Lecture 3 - Regression

Instructor: Prof. Ganesh Ramakrishnan

The Simplest ML Problem: Least Square Regression

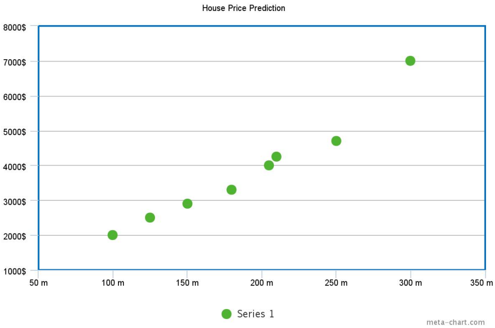
- Curve Fitting: Motivation
  - Error measurement
  - Minimizing Error
- Method of Least Squares

Curve Fitting: Motivation

- Example scenarios:
  - Prices of house to be fitted as a function of the area of the house
  - Temperature of a place to be fitted as a function of its latitude and longitude and time of the year
  - Stock Price (or BSE/Nifty value) to be fitted as a function of Company Earnings
  - Height of students to be fitted as a function of their weight
- One or more observations/parameters in the data are expected to represent the output in the future

Higher you go, the more expensive the house!

- Consider the variation of price (in $) of house with variations in its height (in m) above the ground level
- These are specified as coordinates of the 8 points: $(x_1, y_1), \ldots, (x_8, y_8)$
- Desired: Find a pattern or curve that characterizes the price as a function of the height



Errors and Causes

- (Observable) Data is generally collected through measurements or surveys
  - Surveys can have random human **errors**
  - Measurements are subject to **imprecision** of the measuring or recording instrument
  - **Outliers** due to variability in the measurement or due to some experimental error;
- **Robustness to Errors:** Minimize the effect of error in predicted model
- **Data cleansing**: Outlier handling in a pre-processing step

Curve Fitting: The Process

- *Curve fitting is the process of constructing a curve, or mathematical function, that has the* **best fit** *to a series of data points, possibly subject to constraints.* - Wikipedia

Curve Fitting: The Process

- *Curve fitting is the process of constructing a curve, or mathematical function, that has the* **best fit** *to a series of data points, possibly subject to constraints.* - Wikipedia
- Need quantitative criteria to find the **best fit**
- **Error function** E : curve $f \times$ dataset $\mathcal{D} \longrightarrow \Re$
- Error function must capture the deviation of prediction from expected value

Example

- Consider the two candidate prediction curves in blue and red respectively respectively. Which is the better fit?

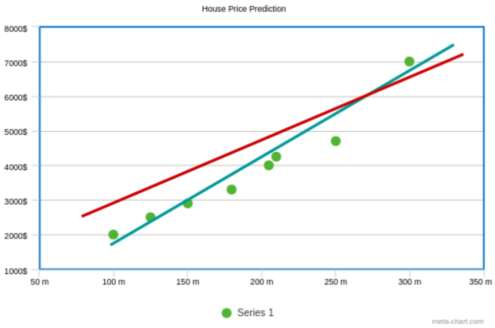


Figure: Price of house *vs.* its height - for illustration purpose only

Question

What are some options for error function $E(f, D)$ that measure the deviation of prediction from expected value?

Examples of E

- $\sum_D f(x_i) - y_i$
- $\sum_D |f(x_i) - y_i|$
- $\sum_D (f(x_i) - y_i)^2$
- $\sum_D (f(x_i) - y_i)^3$
- and many more

Question

Which choice F do you think can give us best fit curve and why?
Hint: Think of these errors as distances.

Squared Error

$$\sum_D (f(x_\mathrm{i}) - y_\mathrm{i})^2$$

- One best fit curve corresponds to f that minimizes the above function. It..
  1. Is continuous and differentiable
  2. Can be visualized as square of Euclidean distance between predicted and observed values
- Mathematical optimization of this function: Topic of following lectures.
- This is the Method of least squares

Regression, More Formally

- Formal Definition
- Types of Regression
- Geometric Interpretation of least square solution

Linear Regression as a canonical example

- **Optimization** (Formally deriving least Square Solution)
- **Regularization** (Ridge Regression, Lasso), **Bayesian Interpretation** (Bayesian Linear Regression)
- **Non-parametric estimation** (Local linear regression),
- **Non-linearity through Kernels** (Support Vector Regression)

Linear Regression with Illustration

- Regression is about learning to predict a set of output variables (*dependent variables*) as a function of a set of input variables (*independent variables*)
- Example
  - A company wants to determine how much it should spend on T.V commercials to increase sales to a desired level y^*
  - **Basis?**

Linear Regression with Illustration

- Regression is about learning to predict a set of output variables (*dependent variables*) as a function of a set of input variables (*independent variables*)
- Example
  - A company wants to determine how much it should spend on T.V commercials to increase sales to a desired level y^*
  - **Basis?** It has previous observations of the form $<x_i,y_i>$,
    - ★ x_i is an instance of money spent on advertisements and y_i was the corresponding observed sale figure

Linear Regression with Illustration

- Regression is about learning to predict a set of output variables (*dependent variables*) as a function of a set of input variables (*independent variables*)
- Example
  - A company wants to determine how much it should spend on T.V commercials to increase sales to a desired level y^*
  - **Basis?** It has previous observations of the form $<x_i, y_i>$,
    - x_i is an instance of money spent on advertisements and y_i was the corresponding observed sale figure
  - Suppose the observations support the following linear approximation

$$y = \beta_0 + \beta_1 * x \tag{1}$$

    Then $x^* = \frac{y^* - \beta_0}{\beta_1}$ can be used to determine the money to be spent
- **Estimation** for Regression: Determine appropriate value for β_0 and β_1 from the past observations

Linear Regression with Illustration

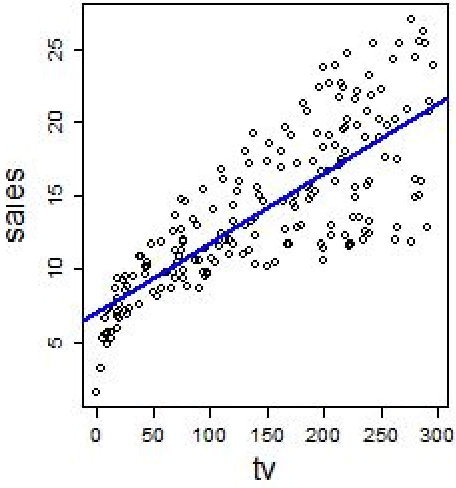


Figure: Linear regression on T.V advertising vs sales figure

What will it mean to have sales as a non-linear function of investment in advertising?

Basic Notation

- Data set: $\mathcal{D} =< \mathbf{x_1}, \mathbf{y_1} >, .., < \mathbf{x_m}, \mathbf{y_m} >$
  - Notation (used throughout the course)
  - m = number of training examples
  - $\mathbf{x's}$ = input/independent variables
  - $\mathbf{y's}$ = output/dependent/'target' variables
  - $(\mathbf{x}, \mathbf{y})$ - a single training example
  - $(\mathbf{x_j}, \mathbf{y_j})$ - specific example (j^{th} training example)
  - j is an index into the training set
- ϕ_i's are the attribute/basis functions, and let

$$\phi = \begin{bmatrix} \phi_1(\mathbf{x_1}) & \phi_2(\mathbf{x_1}) & \ldots\ldots & \phi_p(\mathbf{x_1}) \\ . & & & \\ . & & & \\ \phi_1(\mathbf{x_m}) & \phi_2(\mathbf{x_m}) & \ldots\ldots & \phi_p(\mathbf{x_m}) \end{bmatrix} \tag{2}$$

-

$$\mathbf{y} = \begin{bmatrix} y_1 \\ . \\ y_m \end{bmatrix} \tag{3}$$

Formal Definition

- **General Regression problem**: Determine a function f^* such that $f^*(x)$ is the best predictor for y, with respect to $\mathcal{D}$:

$$f^* = \underset{f \in F}{\text{argmin}}\ E(f, \mathcal{D})$$

  Here, F denotes the class of functions over which the error minimization is performed

- **Parametrized Regression problem**: Need to determine parameters $\mathbf{w}$ for the function $f\big(\phi(\mathbf{x}), \mathbf{w}\big)$ which minimize our error function $E\big(f(\phi(\mathbf{x}), \mathbf{w}), \mathcal{D}\big)$

$$\mathbf{w}^* = \underset{\mathbf{w}}{\text{argmin}} \Big\langle E\big(f(\phi(\mathbf{x}), \mathbf{w}), \mathcal{D}\big) \Big\rangle$$

Types of Regression

- Classified based on the function class and error function
- F is space of linear functions $f(\phi(\mathbf{x}), \mathbf{w}) = \mathbf{w}^T \phi(\mathbf{x}) + b \implies$ Linear Regression
  - Problem is then to determine $\mathbf{w}^*$ such that,

$$\mathbf{w}^* = \underset{\mathbf{w}}{\text{argmin}}\ E(\mathbf{w}, \mathcal{D}) \tag{4}$$

Types of Regression (contd.)

- **Ridge Regression:** A shrinkage parameter (regularization parameter) is added in the error function to reduce discrepancies due to variance
- **Logistic Regression:** Models conditional probability of dependent variable given independent variables and is extensively used in classification tasks

$$f(\phi(\mathbf{x}), \mathbf{w}) = \log \frac{\Pr(\mathbf{y}|\mathbf{x})}{1 - \Pr(\mathbf{y}|\mathbf{x})} = b + \mathbf{w}^T * \phi(\mathbf{x}) \quad (5)$$

- Lasso regression, Stepwise regression and several others

Least Square Solution

- Form of $E()$ should lead to accuracy and tractability
- The squared loss is a commonly used error/loss function. It is the sum of squares of the differences between the actual value and the predicted value

$$E(f, \mathcal{D}) = \sum_{j=1}^{m} (f(x_j) - y_j)^2 \tag{6}$$

- The least square solution for linear regression is obtained as

$$\mathbf{w}^* = \underset{\mathbf{w}}{\text{argmin}} \sum_{j=1}^{m} \left(\sum_{i=1}^{p} (w_i \phi_i(x_j) - y_j)^2 \right) \tag{7}$$

- The minimum value of the squared loss is zero
- If zero were attained at $\mathbf{w}^*$, we would have ....

- The minimum value of the squared loss is zero
- If zero were attained at $\mathbf{w}^*$, we would have $\forall u, \phi^T(x_u)\mathbf{w}^* = \mathbf{y_u}$, or equivalently $\phi\mathbf{w}^* = \mathbf{y}$, where

$$\phi = \begin{bmatrix} \phi_1(x_1) & \dots & \phi_p(x_1) \\ \dots & \dots & \dots \\ \phi_1(x_m) & \dots & \phi_p(x_m) \end{bmatrix}$$

and

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \dots \\ y_m \end{bmatrix}$$

- It has a solution if $\mathbf{y}$ is in the column space (the subspace of R^n formed by the column vectors) of ϕ

- The minimum value of the squared loss is zero
- If zero were NOT attainable at $\mathbf{w}^*$, what can be done?

Geometric Interpretation of Least Square Solution

- Let $\mathbf{y}^*$ be a solution in the column space of ϕ
- The least squares solution is such that the distance between $\mathbf{y}^*$ and $\mathbf{y}$ is minimized
- Therefore...........

Geometric Interpretation of Least Square Solution

- Let $\mathbf{y}^*$ be a solution in the column space of ϕ
- The least squares solution is such that the distance between $\mathbf{y}^*$ and $\mathbf{y}$ is minimized
- Therefore, the line joining $\mathbf{y}^*$ to $\mathbf{y}$ should be orthogonal to the column space

$$\phi\mathbf{w} = \mathbf{y}^* \tag{8}$$

$$(\mathbf{y} - \mathbf{y}^*)^{\mathbf{T}}\phi = \mathbf{0} \tag{9}$$

$$(\mathbf{y}^*)^{\mathbf{T}}\phi = (\mathbf{y})^{\mathbf{T}}\phi \tag{10}$$

$$(\phi \mathbf{w})^{\mathbf{T}} \phi = \mathbf{y}^{\mathbf{T}} \phi \tag{11}$$

$$\mathbf{w}^{\mathbf{T}} \phi^{\mathbf{T}} \phi = \mathbf{y}^{\mathbf{T}} \phi \tag{12}$$

$$\phi^{T} \phi \mathbf{w} = \phi^{\mathbf{T}} \mathbf{y} \tag{13}$$

$$\mathbf{w} = (\phi^{\mathbf{T}} \phi)^{-\mathbf{1}} \mathbf{y} \tag{14}$$

- Here $\phi^T \phi$ is invertible only if ϕ has full column rank

Proof?

Theorem : $\phi^T\phi$ is invertible if and only if ϕ is full column rank

Proof :

Given that ϕ has full column rank and hence columns are linearly independent, we have that $\phi\mathbf{x} = \mathbf{0} \Rightarrow \mathbf{x} = \mathbf{0}$

Assume on the contrary that $\phi^T\phi$ is non invertible. Then $\exists\mathbf{x} \neq \mathbf{0}$ such that $\phi^T\phi\mathbf{x} = \mathbf{0}$

$$\Rightarrow \mathbf{x^T}\phi^\mathbf{T}\phi\mathbf{x} = \mathbf{0}$$
$$\Rightarrow (\phi\mathbf{x})^\mathbf{T}\phi\mathbf{x} = \mathbf{0}$$
$$\Rightarrow \phi\mathbf{x} = \mathbf{0}$$

This is a contradiction. Hence $\phi^T\phi$ is invertible if ϕ is full column rank

If $\phi^T\phi$ is invertible then $\phi\mathbf{x} = \mathbf{0}$ implies $(\phi^T\phi\mathbf{x}) = \mathbf{0}$, which in turn implies $\mathbf{x} = \mathbf{0}$ **, This implies ϕ has full column rank if $\phi^T\phi$ is invertible. Hence, theorem proved**

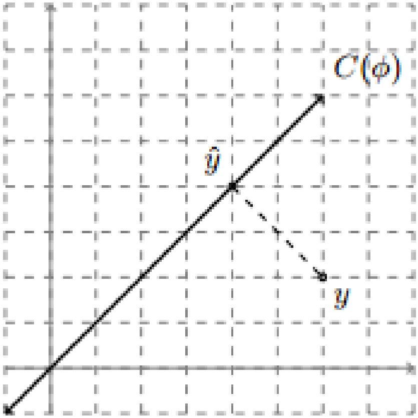


Figure: Least square solution $\mathbf{y}^*$ is the orthogonal projection of y onto column space of ϕ

What is Next?

- Some more questions on the Least Square Linear Regression Model
- More generally: How to minimize a function?
  - Level Curves and Surfaces
  - Gradient Vector
  - Directional Derivative
  - Hyperplane
  - Tangential Hyperplane
- Gradient Descent Algorithm