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1.1 Linear Regression Models

Suppose we have an input vector $\mathbf{X}^{\top} = (X_1, X_2, \dots, X_p)$ and we want to predict a real-valued output Y. The linear regression model has the form

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j.$$
 (1.1)

Typically we have a set of training data $(x_1, y_1) \dots (x_N, y_N)$ from which we can estimate the parameters β by minimizing the error function which we will define next. Each $x_i = (x_{i1}, x_{i2}, \dots, x_{ip})^{\top}$ represents a vector of feature measurements for the ith case. The most popular estimation method is least squares, in which we pick the coefficients β to minimize the residual sum of squares

$$RSS(\beta) = \sum_{i=1}^{N} (y_i - f(x_i))^2$$

$$= \sum_{i=1}^{N} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j \right)^2.$$
(1.2)

To minimize (1.2), we rewrite β by appending $\beta_0 = 1$ at its first element for convenience. Then, we rewrite the residual sum-of-squares as

$$RSS(\beta) = (\mathbf{y} - \mathbf{X}\beta)^{\top} (\mathbf{y} - \mathbf{X}\beta). \tag{1.3}$$

Expanding the above equality, we could obtain

$$RSS(\beta) = \mathbf{y}^{\top} \mathbf{y} - \mathbf{y}^{\top} \mathbf{X} \beta - \beta^{\top} \mathbf{X}^{\top} \mathbf{y} + \beta^{\top} \mathbf{X}^{\top} \mathbf{X} \beta$$
$$= \mathbf{y}^{\top} \mathbf{y} - 2 \mathbf{y}^{\top} \mathbf{X} \beta + \beta^{\top} \mathbf{X}^{\top} \mathbf{X} \beta$$
(1.4)

Differentiating with respect to β we obtain

$$\frac{\partial \text{RSS}}{\partial \beta} = -2\mathbf{y}^{\top} \mathbf{X} + 2\mathbf{X}^{\top} \mathbf{X} \beta$$

$$\frac{\partial^2 \text{RSS}}{\partial \beta \partial \beta^{\top}} = 2\mathbf{X}^{\top} \mathbf{X}.$$
(1.5)







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Since the Hessian $\mathbf{X}^{\top}\mathbf{X}$ is positive definite, we set the first derivative to

$$\mathbf{X}^{\top} \left(\mathbf{y} - \mathbf{X} \beta \right) = 0 \tag{1.6}$$

to obtain the unique solution

$$\hat{\beta} = \left(\mathbf{X}^{\top}\mathbf{X}\right)^{-1}\mathbf{X}^{\top}\mathbf{y}.\tag{1.7}$$

The predicted values at an input vector x_0 are given by $\hat{f}(x_0) = (1 : x_0)^{\top} \hat{\beta}$; the fitted values at the training inputs are

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^{\top}\mathbf{X})^{-1}\mathbf{X}^{\top}\mathbf{y},\tag{1.8}$$

where $\hat{y}_i = \hat{f}(x_i)$.

- 1.2 Conditioning Gaussians
- ${\bf 1.3} \quad {\bf Ridge} \ {\bf Regression} \ / \ {\bf L1} \ {\bf regularized} \ {\bf Linear} \ {\bf Regression}$
- 1.4 L1/L2 Regularization
- 1.5 Multivariate Gaussian
- 1.6 Gaussian Discriminant Analysis
- 1.7 Exponential Family
- 1.8 Solving an Unconstrained Quadratic
- 1.9 SVD, Cholesky, Eigen/Spectral Decompositions
- 1.10 Generalized Linear Models



