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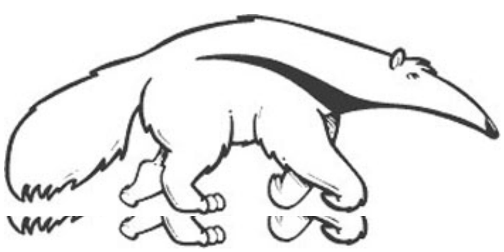
Machine Learning and Data Mining

Linear classification

Prof. Alexander Ihler



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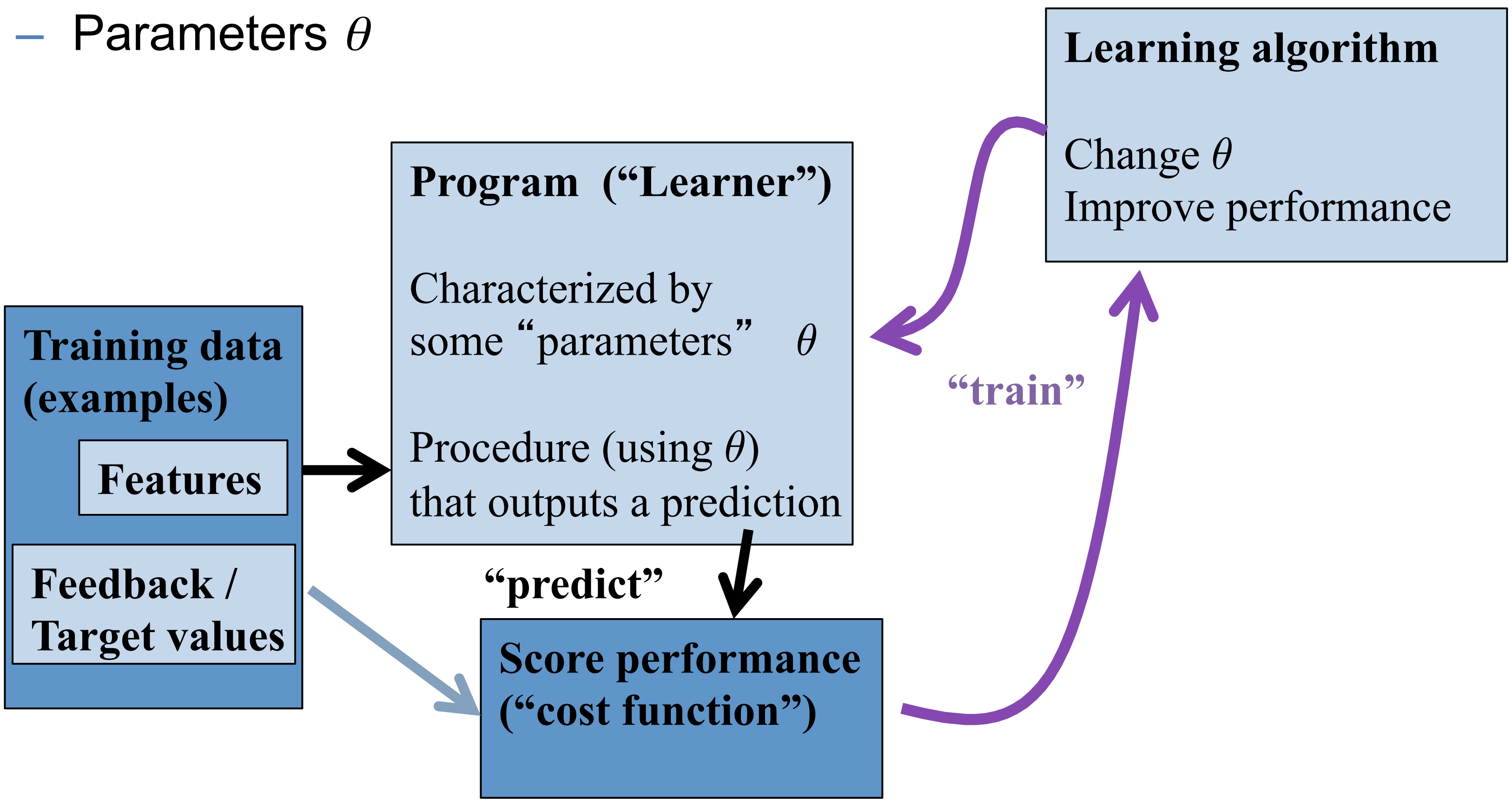
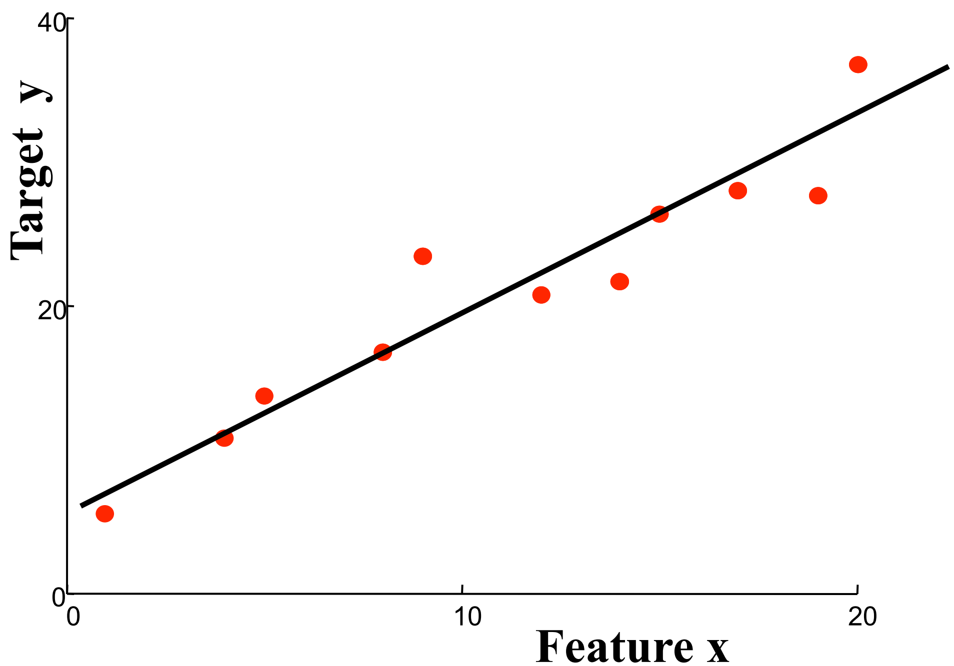
Supervised learning

- Notation
  - Features x
  - Targets y
  - Predictions $\hat{y} = f(x\,;\,\theta)$
  - Parameters θ



Linear regression



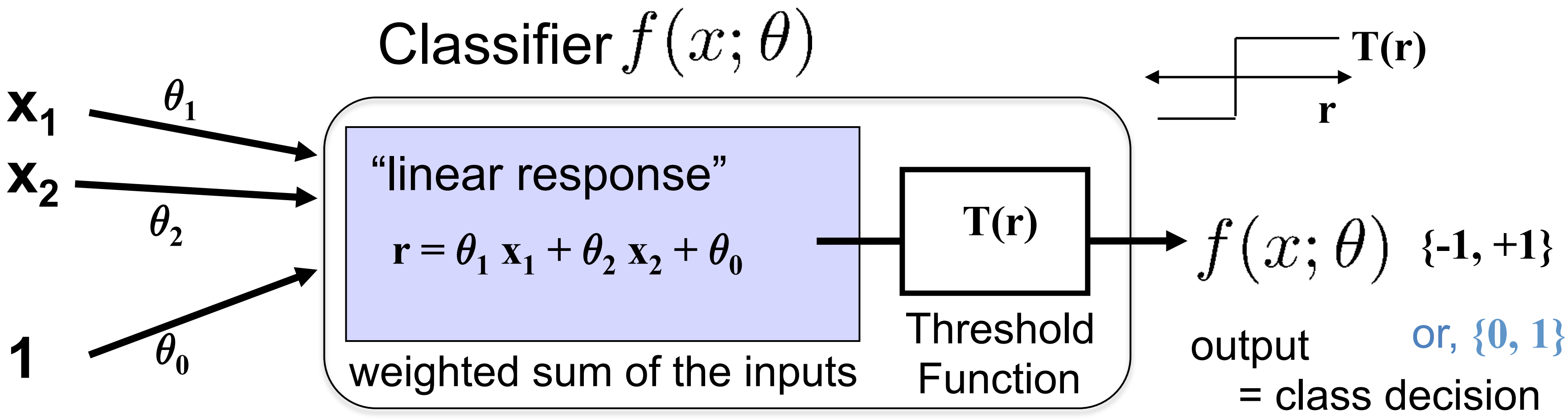
"Predictor":
Evaluate line:

$$r = \theta_0 + \theta_1 x_1$$

return r

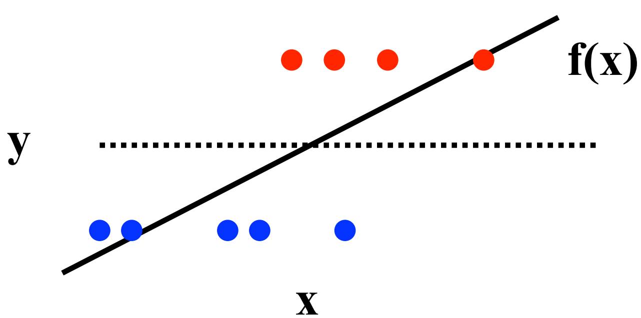
- Contrast with classification
  - Classify: predict discrete-valued target y
  - Initially: "classic" binary { -1, +1} classes; generalize later

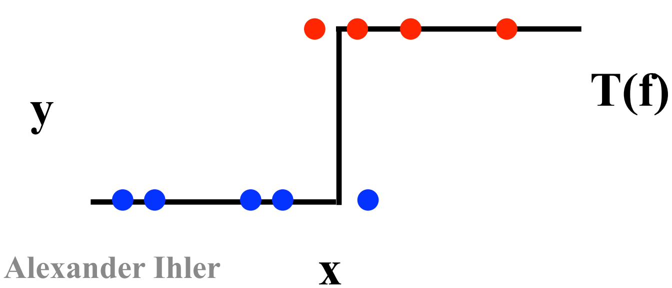
Perceptron Classifier (2 features)




```
r = X.dot( theta.T );          # compute linear response
Yhat = (r > 0)                 # predict class 1 vs 0
Yhat = 2*(r > 0)-1             # or "sign": predict +1 / -1
# Note: typically convert classes to "canonical" values 0,1,…
# then convert back ("learner.classes[c]") after prediction
```

Visualizing for one feature "x":





Perceptrons

- Perceptron = a linear classifier
  - The parameters θ are sometimes called weights ("w")
    - real-valued constants (can be positive or negative)
  - Input features $x_1 \ldots x_n$; define an additional constant input "1"

- A perceptron calculates 2 quantities:
  - 1. A weighted sum of the input features
  - 2. This sum is then thresholded by the T(.) function

- Perceptron: a simple artificial model of human neurons
  - weights = "synapses"
  - threshold = "neuron firing"

Perceptron Decision Boundary

- The perceptron is defined by the decision algorithm:

$$f(x;\theta) = \begin{cases} +1 & \text{if } \theta \cdot x^T > 0 \\ -1 & \text{otherwise} \end{cases}$$

- The perceptron represents a hyperplane decision surface in d-dimensional space
  - A line in 2D, a plane in 3D, etc.

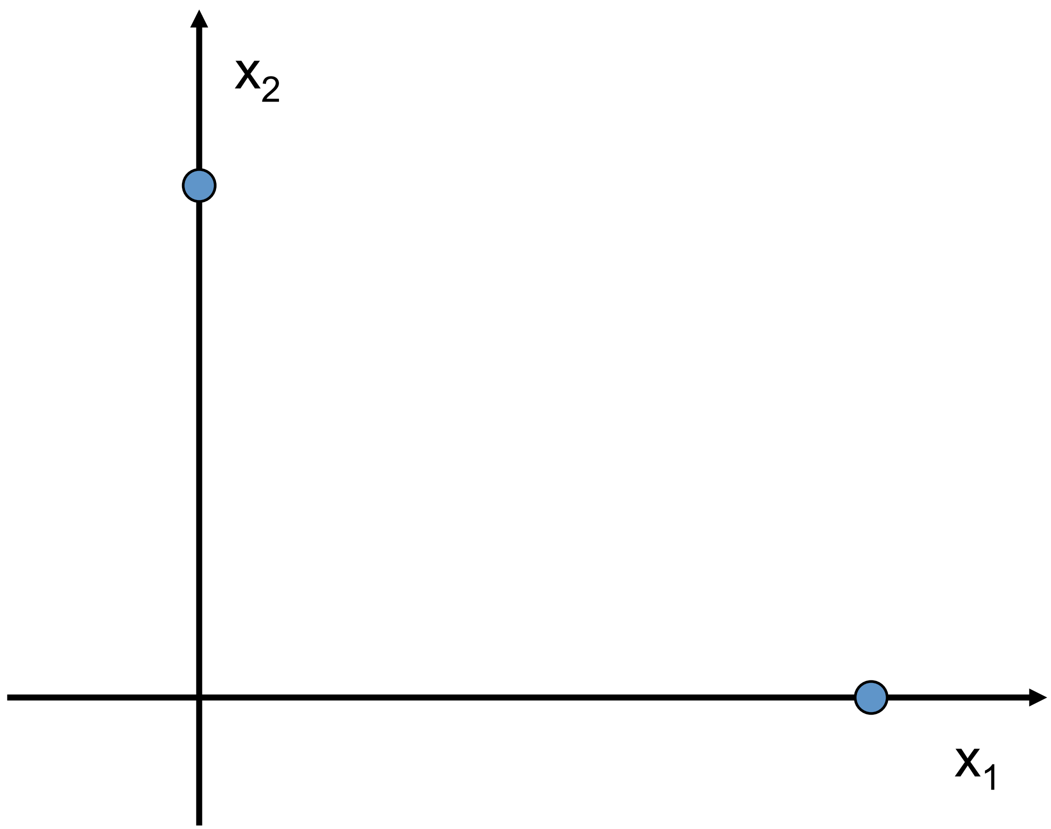
- The equation of the hyperplane is given by

$$\underline{\theta} \cdot \underline{\mathbf{x}}^{\mathbf{T}} = 0$$

This defines the set of points that are on the boundary.

Example, Linear Decision Boundary

$$\underline{\theta} = (\theta_0, \quad \theta_1, \quad \theta_2) \\ = (1, \quad .5, \quad -.5\ )$$



From P. Smyth

Example, Linear Decision Boundary

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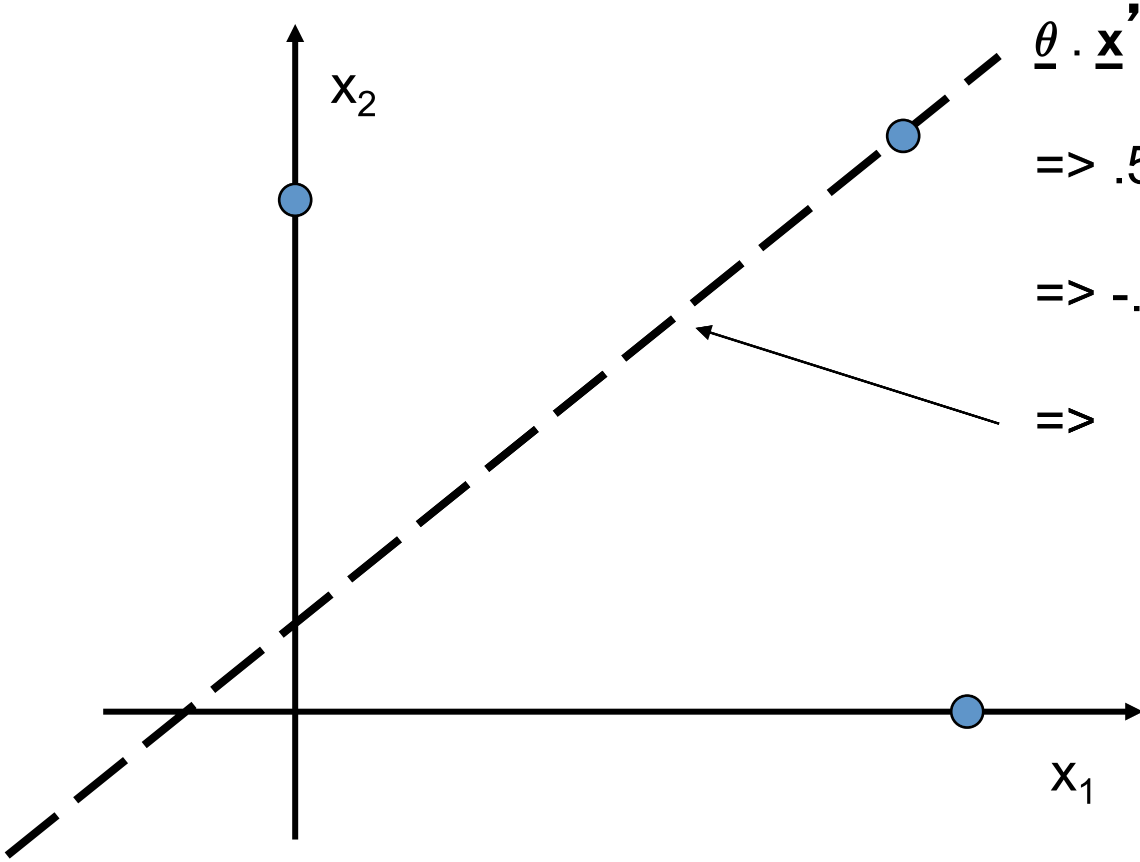

$\underline{\theta} \cdot \underline{\mathbf{x}}' = 0$

$\Rightarrow .5 \cdot x_1 - .5 \cdot x_2 + 1 \cdot 1 = 0$

$\Rightarrow -.5\, x_2 = -.5\, x_1 - 1$

$\Rightarrow \quad x_2 = x_1 + 2$

From P. Smyth

Example, Linear Decision Boundary

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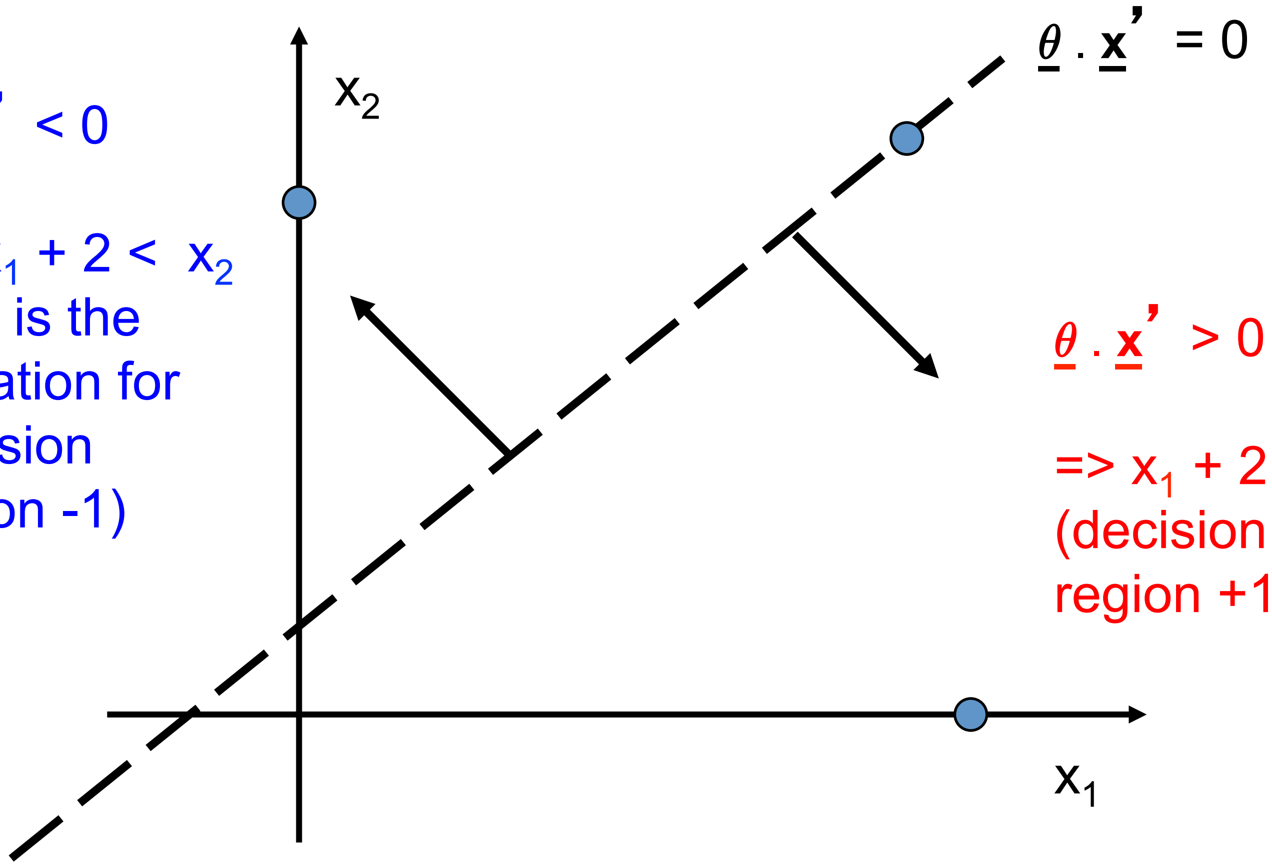


$\underline{\theta} \cdot \underline{\mathbf{x}}' < 0$

$\Rightarrow x_1 + 2 < x_2$
(this is the equation for decision region -1)

$\underline{\theta} \cdot \underline{\mathbf{x}}' > 0$

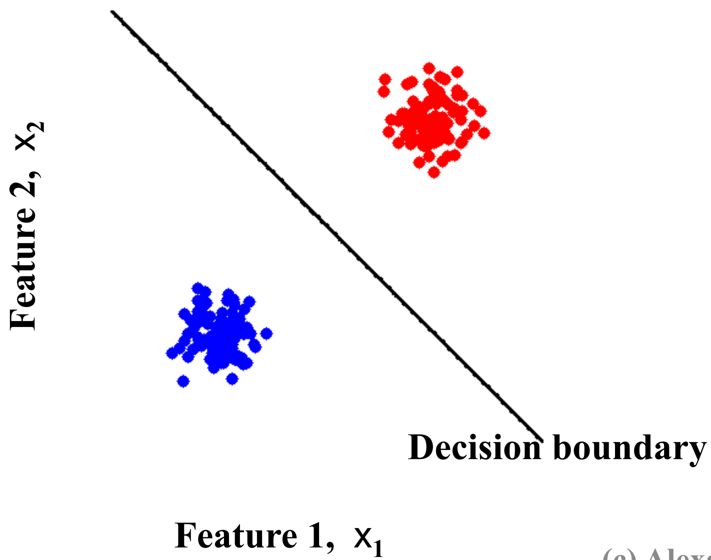
$\Rightarrow x_1 + 2 > x_2$
(decision region +1)

From P. Smyth

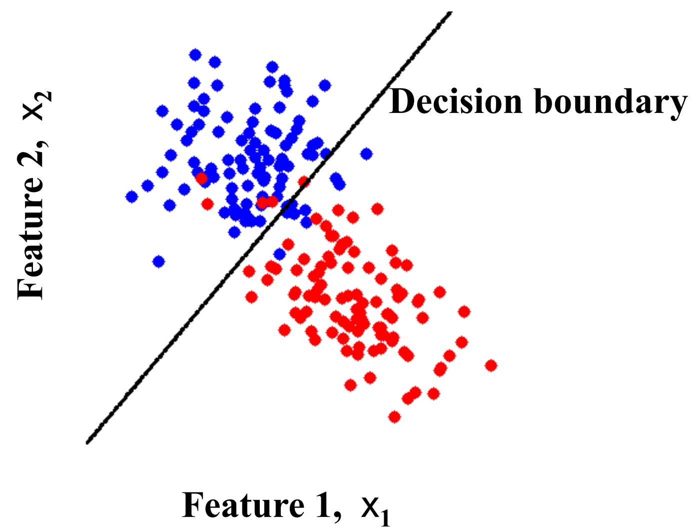
Separability

- A data set is separable by a learner if
  - There is some instance of that learner that correctly predicts all the data points
- Linearly separable data
  - Can separate the two classes using a straight line in feature space
  - in 2 dimensions the decision boundary is a straight line

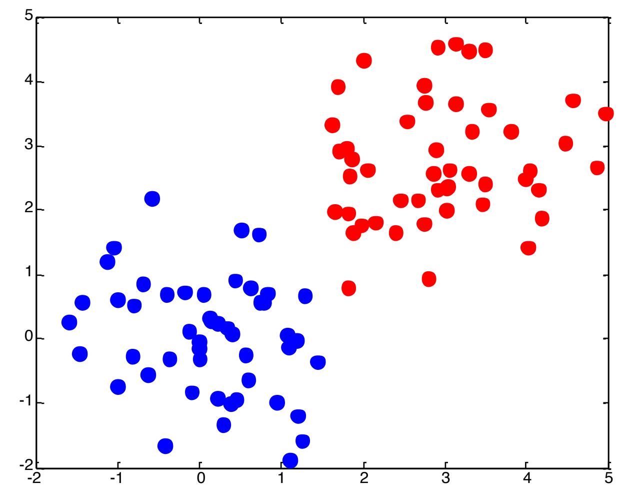
Linearly separable data



Linearly non-separable data

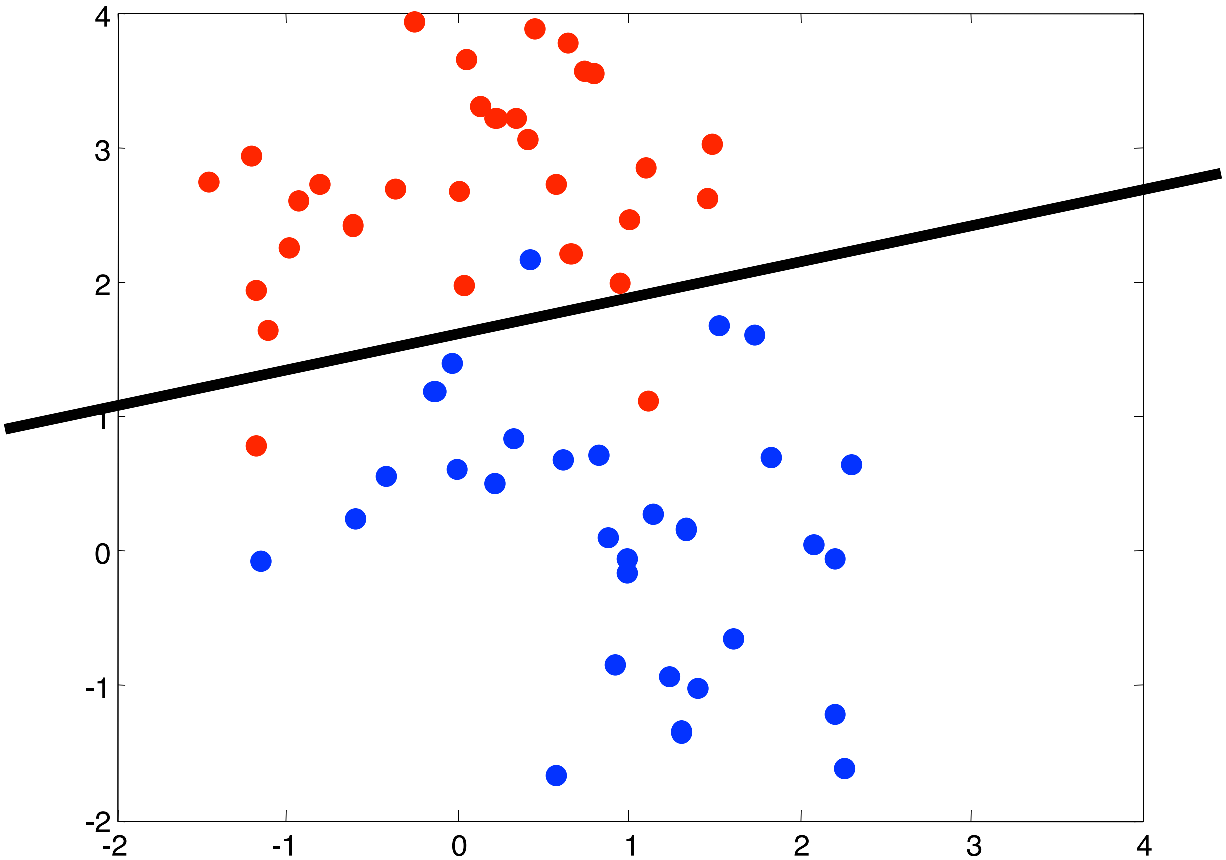


Class overlap

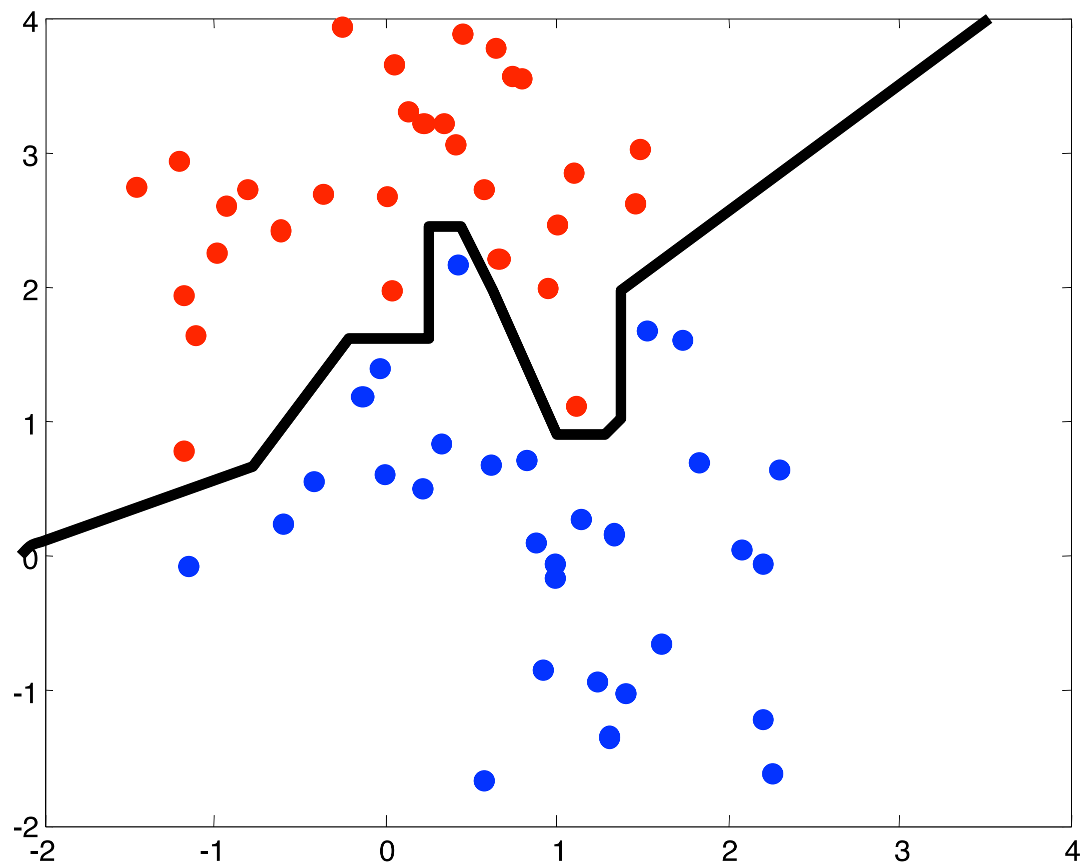


- Classes may not be well-separated
- Same observation values possible under both classes
  - High vs low risk; features {age, income}
  - Benign/malignant cells look similar
  - …
- Common in practice
- May not be able to perfectly distinguish between classes
  - Maybe with more features?
  - Maybe with more complex classifier?
- Otherwise, may have to accept some errors

Another example



Non-linear decision boundary

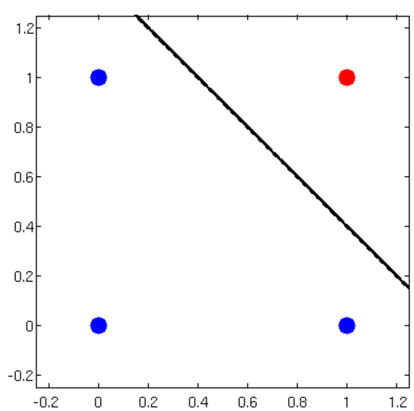


Representational Power of Perceptrons

- What mappings can a perceptron represent perfectly?
  - A perceptron is a linear classifier
  - thus it can represent any mapping that is linearly separable
  - some Boolean functions like AND (on left)
  - but not Boolean functions like XOR (on right)

"AND"

x_1	x_2	y
0	0	-1
0	1	-1
1	0	-1
1	1	1



"XOR"

x_1	x_2	y
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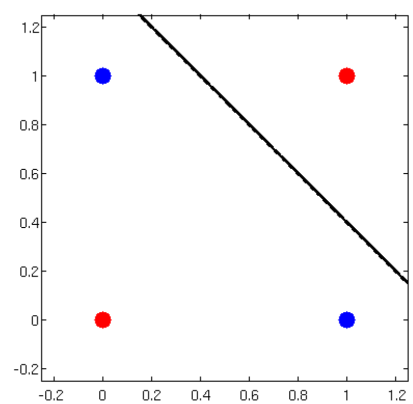
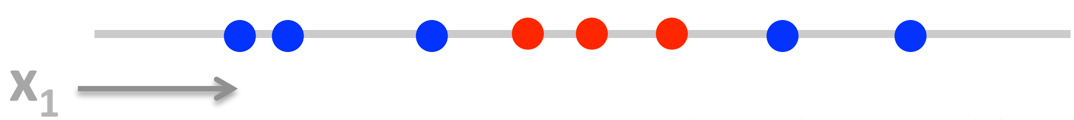


Adding features

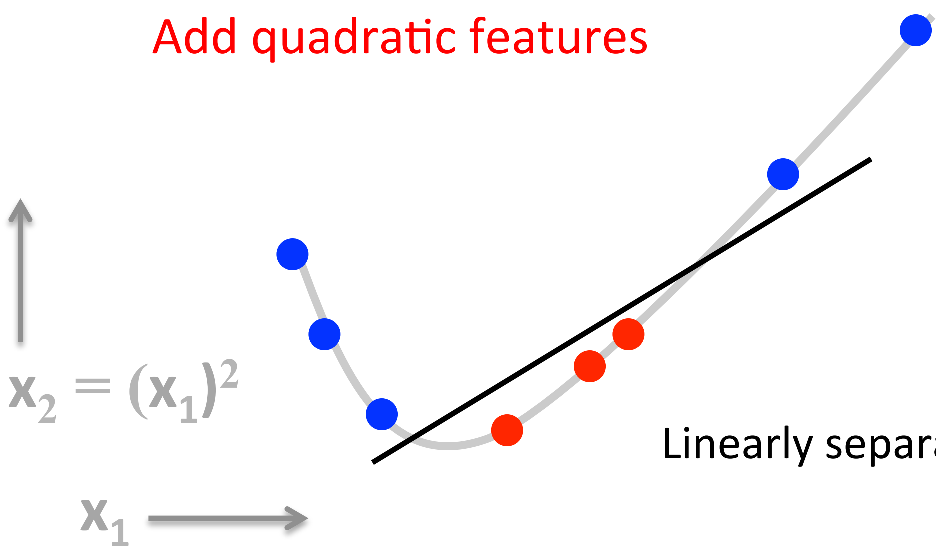
- Linear classifier can't learn some functions

1D example:



Not linearly separable

Add quadratic features



Linearly separable in new features…

Adding features

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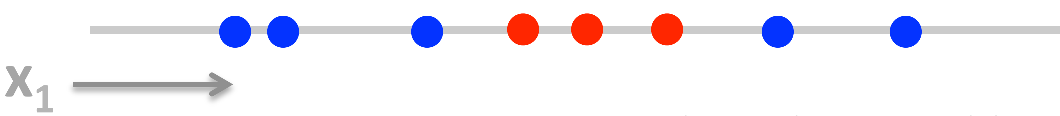
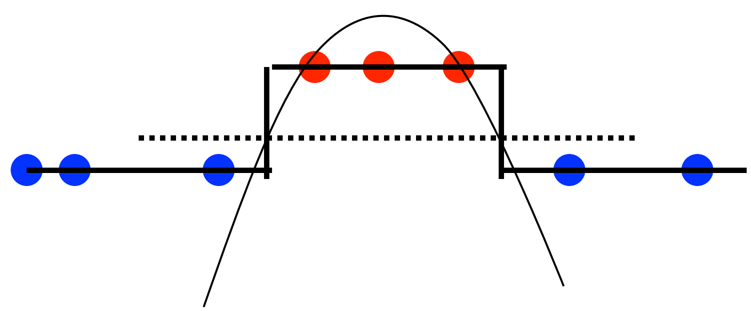


Not linearly separable

Quadratic features, visualized in original feature space:

$$y = T(\, a\, x^2 + b\, x + c\,)$$



More complex decision boundary: $ax^2+bx+c = 0$

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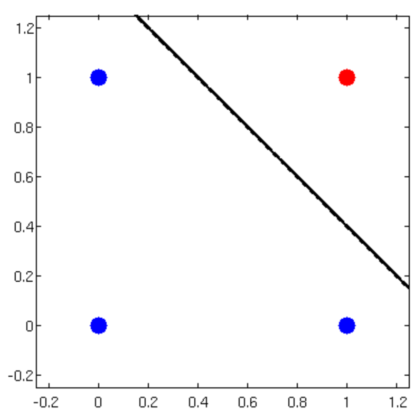

"XOR"

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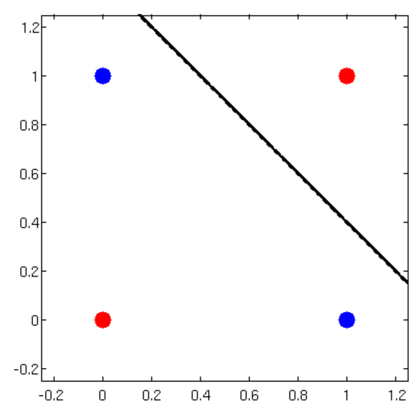

What kinds of functions would we need to learn the data on the right?

Representational Power of Perceptrons

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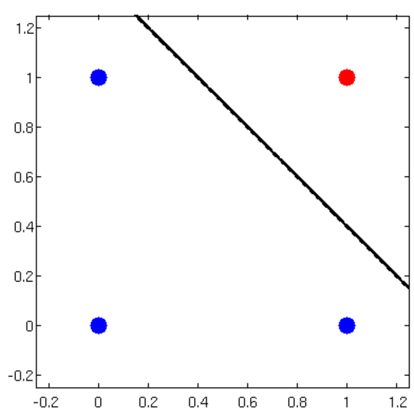

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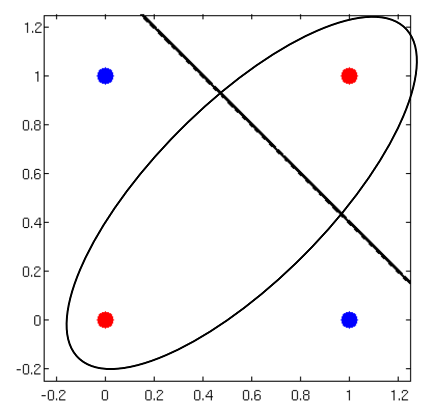


What kinds of functions would we need to learn the data on the right?

Ellipsiodal decision boundary: $a\,x_1^2 + b\,x_1 + c\,x_2^2 + d\,x_2 + e\,x_1x_2 + f = 0$

Feature representations

- Features are used in a linear way
- Learner is dependent on representation

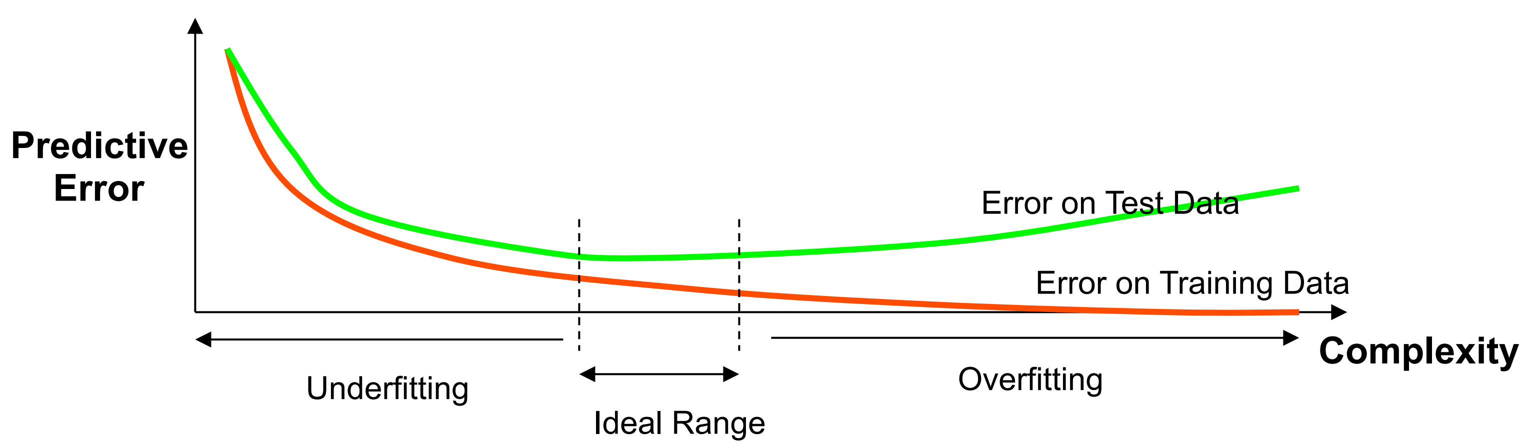
- Ex: discrete features
  - Mushroom surface: {fibrous, grooves, scaly, smooth}
  - Probably not useful to use x = {1, 2, 3, 4}
  - Better: 1-of-K,   x = { [1000], [0100], [0010], [0001] }
  - Introduces more parameters, but a more flexible relationship

Effect of dimensionality

- Data are increasingly separable in high dimension – is this a good thing?

- "Good"
  - Separation is easier in higher dimensions (for fixed # of data m)
  - Increase the number of features, and even a linear classifier will eventually be able to separate all the training examples!

- "Bad"
  - Remember training vs. test error? Remember overfitting?
  - Increasingly complex decision boundaries can eventually get all the training data right, but it doesn't necessarily bode well for test data…



Summary

- Linear classifier ⇔ perceptron
- Linear decision boundary
  - Computing and visualizing
- Separability
  - Limits of the representational power of a perceptron
- Adding features
  - Interpretations
  - Effect on separability
  - Potential for overfitting

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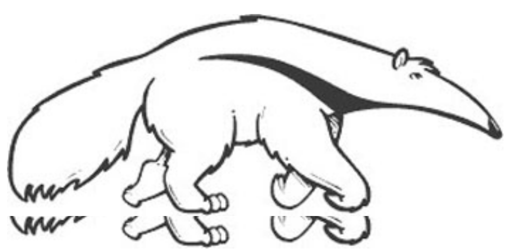
Machine Learning and Data Mining

Linear classification: Learning

Prof. Alexander Ihler



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Learning the Classifier Parameters

- Learning from Training Data:
  - training data = labeled feature vectors
  - Find parameter values that predict well (low error)
    - error is estimated on the training data
    - "true" error will be on future test data

- Define a loss function $J(\underline{\theta})$:
  - Classifier error rate (for a given set of weights $\underline{\theta}$ and labeled data)

- Minimize this loss function   (or, maximize accuracy)
  - An optimization or search problem over the vector $(\theta_1, \theta_2, \theta_0)$

Training a linear classifier

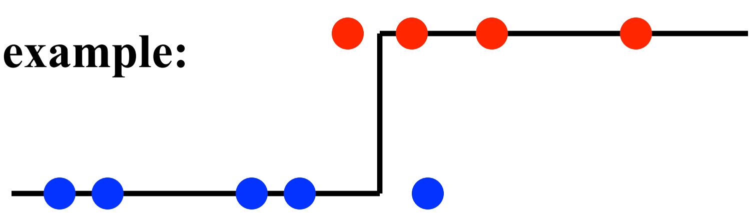
- How should we measure error?
  - Natural measure = "fraction we get wrong" (error rate)

$$\mathrm{err}(\theta) = \frac{1}{m}\sum_i \mathbb{1}\left[y^{(i)} \neq f(x^{(i)};\theta)\right] \quad \text{where} \quad \mathbb{1}\left[y \neq \hat{y}\right] = \begin{cases} 1 & y \neq \hat{y} \\ 0 & \text{o.w.} \end{cases}$$

```
Yhat = np.sign( X.dot( theta.T ) );          # predict class (+1/-1)
err = np.mean( Y != Yhat )                   # count errors: empirical error rate
```

- But, hard to train via gradient descent
  - Not continuous
  - As decision boundary moves, errors change abruptly

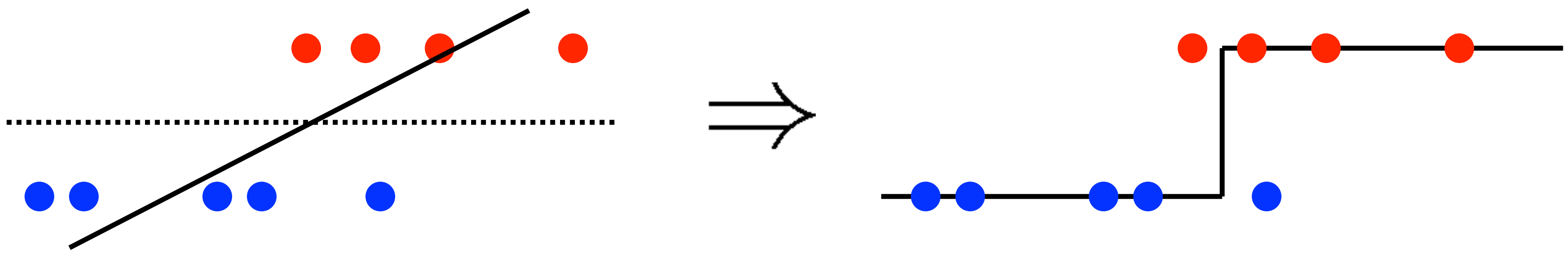
1D example:



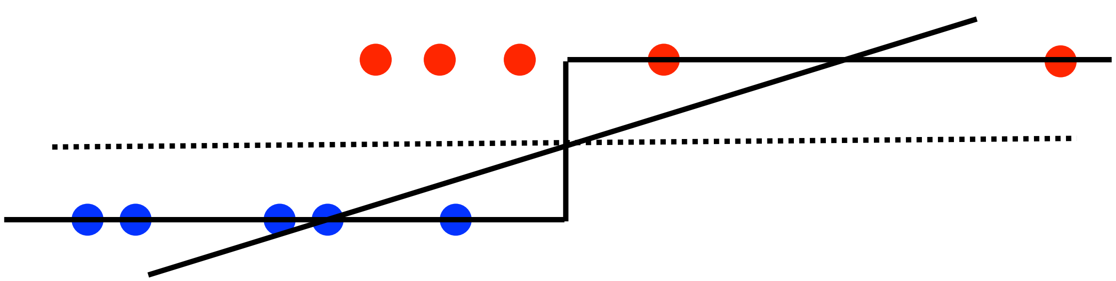
T(f) = -1 if f < 0
T(f) = +1 if f > 0

Linear regression?

- Simple option: set θ using linear regression



- In practice, this often doesn't work so well…
  - Consider adding a distant but "easy" point
  - MSE distorts the solution



Perceptron algorithm

- Perceptron algorithm: an SGD-like algorithm

while $\neg$ done:

for each data point j:

$$\hat{y}^{(j)} = \text{sign}(\theta \cdot x^{(j)})$$ (predict output for point j)

$$\theta \leftarrow \theta + \alpha(y^{(j)} - \hat{y}^{(j)})x^{(j)}$$ ("gradient-like" step)

- Compare to linear regression + MSE cost
  - Identical update to SGD for MSE except error uses thresholded ŷ(j) instead of linear response $\underline{\theta}$ x' so:
  - (1) For correct predictions, y(j) - ŷ(j) = 0
  - (2) For incorrect predictions, y(j) - ŷ(j) = $\pm$ 2

"adaptive" linear regression: correct predictions stop contributing

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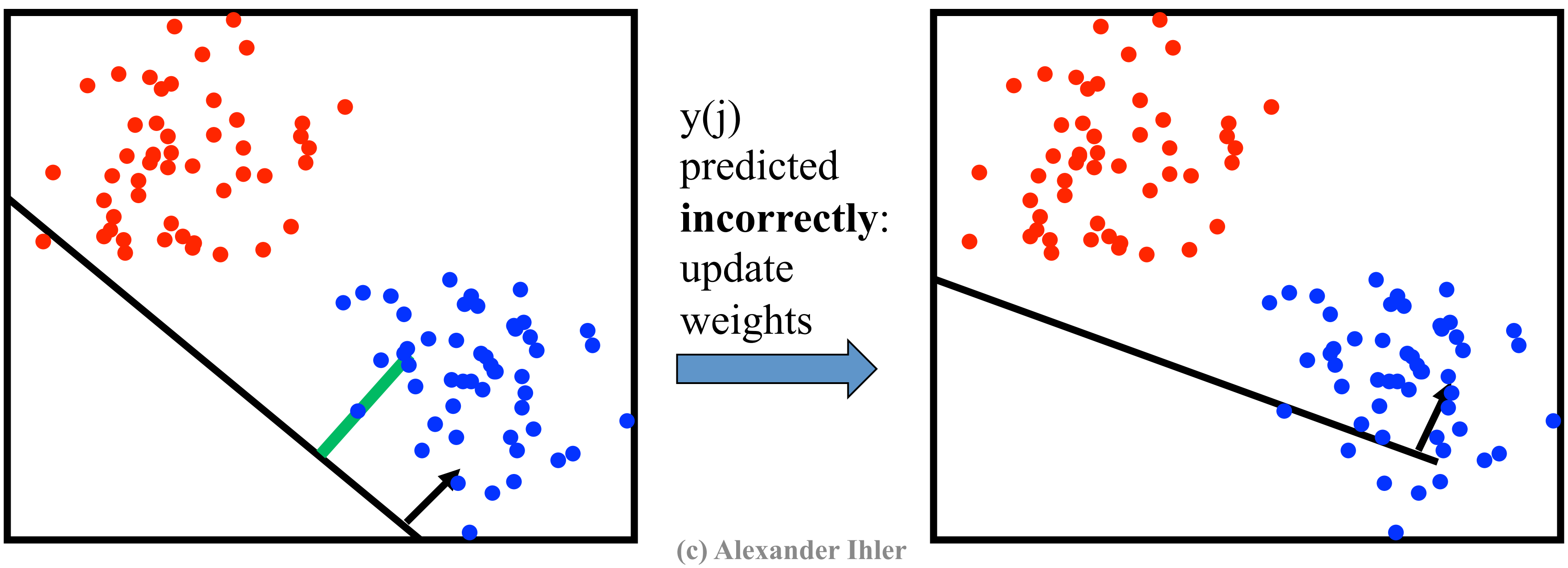

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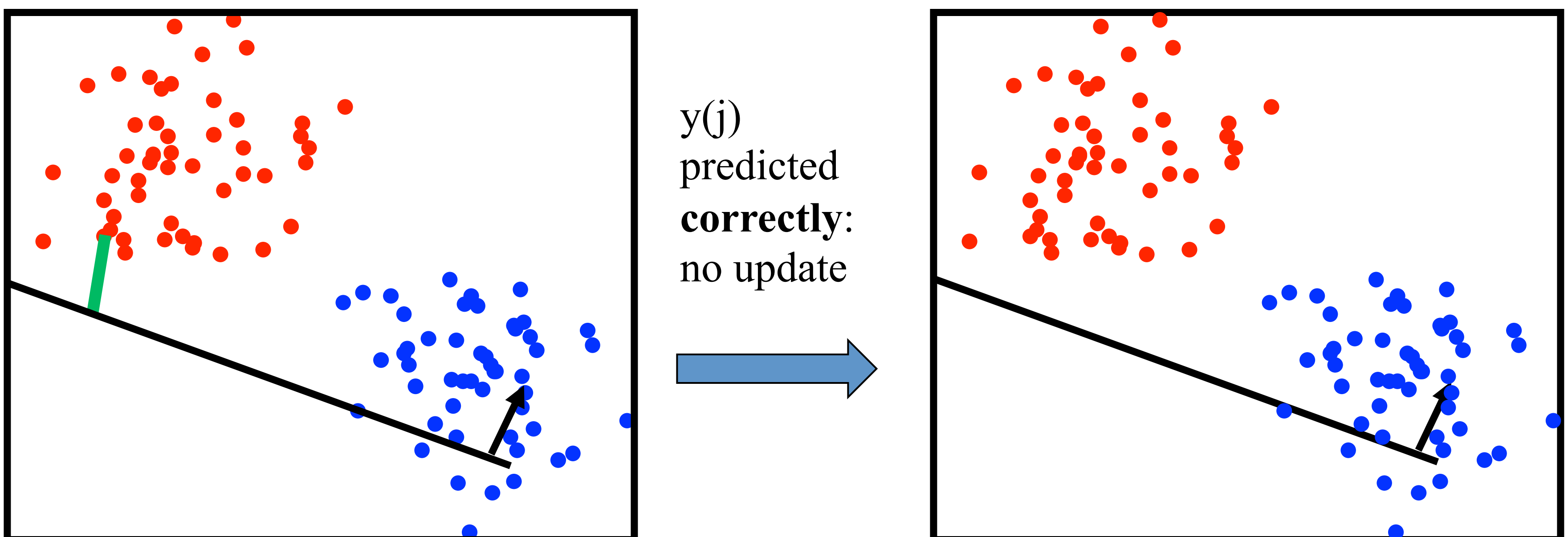

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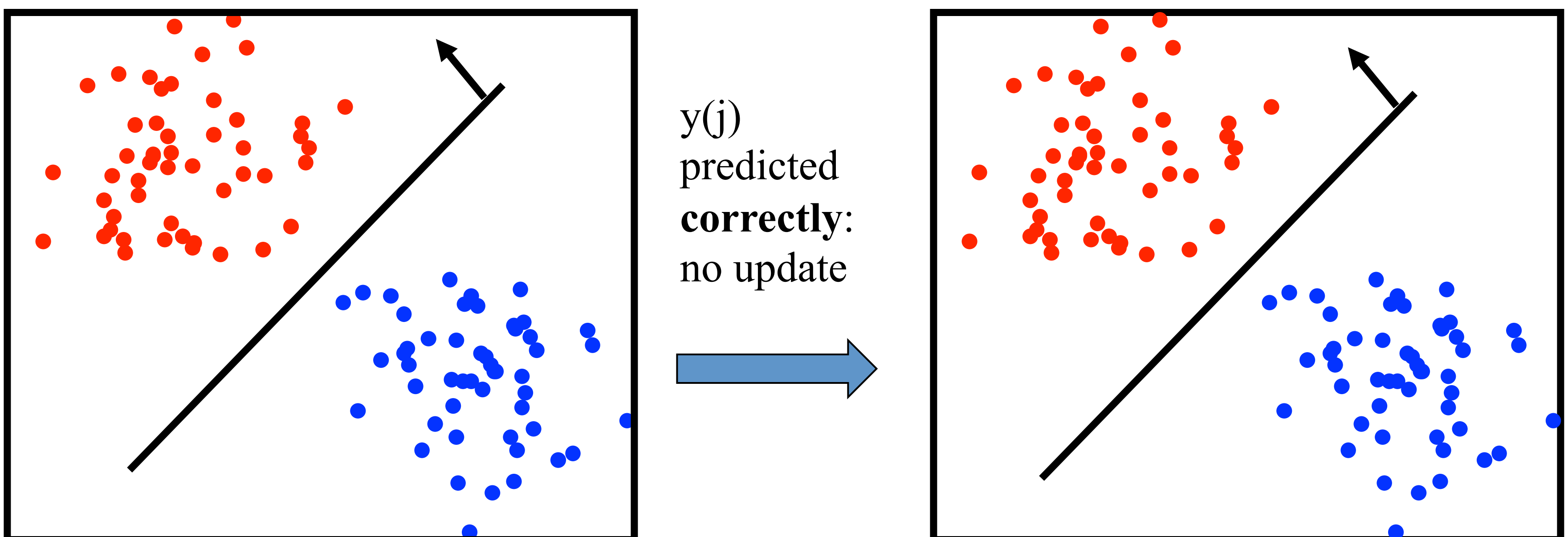
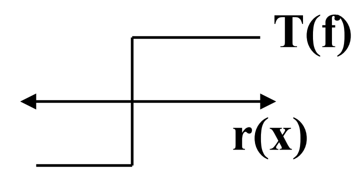
(Converges if data are linearly separable)

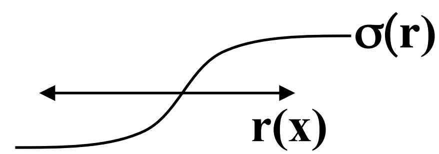


Surrogate loss functions

- Another solution: use a "smooth" loss
  - e.g., approximate the threshold function



  - Usually some smooth function of distance
    - Example: logistic "sigmoid", looks like an "S"



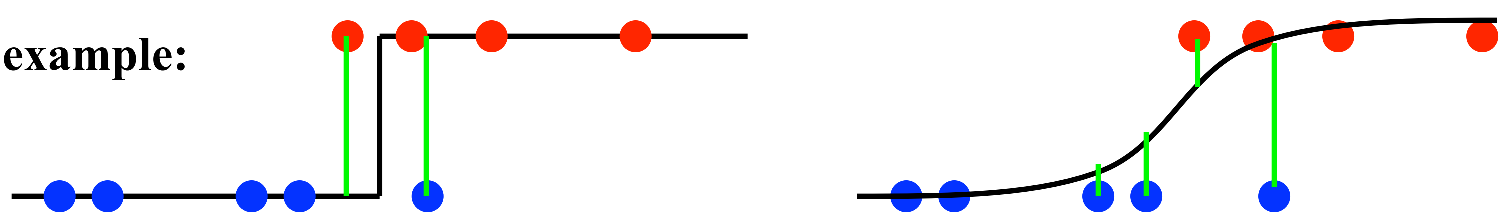
  - Now, measure e.g. MSE

$$J(\underline{\theta}) = \frac{1}{m} \sum_j \Big(\, \sigma(\, r(x^{(j)})\,) - y^{(j)} \, \Big)^2$$

Class y = {0, 1} …

  - Far from the decision boundary: |f(.)| large, small error
  - Nearby the boundary: |f(.)| near 1/2, larger error

1D example:

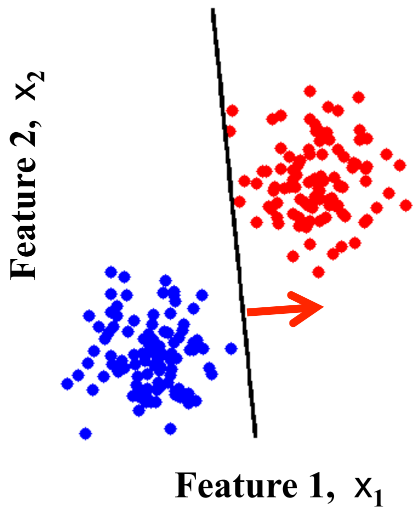


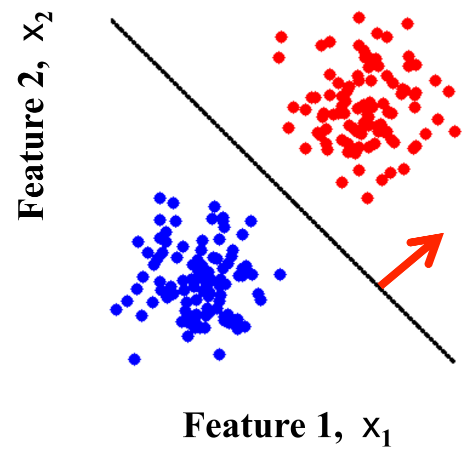
Classification error = 2/9

MSE = $(0^2 + 1^2 + .2^2 + .25^2 + .05^2 + \ldots)/9$

Beyond misclassification rate

- Which decision boundary is “better”?
  - Both have zero training error (perfect training accuracy)
  - But, one of them seems intuitively better…





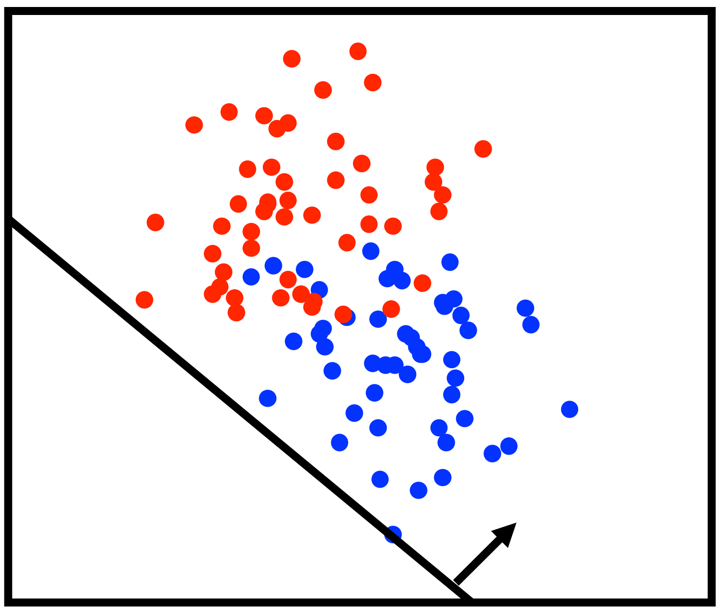
- Side benefit of many “smoothed” error functions
  - Encourages data to be far from the decision boundary
  - See more examples of this principle later...

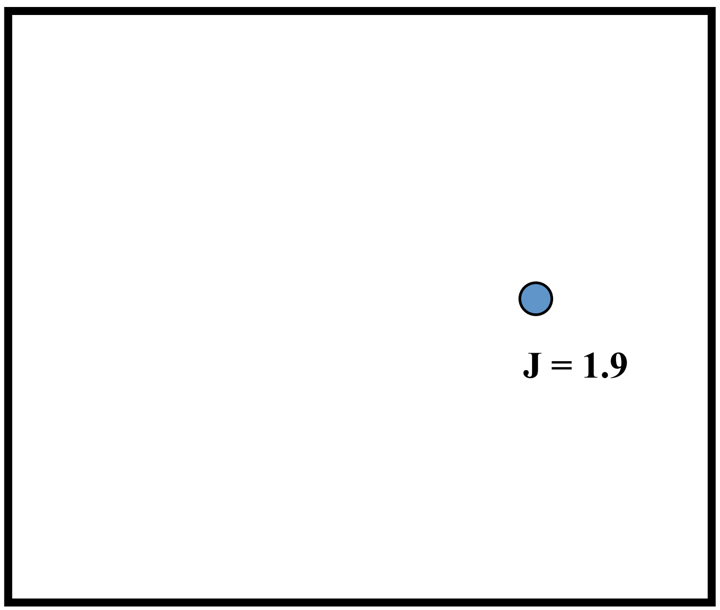
Training the Classifier

- Once we have a smooth measure of quality, we can find the "best" settings for the parameters of

  $r(x_1,x_2) = a^*x_1 + b^*x_2 + c$

- Example: 2D feature space ⇔ parameter space





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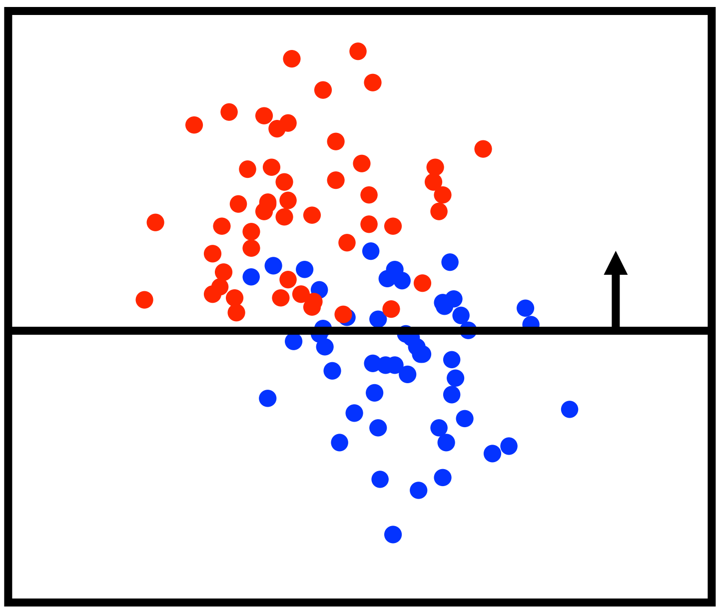

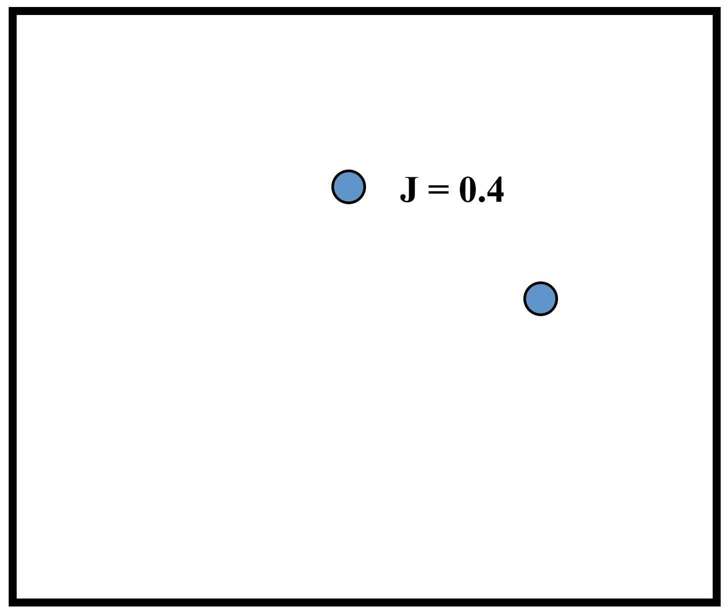

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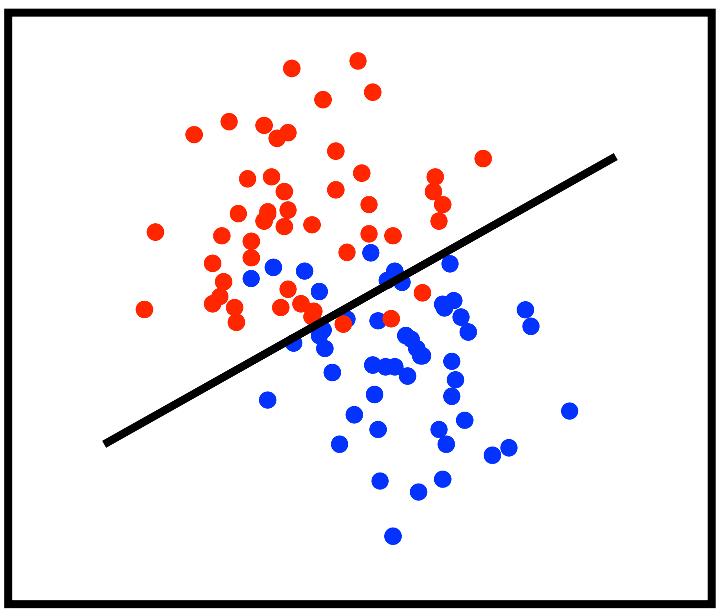
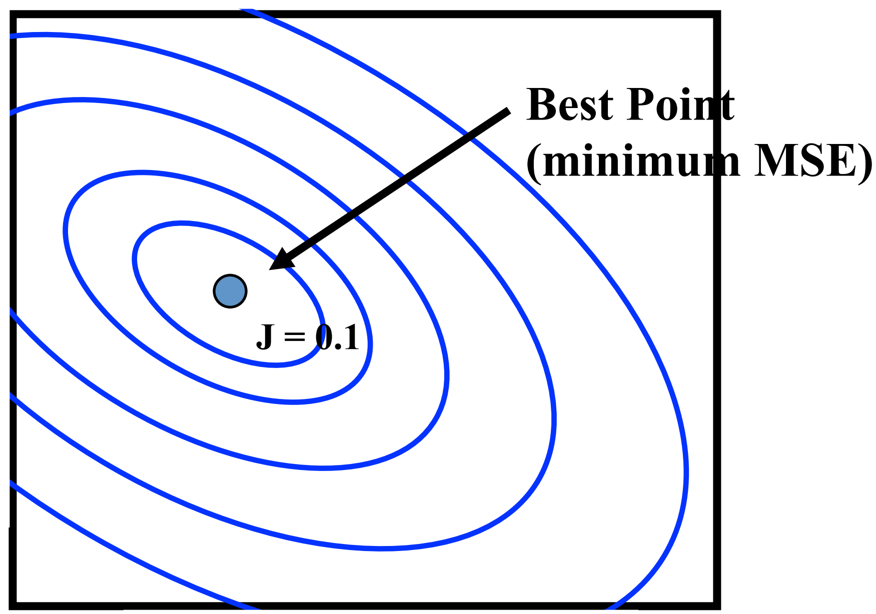
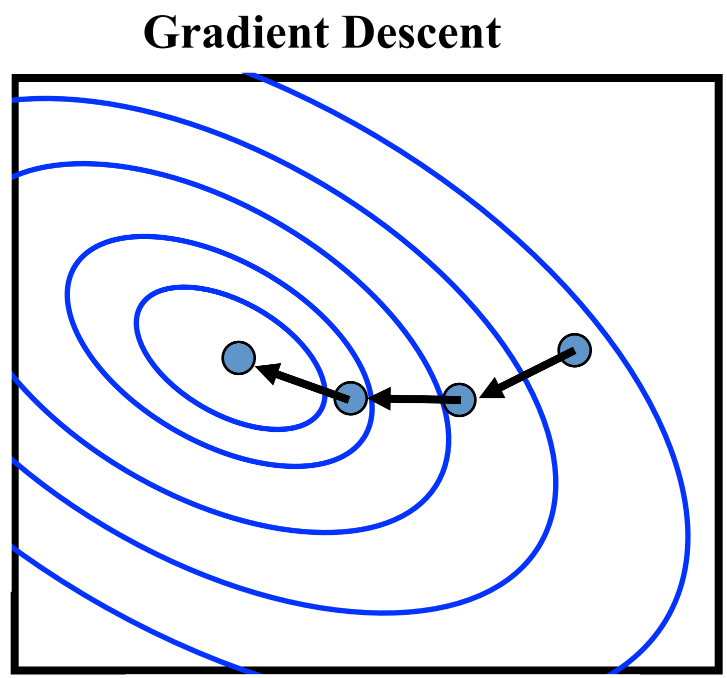




Finding the Best MSE

- As in linear regression, this is now just optimization

- Methods:
  - Gradient descent
    - Improve loss by small changes in parameters ("small" = learning rate)
  - Or, substitute your favorite optimization algorithm…
    - Coordinate descent
    - Stochastic search
    - Genetic algorithms



Gradient Equations

- MSE (note, depends on function σ(.))

$$J(\underline{\theta} = [a,b,c]) = \frac{1}{m}\sum_i \left(\sigma(a x_1^{(i)} + b x_2^{(i)} + c) - y^{(i)} \right)^2$$

- What's the derivative with respect to one of the parameters?
  - Recall the chain rule of calculus:

$$\frac{\partial}{\partial a} f(\, g(\, h(a)\,)\,) = f'(\, g(h(a))\,)\; g'(\, h(a)\,)\; h'(a)$$

$$f(g) = (\, g\,)^2 \quad \Rightarrow \quad f'(g) = 2(g)$$

$$g(h) = \sigma(h) - y \quad \Rightarrow \quad g'(h) = \sigma'(h)$$

$$h(a) = a x_1^{(i)} + b x_2^{(i)} + c \quad \Rightarrow \quad h'(a) = x_1^{(i)}$$

w.r.t. b,c : similar; replace x_1 with x_2 or 1

$$\frac{\partial J}{\partial a} = \frac{1}{m}\sum_i 2\boxed{(\sigma(\theta \cdot x^{(i)}) - y^{(i)})}\;\boxed{\partial\sigma(\theta \cdot x^{(i)})\;\; x_1^{(i)}}$$

Error between class and prediction

Sensitivity of prediction to changes in parameter "a"

Saturating Functions

- Many possible "saturating" functions

- "Logistic" sigmoid (scaled for range [0,1]) is
  $\sigma(z) = 1 / (1 + \exp(-z))$

(z = linear response, $x^T\theta$)

- Derivative (slope of the function at a point z) is
  $\partial\sigma(z) = \sigma(z)\,(1-\sigma(z))$

(to predict:
threshold z at 0 or
threshold $\sigma(z)$ at ½)

- Python Implementation:

```
def sig(z):                               # logistic sigmoid
   return  1.0 / (1.0 + np.exp(-z) ) #   in [0,1]

def dsig(z):                              # its derivative at z
   return  sig(z) * (1-sig(z))
```

For range [-1 , +1]:

$\rho(z) \;\; = 2\,\sigma(z) - 1$

$\partial\rho(z) = 2\,\sigma(z)\,(1-\sigma(z))$

Predict: threshold z or ρ at zero

Logistic regression

- Intepret $\sigma(\underline{\theta}\, x^T)$ as a probability that y = 1
- Use a negative log-likelihood loss function
  - If y = 1, cost is - log Pr[y=1] = - log $\sigma(\underline{\theta}\, x^T)$
  - If y = 0, cost is - log Pr[y=0] = - log (1 - $\sigma(\underline{\theta}\, x^T)$)

- Can write this succinctly:

$$J(\underline{\theta}) = -\frac{1}{m} \sum_i \underbrace{y^{(i)} \log \sigma(\theta \cdot x^{(i)})}_{\textbf{Nonzero only if y=1}} + \underbrace{(1 - y^{(i)}) \log (1 - \sigma(\theta \cdot x^{(i)}))}_{\textbf{Nonzero only if y=0}}$$

Logistic regression

- Intepret $\sigma(\underline{\theta}\, x^T)$ as a probability that y = 1
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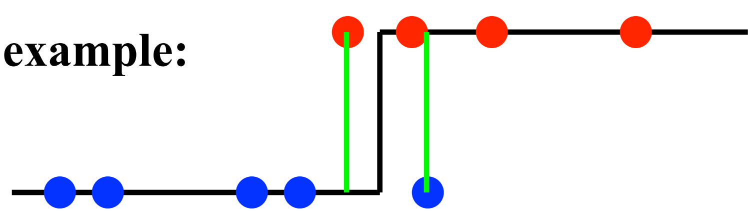
- Can write this succinctly:

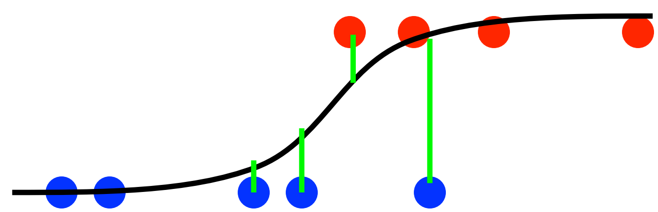
$$J(\underline{\theta}) = -\frac{1}{m}\sum_i y^{(i)} \log \sigma(\theta \cdot x^{(i)}) + (1 - y^{(i)}) \log(1 - \sigma(\theta \cdot x^{(i)}))$$

- Convex! Otherwise similar: optimize J(θ) via …

1D example:



Classification error = MSE = 2/9



NLL = - (log(.99) + log(.97) + …)/9

Gradient Equations

- Logistic neg-log likelihood loss:

$$J(\underline{\theta}) = -\frac{1}{m}\sum_i y^{(i)}\ \log\sigma(\theta\cdot x^{(i)}) + (1-y^{(i)})\log(1-\sigma(\theta\cdot x^{(i)}))$$

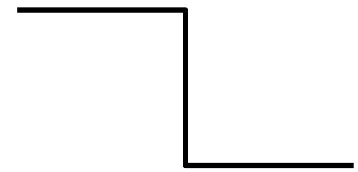
- What’s the derivative with respect to one of the parameters?

$$\frac{\partial J}{\partial a} = -\frac{1}{m}\sum_i y^{(i)}\frac{1}{\sigma(\theta\cdot x^{(i)})}\ \partial\sigma(\theta\cdot x^{(i)})\ x_1^{(i)} + (1-y(i))\ldots$$

$$= -\frac{1}{m}\sum_i y^{(i)}(1-\sigma(\theta\cdot x^{(i)}))\ x_1^{(i)} - (1-y^{(i)})\ldots$$

Surrogate loss functions

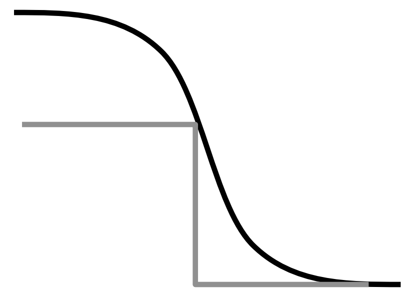
- Replace 0/1 loss $\Delta_i(\theta) = \mathbb{1}\left[T(\theta x^{(i)}) \neq y^{(i)}\right]$
  with something easier:



0 / 1 Loss

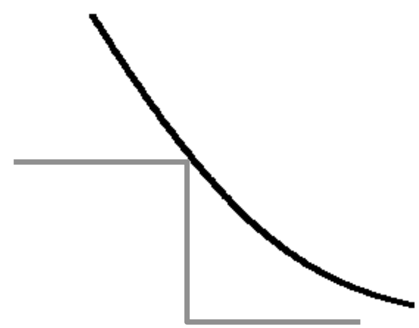
- Logistic MSE

$$J_i(\theta) = 4\left(\sigma(\theta x^{(i)}) - y^{(i)}\right)^2$$



- Logistic Neg Log Likelihood

$$J_i(\underline{\theta}) = -\frac{y^{(i)}}{\log 2} \log \sigma(\theta \cdot x^{(i)}) + \dots$$



Summary

- Linear classifier ⇔ perceptron
- Measuring quality of a decision boundary
  - Error rate (0/1 loss)
  - Logistic sigmoid + MSE criterion
  - Logistic Regression
- Learning the weights of a linear classifer from data
  - Reduces to an optimization problem
  - Perceptron algorithm
  - For MSE or Logistic NLL, we can do gradient descent
  - Gradient equations & update rules

Multi-class linear models

- What about multiple classes? One option:
  - Define one linear response per class
  - Choose class with the largest response

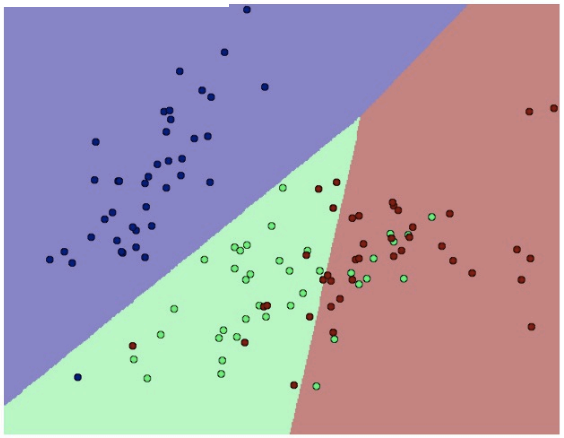
$$\theta = \begin{bmatrix} \theta_{00} & \dots & \theta_{0n} \\ \vdots & \ddots & \vdots \\ \theta_{C0} & \dots & \theta_{Cn} \end{bmatrix}$$

$$f(x;\theta) = \arg\max_c \; \theta_c \cdot x^T$$

  - Boundary between two classes, c vs. c'?

$$= \begin{cases} c & \text{if } \theta_c \cdot x^T > \theta_{c'} x^T \\ c' & \text{otherwise} \end{cases} \quad \Leftrightarrow (\theta_c - \theta_{c'}) x^T > 0$$

    - Linear boundary: $(\theta_c - \theta_{c'})\, x^T = 0$



Multiclass linear models

- More generally, can define a generic linear classifier by

$$f(x\,;\theta) = \arg\max_y \ \theta \cdot \Phi(x, y)$$

- Example: y ∈ {-1, +1}

$$\Phi(x, y) = y \ [1 \ x \ x^2 \ \ \ldots]$$

$$f(x\,;\theta) = \begin{cases} +1 & \theta \cdot [1 \ x \ x^2 \ldots] > -\theta \cdot [1 \ x \ x^2 \ldots] \\ -1 & \text{o.w.} \end{cases}$$

(Standard perceptron rule)

Multiclass linear models

- More generally, can define a generic linear classifier by

$$f(x\,;\theta) = \arg\max_y \; \theta \cdot \Phi(x, y)$$

- Example: y $\in$ {0,1,2,…}

$$\Phi(x,y) = [\;\mathbb{1}[y=0][1\;\;x\;\;x^2\;\;\ldots]\;\;\mathbb{1}[y=1][1\;\;x\;\;x^2\ldots]\ldots]$$

$$\theta = [\;\;[\theta_{00}\;\;\theta_{01}\;\;\theta_{02}\ldots]\quad[\theta_{10}\;\;\theta_{11}\;\;\theta_{12}\ldots]\quad\ldots]$$

(parameters for each class c)

$$f(x\,;\theta) = \arg\max_c \; \theta_{c\cdot} \cdot [1\;\;x\;\;x^2\;\;\ldots]$$

(predict class with largest linear response)

Multiclass perceptron algorithm

- Perceptron algorithm:
  - Make prediction f(x)
  - Increase linear response of true target y; decrease for prediction f

While (~done)

For each data point j:

$f^{(j)} = \arg\max (\underline{\theta}_c * \underline{x}^{(j)})$: predict output for data point j

$\underline{\theta}_f \leftarrow \underline{\theta}_f - \alpha\, \underline{x}^{(j)}$: decrease response of class $f^{(j)}$ to $x^{(j)}$

$\underline{\theta}_y \leftarrow \underline{\theta}_y + \alpha\, \underline{x}^{(j)}$: increase response of true class $y^{(j)}$

– More general form update:

$$f(x\,;\theta) = \arg\max_y \; \theta \cdot \Phi(x,y)$$

$$\theta \leftarrow \theta + \alpha\big(\Phi(x,y) - \Phi(x,f(x))\big)$$

Multilogit regression

- Define the probability of each class:

$$p(Y = y|X = x) = \frac{\exp(\theta_y \cdot x^T)}{\sum_c \exp(\theta_c \cdot x^T)}$$

(Y binary = logistic regression)

- Then, the NLL loss function is:

$$J(\theta) = -\frac{1}{m}\sum_i \log p(y^{(i)}|x^{(i)}) = -\frac{1}{m}\sum_i \left[\theta_{y^{(i)}} \cdot x^{(i)} - \log \sum_c \exp(\theta_c \cdot x^{(i)})\right]$$

  – P: “confidence” of each class
    - Soft decision value
  – Decision: predict most probable
    - Linear decision boundary
  – Convex loss function