# CSC 411: Lecture 02: Linear Regression

Class based on Raquel Urtasun & Rich Zemel's lectures

Sanja Fidler

University of Toronto

Jan 13, 2016

(Most plots in this lecture are from Bishop's book)

# Problems for Today

- What should I watch this Friday?

# Problems for Today

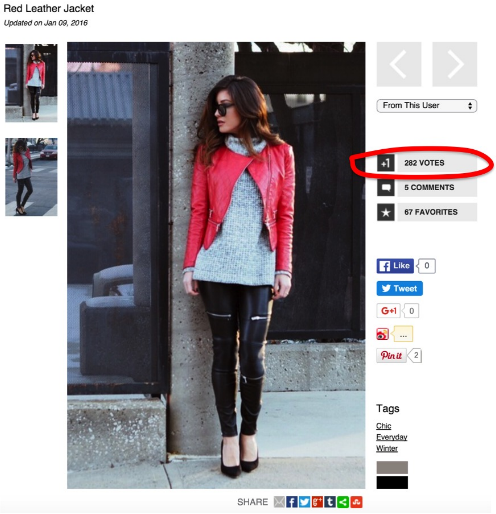
- What should I watch this Friday?

# Problems for Today

- **Goal**: Predict movie rating automatically!

# Problems for Today

- **Goal:** How many followers will I get?



# Problems for Today

- **Goal:** Predict the price of the house

# Regression

- What do all these problems have in common?

# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these $t$

    (eg, a rating: a real number between 0-10, # of followers, house price)

# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these $t$

    (eg, a rating: a real number between 0-10, # of followers, house price)
- What do I need in order to predict these outputs?

  Predicting continuous outputs is called regression

# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these $t$
    (eg, a rating: a real number between 0-10, # of followers, house price)
- What do I need in order to predict these outputs?
  Predicting continuous outputs is called regression
  - Features (inputs), we'll call these $x$ (or $\mathbf{x}$ if vectors)

# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these $t$
    (eg, a rating: a real number between 0-10, # of followers, house price)
- What do I need in order to predict these outputs?
  Predicting continuous outputs is called regression
  - Features (inputs), we'll call these $x$ (or $\mathbf{x}$ if vectors)
  - Training examples, many $x^{(i)}$ for which $t^{(i)}$ is known (eg, many movies for which we know the rating)

# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these $t$

    (eg, a rating: a real number between 0-10, # of followers, house price)
- What do I need in order to predict these outputs?

  Predicting continuous outputs is called regression
  - Features (inputs), we'll call these $x$ (or $\mathbf{x}$ if vectors)
  - Training examples, many $x^{(i)}$ for which $t^{(i)}$ is known (eg, many movies for which we know the rating)
  - A model, a function that represents the relationship between $x$ and $t$

# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these $t$
    (eg, a rating: a real number between 0-10, # of followers, house price)
- What do I need in order to predict these outputs?
  Predicting continuous outputs is called regression
  - Features (inputs), we'll call these $x$ (or $\mathbf{x}$ if vectors)
  - Training examples, many $x^{(i)}$ for which $t^{(i)}$ is known (eg, many movies for which we know the rating)
  - A model, a function that represents the relationship between $x$ and $t$
  - A loss or a cost or an objective function, which tells us how well our model approximates the training examples

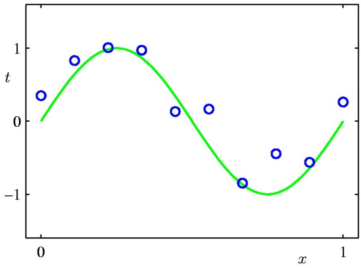
# Regression

- What do all these problems have in common?
  - Continuous outputs, we'll call these $t$
    (eg, a rating: a real number between 0-10, # of followers, house price)
- What do I need in order to predict these outputs?
  Predicting continuous outputs is called regression
  - Features (inputs), we'll call these $x$ (or $\mathbf{x}$ if vectors)
  - Training examples, many $x^{(i)}$ for which $t^{(i)}$ is known (eg, many movies for which we know the rating)
  - A model, a function that represents the relationship between $x$ and $t$
  - A loss or a cost or an objective function, which tells us how well our model approximates the training examples
  - Optimization, a way of finding the parameters of our model that minimizes the loss function

# Today: Linear Regression

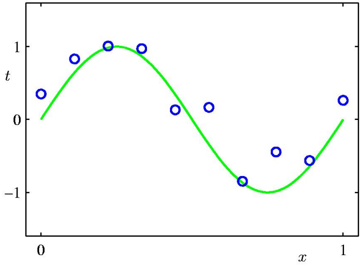
- Linear regression
  - continuous outputs
  - simple model (linear)
- Introduce key concepts:
  - loss functions
  - generalization
  - optimization
  - model complexity
  - regularization

# Simple 1-D regression




- Circles are data points (i.e., training examples) that are given to us

# Simple 1-D regression

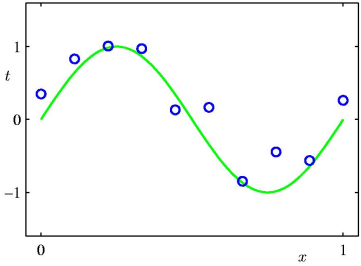



- Circles are data points (i.e., training examples) that are given to us
- The data points are uniform in $x$, but may be displaced in $y$

$$t(x) = f(x) + \epsilon$$

with $\epsilon$ some noise

# Simple 1-D regression

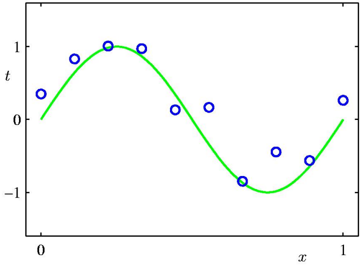



- Circles are data points (i.e., training examples) that are given to us
- The data points are uniform in $x$, but may be displaced in $y$

$$t(x) = f(x) + \epsilon$$

  with $\epsilon$ some noise
- In green is the "true" curve that we don't know

# Simple 1-D regression

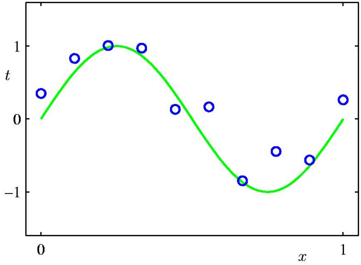



- Circles are data points (i.e., training examples) that are given to us
- The data points are uniform in $x$, but may be displaced in $y$

$$t(x) = f(x) + \epsilon$$

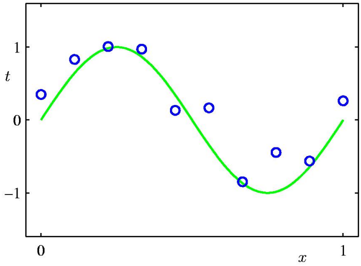
  with $\epsilon$ some noise
- In green is the "true" curve that we don't know
- Goal: We want to fit a curve to these points

# Simple 1-D regression



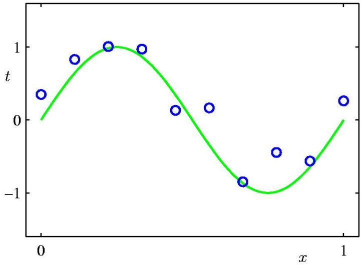

- Key Questions:

# Simple 1-D regression



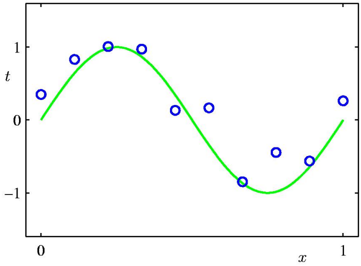

- Key Questions:
  - How do we parametrize the model?

# Simple 1-D regression




- Key Questions:
  - How do we parametrize the model?
  - What loss (objective) function should we use to judge the fit?

# Simple 1-D regression



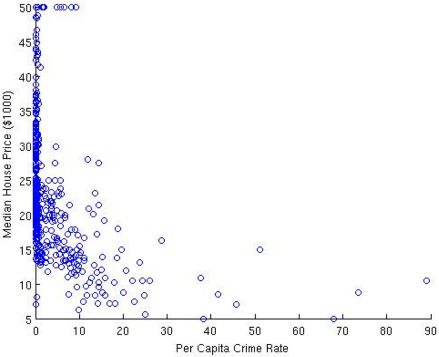

- Key Questions:
  - How do we parametrize the model?
  - What loss (objective) function should we use to judge the fit?
  - How do we optimize fit to unseen test data (generalization)?

# Example: Boston Housing data

- Estimate median house price in a neighborhood based on neighborhood statistics

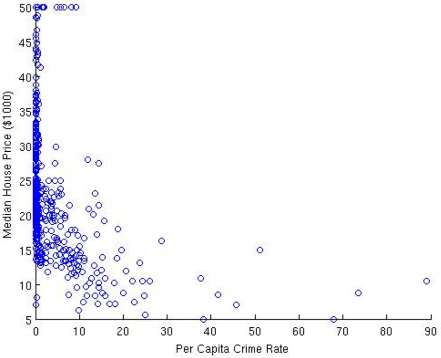
# Example: Boston Housing data

- Estimate median house price in a neighborhood based on neighborhood statistics
- Look at first possible attribute (feature): per capita crime rate



# Example: Boston Housing data

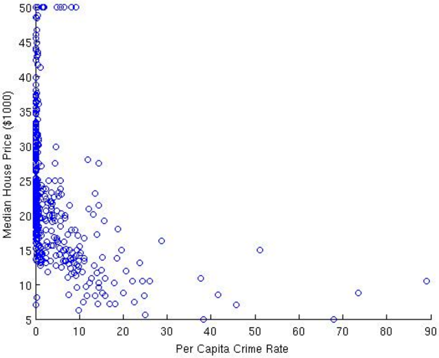
- Estimate median house price in a neighborhood based on neighborhood statistics
- Look at first possible attribute (feature): per capita crime rate




- Use this to predict house prices in other neighborhoods

# Example: Boston Housing data

- Estimate median house price in a neighborhood based on neighborhood statistics
- Look at first possible attribute (feature): per capita crime rate




- Use this to predict house prices in other neighborhoods
- Is this a good input (attribute) to predict house prices?

# Represent the Data

- Data is described as pairs $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$
  - $x \in \mathbb{R}$ is the input feature (per capita crime rate)
  - $t \in \mathbb{R}$ is the target output (median house price)
  - $^{(i)}$ simply indicates the training examples (we have $N$ in this case)

# Represent the Data

- Data is described as pairs $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$
  - $x \in \mathbb{R}$ is the input feature (per capita crime rate)
  - $t \in \mathbb{R}$ is the target output (median house price)
  - $^{(i)}$ simply indicates the training examples (we have $N$ in this case)
- Here $t$ is continuous, so this is a regression problem

# Represent the Data

- Data is described as pairs $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$
  - $x \in \mathbb{R}$ is the input feature (per capita crime rate)
  - $t \in \mathbb{R}$ is the target output (median house price)
  - $^{(i)}$ simply indicates the training examples (we have $N$ in this case)
- Here $t$ is continuous, so this is a regression problem
- Model outputs $y$, an estimate of $t$

$$y(x) = w_0 + w_1 x$$

# Represent the Data

- Data is described as pairs $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$
  - $x \in \mathbb{R}$ is the input feature (per capita crime rate)
  - $t \in \mathbb{R}$ is the target output (median house price)
  - $^{(i)}$ simply indicates the training examples (we have $N$ in this case)
- Here $t$ is continuous, so this is a regression problem
- Model outputs $y$, an estimate of $t$

$$y(x) = w_0 + w_1 x$$

- What type of model did we choose?

# Represent the Data

- Data is described as pairs $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$
  - $x \in \mathbb{R}$ is the input feature (per capita crime rate)
  - $t \in \mathbb{R}$ is the target output (median house price)
  - $^{(i)}$ simply indicates the training examples (we have $N$ in this case)
- Here $t$ is continuous, so this is a regression problem
- Model outputs $y$, an estimate of $t$

$$y(x) = w_0 + w_1 x$$

- What type of model did we choose?
- Divide the dataset into training and testing examples

# Represent the Data

- Data is described as pairs $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$
  - $x \in \mathbb{R}$ is the input feature (per capita crime rate)
  - $t \in \mathbb{R}$ is the target output (median house price)
  - $^{(i)}$ simply indicates the training examples (we have $N$ in this case)
- Here $t$ is continuous, so this is a regression problem
- Model outputs $y$, an estimate of $t$

$$y(x) = w_0 + w_1 x$$

- What type of model did we choose?
- Divide the dataset into training and testing examples
  - Use the training examples to construct hypothesis, or function approximator, that maps $x$ to predicted $y$

# Represent the Data

- Data is described as pairs $\mathcal{D} = \{(x^{(1)}, t^{(1)}), \cdots, (x^{(N)}, t^{(N)})\}$
  - $x \in \mathbb{R}$ is the input feature (per capita crime rate)
  - $t \in \mathbb{R}$ is the target output (median house price)
  - $^{(i)}$ simply indicates the training examples (we have $N$ in this case)
- Here $t$ is continuous, so this is a regression problem
- Model outputs $y$, an estimate of $t$

$$y(x) = w_0 + w_1 x$$

- What type of model did we choose?
- Divide the dataset into training and testing examples
  - Use the training examples to construct hypothesis, or function approximator, that maps $x$ to predicted $y$
  - Evaluate hypothesis on test set

# Noise

- A simple model typically does not exactly fit the data – lack of fit can be considered noise

# Noise

- A simple model typically does not exactly fit the data – lack of fit can be considered noise
- Sources of noise:

# Noise

- A simple model typically does not exactly fit the data – lack of fit can be considered noise
- Sources of noise:
  - Imprecision in data attributes (input noise, eg noise in per-capita crime)

# Noise

- A simple model typically does not exactly fit the data – lack of fit can be considered noise
- Sources of noise:
  - Imprecision in data attributes (input noise, eg noise in per-capita crime)
  - Errors in data targets (mis-labeling, eg noise in house prices)

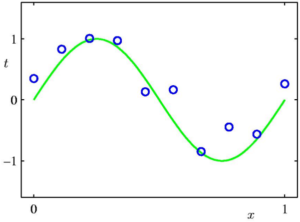
# Noise

- A simple model typically does not exactly fit the data – lack of fit can be considered noise
- Sources of noise:
  - Imprecision in data attributes (input noise, eg noise in per-capita crime)
  - Errors in data targets (mis-labeling, eg noise in house prices)
  - Additional attributes not taken into account by data attributes, affect target values (latent variables). In the example, what else could affect house prices?

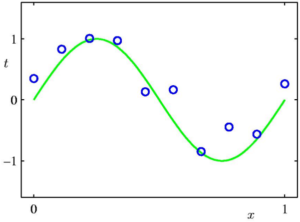
# Noise

- A simple model typically does not exactly fit the data – lack of fit can be considered noise
- Sources of noise:
  - Imprecision in data attributes (input noise, eg noise in per-capita crime)
  - Errors in data targets (mis-labeling, eg noise in house prices)
  - Additional attributes not taken into account by data attributes, affect target values (latent variables). In the example, what else could affect house prices?
  - Model may be too simple to account for data targets

# Least-Squares Regression



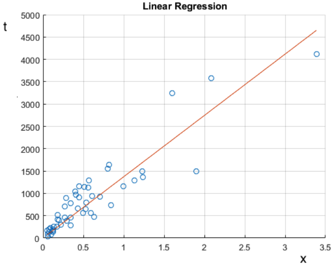
# Least-Squares Regression




- Define a model

$$y(x) = \text{function}(x, \mathbf{w})$$

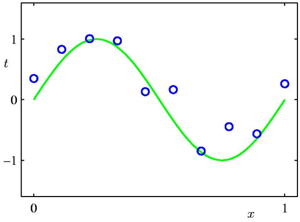
# Least-Squares Regression




- Define a model

$$\text{Linear:} \qquad y(x) = w_0 + w_1 x$$

# Least-Squares Regression



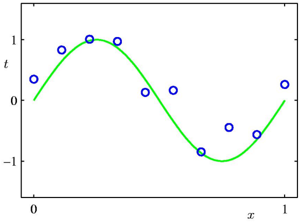

- Define a model

Linear: $y(x) = w_0 + w_1 x$

- Standard loss/cost/objective function measures the squared error between $y$ and the true value $t$

$$\ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - y(x^{(n)})]^2$$

# Least-Squares Regression



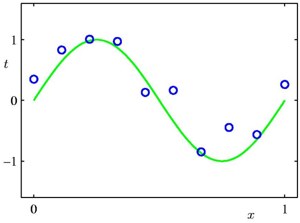

- Define a model

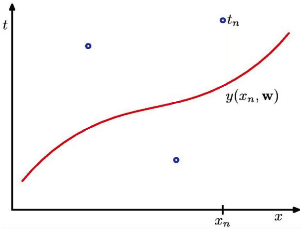
$$\text{Linear:} \qquad y(x) = w_0 + w_1 x$$

- Standard loss/cost/objective function measures the squared error between $y$ and the true value $t$

$$\text{Linear model:} \qquad \ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2$$

# Least-Squares Regression




- Define a model

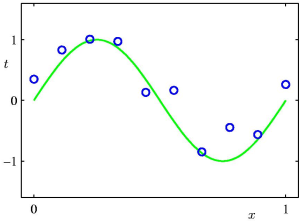
$$\text{Linear:} \qquad y(x) = w_0 + w_1 x$$

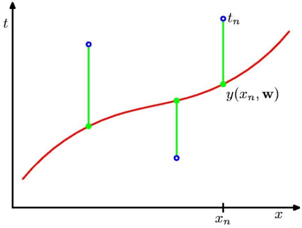
- Standard loss/cost/objective function measures the squared error between $y$ and the true value $t$

$$\text{Linear model:} \qquad \ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2$$

- For a particular hypothesis ($y(x)$ defined by a choice of $\mathbf{w}$, drawn in red), what does the loss represent geometrically?

# Least-Squares Regression




- Define a model

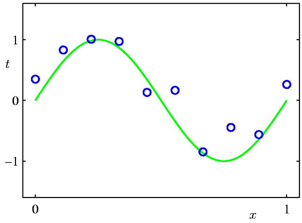
$$\text{Linear:} \qquad y(x) = w_0 + w_1 x$$

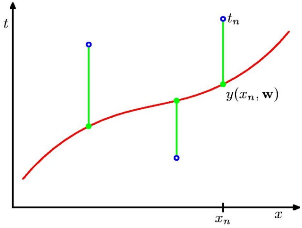
- Standard loss/cost/objective function measures the squared error between $y$ and the true value $t$

$$\text{Linear model:} \qquad \ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2$$

- The loss for the red hypothesis is the **sum of the squared vertical errors** (squared lengths of green vertical lines)

# Least-Squares Regression




- Define a model

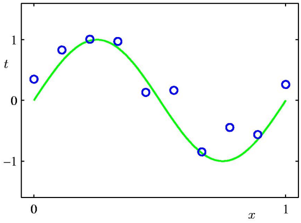
$$\text{Linear:} \qquad y(x) = w_0 + w_1 x$$

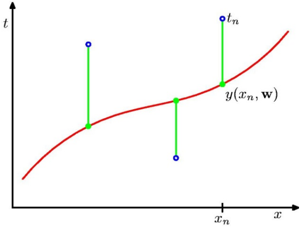
- Standard loss/cost/objective function measures the squared error between $y$ and the true value $t$

$$\text{Linear model:} \qquad \ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2$$

- How do we obtain weights $\mathbf{w} = (w_0, w_1)$?

# Least-Squares Regression




- Define a model

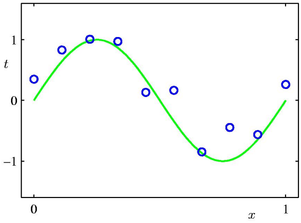
$$\text{Linear:} \qquad y(x) = w_0 + w_1 x$$

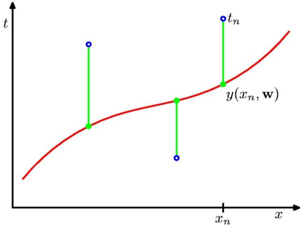
- Standard loss/cost/objective function measures the squared error between $y$ and the true value $t$

$$\text{Linear model:} \qquad \ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2$$

- How do we obtain weights $\mathbf{w} = (w_0, w_1)$? Find $\mathbf{w}$ that minimizes loss $\ell(\mathbf{w})$

# Least-Squares Regression




- Define a model

$$\text{Linear:} \qquad y(x) = w_0 + w_1 x$$

- Standard loss/cost/objective function measures the squared error between $y$ and the true value $t$

$$\text{Linear model:} \qquad \ell(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2$$

- How do we obtain weights $\mathbf{w} = (w_0, w_1)$?
- For the linear model, what kind of a function is $\ell(\mathbf{w})$?

# Optimizing the Objective

- One straightforward method: gradient descent

# Optimizing the Objective

- One straightforward method: gradient descent
  - initialize $\mathbf{w}$ (e.g., randomly)

# Optimizing the Objective

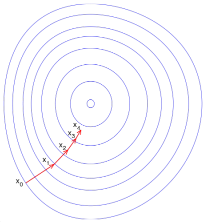
- One straightforward method: gradient descent
  - initialize $\mathbf{w}$ (e.g., randomly)
  - repeatedly update $\mathbf{w}$ based on the gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \lambda \frac{\partial \ell}{\partial \mathbf{w}}$$

# Optimizing the Objective

- One straightforward method: gradient descent
  - initialize $\mathbf{w}$ (e.g., randomly)
  - repeatedly update $\mathbf{w}$ based on the gradient

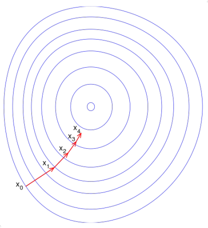
$$\mathbf{w} \leftarrow \mathbf{w} - \lambda \frac{\partial \ell}{\partial \mathbf{w}}$$



# Optimizing the Objective

- One straightforward method: gradient descent
  - initialize $\mathbf{w}$ (e.g., randomly)
  - repeatedly update $\mathbf{w}$ based on the gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \lambda \frac{\partial \ell}{\partial \mathbf{w}}$$

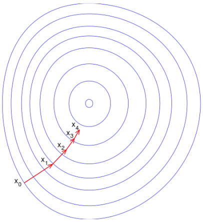



- $\lambda$ is the learning rate

# Optimizing the Objective

- One straightforward method: gradient descent
  - initialize $\mathbf{w}$ (e.g., randomly)
  - repeatedly update $\mathbf{w}$ based on the gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \lambda \frac{\partial \ell}{\partial \mathbf{w}}$$



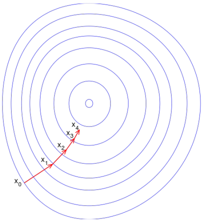

- $\lambda$ is the learning rate
- For a single training case, this gives the LMS update rule:

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda(t^{(n)} - y(x^{(n)}))x^{(n)}$$

# Optimizing the Objective

- One straightforward method: gradient descent
  - initialize **w** (e.g., randomly)
  - repeatedly update **w** based on the gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \lambda \frac{\partial \ell}{\partial \mathbf{w}}$$




- $\lambda$ is the learning rate
- For a single training case, this gives the LMS update rule:

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda \underbrace{\left(t^{(n)} - y(x^{(n)})\right)}_{\text{error}} x^{(n)}$$

- Note: As error approaches zero, so does the update (**w** stops changing)

# Optimizing Across Training Set

- Two ways to generalize this for all examples in training set:

# Optimizing Across Training Set

- Two ways to generalize this for all examples in training set:
   1. Batch updates: sum or average updates across every example $n$, then change the parameter values

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda \sum_{n=1}^{N} (t^{(n)} - y(x^{(n)}))x^{(n)}$$

# Optimizing Across Training Set

- Two ways to generalize this for all examples in training set:
  1. Batch updates: sum or average updates across every example $n$, then change the parameter values

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda \sum_{n=1}^{N} (t^{(n)} - y(x^{(n)}))x^{(n)}$$

  2. Stochastic/online updates: update the parameters for each training case in turn, according to its own gradients

---

**Algorithm 1** Stochastic gradient descent

---

1: Randomly shuffle examples in the training set
2: **for** $i = 1$ to $N$ **do**
3: Update:

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda (t^{(i)} - y(x^{(i)}))x^{(i)} \qquad \text{(update for a linear model)}$$

4: **end for**

---

# Optimizing Across Training Set

- Two ways to generalize this for all examples in training set:
  1. Batch updates: sum or average updates across every example $n$, then change the parameter values

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda \sum_{n=1}^{N} (t^{(n)} - y(x^{(n)}))x^{(n)}$$

  2. Stochastic/online updates: update the parameters for each training case in turn, according to its own gradients

  - Underlying assumption: sample is independent and identically distributed (i.i.d.)

# Analytical Solution?

- For some objectives we can also find the optimal solution analytically
- This is the case for linear least-squares regression
- How?

# Analytical Solution?

- For some objectives we can also find the optimal solution analytically
- This is the case for linear least-squares regression
- How?
- Compute the derivatives of the objective wrt $\mathbf{w}$ and equate with 0

# Analytical Solution?

- For some objectives we can also find the optimal solution analytically
- This is the case for linear least-squares regression
- How?
- Compute the derivatives of the objective wrt **w** and equate with 0
- Define:

$$\mathbf{t} = [t^{(1)}, t^{(2)}, \ldots, t^{(N)}]^T$$

$$\mathbf{X} = \begin{bmatrix} 1, x^{(1)} \\ 1, x^{(2)} \\ \ldots \\ 1, x^{(N)} \end{bmatrix}$$

- Then:

$$\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{t}$$

(work it out!)

# Multi-dimensional Inputs

- One method of extending the model is to consider other input dimensions

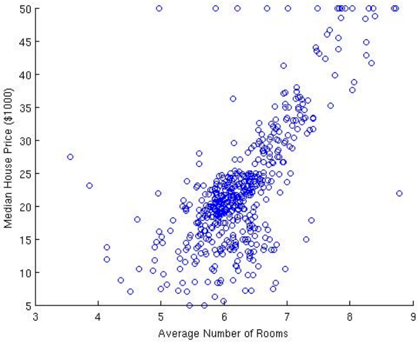
$$y(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2$$

# Multi-dimensional Inputs

- One method of extending the model is to consider other input dimensions

$$y(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2$$

- In the Boston housing example, we can look at the number of rooms



# Linear Regression with Multi-dimensional Inputs

- Imagine now we want to predict the median house price from these multi-dimensional observations

# Linear Regression with Multi-dimensional Inputs

- Imagine now we want to predict the median house price from these multi-dimensional observations
- Each house is a data point $n$, with observations indexed by $j$:

$$\mathbf{x}^{(n)} = \left(x_1^{(n)}, \cdots, x_j^{(n)}, \cdots, x_d^{(n)}\right)$$

# Linear Regression with Multi-dimensional Inputs

- Imagine now we want to predict the median house price from these multi-dimensional observations
- Each house is a data point $n$, with observations indexed by $j$:

$$\mathbf{x}^{(n)} = \left(x_1^{(n)}, \cdots, x_j^{(n)}, \cdots, x_d^{(n)}\right)$$

- We can incorporate the bias $w_0$ into $\mathbf{w}$, by using $x_0 = 1$, then

$$y(\mathbf{x}) = w_0 + \sum_{j=1}^{d} w_j x_j = \mathbf{w}^T \mathbf{x}$$

# Linear Regression with Multi-dimensional Inputs

- Imagine now we want to predict the median house price from these multi-dimensional observations
- Each house is a data point $n$, with observations indexed by $j$:

$$\mathbf{x}^{(n)} = \left(x_1^{(n)}, \cdots, x_j^{(n)}, \cdots, x_d^{(n)}\right)$$

- We can incorporate the bias $w_0$ into $\mathbf{w}$, by using $x_0 = 1$, then

$$y(\mathbf{x}) = w_0 + \sum_{j=1}^{d} w_j x_j = \mathbf{w}^T \mathbf{x}$$

- We can then solve for $\mathbf{w} = (w_0, w_1, \cdots, w_d)$. How?

# Linear Regression with Multi-dimensional Inputs

- Imagine now we want to predict the median house price from these multi-dimensional observations
- Each house is a data point $n$, with observations indexed by $j$:

$$\mathbf{x}^{(n)} = \left(x_1^{(n)}, \cdots, x_j^{(n)}, \cdots, x_d^{(n)}\right)$$

- We can incorporate the bias $w_0$ into $\mathbf{w}$, by using $x_0 = 1$, then

$$y(\mathbf{x}) = w_0 + \sum_{j=1}^{d} w_j x_j = \mathbf{w}^T \mathbf{x}$$

- We can then solve for $\mathbf{w} = (w_0, w_1, \cdots, w_d)$. How?
- We can use gradient descent to solve for each coefficient, or compute $\mathbf{w}$ analytically (how does the solution change?)

# More Powerful Models?

- What if our linear model is not good? How can we create a more complicated model?

# Fitting a Polynomial

- What if our linear model is not good? How can we create a more complicated model?
- We can create a more complicated model by defining input variables that are combinations of components of $\mathbf{x}$

# Fitting a Polynomial

- What if our linear model is not good? How can we create a more complicated model?
- We can create a more complicated model by defining input variables that are combinations of components of $\mathbf{x}$
- Example: an $M$-th order polynomial function of one dimensional feature $x$:

$$y(x, \mathbf{w}) = w_0 + \sum_{j=1}^{M} w_j x^j$$

where $x^j$ is the $j$-th power of $x$

# Fitting a Polynomial

- What if our linear model is not good? How can we create a more complicated model?
- We can create a more complicated model by defining input variables that are combinations of components of $\mathbf{x}$
- Example: an $M$-th order polynomial function of one dimensional feature $x$:

$$y(x, \mathbf{w}) = w_0 + \sum_{j=1}^{M} w_j x^j$$

  where $x^j$ is the $j$-th power of $x$
- We can use the same approach to optimize for the weights $\mathbf{w}$

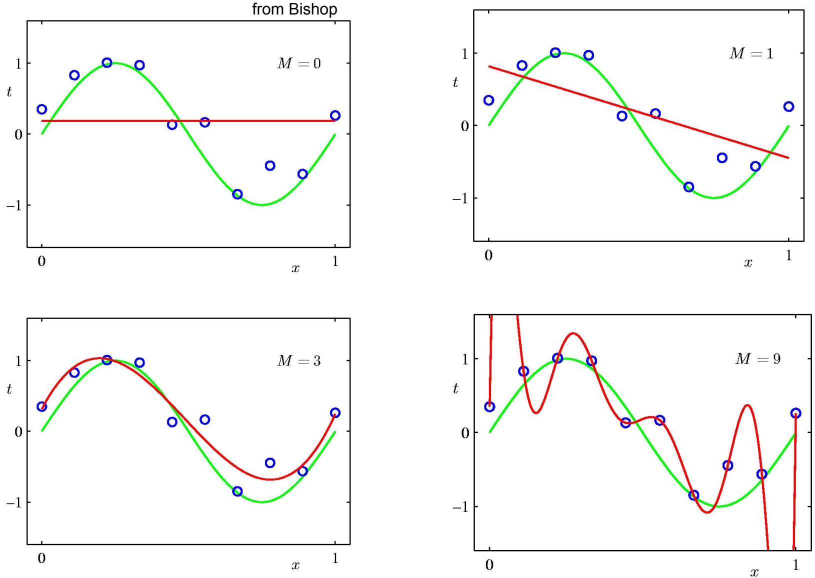
# Fitting a Polynomial

- What if our linear model is not good? How can we create a more complicated model?
- We can create a more complicated model by defining input variables that are combinations of components of $\mathbf{x}$
- Example: an $M$-th order polynomial function of one dimensional feature $x$:

$$y(x, \mathbf{w}) = w_0 + \sum_{j=1}^{M} w_j x^j$$

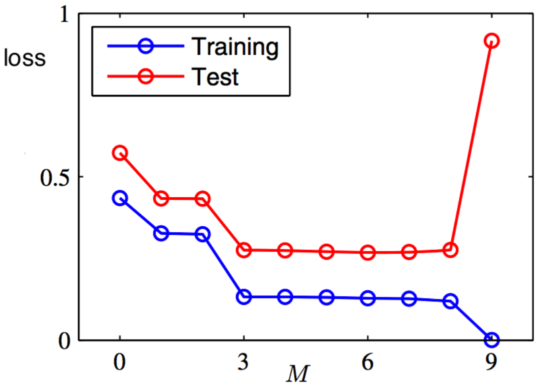
  where $x^j$ is the $j$-th power of $x$
- We can use the same approach to optimize for the weights $\mathbf{w}$
- How do we do that?

# Which Fit is Best?



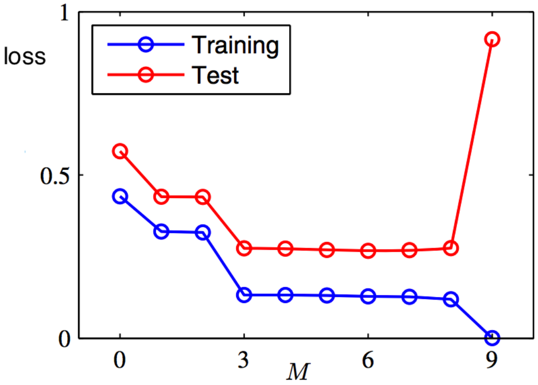
# Generalization

- Generalization = model's ability to predict the held out data
- What is happening?



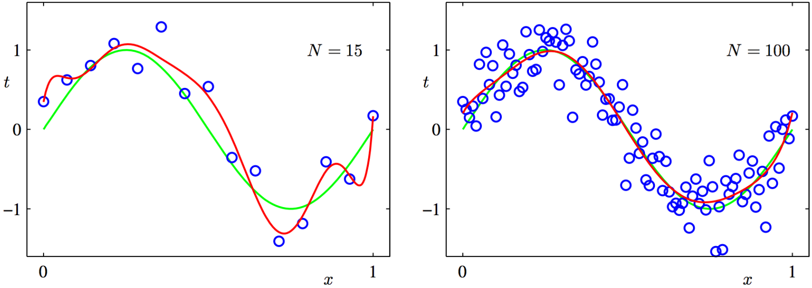
# Generalization

- Generalization = model's ability to predict the held out data
- What is happening?
- Our model with $M = 9$ overfits the data (it models also noise)



# Generalization

- Generalization = model's ability to predict the held out data
- What is happening?
- Our model with $M = 9$ overfits the data (it models also noise)
- Not a problem if we have lots of training examples



# Generalization

- Generalization = model's ability to predict the held out data
- What is happening?
- Our model with $M = 9$ overfits the data (it models also noise)
- Let's look at the estimated weights for various $M$ in the case of fewer examples

| | $M = 0$ | $M = 1$ | $M = 6$ | $M = 9$ |
|---|---|---|---|---|
| $w_0^\star$ | 0.19 | 0.82 | 0.31 | 0.35 |
| $w_1^\star$ | | -1.27 | 7.99 | 232.37 |
| $w_2^\star$ | | | -25.43 | -5321.83 |
| $w_3^\star$ | | | 17.37 | 48568.31 |
| $w_4^\star$ | | | | -231639.30 |
| $w_5^\star$ | | | | 640042.26 |
| $w_6^\star$ | | | | -1061800.52 |
| $w_7^\star$ | | | | 1042400.18 |
| $w_8^\star$ | | | | -557682.99 |
| $w_9^\star$ | | | | 125201.43 |

# Generalization

- Generalization = model's ability to predict the held out data
- What is happening?
- Our model with $M = 9$ overfits the data (it models also noise)
- Let's look at the estimated weights for various $M$ in the case of fewer examples
- The weights are becoming huge to compensate for the noise

# Generalization

- Generalization = model's ability to predict the held out data
- What is happening?
- Our model with $M = 9$ overfits the data (it models also noise)
- Let's look at the estimated weights for various $M$ in the case of fewer examples
- The weights are becoming huge to compensate for the noise
- One way of dealing with this is to encourage the weights to be small (this way no input dimension will have too much influence on prediction). This is called regularization.

# Regularized Least Squares

- Increasing the input features this way can complicate the model considerably

# Regularized Least Squares

- Increasing the input features this way can complicate the model considerably
- Goal: select the appropriate model complexity automatically

# Regularized Least Squares

- Increasing the input features this way can complicate the model considerably
- Goal: select the appropriate model complexity automatically
- Standard approach: regularization

$$\tilde{\ell}(\mathbf{w}) = \sum_{n=1}^{N}[t^{(n)} - (w_0 + w_1 x^{(n)})]^2 + \alpha \mathbf{w}^T \mathbf{w}$$

# Regularized Least Squares

- Increasing the input features this way can complicate the model considerably
- Goal: select the appropriate model complexity automatically
- Standard approach: regularization

$$\tilde{\ell}(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2 + \alpha \mathbf{w}^T \mathbf{w}$$

- Intuition: Since we are minimizing the loss, the second term will encourage smaller values in **w**

# Regularized Least Squares

- Increasing the input features this way can complicate the model considerably
- Goal: select the appropriate model complexity automatically
- Standard approach: regularization

$$\tilde{\ell}(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2 + \alpha \mathbf{w}^T \mathbf{w}$$

- Intuition: Since we are minimizing the loss, the second term will encourage smaller values in **w**
- The penalty on the squared weights is known as ridge regression in statistics

# Regularized Least Squares

- Increasing the input features this way can complicate the model considerably
- Goal: select the appropriate model complexity automatically
- Standard approach: regularization

$$\tilde{\ell}(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2 + \alpha \mathbf{w}^T \mathbf{w}$$

- Intuition: Since we are minimizing the loss, the second term will encourage smaller values in **w**
- The penalty on the squared weights is known as ridge regression in statistics
- Leads to a modified update rule for gradient descent:

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda [\sum_{n=1}^{N} (t^{(n)} - y(x^{(n)})) x^{(n)} - \alpha \mathbf{w}]$$

# Regularized Least Squares

- Increasing the input features this way can complicate the model considerably
- Goal: select the appropriate model complexity automatically
- Standard approach: regularization

$$\tilde{\ell}(\mathbf{w}) = \sum_{n=1}^{N} [t^{(n)} - (w_0 + w_1 x^{(n)})]^2 + \alpha \mathbf{w}^T \mathbf{w}$$

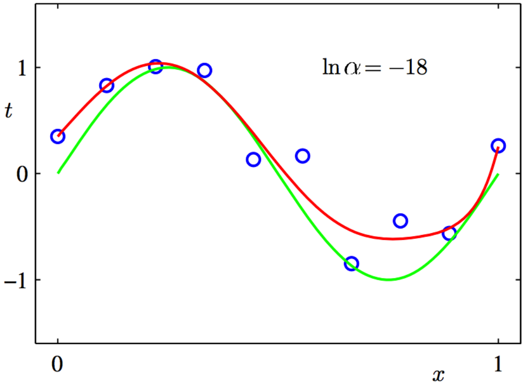
- Intuition: Since we are minimizing the loss, the second term will encourage smaller values in $\mathbf{w}$
- The penalty on the squared weights is known as ridge regression in statistics
- Leads to a modified update rule for gradient descent:

$$\mathbf{w} \leftarrow \mathbf{w} + 2\lambda [\sum_{n=1}^{N} (t^{(n)} - y(x^{(n)})) x^{(n)} - \alpha \mathbf{w}]$$

- Also has an analytical solution: $\mathbf{w} = (\mathbf{X}^T \mathbf{X} + \alpha \mathbf{I})^{-1} \mathbf{X}^T \mathbf{t}$ (verify!)

# Regularized least squares

- Better generalization
- Choose $\alpha$ carefully



# 1-D regression illustrates key concepts

- Data fits – is linear model best (model selection)?

# 1-D regression illustrates key concepts

- Data fits – is linear model best (model selection)?
  - Simple models may not capture all the important variations (signal) in the data: underfit

# 1-D regression illustrates key concepts

- Data fits – is linear model best (model selection)?
  - Simple models may not capture all the important variations (signal) in the data: underfit
  - More complex models may overfit the training data (fit not only the signal but also the noise in the data), especially if not enough data to constrain model

# 1-D regression illustrates key concepts

- Data fits – is linear model best (model selection)?
  - Simple models may not capture all the important variations (signal) in the data: underfit
  - More complex models may overfit the training data (fit not only the signal but also the noise in the data), especially if not enough data to constrain model
- One method of assessing fit: test generalization = model's ability to predict the held out data

# 1-D regression illustrates key concepts

- Data fits – is linear model best (model selection)?
  - Simple models may not capture all the important variations (signal) in the data: underfit
  - More complex models may overfit the training data (fit not only the signal but also the noise in the data), especially if not enough data to constrain model
- One method of assessing fit: test generalization = model's ability to predict the held out data
- Optimization is essential: stochastic and batch iterative approaches; analytic when available

# So...

- Which movie will you watch?