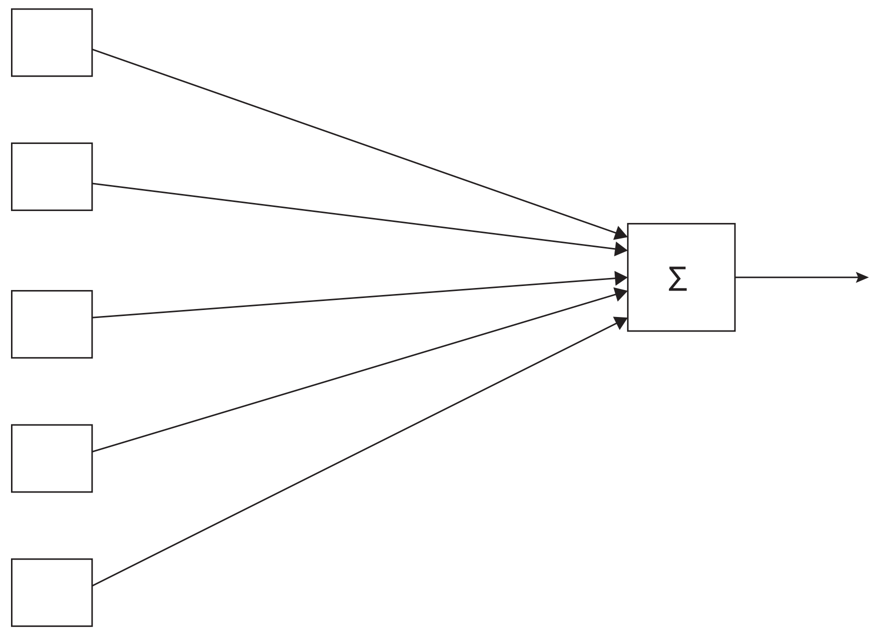
- General idea:

1. Encode class label using a real number t.
   - e.g., "positive" = 1, "negative" = 0 or "negative" = -1.
   - This is the first example we see of *embedding*.
2. Measure error or **loss** by comparing continuous linear output y and class label code t.
3. Obvious loss function is 0-1:
   0 if prediction correct, 1 otherwise.
4. In practice use *convex* upper bounds on 0-1 loss:
   $loss(y,t) \geq 0$ if prediction correct
   $loss(y,t) \geq 1$ if prediction false

Perceptrons

- Perceptrons are a precursor to neural nets.
  - Analog implementation by Rosenblatt in the 1950s





The Perceptron Error Function

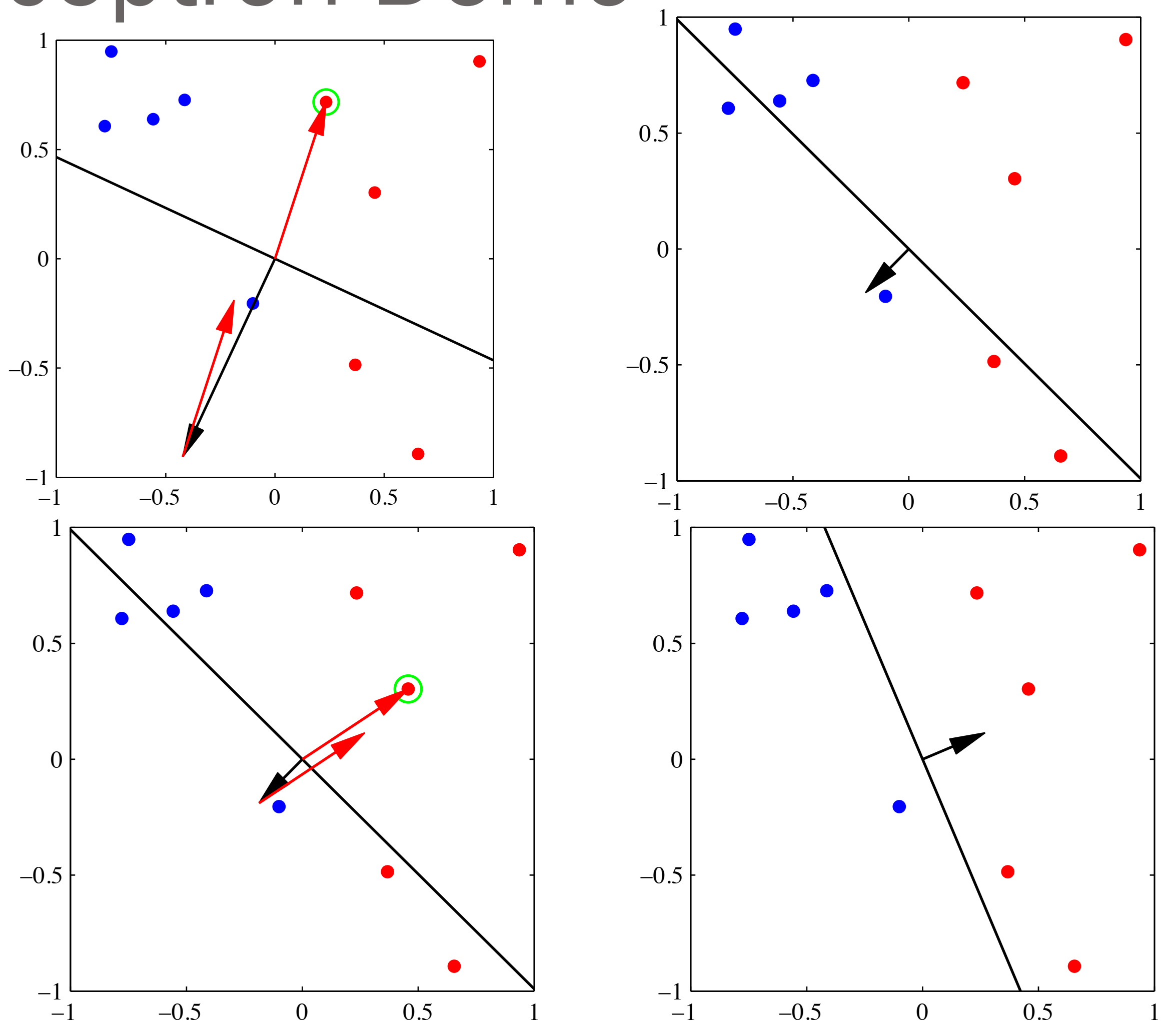
- Let y = 1 for positive class, y = -1 for negative
- An example is misclassified if and only if $(x_j \cdot \boldsymbol{w})\boldsymbol{y_j}<0$
  - Exercise: Take a moment to verify this.
- <u>Perceptron Error</u> (fixed dataset *D*)

  $$E(\boldsymbol{w}) = \sum_{j \in M} (x_j \cdot \boldsymbol{w})\boldsymbol{y_j}$$

  where *M* is the set of misclassified inputs, the **mistakes**.
- Exercise: find the gradient of the error function for a single input $\mathbf{x}_j$.
- Solution:
  - 0 if $\mathbf{x}_j$ is correctly classified.
  - $-\ \mathbf{x}_j\mathbf{y}_j$ o.w.
- What is the gradient descent weight update formula?

Perceptron Demo

weight vector = black



Perceptron Learning Analysis

- **Theorem** If the classes are linearly separable, the perceptron learning algorithm converges to a weight vector that separates them.
- Number of steps to convergence has a theoretical upper bound.
  - In deep learning, usually no bound
- Sensitive to initialization.
- If classes are not linearly separable (e.g. X-OR), typically fails to converge.

Least-Squares Error Function

- Venerable idea (19^{th} century)

1. For each data point, find the difference between predicted and observed value
2. Square the difference
3. Sum/average the squared differences

- Does not work well for classification problems
  - But widely used for regression

$$E(\boldsymbol{w}) = 1/2 \sum_{j} ((x_j \cdot \boldsymbol{w}) - \boldsymbol{y_j})^2$$

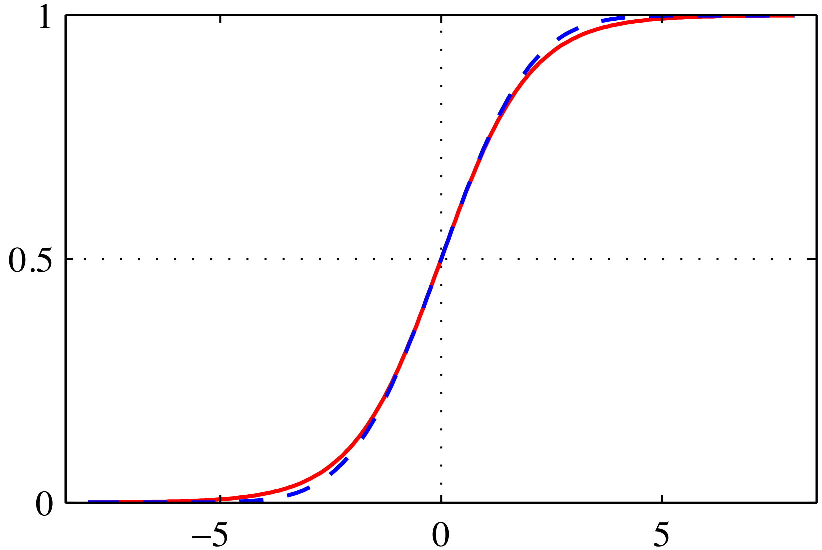
Logistic Regression

From Values to Probabilities

- Key idea: instead of predicting a class label, predict the *probability of a class label*.
- E.g., p+ = P(class is positive | features)
  p- = P(class is negative | features)
- Naturally a continuous quantity.
- How to turn a real number y into a probability p+?

The Logistic Sigmoid Function

- Definition: $$\sigma(y) = \frac{1}{1+\exp(-y)}$$
- Squeezes the real line into $[0,1]$.
- Differentiable: $$\frac{d\sigma}{dy} = \sigma(1-\sigma)$$ (nice exercise)



Soft threshold interpretation

- If $y > 0$, $\sigma(y)$ goes to 1 very quickly.
- If $y < 0$, $\sigma(y)$ goes to 0 very quickly.

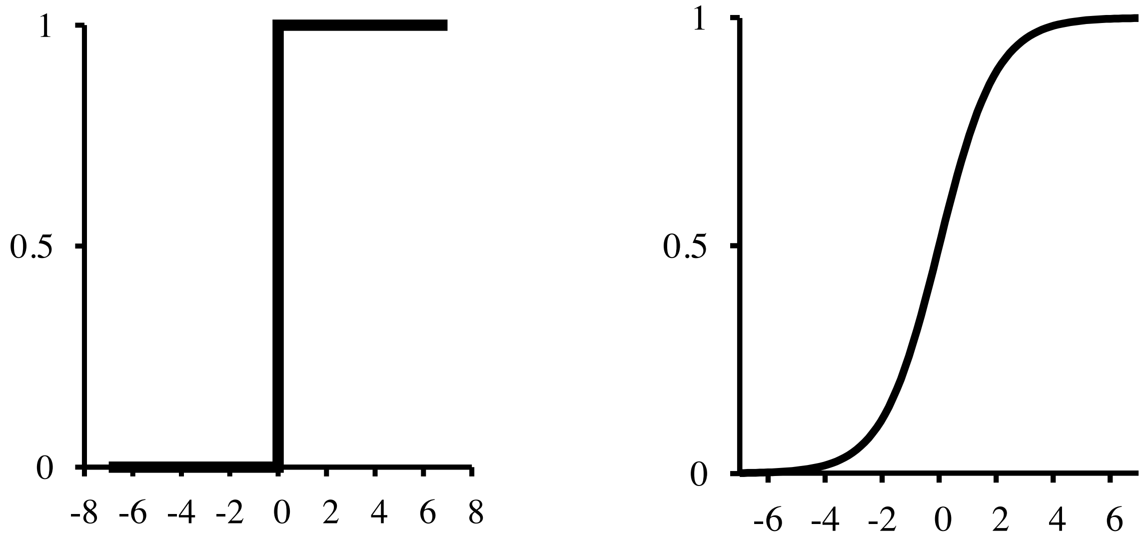


Figure Russell and Norvig 18.17

Probabilistic Interpretation

- The sigmoid can be interpreted in terms of the **class odds** p+/(1-p+).
- Exercise: Show the following implication for the class odds:

$$p^{+} = \frac{1}{1+\exp(-y)} \Rightarrow \frac{p^{+}}{1-p^{+}} = \exp(y)$$

- Therefore $y = \ln(\frac{p^{+}}{1-p^{+}}) =$ the **log class odds**.

Logistic Regression

- In logistic regression, the log-class odds are a linear function of the input features:

$$\ln\left(\frac{p^{+}}{1-p^{+}}\right) = \mathbf{x} \bullet \mathbf{w}$$

- Learning logistic regression is conceptually similar to linear regression.
- Log-linear (or exponential) models are the "nicest" general family of statistical models.

Logistic Regression: Maximum Likelihood

- Notation: the probability that the n-th input example is positive = p_n^+ which depends on a weight vector **w**.
- Positive example has $y_j = 1$, negative $y_j = 0$.
- Then the likelihood assigned to N independent training data is

$$p(\boldsymbol{y};\boldsymbol{w}) = \prod_{j=1}^{N} (\boldsymbol{p}_j^+)^{\boldsymbol{y}_j} \, (\mathbf{1} - \boldsymbol{p}_j^+)^{\boldsymbol{y}_j}$$

➢ The <u>cross-entropy error</u>

$$\mathrm{E}(\boldsymbol{w}) = -\ln p(\boldsymbol{y};\boldsymbol{w}) =$$

$$-\sum_{j=1}^{N} \boldsymbol{y}_j \boldsymbol{ln}(\boldsymbol{p}_j^+) + (\mathbf{1} - \boldsymbol{y}_j)\boldsymbol{ln}(\mathbf{1} - \boldsymbol{p}_j^+)$$

- Equivalent to minimizing the KL divergence between the predicted class probabilities and the observed class frequencies.

Weight Learning

- Homework Exercise: find the gradient of the cross-entropy error function wrt a single input $\mathbf{x}_n$

$$\mathrm{E}(\boldsymbol{w}) = -\sum_{j=1}^{N} \boldsymbol{y_j ln(p_j^+) + (1 - y_j) ln(1 - p_j^+)}$$

- Hint: recall that $\frac{d\sigma}{dy} = \sigma(1-\sigma)$
- No closed form minimum since p_j^+ is non-linear function of input features.
- Can use gradient descent. See Stanford Demo with softmax.
- Better approach: Use Iterative Reweighted Least Squares (IRLS).

Example logistic regression model learned on non-separable data

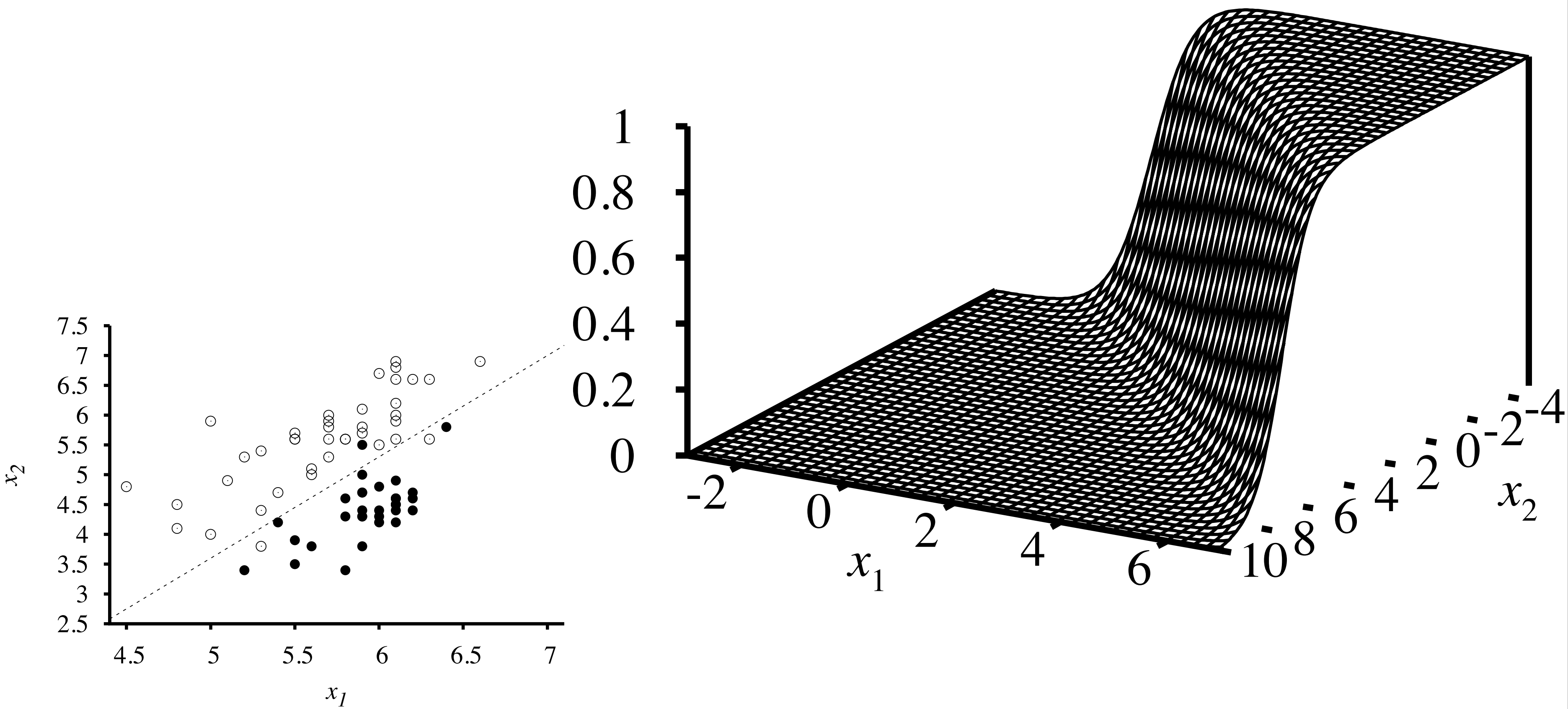
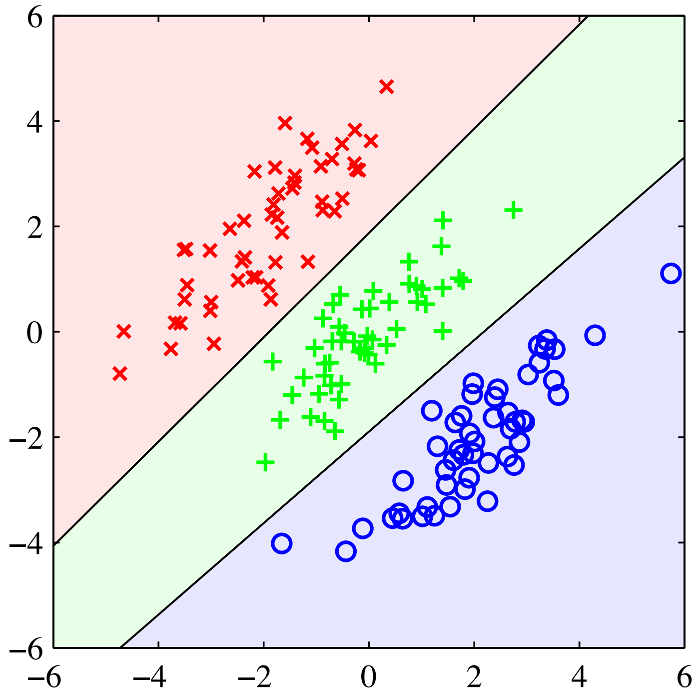


Figure Russell and Norvig 18.17

Multi-Class Example

- Logistic regression can be extended to multiple classes.
- Here's a picture of what decision boundaries can look like.



Multi-Class Problems and the SoftMax Function

- Generic multi-class probabilistic prediction

1. Build prediction models $y_1(\mathbf{x}), y_2(\mathbf{x}), .. y_k(\mathbf{x})$, one for each of the k classes.
2. Transform the numbers into probabilities:
   1. Map each $y_i(\mathbf{x})$ to $\exp\{y_i(\mathbf{x})\}$
   2. Divide by the sum:
      $\boldsymbol{\sigma}(\mathbf{x})_j = \exp\{y_j(\mathbf{x})\} / \boldsymbol{\Sigma} i \exp\{y_i(\mathbf{x})\}$

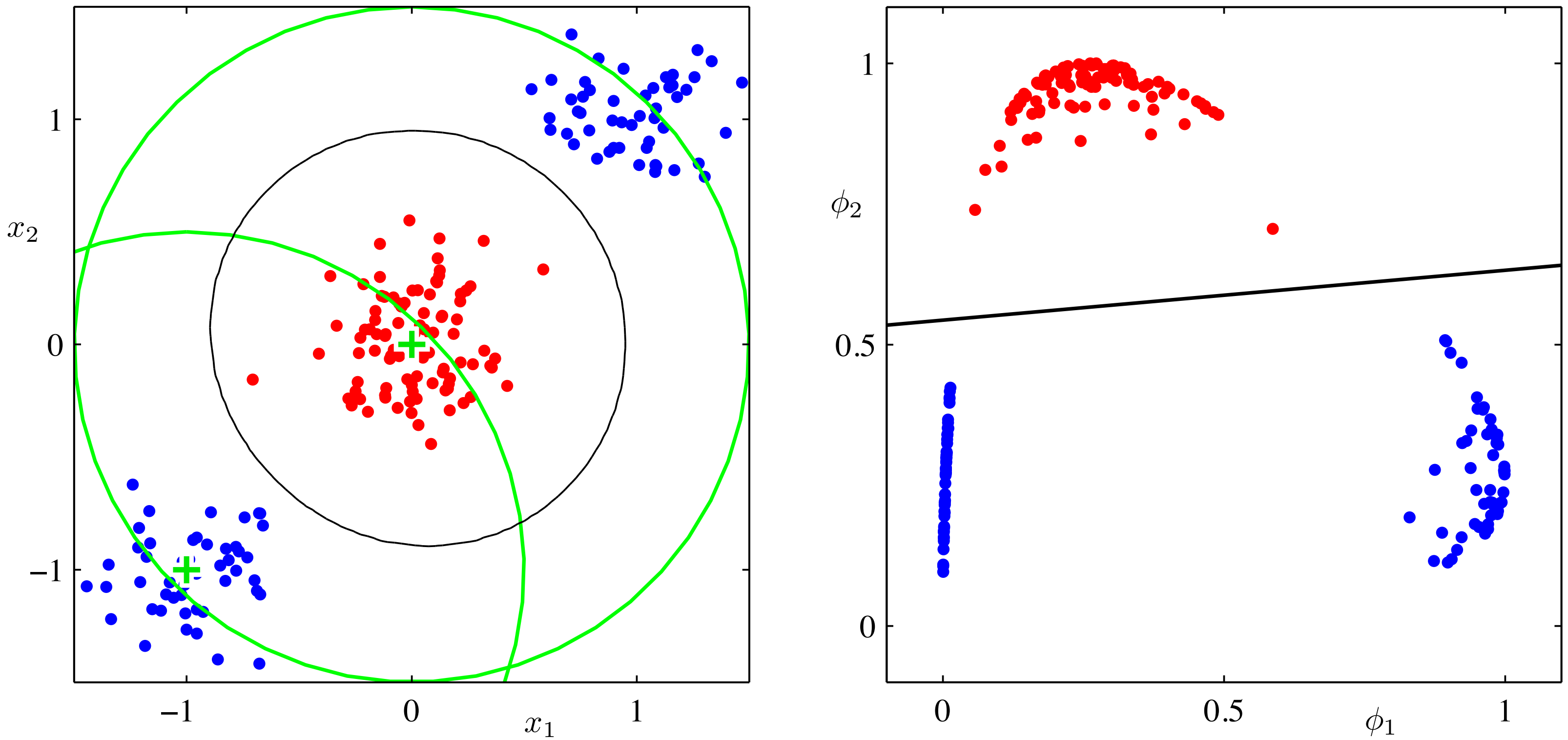
Linear Algebra Notation

- Suppose we build 10 linear models $y_1(\mathbf{x}), y_2(\mathbf{x}), .. y_{10}(\mathbf{x})$, for 10 classes.
- For a data matrix $\mathbf{X}$, the linear model predictions for each data point can be written like this (including the bias terms)
  $\mathbf{Y} = \mathbf{XW} + \mathbf{B}$
- What are the dimensions of $\mathbf{X}, \mathbf{W}, \mathbf{Y}, \mathbf{B}$ and what do they represent?

Feature Transformations

Basis Functions

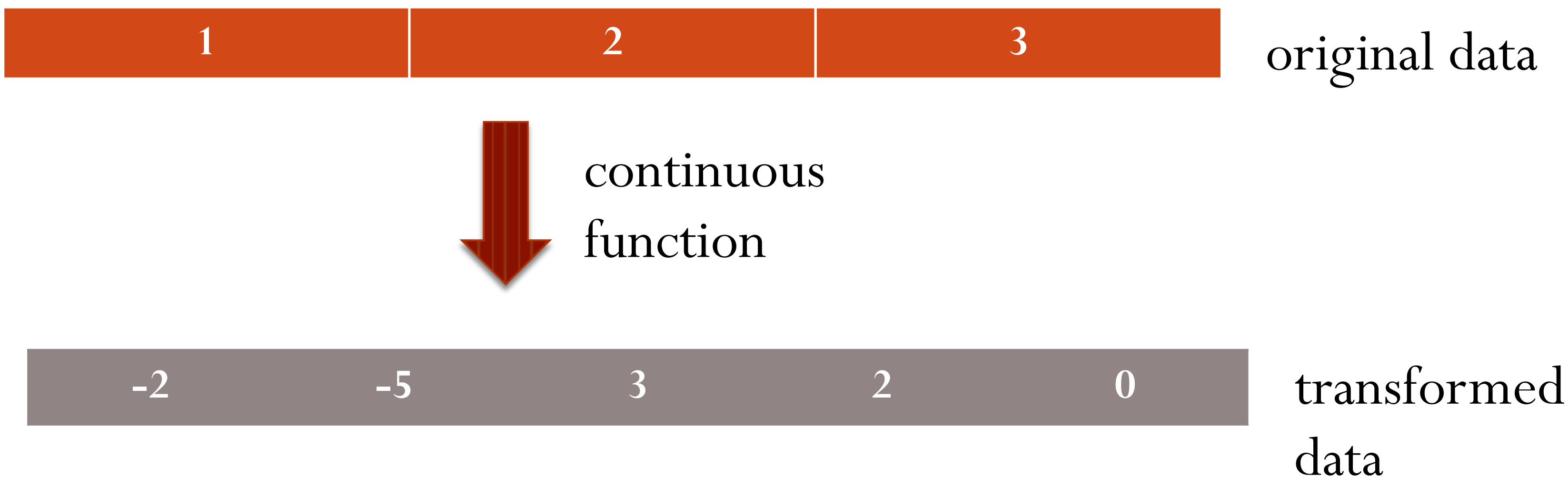
Example



- $\varphi_1(x_1,x_2)$ measures distance from left green cross
- $\varphi_2(x_1,x_2)$ measures closeness to centre green cross
- [3D demo]

Figure Bishop 4.12 see also

Visualize Transformation



Transformations can keep/increase/decrease original dimensionality

Summary I

- Linear classification: learn a linear function of features that separates positive and negative classes.
- Find feature weights by minimizing an error function.
- Different error functions used:
  - perceptron
  - cross-entropy (logistic regression)
  - max-margin (support vector machines, not discussed)
  - Least squares (for regression not classification)
- If classes are not linearly separable, no linear classifier is 100% accurate.
- Options:
  - use the best line you can $\longrightarrow$ logistic regression
  - use non-linear prediction function $\longrightarrow$ neural nets

Looking Ahead to Deep Learning

- Neural nets:
  - Hidden layers transform the input features
  - Output nodes perform linear classification/regression on the transformed features
- Deep neural nets: transform input features, transform the transformed features, …., again and again
- The transformations are *learned* not fixed