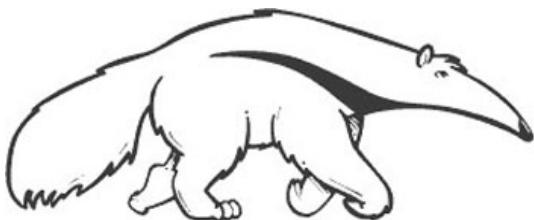


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CS178: Machine Learning and Data Mining

Linear Classification

Prof. Alexander Ihler



Machine Learning

Linear Classification with Perceptrons

Perceptron Learning

Gradient-Based Classifier Learning

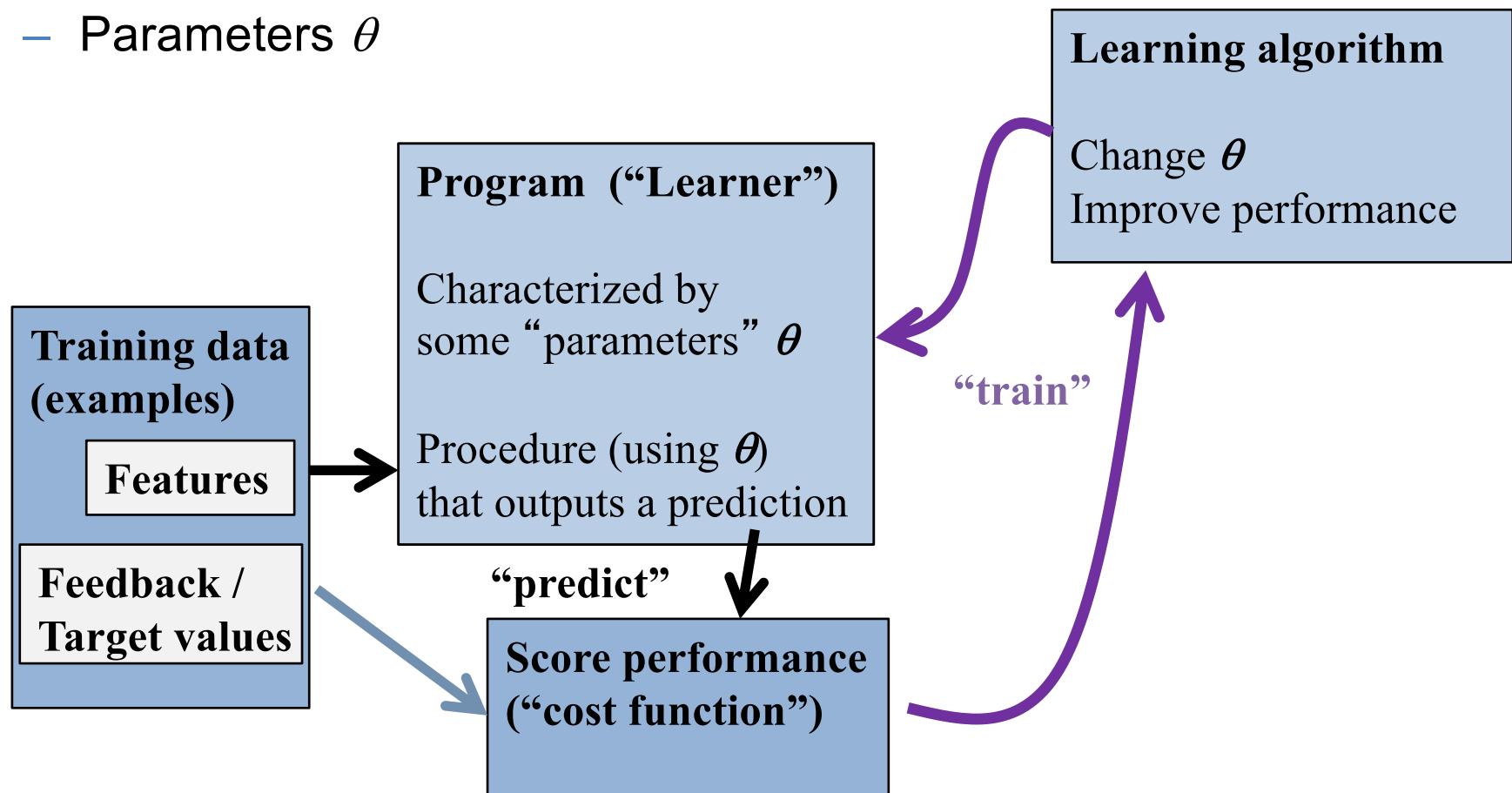
Multi-Class Classification

Regularization for Linear Classification

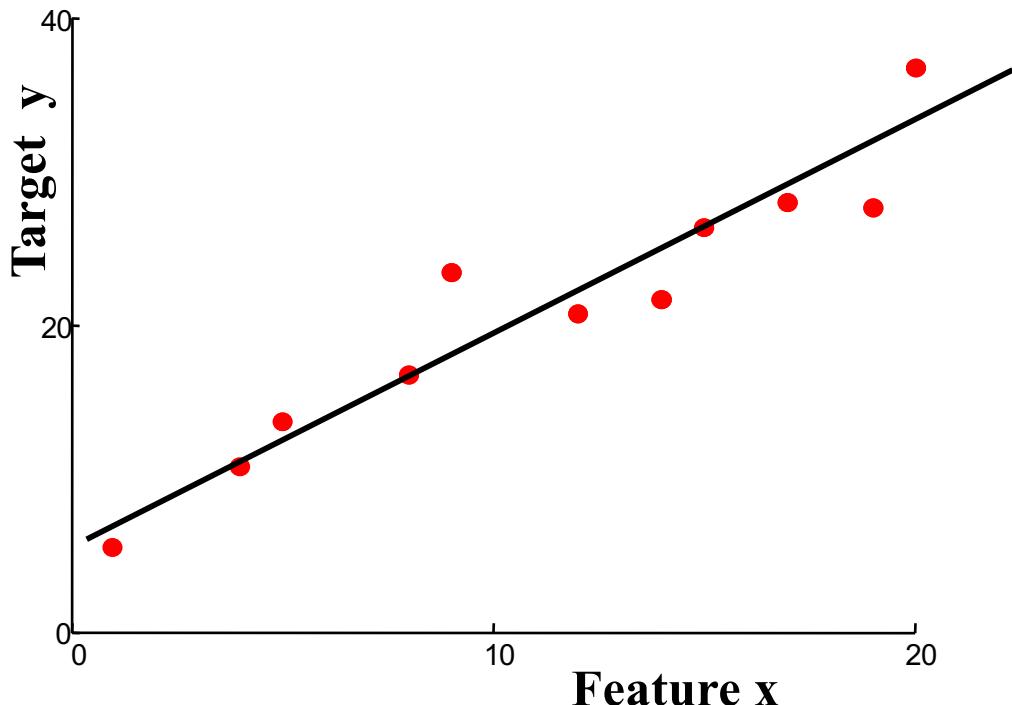
Supervised learning

- Notation

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



Linear regression



“Predictor”:

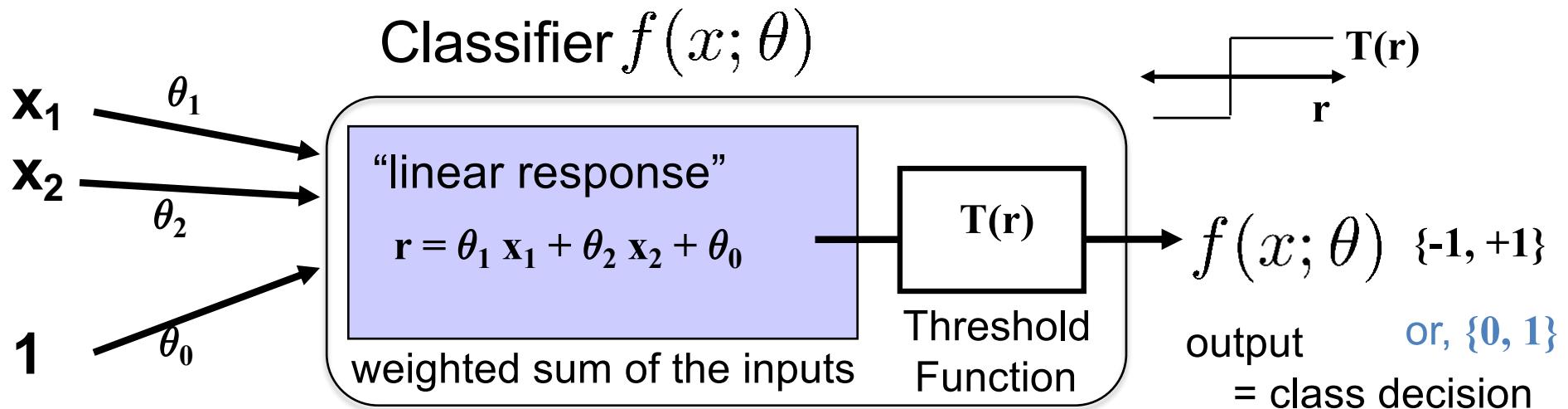
Evaluate line:

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

return r

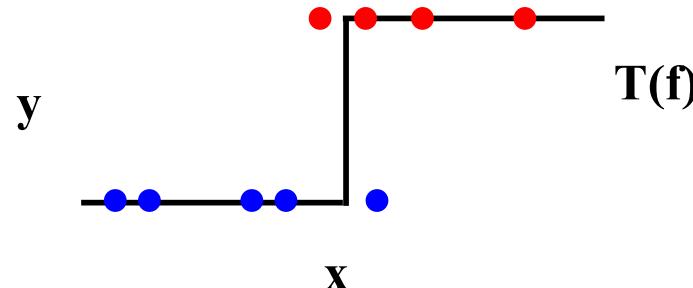
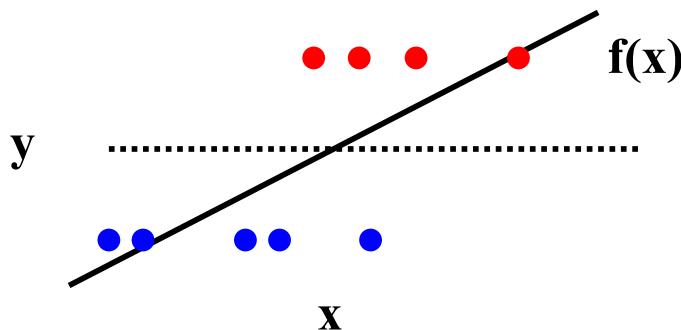
- Contrast with classification
 - Classify: predict discrete-valued target y
 - Initially: “classic” binary { -1, +1} classes; generalize later

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 $x_1 \dots x_n$ are arbitrary numbers
 - Define an additional constant input feature $x_0=1$
- A perceptron calculates 2 quantities:
 - 1. A weighted sum of the input features
 - 2. This sum is then thresholded by the $T(\cdot)$ 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:

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

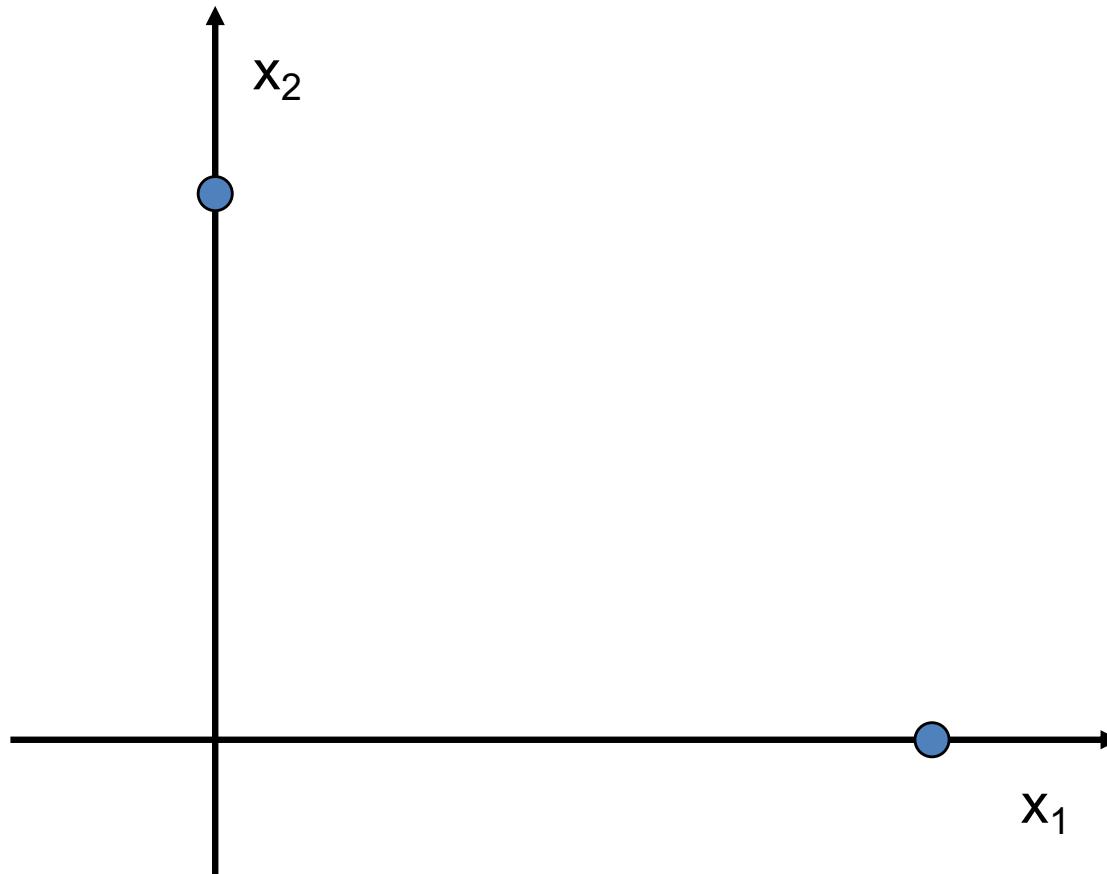
- The perceptron represents a hyperplane decision surface in d-dimensional space
 - A line in 2D, a plane in 3D, etc.
- The equation of the hyperplane is given by

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

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

Example, Linear Decision Boundary

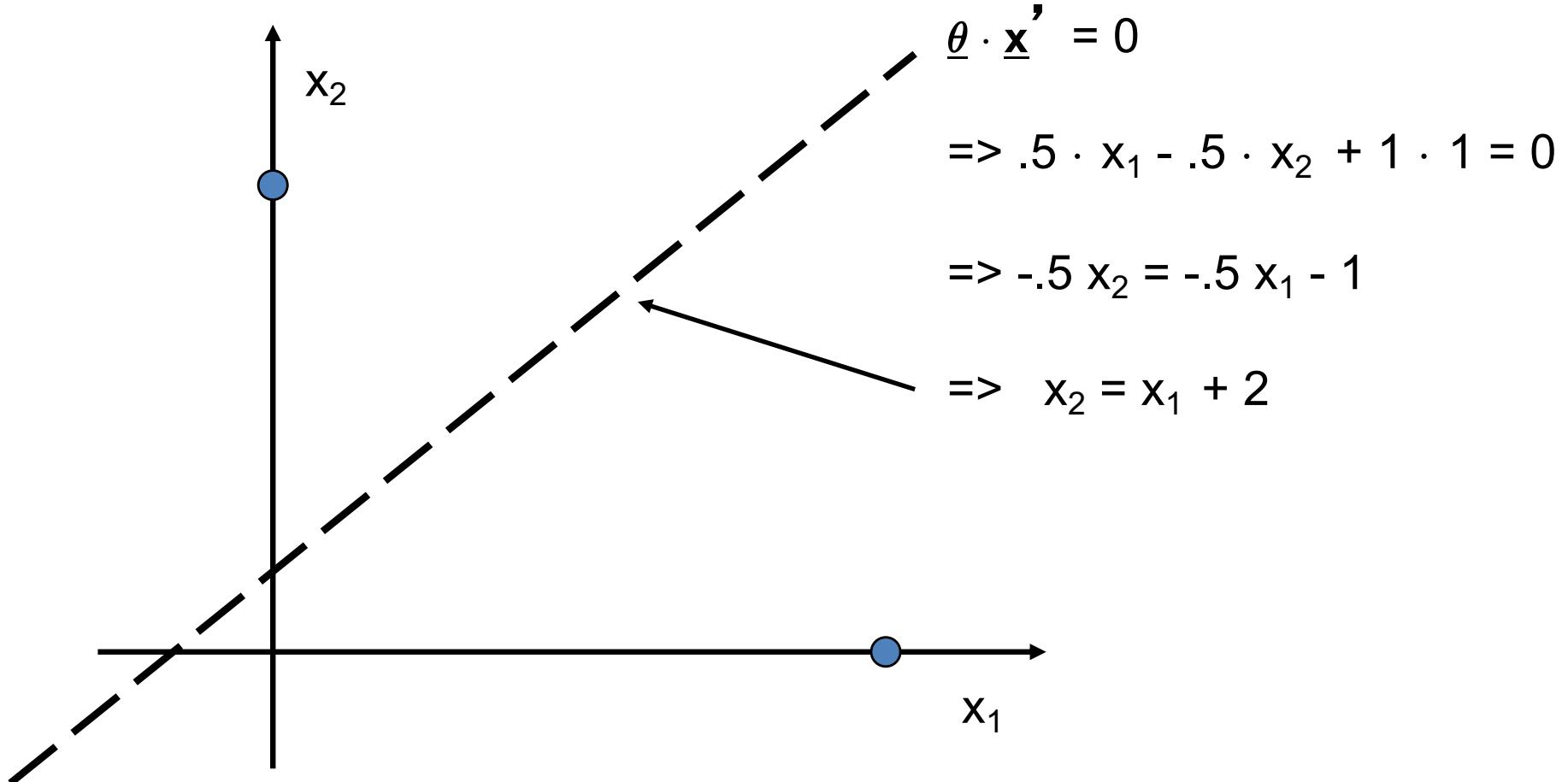
$$\begin{aligned}\underline{\theta} &= (\theta_0, \theta_1, \theta_2) \\ &= (1, .5, -.5)\end{aligned}$$



From P. Smyth

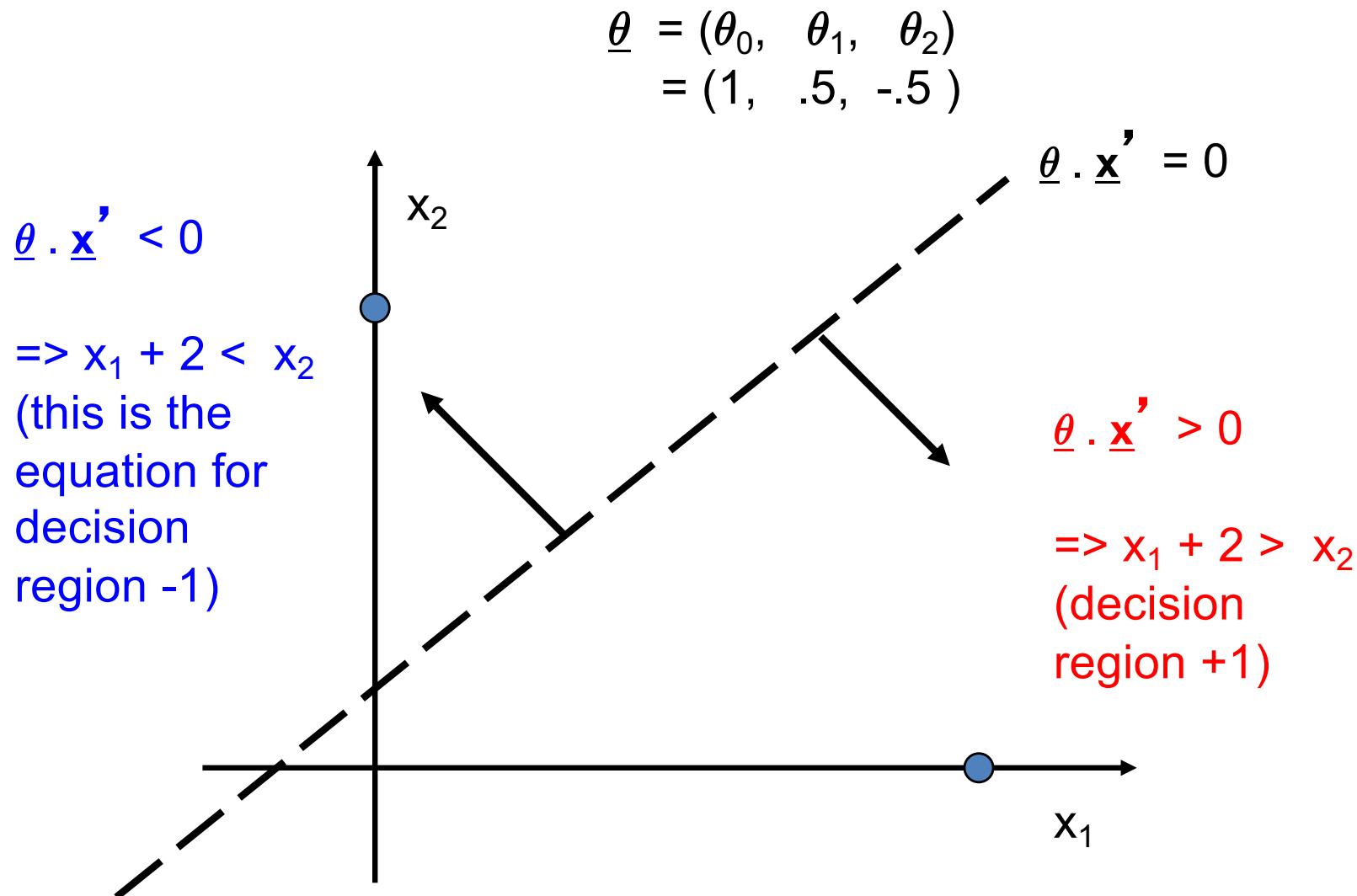
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Example, Linear Decision Boundary

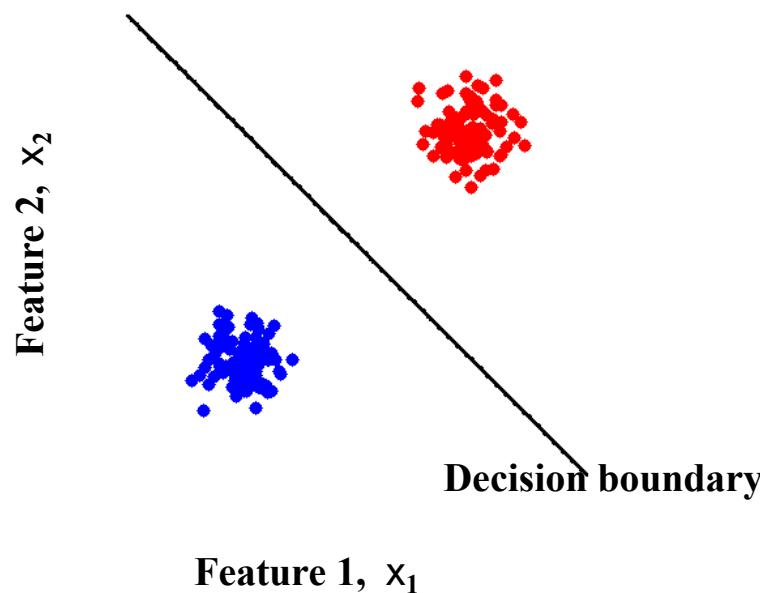


From P. Smyth

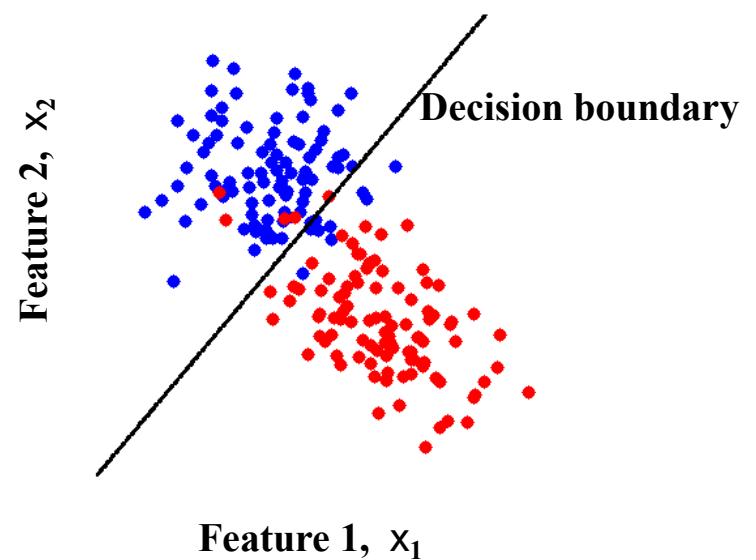
Separability

- 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

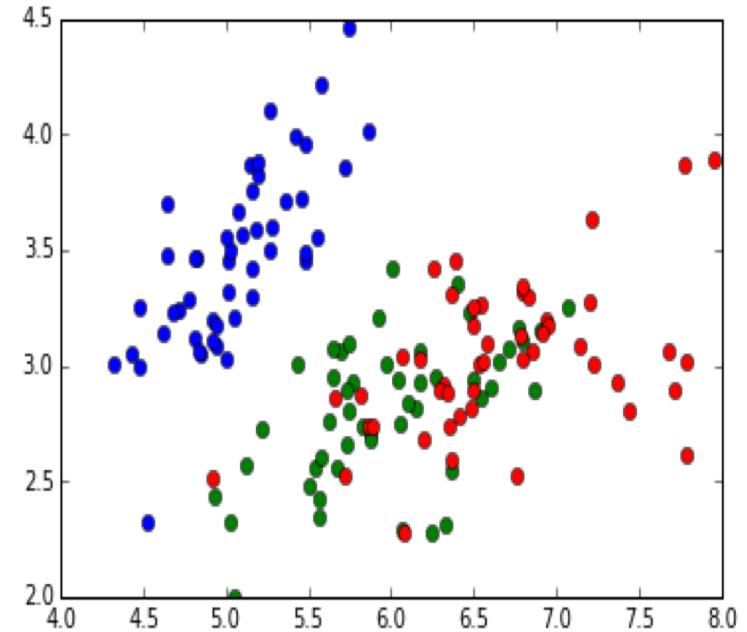


Linearly non-separable data

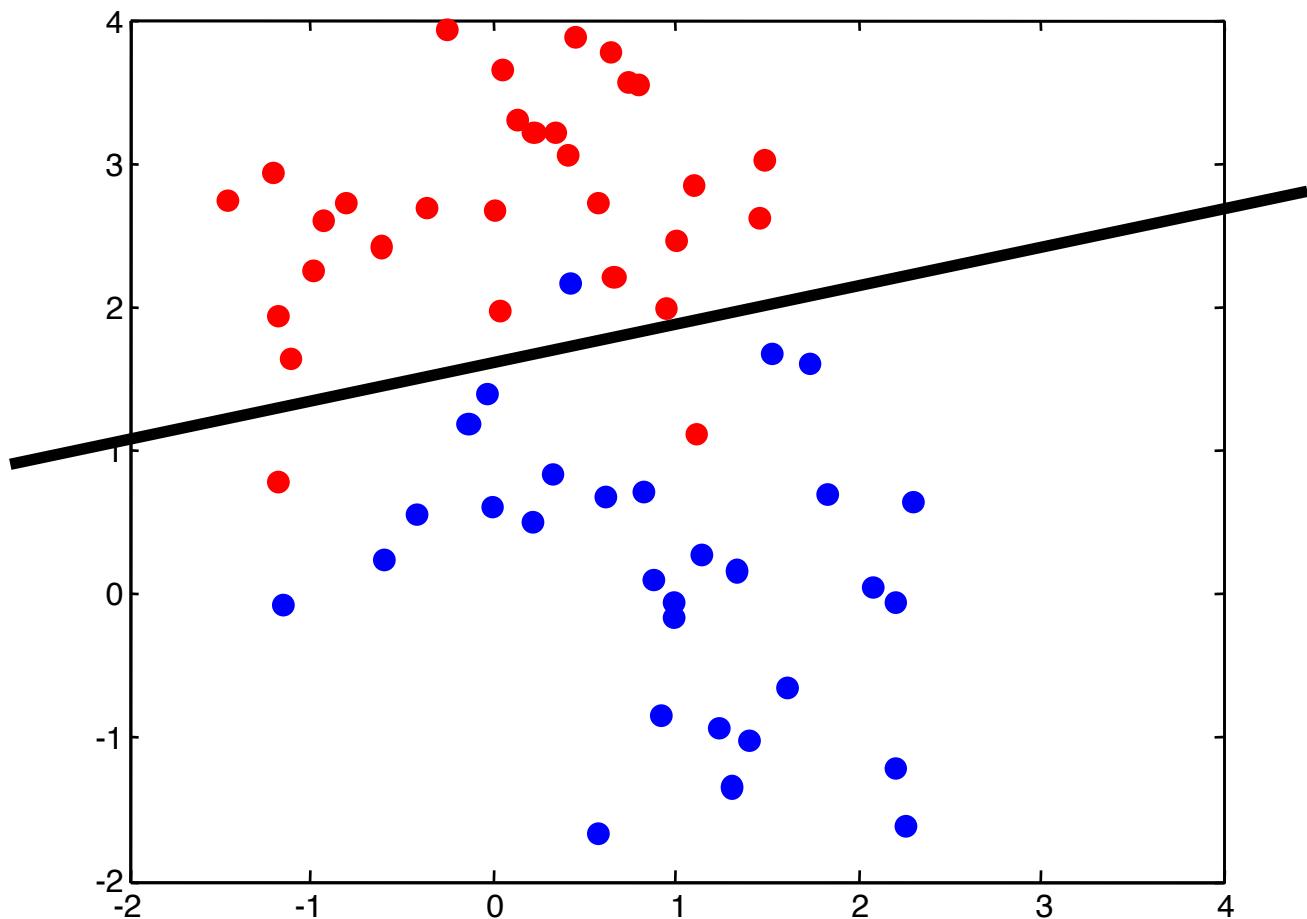


Class overlap

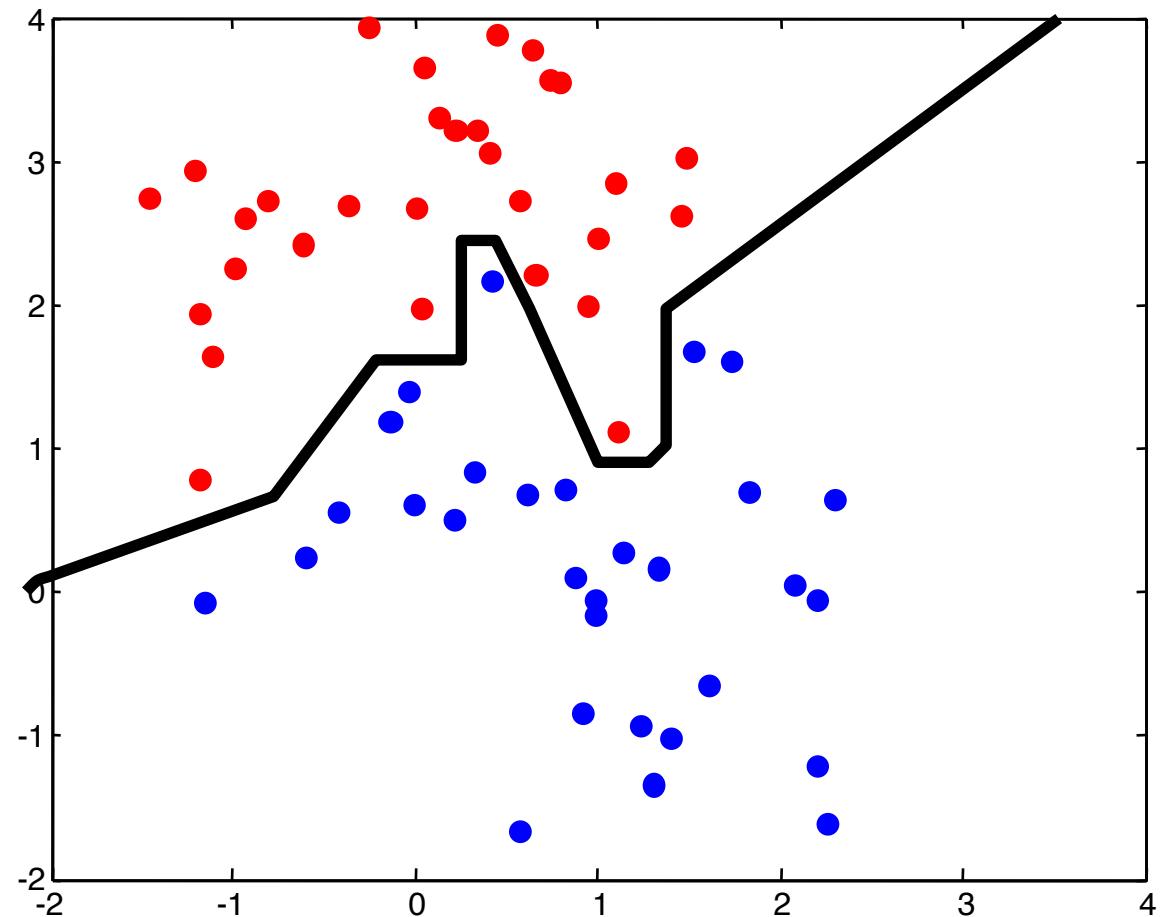
- Classes may not be well-separated
- Same observation values possible under both classes
 - High vs low risk; features {age, income}
 - Benign/malignant cells look similar
 - ...
- Common in practice
- May not be able to perfectly distinguish between classes
 - Maybe with more features?
 - Maybe with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



Another example



Non-linear decision boundary

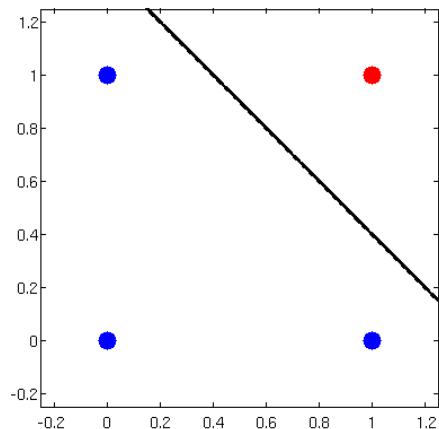


Representational Power of Perceptrons

- 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)

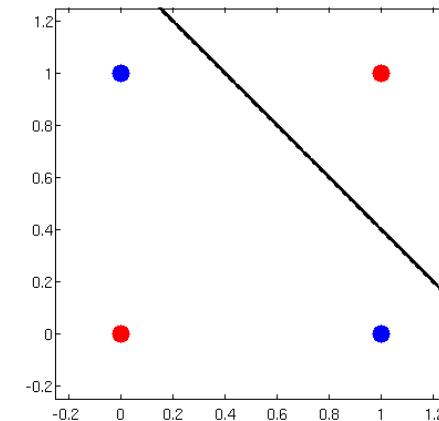
“AND”

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



“XOR”

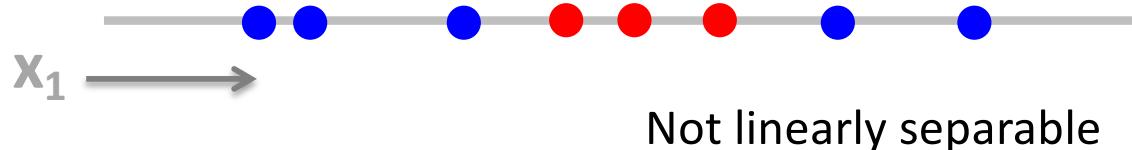
x_1	x_2	y
0	0	1
0	1	-1
1	0	-1
1	1	1



Adding features

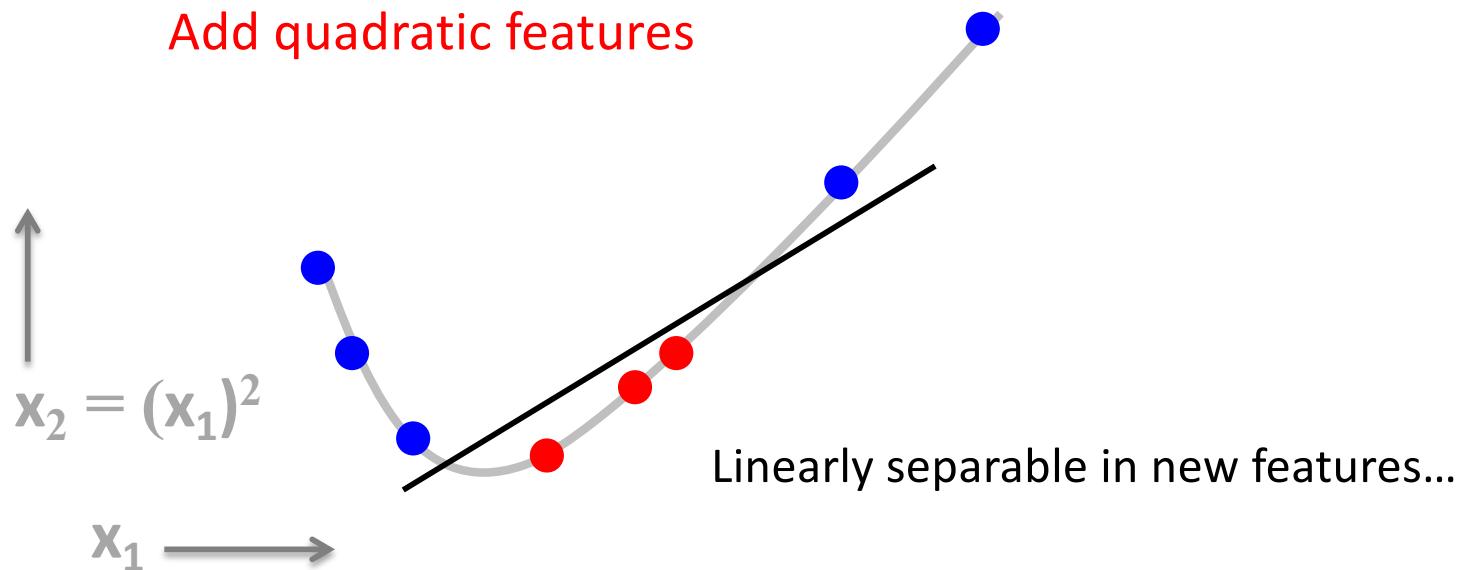
- Linear classifier can't learn some functions

1D example:



Not linearly separable

Add quadratic features

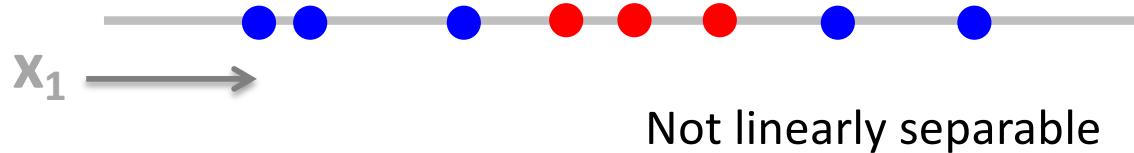


Linearly separable in new features...

Adding features

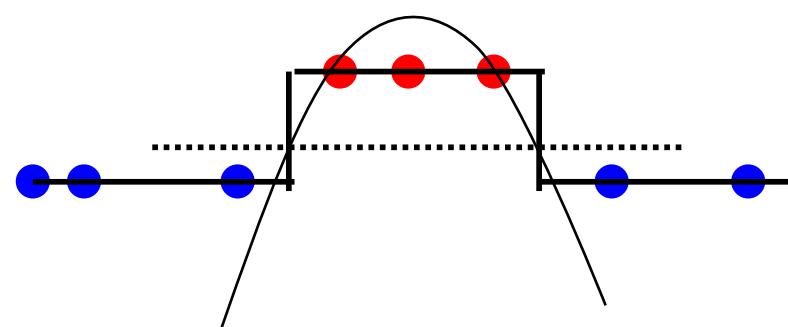
- Linear classifier can't learn some functions

1D example:



Quadratic features, visualized in original feature space:

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



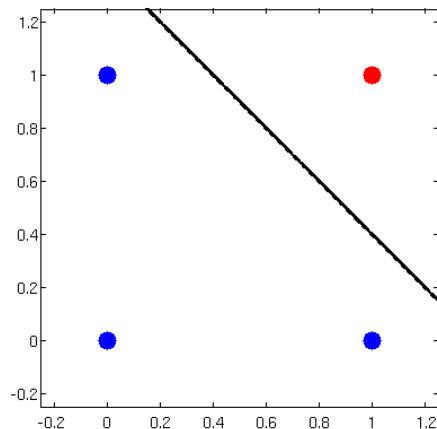
More complex decision boundary: $ax^2+bx+c = 0$

Representational Power of Perceptrons

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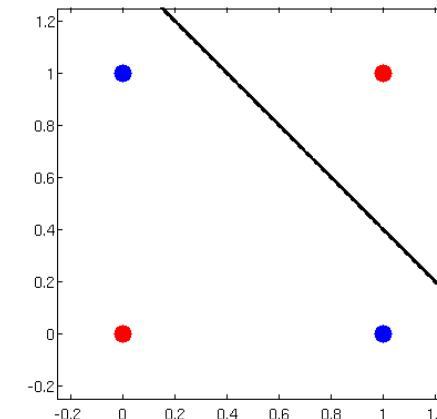
“AND”

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



“XOR”

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



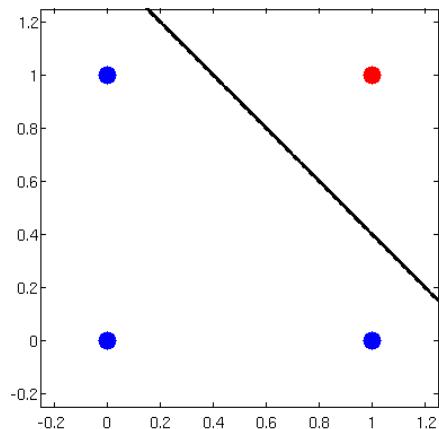
What kinds of functions would we need to learn the data on the right?

Representational Power of Perceptrons

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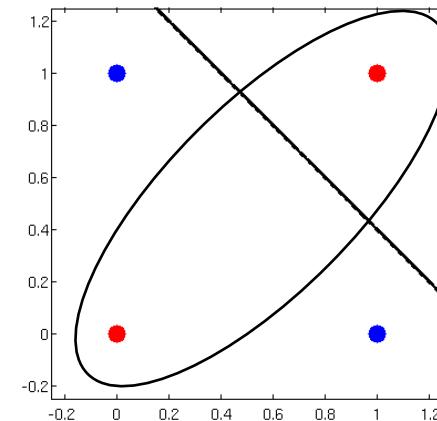
“AND”

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



“XOR”

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



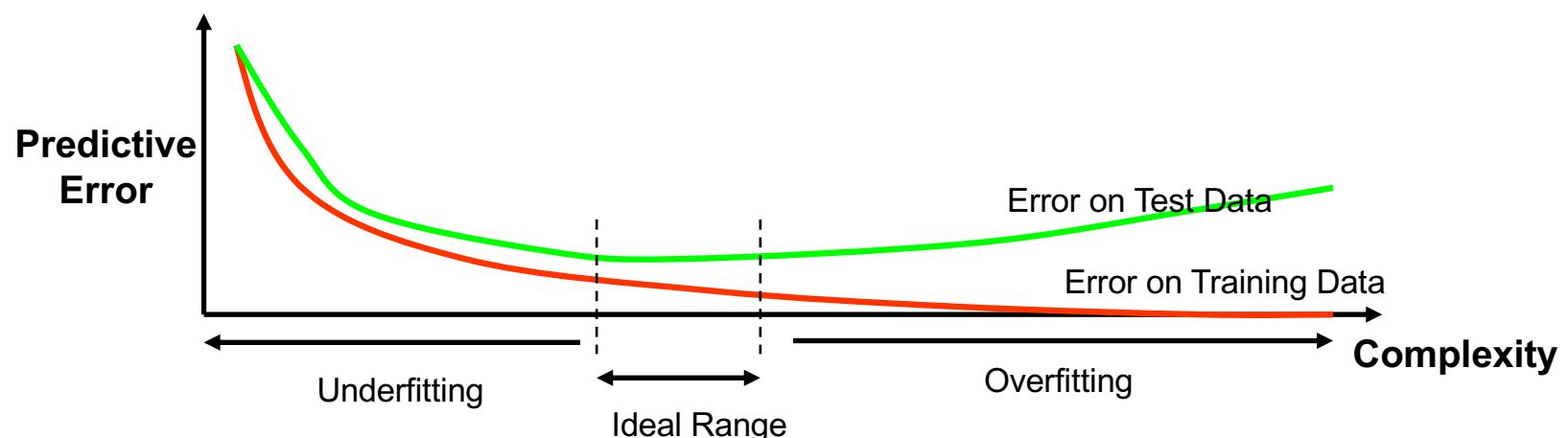
What kinds of functions would we need to learn the data on the right?
Ellipsiodal decision boundary: $a x_1^2 + b x_1 + c x_2^2 + d x_2 + e x_1 x_2 + f = 0$

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 \Leftrightarrow 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

Machine Learning

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Regularization for Linear Classification

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 $(\theta_0, \theta_1, \theta_2, \dots)$

Training a linear classifier

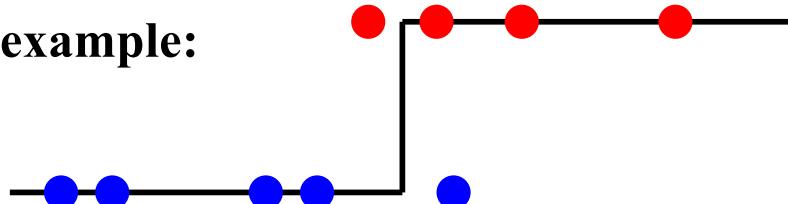
- How should we measure error?
 - Natural measure = “fraction we get wrong” (error rate)

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

```
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

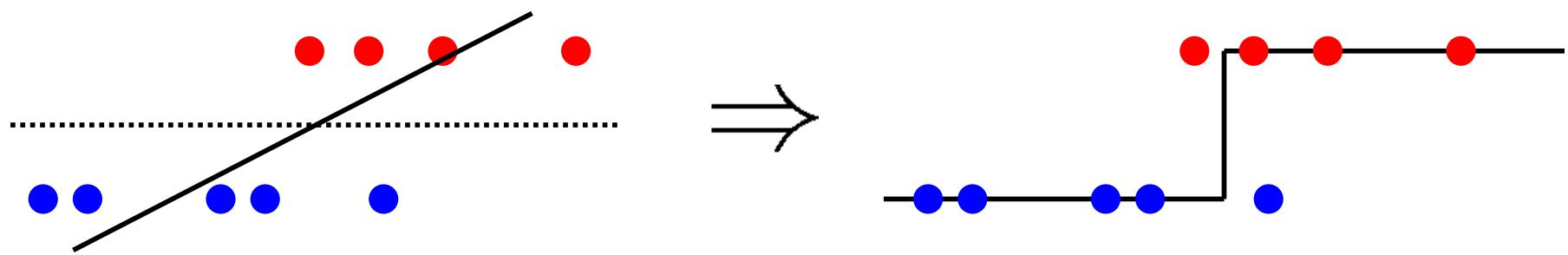
1D example:



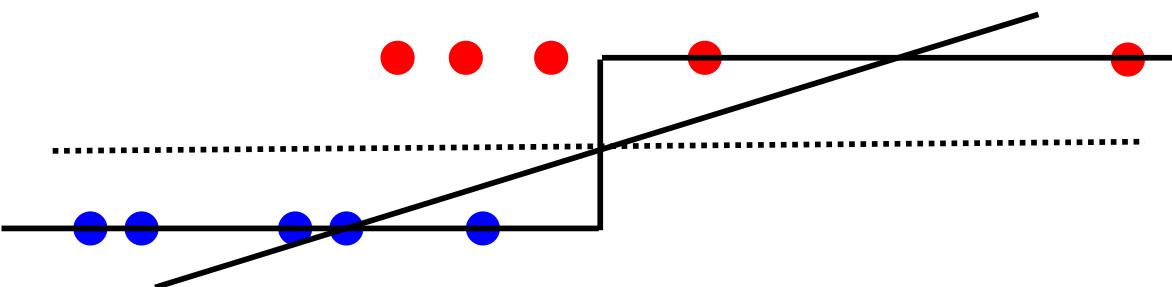
$$\begin{aligned} T(f) &= -1 \text{ if } f < 0 \\ T(f) &= +1 \text{ if } f \geq 0 \end{aligned}$$

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 :

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

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

- Compare to linear regression + MSE cost

– Identical update to SGD for MSE except error uses thresholded $\hat{y}(j)$ instead of linear response $\underline{\theta} \cdot x$:

– (1) For correct predictions, $y(j) - \hat{y}(j) = 0$

– (2) For incorrect predictions, $y(j) - \hat{y}(j) = \pm 2$

“adaptive” linear regression: correct predictions stop contributing

Perceptron algorithm

- Perceptron algorithm: an SGD-like algorithm

while \neg done:

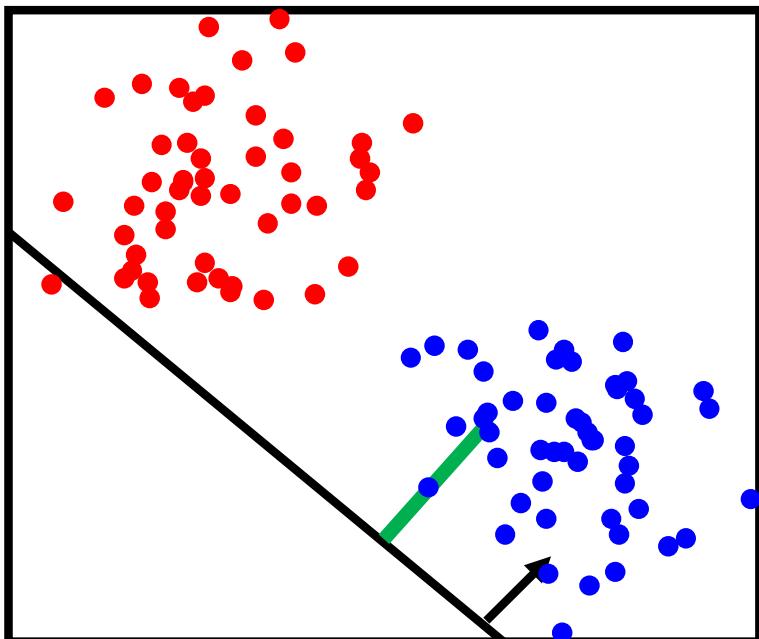
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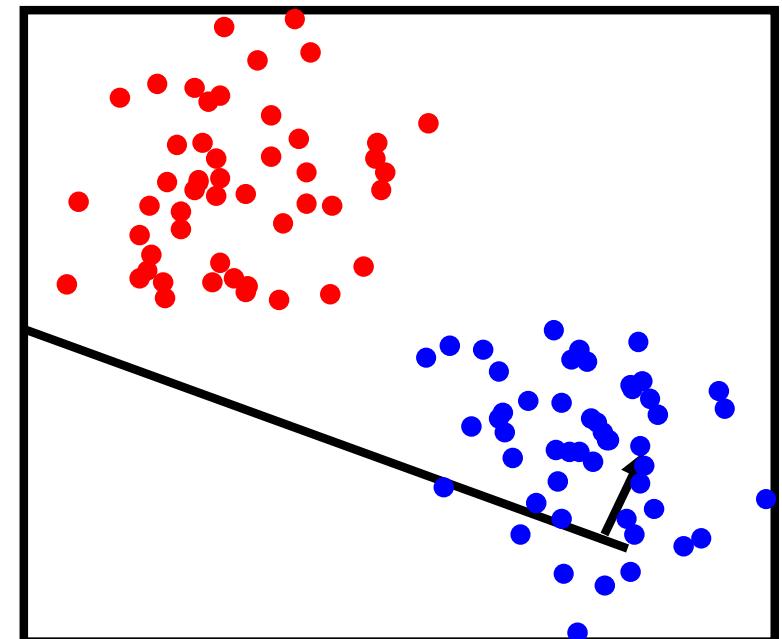
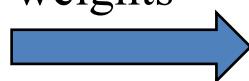
(predict output for point j)

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

("gradient-like" step)



$y(j)$
predicted
incorrectly:
update
weights



Perceptron algorithm

- Perceptron algorithm: an SGD-like algorithm

while \neg done:

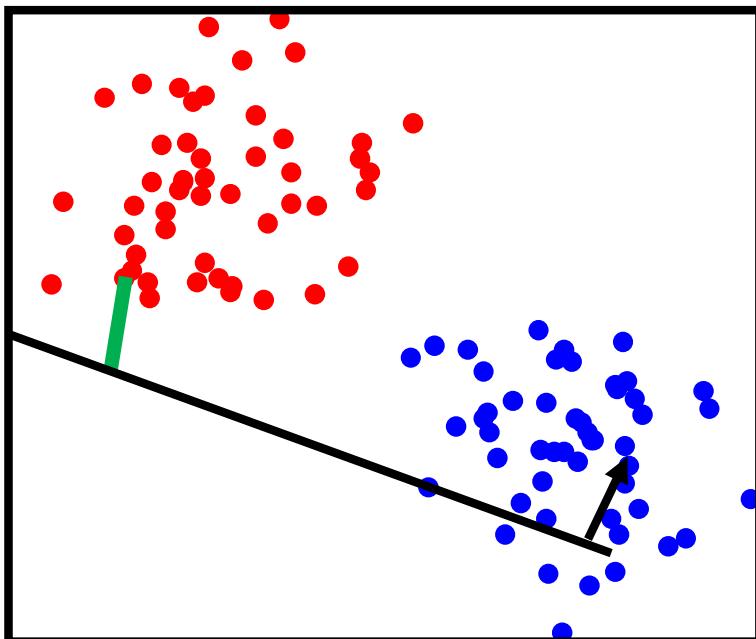
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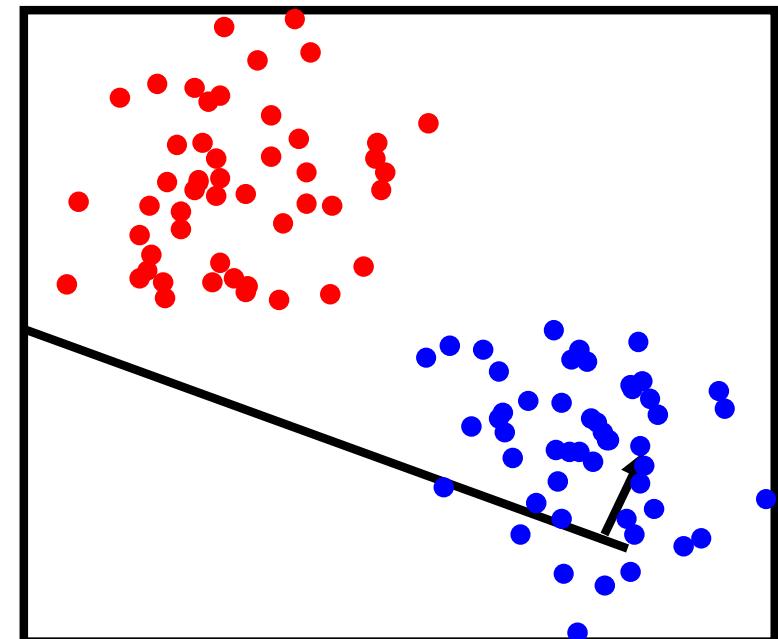
(predict output for point j)

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

("gradient-like" step)



$y(j)$
predicted
correctly:
no update



Perceptron algorithm

- Perceptron algorithm: an SGD-like algorithm

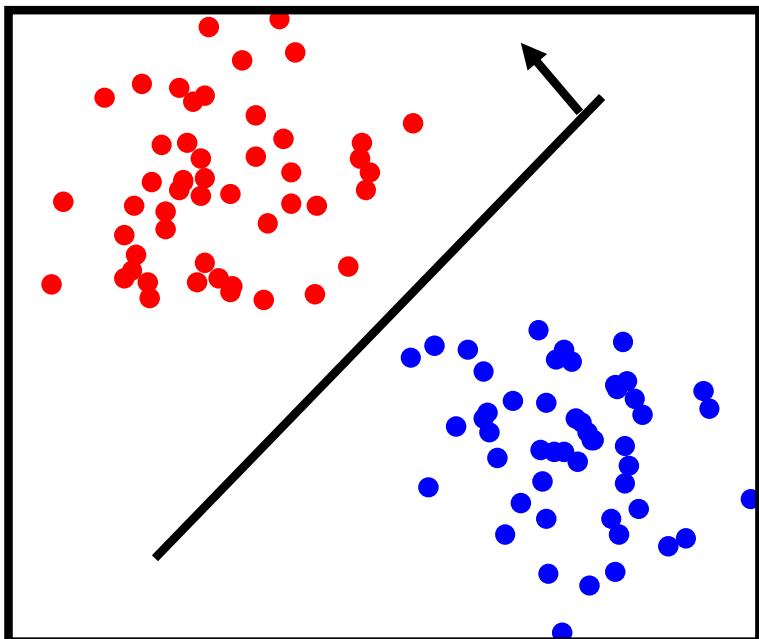
while \neg done:

for each data point j :

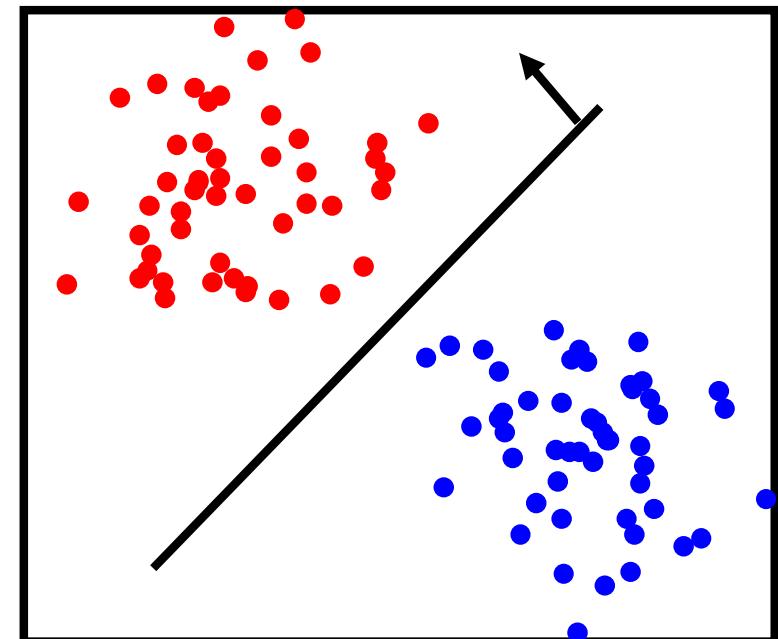
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(Converges if data are linearly separable)



$y(j)$
predicted
correctly:
no update



Perceptron MARK 1 Computer



Frank Rosenblatt, late 1950s

Machine Learning

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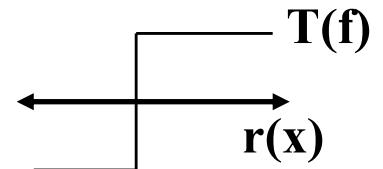
Multi-Class Classification

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Surrogate loss functions

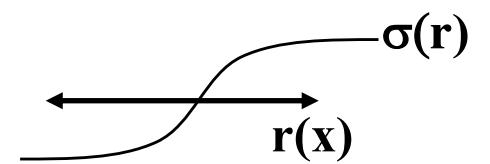
- Another solution: use a “smooth” loss

- e.g., approximate the threshold function



- Usually some smooth function of distance

- Example: logistic “sigmoid”, looks like an “S”



- Now, measure e.g. MSE

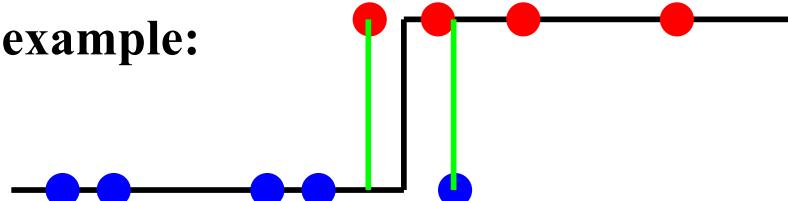
$$J(\underline{\theta}) = \frac{1}{m} \sum_j \left(\sigma(r(x^{(j)})) - y^{(j)} \right)^2$$

Class $y = \{0, 1\} \dots$

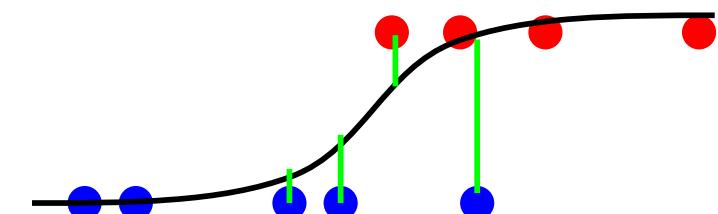
- Far from the decision boundary: $|f(.)|$ large, small error

- Nearby the boundary: $|f(.)|$ near 1/2, larger error

1D example:



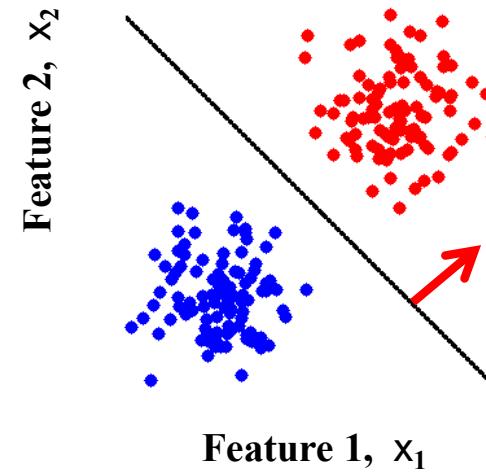
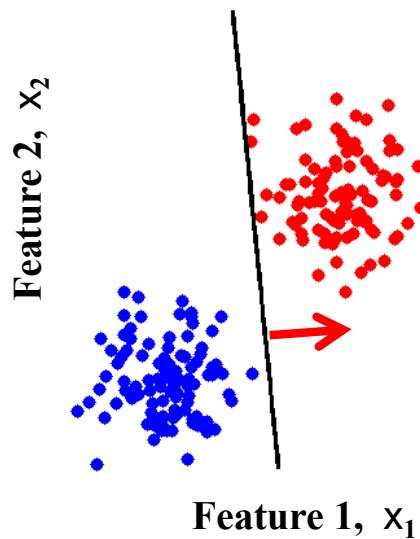
Classification error = 2/9



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

Beyond misclassification rate

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



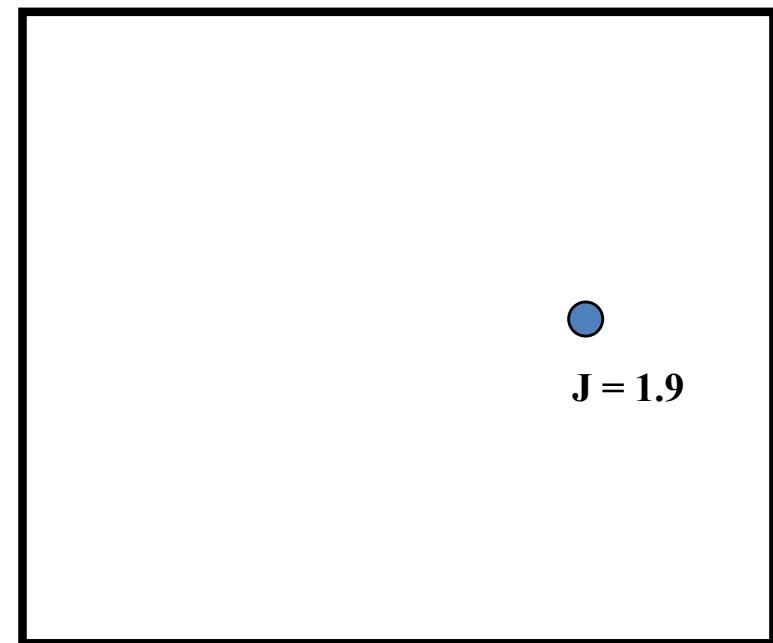
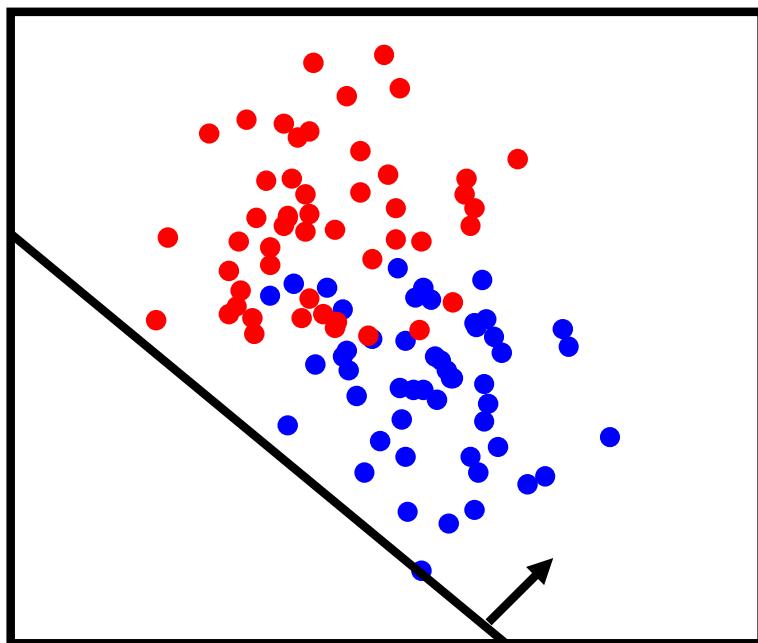
- Side benefit of many “smoothed” error functions
 - Encourages data to be far from the decision boundary
 - See more examples of this principle later...

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 \Leftrightarrow parameter space

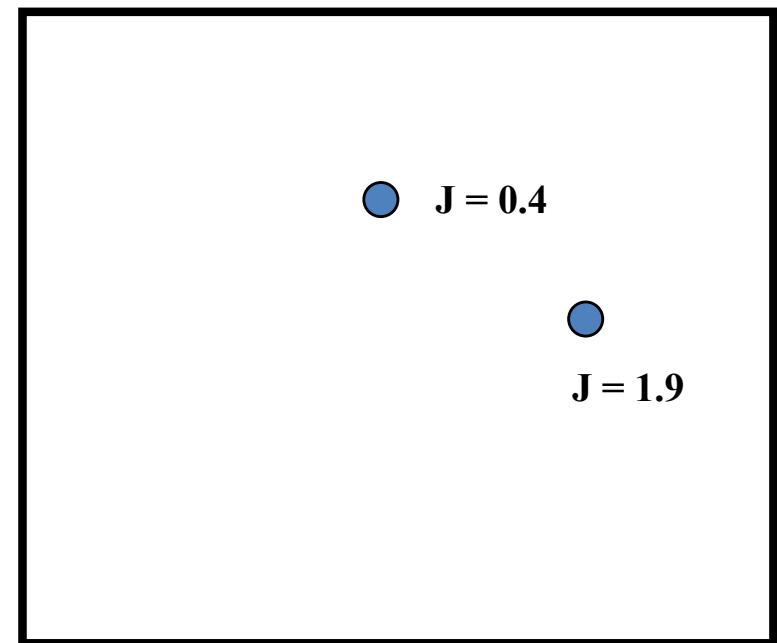
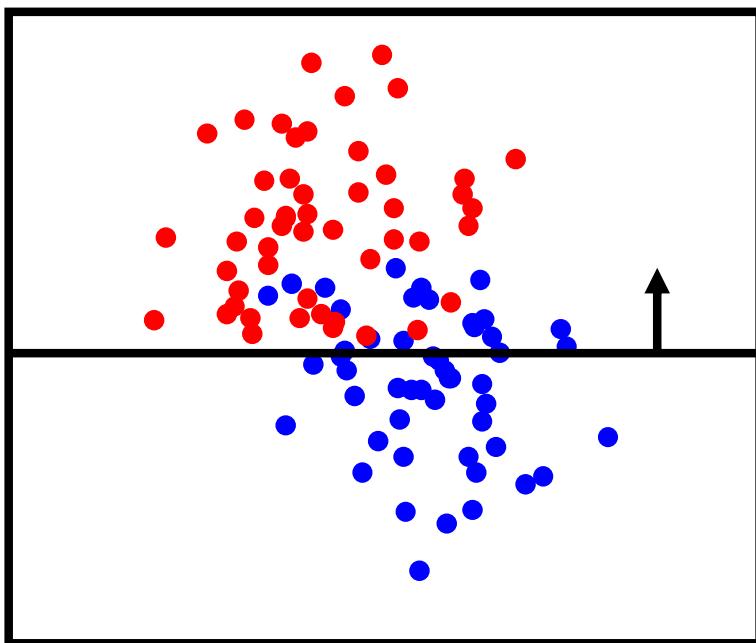


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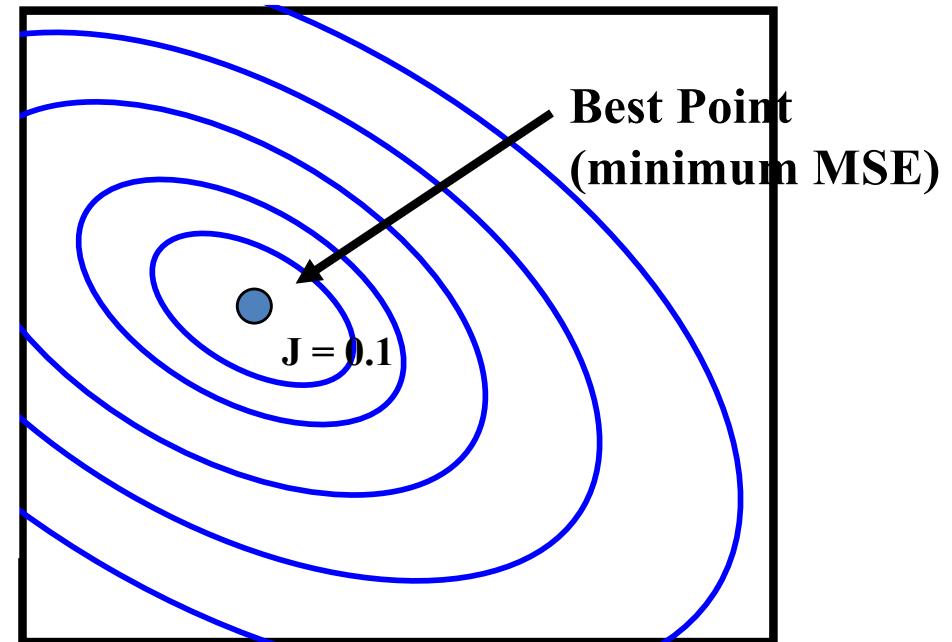
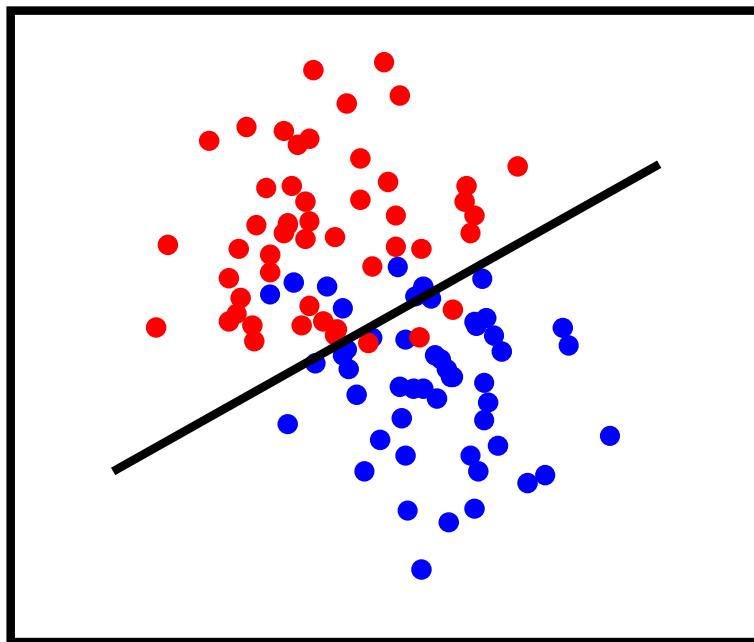


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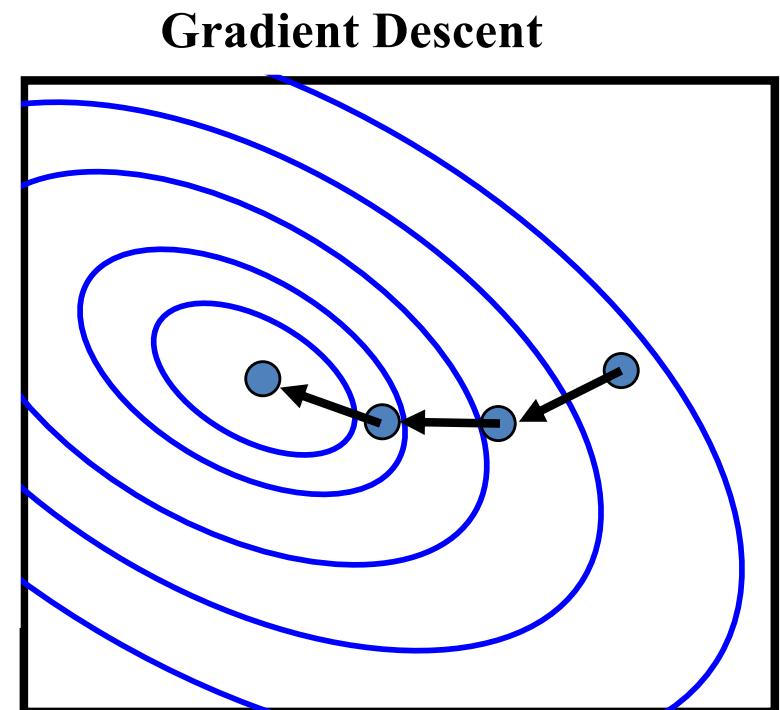
$$r(x_1, x_2) = a^*x_1 + b^*x_2 + c$$

- Example: 2D feature space \Leftrightarrow parameter space



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



Gradient Equations

- MSE (note, depends on function $\sigma(\cdot)$)

$$J(\underline{\theta} = [a, b, c]) = \frac{1}{m} \sum_i (\sigma(ax_1^{(i)} + bx_2^{(i)} + c) - y^{(i)})^2$$

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

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

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

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

$$h(a) = ax_1^{(i)} + bx_2^{(i)} + c \Rightarrow h'(a) = x_1^{(i)}$$

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

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

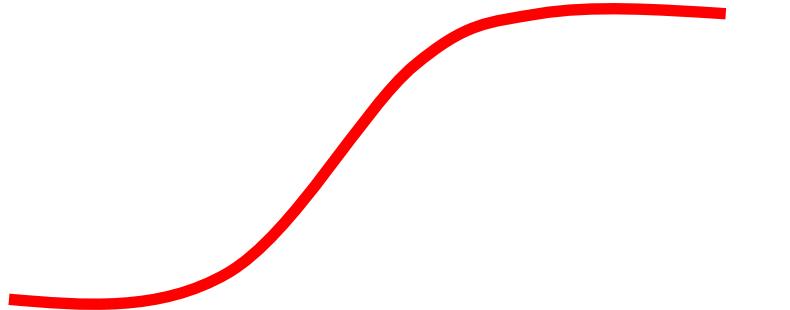
Error between class and prediction Sensitivity of prediction to changes in parameter "a"

Saturating Functions

- Many possible “saturating” functions
- “Logistic” sigmoid (scaled for range [0,1]) is
$$\sigma(z) = 1 / (1 + \exp(-z))$$
- Derivative (slope of the function at a point z) is
$$\partial\sigma(z) = \sigma(z) (1-\sigma(z))$$
- 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))
```



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

(to predict:
threshold z at 0 or
threshold $\sigma(z)$ at $\frac{1}{2}$)

For range [-1, +1]:

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

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

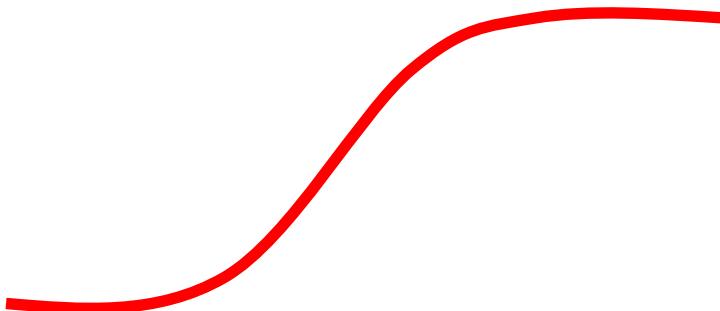
Predict: threshold z or ρ at zero

Class posterior probabilities

- Useful to also know class *probabilities*
- Some notation
 - $p(y=0)$, $p(y=1)$ – class *prior* probabilities
 - How likely is each class in general?
 - $p(x | y=c)$ – class conditional probabilities
 - How likely are observations “x” in that class?
 - $p(y=c | x)$ – class posterior probability
 - How likely is class c *given* an observation x?
- We can compute posterior using Bayes’ rule
 - $p(y=c | x) = p(x|y=c) p(y=c) / p(x)$
- Compute $p(x)$ using sum rule / law of total prob.
 - $p(x) = p(x|y=0) p(y=0) + p(x|y=1)p(y=1)$

Class posterior probabilities

- Consider comparing two classes
 - $p(x | y=0) * p(y=0)$ vs $p(x | y=1) * p(y=1)$
 - Write probability of each class as
 - $$\begin{aligned} p(y=0 | x) &= p(y=0, x) / p(x) \\ &= p(y=0, x) / (p(y=0,x) + p(y=1,x)) \\ &= 1 / (1 + \exp(-a)) \quad (***) \end{aligned}$$
 - $a = \log [p(x|y=0) p(y=0) / p(x|y=1) p(y=1)]$
 - (**) called the logistic function, or logistic sigmoid.



Gaussian models and Logistics

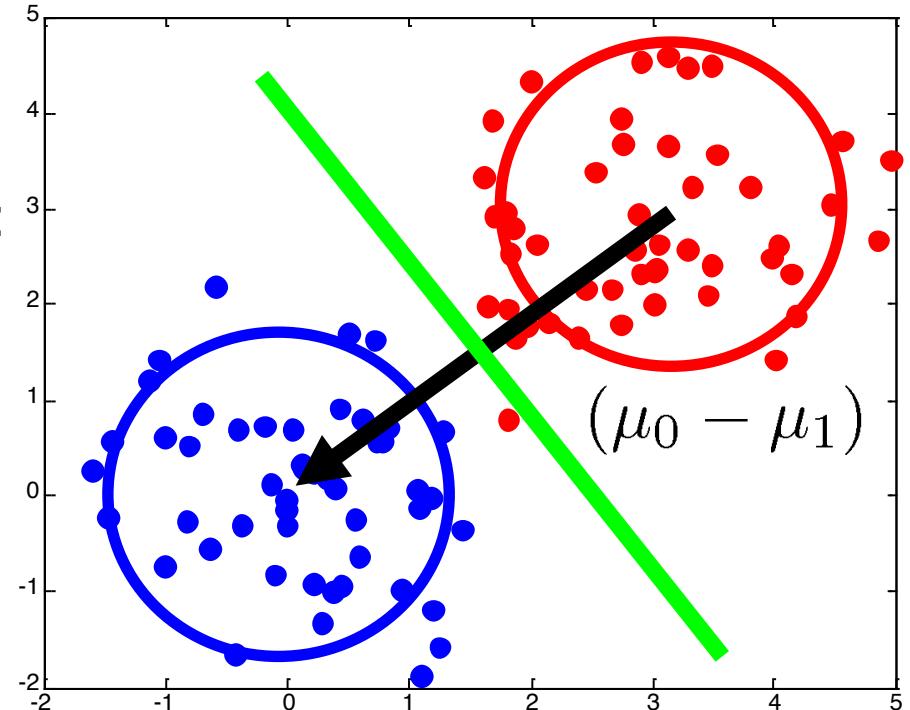
- For Gaussian models with equal covariances

$$\mathcal{N}(\underline{x} ; \underline{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}} |\Sigma|^{-1/2} \exp \left\{ -\frac{1}{2} (\underline{x} - \underline{\mu})^T \Sigma^{-1} (\underline{x} - \underline{\mu}) \right\}$$

$$0 < \log \frac{p(x|y=0)}{p(x|y=1)} \frac{p(y=0)}{p(y=1)} = (\mu_0 - \mu_1)^T \Sigma^{-1} x + constants$$

The probability of each class is given by:

$$p(y=0 | x) = \text{Logistic}(w^T x + b)$$



Logistic regression

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

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

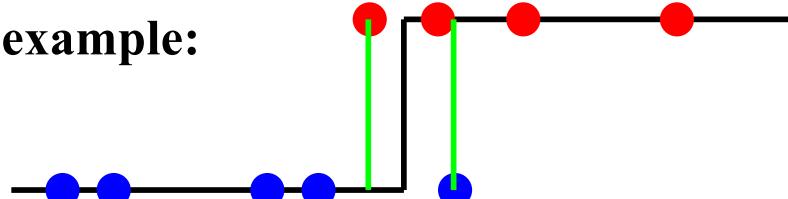
Logistic regression

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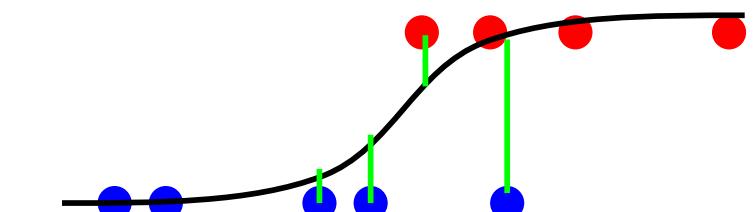
$$J(\underline{\theta}) = -\frac{1}{m} \left(\sum_i y^{(i)} \log \sigma(\underline{\theta} \cdot x^{(i)}) + (1-y^{(i)}) \log(1-\sigma(\underline{\theta} \cdot x^{(i)})) \right)$$

- Convex! Otherwise similar: optimize $J(\underline{\theta})$ via ...

1D example:



Classification error = MSE = 2/9



NLL = - (log(.99) + log(.97) + ...)/9

Gradient Equations

- Logistic neg-log likelihood loss:

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

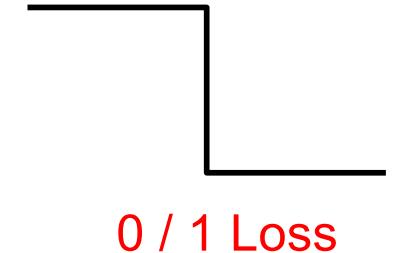
- What's the derivative with respect to one of the parameters?

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

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

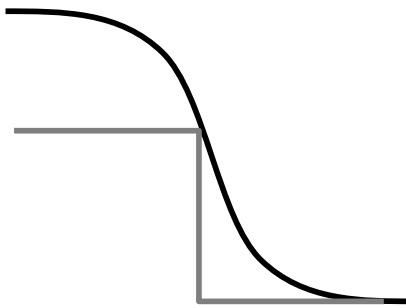
Surrogate loss functions

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



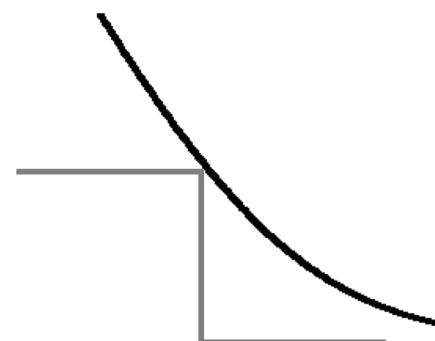
- Logistic MSE

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



- Logistic Neg Log Likelihood

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



Summary

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

Machine Learning

Linear Classification with Perceptrons

Perceptron Learning

Gradient-Based Classifier Learning

Multi-Class Classification

Regularization for Linear Classification

Multi-class linear models

- What about multiple classes? One option:

- Define one linear response per class
 - Choose class with the largest response

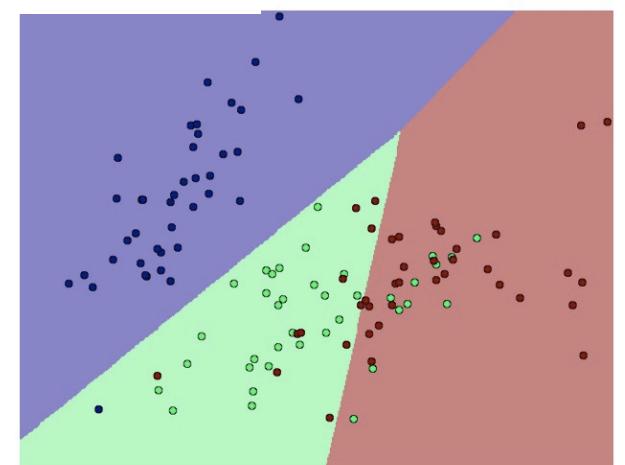
$$f(x; \theta) = \arg \max_c \theta_c \cdot x^T$$

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

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

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

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



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 :

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

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

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

Multilogit regression

- Define the probability of each class:

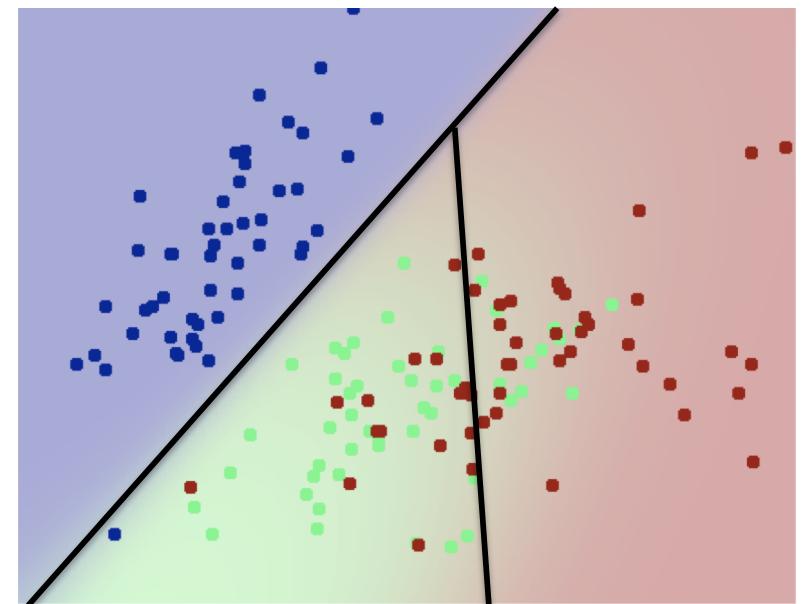
$$p(Y = y|X = x) = \frac{\exp(\theta_y \cdot x^T)}{\sum_c \exp(\theta_c \cdot x^T)}$$

(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



Machine Learning

Linear Classification with Perceptrons

Perceptron Learning

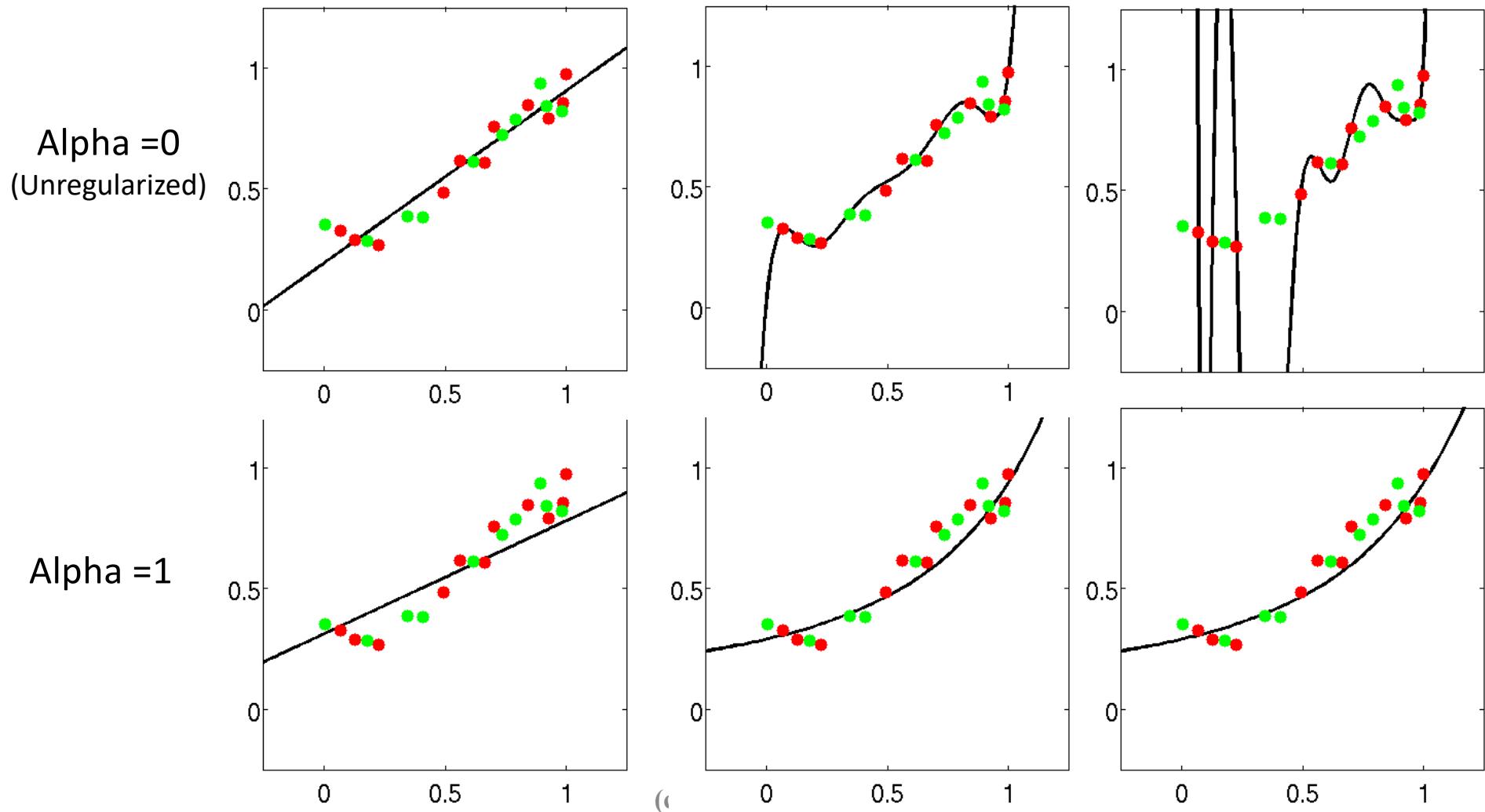
Gradient-Based Classifier Learning

Multi-Class Classification

Regularization for Linear Classification

Regularization

- Reminder: Regularization for linear regression



Regularized logistic regression

- Interpret $\sigma(\underline{\theta} \cdot x^T)$ as a probability that $y = 1$
- Use a negative log-likelihood loss function
 - If $y = 1$, cost is $-\log \Pr[y=1] = -\log \sigma(\underline{\theta} \cdot x^T)$
 - If $y = 0$, cost is $-\log \Pr[y=0] = -\log (1 - \sigma(\underline{\theta} \cdot x^T))$
- Minimize weighted sum of negative log-likelihood and a regularizer that encourages small weights:

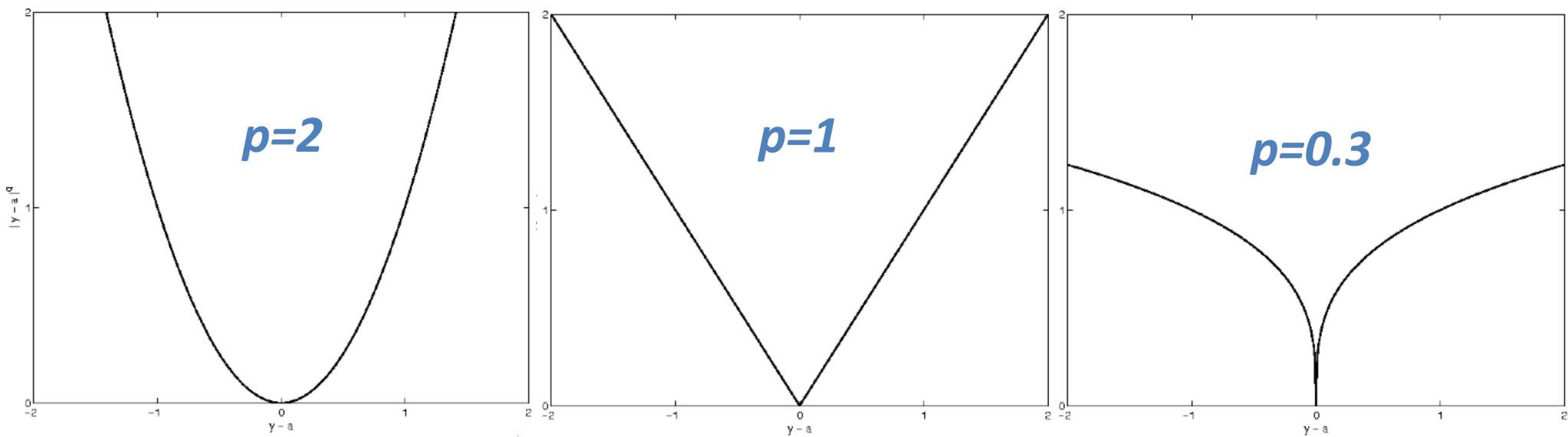
$$J(\underline{\theta}) = -\frac{1}{m} \left(\sum_i y^{(i)} \underbrace{\log \sigma(\underline{\theta} \cdot x^{(i)})}_{\text{Nonzero only if } y=1} + (1-y^{(i)}) \underbrace{\log(1-\sigma(\underline{\theta} \cdot x^{(i)}))}_{\text{Nonzero only if } y=0} \right)$$

$$+ \alpha \|\underline{\theta}\|_p$$

Different regularization functions

- In general, for the L_p regularizer:

$$\left(\sum_i |\theta_i|^p \right)^{\frac{1}{p}} = ||\theta||_p$$

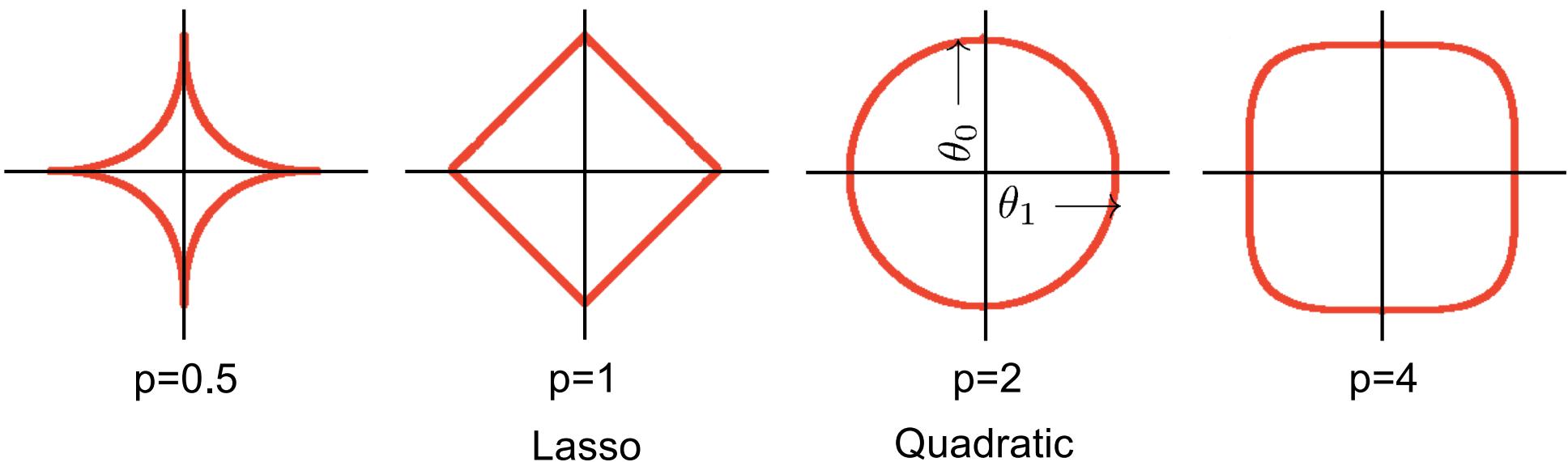


Different regularization functions

- In general, for the L_p regularizer:

$$\left(\sum_i |\theta_i|^p \right)^{\frac{1}{p}} = \|\theta\|_p$$

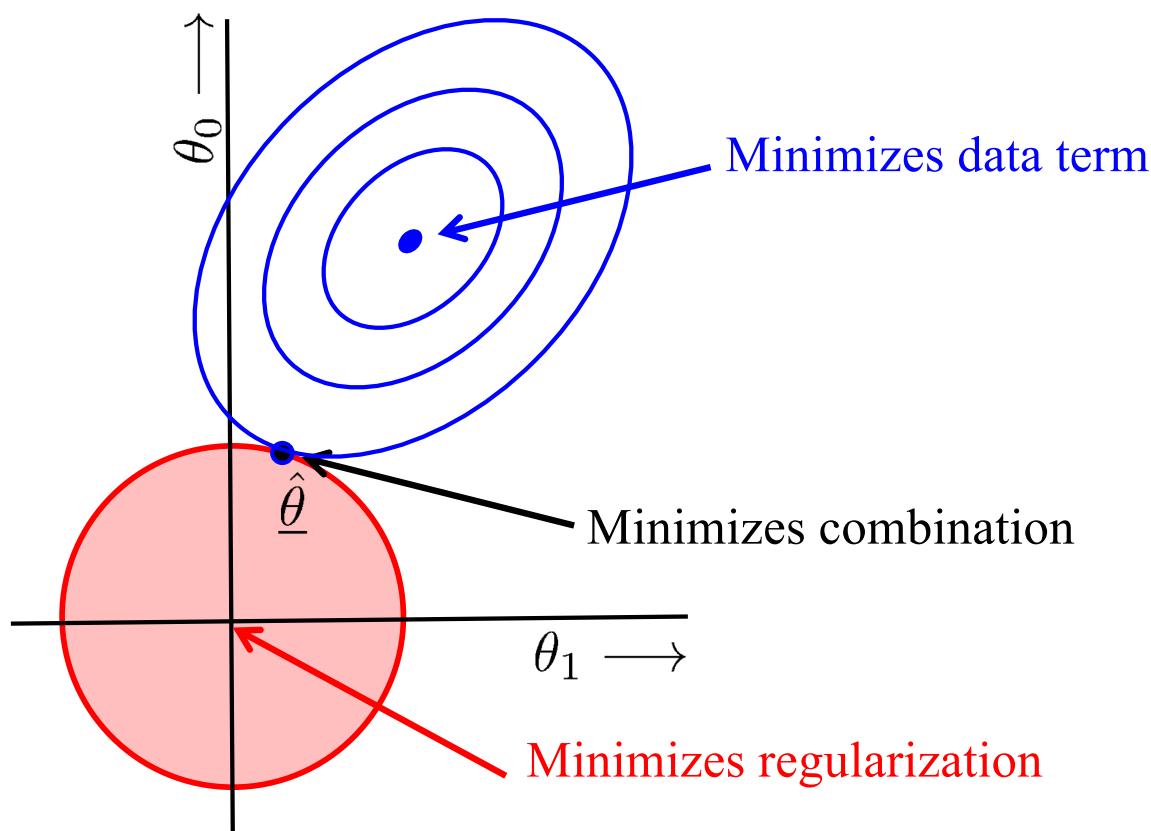
Isosurfaces: $\|\theta\|_p = \text{constant}$



L_0 = limit as p goes to 0 : “number of nonzero weights”, a natural notion of complexity

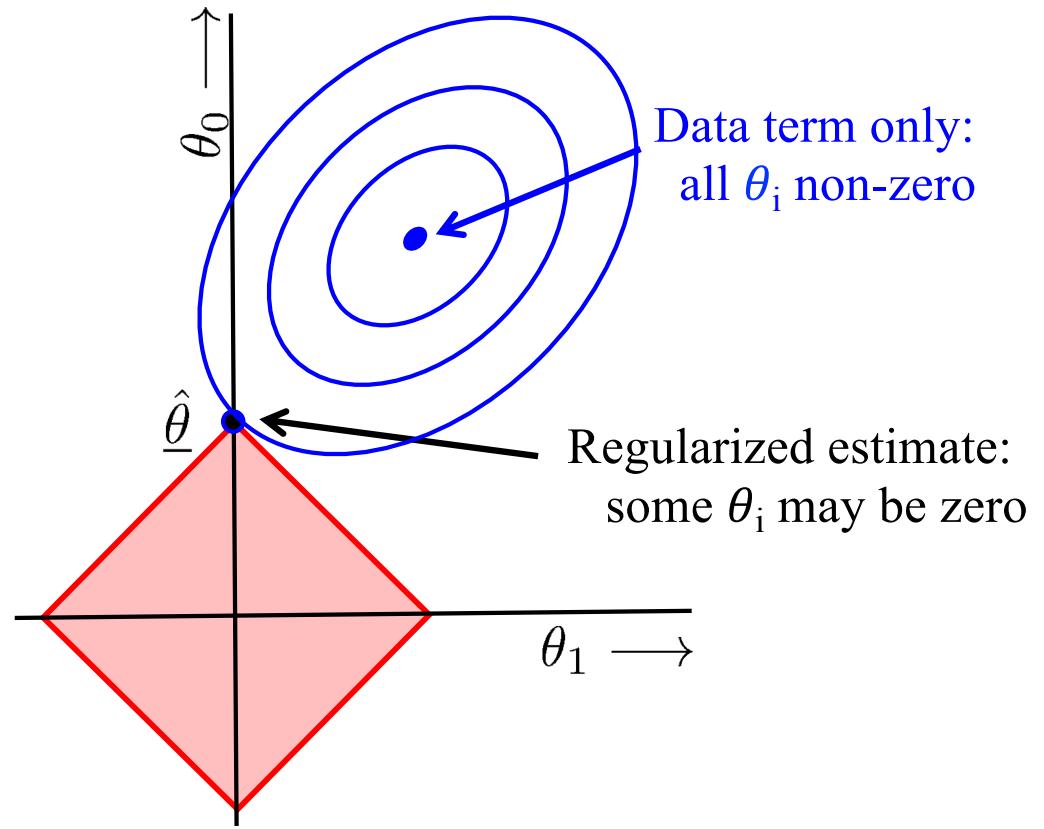
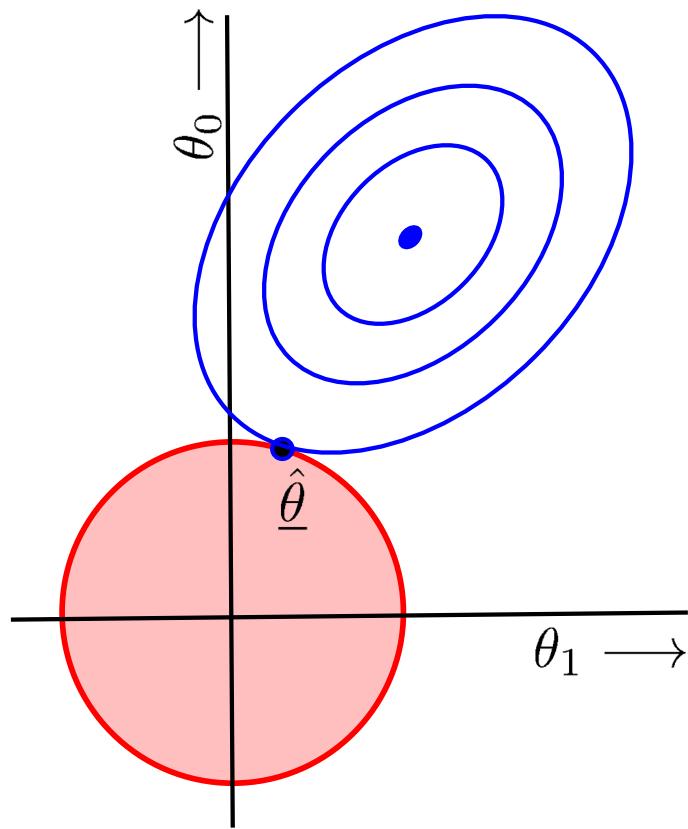
Regularization: L_2 vs L_1

- Estimate balances data term & regularization term



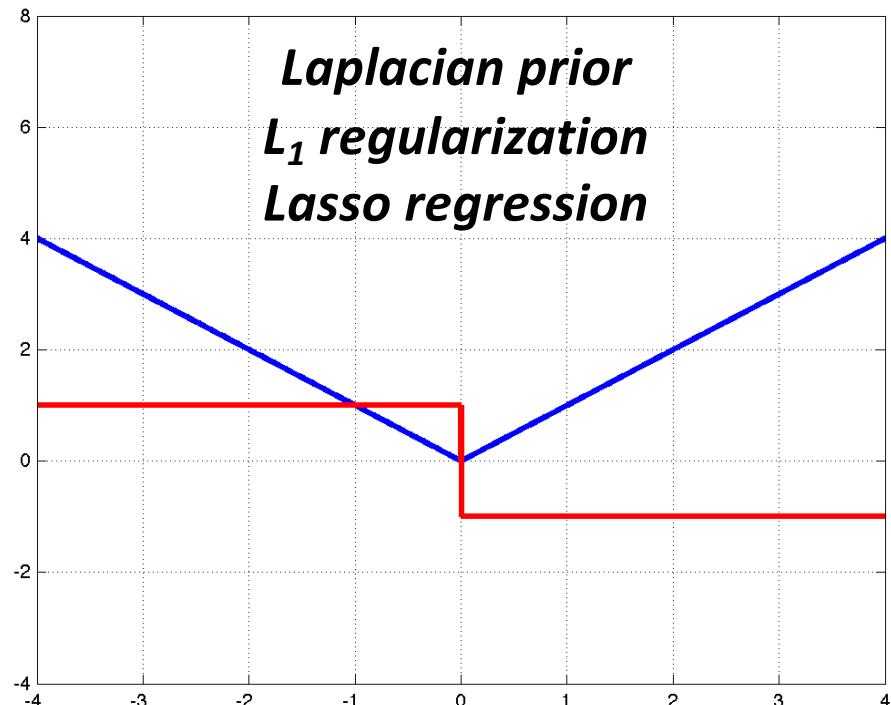
Regularization: L_2 vs L_1

- Estimate balances data term & regularization term
- Lasso tends to generate sparser solutions than a quadratic regularizer.



Gradient-Based Optimization

- L_2 makes (all) coefficients smaller
- L_1 makes (some) coefficients exactly zero: **feature selection**

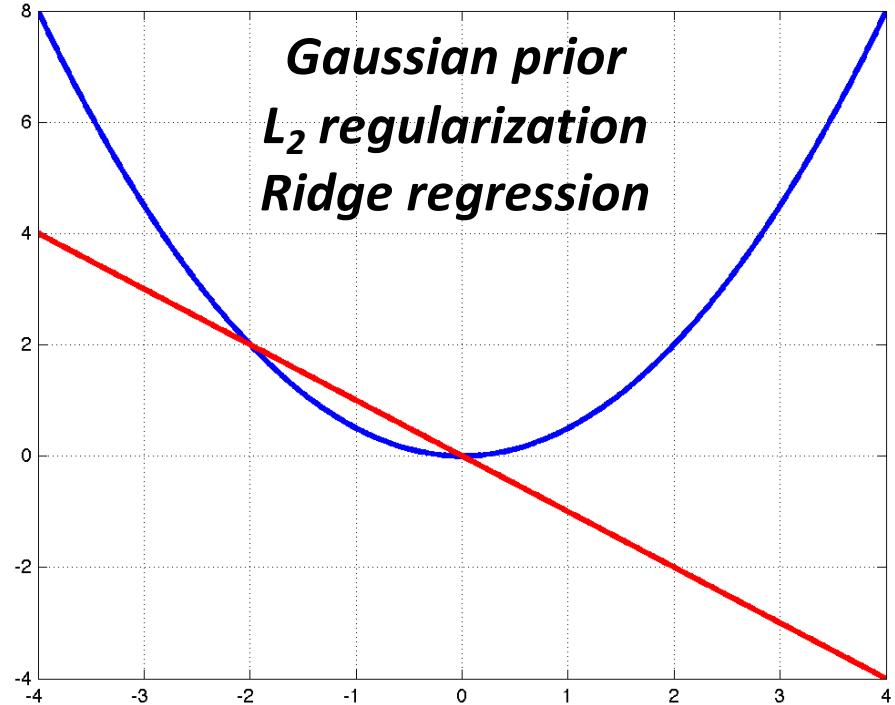


Objective Function:

$$f(\theta_i) = |\theta_i|^p$$

Negative Gradient:

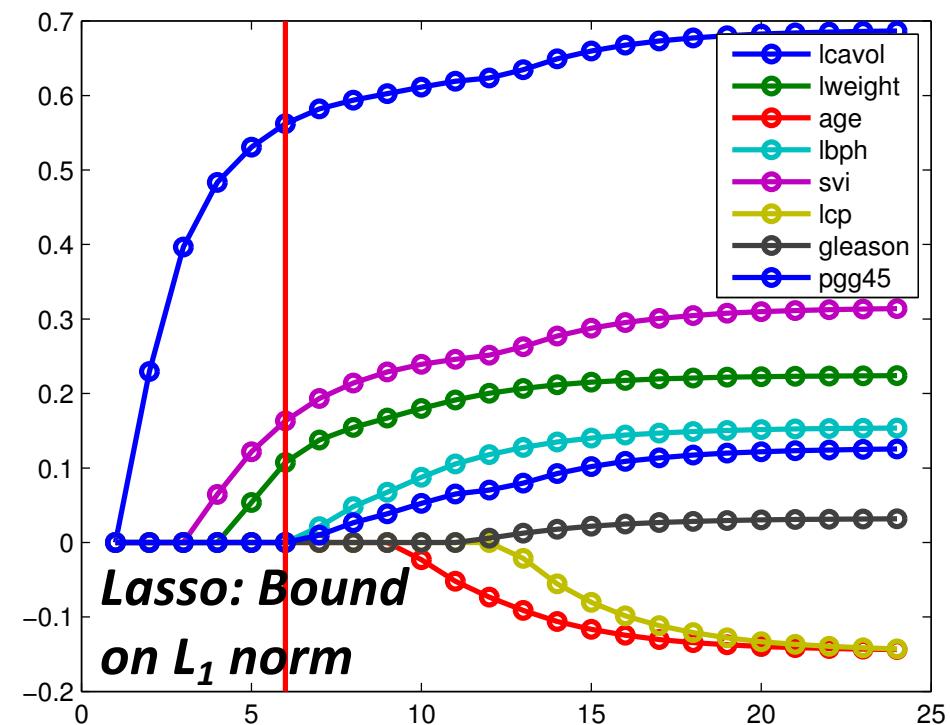
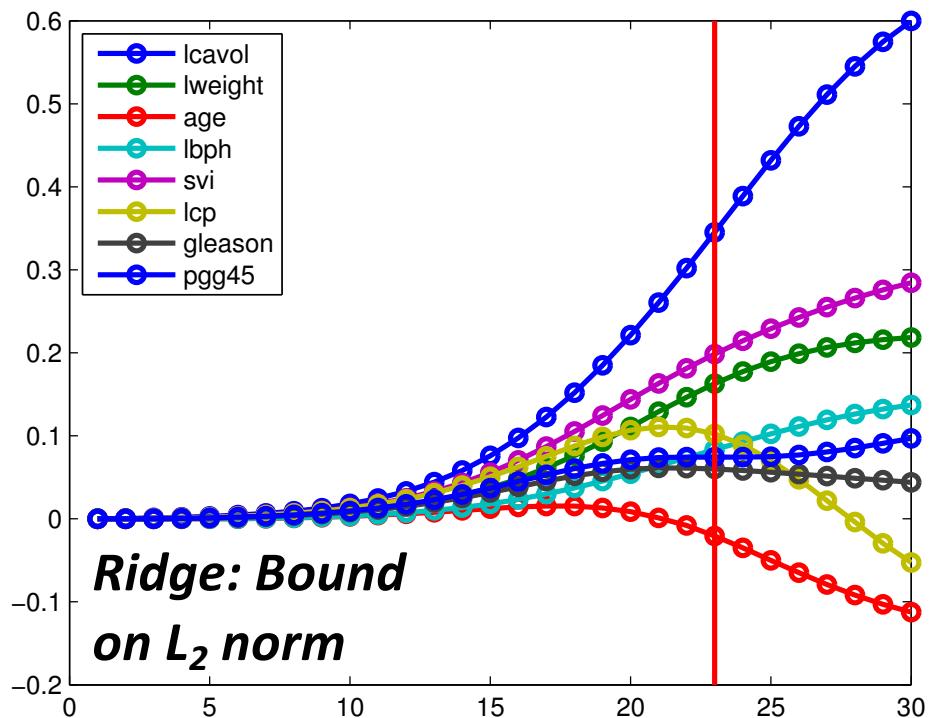
$$-f'(\theta_i)$$



(Informal intuition: Gradient of L₁ objective not defined at zero)

Regularization Paths

Prostate Cancer Dataset with M=67, N=8



- Horizontal axis increases bound on weights (less regularization, smaller α)
- For each bound, plot values of estimated feature weights
- Vertical lines are models chosen by cross-validation