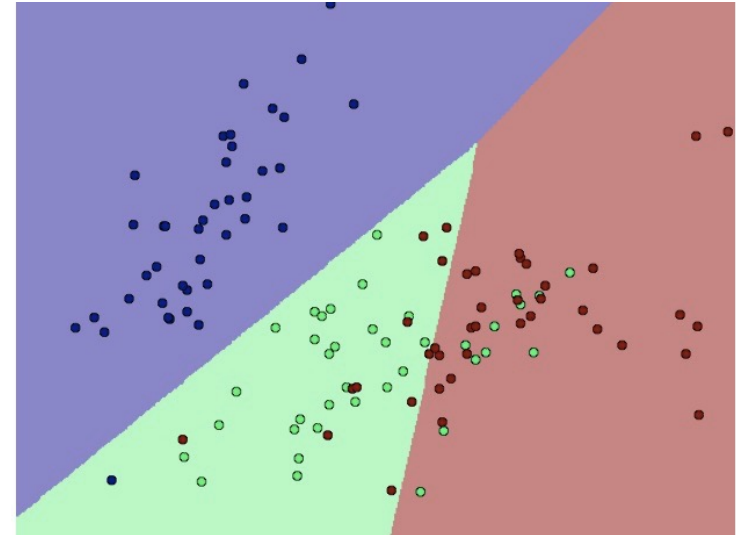
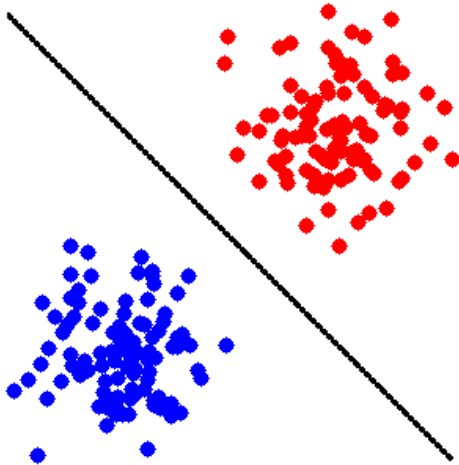


CS273A: Linear Classifiers



Prof. Alexander Ihler
Fall 2023

Linear Classifiers

Linear Classification with Perceptrons

Perceptron Learning

Gradient-Based Classifier Learning

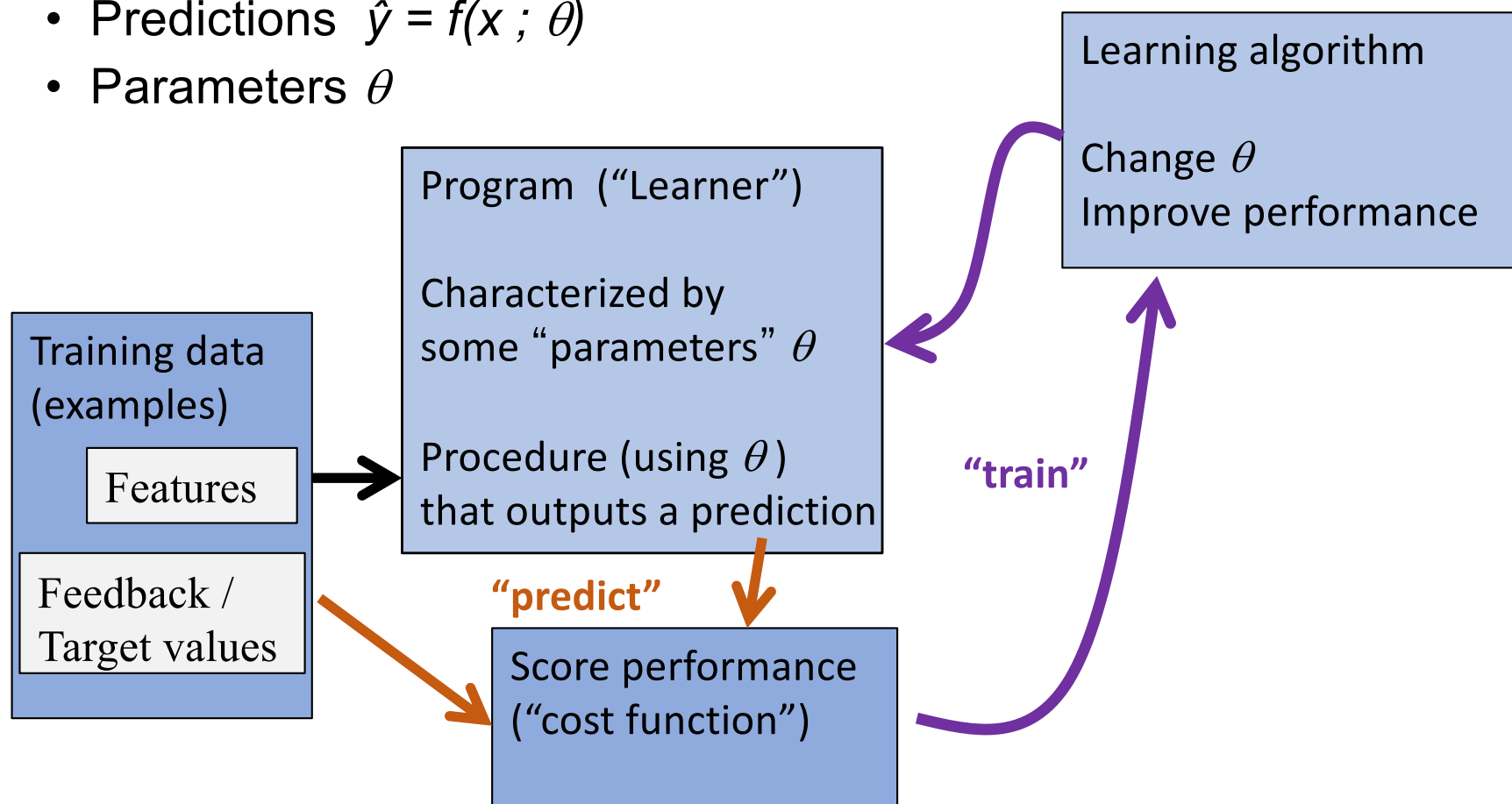
Multi-Class Classification

Regularization for Linear Classifiers

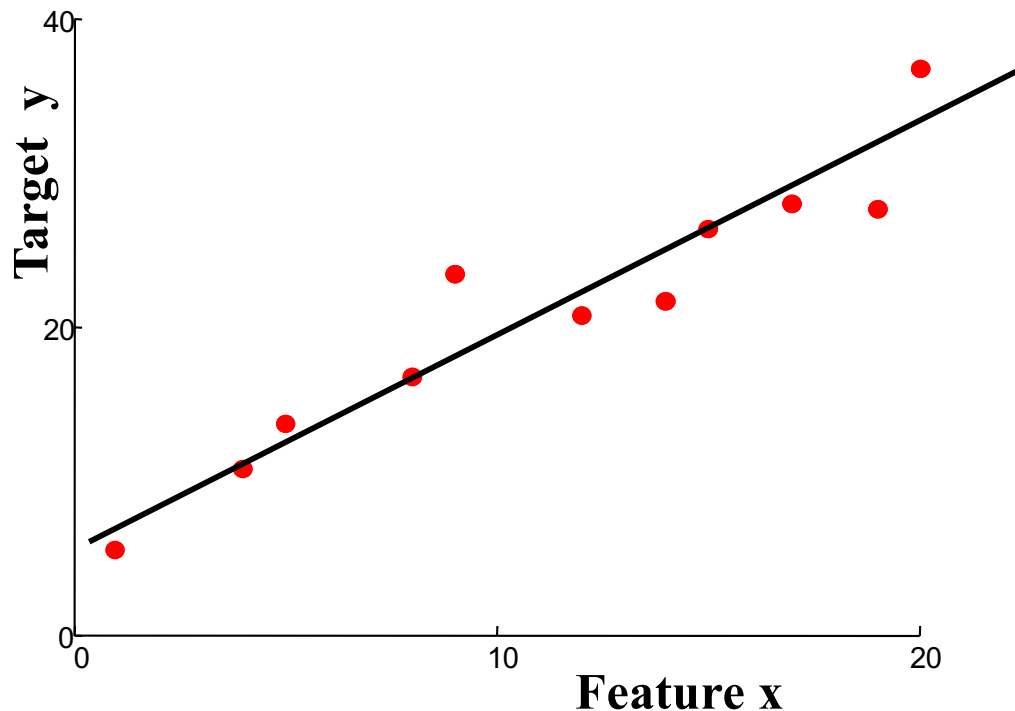
Supervised Learning

- Notation

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



Linear Regression



“Predictor”:

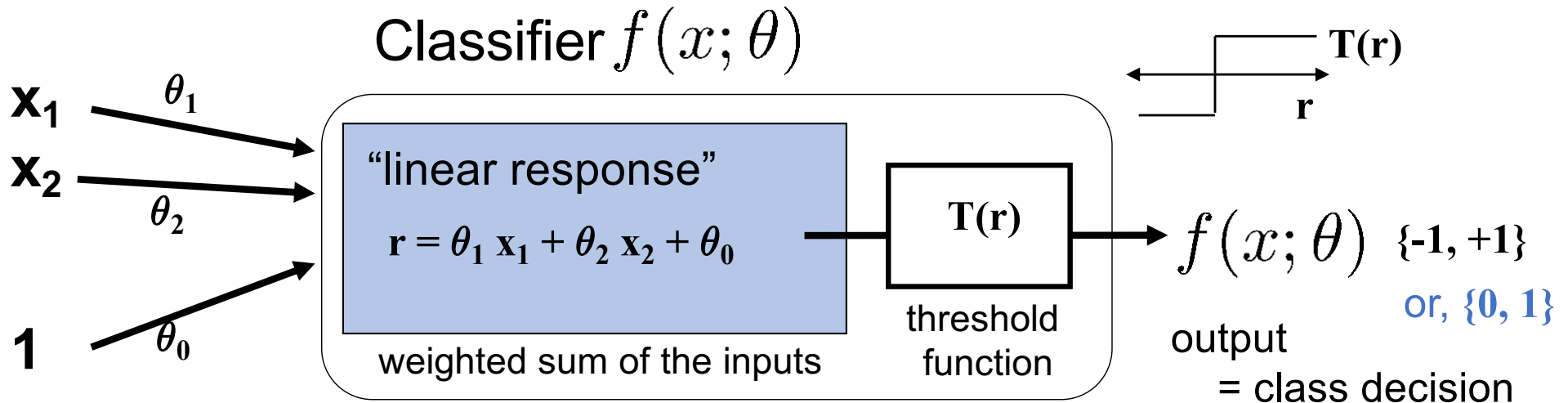
Evaluate line:

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

return r

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

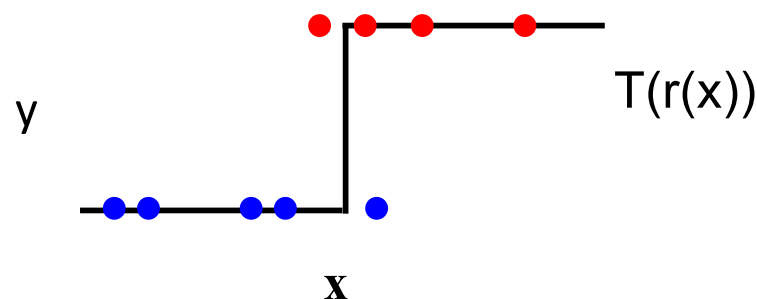
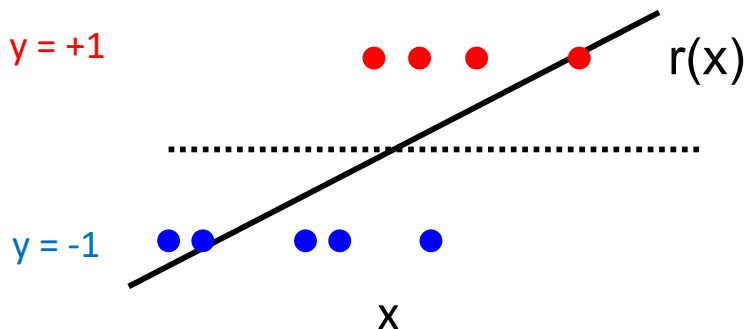
Perceptron Classifier (2 Features)



```

r = X @ theta.T           # compute linear response
Yhat = 1*(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”:



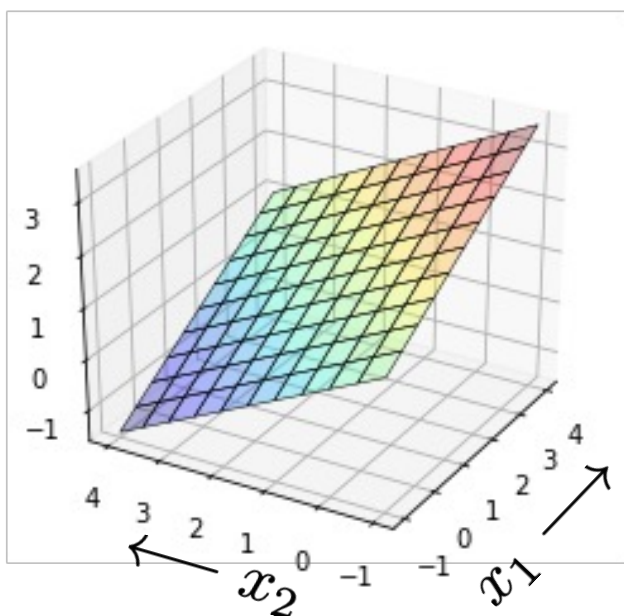
Perceptrons

- 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:
 1. A weighted sum of the input features (“linear response”)
 2. The sum is then thresholded by the $T(\cdot)$ function (“decision”)
- Perceptron: a simple artificial model of human neurons
 - weights = “synapses”
 - threshold = “neuron firing”

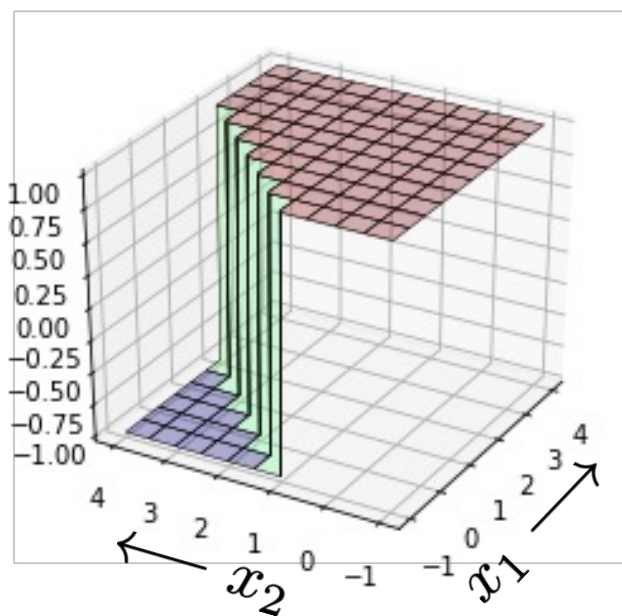
Perceptron Decision Boundary

- The perceptron is defined by the decision algorithm:

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



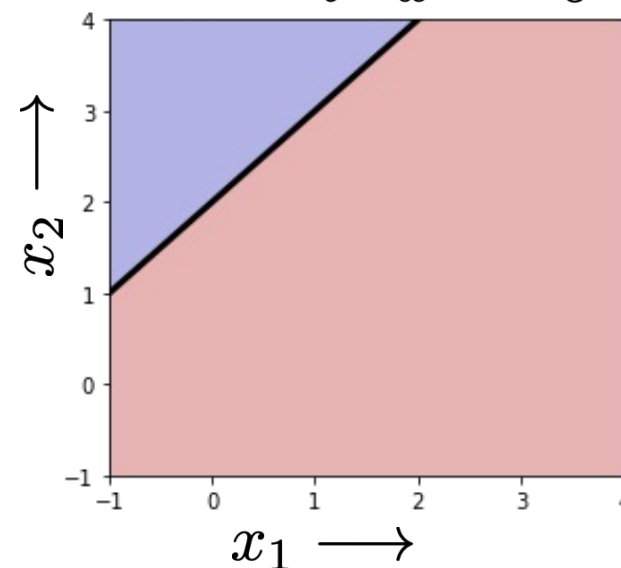
Linear response $r(x)$



Decision $f(x) = T(r(x))$

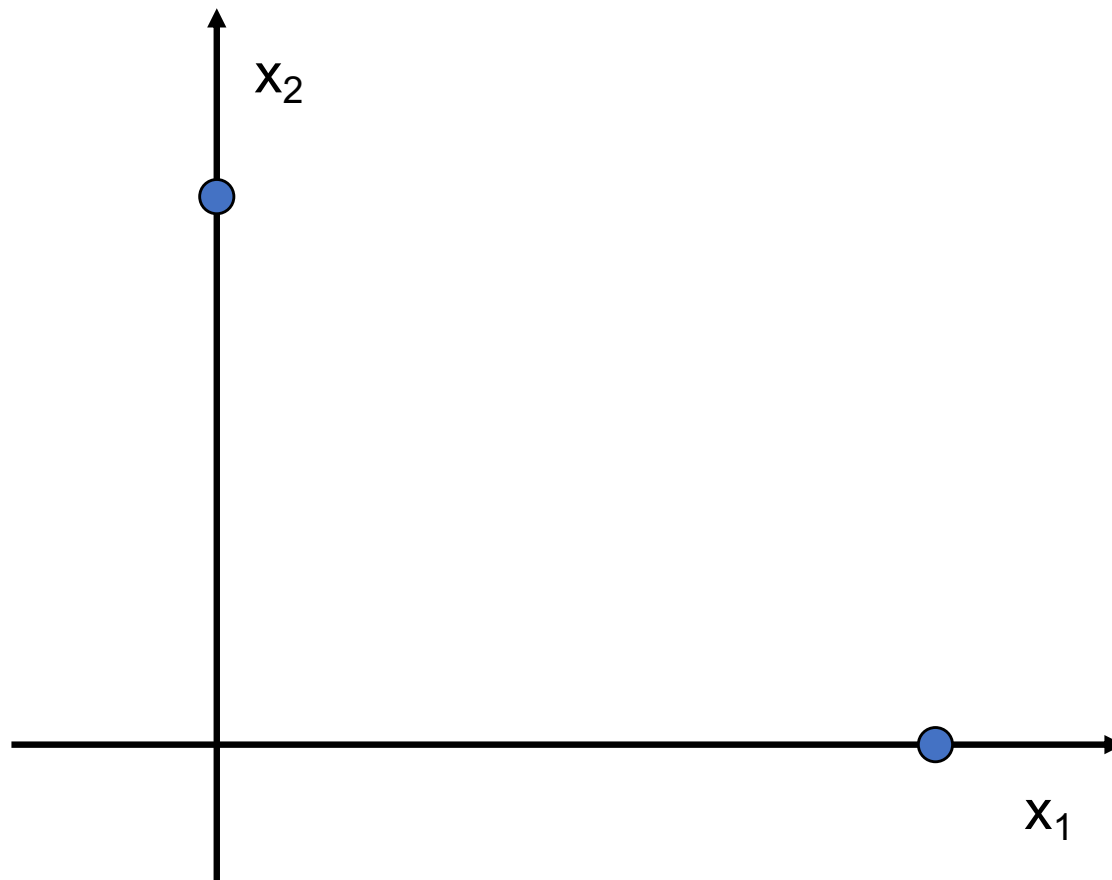
Decision boundary:

$$\theta \cdot x^T = 0$$



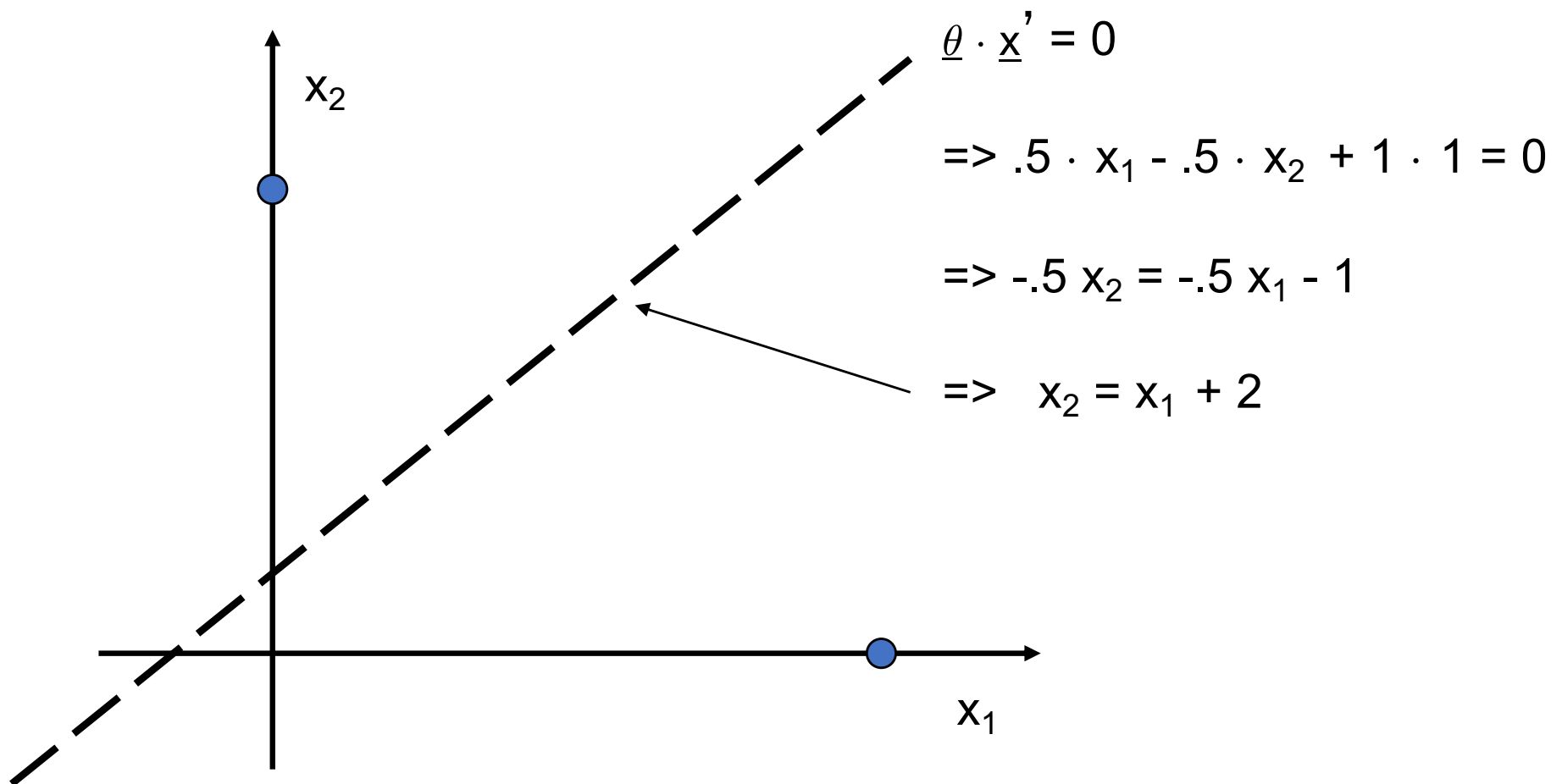
Example, Linear Decision Boundary

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



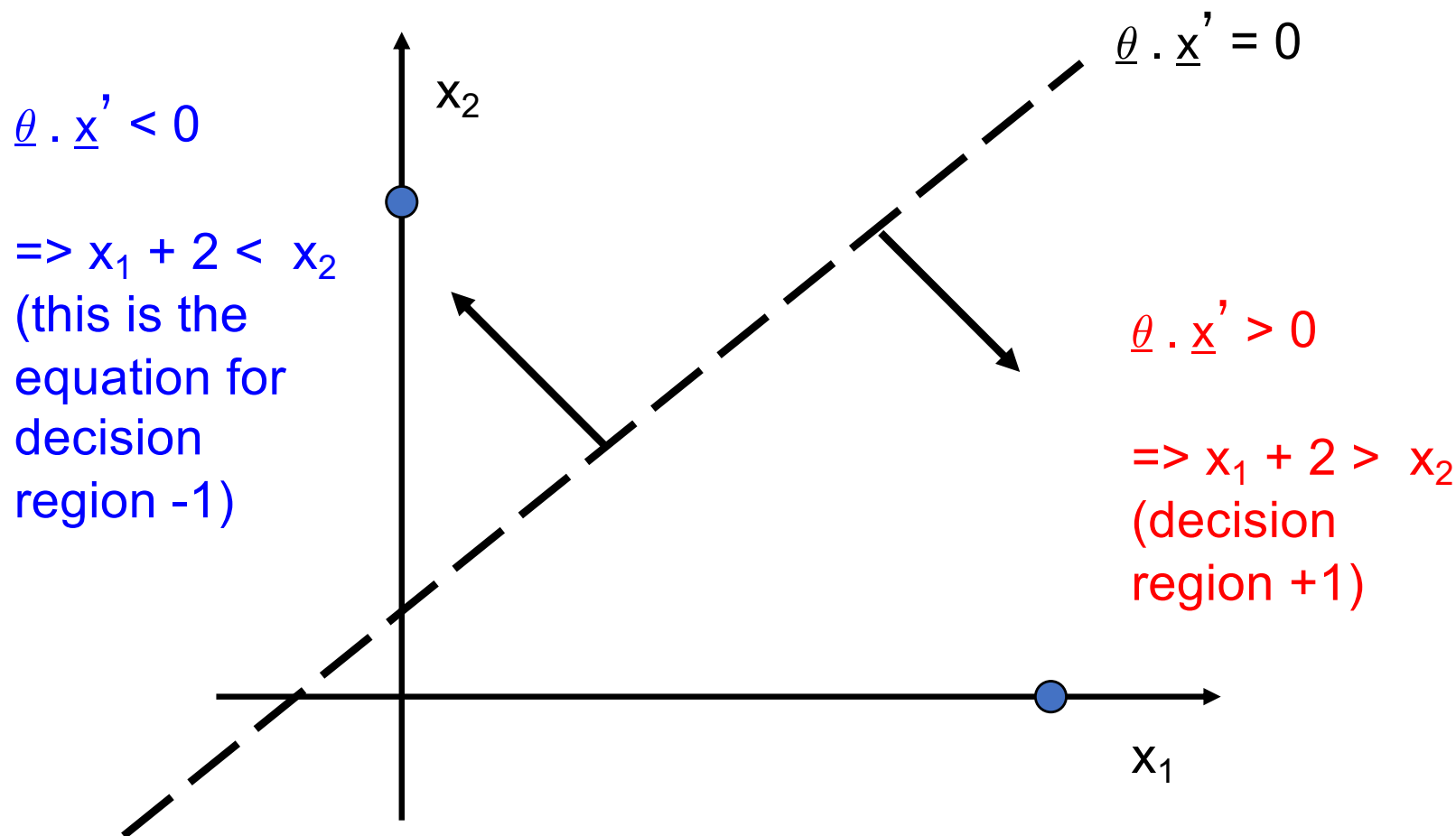
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Example, Linear Decision Boundary

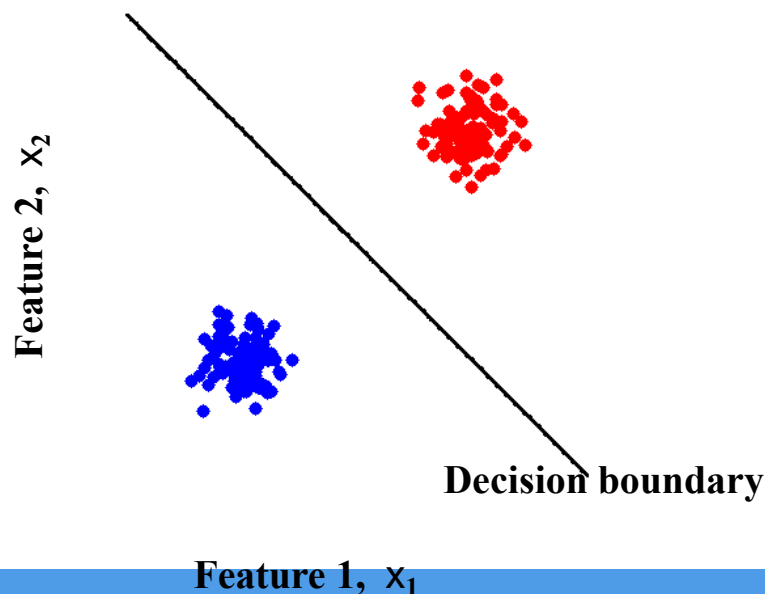
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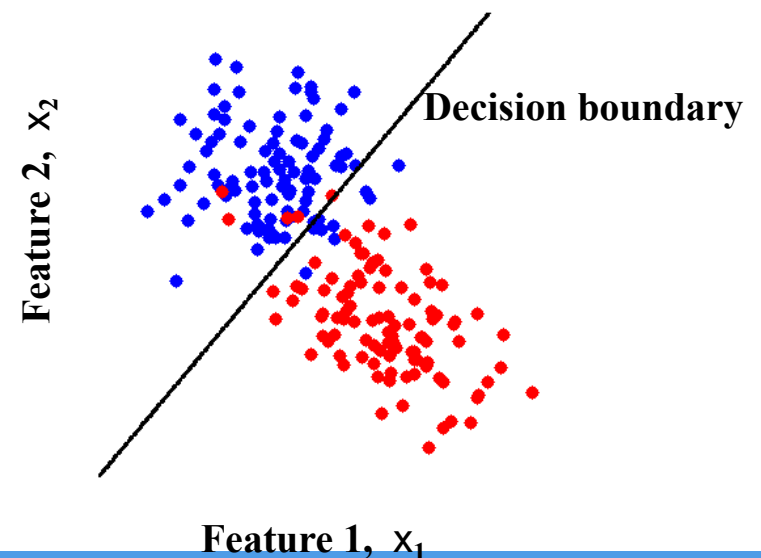
Separability

- 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 hyperplane in feature space
 - in 2 dimensions the decision boundary is a straight line

Linearly separable data

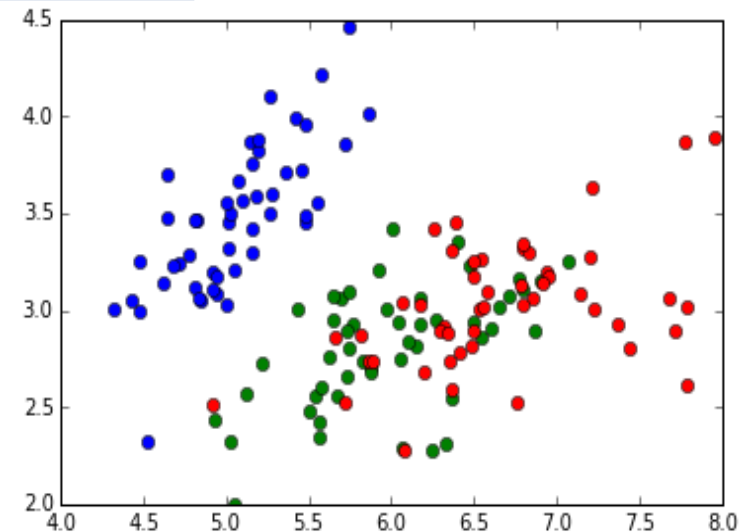


Linearly non-

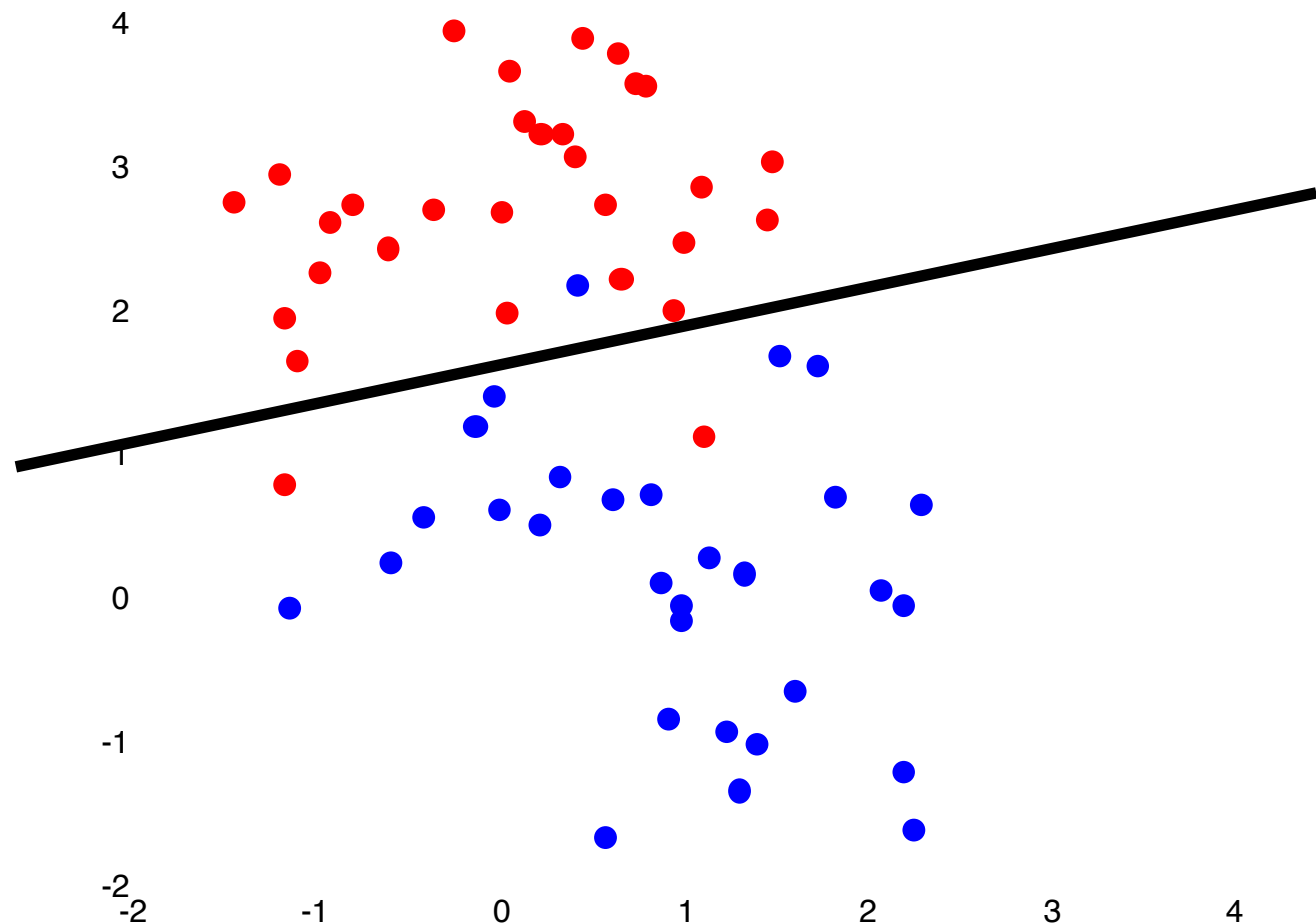


Class overlap

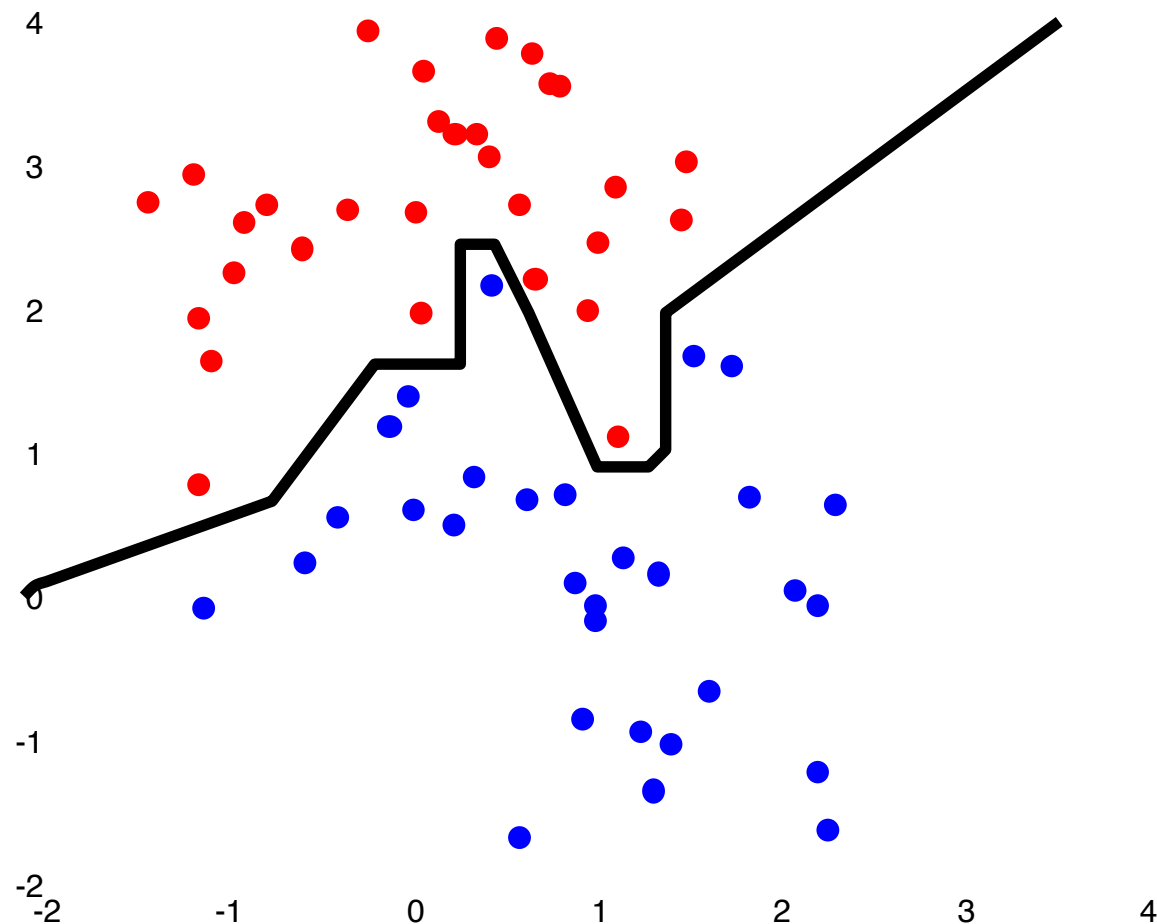
- Classes may not be well-separated
- Same observation values possible under both classes
 - High vs low risk; features {age, income}
 - Benign/malignant cells look similar
 - ...
- Common in practice
- May not be able to perfectly distinguish between classes
 - Maybe with more features?
 - Maybe with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



Another example



Non-linear decision boundary

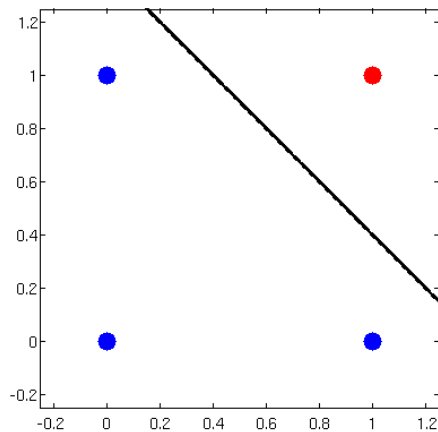


Representational Power of Perceptrons

- 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)

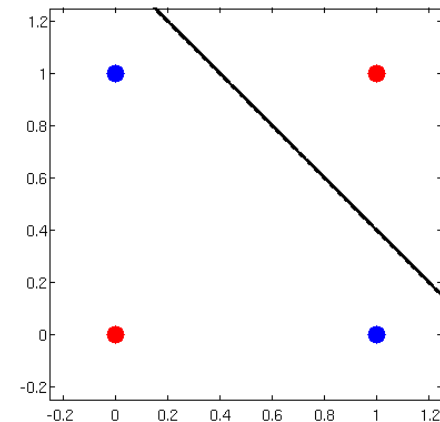
“AND”

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



“XOR”

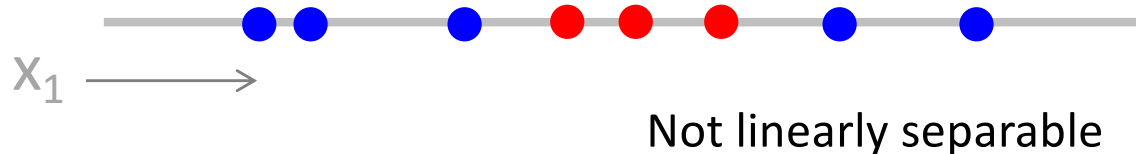
x_1	x_2	y
0	0	1
0	1	-1
1	0	-1
1	1	1



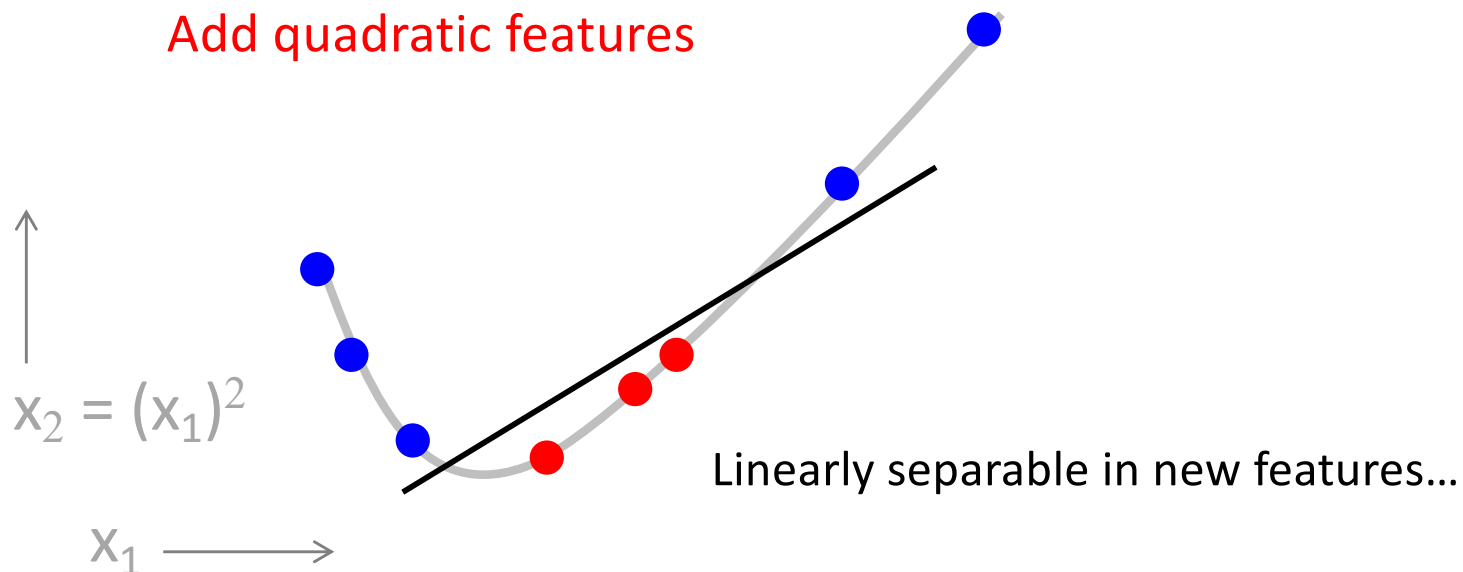
Adding features

- Linear classifier can't learn some functions

1D example:



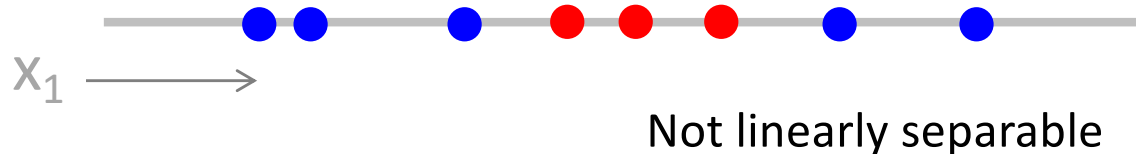
Add quadratic features



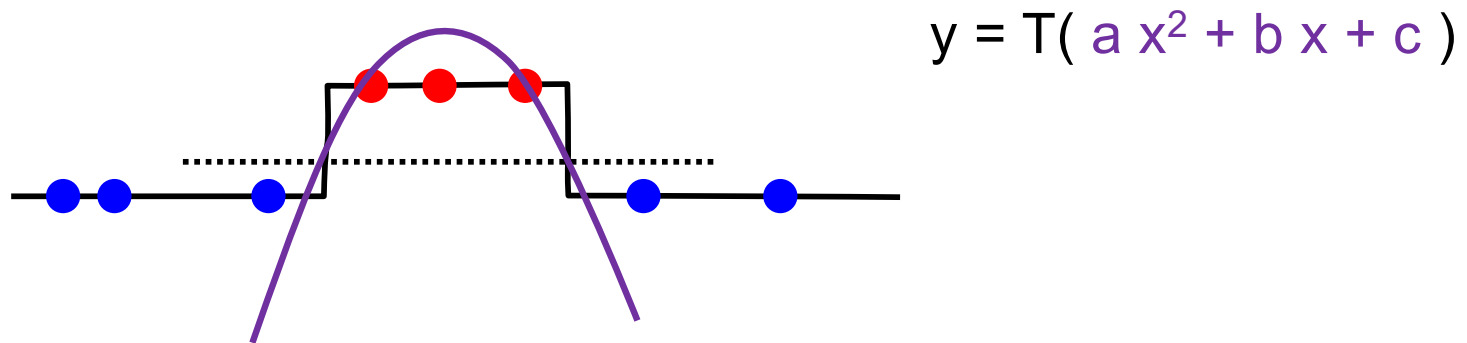
Adding features

- Linear classifier can't learn some functions

1D example:



Quadratic features, visualized in original feature space:



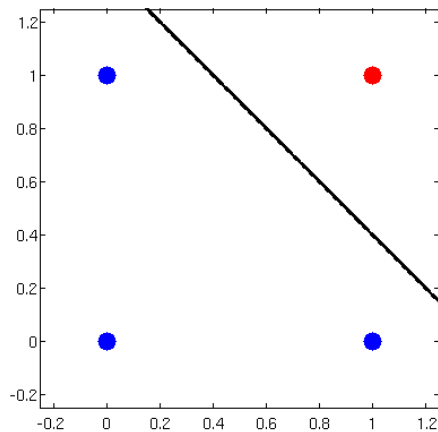
More complex decision boundary: $ax^2+bx+c = 0$

Representational Power of Perceptrons

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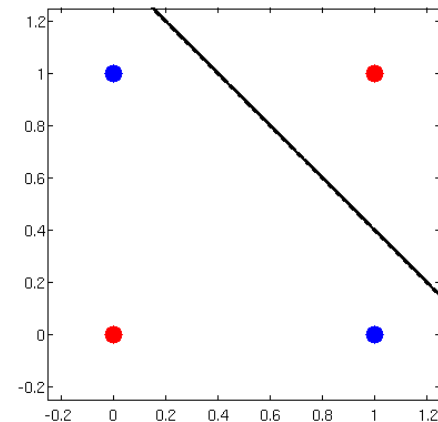
“AND”

x_1	x_2	y
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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



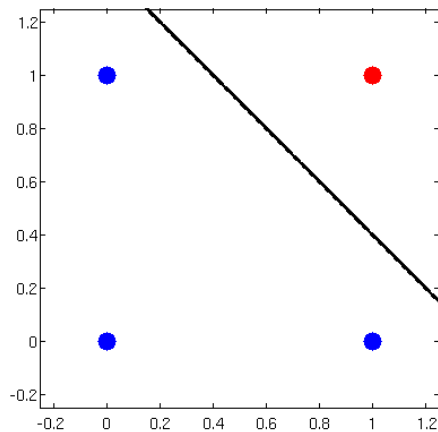
What kinds of functions could we use to learn the data on the right?

Representational Power of Perceptrons

- What mappings can a perceptron represent perfectly?
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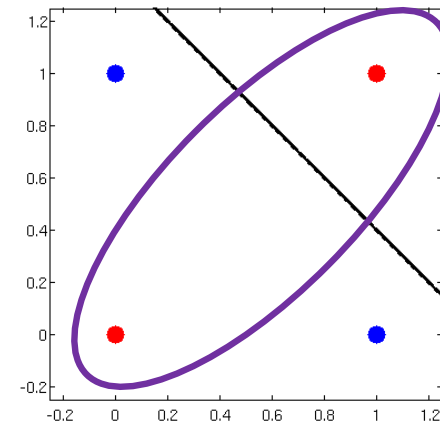
“AND”

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 could we use to learn the data on the right?

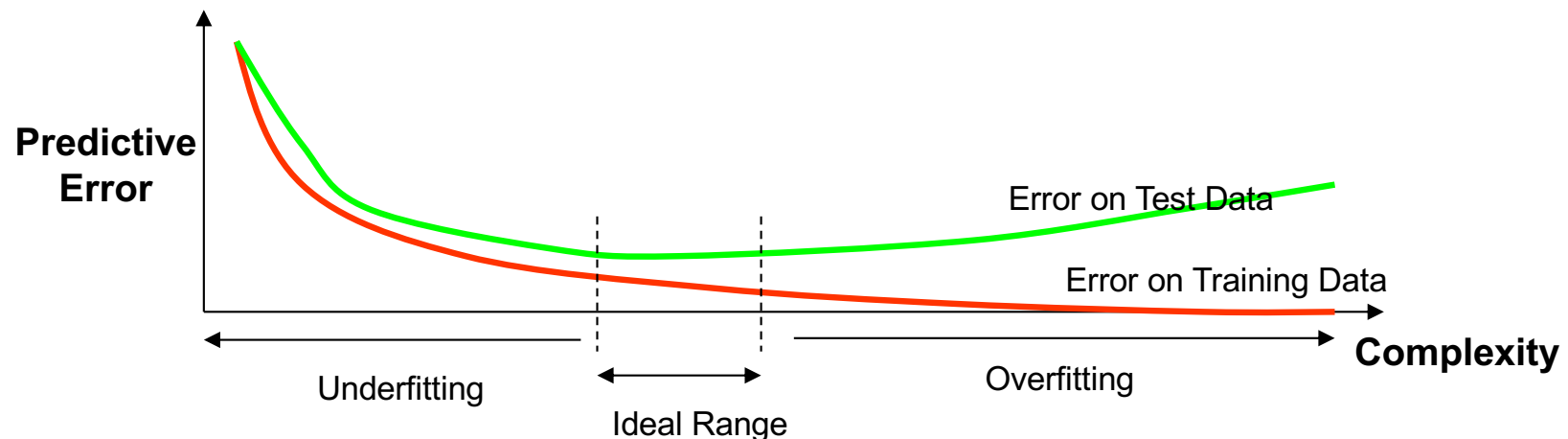
Ellipsoidal decision boundary: $a x_1^2 + b x_1 + c x_2^2 + d x_2 + e x_1 x_2 + f = 0$

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

Linear Classifiers

Linear Classification with Perceptrons

Perceptron Learning

Gradient-Based Classifier Learning

Multi-Class Classification

Regularization for Linear Classifiers

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

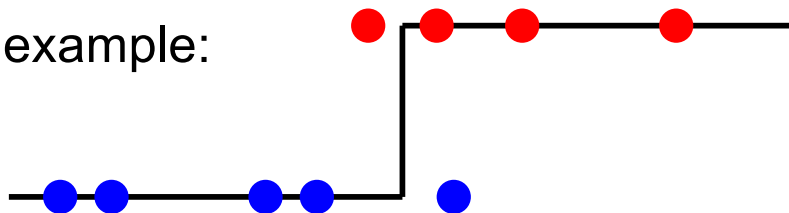
- How should we measure error?
 - Natural measure = “fraction we get wrong” (error rate)

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

```
Yhat = np.sign( X @ 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

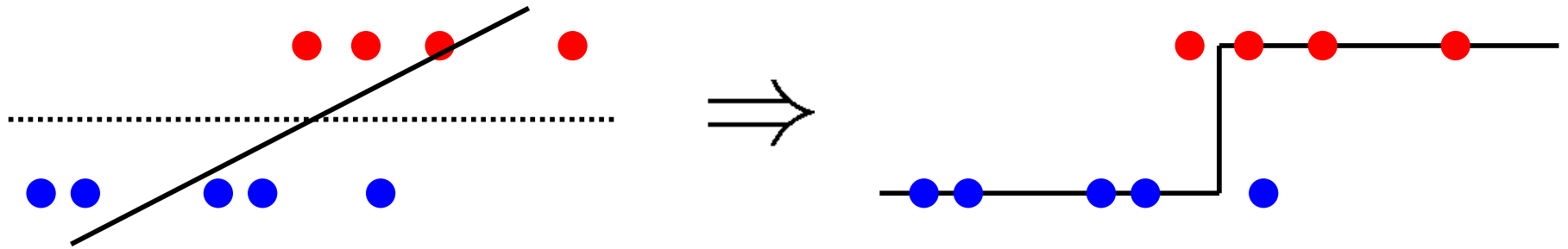
1D example:



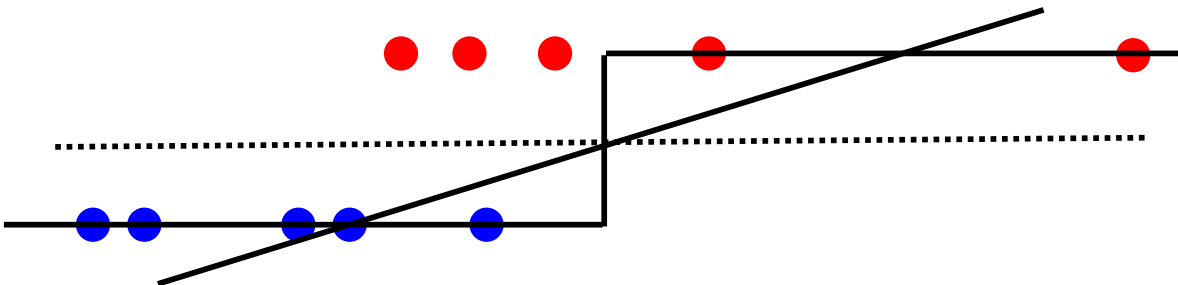
$$\begin{aligned} T(r(x)) &= -1 & \text{if } r(x) < 0 \\ T(r(x)) &= +1 & \text{if } r(x) > 0 \end{aligned}$$

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 $\theta \cdot x^{(j)}$:
 - (1) For correct predictions, $y^{(j)} - \hat{y}^{(j)} = 0$
 - (2) For incorrect predictions, $y^{(j)} - \hat{y}^{(j)} = \pm 1$

“adaptive” linear regression: correct predictions stop contributing

Perceptron algorithm

- Perceptron algorithm: an SGD-like algorithm

while \neg done:

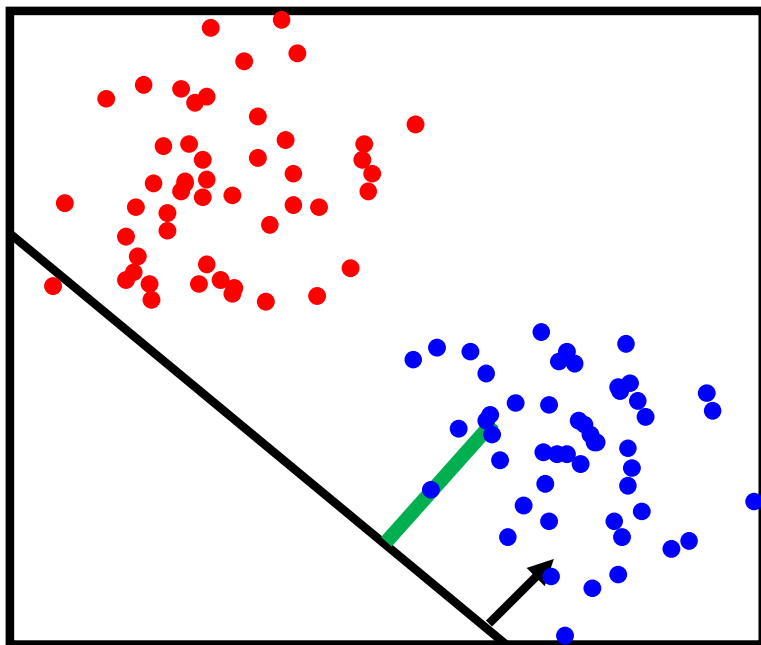
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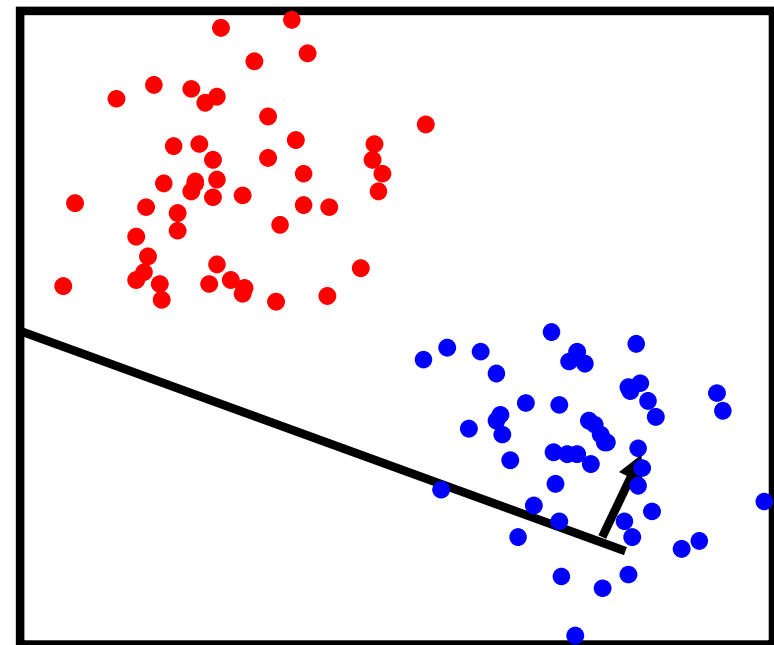
(predict output for point j)

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

(“gradient-like” step)



$y(j)$
predicted
incorrectly:
update
weights



Perceptron algorithm

- Perceptron algorithm: an SGD-like algorithm

while \neg done:

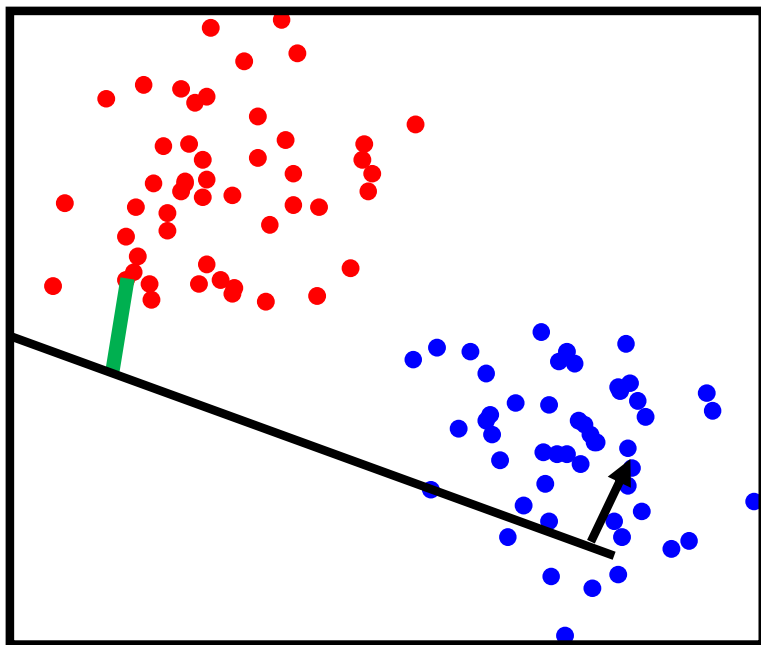
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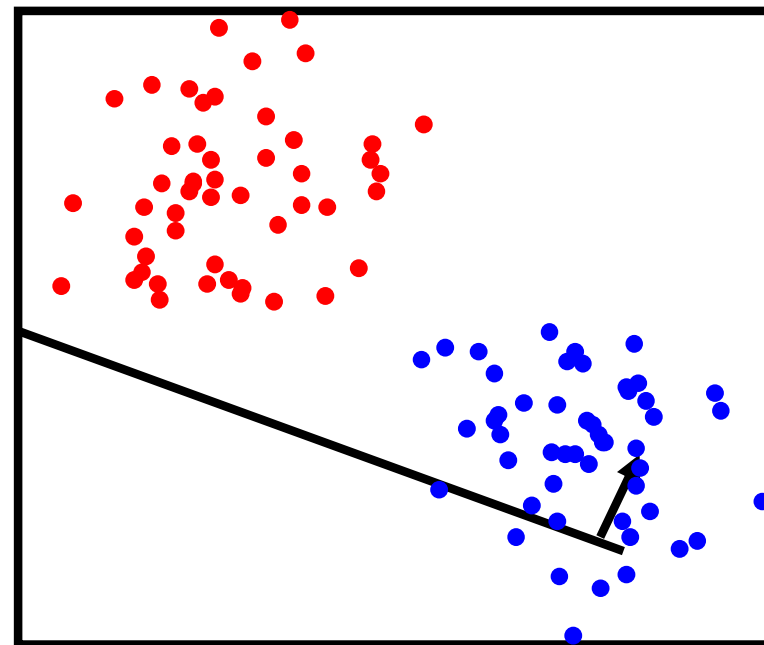
(predict output for point j)

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

(“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 :

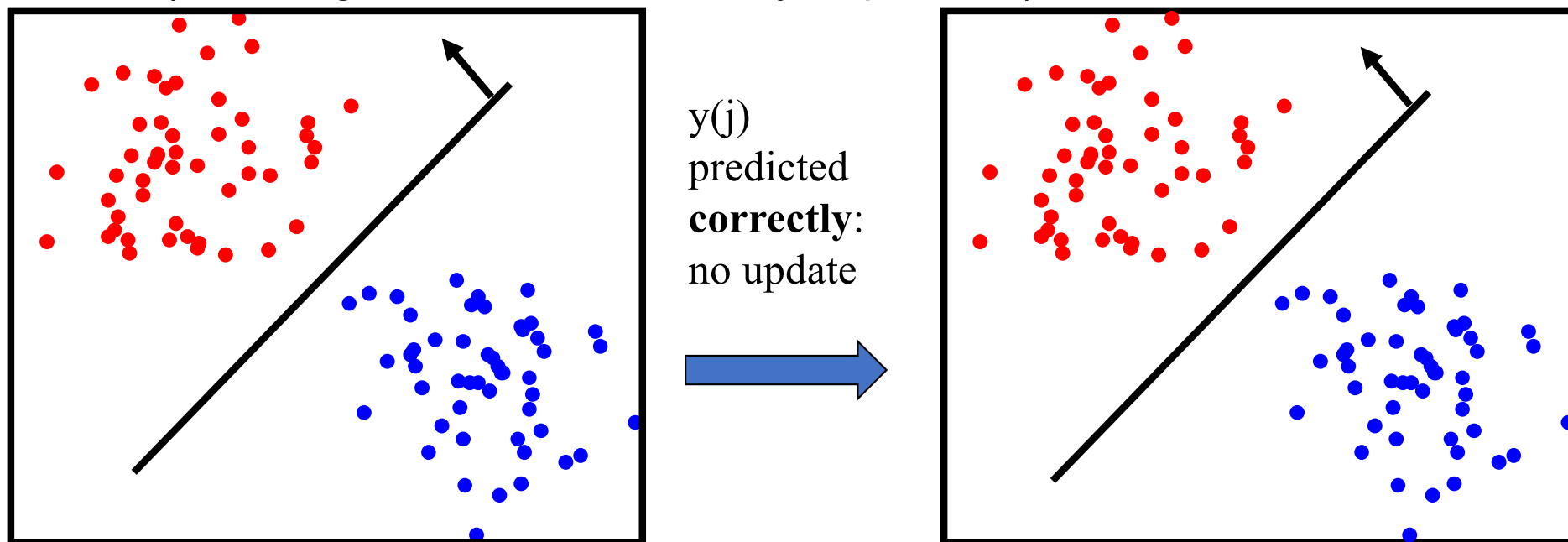
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(predict output for point j)

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

(“gradient-like” step)

(Converges if data are linearly separable)



Perceptron MARK 1 Computer



Frank Rosenblatt, late 1950s

Linear Classifiers

Linear Classification with Perceptrons

Perceptron Learning

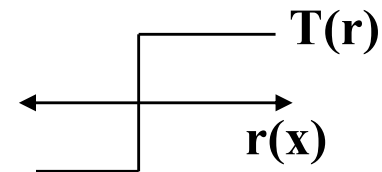
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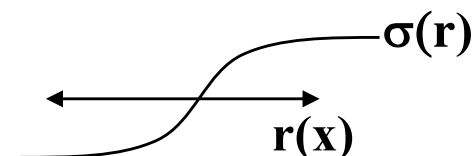
Regularization for Linear Classifiers

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”



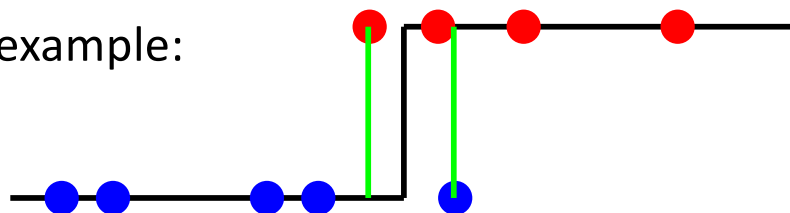
- Now, measure e.g. MSE

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

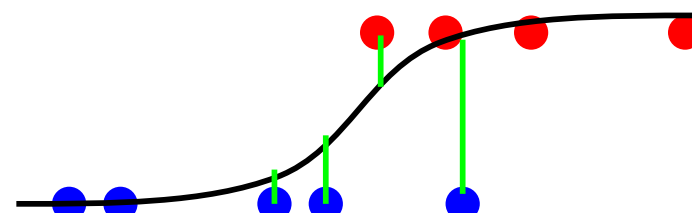
Class $y = \{0, 1\} \dots$

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

1D example:



Classification error = $2/9$



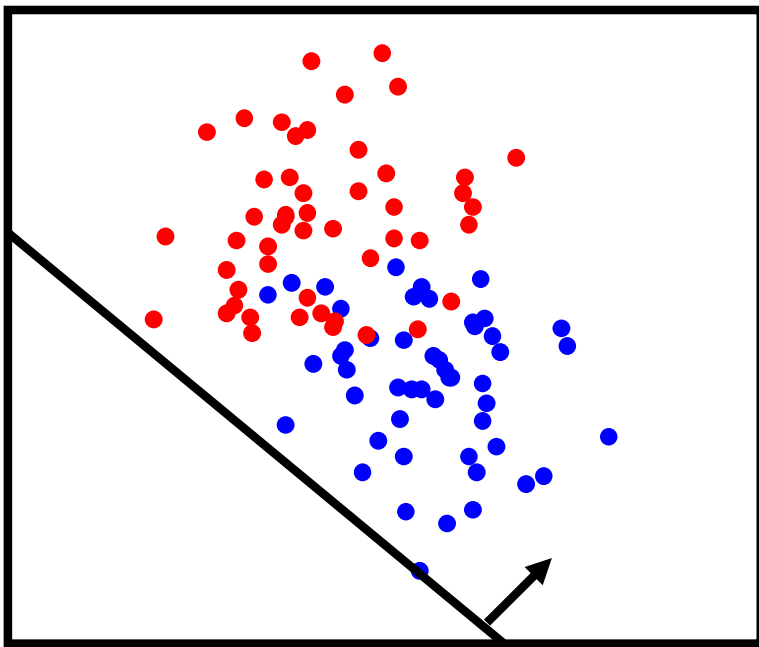
MSE = $(0^2 + .1^2 + .2^2 + .25^2 + .05^2 + \dots)/9$

Training the Classifier

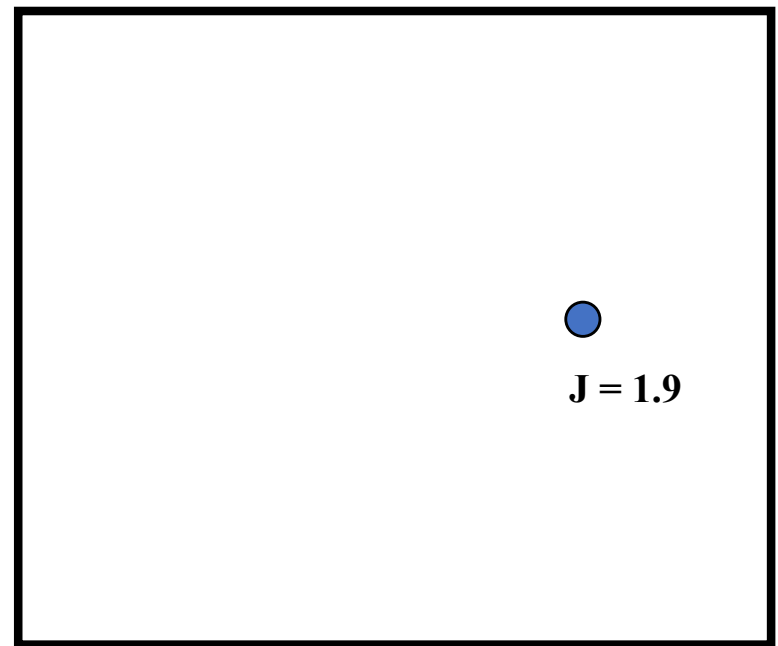
- Once we have a smooth measure of quality, we can find the “best” settings for the parameters of

$$r(x_1, x_2) = a \cdot x_1 + b \cdot x_2 + c$$

- Example: 2D feature space



parameter space

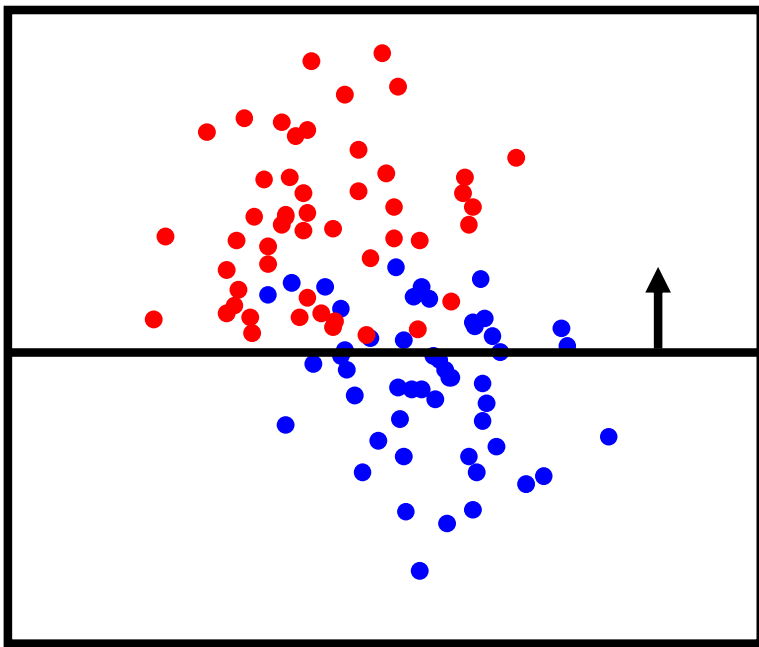


Training the Classifier

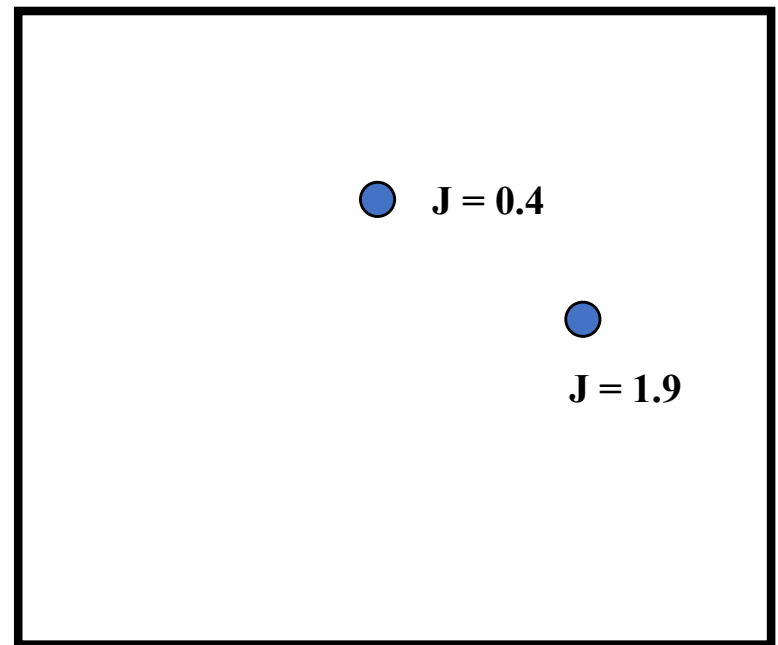
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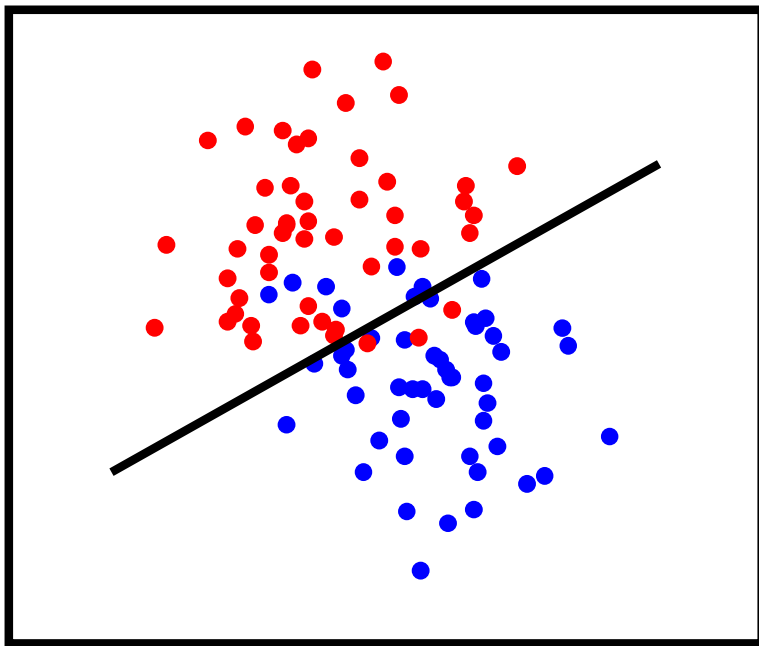


Training the Classifier

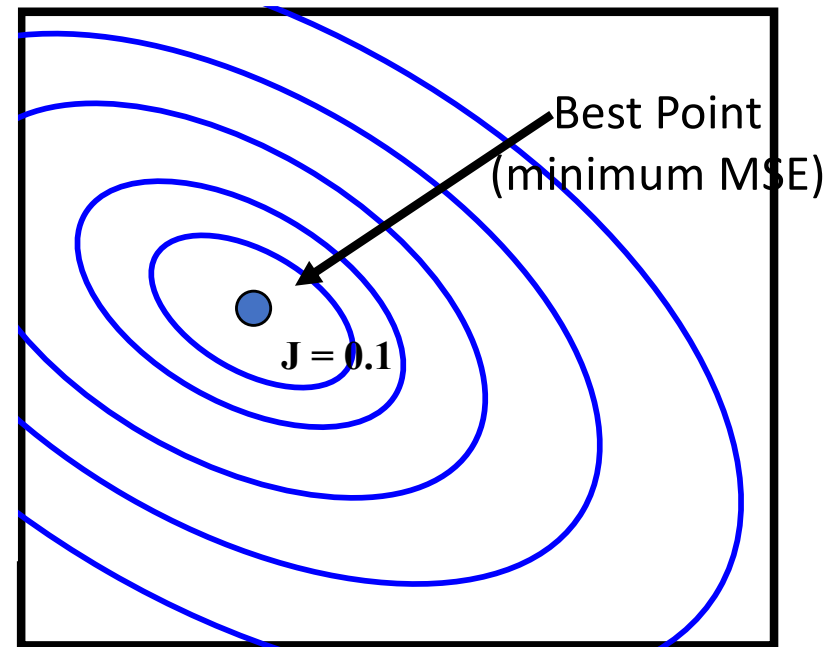
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- Example: 2D feature space



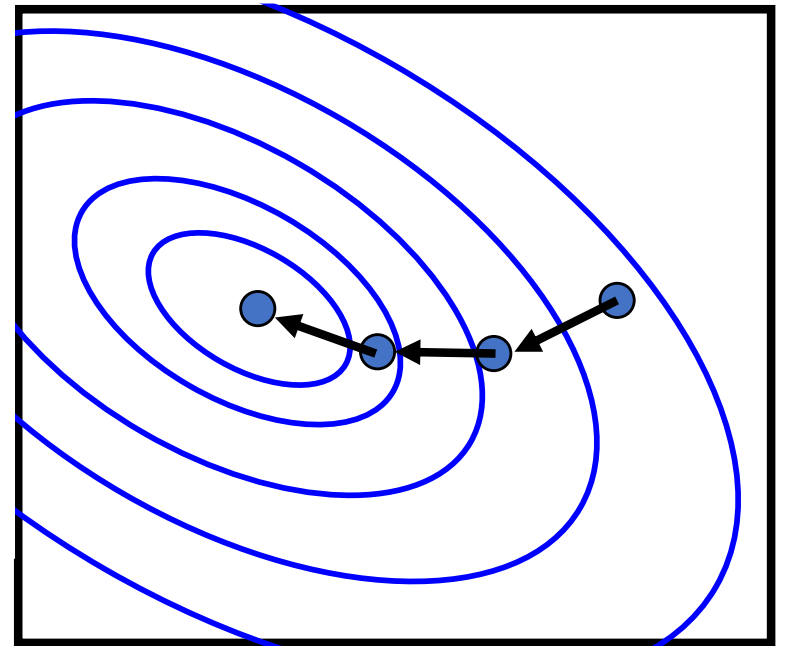
parameter space



Finding the Best MSE

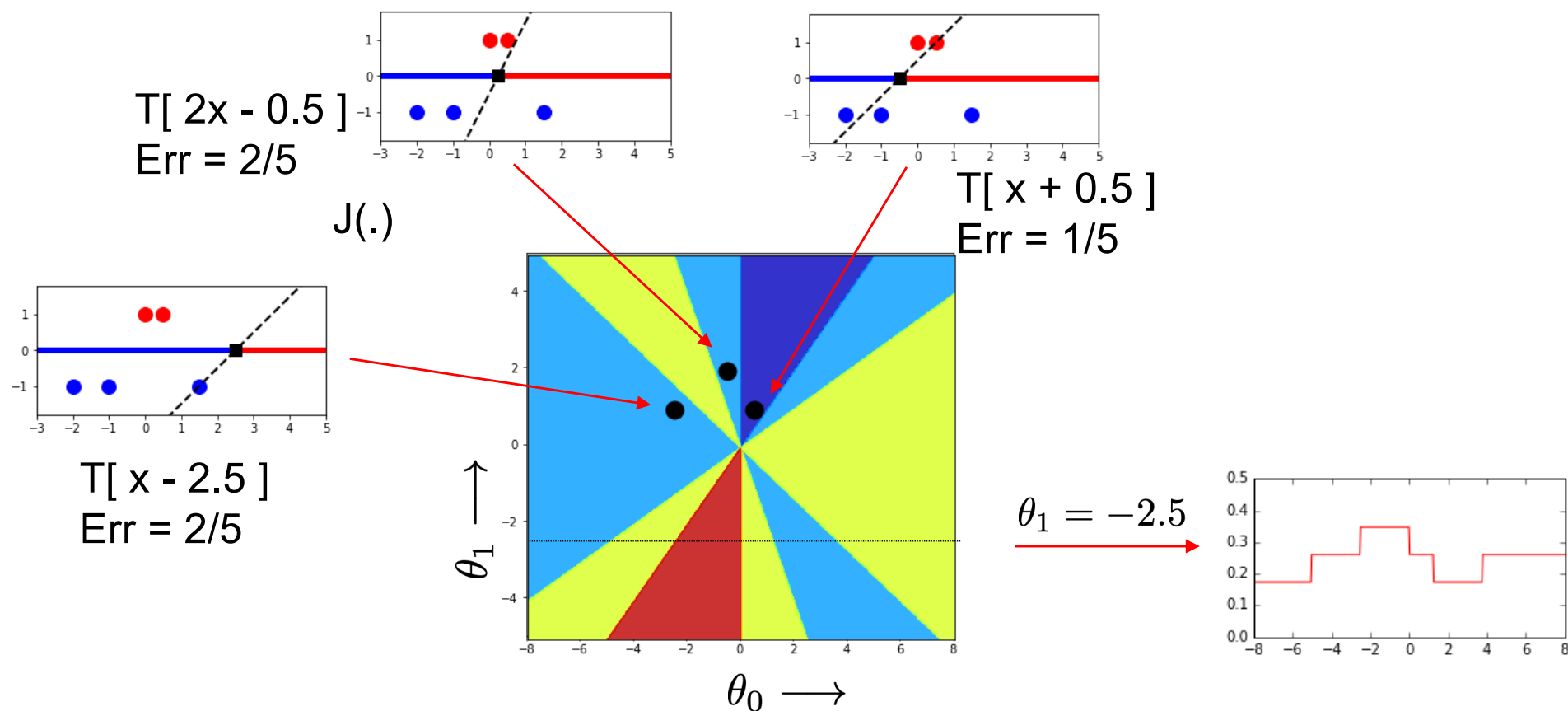
- As in linear regression, this is now just optimization
- Methods:
 - Gradient descent
 - Improve loss by small changes in parameters (“small” = learning rate)
 - Or, substitute your favorite optimization algorithm...
 - Coordinate descent
 - Stochastic search

Gradient Descent



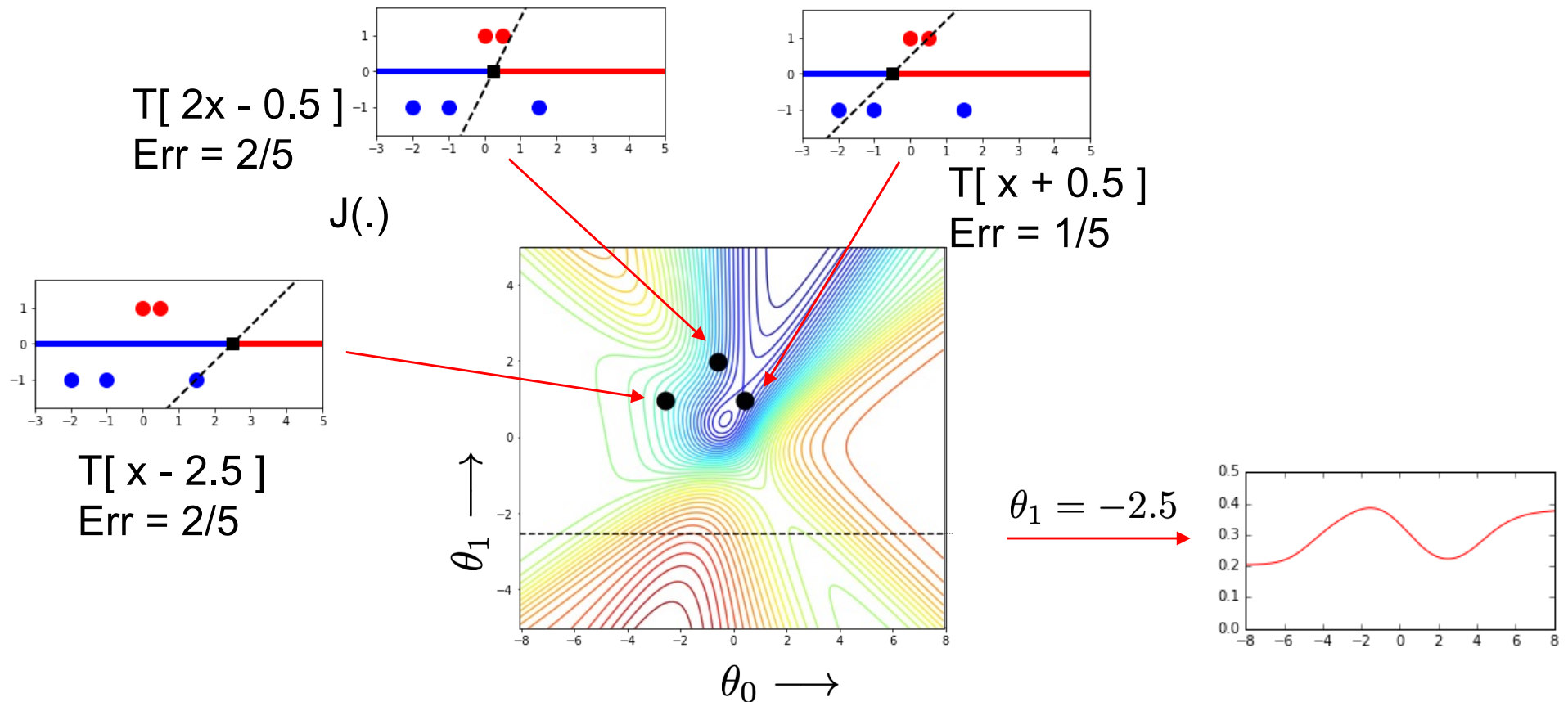
0/1 (Error Rate) Loss Example

- Data set: one feature, 5 data points



Logistic MSE Surrogate

- Smoother version of 0/1 Loss



Gradient Equations

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

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

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

- Recall the chain rule of calculus:

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

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

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

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

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

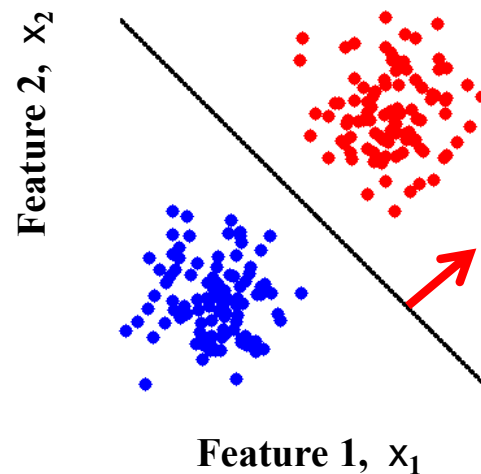
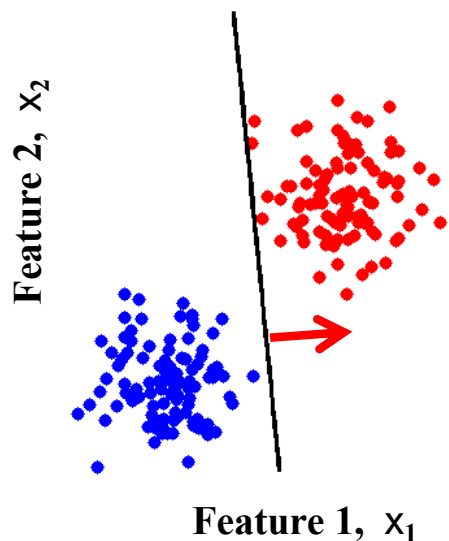
$$\frac{\partial J}{\partial a} = \frac{1}{m} \sum_i 2(\sigma(\theta \cdot x^{(i)}) - y^{(i)}) \partial \sigma(\theta \cdot x^{(i)}) x_1^{(i)}$$

Error between class and prediction

Sensitivity of prediction to changes in parameter "a"

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...

Saturating Functions

- Many possible “saturating” functions

- “Logistic” sigmoid (scaled for range [0,1]) is

$$\sigma(z) = 1 / (1 + \exp(-z))$$

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

- 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 $\frac{1}{2}$)

- 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

- Interpret $\sigma(\underline{\theta} x^T)$ 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:

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

Logistic regression

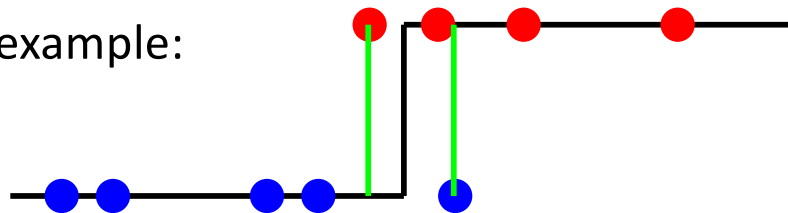
- Interpret $\sigma(\underline{\theta} \cdot \mathbf{x}^T)$ as a probability that $y = 1$
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 - If $y = 1$, cost is $-\log \Pr[y=1] = -\log \sigma(\underline{\theta} \cdot \mathbf{x}^T)$
 - If $y = 0$, cost is $-\log \Pr[y=0] = -\log (1 - \sigma(\underline{\theta} \cdot \mathbf{x}^T))$

- Can write this succinctly:

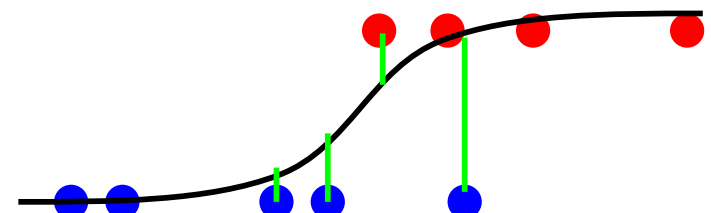
$$J(\underline{\theta}) = -\frac{1}{m} \left(\sum_i y^{(i)} \log \sigma(\underline{\theta} \cdot \mathbf{x}^{(i)}) + (1 - y^{(i)}) \log (1 - \sigma(\underline{\theta} \cdot \mathbf{x}^{(i)})) \right)$$

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

1D example:



Classification error = 2/9



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

Gradient Equations

- Logistic neg-log likelihood loss:

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

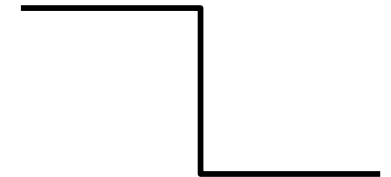
- What's the derivative with respect to one of the parameters?

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

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

Surrogate loss functions

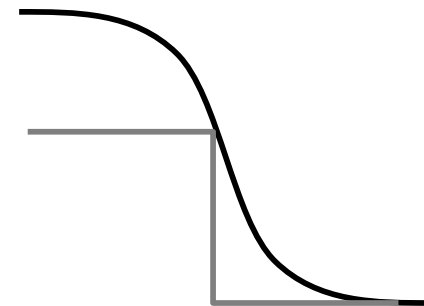
- Replace 0/1 loss $\Delta_i(\theta) = \mathbb{1}[T(\theta x^{(i)}) \neq y^{(i)}]$ with something easier:



0 / 1 Loss

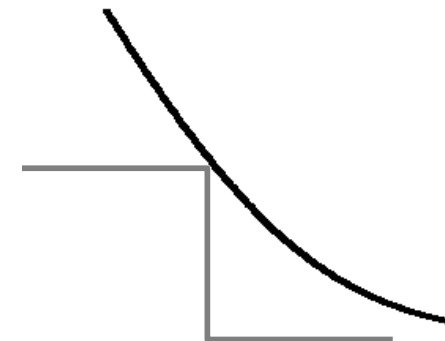
- Logistic MSE

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



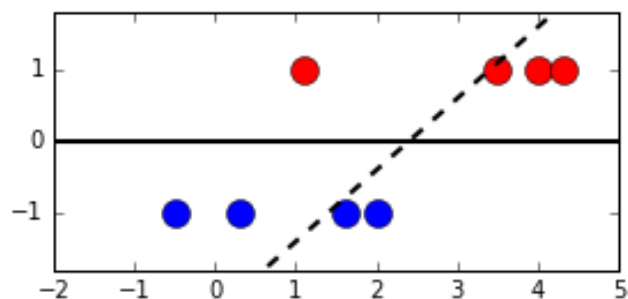
- Logistic Neg Log Likelihood

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

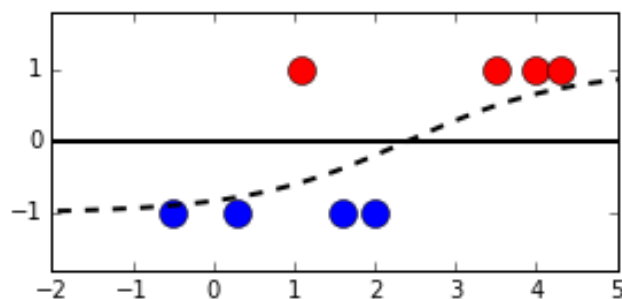


Surrogate loss functions

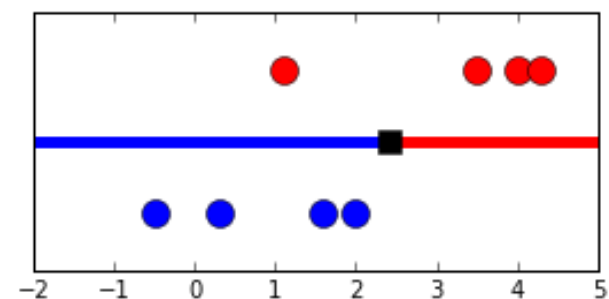
$$\theta = [-2.4, 1.0]$$



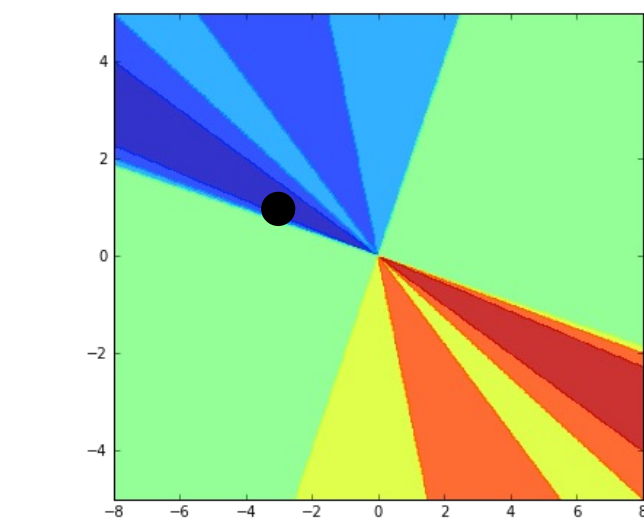
Linear response: $r(x)$



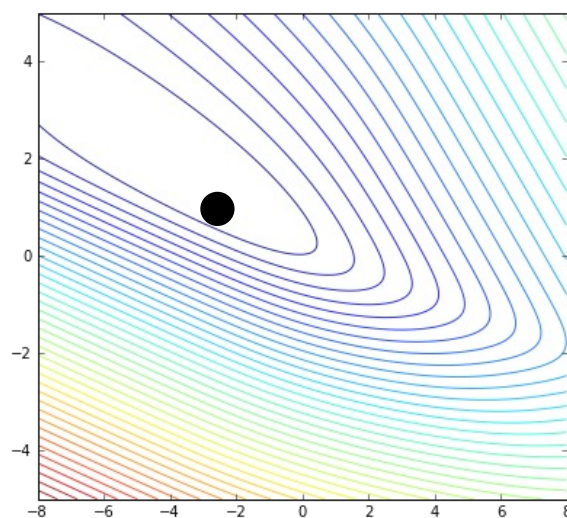
Saturating response: $\rho(r(x))$



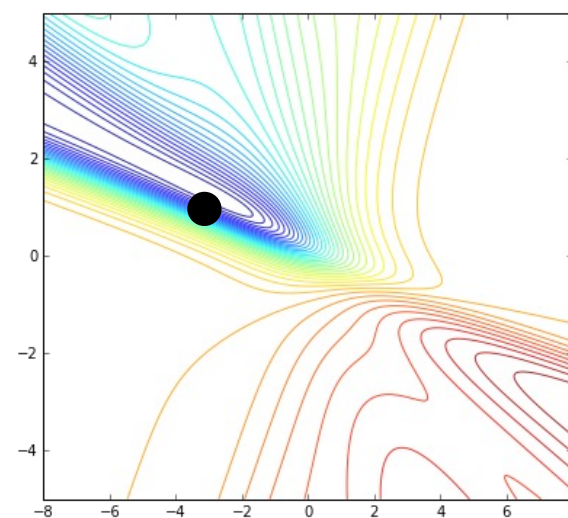
Decision function: $T(r(x))$



$J(\theta)$
0/1 Loss



Logistic NLL



Logistic MSE

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

Linear Classifiers

Linear Classification with Perceptrons

Perceptron Learning

Gradient-Based Classifier Learning

Multi-Class Classification

Regularization for Linear Classifiers

Multi-class linear models

- What about multiple classes? One option:

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

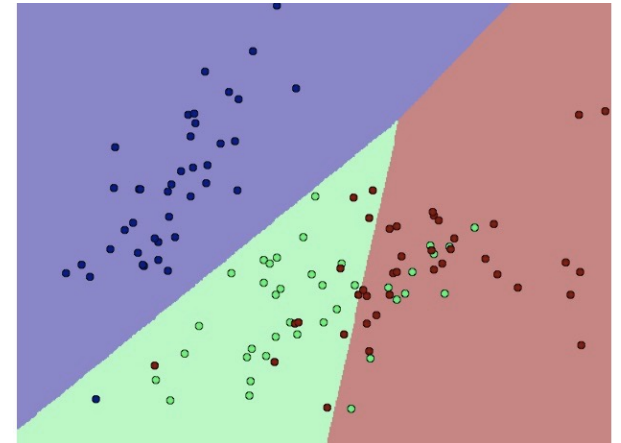
$$f(x; \theta) = \arg \max_c \theta_c \cdot x^T$$

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

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

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

- 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 \neg done:

for each data point j :

$f^{(j)} = \arg \max_c (\theta_c \cdot x^{(j)})$ Predict output for data point j

$\theta_{f^{(j)}} \leftarrow \theta_{f^{(j)}} - \alpha x^{(j)}$ Decrease response of class f on data $x^{(j)}$

$\theta_{y^{(j)}} \leftarrow \theta_{y^{(j)}} + \alpha x^{(j)}$ Increase response of class y on data $x^{(j)}$

If prediction “ f ” matches true class “ y ”, no update

Otherwise, makes it more likely that “ y ” will have the largest response next time

Multilogit regression

- Define the probability of each class:

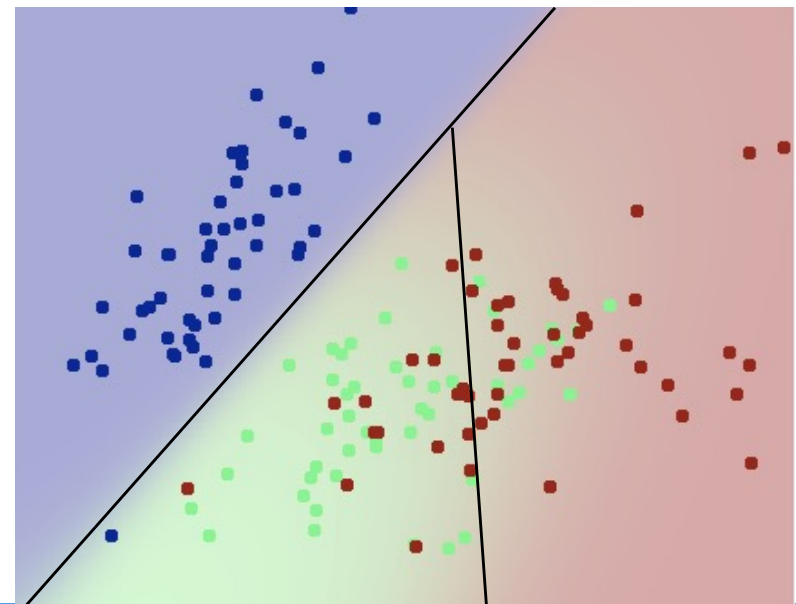
$$p(Y = y|X = x) = \frac{\exp(\theta_y \cdot x^T)}{\sum_c \exp(\theta_c \cdot x^T)}$$

(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



Linear Classifiers

Linear Classification with Perceptrons

Perceptron Learning

Gradient-Based Classifier Learning

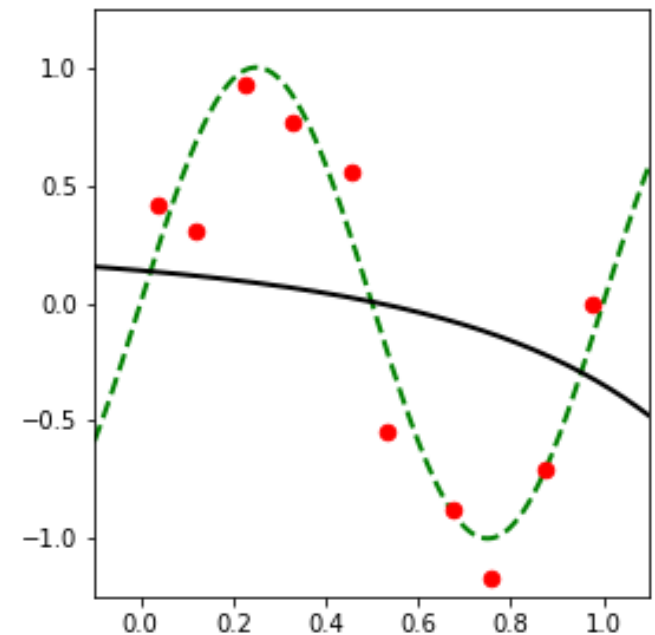
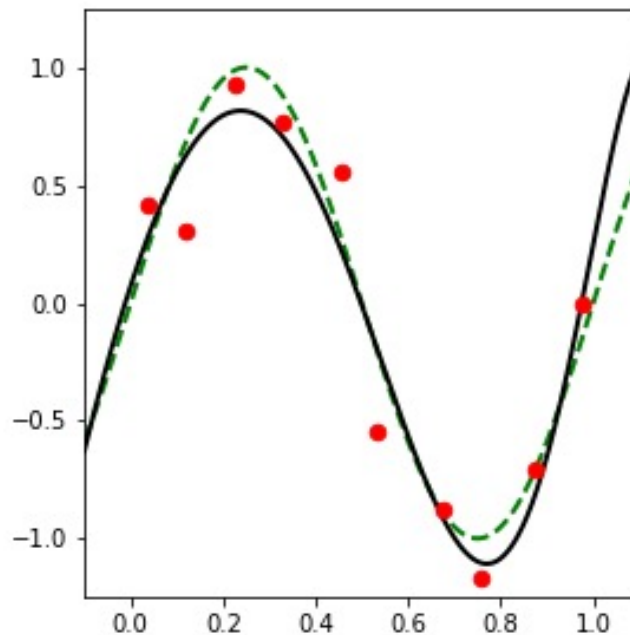
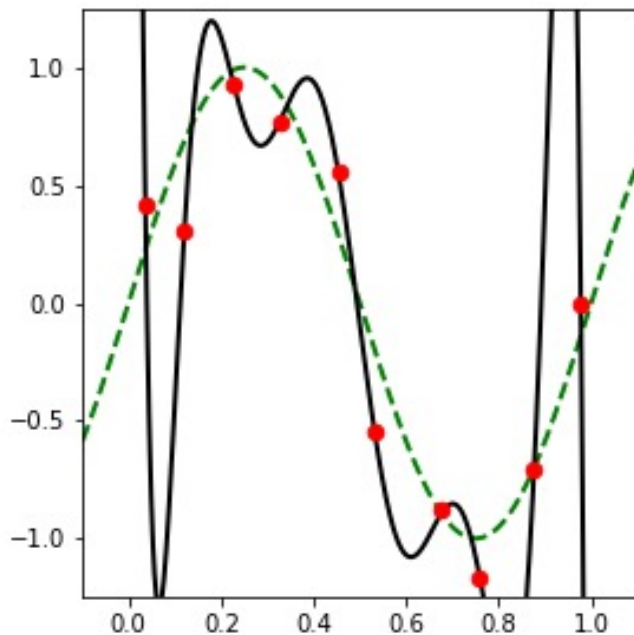
Multi-Class Classification

Regularization for Linear Classifiers

Regularization

- Reminder: Regularization for linear regression
 - Encourage models with small parameter values
 - Can reduce overfitting (by reducing variance)

Degree-9 polynomial fit



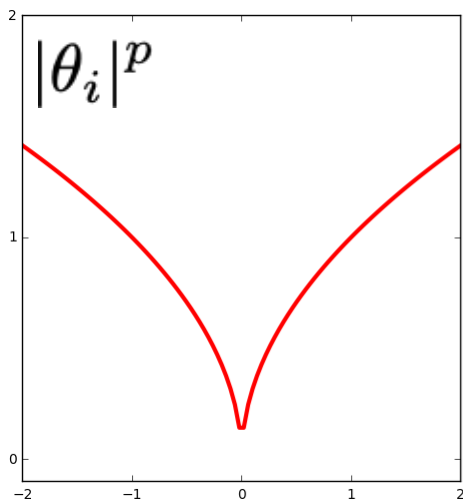
Regularized logistic regression

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

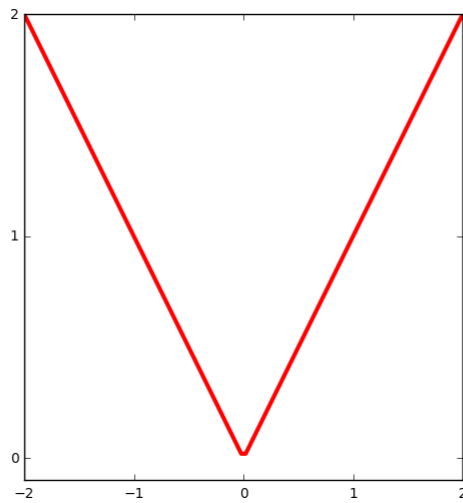
$$J(\underline{\theta}) = -\frac{1}{m} \left(\sum_i \underbrace{y^{(i)} \log \sigma(\underline{\theta} \cdot \mathbf{x}^{(i)})}_{\text{Nonzero only if } y=1} + \underbrace{(1-y^{(i)}) \log (1 - \sigma(\underline{\theta} \cdot \mathbf{x}^{(i)}))}_{\text{Nonzero only if } y=0} \right) + \alpha \|\underline{\theta}\|_p$$

Different regularization functions

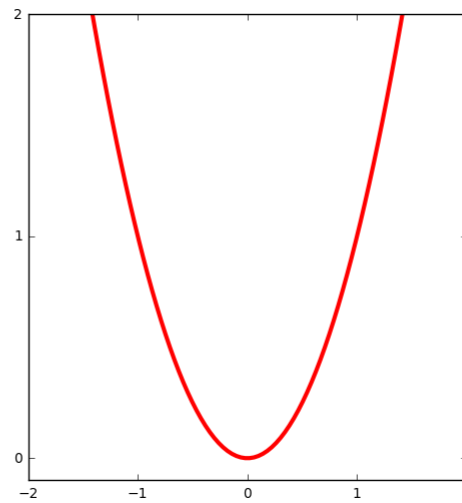
- More generally, for the L_p regularizer: $\left(\sum_i |\theta_i|^p \right)^{\frac{1}{p}}$



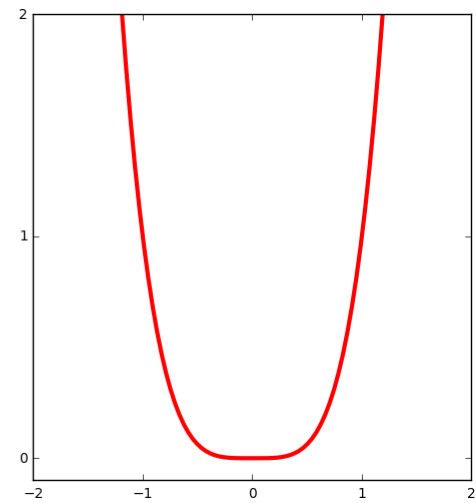
$p=0.5$



$p=1$



$p=2$



$p=4$



Penalize small non-zero parameters more
Prefer some parameters exactly zero;
a few big parameters are OK

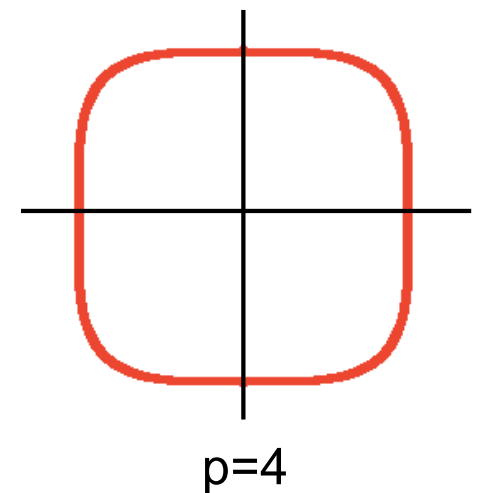
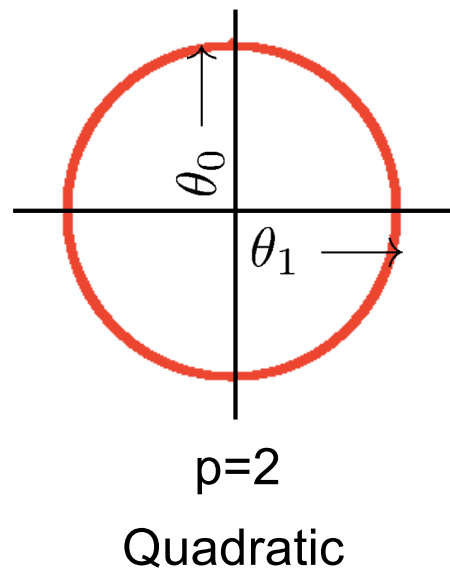
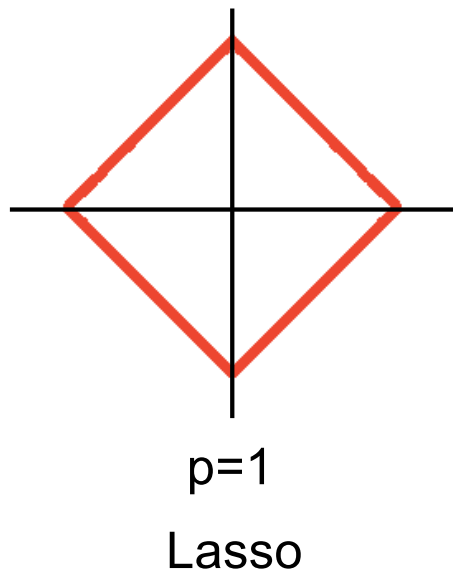
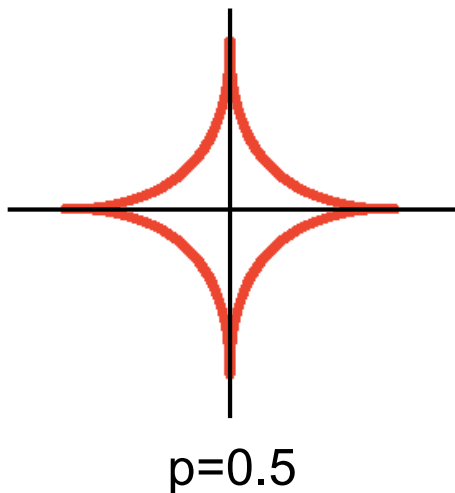


Penalize small non-zero parameters less,
but big parameter values a lot
Prefer lots of small weights, no big weights

Different regularization functions

- More generally, for the L_p regularizer: $\left(\sum_i |\theta_i|^p \right)^{\frac{1}{p}}$

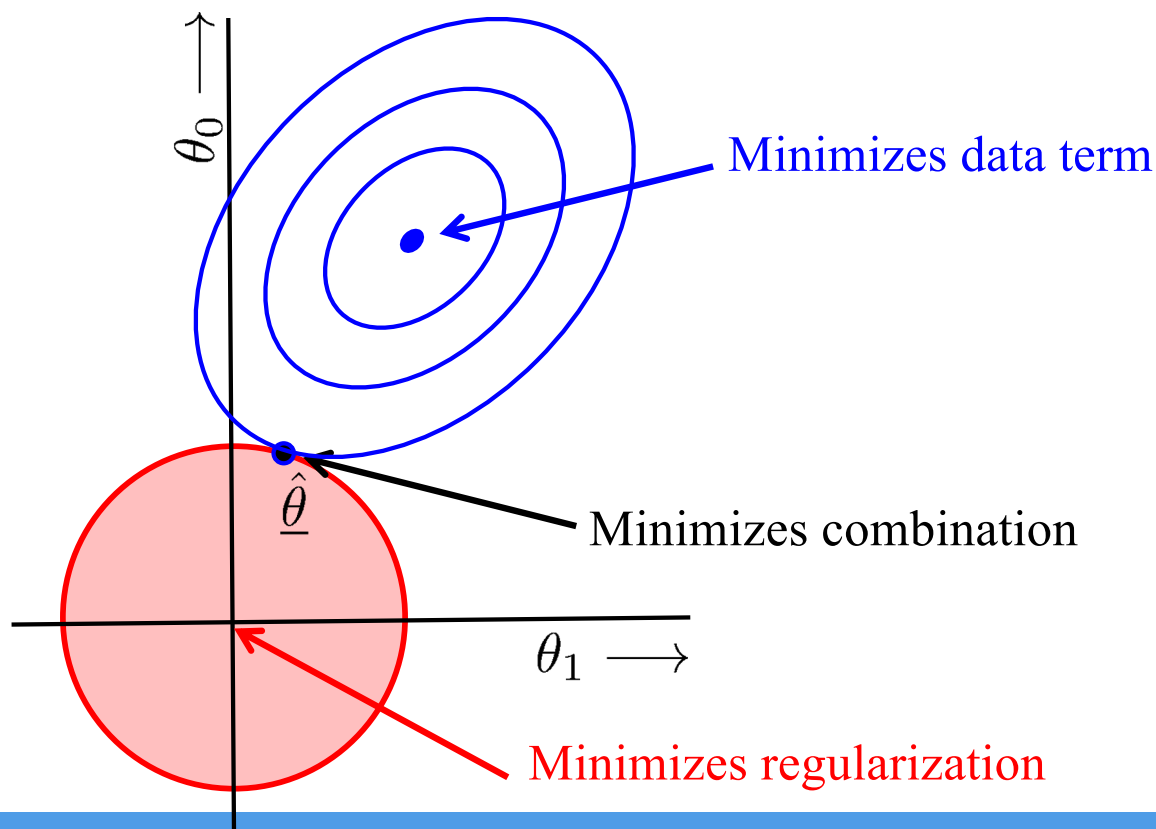
Isosurfaces: $\|\theta\|_p = \text{constant}$



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

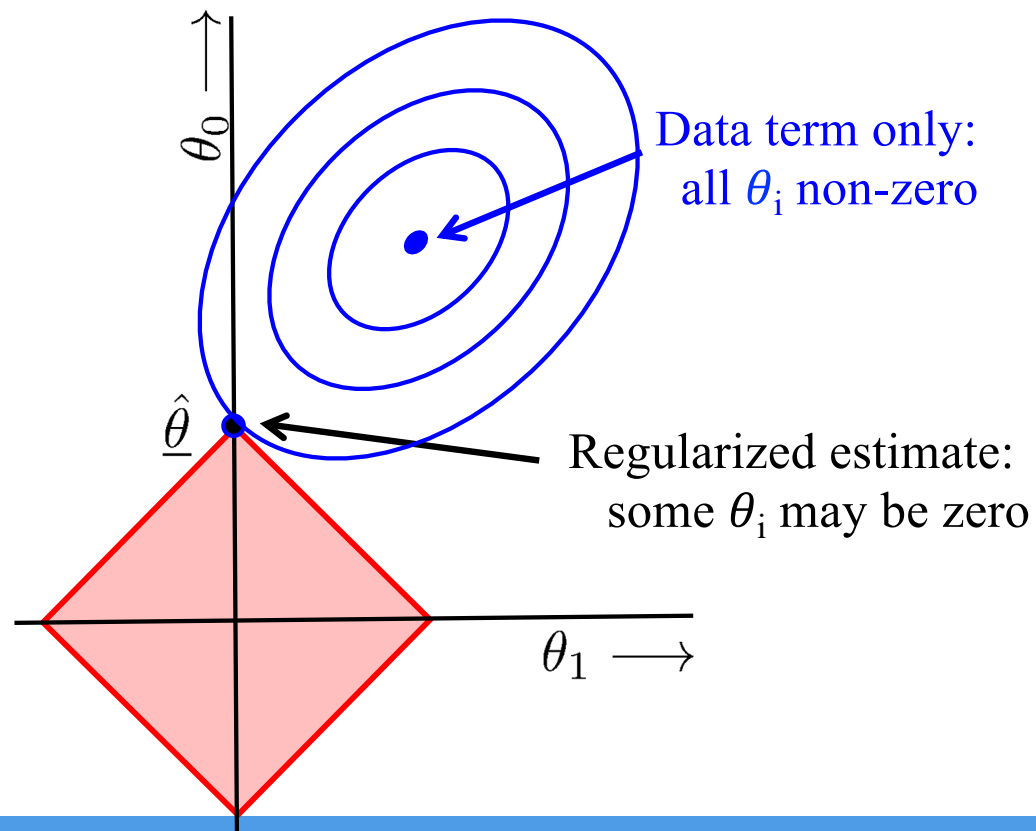
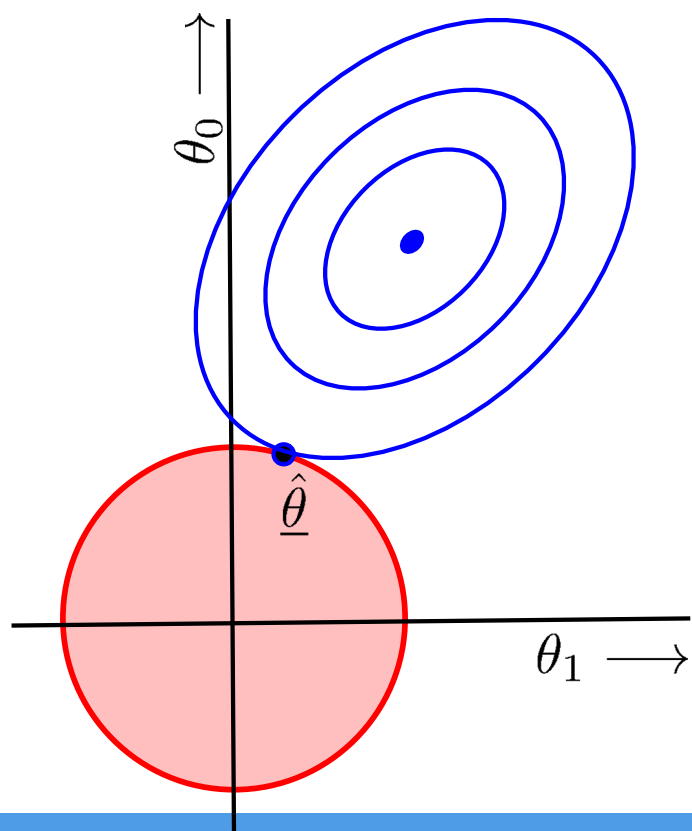
Regularization: L2 vs L1

- Estimate balances data term & regularization term



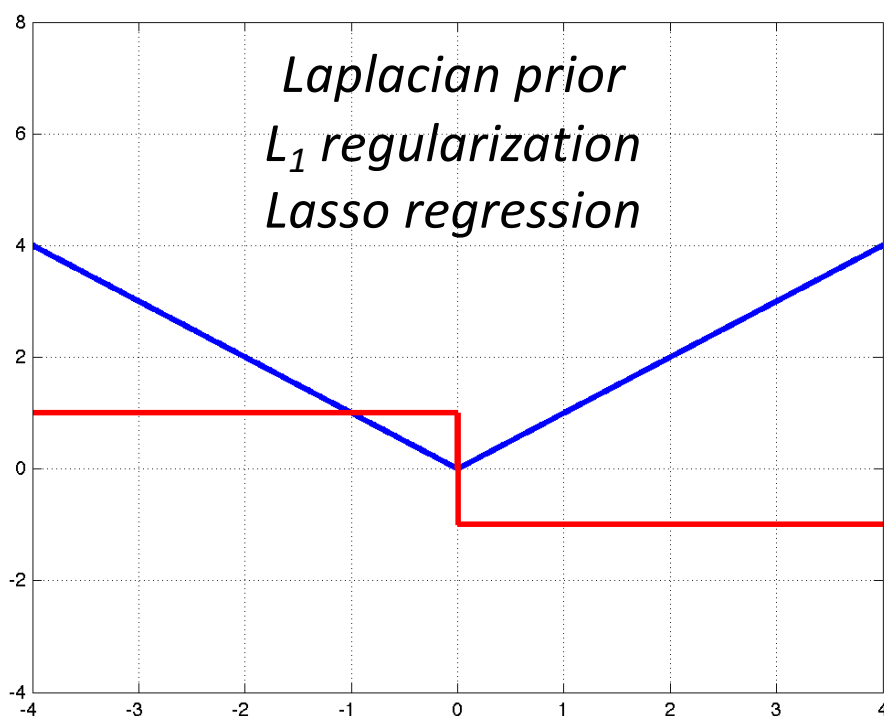
Regularization: L2 vs L1

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



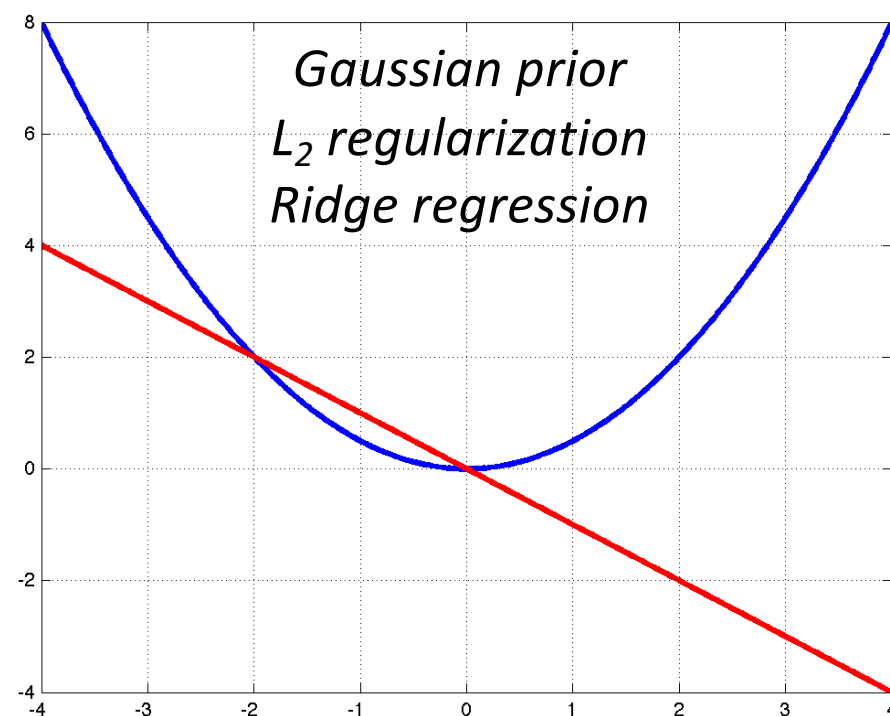
Gradient-Based Optimization

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



Objective Function:

Negative Gradient:



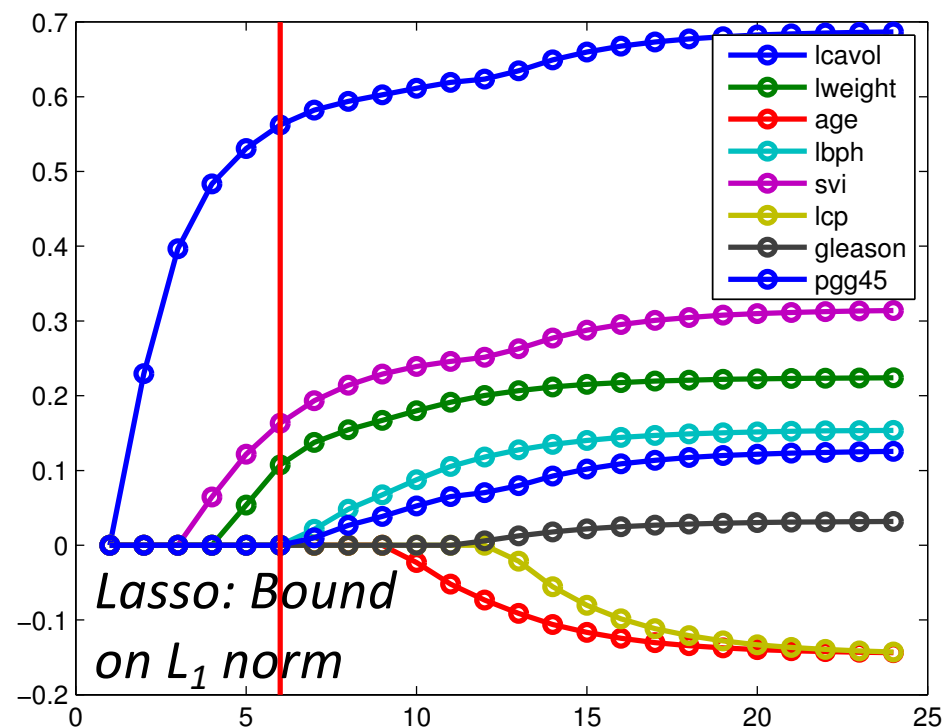
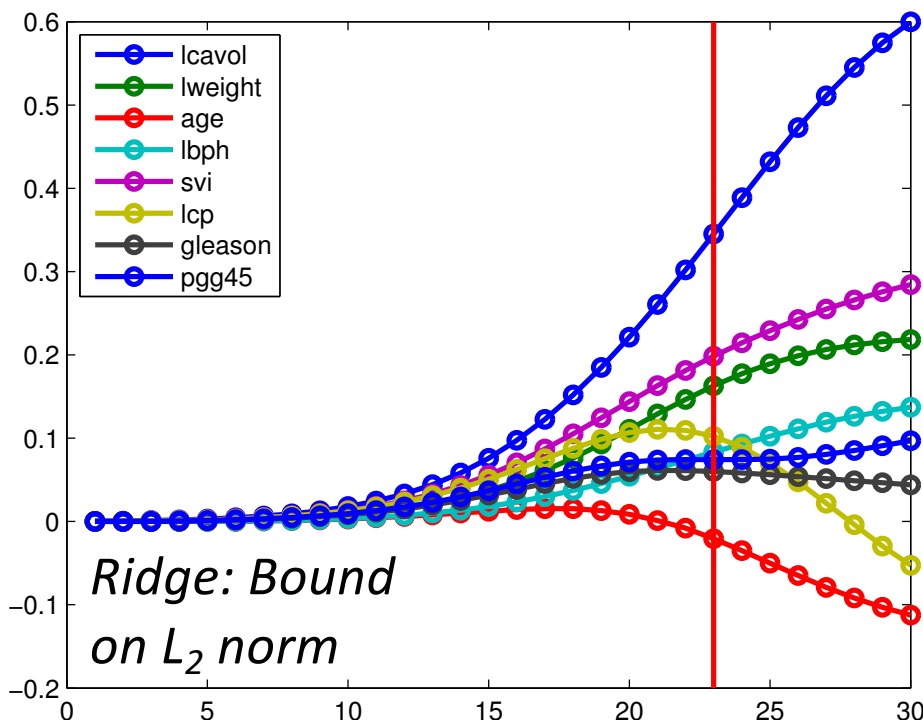
$$f(\theta_i) = |\theta_i|^p$$

$$-f'(\theta_i)$$

(Informal intuition: Gradient of L_1 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