CS184A/284A
AI in Biology and Medicine

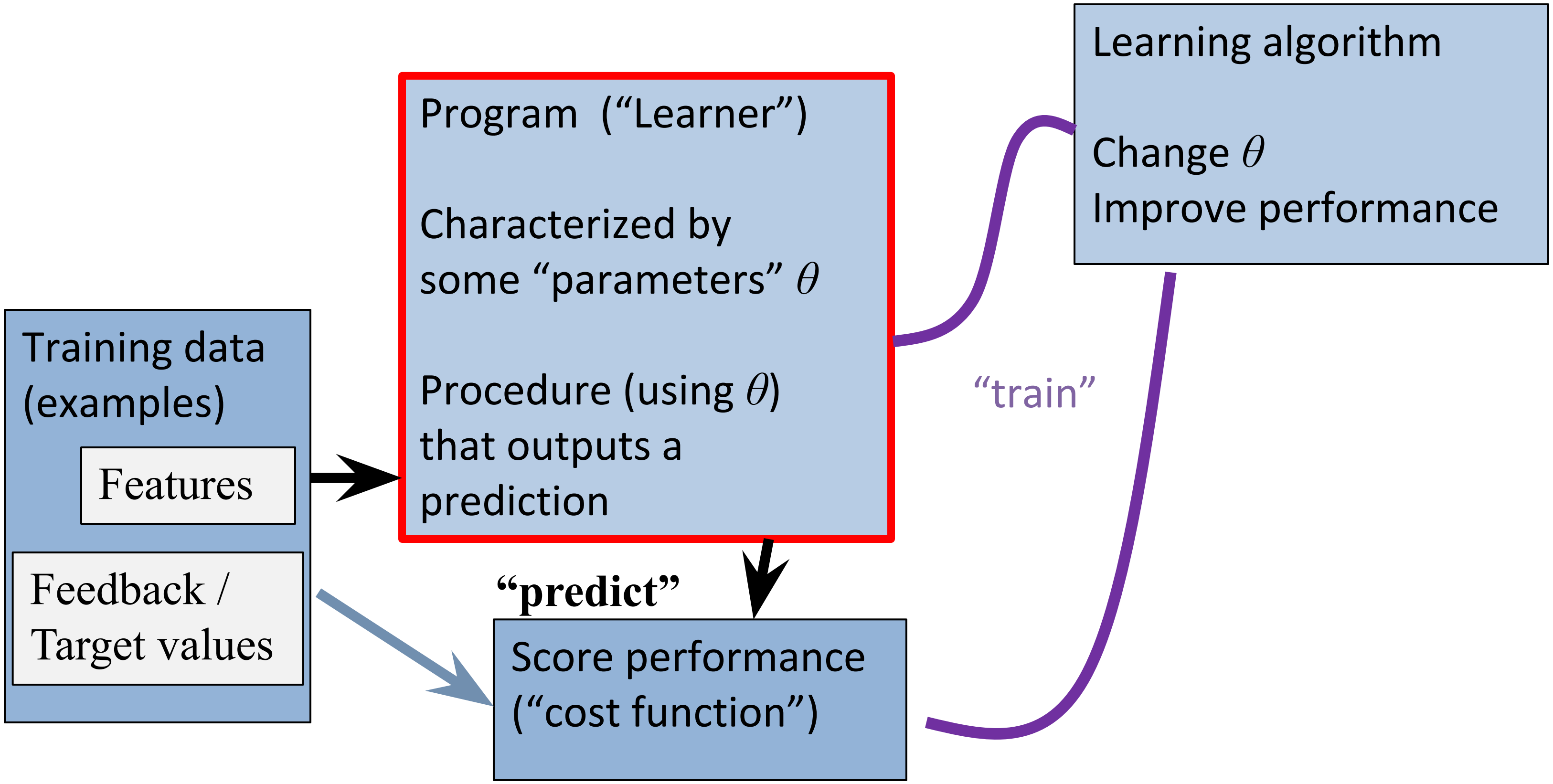
Linear Regression

Machine Learning

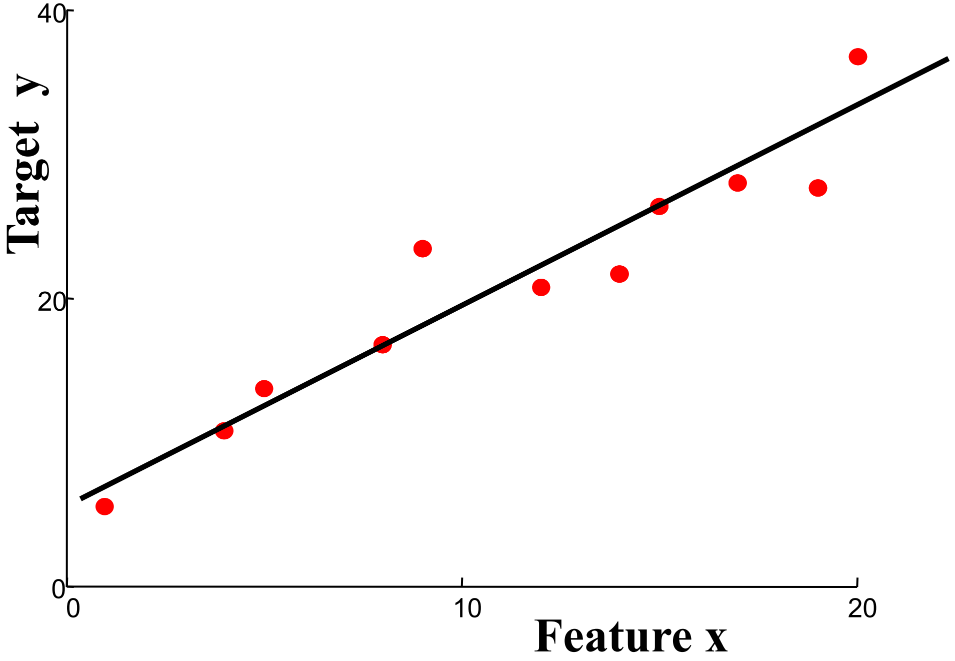
- **Linear Regression via Least Squares**
- Gradient Descent Algorithms
- Direct Minimization of Squared Error
- Regression with Non-linear Features
- Bias, Variance, & Validation
- Regularized Linear Regression

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

- Define form of function f(x) explicitly
- Find a good f(x) within that family

Notation

$$\hat{y}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \dots$$

Define "feature" $x_0 = 1$ (constant)

Then

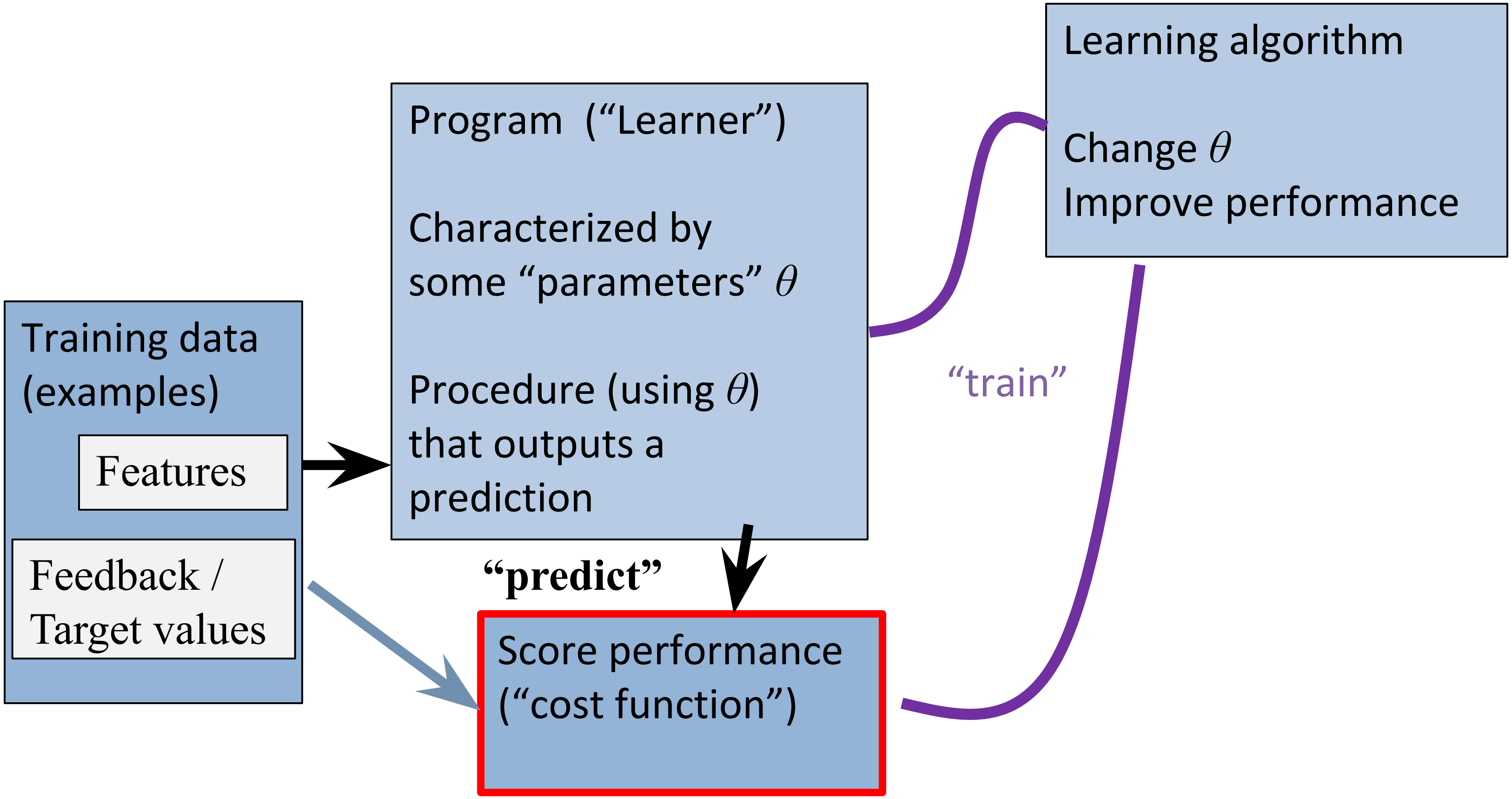
$$\hat{y}(x) = \theta \, x^T$$

$$\underline{\theta} = [\theta_0, \dots, \theta_n]$$

$$\underline{x} = [1, x_1, \dots, x_n]$$

Supervised learning

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



Program ("Learner")

Characterized by some "parameters" θ

Procedure (using θ) that outputs a prediction

Learning algorithm

Change θ

Improve performance

Training data (examples)

Features

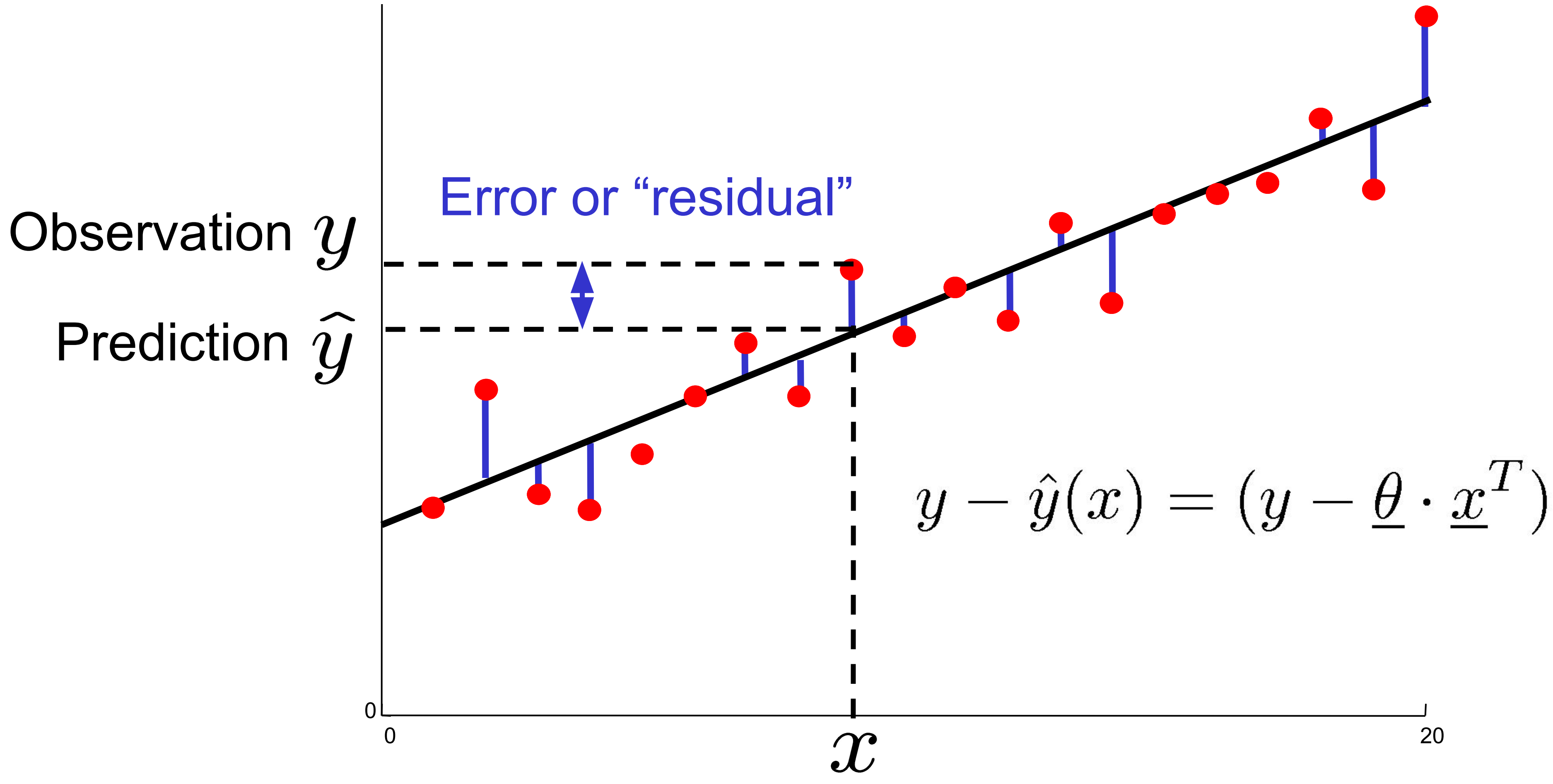
Feedback / Target values

"predict"

"train"

Score performance ("cost function")

Measuring error



$$y - \hat{y}(x) = (y - \underline{\theta} \cdot \underline{x}^T)$$

Mean squared error

- How can we quantify the error?

$$\text{MSE},\ J(\underline{\theta}) = \frac{1}{m}\sum_j (y^{(j)} - \hat{y}(x^{(j)}))^2$$

$$= \frac{1}{m}\sum_j (y^{(j)} - \underline{\theta}\cdot\underline{x}^{(j)T})^2$$

- Could choose something else, of course…
  - Computationally convenient (more later)
  - Measures the variance of the residuals
  - Corresponds to likelihood under Gaussian model of “noise”

$$\mathcal{N}(y\ ;\ \mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left\{-\frac{1}{2\sigma^2}(y-\mu)^2\right\}$$

MSE cost function

- Rewrite using matrix form

$$\text{MSE},\ J(\underline{\theta}) = \frac{1}{m}\sum_j \left(y^{(j)} - \hat{y}(x^{(j)})\right)^2$$

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

$$\underline{\theta} = [\theta_0, \ldots, \theta_n]$$

$$\underline{y} = \left[y^{(1)} \ldots, y^{(m)}\right]^T$$

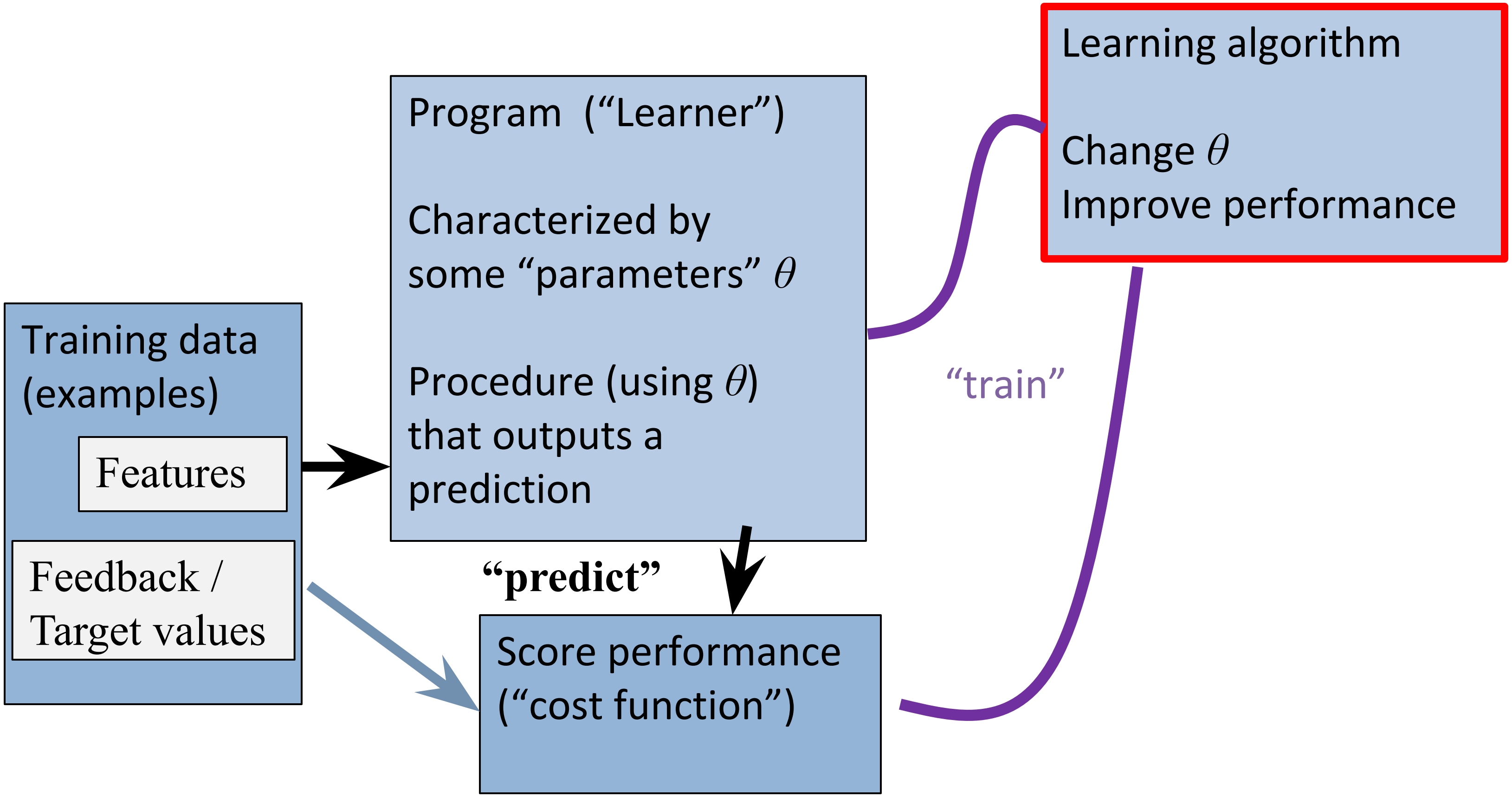
$$\underline{X} = \begin{bmatrix} x_0^{(1)} & \ldots & x_n^{(1)} \\ \vdots & \ddots & \vdots \\ x_0^{(m)} & \ldots & x_n^{(m)} \end{bmatrix}$$

$$J(\underline{\theta}) = \frac{1}{m}(\underline{y}^T - \underline{\theta}\,\underline{X}^T)\cdot(\underline{y}^T - \underline{\theta}\,\underline{X}^T)^T$$

```
# Python / NumPy:
e = Y – X.dot( theta.T );
J = e.T.dot( e ) / m  # = np.mean( e ** 2 )
```

Supervised learning

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



Learning algorithm

Change θ

Improve performance

Program (“Learner”)

Characterized by some “parameters” θ

Procedure (using θ) that outputs a prediction

Training data (examples)

Features

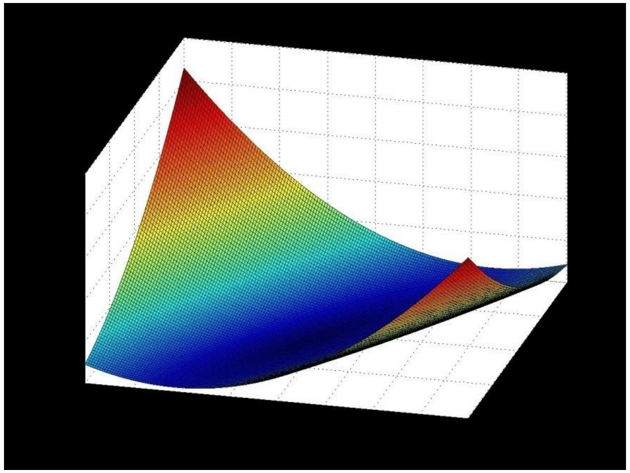
Feedback / Target values

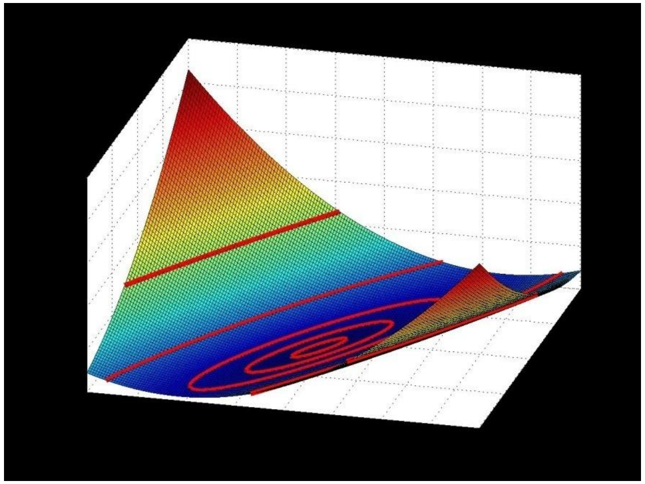
“train”

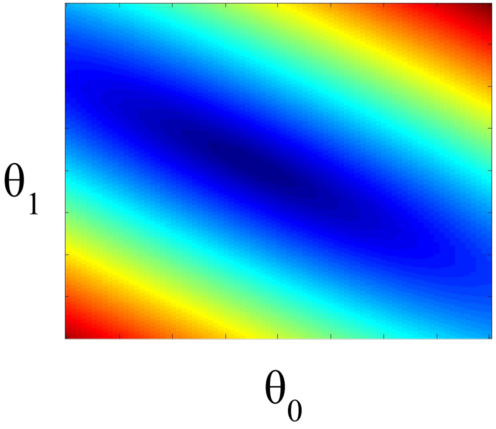
“predict”

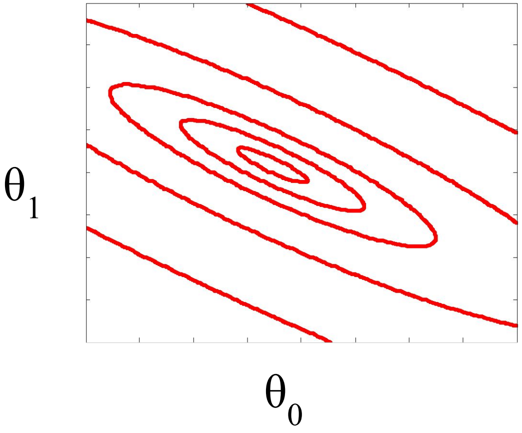
Score performance (“cost function”)

Visualizing the cost function





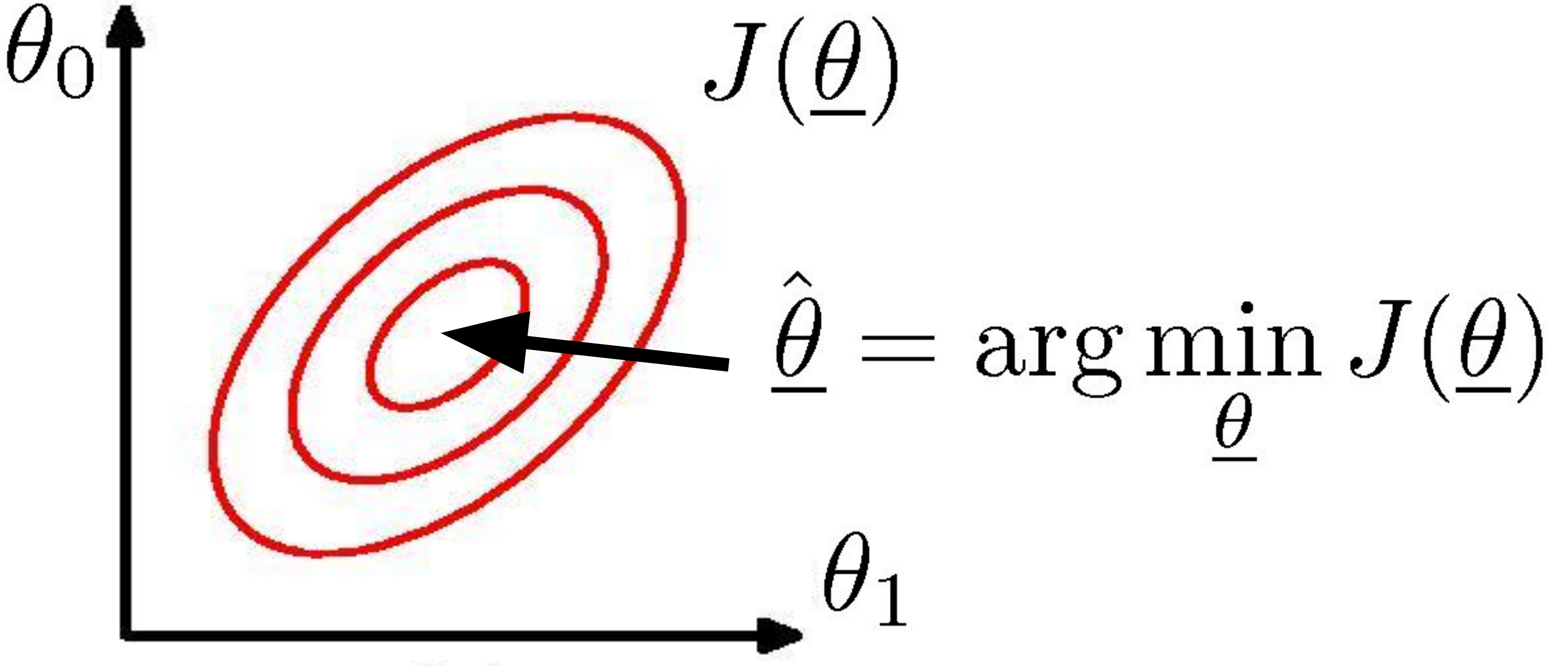




Finding good parameters

- Want to find parameters which minimize our error…

- Think of a cost “surface”: error residual for that θ …



$$\underline{\hat{\theta}} = \arg\min_{\underline{\theta}} J(\underline{\theta})$$

Machine Learning

Linear Regression via Least Squares

Gradient Descent Algorithms

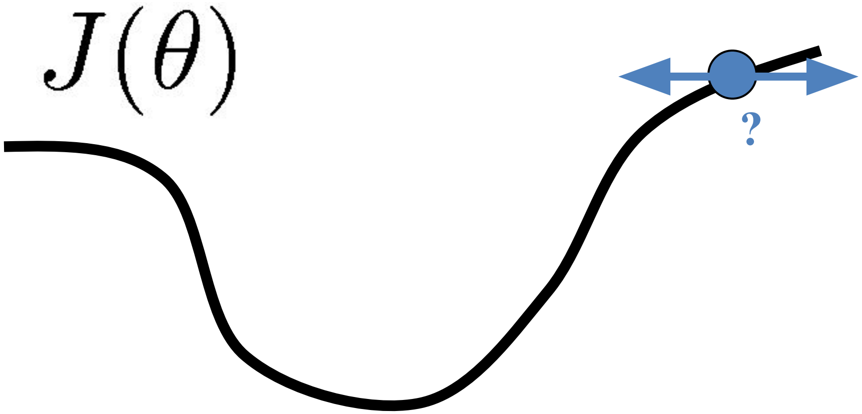
Direct Minimization of Squared Error

Regression with Non-linear Features

Bias, Variance, & Validation

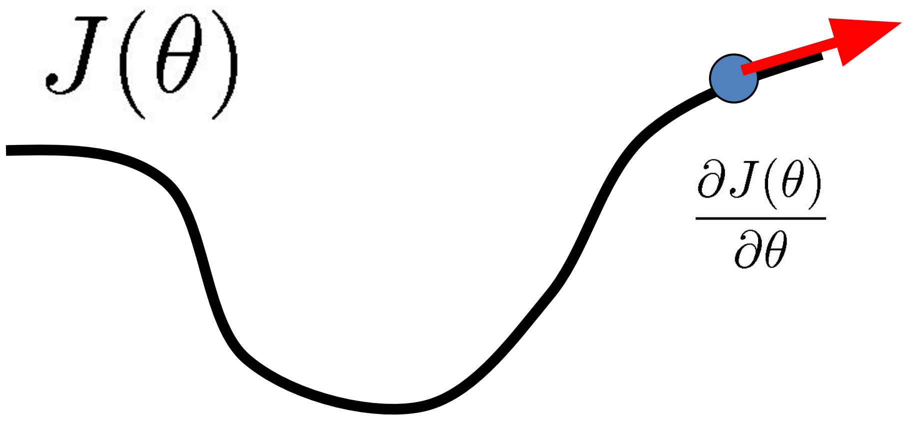
Regularized Linear Regression

Gradient descent



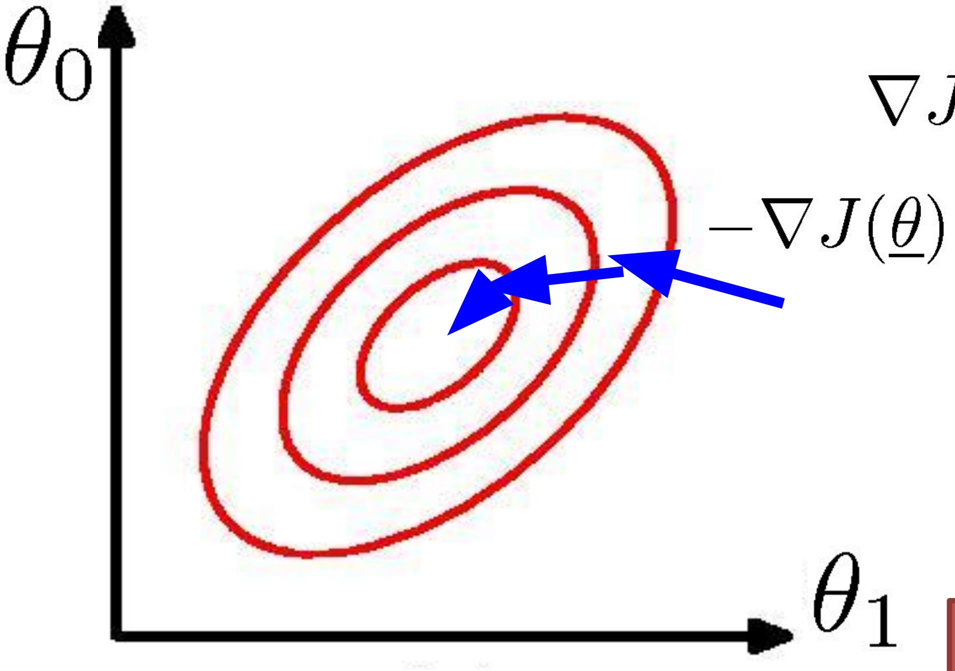
- How to change θ to improve J(θ)?
- Choose a direction in which J(θ) is decreasing

Gradient descent



- How to change θ to improve J(θ)?
- Choose a direction in which J(θ) is decreasing
- Derivative $\frac{\partial J(\theta)}{\partial \theta}$
- Positive => increasing
- Negative => decreasing

Gradient descent in more dimensions



- Gradient vector

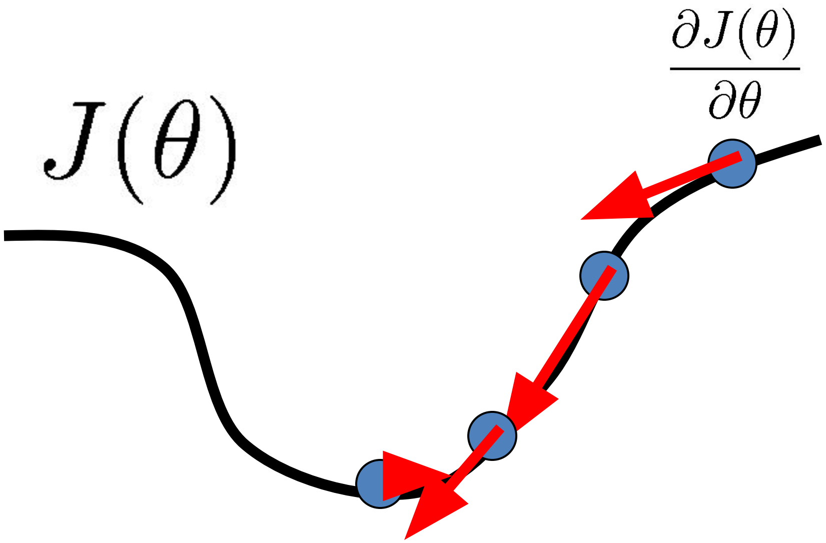
$$\nabla J(\underline{\theta}) = \left[\frac{\partial J(\underline{\theta})}{\partial \theta_0} \quad \frac{\partial J(\underline{\theta})}{\partial \theta_1} \quad \ldots \right]$$

Indicates direction of steepest ascent
(negative = steepest descent)

Gradient descent

- Initialization
- Step size α
  - Can change over iterations
- Gradient direction
- Stopping condition

```
Initialize $\theta$
Do{
 $\theta \leftarrow \theta - \alpha\nabla_\theta J(\theta)$
} while ($\alpha\|\nabla_\theta J\| > \varepsilon$)
```



Gradient for the MSE

- MSE

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

- ∇ J = ?

$$J(\underline{\theta}) = \frac{1}{m} \sum_j (\overbrace{y^{(j)} - \theta_0 \underline{x}_0^{(j)} - \theta_1 \underline{x}_1^{(j)} - \ldots}^{e_j(\theta)})^2$$

$$\frac{\partial J}{\partial \theta_0} = \frac{\partial}{\partial \theta_0} \frac{1}{m} \sum_j (\ e_j(\theta)\ )^2$$

$$= \frac{1}{m} \sum_j \ \frac{\partial}{\partial \theta_0} (\ e_j(\theta)\ )^2$$

$$= \frac{1}{m} \sum_j \ 2 e_j(\theta)\ \frac{\partial}{\partial \theta_0} e_j(\theta)$$

$$\frac{\partial}{\partial \theta_0} e_j(\theta) = \underbrace{\frac{\partial}{\partial \theta_0} y^{(j)}}_{\mathbf{0}} - \frac{\partial}{\partial \theta_0} \theta_0 x_0^{(j)} - \underbrace{\frac{\partial}{\partial \theta_0} \theta_1 x_1^{(j)}}_{\mathbf{0}} - \ldots$$

$$= -x_0^{(j)}$$

Gradient for the MSE

- MSE

$$J(\underline{\theta}) = \frac{1}{m} \sum_j (y^{(j)} - \underline{\theta} \cdot \underline{x}^{(j)T})^2$$

- ∇ J = ?

$$J(\underline{\theta}) = \frac{1}{m} \sum_j (\overbrace{y^{(j)} - \theta_0 \underline{x}_0^{(j)} - \theta_1 \underline{x}_1^{(j)} - \ldots}^{e_j(\theta)})^2$$

$$\nabla J(\underline{\theta}) = \left[\quad \frac{\partial J}{\partial \theta_0} \qquad \qquad \frac{\partial J}{\partial \theta_1} \qquad \ldots \right]$$

$$= \left[\frac{2}{m} \sum_j -e_j(\theta) x_0^{(j)} \quad \frac{2}{m} \sum_j -e_j(\theta) x_1^{(j)} \qquad \ldots \right]$$

Gradient descent

- Initialization
- Step size α
  - Can change over iterations
- Gradient direction
- Stopping condition

```
Initialize $\theta$
Do{
 $\theta \leftarrow \theta - \alpha \nabla_\theta J(\theta)$
} while ($\alpha \| \nabla_\theta J \| > \varepsilon$)
```

$$J(\underline{\theta}) = \frac{1}{m} \sum_j (y^{(j)} - \underline{\theta} \cdot \underline{x}^{(j)^T})^2$$

$$\nabla J(\underline{\theta}) = -\frac{2}{m} \sum_j (\underbrace{y^{(j)} - \underline{\theta} \cdot \underline{x}^{(j)^T}}_{\text{Error magnitude \& direction for datum j}}) \cdot \underbrace{[x_0^{(j)}\, x_1^{(j)} \, \ldots]}_{\text{Sensitivity to each param}}$$

Derivative of MSE

- Rewrite using matrix form

$$\nabla J(\underline{\theta}) = -\frac{2}{m}\sum_j (\underbrace{y^{(j)} - \underline{\theta}}_{\text{Error magnitude \& direction for datum j}} \cdot \underline{x}^{(j)^T}) \cdot [\underbrace{x_0^{(j)} x_1^{(j)}}_{\text{Sensitivity to each } \theta_i} \ldots]$$

$$\underline{\theta} = [\theta_0, \ldots, \theta_n]$$

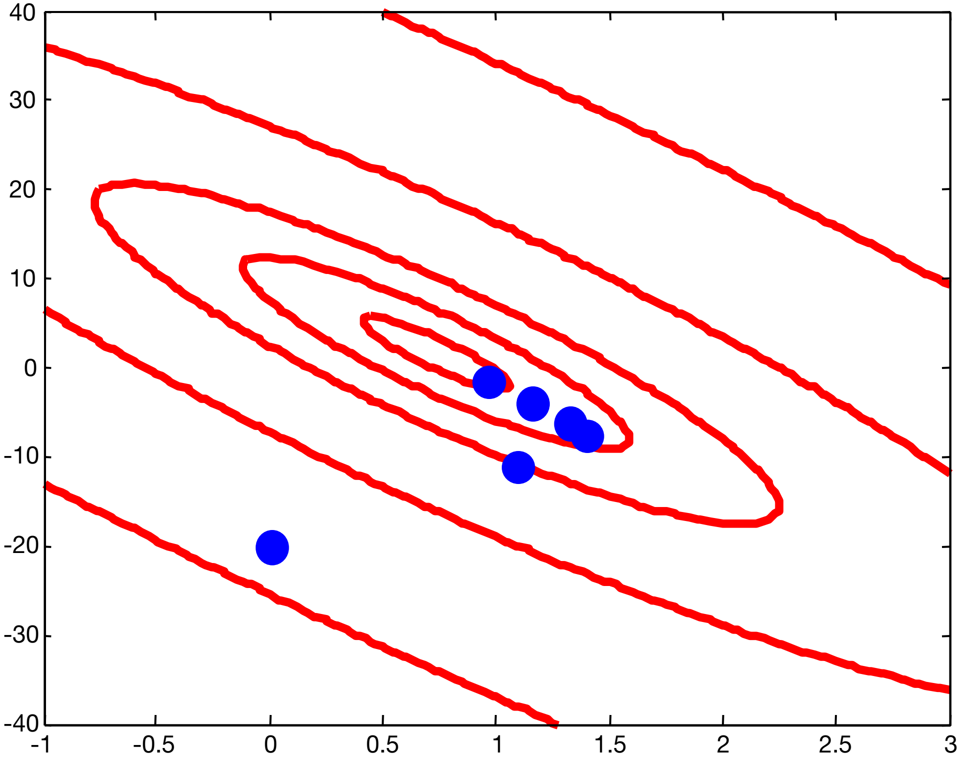
$$\underline{y} = \left[y^{(1)} \ldots, y^{(m)}\right]^T$$

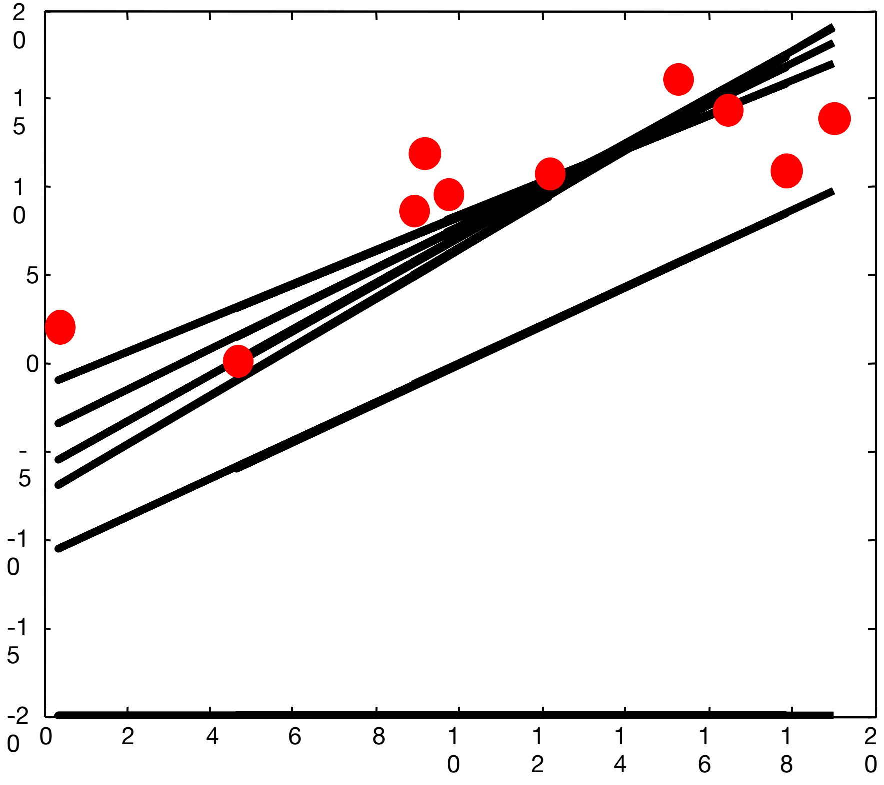
$$\underline{X} = \begin{bmatrix} x_0^{(1)} & \ldots & x_n^{(1)} \\ \vdots & \ddots & \vdots \\ x_0^{(m)} & \ldots & x_n^{(m)} \end{bmatrix}$$

$$\nabla J(\underline{\theta}) = -\frac{2}{m}(\underline{y}^T - \underline{\theta}\underline{X}^T) \cdot \underline{X}$$

```
e = Y – X.dot( theta.T ) # error residual
DJ = - e.dot(X) * 2.0/m  # compute the gradient
theta -= alpha * DJ       # take a step
```

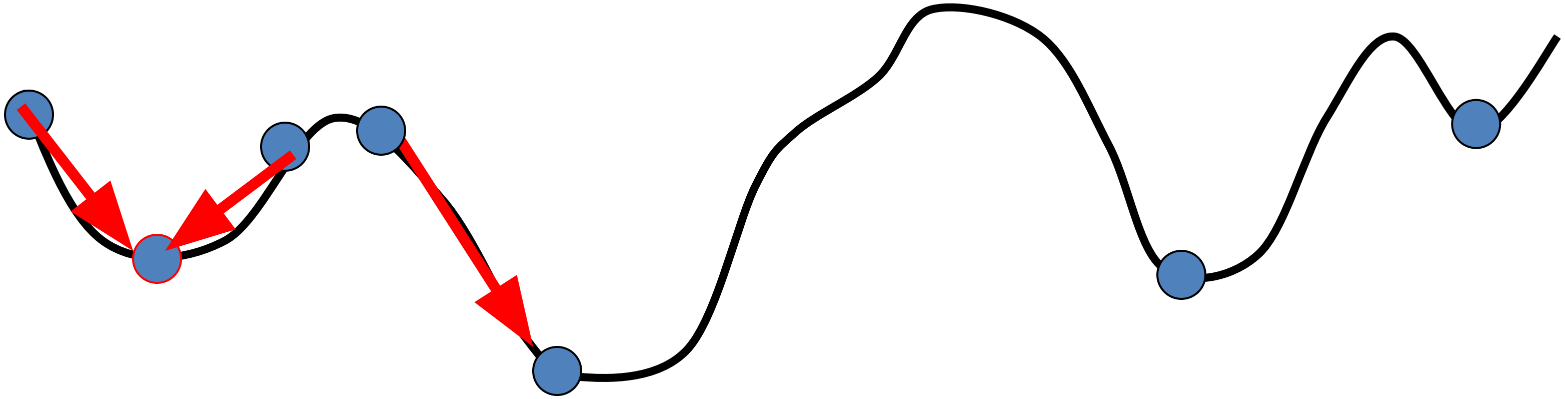
Gradient descent on cost function





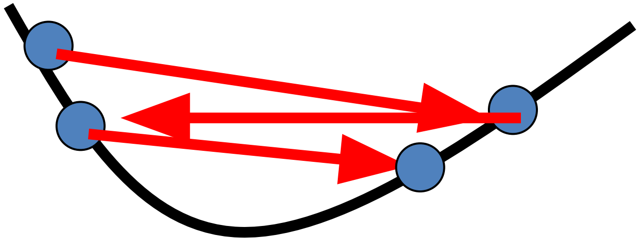
Comments on gradient descent

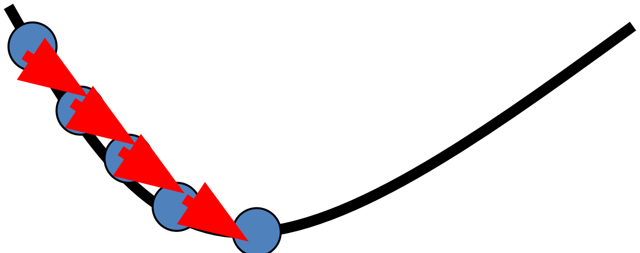
- Very general algorithm
  - We'll see it many times
- Local minima
  - Sensitive to starting point



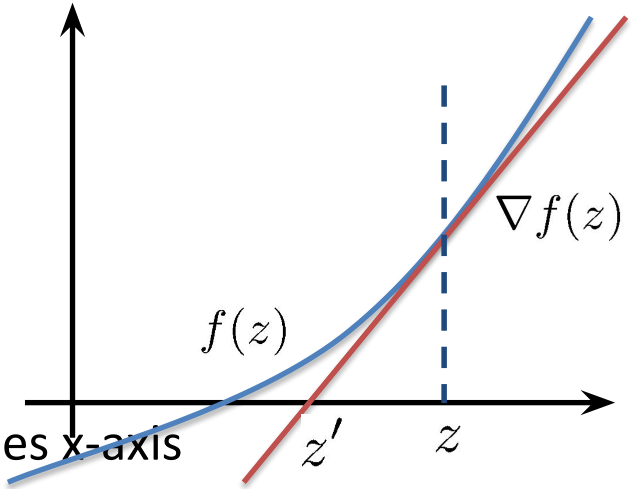
Comments on gradient descent

- Very general algorithm
  - We'll see it many times
- Local minima
  - Sensitive to starting point
- Step size
  - Too large? Too small? Automatic ways to choose?
  - May want step size to decrease with iteration
  - Common choices:
    - Fixed
    - Linear: C/(iteration)
    - Line search / backoff (Armijo, etc.)
    - Newton's method





Newton’s method



- Want to find the roots of f(x)
  - “Root”: value of x for which f(x)=0
- Initialize to *some* point x
- Compute the tangent at x & compute where it crosses x-axis

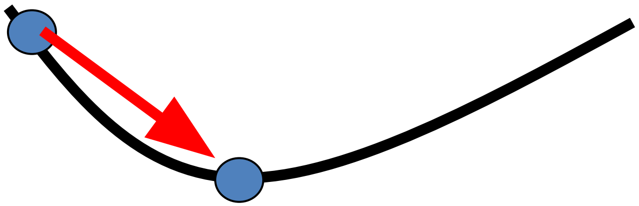
$$\nabla f(z) = \frac{0 - f(z)}{z' - z} \quad \Rightarrow \quad z' = z - \frac{f(z)}{\nabla f(z)}$$

- Optimization: find roots of rJ(μ)

$$\nabla\nabla J(\theta) = \frac{0 - \nabla J(\theta)}{\theta' - \theta} \quad \Rightarrow \quad \theta' = \theta - \frac{\nabla J(\theta)}{\nabla\nabla J(\theta)}$$

(“Step size” ¸ = 1/rrJ ; inverse curvature)

  - If converges, usually very fast
  - Works well for smooth, non-pathological functions, locally quadratic
  - For n large, may be computationally hard: O(n^2) storage, O(n^3) time



(Multivariate:
r J(μ) = gradient vector
r^2 J(μ) = matrix of 2nd derivatives
a/b = a b^{-1}, matrix inverse)

Stochastic / Online gradient descent

- MSE

$$J(\underline{\theta}) = \frac{1}{m}\sum_j J_j(\underline{\theta}), \qquad J_j(\underline{\theta}) = (y^{(j)} - \underline{\theta}\cdot \underline{x}^{(j)\,T})^2$$

- Gradient

$$\nabla J(\underline{\theta}) = \frac{1}{m}\sum_j \nabla J_j(\underline{\theta}) \qquad \nabla J_j(\underline{\theta}) = (y^{(j)} - \underline{\theta}\cdot \underline{x}^{(j)\,T}) \cdot [x_0^{(j)} x_1^{(j)} \ldots]$$

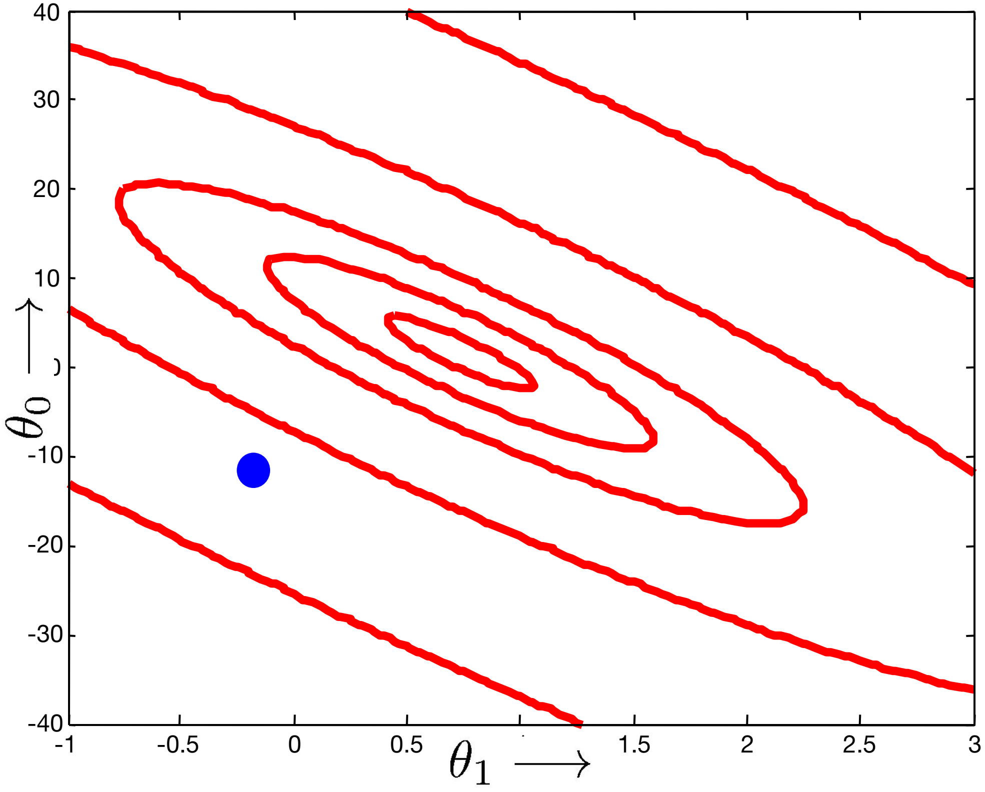
- Stochastic (or “online”) gradient descent:
  - Use updates based on individual datum j, chosen at random
  - At optima, $\mathbb{E}\big[\nabla J_j(\underline{\theta})\big] = \nabla J(\underline{\theta}) = 0$

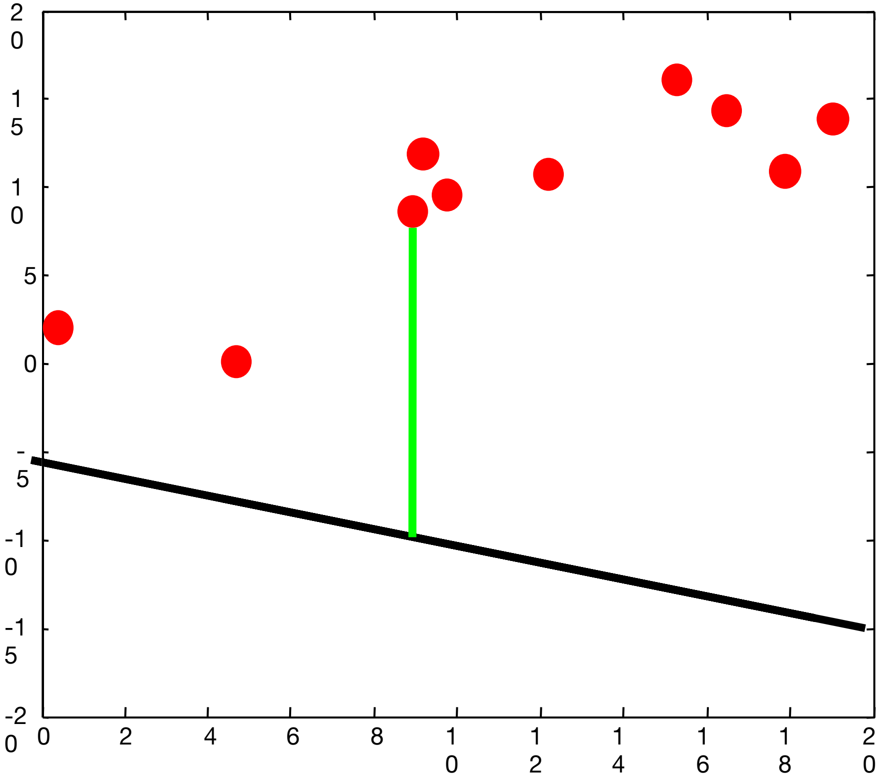
    (average over the data)

Online gradient descent

- Update based on one datum, and its residual, at a time

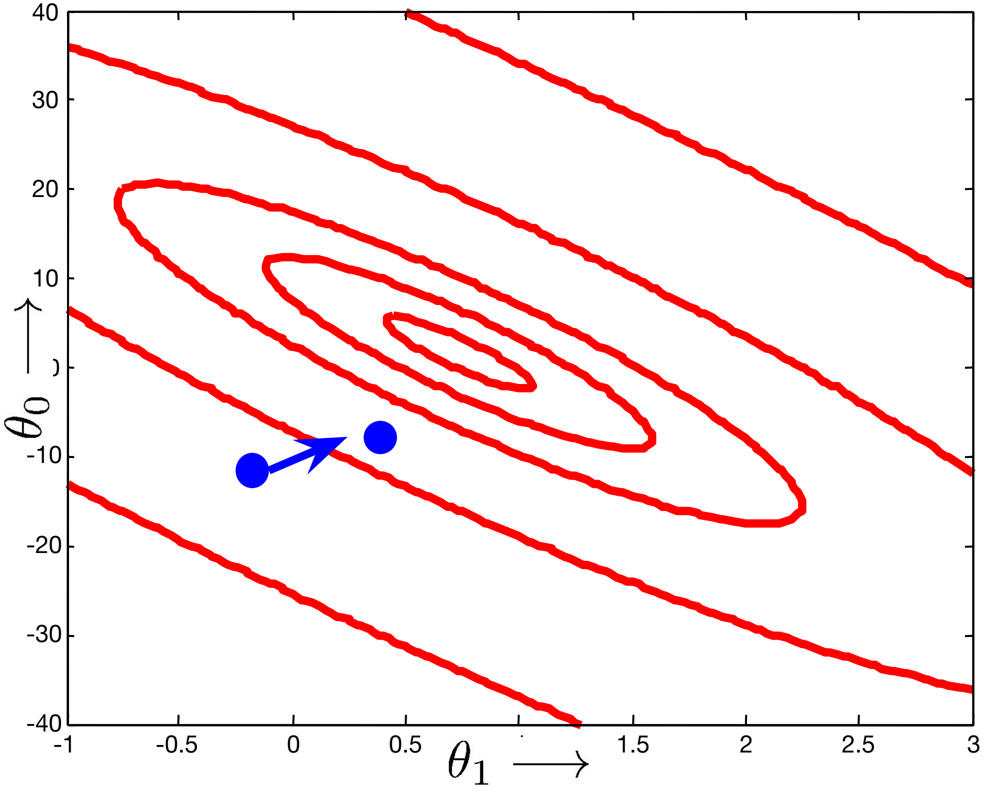
```
Initialize θ
Do {
 for j=1:m
   θ ← θ - $\alpha \nabla_{\theta} J_j(\theta)$
} while (not done)
```

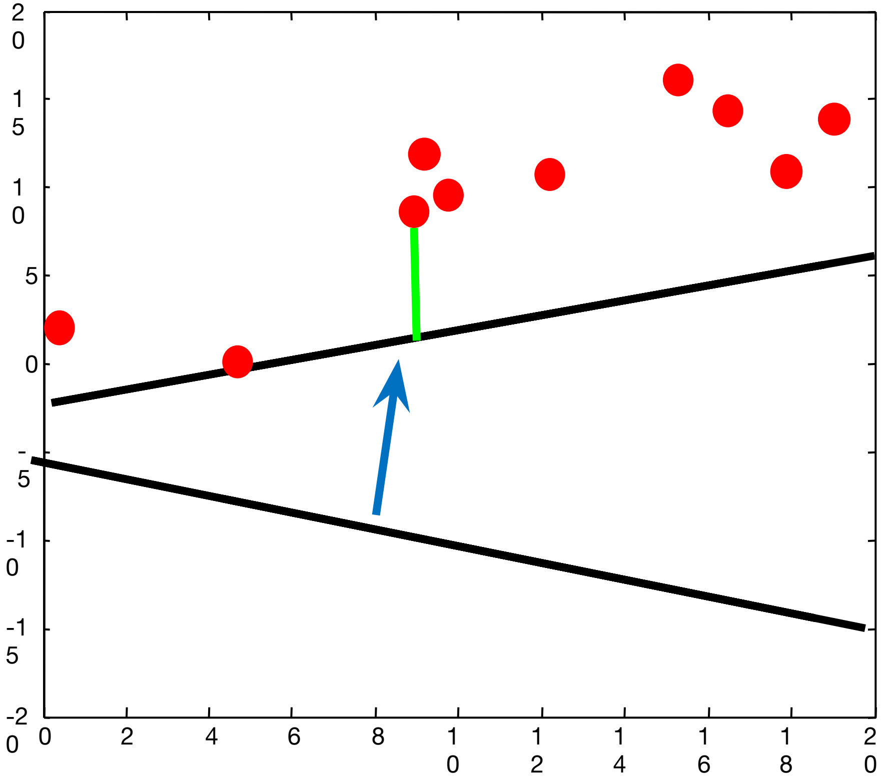




Online gradient descent

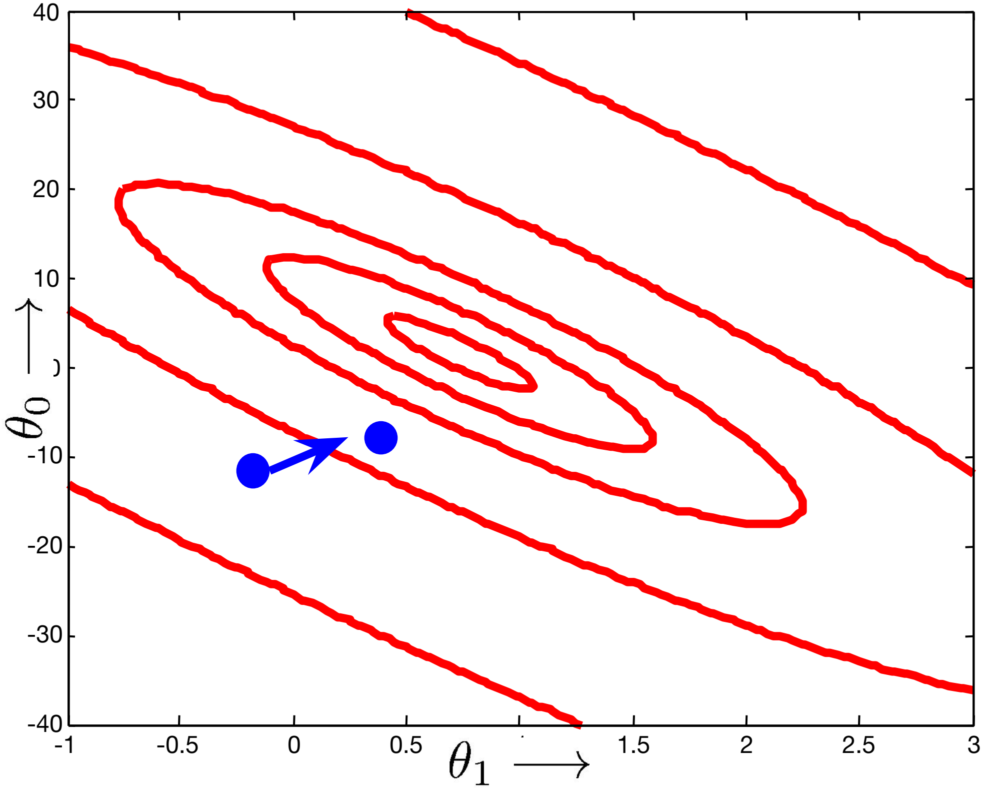
```
Initialize θ
Do {
 for j=1:m
   $θ \leftarrow θ - α\nabla_θ J_j(θ)$
} while (not done)
```

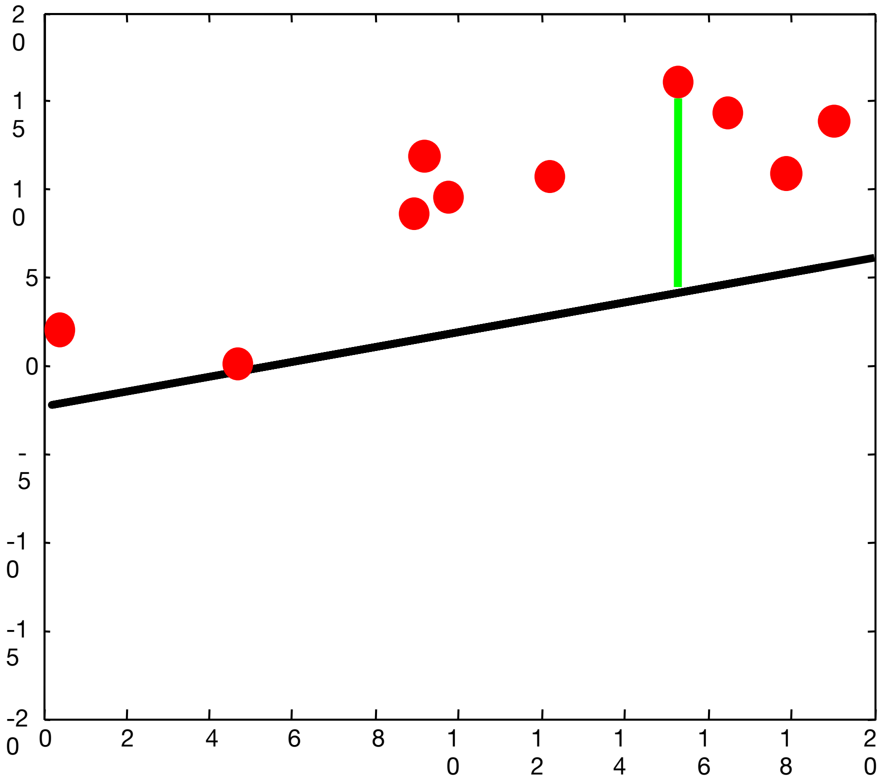




Online gradient descent

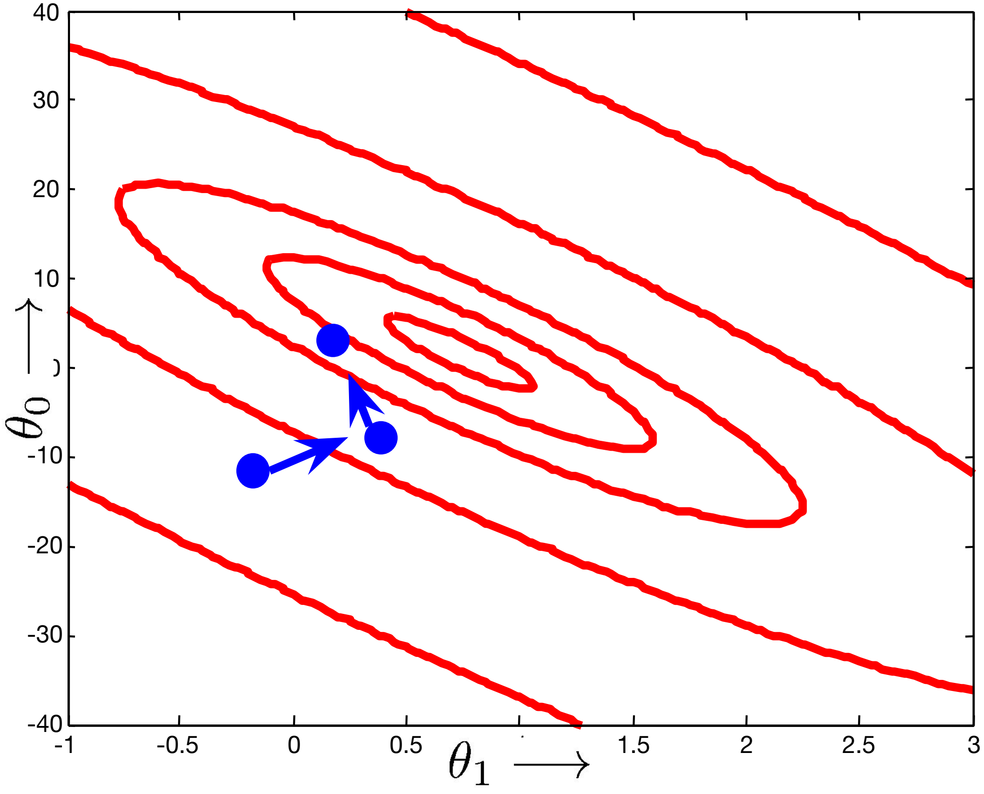
```
Initialize $\theta$
Do {
 for j=1:m
   $\theta \leftarrow \theta -$
   $\alpha \nabla_\theta J_j(\theta)$
} while (not done)
```

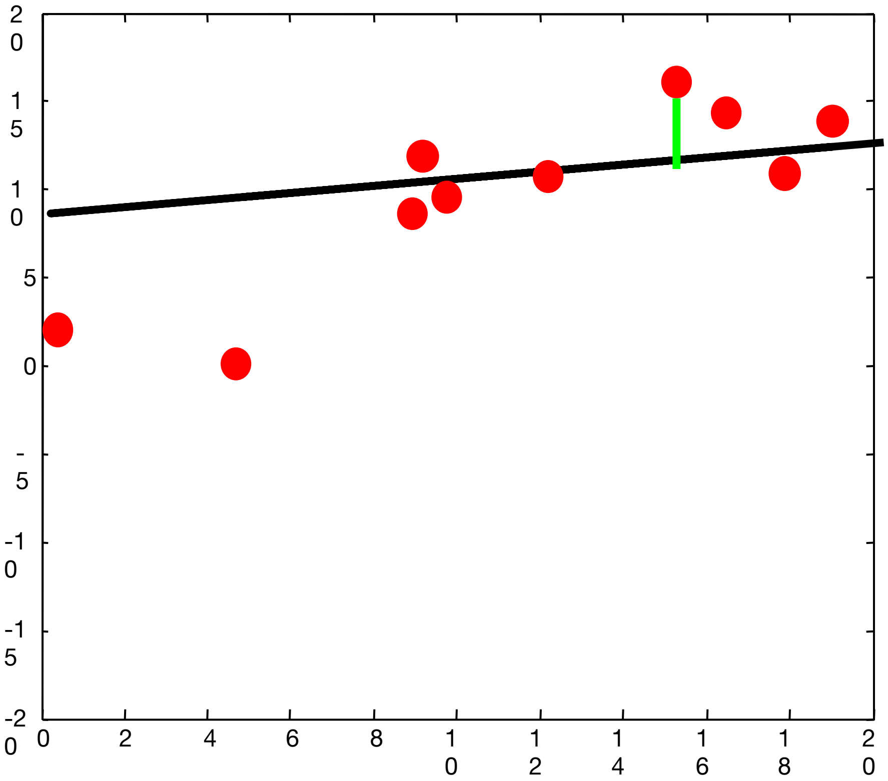




Online gradient descent

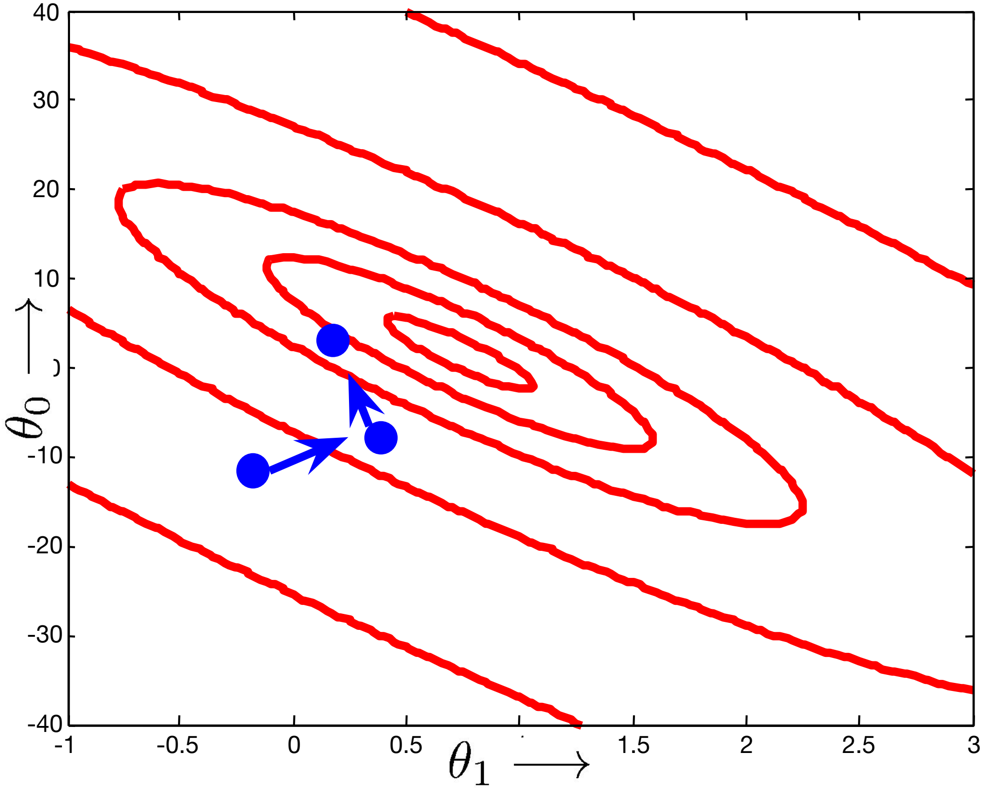
```
Initialize $\theta$
Do {
 for j=1:m
   $\theta \leftarrow \theta - \alpha \nabla_\theta J_j(\theta)$
} while (not done)
```

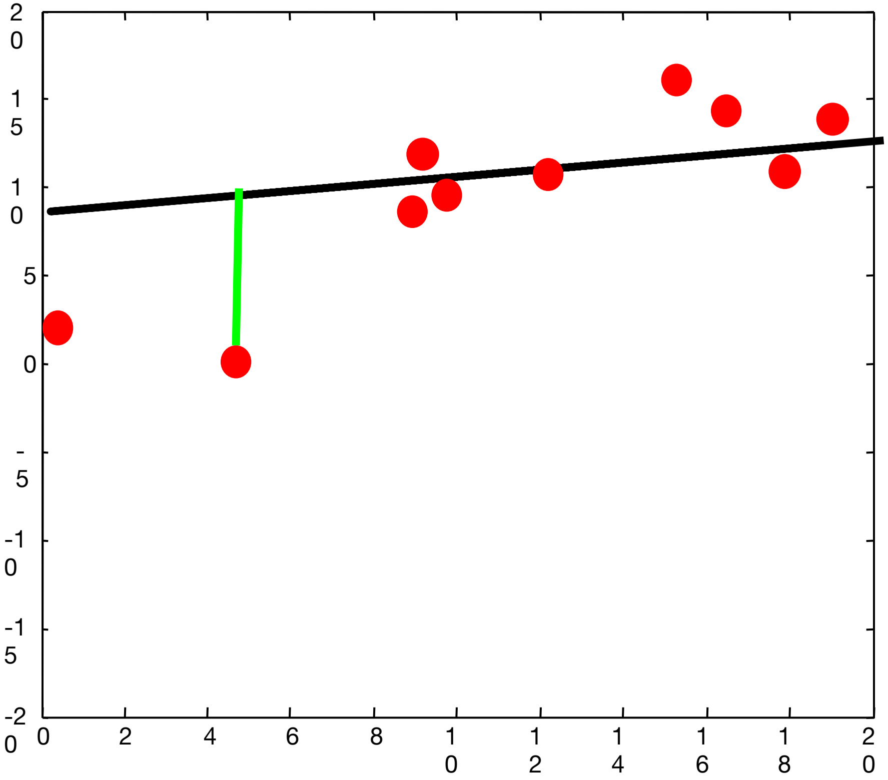




Online gradient descent

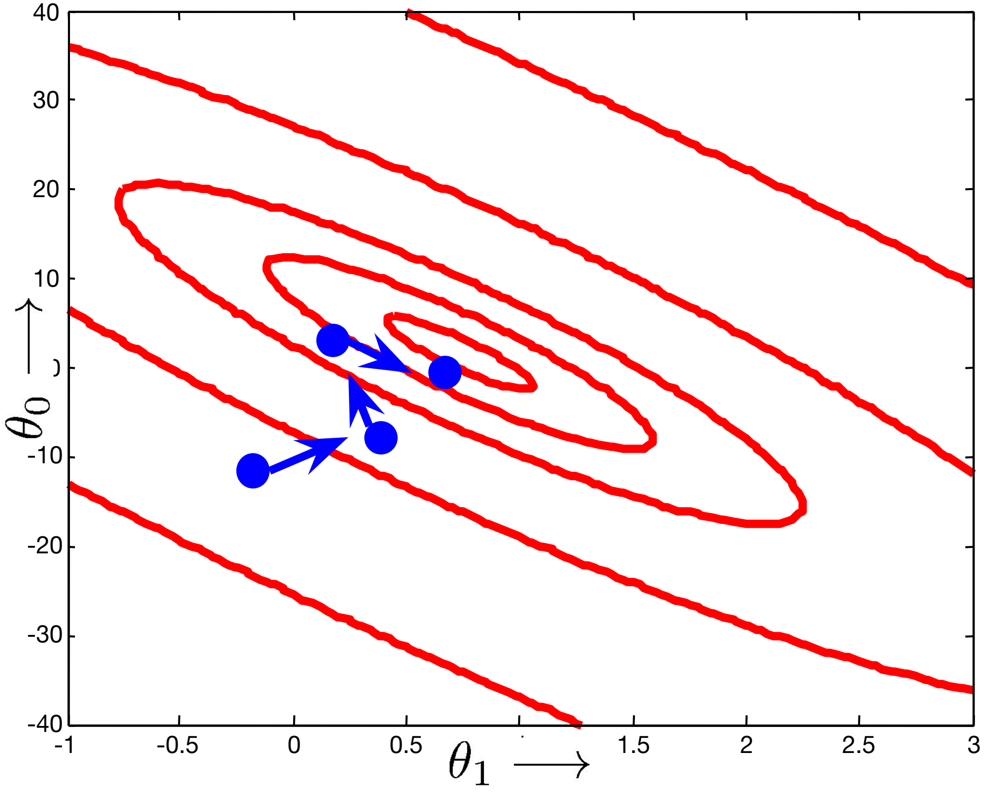
```
Initialize θ
Do {
 for j=1:m
   $\theta \leftarrow \theta - \alpha \nabla_\theta J_j(\theta)$
} while (not done)
```

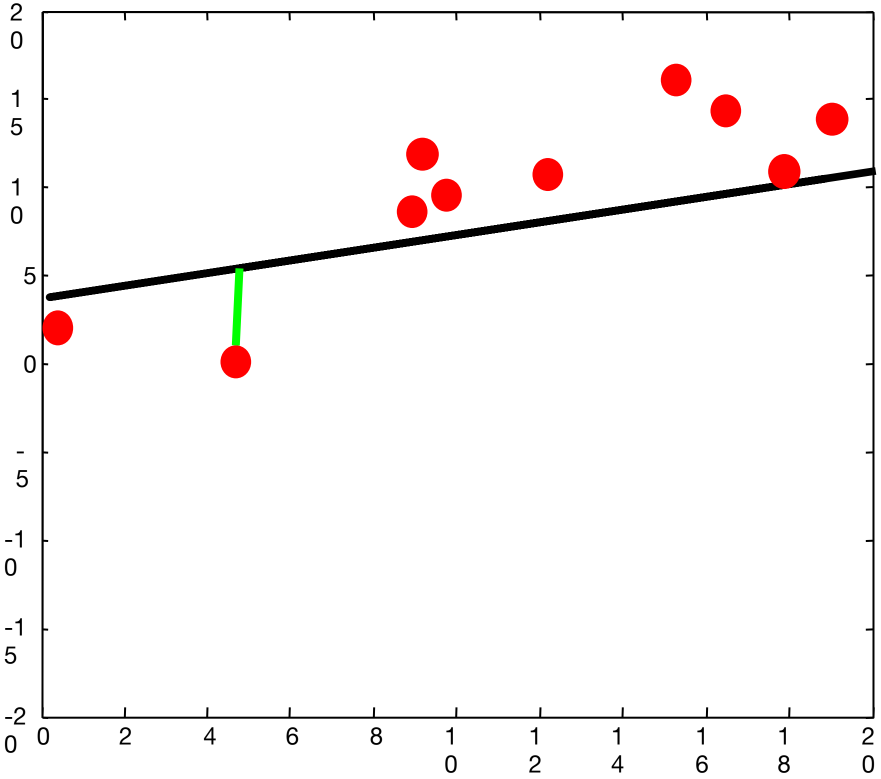




Online gradient descent

```
Initialize θ
Do {
 for j=1:m
   $\theta \leftarrow \theta - \alpha \nabla_\theta J_j(\theta)$
} while (not done)
```





Online gradient descent

```
Initialize $\theta$
Do {
 for j=1:m
   $\theta \leftarrow \theta - \alpha \nabla_\theta J_j(\theta)$
} while (not done)
```

- Benefits
  - Lots of data = many more updates per pass
  - Computationally faster
- Disadvantages
  - No longer strictly “descent”
  - Stopping conditions may be harder to evaluate

(Can use “running estimates” of J(.), etc.)

$$J_j(\underline{\theta}) = (y^{(j)} - \underline{\theta} \cdot \underline{x}^{(j)\,T})^2$$

$$\nabla J_j(\underline{\theta}) = -2(y^{(j)} - \underline{\theta} \cdot \underline{x}^{(j)\,T}) \cdot [x_0^{(j)} x_1^{(j)} \ldots]$$

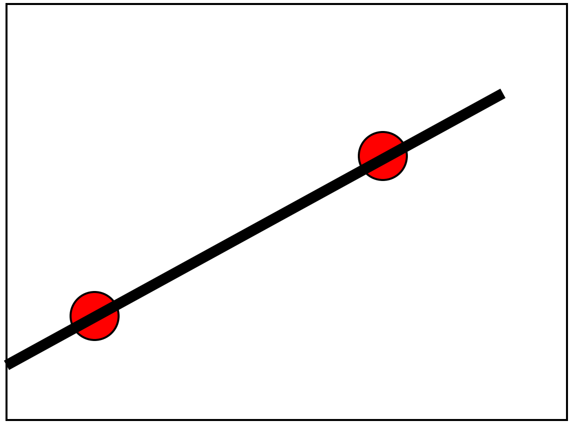
Machine Learning

- Linear Regression via Least Squares
- Gradient Descent Algorithms
- **Direct Minimization of Squared Error**
- Regression with Non-linear Features
- Bias, Variance, & Validation
- Regularized Linear Regression

MSE Minimum

- Consider a simple problem
  - One feature, two data points
  - Two unknowns: θ_0, θ_1
  - Two equations:

$$y^{(1)} = \theta_0 + \theta_1 x^{(1)}$$
$$y^{(2)} = \theta_0 + \theta_1 x^{(2)}$$



- Can solve this system directly:

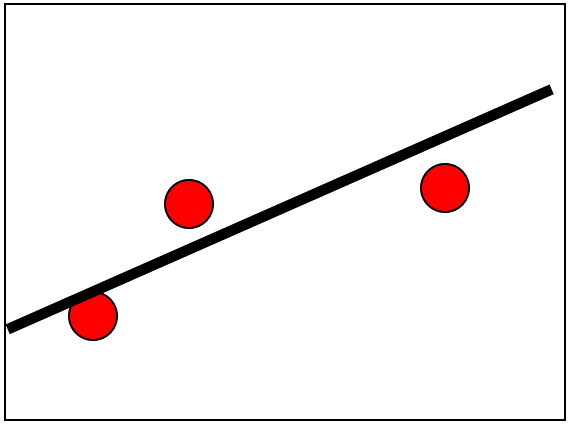
$$\underline{y}^T = \underline{\theta}\,\underline{X}^T \qquad \Rightarrow \qquad \underline{\hat{\theta}} = y^T (\underline{X}^T)^{-1}$$

- However, most of the time, m > n
  - There may be no linear function that hits all the data exactly
  - Instead, solve directly for minimum of MSE function

MSE Minimum

- Simplify with some algebra:

$$\nabla J(\underline{\theta}) = -\frac{2}{m}(\underline{y}^T - \underline{\theta X^T}) \cdot \underline{X} \quad = \quad \underline{0}$$



$$\begin{aligned} \underline{y}^T \, \underline{X} - \underline{\theta X}^T \cdot \underline{X} \quad &= \quad \underline{0} \\ \underline{y}^T \, \underline{X} = \underline{\theta X}^T &\cdot \underline{X} \\ \underline{\theta} \quad = \quad \underline{y}^T \, \underline{X}&(\underline{X}^T \, \underline{X})^{-1} \end{aligned}$$

- X (X^T X)$^{-1}$ is called the “pseudo-inverse”

- If X^T is square and full rank, this is the inverse
- If m > n: overdetermined; gives minimum MSE fit

Matlab MSE

- This is easy to solve in Matlab…

$$\underline{\theta} \quad = \quad \underline{y}^T \, \underline{X}(\underline{X}^T \, \underline{X})^{-1}$$

```
%  y = [y1 ; … ; ym]
%  X = [x1_0 … x1_m ; x2_0 … x2_m ; …]


% Solution 1: "manual"
   th = y' * X * inv(X' * X);


% Solution 2: "mrdivide"
   th = y' / X'; % th*X' = y  =>  th = y/X'
```

Python MSE

- This is easy to solve in Python / NumPy…

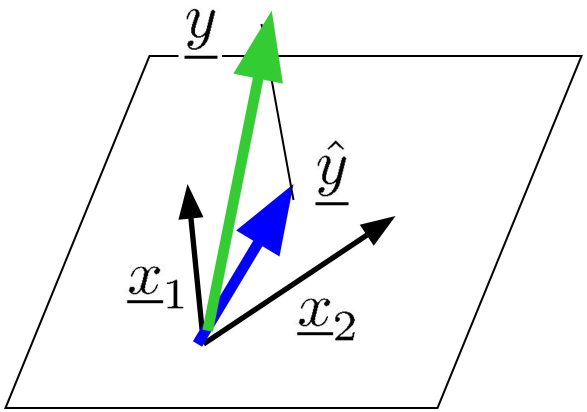
$$\underline{\theta} \quad = \quad \underline{y}^T \, \underline{X} (\underline{X}^T \, \underline{X})^{-1}$$

```
#  y = np.matrix( [[y1], … , [ym]] )
#  X = np.matrix( [[x1_0 … x1_n], [x2_0 … x2_n],
…] )

# Solution 1: “manual”
   th = y.T * X * np.linalg.inv(X.T * X)


# Solution 2: “least squares solve”
   th = np.linalg.lstsq(X, Y)
```

Normal equations

$$\nabla J(\underline{\theta}) = 0 \quad \Rightarrow \quad (\underline{y}^T - \underline{\theta X}^T) \cdot \underline{X} \quad = \quad \underline{0}$$

- Interpretation:
  - (y - θ X) = (y - yhat) is the vector of errors in each example
  - X are the features we have to work with for each example
  - Dot product = 0: orthogonal

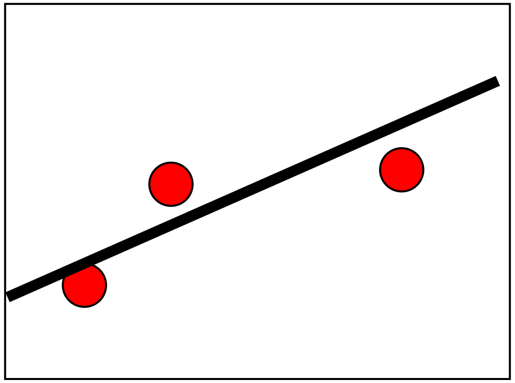


$$\underline{y}^T = [y^{(1)} \ldots y^{(m)}]$$
$$\underline{x}_i = [x_i^{(1)} \ldots x_i^{(m)}]$$

Normal equations

$$\nabla J(\underline{\theta}) = 0 \quad \Rightarrow \quad (\underline{y}^T - \underline{\theta X}^T) \cdot \underline{X} \quad = \quad \underline{0}$$

- Interpretation:
  - (y - θ X) = (y - yhat) is the vector of errors in each example
  - X are the features we have to work with for each example
  - Dot product = 0: orthogonal
- Example:



$$\underline{y} = [1 \quad 3 \quad 3]^T$$

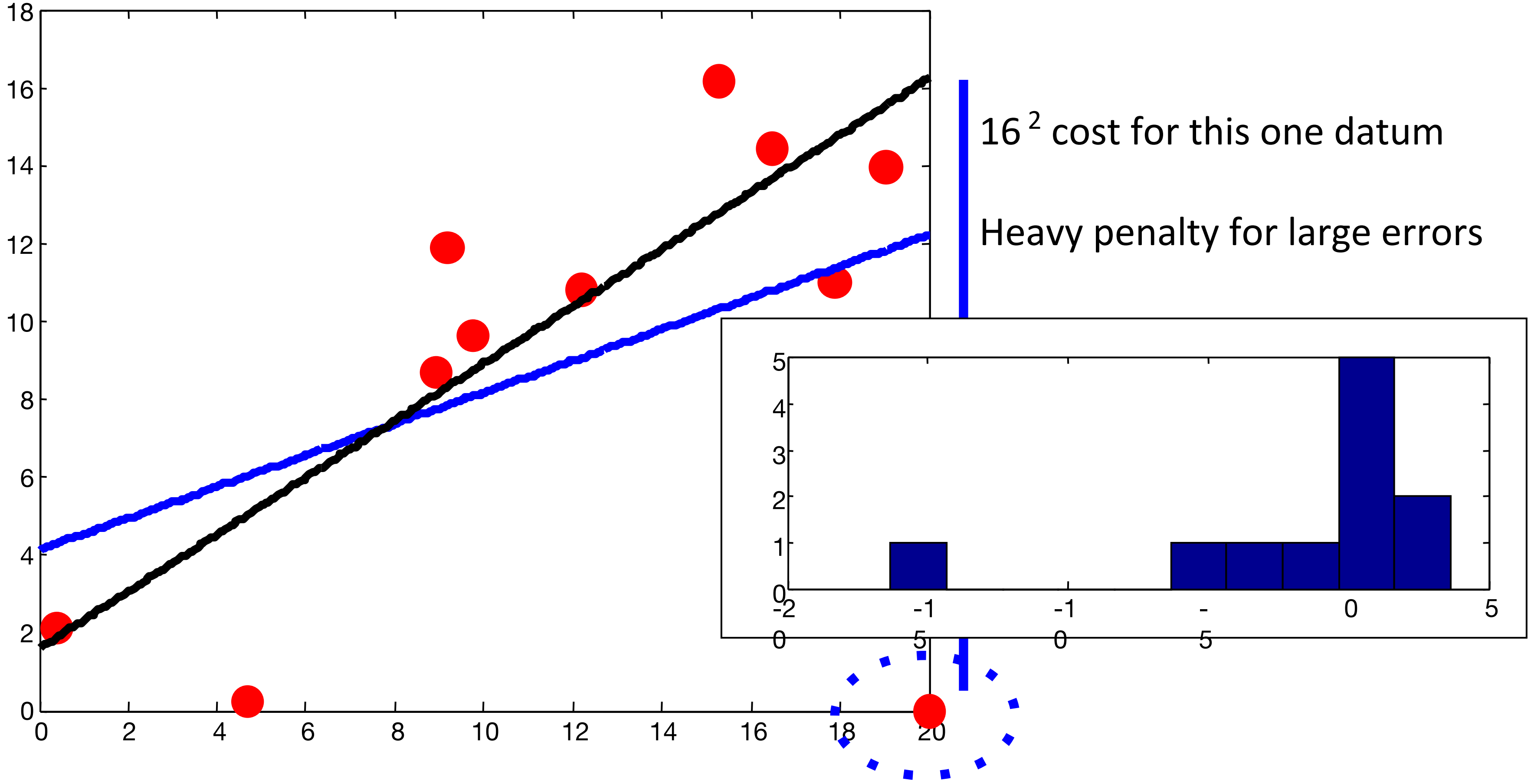
$$\underline{x}_0 = [1 \quad 1 \quad 1]^T \qquad \theta = [1.00 \quad 0.57]$$

$$\underline{x}_1 = [1 \quad 2 \quad 4]^T$$

$$\underline{e} = (y - \hat{y}) = [-0.57 \quad 0.85 \quad -0.28]^T$$

Effects of MSE choice

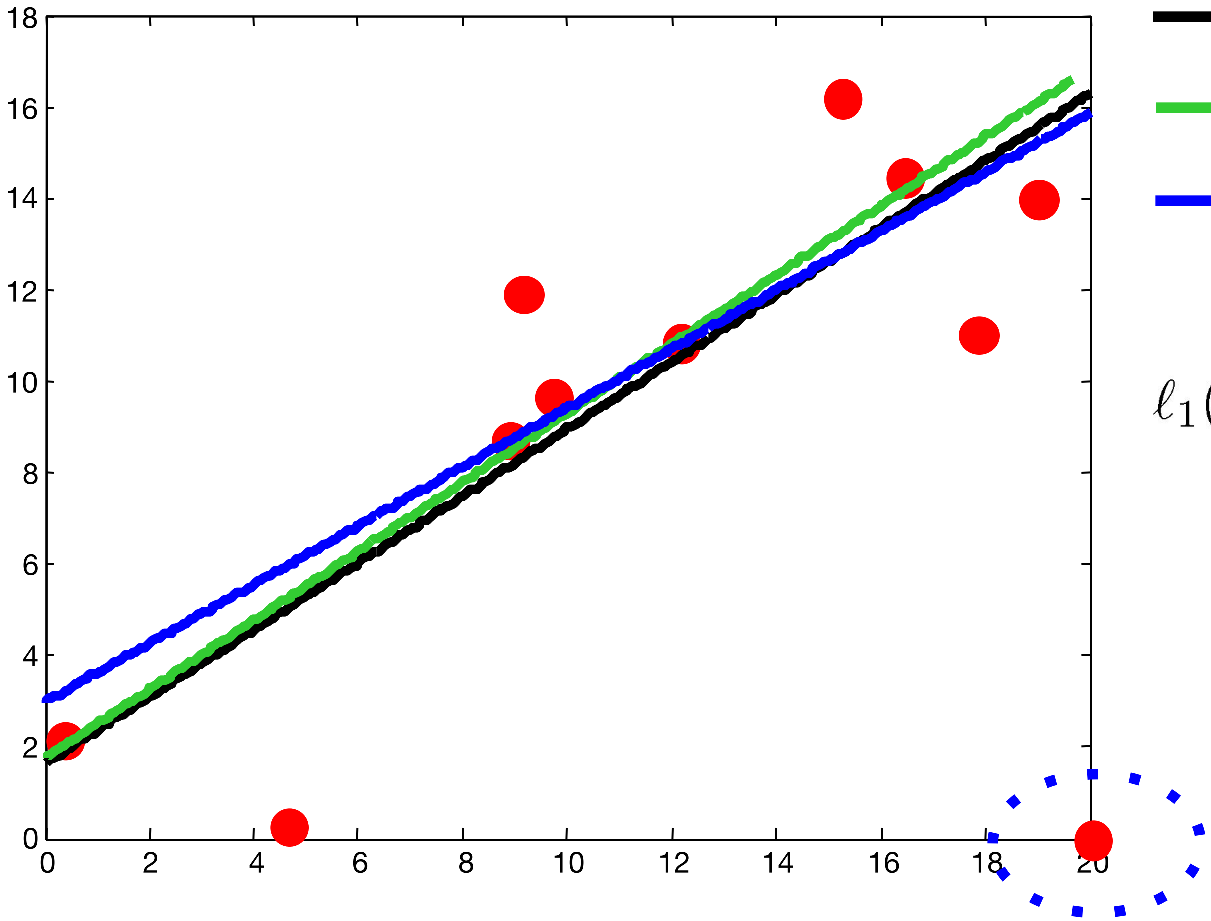
- Sensitivity to outliers



16^2 cost for this one datum

Heavy penalty for large errors

L1 error: Mean Absolute Error



$$\ell_1(\underline{\theta}) = \sum_j |y^{(j)} - \hat{y}(x^{(j)})|$$

$$= \sum_j |y - \underline{\theta} \cdot \underline{x}^T|$$

Cost functions for regression

$\ell_2 \ : \ (y - \hat{y})^2$ **(MSE)**

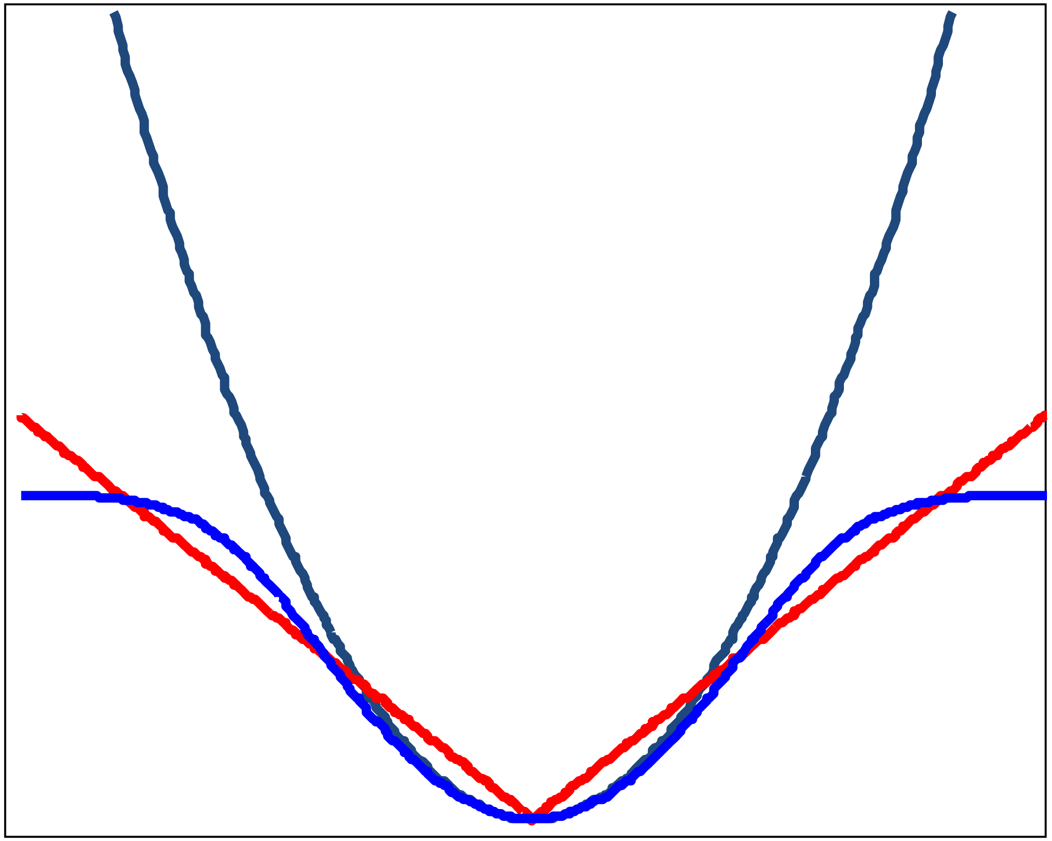
$\ell_1 \ : \ |y - \hat{y}|$ **(MAE)**

Something else entirely…

$c - \log(\exp(-(y - \hat{y})^2) + c)$

(???)

Arbitrary functions cannot be solved in closed form
- use gradient descent

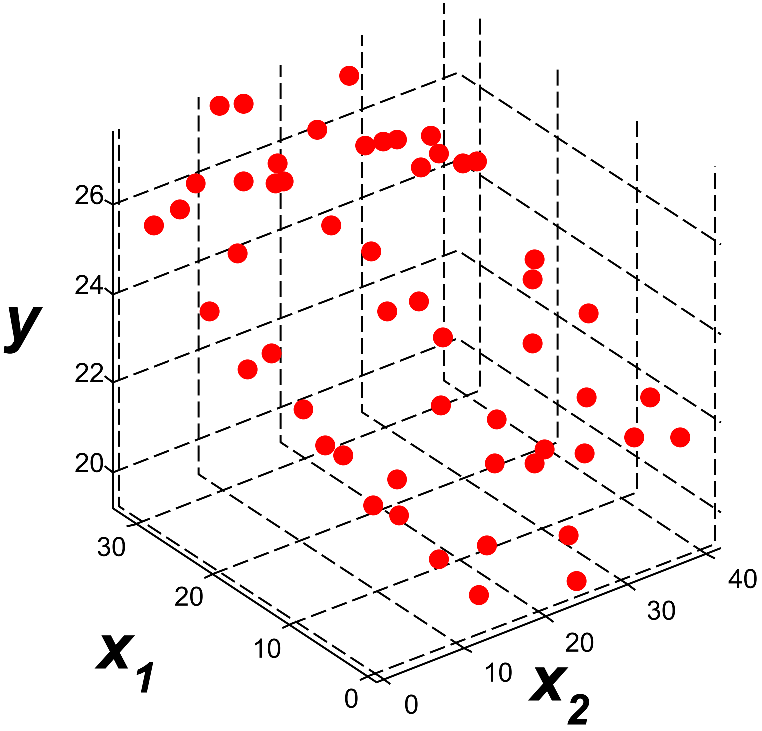


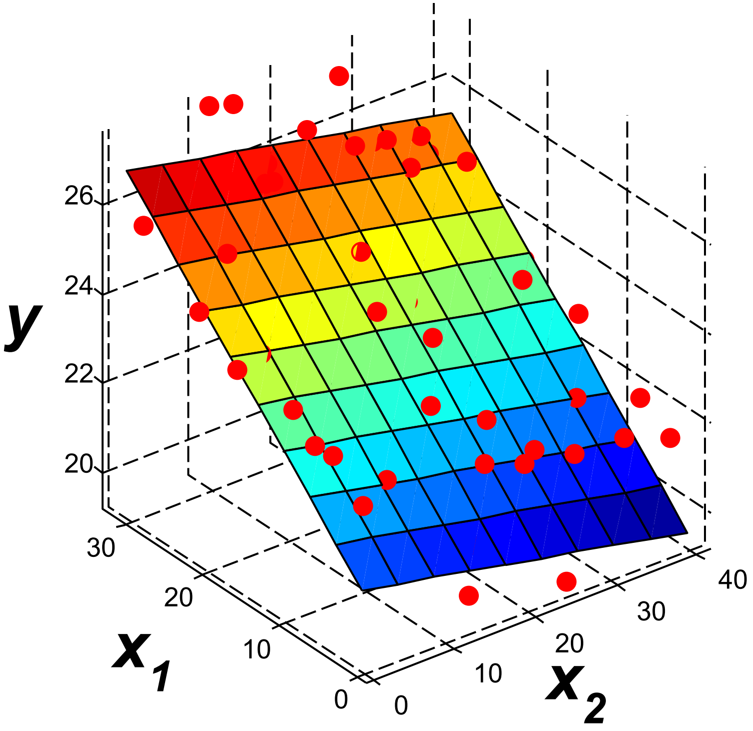
$\leftarrow (y - \hat{y}) \rightarrow$

Machine Learning

- Linear Regression via Least Squares
- Gradient Descent Algorithms
- Direct Minimization of Squared Error
- **Regression with Non-linear Features**
- Bias, Variance, & Validation
- Regularized Linear Regression

More dimensions?





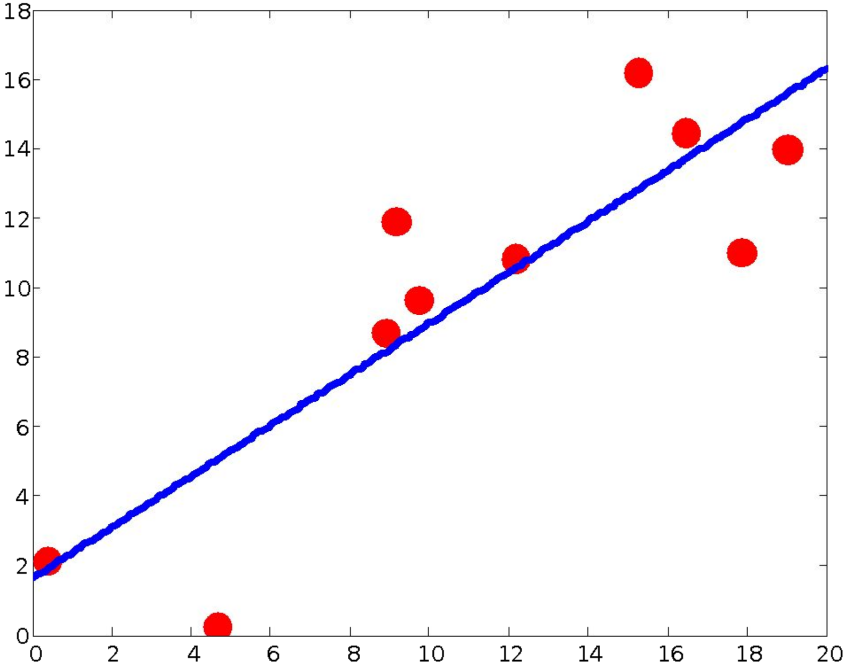
$$\underline{\theta} = [\theta_0 \ \theta_1 \ \theta_2]$$

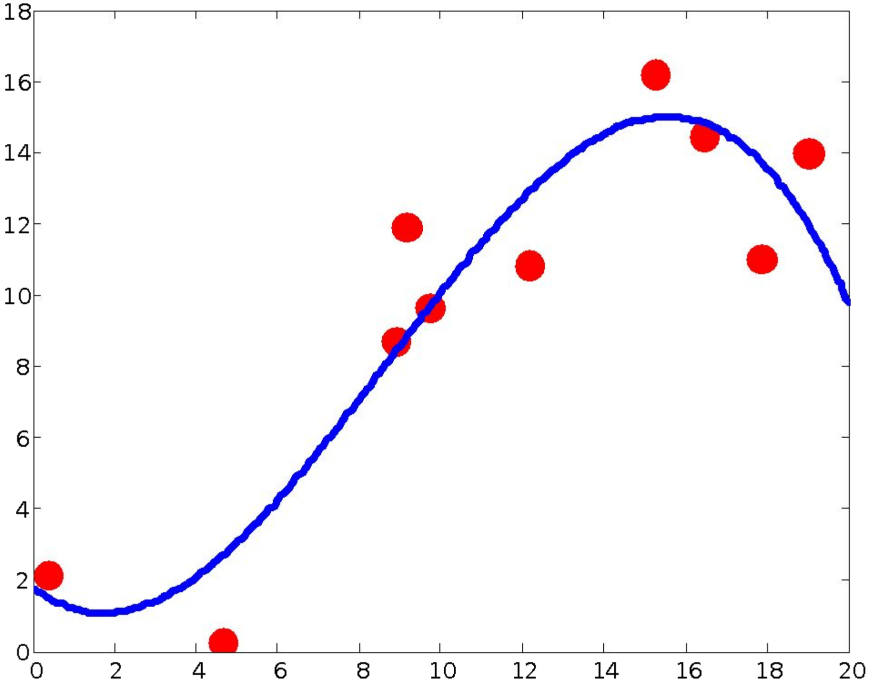
$$\underline{x} = [1 \ x_1 \ x_2]$$

$$\hat{y}(x) = \underline{\theta} \cdot \underline{x}^T$$

Nonlinear functions

- What if our hypotheses are not lines?
    - Ex: higher-order polynomials





Nonlinear functions

- Single feature x, predict target y:

$$D = \{(x^{(j)}, y^{(j)})\}$$

$$\Downarrow$$

Add features:

$$D = \{([x^{(j)}, (x^{(j)})^2, (x^{(j)})^3], y^{(j)})\}$$

$$\hat{y}(x) = \theta_0 + \theta_1\, x + \theta_2\, x^2 + \theta_3\, x^3$$

$$\Downarrow$$

$$\hat{y}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3$$

Linear regression in new features

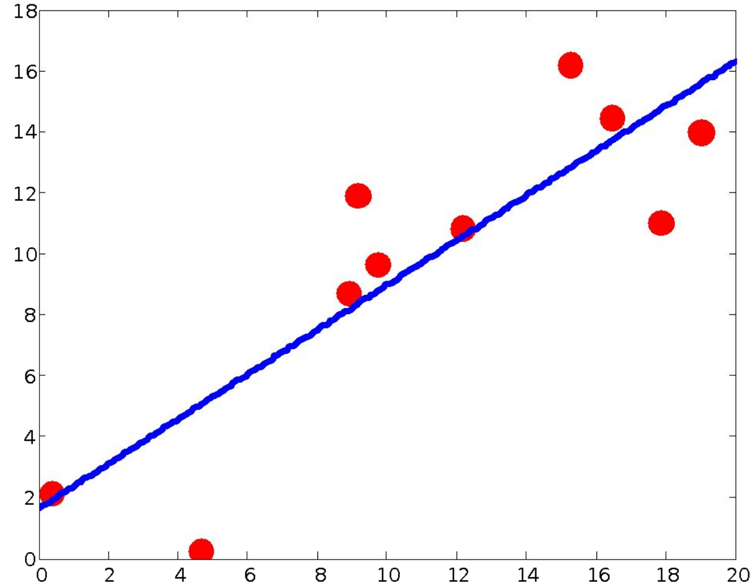
- Sometimes useful to think of “feature transform”

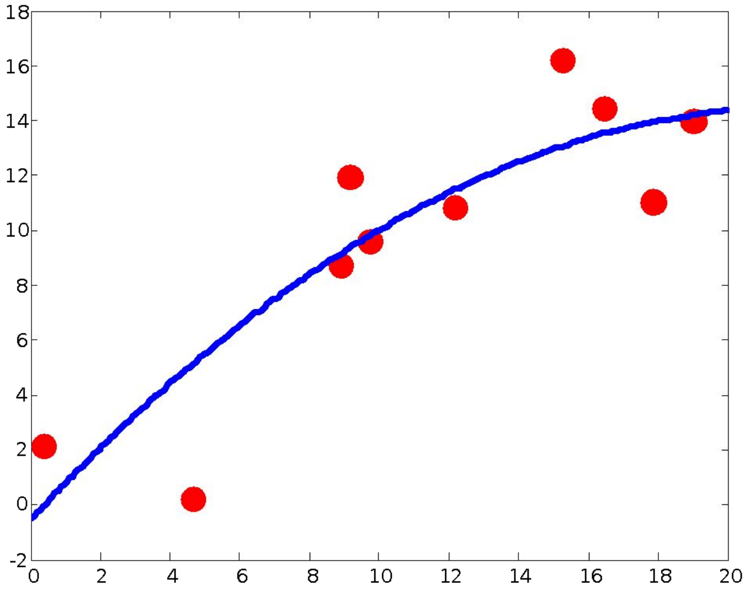
$$\Phi(x) = \left[1\,,\, x\,,\, x^2\,,\, x^3\,,\, \ldots\right]$$

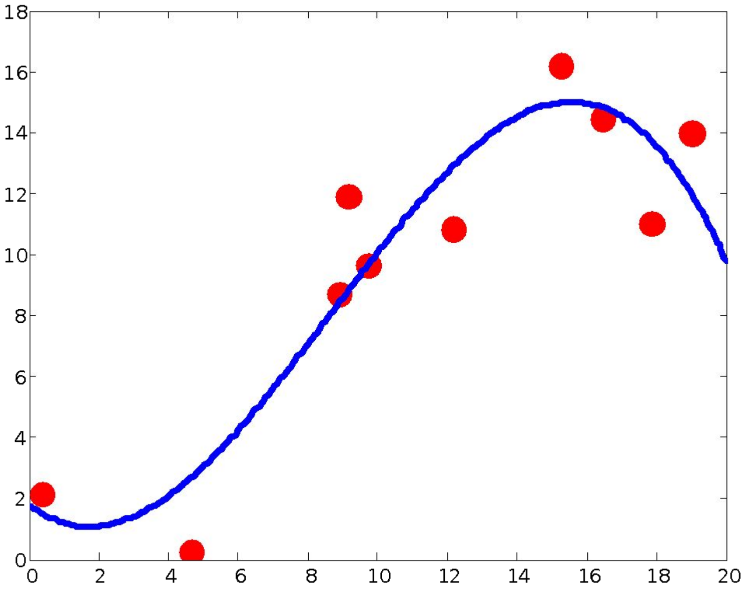
$$\hat{y}(x) = \underline{\theta} \cdot \Phi(x)$$

Higher-order polynomials

- Fit in the same way
- More “features”







Features

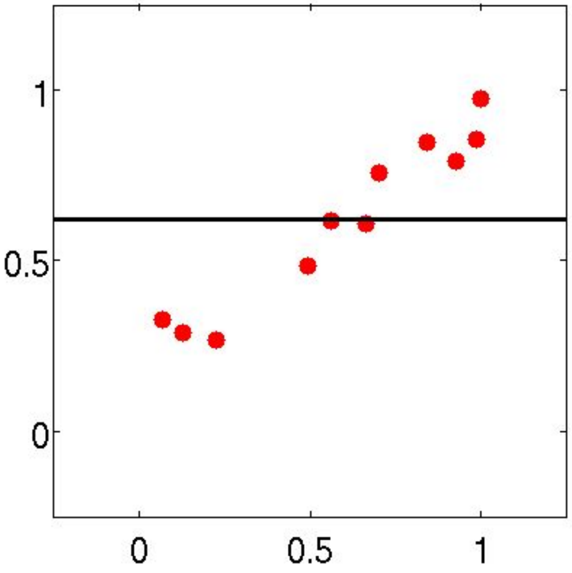
- In general, can use any features we think are useful

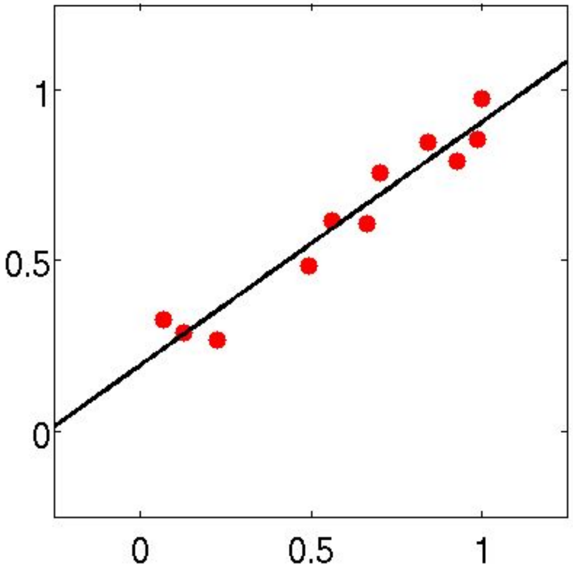
- Other information about the problem
  - Anything you can encode as fixed-length vectors of numbers
- Polynomial functions
  - Features $[1, x, x^2, x^3, \ldots]$
- Other functions
  - $1/x$, $\mathrm{sqrt}(x)$, $x_1 * x_2$, …

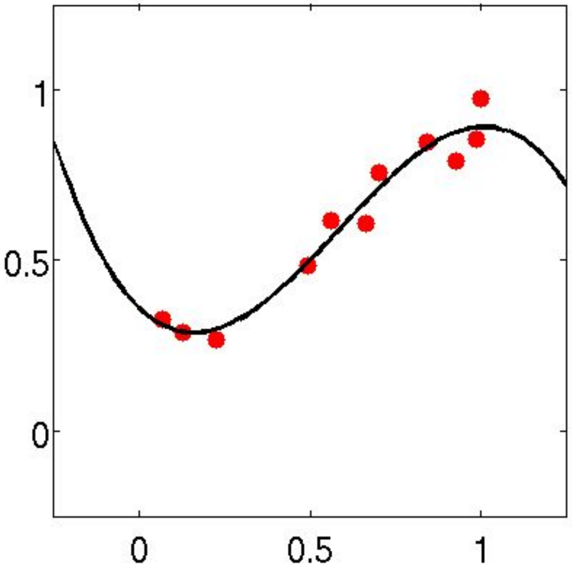
- “Linear regression” = linear in the parameters
  - Features we can make as complex as we want!

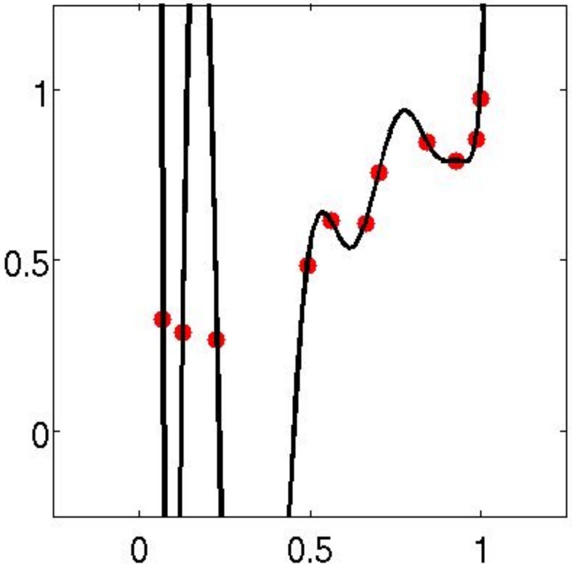
Higher-order polynomials

- Are more features better?
- “Nested” hypotheses
  - 2nd order more general than 1st,
  - 3rd order more general than 2nd, …
- Fits the observed data better



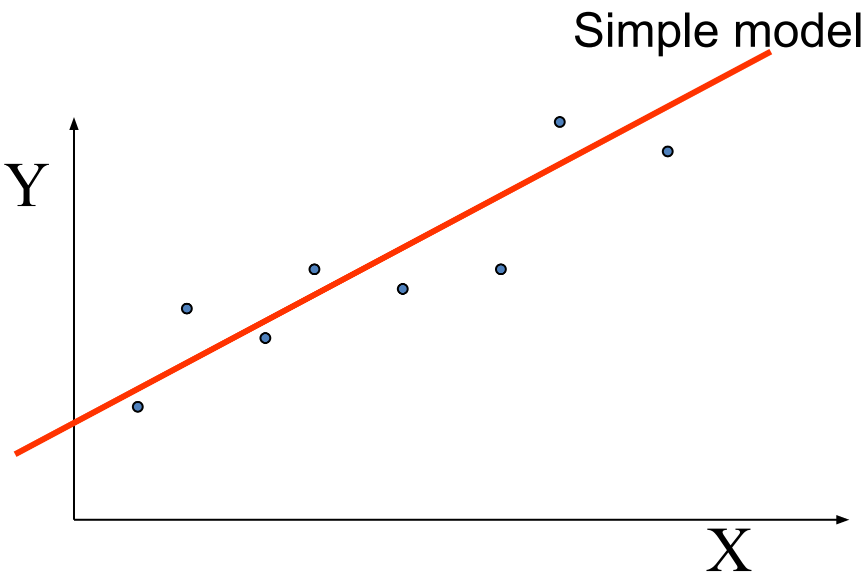


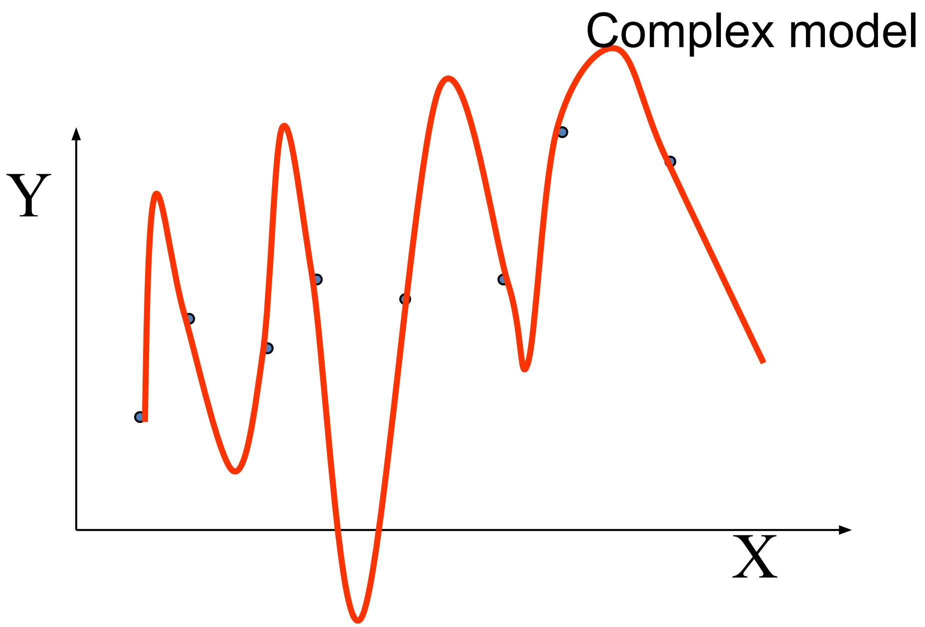




Overfitting and complexity

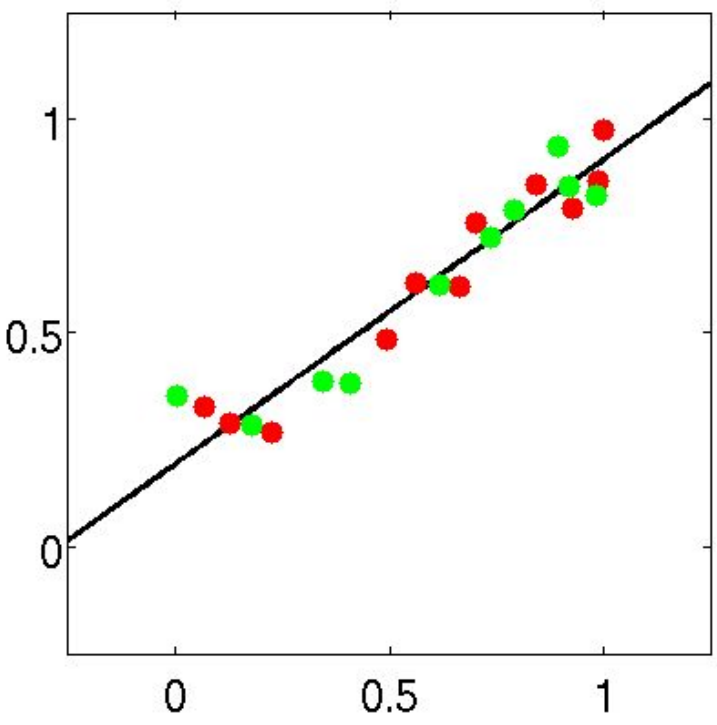
- More complex models will always fit the training data better
- But they may “overfit” the training data, learning complex relationships that are not really present

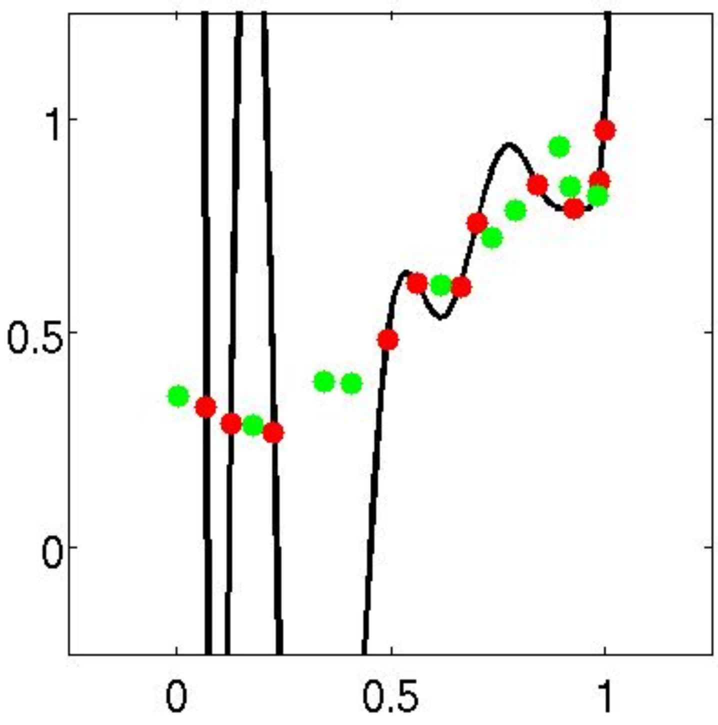




Test data

- After training the model
- Go out and get more data from the world
  - New observations (x,y)
- How well does our model perform?

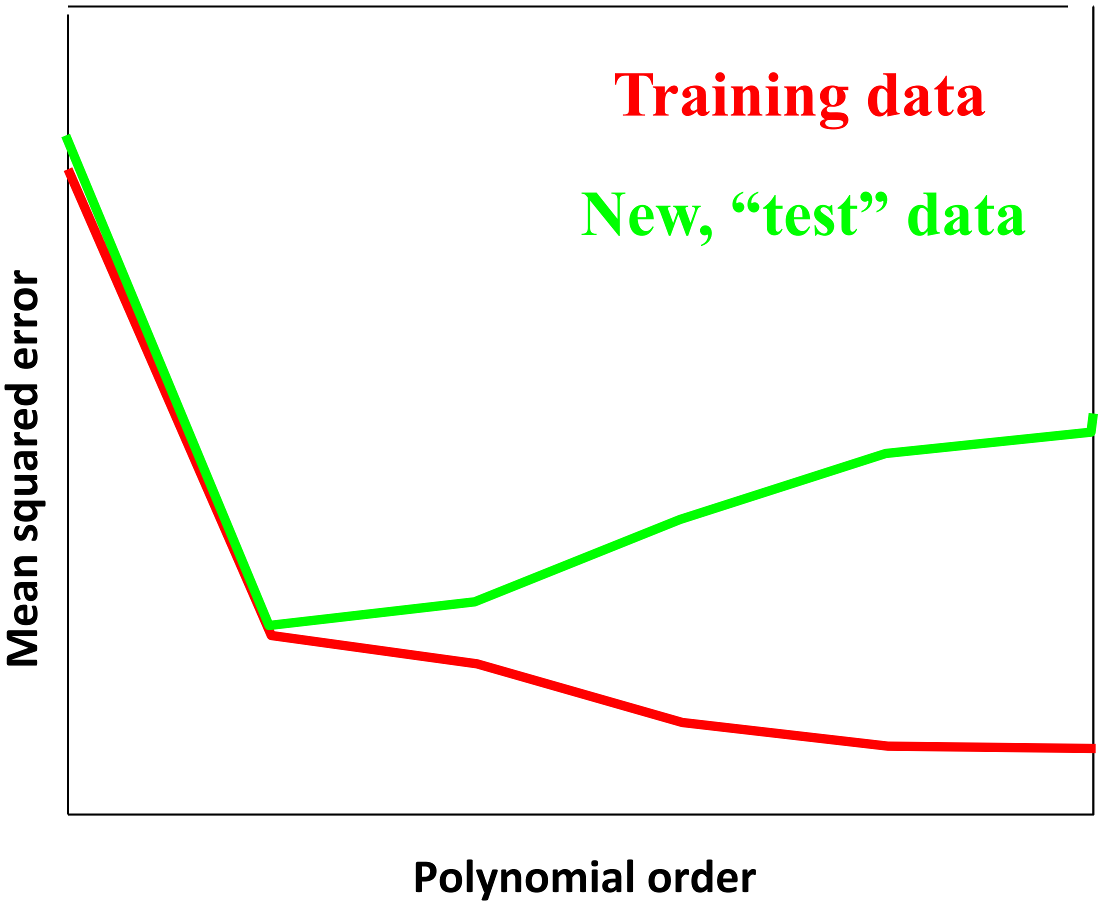




Training versus test error

- Plot MSE as a function of model complexity
  - Polynomial order
- Decreases
  - More complex function fits training data better
- What about new data?

  - 0^{th} to 1^{st} order
    - Error decreases
    - Underfitting
  - Higher order
    - Error increases
    - Overfitting



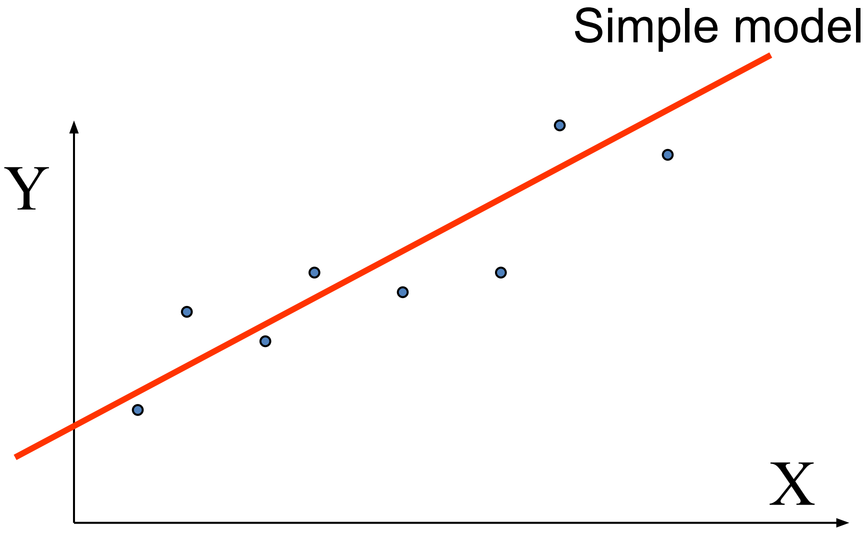
Machine Learning

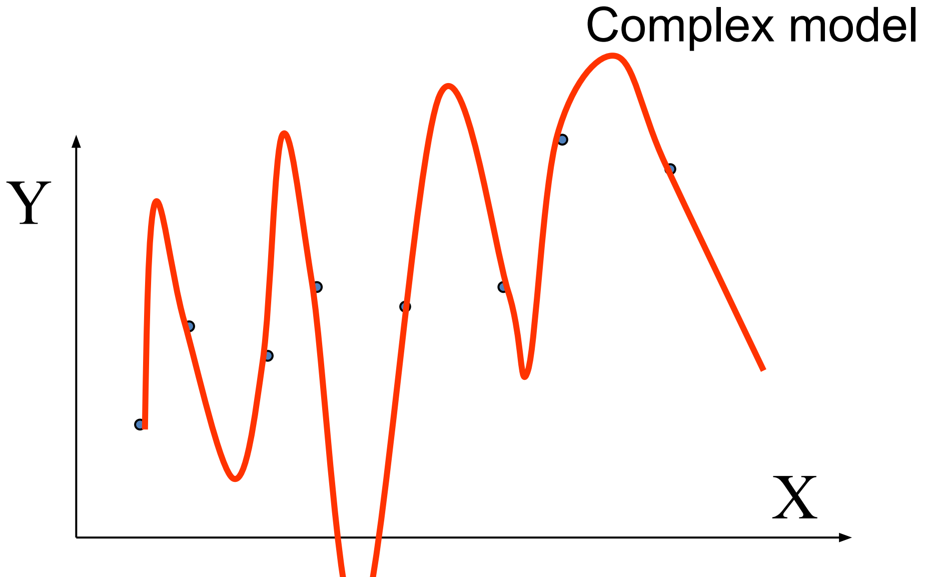
- Linear Regression via Least Squares
- Gradient Descent Algorithms
- Direct Minimization of Squared Error
- Regression with Non-linear Features
- **Bias, Variance, & Validation**
- Regularized Linear Regression

Inductive bias

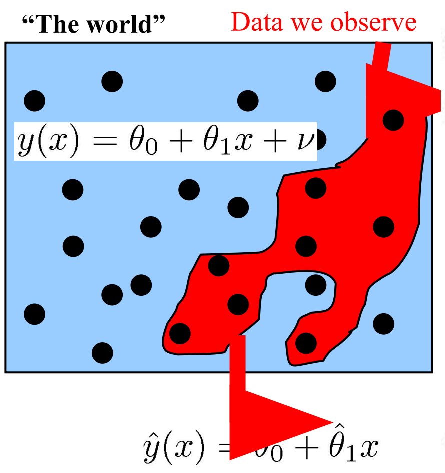
- The assumptions needed to predict examples we haven't seen
- Makes us "prefer" one model over another
- Polynomial functions; smooth functions; etc

- Some bias is necessary for learning!





Bias & variance



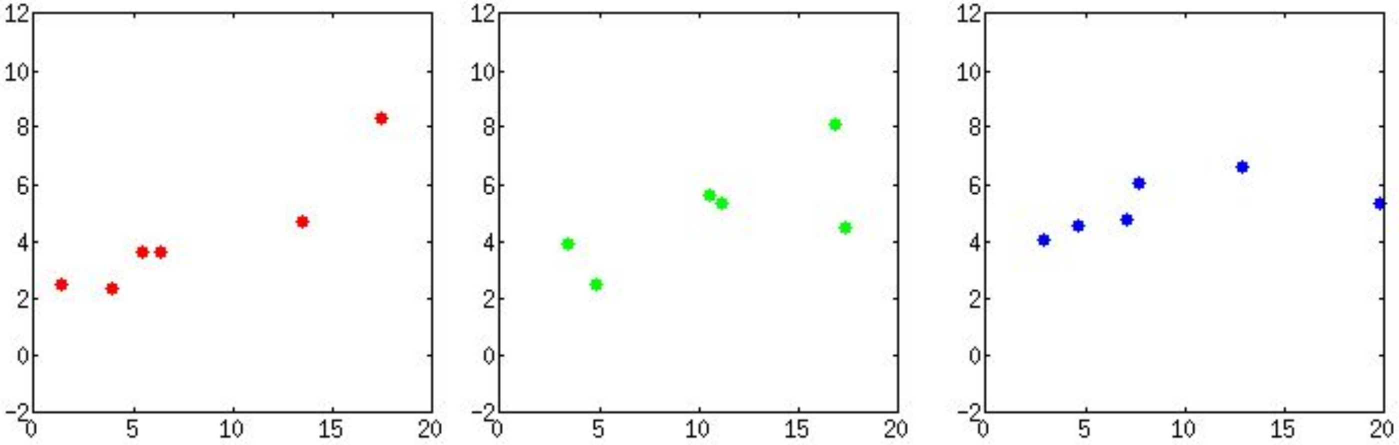
“The world”

Data we observe

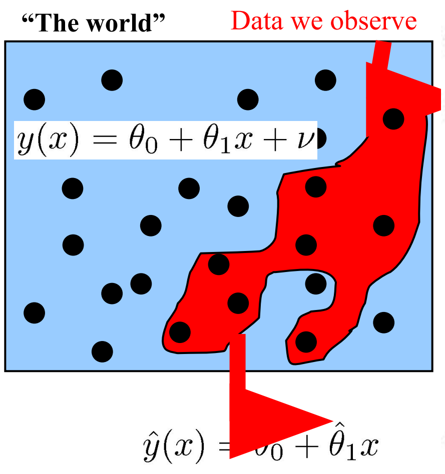
$y(x) = \theta_0 + \theta_1 x + \nu$

$\hat{y}(x) = \hat{\theta}_0 + \hat{\theta}_1 x$

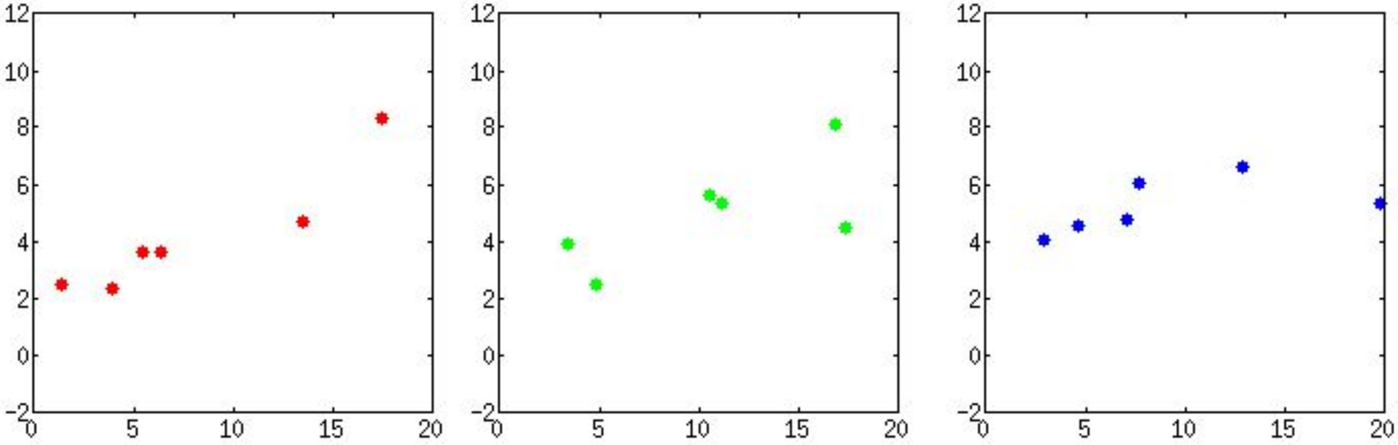
Three different possible data sets:



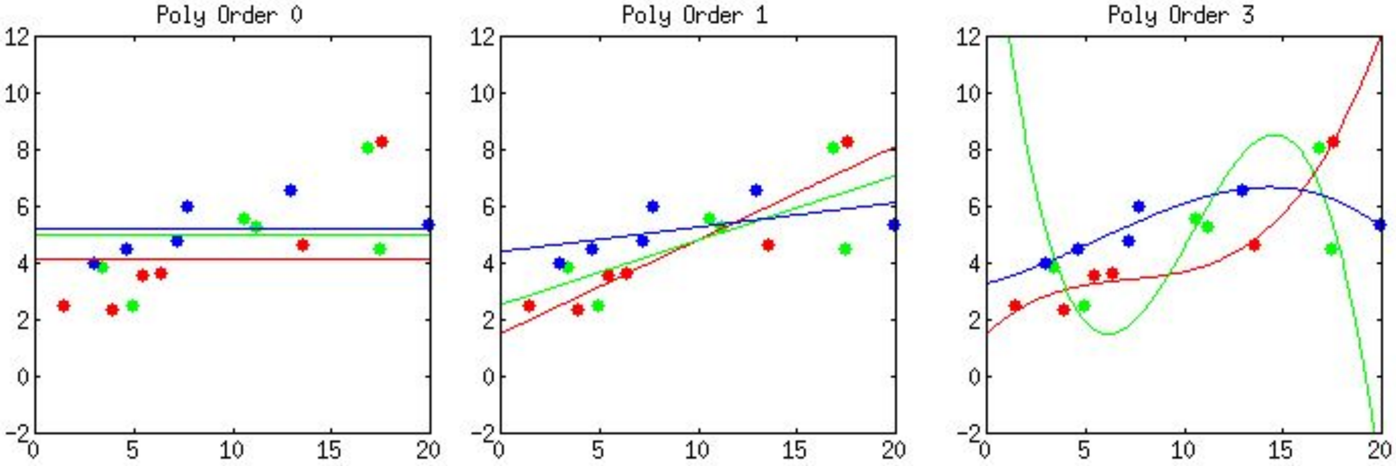
Bias & variance


"The world"
Data we observe
$y(x) = \theta_0 + \theta_1 x + \nu$
$\hat{y}(x) = \hat{\theta}_0 + \hat{\theta}_1 x$

Three different possible data sets:



Each would give different predictors for any polynomial degree:



Detecting overfitting

- Overfitting effect
  - Do better on training data than on future data
  - Need to choose the “right” complexity

- One solution: “Hold-out” data
- Separate our data into two sets
  - Training
  - Test
- Learn only on training data
- Use test data to estimate generalization quality
  - Model selection

- All good competitions use this formulation
  - Often multiple splits: one by judges, then another by you

Model selection

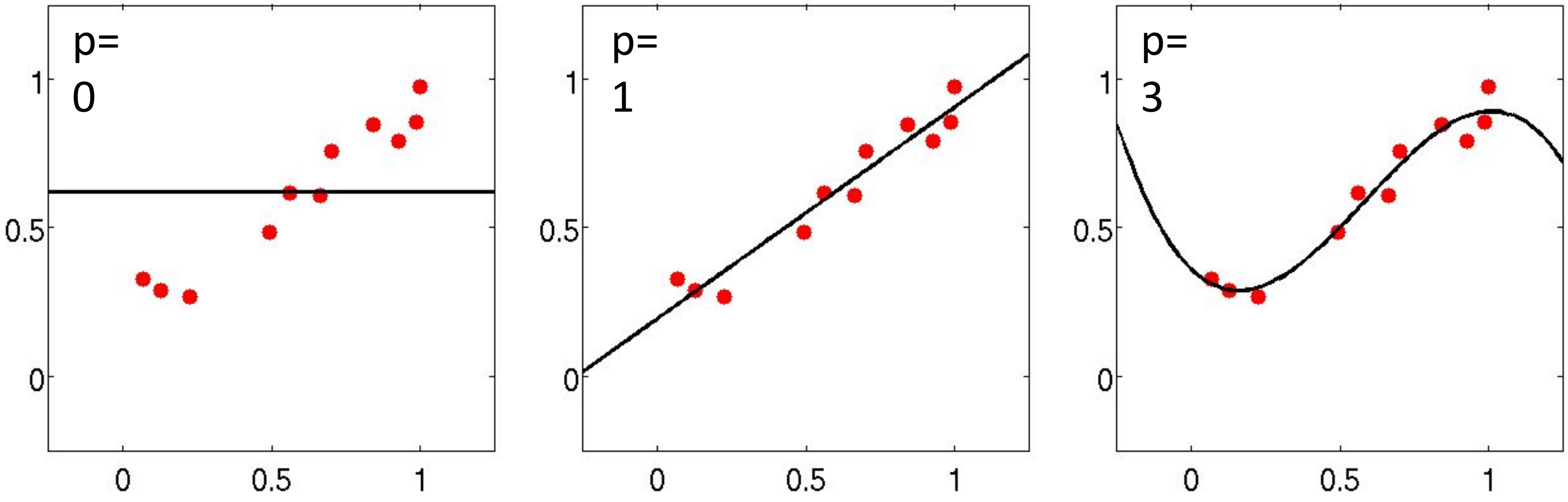
- Which of these models fits the data best?
  - p=0 (constant); p=1 (linear); p=3 (cubic); …
- Or, should we use KNN? Other methods?

- Model selection problem
  - Can't use training data to decide (esp. if models are nested!)

- Want to estimate

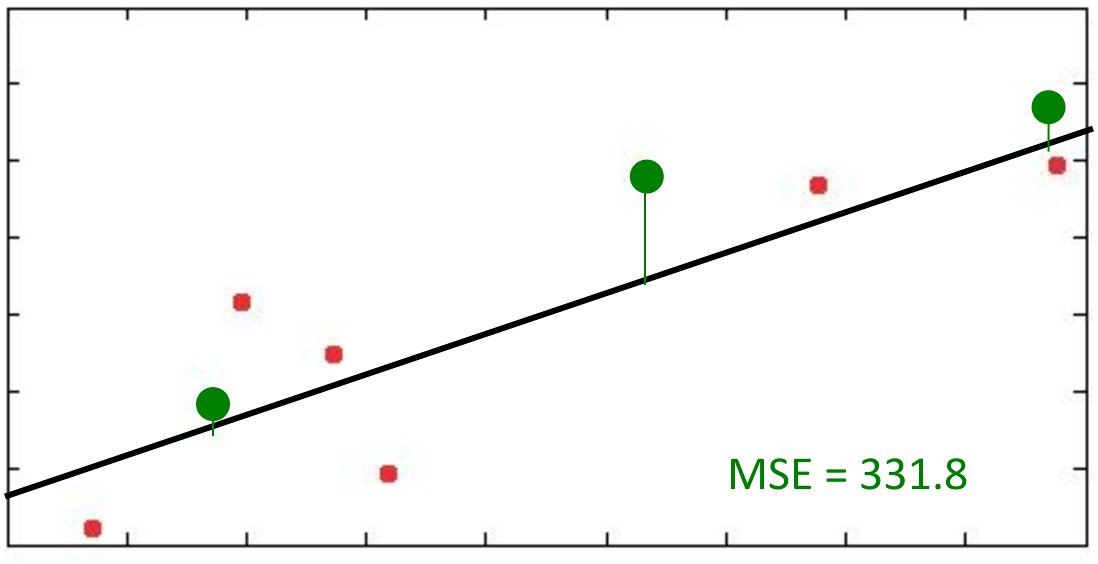
$$\mathbb{E}_{(x,y)}[J(y, \hat{y}(x\,;\; D))]$$

J = loss function (MSE)
D = training data set



Hold-out method

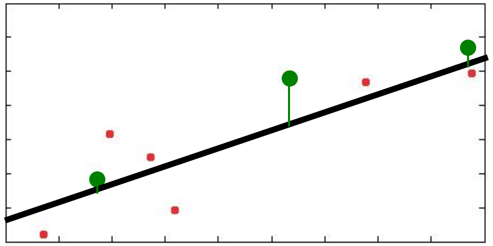
- Validation data
  - “Hold out” some data for evaluation (e.g., 70/30 split)
  - Train only on the remainder
- Some problems, if we have few data:
  - Few data in hold-out: noisy estimate of the error
  - More hold-out data leaves less for training!



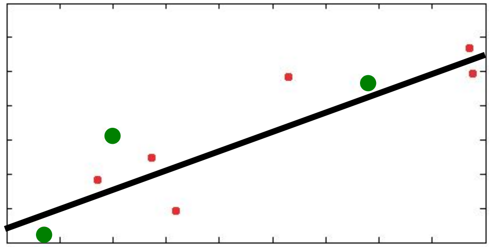
	$x^{(i)}$	$y^{(i)}$
Training data	88	79
	32	-2
	27	30
	68	73
	7	-16
	20	43
Validation data	53	77
	17	16
	87	94

Cross-validation method

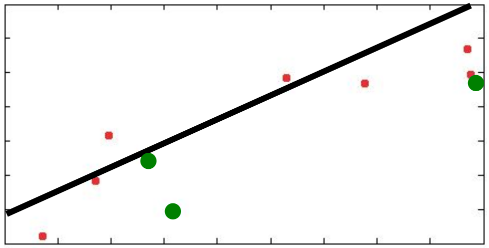
- K-fold cross-validation
  - Divide data into K disjoint sets
  - Hold out one set (= M / K data) for evaluation
  - Train on the others (= M*(K-1) / K data)



Split 1:
MSE = 331.8



Split 2:
MSE = 361.2



Split 3:
MSE = 669.8

3-Fold X-Val MSE
= 464.1

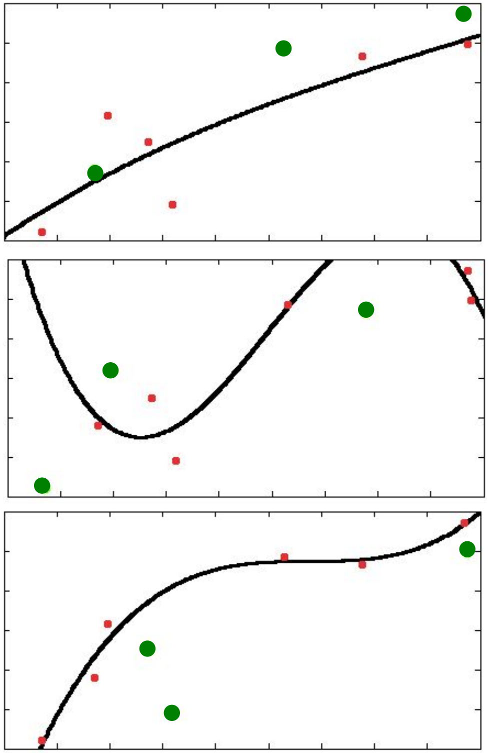
Training data

Validation data

$x^{(i)}$	$y^{(i)}$
88	79
32	-2
27	30
68	73
7	-16
20	43
53	77
17	16
87	94

Cross-validation method

- K-fold cross-validation
  - Divide data into K disjoint sets
  - Hold out one set (= M / K data) for evaluation
  - Train on the others (= M*(K-1) / K data)



Split 1:
MSE = 280.5

Split 2:
MSE = 3081.3

Split 3:
MSE = 1640.1

3-Fold X-Val MSE
= 1667.3

Training
data

Validation
data

$x^{(i)}$	$y^{(i)}$
88	79
32	-2
27	30
68	73
7	-16
20	43
53	77
17	16
87	94

Cross-validation

- Advantages:
  - Lets us use more (M) validation data

    (= less noisy estimate of test performance)

- Disadvantages:
  - More work
    - Trains K models instead of just one
  - Doesn't evaluate any *particular* predictor
    - Evaluates K different models & averages
    - Scores *hyperparameters / procedure*, not an actual, specific predictor!

- Also: still estimating error for M' < M data…

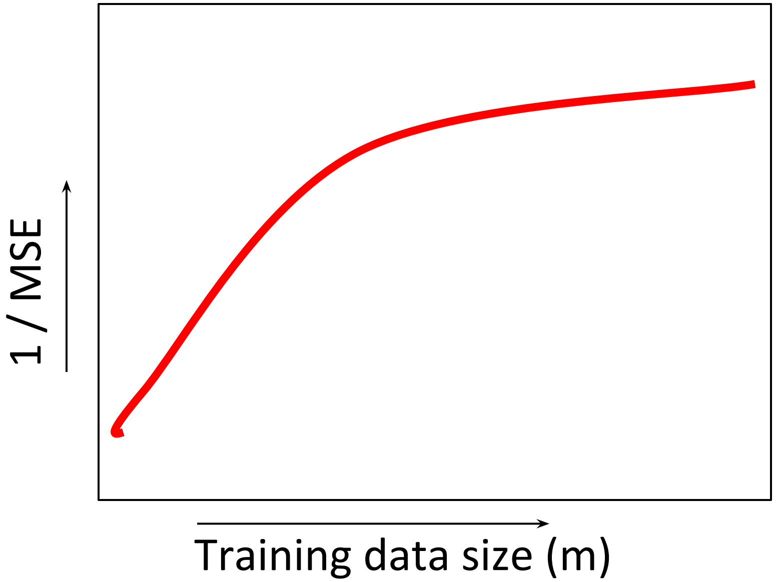
Learning curves

- Plot performance as a function of training size
  - Assess impact of fewer data on performance

    Ex: MSE0 - MSE (regression)

    or 1-Err (classification)

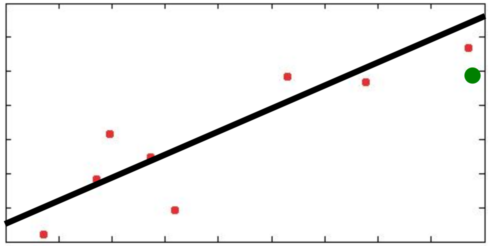
- Few data
  - More data significantly improve performance
- “Enough” data
  - Performance saturates



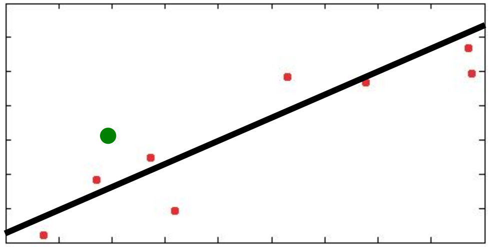
- If slope is high, decreasing *m* (for validation / cross-validation) might have a big impact…

Leave-one-out cross-validation

- When K=M (# of data), we get
  - Train on all data except one
  - Evaluate on the left-out data
  - Repeat M times (each data point held out once) and average



MSE = …



MSE = …

⋮

➡ LOO X-Val MSE = …

Training data

Validation data

$x^{(i)}$	$y^{(i)}$
88	79
32	-2
27	30
68	73
7	-16
20	43
53	77
17	16
87	94

Cross-validation Issues

- Need to balance:
  - Computational burden (multiple trainings)
  - Accuracy of estimated performance / error
- Single hold-out set:
  - Estimates performance with M' < M data (important? learning curve?)
  - Need enough data to trust performance estimate
  - Estimates performance of a particular, trained learner
- K-fold cross-validation
  - K times as much work, computationally
  - Better estimates, still of performance with M' < M data
- Leave-one-out cross-validation
  - M times as much work, computationally
  - M' = M-1, but overall error estimate may have high variance

Machine Learning

Linear Regression via Least Squares

Gradient Descent Algorithms

Direct Minimization of Squared Error

Regression with Non-linear Features

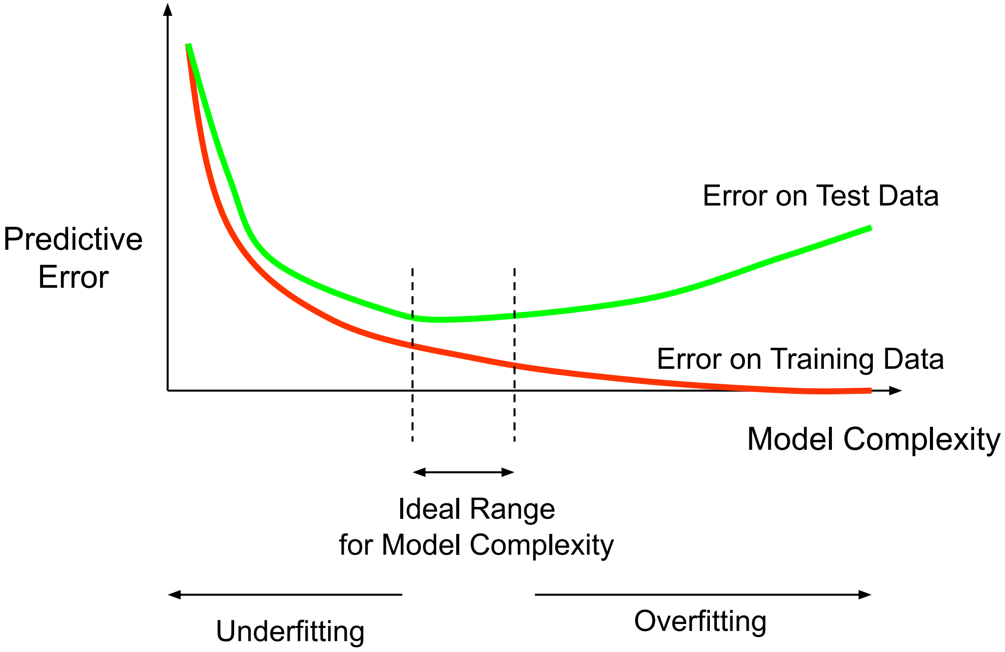
Bias, Variance, & Validation

Regularized Linear Regression

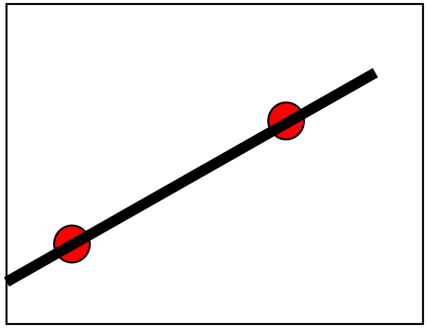
What to do about under/overfitting?

- Ways to increase complexity?
  - Add features, parameters
  - We'll see more…

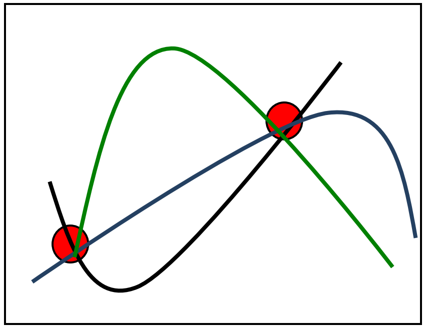
- Ways to decrease complexity?
  - Remove features ("feature selection")
  - "Fail to fully memorize data"
    - Partial training
    - Regularization



Linear regression



- Linear model, two data

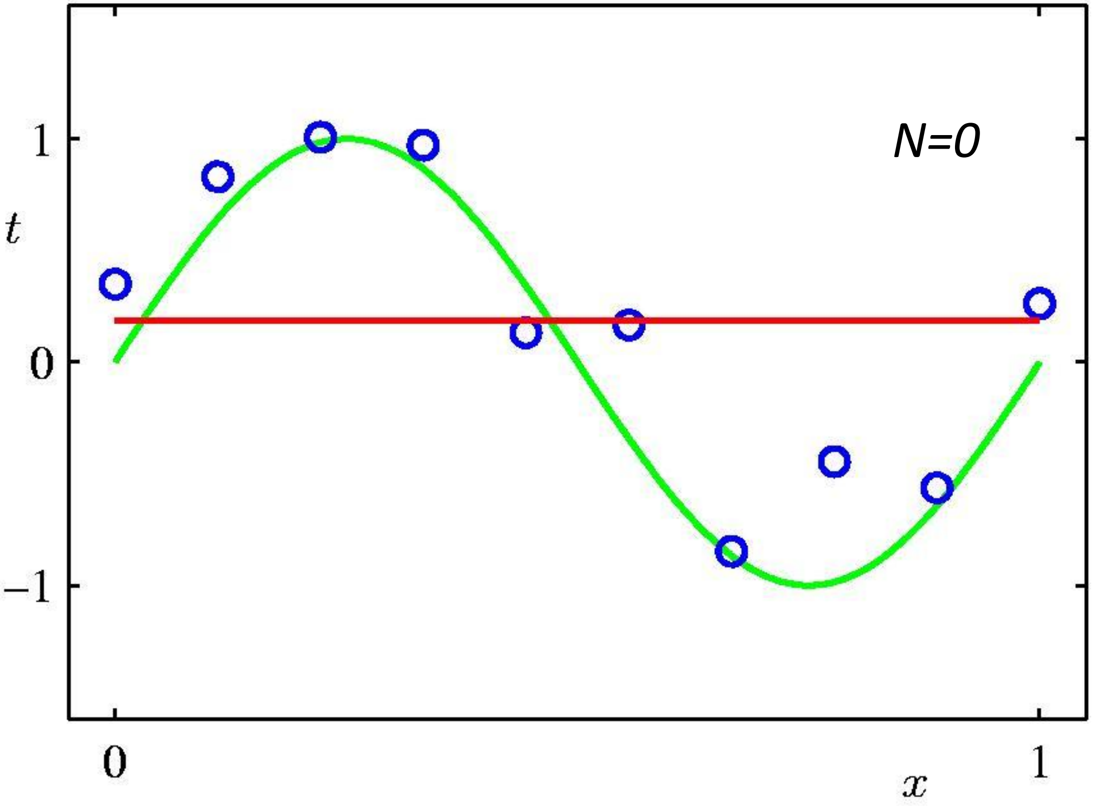


- Quadratic model, two data?
  - Infinitely many settings with zero error
  - How to choose among them?
- Higher order coefficients = 0?
  - Uses knowledge of where features came from…
- Could choose e.g. minimum magnitude:

$$\min \underline{\theta \theta}^T \quad s.t. \quad J(\underline{\theta}) = 0$$

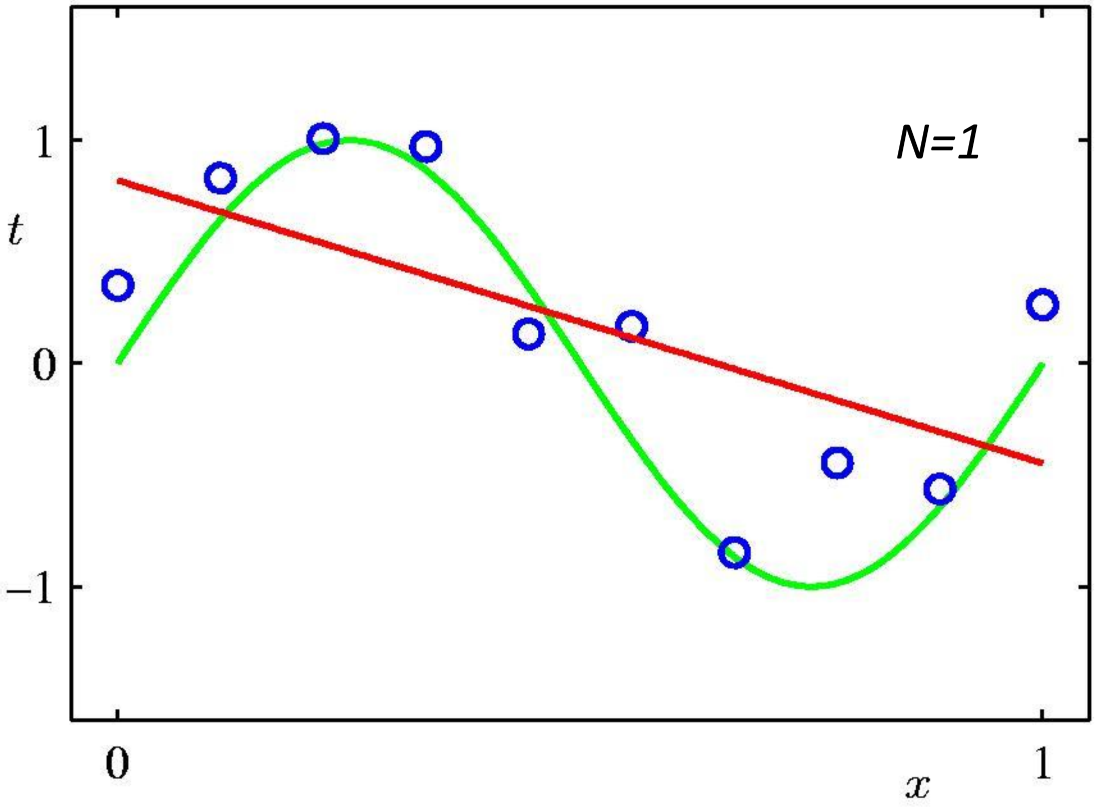
- A type of *bias*: tells us which models to prefer

0^{th} Order Polynomial

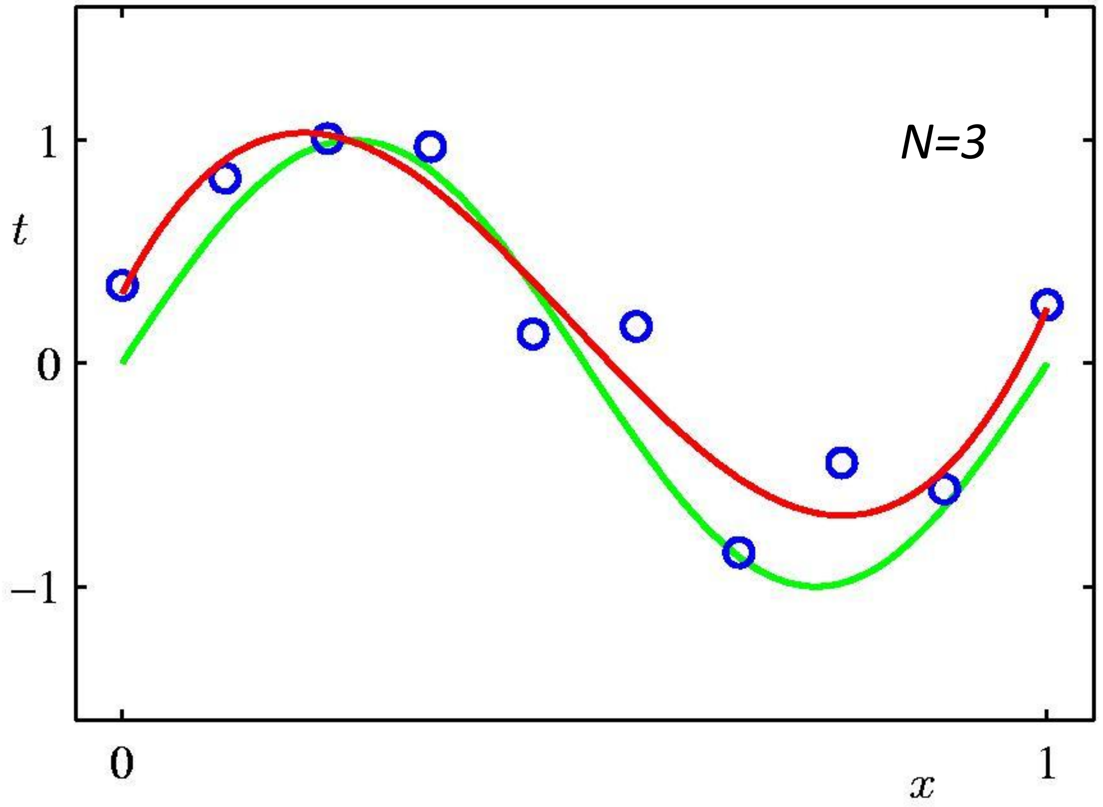


N=0

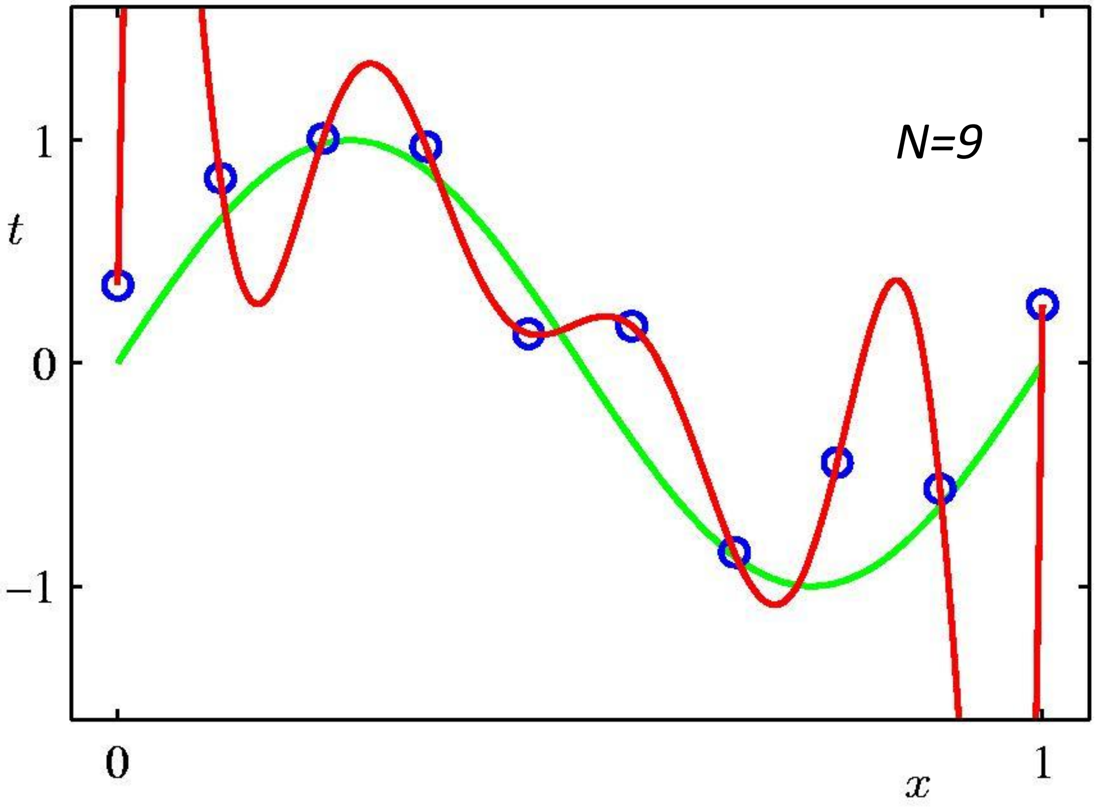
1st Order Polynomial



3^{rd} Order Polynomial

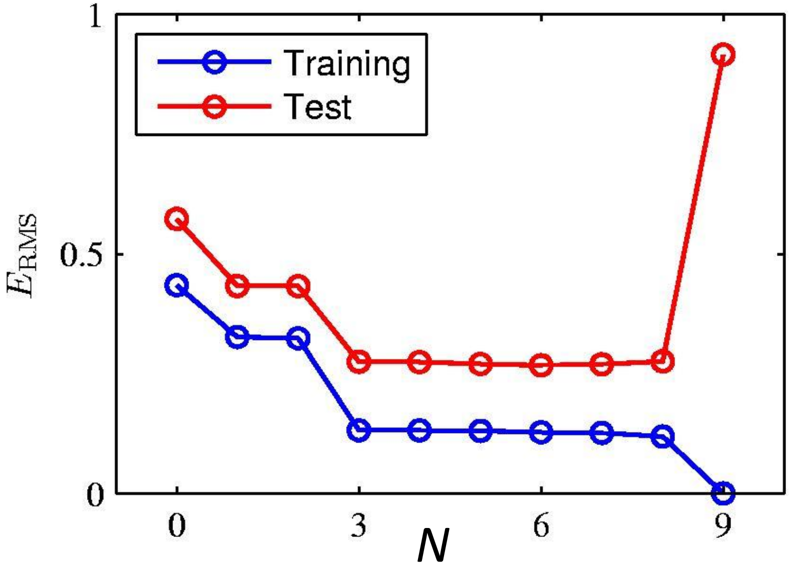


9^{th} Order Polynomial



Estimated Polynomial Coefficients

	N=0	*N=1*	*N=3*	*N=9*
Estimated Regression Coeffients θ	0.19	0.82	0.31	0.35
		-1.27	7.99	232.37
			-25.43	-5321.83
			17.37	48568.31
				-231639.30
				640042.26
				-1061800.52
				1042400.18
				-557682.99
				125201.43



Regularization

- Can modify our cost function J to add "preference" for certain parameter values

$$J(\underline{\theta}) = \frac{1}{2}(\underline{y} - \underline{\theta}\,\underline{X}^T) \cdot (\underline{y} - \underline{\theta}\,\underline{X}^T)^T + \alpha\,\theta\theta^T$$

L$_2$ penalty:
"Ridge regression"

$$\theta\theta^T = \sum_i \theta_i^2$$

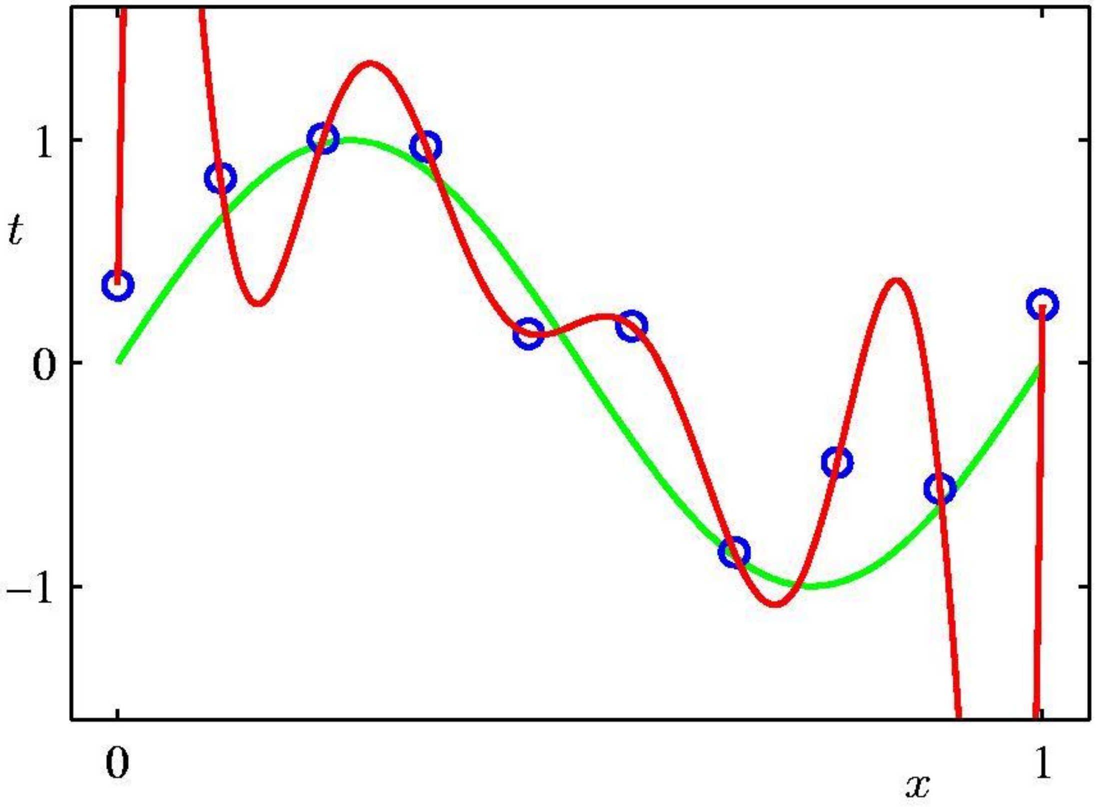
- New solution (derive the same way)

$$\underline{\theta} \quad = \quad \underline{y}\,\underline{X}(\underline{X}^T\,\underline{X} + \alpha I)^{-1}$$

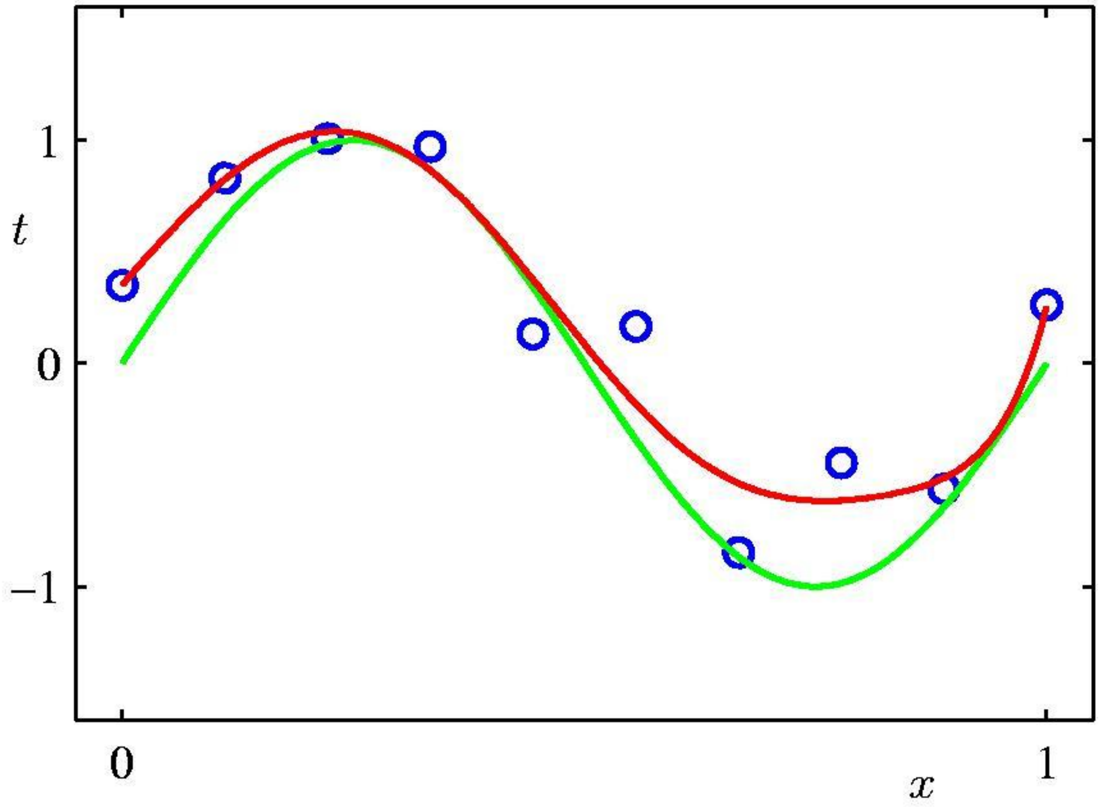
  - Problem is now well-posed for any degree

- Notes:
  - "Shrinks" the parameters toward zero
  - Alpha large: we prefer small theta to small MSE
  - Regularization term is independent of the data: paying more attention reduces our model variance

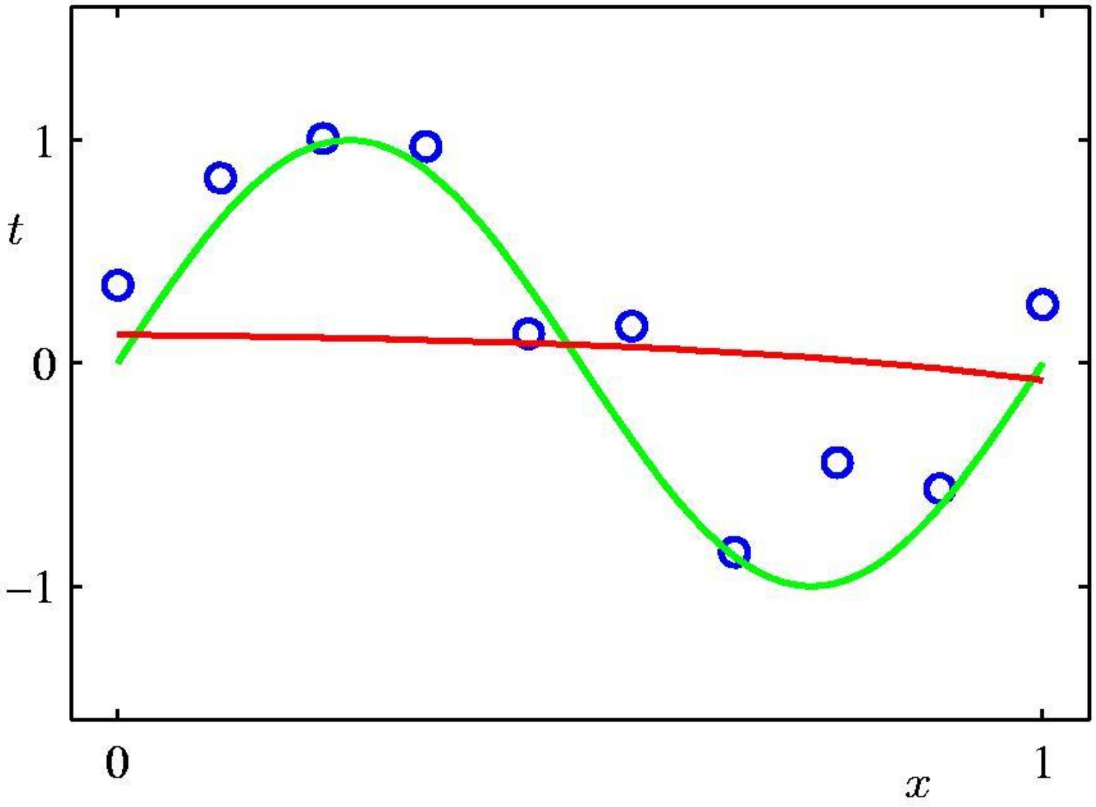
Regression: Zero Regularization



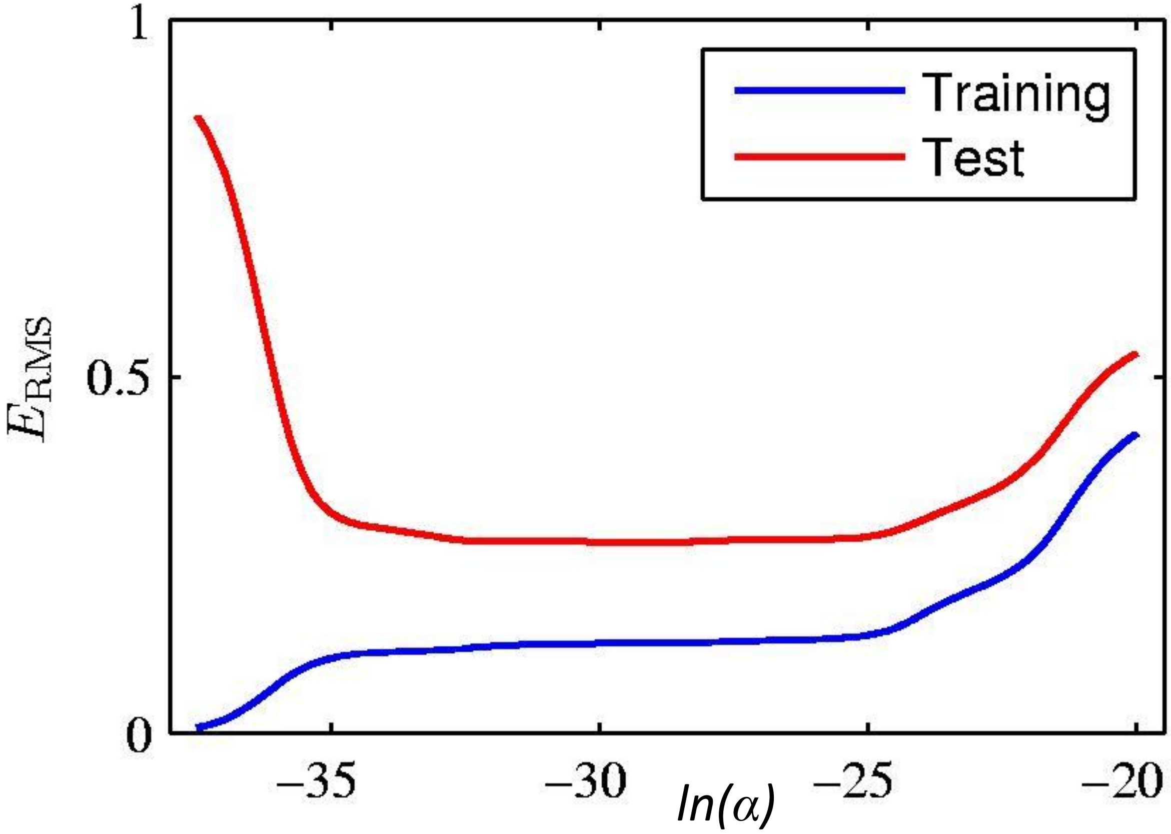
Regression: Moderate Regularization



Regression: Big Regularization



Impact of Regularization Parameter



Estimated Polynomial Coefficients

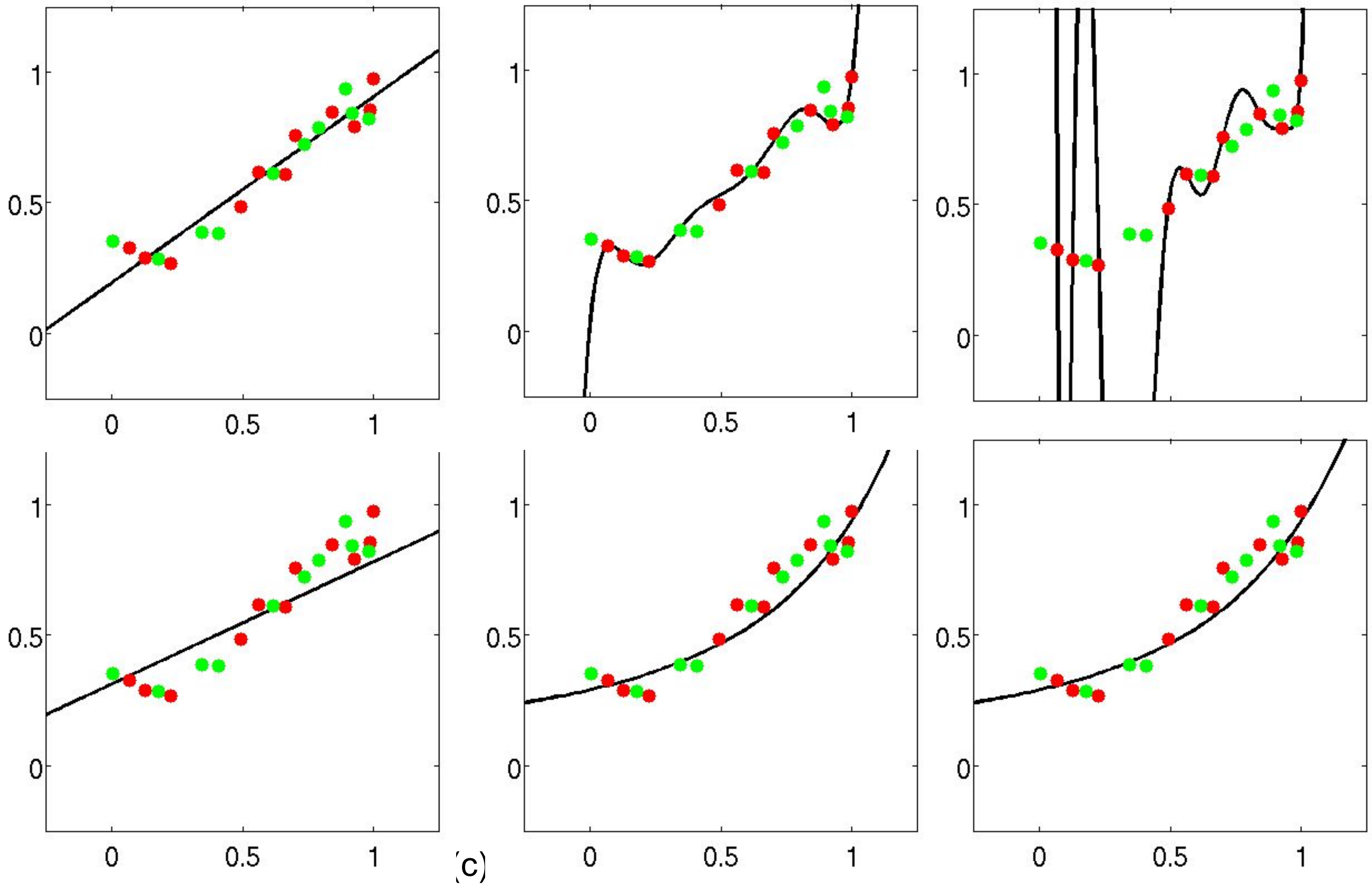
	α zero	α medium	α big
Estimated Regression Coeffients θ	0.35	0.35	0.13
	232.37	4.74	-0.05
	-5321.83	-0.77	-0.06
	48568.31	-31.97	-0.05
	-231639.30	-3.89	-0.03
	640042.26	55.28	-0.02
	-1061800.52	41.32	-0.01
	1042400.18	-45.95	-0.00
	-557682.99	-91.53	0.00
	125201.43	72.68	0.01

Regularization

- Compare between unreg. & reg. results

Alpha =0
(Unregularized)

Alpha =1

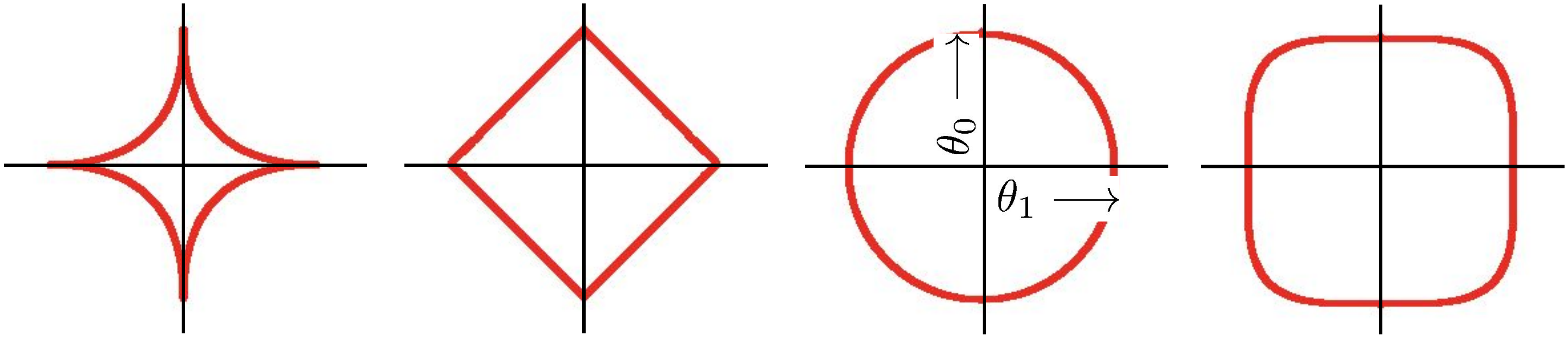


Different regularization functions

- More generally, for the L_p regularizer:

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

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



p=0.5

p=1
Lasso

p=2
Quadratic

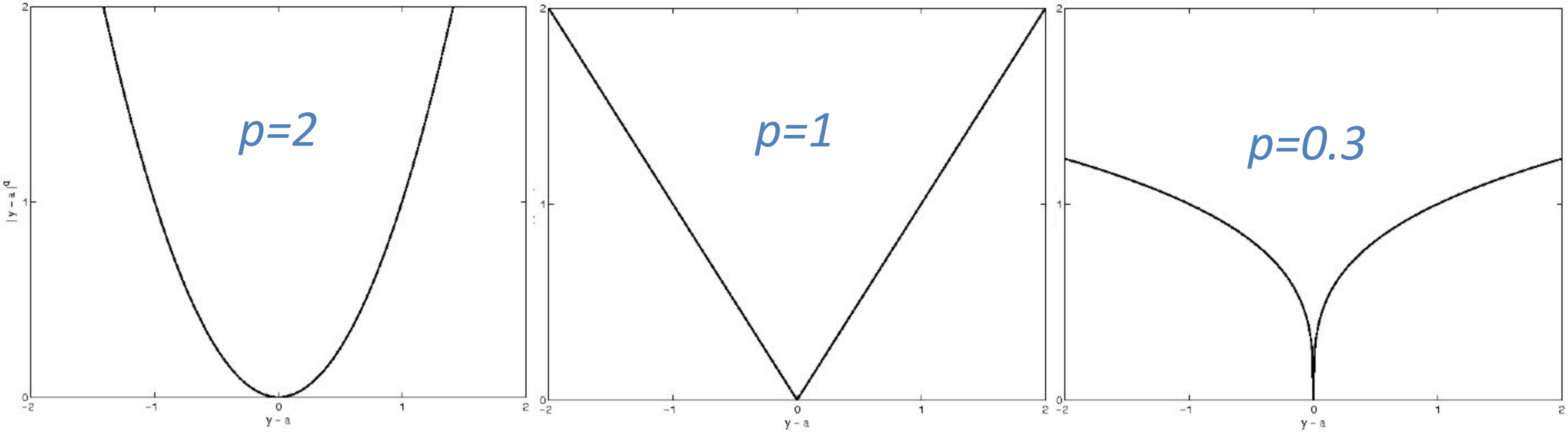
p=4

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

Different regularization functions

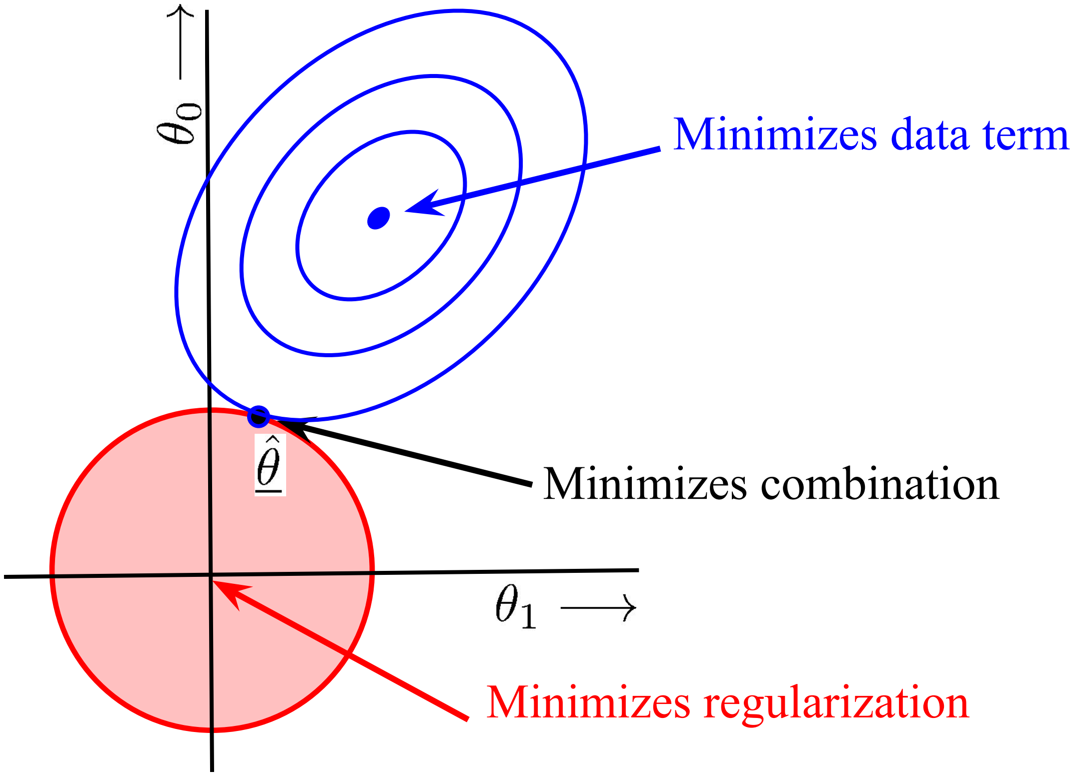
- More generally, for the L_p regularizer:

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



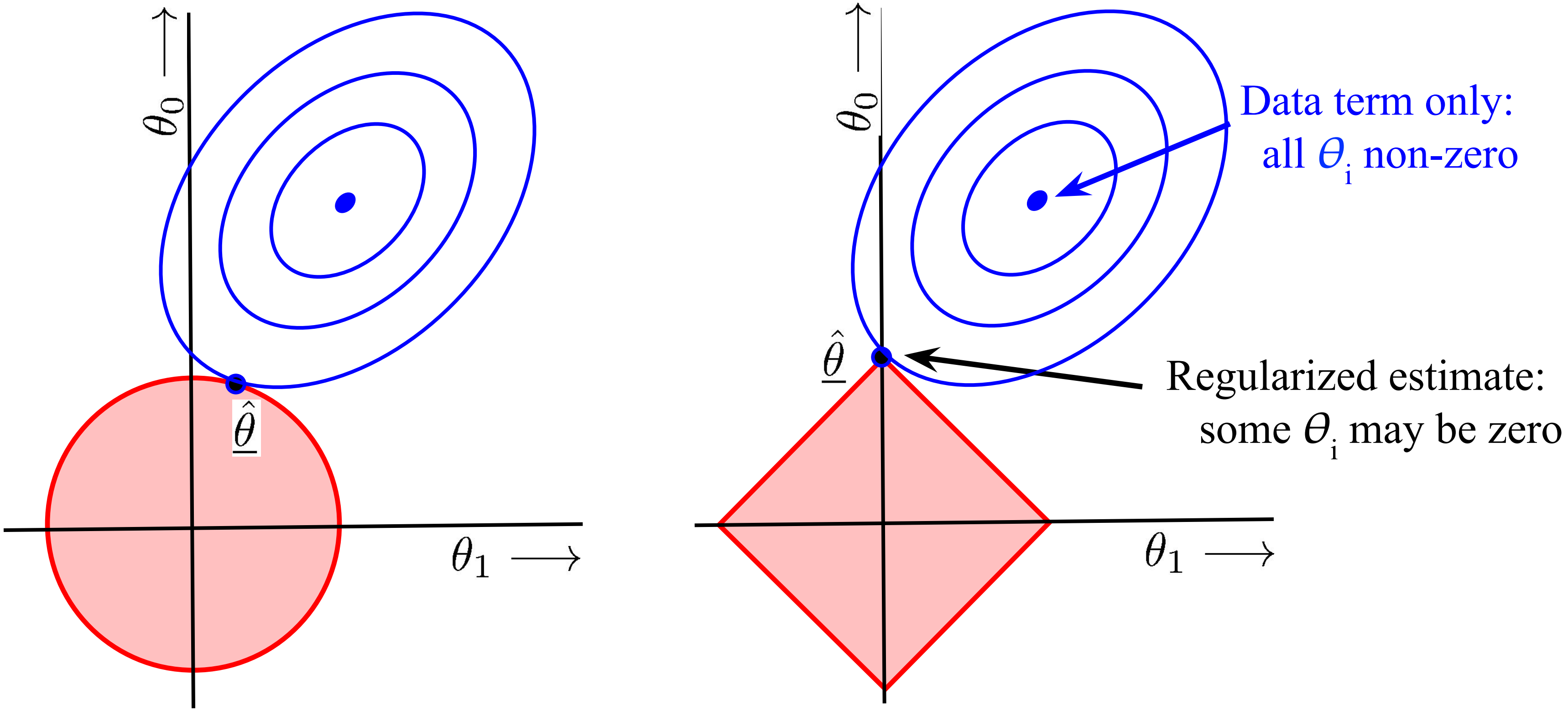
Regularization: L_2 vs L_1

- 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.

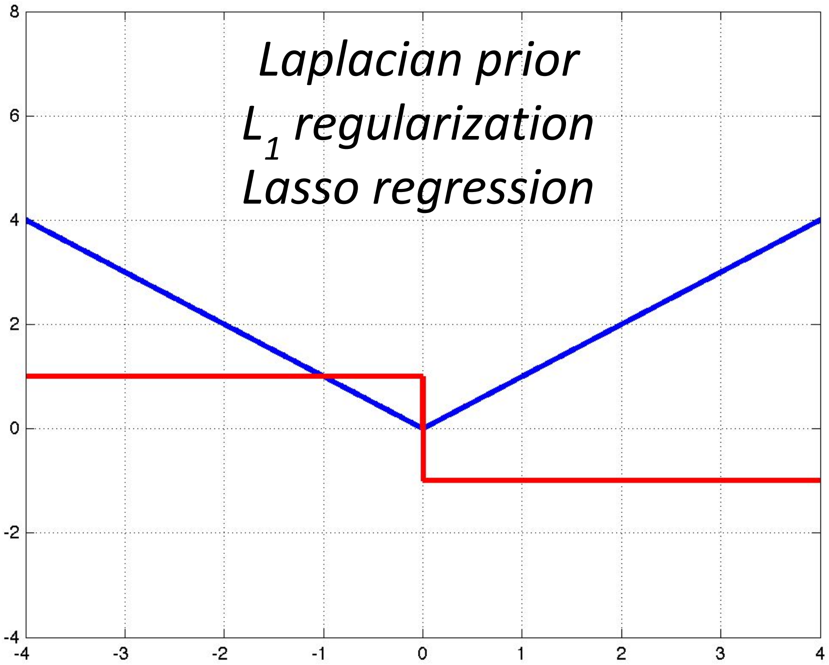

$\theta_0 \longrightarrow$
$\hat{\underline{\theta}}$
$\theta_1 \longrightarrow$
$\theta_0 \longrightarrow$
$\hat{\underline{\theta}}$
$\theta_1 \longrightarrow$

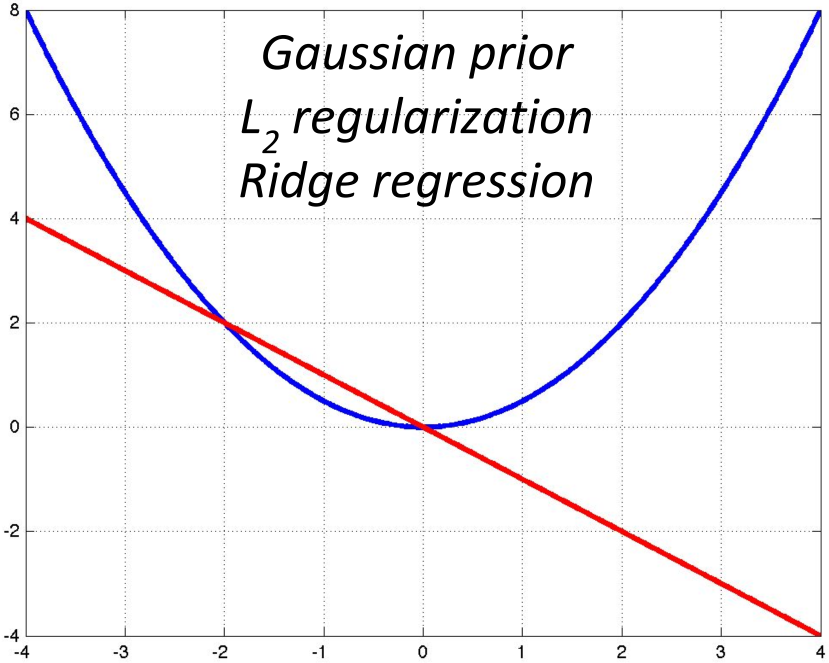
Data term only: all θ_i non-zero

Regularized estimate: some θ_i may be zero

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 L_1 objective not defined at zero)