Regression

Linear Regression

1. Form

$$Y = \mathbf{X}\beta + \epsilon$$

where $Y = (y_1, y_2, \dots, y_n)^T$, $\beta = (\beta_1, \beta_2, \dots, \beta_p)^T$ and $\mathbf{X}$ is the data matrix with an extra column of ones on the left to account for the intercept.

2. Assumptions

- Linear relationship
- Multivariate normality + Independence + Constant variance

$$\epsilon \overset{iid}{\sim} N(0, \sigma^2)$$

Assumptions	Diagnosis	Solutions
Linearity	Scatter plot	1. Apply a nonlinear transformation; 2. Try a nonlinear form to fit
Normality	QQ plot of residuals/non-parametric tests(KS or AD test)	Box-cox transformation on dependent variable
Independence	Residual vs time/Durbin Watson test/VIF	1. Time series model like ARCH, ARMA or ARIMA; 2. Ridge Regression/Lasso Regression
Constant Variance	Residual vs predicted values	Log transformation

Ref: http://people.duke.edu/~rnau/testing.htm

3. Loss Function & Estimation

$$RSS = \Sigma_{i=1}^{n}(y_i - X_i\beta)^2$$

The goal is to minimize RSS. The mean square estimation of β is:

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

This only exists when $\mathbf{X}^T X$ is invertible. This requires $n \geq p$ (because if a matrix is invertible, it should be full rank).

- What if $n \leq p$?

  We could introduce **L2 regulariation** to solve the problem. Then the estimator would become

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T Y$$

Ref: https://zhuanlan.zhihu.com/p/44612139

- In practise: it would take long time to solve the inverse for a matrix with high dimension, therefore, we always use gradient descent to get the estimator in practise.

4. Goodness of Fit

- F-test: test whether a group of variables is important
- T-test: test whether a variable is important
- Variable selection:
  - Forward: start from a null model, include variables one at a time, minimize the RSS at each step.
  - Backward: start from a full model, eliminate variables one at a time, choosing the one with the largest t-test p-value at each step.
  - Mixed: start from a null model, include variables one at a time, minimizing the RSS at each step. If the p-value for some variables goes beyond a threshold, eliminate that variable.
- Model selection: AIC/BIC
- R square: $corr^2(Y, \hat{Y})$ always increases as we add more variables.
- RSE: residual standard error does not always imporve with more predictors:

$$RSE = \sqrt{\frac{1}{n-p-1}RSS}$$

- MSE:

$$MSE = \frac{1}{n}RSS$$

5. Additionals

- How to encode dummy variables?

  Different ways of encoding would bring different interpretations for parameters. In order to get corresponding results, we have to carefully encode our dummy variables.

- How to solve overfitting problem when variables are too many ?
  - regularization
  - variable selection
  - dimension reduction (feature extraction)

Ridge Regression

As we mentioned above, least squares for linear regression only works if $X^T X$ is invertible. And when $X^T X$ is almost invertible, the OLS estimator would be **numerically unstable (non-unique solution) which would lead to high variance of predictions**. Moreover, for high dimensional data, the data matrix is often sparse in which OLS does not perform as we expect.

In order to solve these issues, we could introduce L2 regularization to **make the almost singular matrix to be regular**.

1. Loss function & Estimation

Actually, ridge regression is a modificaiton of linear regression. We try to make estimators more robust if $X^T X$ is almost singular. The loss function of ridge regression is

$$Loss = (Y - X\beta)^T (Y - X\beta) + \lambda \beta^T \beta$$

The first part of ridge loss function is same to linear regression while the second part is called penalty term/L2 regulariation. By deriativating, we could get the closed-form solution of miminizing the loss function is

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T Y$$

2. Tuning λ

Comparing with linear regression, the estimator of ridge regression is biased but it does decrease the variance of predictions since it solves the singularity issue. In ridge regression, λ controls the trade-off between bias and variance. We could tune λ by using cross-validation.

3. Additional

- What benefits could it bring?
  - Estimators become more numerically stable.
  - Estimators shrink globally which means we expect to get a simpler model.
  - The simpler model, the less chance to overfit.
  - The variance of predictions become smaller.
- Do we have to preprocess our dataset when different variables has different scale?

  Yes. For linear regression, the scale difference between variables could be represented well in estimators. However, it's not the case in ridge regression. In order to prevent penalizing some coefficients more than others, we'd better to scale each variable such that it has sample variance 1 before runing the regression.

Lasso Regression

1. Loss Function & Estimator

Similarily, Lasso regression introduces L1 regulariation as the penalty term.

$$Loss = (Y - X\beta)^T (Y - X\beta) + \lambda \Sigma_{j=1}^{p} |\beta_j|$$

For lasso regression, there is no closed-form solution, so we have to use numerical optimization.

2. Estimator

- Closed-form solution

Since the loss function of lass regression is non-derivative at $x = 0$, we said that there is no closed-form solution above. However, if we add an assumption $X^T X = \mathbf{I}$, then things will be different.

In this case, we could expand the loss function

$$\begin{aligned} Loss &= Y^T Y - 2\beta^T X^T Y + \beta^T \beta + \lambda \Sigma_{j=1}^{p} |\beta_j| \\ &= C - 2\beta^T X^T Y + \beta^T \beta + \lambda \Sigma_{j=1}^{p} |\beta_j| \end{aligned}$$

And if $X^T X = \mathbf{I}$, we could get $\hat{\beta}^{OLS} = X^T Y$. So

$$\begin{aligned} Loss &= C - 2\beta^T \beta^{OLS} + \beta^T \beta + \lambda \Sigma_{j=1}^{p} |\beta_j| \\ &= C + \Sigma_{j=1}^{p} (-2\beta_j \beta_j^{OLS} + \beta_j^2 + \lambda |\beta_j|) \end{aligned}$$

Minimizing the loss function actually equivalent to minimizing $-2\beta_j \beta_j^{OLS} + \beta_j^2 + \lambda |\beta_j|$. Then we could get the closed-form case-by-case, the solution would be

$$\hat{\beta}_j^{LASSO} = sign(\hat{\beta}_j^{OLS})(|\hat{\beta}_j^{OLS}| - \frac{\lambda}{2})^+$$

Ref: *https://stats.stackexchange.com/questions/17781/derivation-of-closed-form-lasso-solution* & https://blog.csdn.net/zhili8866/article/details/53408839

- Coordinate Descent

  The core idea of coordinate descent is that in each step, we take β_{-j} as constant variables and then only get the best solution of β_j. We'll iterate this process till all weights converge.

  Derivation see in https://courses.cs.washington.edu/courses/cse446/17wi/slides/lasso.pdf

- Least Angle Regression

  please read https://www.cnblogs.com/pinard/p/6018889.html

3. Difference between L1 & L2 regulariztion

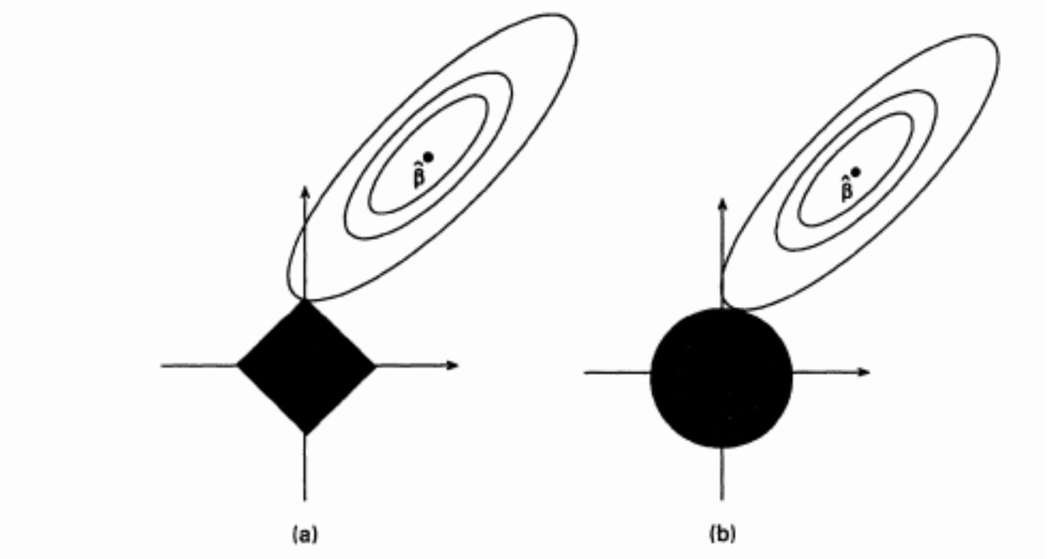


Fig. 2. Estimation picture for (a) the lasso and (b) ridge regression

L2 shrinks all the coefficients to a non-zero value. However, L1 shrinks some of the coefficients all the way to zero. Therefore, Lasso regression could be took as a method of variable selection.

4. Additionals

- When some of coefficients are non-zero values, the bias, variance and MSE are lower for the lasso. While if most of coefficients are non-zero values, ridge regression would have a smaller variance than lasso.
- In bayesian interpretations, β_{ridge} is the posterior mean with a Normal prior on β while β_{lasso} is the posterior mean with a Laplace prior on β.
- What is the proper way of pre-processing dataset before lasso regression?
  - Centerize: one thing have to be stated out is that **the result of centering the variables means that there is no longer an intercept**. Whether we have to centerize our data depends on if we need an intercept in the model.
  - Scaling: in most of cases, we'd better scale our dataset for a better convergence.

Classification

Logistic Regression

Logistic regression is a method of classification which means its dependent variable should be qualitive.

1. Form

$$y = \frac{1}{1 + e^{-(\mathbf{w}^T\mathbf{x}+b)}}$$

where $y = P(y = 1|\mathbf{x})$. The form could be also written as

$$ln\frac{p}{1-p} = w^T\mathbf{x} + b$$

we call $\frac{p}{1-p}$ as **odds** and $ln\frac{p}{1-p}$ as **logit**.

2. Loss Function & Estimation

$$Loss = \frac{1}{m}\Sigma_{i=1}^{m} - y_i log(\hat{y}_i) - (1 - y_i)log(1 - \hat{y}_i)$$

Here we use logarithmic loss function (a.k.a 0-1 classification form of cross entropy) as our loss function. And **minimizing this loss function is actually equivalent to maximizing the log-likelihood**.

- Why don't we use MSE as loss function?

  If we use MSE as loss function, the deriative of the loss function must include the deriative of sigmoid.

$$loss' = (\hat{y} - y)sigmoid'x$$

And we know the deriative of sigmoid would be 0 when x is big which would lead to **gradient vanishing** issue. However, logarithmic loss function would not have this problem. The derivative of logarithmic loss function looks as below

$$loss' = \frac{1}{N}\Sigma_{i=1}^{N} x_i(y_i - p(x_i))$$

The advantage of logarithmic loss function is that when the predicted value is far away from the truth, graident would become big and then the training process would be speeded up.

- How to estimate parameters?
  - Gradient Descent: first-order deriative

$$w^{t+1} = w^t - \alpha\frac{\partial L}{\partial w^t}$$

  - Newton's algorithm: second-order deriative

$$w^{t+1} = w^t - \alpha\frac{L'}{L''}$$

3. Additionals

- Is it linear or non-linear classfication?

  Logistic regression is a linear classifier because the predicted log-odds could be formed as a linear function of x. However, non-linear classfication, such as neural networks, there is no way to summarize the output of a neural network in terms of a linear function of x.

- Can it apply to multi-classes problem?

  Yes. As for k-classes problem, we could fit k-1 logistic regression models to classify k-classes.

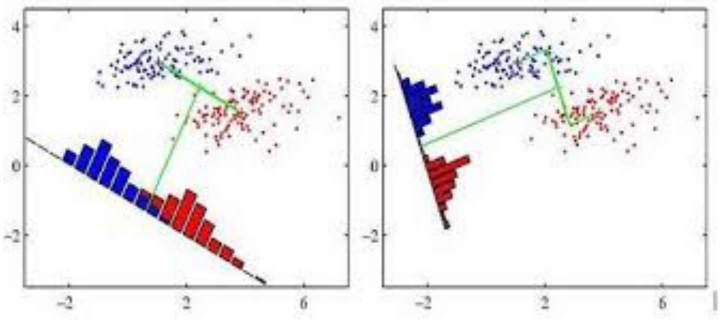
- Can it be used to non-linear problem?

  Yes. Think about Kernel used in SVM. For non-linear problem, we could fit kernel logistic regression.

Linear Discriminant Analysis (LDA)

1. Goal

The goal of LDA (binary case) is that : given dataset, we need to find a line $y = w^T x$ which could make the projection of same class points to be close to each other and conversely the projection of different class points to be as far as possible.



Another equivalent explanation is: we have to make the covariance of same class points to be as small as possible, in the meanwhile, the center of different classes to be as far as possible. This explaination could be easier to understant if we take the normality assumption of LDA into account.

2. Loss Function & Estimation

Based on the goal of LDA, we could construct a loss function like

$$\begin{aligned} Loss &= \frac{||w^T\mu_0 - w^T\mu_1||_2^2}{w^T\Sigma_0 w + w^T\Sigma_1 w} \\ &= \frac{w^T(\mu_0-\mu_1)(\mu_0-\mu_1)^T w}{w^T(\Sigma_0+\Sigma_1)w} \end{aligned}$$

Here, we could let $S_w = \Sigma_0 + \Sigma_1$ and $S_b = (\mu_0-\mu_1)(\mu_0-\mu_1)^T$.

According to Lagrange multiplier and the property of vector dot product (dot product is scalar which has no direction), we could get

$$w = S_w^{-1}(\mu_0 - \mu_1)$$

In practise, considering the stability of results, we usually apply SVD on S_w to get its inverse.

3. Bayesian Explanation

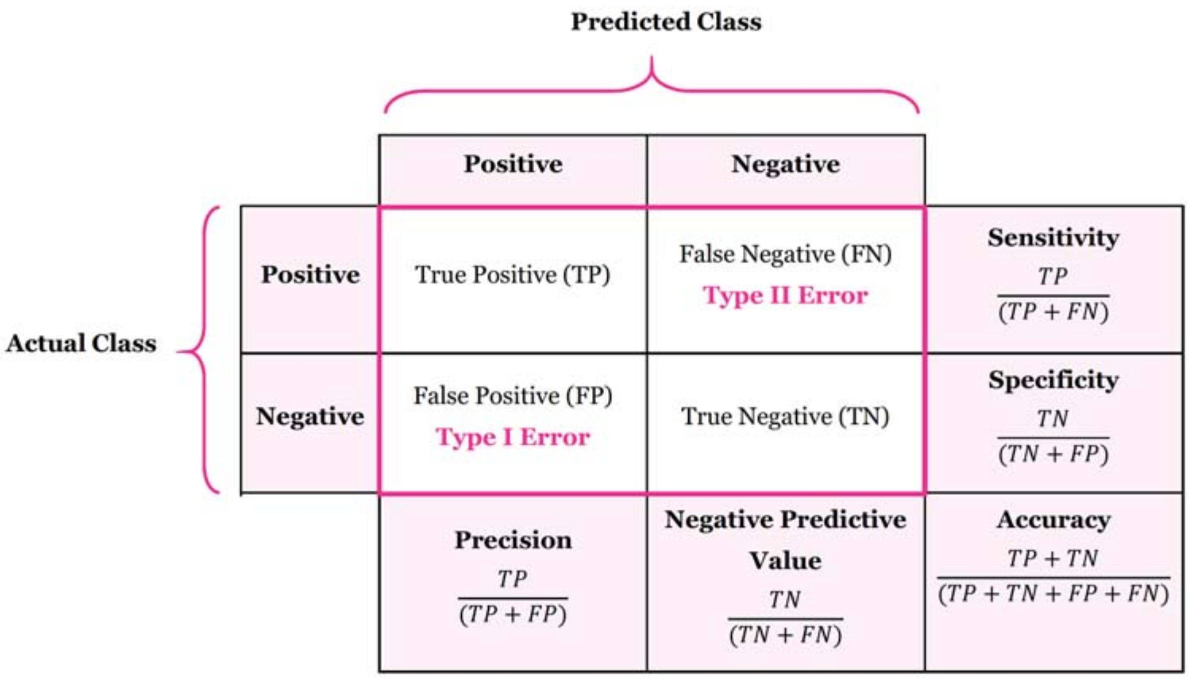
- What we want to know:

$$\hat{P}(Y=k|X=x) = \frac{\hat{P}(X=x|Y=k)\hat{P}(Y=k)}{\Sigma_j \hat{P}(X=x|Y=j)\hat{P}(Y=j)}$$

- What we suppose:
  - Suppose $P(X=x|Y=k) = f_k(x)$ to be a **multivariate normal distribution**.
  - Suppose the convariance matrix is same to all categories.
  - Suppose we know $P(Y=k) = \pi_k$ exactly.
- After expanding RHS of the equation, we could know that LDA has linear decision boundaries.
- How about QDA?
  - QDA is a non-linear classifier.
  - It **does not** require the convariance matrix is same to all categories.

4. Evaluation

- Confusion Matrix



		Predicted Class		
		Positive	Negative	
Actual Class	Positive	True Positive (TP)	False Negative (FN) **Type II Error**	**Sensitivity** $\frac{TP}{(TP+FN)}$
	Negative	False Positive (FP) **Type I Error**	True Negative (TN)	**Specificity** $\frac{TN}{(TN+FP)}$
		Precision $\frac{TP}{(TP+FP)}$	**Negative Predictive Value** $\frac{TN}{(TN+FN)}$	**Accuracy** $\frac{TP+TN}{(TP+TN+FP+FN)}$

  - Type I Error: reject the true null hypothesis.
  - Type II Error: fail to reject the false null hypothesis.

  Note: threshold is the hidden parameter needs to be careful.

- ROC curves
  - Display the performance of the method for any choice of threshold. That means, we could use it as a method of choosing best-fit threshold.
  - The area under the curver (AUC) measures the quality of the classifier. The closer AUC is to 1, the better.

5. Multi-class LDA

As for N classes, $i-th$ class has m_i samples. We could define the global scatter matrix:

$$\begin{aligned} S_t &= S_b + S_w \\ &= \Sigma_{i=1}^{m}(x_i-\mu)(x_i-\mu)^T \end{aligned}$$

And we could also define:

$$S_w = \Sigma_{i=1}^{N}\Sigma_{x\in X_i}(x_i-\mu_i)(x_i-\mu_i)^T$$

Then we have

$$\begin{aligned} S_b &= S_t - S_w \\ &= \Sigma_{i=1}^{N} m_i(\mu_i-\mu)(\mu_i-\mu)^T \end{aligned}$$

Similar to binary case, we have to maximize $\frac{tr(W^T S_b W)}{tr(W^T S_w W)}$. In the end, we have to solve $S_b W = \lambda S_w W$.

The closed-form solution of W is the matrix composed of the top d' eigenvectors having the d largest eigenvalues of $S_w^{-1}S_b$. Here, $d' \le N-1$.

Note: since we could take W as a project matrix and d' is always smaller than the original dimension d, in this way, LDA is also an useful way of dimension reduction.

Two Main Issues on Classification

- How to train build a multi-classes classifier?
  - One vs One: N(N-1)/2 binary classifiers + vote
  - One vs Rest: N binary classifiers
  - Many vs Many: Error correcting output codes + compute distance
- Imbalance dataset (ex: 0 dataset is larger than 1)
  - undersampling: eliminate some 0 samples.
  - oversampling: add some 1 samples. For example, SMOTE

    Note: here we could not simply resample 1s because it could lead to overfitting.
  - Threshold-moving: changing threshold of binary classifier.