

Introduction to Regression

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1 Definitions

1. $x \in \mathfrak{R}$ means that the variable x is a member of the real numbers.
2. $\mathbf{x} \in \mathfrak{R}^d$ means that the d elements of the vector $\mathbf{x} = (x_1, \dots, x_d)$ all are members of the real numbers.
3. If \mathbf{x} is a random variable, then every sample of \mathbf{x} is generated from some density function $D(\mathbf{x})$.
4. A random variable \mathbf{x} is independently and identically distributed (iid) if each sample of \mathbf{x} is independent from all other samples, and each is drawn from the same density function $D(\mathbf{x})$.
5. A distribution is stationary if it doesn't change over time.
6. Expected value of \mathbf{x} is defined by:

$$\bar{\mathbf{x}} = E[\mathbf{x}] = \int_{-\infty}^{+\infty} \mathbf{x} D(\mathbf{x}) d\mathbf{x}$$

An unbiased estimate of $E[\mathbf{x}]$ can be obtained from N samples of \mathbf{x} (from $D(\mathbf{x})$), denoted by $\mathbf{x}_1, \dots, \mathbf{x}_N$ as follows

$$\hat{\bar{\mathbf{x}}} = \frac{1}{N} \sum_{i=1}^N \mathbf{x}_i$$

7. $\hat{\bar{\mathbf{x}}}$ is an unbiased estimate of $\bar{\mathbf{x}}$ means that $E[\hat{\bar{\mathbf{x}}}] = \bar{\mathbf{x}}$.
8. Variance of x is defined by:

$$\sigma^2 = V[x] = E[(x - \bar{x})^2]$$

The standard deviation is given by the square root of the above, or σ . An unbiased estimate of $V[x]$ can be obtained from N samples of x , once more symbolized by x_1, \dots, x_N as follows:

$$\hat{V}[x] = \frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2$$

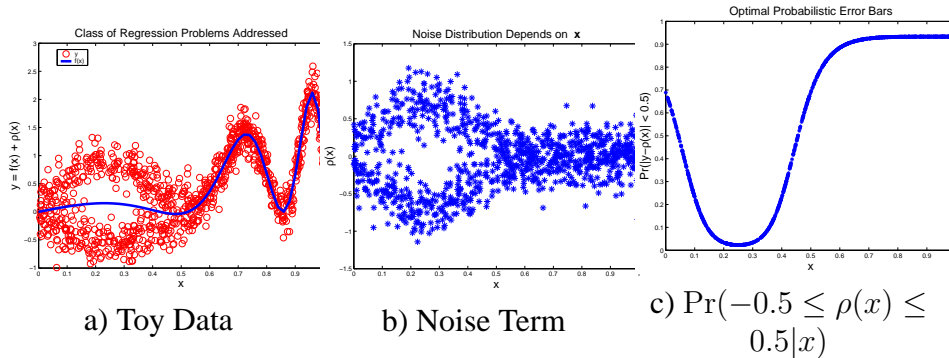


Figure 1: The noise term is a function of the input x and it is not Gaussian.

2 Assumptions on Data

Let $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$ be a set of N training examples, where $\mathbf{x} \in \mathfrak{R}^d$ are independently and identically distributed (iid) from some stationary distribution $D(\mathbf{x})$. The standard regression function formulation assumes that the outputs $y \in \mathfrak{R}$ are generated from:

$$y = f(\mathbf{x}) + \rho$$

where $f(\mathbf{x}) \in \mathfrak{R}$ is a real valued function defined on $\mathbf{x} \in \mathfrak{R}^d$, and ρ is a random variable with mean zero (i.e. $E[\rho] = 0$) and finite variance (i.e. $V[\rho] = c, 0 \leq c < \infty, c \in \mathfrak{R}$). This regression formulation assumes that $E[\rho]$ and $V[\rho]$ are independent of \mathbf{x} .

A more general data model, which is generally NOT assumed, would allow ρ be a function of \mathbf{x} . This assumes that $y \in \mathfrak{R}$ is generated from:

$$y = f(\mathbf{x}) + \rho(\mathbf{x}) \quad (1)$$

where the random variable ρ has $E[\rho(\mathbf{x})] = 0$ and $V[\rho(\mathbf{x})] = c(\mathbf{x}), 0 \leq c(\mathbf{x}) < \infty, c(\mathbf{x}) \in \mathfrak{R}$. Figure 1a shows a regression function where the noise changes as a function of the input \mathbf{x} . This noise term is shown in Figure 1b. The variation, as a function of \mathbf{x} , in the probability that the noise term lies between -0.5 and 0.5 , is shown in Figure 1c. Note that the noise is constant for $x > 0.7$.

Training data inputs can be represented in matrix form. For N training example of d dimensional inputs:

$$\begin{pmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_N^T \end{pmatrix} = \begin{pmatrix} x_{11} & \cdots & x_{1d} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{Nd} \end{pmatrix}$$

3 Regression Models

3.1 Linear Least Squares Regression

For data with d inputs, the model is assumed to have the following form:

$$\hat{y} = \hat{f}(\mathbf{x}) = \hat{\beta}_0 + \sum_{j=1}^d \hat{\beta}_j x_j = \hat{\beta}_0 + (\hat{\beta}_1, \dots, \hat{\beta}_d) \mathbf{x}^T$$

where $\beta = (\hat{\beta}_0, \dots, \hat{\beta}_d)^T$ are the model coefficients that are estimated from the training data. In *Least Squares Regression*, the model coefficients are chosen to minimize the following error metric (called Residual Sum of Squares (RSS)) on the training data $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$:

$$\begin{aligned} RSS(\beta) &= \sum_{i=1}^N (y_i - \hat{f}(\mathbf{x}_i))^2 \\ &= \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^d \beta_j x_{ij} \right)^2 \\ &= (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \end{aligned}$$

where $\mathbf{y} = (y_1, \dots, y_N)^T$ and

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1d} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_{N1} & \cdots & x_{Nd} \end{pmatrix}$$

RSS is a quadratic function and can be solved by differentiating with respect to β , setting the resulting equation to zero (which is where the minimum is), and solving for β . Differentiating we get:

$$\frac{\partial RSS}{\partial \beta} = -2\mathbf{X}^T (\mathbf{y} - \mathbf{X}\beta)$$

Assuming that \mathbf{X} is nonsingular (and hence $(\mathbf{X}^T \mathbf{X})^{-1}$ exists), setting to zero gives:

$$\mathbf{X}^T (\mathbf{y} - \mathbf{X}\beta) = 0$$

Solving for β gives:

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

The predicted model outputs for the training data are then given by:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\beta} = \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

3.1.1 Parameter Inference

If we assume that the training data is generated from a function that has *exactly* the following form:

$$y = \beta_0 + \sum_{j=1}^d \beta_j x_j + \varepsilon$$

where ε is a Gaussian Noise term (i.e. Normally distributed) with $E[\varepsilon] = 0$ and finite variance σ^2 , then we can make a number of interesting conclusions about the parameters $\hat{\beta}$. Under these assumptions, $\hat{\beta}$ is generated from a $d + 1$ dimensional Normal Distribution, allowing Hypothesis testing on $\hat{\beta}$ (i.e. is $\hat{\beta}_j$ zero, and what is the probability that it falls in some range of values). You will not be tested on this, but if you are interested in details, any text on Regression Analysis will do. Also see Chapter 3 of [1].

3.2 Regularization or Shrinkage Least Squares Methods

If any two inputs are well correlated, then $(\mathbf{X}^T \mathbf{X})^{-1}$ will not exist. You can calculate the correlation coefficient κ between any two variables x_i and x_j using:

$$\kappa = \frac{Cov(x_i, x_j)}{\sigma_i \sigma_j}$$

where σ_1 and σ_j are the standard deviation of x_i and x_j respectively, and the covariance $Cov(x_i, x_j)$ is given by:

$$Cov(x_i, x_j) = E[(x_i - \bar{x}_i)(x_j - \bar{x}_j)]$$

Note that $-1 \leq \kappa \leq 1$ and $(\mathbf{X}^T \mathbf{X})^{-1}$ will not exist if $|\kappa|$ is close to 1.

When $(\mathbf{X}^T \mathbf{X})^{-1}$ is singular, regularization methods can be used to find the model coefficients $\hat{\beta}$. Two commonly used regularization methods are Ridge regression and Lasso Regression.

3.2.1 Ridge Regression

In Ridge Regression, given training data $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$, the ridge model coefficients $\hat{\beta}^{ridge}$ are defined as follows:

$$\hat{\beta}^{ridge} = \arg \min_{\beta} \left\{ \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^d \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^d \beta_j^2 \right\}$$

This is equivalent to the following optimization problem:

$$\begin{aligned} \hat{\beta}^{ridge} &= \arg \min_{\beta} \left\{ \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^d \beta_j x_{ij} \right)^2 \right\} \\ &\text{subject to: } \sum_{j=1}^d \beta_j^2 \leq s \\ &s > 0 \end{aligned}$$

Obtaining the ridge model coefficients $\hat{\beta}^{ridge}$ is relatively straight forward. One way is to center all your inputs by replacing x_{ij} with $x_{ij} - \bar{x}_j$. The coefficients $(\hat{\beta}_1^{ridge}, \dots, \hat{\beta}_d^{ridge})$ are given by

$$(\hat{\beta}_1^{ridge}, \dots, \hat{\beta}_d^{ridge})^T = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

where \mathbf{I} is the d by d identity matrix, and \mathbf{X} contains the centered data points as follows:

$$\mathbf{X} = \begin{pmatrix} x_{11} - \bar{x}_1 & \dots & x_{1d} - \bar{x}_d \\ \vdots & \ddots & \vdots \\ x_{N1} - \bar{x}_1 & \dots & x_{Nd} - \bar{x}_d \end{pmatrix}$$

Then the offset coefficient is obtained by the following equation:

$$\hat{\beta}_0^{ridge} = \bar{y} - (\hat{\beta}_1^{ridge}, \dots, \hat{\beta}_d^{ridge}) \bar{\mathbf{x}}^T = \left[\frac{1}{N} \sum_{i=1}^N y_i \right] - \left[\sum_{j=1}^d \bar{x}_j \hat{\beta}_j^{ridge} \right]$$

3.2.2 Lasso Regression

In Lasso Regression, given training data $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)\}$, the lasso model coefficients $\hat{\beta}^{lasso}$ are calculate as follows:

$$\hat{\beta}^{lasso} = \arg \min_{\beta} \left\{ \sum_{i=1}^N \left(y_i - \beta_0 - \sum_{j=1}^d \beta_j x_{ij} \right)^2 \right\}$$

$$\text{subject to: } \sum_{j=1}^d |\beta_j| \leq s$$

$$s > 0$$

Therefore, the main difference between Lasso and Ridge is that Lasso measures shrinkage by $\sum |\beta|$ while ridge uses $\sum \beta^2$. For Lasso, this has the interesting and desirable effect of setting β coefficients to zero. This is not true for Ridge Regression. However, Ridge regression is easy to solve, while Lasso has has been computationally expensive until very recently (see <http://www-stat.stanford.edu/~hastie/Papers/LARS/>).

3.3 Non-Linear Least Squares Regression

3.3.1 Standard Nonlinear Formulations

When the problem is believed to be non-linear, the following model structure can be used:

$$\hat{y} = \hat{f}(\mathbf{x}) = \hat{\beta}_0 + \sum_{j=1}^p \hat{\beta}_j \varphi_j(\mathbf{x}) = \hat{\beta}_0 + (\hat{\beta}_1, \dots, \hat{\beta}_p) \Phi(\mathbf{x})^T$$

Where the p basis functions $\Phi(\mathbf{x}) = (\varphi_1(\mathbf{x}), \dots, \varphi_p(\mathbf{x}))^T$ are nonlinear functions of the inputs \mathbf{x} . Examples include $\varphi_1(\mathbf{x}) = x_1 x_2$, $\varphi_2(\mathbf{x}) = x_1^2$, $\varphi_3(\mathbf{x}) = \sin(x_3)$, etc.

The model coefficients $\beta = (\hat{\beta}_0, \dots, \hat{\beta}_p)^T$ can be obtained using the same techniques described above with the following differences. For standard least squares regression the \mathbf{X} matrix becomes:

$$X = \begin{pmatrix} 1 & \varphi_1(\mathbf{x}_1) & \cdots & \varphi_p(\mathbf{x}_1) \\ \vdots & \vdots & \vdots & \vdots \\ 1 & \varphi_1(\mathbf{x}_N) & \cdots & \varphi_p(\mathbf{x}_N) \end{pmatrix}$$

For ridge regression, the \mathbf{X} matrix becomes:

$$\mathbf{X} = \begin{pmatrix} \varphi_1(\mathbf{x}_1) - \bar{\varphi}_1 & \cdots & \varphi_p(\mathbf{x}_1) - \bar{\varphi}_p \\ \vdots & \ddots & \vdots \\ \varphi_1(\mathbf{x}_N) - \bar{\varphi}_1 & \cdots & \varphi_p(\mathbf{x}_N) - \bar{\varphi}_p \end{pmatrix}$$

where

$$\bar{\varphi}_j = \frac{1}{N} \sum_{i=1}^N \varphi_j(\mathbf{x}_i)$$

3.3.2 Kernel Regression

The problem with the standard non-linear regression as posed above is that there are infinitely many possibilities for the nonlinear basis functions $\phi_j(\mathbf{x})$, and choosing which to use and how many can become computationally expensive. In kernel regression, the basis functions are restricted to be kernels of the following form:

$$\varphi_i(\mathbf{x}) = K(\mathbf{x}_i, \mathbf{x})$$

where \mathbf{x}_i for $i = 1, \dots, N$ are training example inputs. Therefore, the kernel model looks like:

$$\hat{y} = \hat{\beta}_0 + \sum_{i=1}^N \hat{\beta}_i K(\mathbf{x}_i, \mathbf{x}) \quad (2)$$

Typically used kernel functions include the Gaussian Kernel:

$$K(\mathbf{a}, \mathbf{b}) = \exp\left[-\frac{\|\mathbf{a} - \mathbf{b}\|^2}{2\sigma^2}\right]$$

where $\mathbf{a}, \mathbf{b} \in \mathfrak{R}^d$, the kernel parameter is $\sigma > 0$, and

$$\|\mathbf{a} - \mathbf{b}\|^2 = \sum_{j=1}^d (a_j - b_j)^2$$

The polynomial kernel:

$$K(\mathbf{a}, \mathbf{b}) = (q + \mathbf{a}^T \mathbf{b})^k$$

where $\mathbf{a}, \mathbf{b} \in \mathfrak{R}^d$, the kernel parameter are $k = 1, 2, 3, \dots$ and $q \in \mathfrak{R}$. (**QUESTION:** What happens when $k = 1$ and $q = 0$?) The sigmoid Kernel:

$$K(\mathbf{a}, \mathbf{b}) = \tanh(\kappa \mathbf{a}^T \mathbf{b} + \theta)$$

where $\mathbf{a}, \mathbf{b} \in \mathfrak{R}^d$, the kernel parameter are $\kappa \in \mathfrak{R}$ and $\theta \in \mathfrak{R}$.

For kernel ridge regression, the \mathbf{X} matrix becomes:

$$\mathbf{X} = \begin{pmatrix} K(\mathbf{x}_1, \mathbf{x}_1) - \bar{\varphi}_1 & \dots & K(\mathbf{x}_1, \mathbf{x}_N) - \bar{\varphi}_N \\ \vdots & \ddots & \vdots \\ K(\mathbf{x}_N, \mathbf{x}_1) - \bar{\varphi}_1 & \dots & K(\mathbf{x}_N, \mathbf{x}_N) - \bar{\varphi}_N \end{pmatrix} \quad (3)$$

where

$$\bar{\varphi}_j = \frac{1}{N} \sum_{i=1}^N K(\mathbf{x}_j, \mathbf{x}_i) \quad (4)$$

Then the offset coefficient is obtained by the following equation:

$$\hat{\beta}_0^{ridge} = \left[\frac{1}{N} \sum_{i=1}^N y_i \right] - \left[\sum_{j=1}^N \bar{\varphi}_j \hat{\beta}_j^{ridge} \right] \quad (5)$$

Ridge regression is often used to solve for the model coefficients, and this framework is called *Kernel Ridge Regression*. Kernel Ridge Regression is a powerful tool for building nonlinear regression models, often outperforming other techniques.

4 Practical Considerations

There are a number of practical considerations when building regression models. These include:

1. Scale all inputs to the same range. Usually -1 to $+1$ before building the model.
2. Get rid of highly correlated inputs.
3. Feature (i.e. input) selection. Features that do not improve the model should be discarded. Lasso regression is a good method for feature selection. We will cover others in class. See Chapter 3 of [1].

5 Other Regression Formulations

We will cover a number of other regression formulations in class. These include Gaussian Process Regression, Support Vector Regression, Regression Trees, Nearest Neighbor Regression, and Random Forests.

References

- [1] T. Hastie, R. Tibshirani, and J. Friedman. *The Elements of Statistical Learning: data mining, inference and prediction*. Springer, 2001.