

Regression

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Recap

- Supervised (Classification and Regression) vs Unsupervised Learning
 - ▶ Three canonical learning problems
- What is data and how to predict
 - ▶ More on this today in the context of regression
- Squared Error

Agenda

- What is Regression
- Formal Defintion
- Types of Regression
- Least Square Solution
- Geometric Interpretation of least square solution

Regression

- Finding correlation between a set of output variables and a set of input variables
- Input variables are called *independent variables*
- Output variables are called *dependent variables*

Examples

- A company wants to know how much money they need to spend on T.V advertising to increase sales to a desired level, say y^*
- They have previous data of form $\langle x_i, y_i \rangle$, where x_i is money spent on advertising and y_i are sale figures
- They now fit the data with a function, lets say linear function

$$y = \beta_0 + \beta_1 * x \quad (1)$$

and then find the money they need to spend using this function

- Regression problem is to find the appropriate function and its coefficients

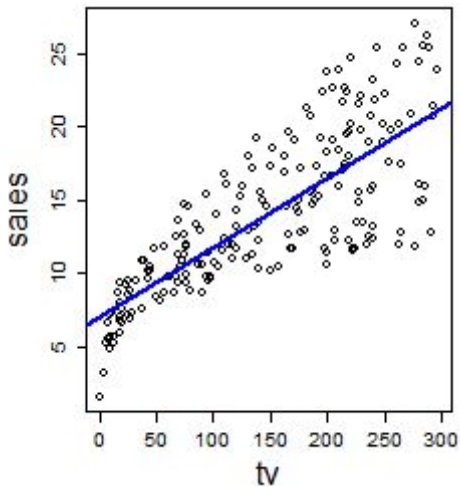


Figure: Linear regression on T.V advertising vs sales figure

What if sales is a non-linear function of advertising?

Formal Definition

- Two sets of variables: $x \in \mathcal{R}^N$ (independent) and $y \in \mathcal{R}^k$ (dependent)
- D is a set of m data points: $\langle x_1, y_1 \rangle, \langle x_2, y_2 \rangle, \dots, \langle x_m, y_m \rangle$
- $\epsilon(f, D)$: An error function, designed to reflect the discrepancy between the predicted value $f(x_i)$ and $y_i \forall i$
- Regression problem: Determine a function f^* such that $f^*(x)$ is the best predictor for y , with respect to D ,

$$f^* = \underset{f \in F}{\operatorname{argmin}} \epsilon(f, D) \quad (2)$$

where, F denotes the class of functions over which the optimization is performed

Types of Regression

- Depends on the function class and error function
- Linear Regression : establishes a relationship between dependent variable (Y) and one or more independent variables (X) using a best fit straight line, i.e

$$Y = a + b * X \quad (3)$$

- ▶ Here F is of the form $\sum_{i=1}^p w_i \phi_i(x)$, where ϕ_i are called basis functions
- ▶ Problem is to find w^* where

$$w^* = \underset{w}{\operatorname{argmin}} \epsilon(w, D) \quad (4)$$

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

$$\log \frac{p(y|x)}{1 - p(y|x)} = \beta_0 + \beta * x \quad (5)$$

- Lasso regression, Stepwise regression and many more

Least Square Solution

- Form of ϵ plays a major role in the accuracy and tractability of the optimization problem
- 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

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

- The least square solution for linear regression is given by

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{j=1}^m \left(\sum_{i=1}^p (\mathbf{w}_i \phi_i(\mathbf{x}_j) - y_j)^2 \right) \quad (7)$$

- 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 $\forall u, \phi^T(x_u)\mathbf{w}^* = y_u$, 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

$$\phi \mathbf{w} = \mathbf{y}^* \quad (8)$$

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

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

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

$$\mathbf{w}^T \phi^T \phi = \mathbf{y}^T \phi \quad (12)$$

$$\phi^T \phi \mathbf{w} = \phi^T \mathbf{y} \quad (13)$$

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

- 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 $\phi^T\phi\mathbf{x} = \mathbf{0}$

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

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

$$\Rightarrow \phi\mathbf{x} = \mathbf{0}$$

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**

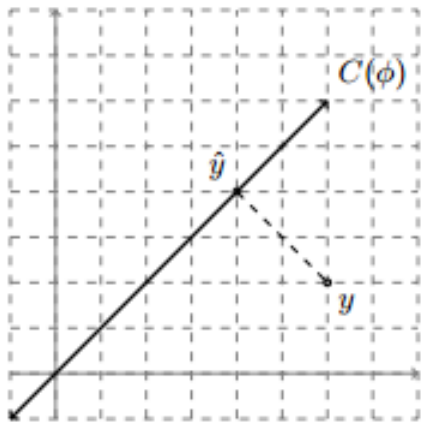


Figure: Least square solution \hat{y}^* is the orthogonal projection of y onto column space of ϕ