Introduction to Big Data Analysis
Regression

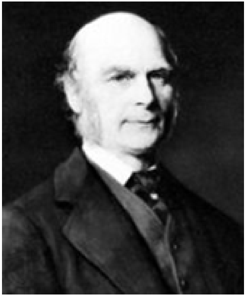
Zhen Zhang

Southern University of Science and Technology

Outlines

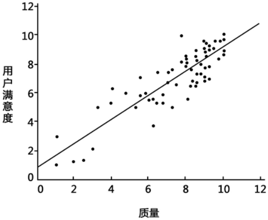
Regression

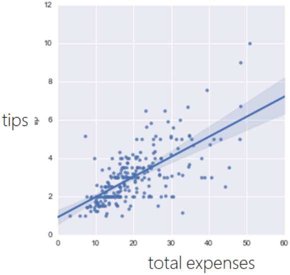
- Proposed by Francis Galton (left) and Karl Pearson (right), in the publication "Regression towards mediocrity in hereditary "
- The characteristics (e.g., height) in the offspring regress towards a mediocre point (mean) of that of their parents
- Generalization : predict the dependent variables y from the independent variables $\mathbf{x}$: $y = f(\mathbf{x})$ or $y = E[y|\mathbf{x}]$



Applications

- Predict medical expenses from the individual profiles of the patients
- Predict the scores on Douban from the quality of the movies
- Predict the tips from the total expenses



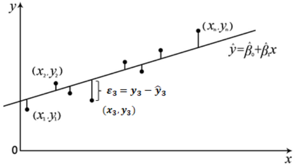


Outlines

Univariate Linear Model

- Linear model : $y = w_0 + w_1 x + \epsilon$, where w_0 and w_1 are regression coefficients, ϵ is the error or noise
- Assume $\epsilon \sim \mathcal{N}(0, \sigma^2)$, where σ^2 is a fixed but unknown variance ; then $y|x \sim \mathcal{N}(w_0 + w_1 x, \sigma^2)$
- Assume the samples $\{x_i, y_i\}_{i=1}^n$ are generated from this conditional distribution, i.e., $y_i|x_i \sim \mathcal{N}(w_0 + w_1 x_i, \sigma^2)$
- Intuitively, find the best straight line (w_0 and w_1) such that the sample points fit it well, i.e., the residuals are minimized,

$$(\hat{w}_0, \hat{w}_1) = \arg\min_{w_0, w_1} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_i)^2$$

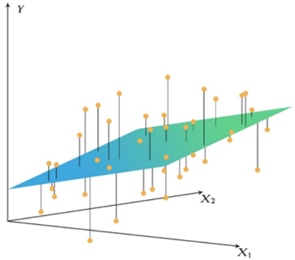


Multivariate Linear Model

- Linear model : $y = f(\mathbf{x}) + \epsilon = w_0 + w_1 x_1 + \cdots + w_p x_p + \epsilon$, where $w_0, w_1, \ldots, w_p$ are regression coefficients, $\mathbf{x} = (x_1, \ldots, x_p)^T$ is the input vector whose components are independent variables or attribute values, $\epsilon \sim \mathcal{N}(0, \sigma^2)$ is the noise
- For the size n samples $\{(\mathbf{x}_i, y_i)\}_{i=1}^n$, let $\mathbf{y} = (y_1, \ldots, y_n)^T$ be the response or dependent variables, $\mathbf{w} = (w_0, w_1, \ldots, w_p)^T$, $\mathbf{X} = [\mathbf{1}_n, (\mathbf{x}_1, \ldots, \mathbf{x}_n)^T] \in \mathbb{R}^{n \times (p+1)}$, and $\boldsymbol{\varepsilon} = (\epsilon_1, \ldots, \epsilon_n)^T \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n)$.

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\varepsilon}$$

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \cdots & x_{1p} \\ 1 & x_{21} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \cdots & x_{np} \end{pmatrix}$$

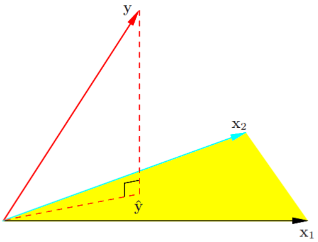


Least Square (LS)

- Minimize the total residual sum-of-squares :
  $RSS(\mathbf{w}) = \sum_{i=1}^{n}(y_i - w_0 - w_1 x_1 - \cdots - w_p x_p)^2 = \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2$
- When $\mathbf{X}^T\mathbf{X}$ is invertible, the minimizer $\hat{\mathbf{w}}$ satisfies

$$\nabla_{\mathbf{w}} RSS(\hat{\mathbf{w}}) = 0 \quad \Rightarrow \quad \hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

- The prediction $\hat{\mathbf{y}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} = \mathbf{P}\mathbf{y}$ is a projection of $\mathbf{y}$ onto the linear space spanned by the column vectors of $\mathbf{X}$; $\mathbf{P} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is the projection matrix satisfying $\mathbf{P}^2 = \mathbf{P}$



Maximal Likelihood Estimate (MLE)

- A probabilistic viewpoint : $y|\mathbf{x} \sim \mathcal{N}(w_0 + w_1 x_1 + \cdots + w_p x_p, \sigma^2)$
- Likelihood function : $L(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \mathrm{P}(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \Pi_{i=1}^{n} \mathrm{P}(y_i|\mathbf{x}_i, \mathbf{w})$ with $\mathrm{P}(y_i|\mathbf{x}_i, \mathbf{w}) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i - w_0 - w_1 x_{i1} - \cdots - w_p x_{ip})^2}{2\sigma^2}}$
- Maximal likelihood estimate : given the samples from some unknown parametric distribution, find the parameters such that the samples the most probably seem to be drawn from that distribution, i.e., $\hat{\mathbf{w}} = \arg\max_{\mathbf{w}} L(\mathbf{w}; \mathbf{X}, \mathbf{y})$
- Equivalent to maximize the log-likelihood function $l(\mathbf{w}; \mathbf{X}, \mathbf{y}) = \log L(\mathbf{w}; \mathbf{X}, \mathbf{y}) = -n\log(\sqrt{2\pi}\sigma) - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_{i1} - \cdots - w_p x_{ip})^2$
- The same minimizer as LS : $\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

Projection by Orthogonalization

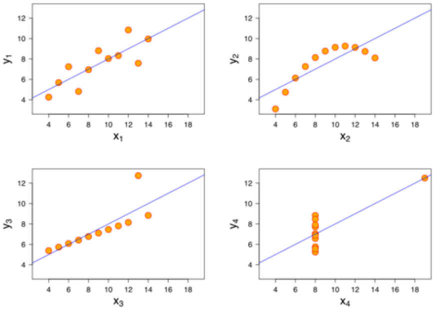
- Another useful formulation : let $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$, $\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i$, then OLS can be formulated by using the centralized data $\{\tilde{\mathbf{x}}_i, \tilde{y}_i\}_{i=1}^{n} = \{\mathbf{x}_i - \bar{\mathbf{x}}, y_i - \bar{y}\}_{i=1}^{n}$, $RSS(\tilde{\mathbf{w}}) = \sum_{i=1}^{n}(\tilde{y}_i - w_1\tilde{x}_{i1} - \cdots - w_p\tilde{x}_{ip})^2 = \|\tilde{\mathbf{y}} - \tilde{\mathbf{X}}\tilde{\mathbf{w}}\|_2^2$, with $\hat{w}_0 = \bar{y} - \hat{\tilde{\mathbf{w}}}^T\bar{\mathbf{x}}$
- Ordinary least square (OLS) prediction $\hat{\mathbf{y}} = \mathbf{P}\mathbf{y}$ is the projection of $\mathbf{y}$ on the linear space spanned by the columns of $\mathbf{X}$, i.e., $\mathcal{X} = \mathrm{Span}\{\mathbf{x}_{\cdot,0}, \mathbf{x}_{\cdot,1}, \ldots, \mathbf{x}_{\cdot,p}\}$, recall that $\mathbf{x}_{\cdot,0} = \mathbf{1}_n$
- If $\{\mathbf{x}_{\cdot,0}, \mathbf{x}_{\cdot,1}, \ldots, \mathbf{x}_{\cdot,p}\}$ forms a set of orthonormal basis, then $\hat{\mathbf{y}} = \sum_{i=0}^{p} < \mathbf{y}, \mathbf{x}_{\cdot,i} > \mathbf{x}_{\cdot,i}$
- If not, we can first do orthogonalization by Gram-Schmidt procedure for the set $\{\mathbf{x}_{\cdot,0}, \mathbf{x}_{\cdot,1}, \ldots, \mathbf{x}_{\cdot,p}\}$
- Similar orthogonalization procedures can be done by QR decomposition or SVD of the matrix $\mathbf{X}^T\mathbf{X}$ (classic topics in numerical linear algebra)

Regression by Successive Orthogonalization

- The expansion of $\mathbf{y}$ on the standard orthonormal basis after Gram-Schmidt procedure can be summarised in the following algorithm :
  1. Initialize $\mathbf{z}_0 = \mathbf{x}_0 = \mathbf{1}_n$
  2. For $j = 1, \ldots, p$:
     Regress $\mathbf{x}_j$ on $\{\mathbf{z}_0, \ldots, \mathbf{z}_{j-1}\}$ to produce coefficients $\hat{\gamma}_{lj} = < \mathbf{z}_l, \mathbf{x}_j > / < \mathbf{z}_l, \mathbf{z}_l >$ with $l = 0, \ldots, j-1$ and residual vectors $\mathbf{z}_j = \mathbf{x}_j - \sum_{k=0}^{j-1} \hat{\gamma}_{kj} \mathbf{z}_k$
  3. Regress $\mathbf{y}$ on the residual $\mathbf{z}_p$ to give the estimate $\hat{w}_p$
- If $\mathbf{x}_p$ is highly correlated with some of the other $\mathbf{x}_k$'s, the residual vector $\mathbf{z}_p$ will be close to zero ; in such situation, the coefficient $\hat{w}_p$ with small Z-score $\frac{\hat{w}_p}{\hat{\sigma}_p}$ could be thrown out, where $\hat{\sigma}_p^2 = \frac{\hat{\sigma}^2}{\|\mathbf{z}_p\|_2^2}$ is an estimate of $\mathrm{Var}(\hat{w}_p) = \frac{\sigma^2}{\|\mathbf{z}_p\|_2^2}$

Shortcomings of Fitting Nonlinear Data

- Evaluating the model by Coefficient of Determination R^2 :
  $R^2 := 1 - \frac{SS_{res}}{SS_{tot}} (= \frac{SS_{reg}}{SS_{tot}}$ for linear regression), where
  $SS_{tot} = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the total sum of squares,
  $SS_{reg} = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$ is the regression sum of squares, and
  $SS_{res} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ is the residual sum of squares.
- The larger the R^2, the better the model



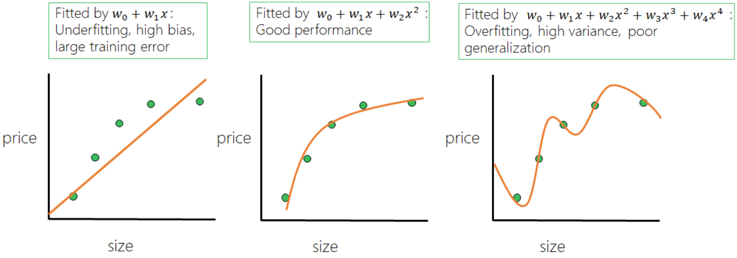
Multicolinearity

- If the columns of $\mathbf{X}$ are almost linearly dependent, i.e., multicolinearity, then $\det(\mathbf{X}^T\mathbf{X}) \approx 0$, the diagonal entries in $(\mathbf{X}^T\mathbf{X})^{-1}$ is quite large. This implies the variances of $\hat{\mathbf{w}}$ get large, and the estimate is not accurate
- Eg : 10 samples are drawn from the true model $y = 10 + 2x_1 + 3x_2 + \epsilon$; the LS estimator is $\hat{w}_0 = 11.292$, $\hat{w}_1 = 11.307$, $\hat{w}_2 = -6.591$, far from the true coefficients ; correlation coefficient is $r_{12} = 0.986$
- Remedies : ridge regression, principal component regression, partial least squares regression, etc.

No.	1	2	3	4	5	6	7	8	9	10
x_1	1.1	1.4	1.7	1.7	1.8	1.8	1.9	2.0	2.3	2.4
x_2	1.1	1.5	1.8	1.7	1.9	1.8	1.8	2.1	2.4	2.5
ε_i	0.8	-0.5	0.4	-0.5	0.2	1.9	1.9	0.6	-1.5	-1.5
y_i	16.3	16.8	19.2	18.0	19.5	20.9	21.1	20.9	20.3	22.0

Overfitting

- Easily to be overfitted when introducing more variables, e.g., regress housing price with housing size
- The high degree model also fits the noises in the training data, so generalizes poorly to new data
- Remedy : regularization

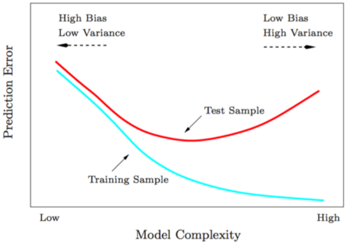


Bias-Variance Decomposition

- Bias-variance decomposition of generalization error in L^2 loss :

$$\mathrm{E}_{train} R_{exp}(\hat{f}(\mathbf{x})) = \mathrm{E}_{train}\mathrm{E}_P[(y-\hat{f}(\mathbf{x}))^2|\mathbf{x}] = \underbrace{\mathrm{Var}(\hat{f}(\mathbf{x}))}_{\text{variance}} + \underbrace{\mathrm{Bias}^2(\hat{f}(\mathbf{x}))}_{\text{bias}} + \underbrace{\sigma^2}_{\text{noise}}$$

  where $P = P(y|\mathbf{x})$ is the conditional probability of y given $\mathbf{x}$
- Bias : $\mathrm{Bias}(\hat{f}(\mathbf{x})) = \mathrm{E}_{train}\hat{f}(\mathbf{x}) - f(\mathbf{x})$ is the average accuracy of prediction for the model (deviation from the truth)
- Variance : $\mathrm{Var}(\hat{f}(\mathbf{x})) = \mathrm{E}_{train}(\hat{f}(\mathbf{x}) - \mathrm{E}_{train}\hat{f}(\mathbf{x}))^2$ is the variability of the model prediction due to different data set (stability)



Bias-Variance Decomposition (Derivation)

Model $y = f(\mathbf{x}) + \epsilon$, with $\mathrm{E}(\epsilon) = 0$ and $\mathrm{Var}(\epsilon) = \sigma^2$ (system error)

$$
\begin{aligned}
\mathrm{E}_{train} R_{exp}(\hat{f}(\mathbf{x})) =& \mathrm{E}_P[(y - f(\mathbf{x}))^2 | \mathbf{x}] + \mathrm{E}_{train}[(f(\mathbf{x}) - \hat{f}(\mathbf{x}))^2] \\
& + 2 \underbrace{\mathrm{E}_{train}\mathrm{E}_P[(y - f(\mathbf{x}))(f(\mathbf{x}) - \hat{f}(\mathbf{x}))|\mathbf{x}]}_{\text{vanishes since } \mathrm{E}_P(y - f(\mathbf{x})|\mathbf{x}) = 0} \\
=& \sigma^2 + \mathrm{E}_{train}[(f(\mathbf{x}) - \mathrm{E}_{train}\hat{f}(\mathbf{x}))^2] + \mathrm{E}_{train}[(\mathrm{E}_{train}\hat{f}(\mathbf{x}) - \hat{f}(\mathbf{x}))^2] \\
& + 2 \underbrace{\mathrm{E}_{train}[(f(\mathbf{x}) - \mathrm{E}_{train}\hat{f}(\mathbf{x}))(\mathrm{E}_{train}\hat{f}(\mathbf{x}) - \hat{f}(\mathbf{x}))]}_{\text{vanishes since } \mathrm{E}_{train}[\mathrm{E}_{train}\hat{f}(\mathbf{x}) - \hat{f}(\mathbf{x})] = 0} \\
=& \sigma^2 + \mathrm{Bias}^2(\hat{f}(\mathbf{x})) + \mathrm{Var}(\hat{f}(\mathbf{x}))
\end{aligned}
$$

The more complicated the model, the lower the bias, but the higher the variance.

Outlines

Regularization by Subset Selection

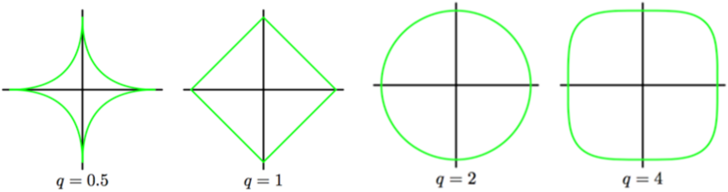
- In high dimensions, the more the input attributes, the larger the variance
- Shrinking some coefficients or setting them to zero can reduce the overfitting
- Using less input variables also help interpretation with the most important variables
- Subset selection： retaining only a subset of the variables, while eliminating the rest variables from the model
- Best-subset selection : find for each $k \in \{0, 1, \ldots, p\}$ the subset $S_k \subset \{1, \ldots, p\}$ of size k that gives the smallest $RSS(\mathbf{w}) = \sum_{i=1}^{n}(y_i - w_0 - \sum_{j \in S_k} w_j x_{ij})^2$

Regularization by Penalties

- Add a penalty term, in general l_q-norm

$$\sum_{i=1}^{n}(y_i - w_0 - w_1x_1 - \cdots - w_px_p)^2 + \lambda\|\mathbf{w}\|_q^q$$
$$= \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_q^q$$

- $q = 2$: ridge regression
- $q = 1$: LASSO regression



Ridge Regression

- The optimization problem turns to be

$$\begin{aligned}\hat{\mathbf{w}} &= \arg\min_{\mathbf{w}} \sum_{i=1}^{n} (y_i - w_0 - w_1 x_1 - \cdots - w_p x_p)^2 + \lambda \|\mathbf{w}\|_2^2 \\ &= \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda \|\mathbf{w}\|_2^2\end{aligned}$$

- $\lambda \geqslant 0$ is a fixed parameter which has to be tuned by cross-validation
- Equivalent to the constraint minimization problem :

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2, \qquad \text{subject to} \qquad \|\mathbf{w}\|_2 \leqslant \mu,$$

  where $\mu \geqslant 0$ is a prescribed threshold (tuning parameter)
- The large λ corresponds to the small μ.

Solving Ridge Regression

- Easy to show that $\hat{\mathbf{w}}^{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I}_{p+1})^{-1}\mathbf{X}^T\mathbf{y}$
- The estimator is also a projection of $\mathbf{y}$: $\hat{\mathbf{y}}^{ridge} = \mathbf{X}(\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I}_{p+1})^{-1}\mathbf{X}^T\mathbf{y}$
- $\mathbf{X}$ can be diagonalized by SVD : $\mathbf{X} = \mathbf{PDQ}$ with $\mathbf{D} = \mathrm{diag}(\nu_1, \ldots, \nu_{p+1})$, and $\mathbf{P} \in \mathbb{R}^{n\times(p+1)}$, $\mathbf{Q} \in \mathbb{R}^{(p+1)\times(p+1)}$ being orthogonal matrices ($\mathbf{P}^T\mathbf{P} = \mathbf{I}_{p+1}$)
- $\hat{\mathbf{y}}^{ridge} = \mathbf{P}\mathrm{diag}(\frac{\nu_1^2}{\nu_1^2+\lambda}, \ldots, \frac{\nu_{p+1}^2}{\nu_{p+1}^2+\lambda})\mathbf{P}^T\mathbf{y}$, while $\hat{\mathbf{y}}^{OLS} = \mathbf{PP}^T\mathbf{y}$
- In the spectral space, the ridge regression estimator is a shrinkage of the OLS estimator ($\lambda = 0$)

Bayesian Viewpoint of Ridge Regression

- Given $\mathbf{X}$ and $\mathbf{w}$, the conditional distribution of $\mathbf{y}$ is $\mathrm{P}(\mathbf{y}|\mathbf{X},\mathbf{w}) = \mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2\mathbf{I}) \propto \exp\big(-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\mathbf{w})^T(\mathbf{y}-\mathbf{X}\mathbf{w})\big)$
- In addition, assume $\mathbf{w}$ has a prior distribution $\mathrm{P}(\mathbf{w}) = \mathcal{N}(\mu_0, \mathbf{\Lambda}_0) \propto \exp\big(-\frac{1}{2}(\mathbf{w}-\mu_0)^T\Lambda_0^{-1}(\mathbf{w}-\mu_0)\big)$
- By Bayes theorem, the posterior distribution of $\mathbf{w}$ given the data $\mathbf{X}$ and $\mathbf{y}$ is

$$
\begin{aligned}
\mathrm{P}(\mathbf{w}|\mathbf{X},\mathbf{y}) &\propto \mathrm{P}(\mathbf{y}|\mathbf{X},\mathbf{w})\mathrm{P}(\mathbf{w}) \\
&\propto \exp\Big(-\frac{1}{2\sigma^2}(\mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w} - 2\mathbf{y}^T\mathbf{X}\mathbf{w}) \\
&\qquad - \frac{1}{2}(\mathbf{w}^T\mathbf{\Lambda}_0^{-1}\mathbf{w} - 2\mu_0^T\mathbf{\Lambda}_0^{-1}\mathbf{w})\Big) \\
&\propto \exp\Big(-\frac{1}{2}(\mathbf{w}-\mu_m)^T\Lambda_m^{-1}(\mathbf{w}-\mu_m)\Big)
\end{aligned}
$$

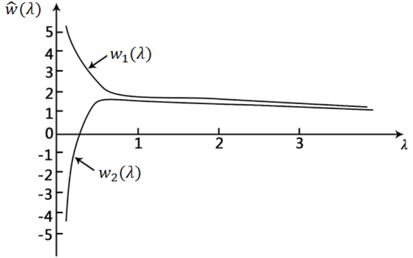
where $\Lambda_m = (\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{X} + \mathbf{\Lambda}_0^{-1})^{-1}$ and $\mu_m = \mathbf{\Lambda}_m(\frac{1}{\sigma^2}\mathbf{X}^T\mathbf{y} + \mathbf{\Lambda}_0^{-1}\mu_0)$

- If $\mu_0 = 0$ and $\mathbf{\Lambda}_0 = \frac{\sigma^2}{\lambda}\mathbf{I}_{p+1}$, then $\hat{\mathbf{w}} = \mu_m = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}_{p+1})^{-1}\mathbf{X}^T\mathbf{y}$ maximizes the posterior probability $\mathrm{P}(\mathbf{w}|\mathbf{X},\mathbf{y})$

Ridge Trace

- The functional plot of $\hat{\mathbf{w}}^{ridge}(\lambda)$ with λ is called ridge trace
- The large variations in ridge trace indicate the multicolinearity in variables
- When $\lambda \in (0, 0.5)$, the ridge traces have large variations, it suggests to choose $\lambda = 1$

λ	0	0.1	0.15	0.2	0.3	0.4	0.5	1.0	1.5	2.0	3.0
$\hat{w}_1^{ridge}(\lambda)$	11.31	3.48	2.99	2.71	2.39	2.20	2.06	1.66	1.43	1.27	1.03
$\hat{w}_2^{ridge}(\lambda)$	-6.59	0.63	1.02	1.21	1.39	1.46	1.49	1.41	1.28	1.17	0.98



LASSO Regression

- Proposed by R. Tibshirani, short for "Least Absolute **Shrinkage and Selection** Operator"
- Can be used to estimate the coefficients and select the important variables simultaneously
- Reduce the model complexity, avoid overfitting, and improve the generalization ability
- Also improve the model interpretability

Regression Shrinkage and Selection via the Lasso - jstor
https://www.jstor.org/stable/2346178 ▾ 翻译此页
作者：R Tibshirani - 1996 - 被引用次数：27385 - 相关文章
Regression Shrinkage and Selection via the Lasso. By ROBERT TIBSHIRANIt. University of Toronto, Canada. [Received January 1994. Revised January 1995].

LASSO Formulation

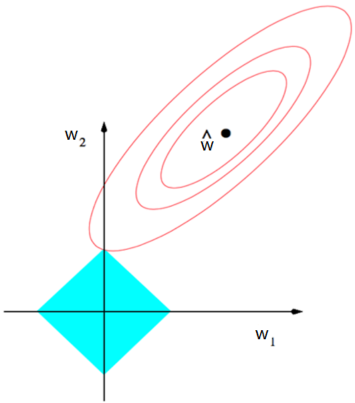
- The optimization problem

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} E(\mathbf{w})$$
$$E(\mathbf{w}) = \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_1$$

- Equivalent to the constraint minimization problem :

$$\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2,$$
$$\text{subject to} \quad \|\mathbf{w}\|_1 \leqslant \mu,$$

- The large λ corresponds to the small μ.
- The optimal solution is sparse with $\hat{w}_2 = 0$

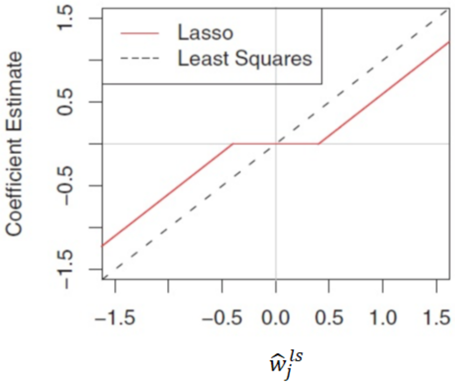


Solving LASSO Regression

- Assume $\mathbf{X}^T\mathbf{X} = \mathbf{I}_{p+1}$, then $\hat{\mathbf{w}}^{OLS} = \mathbf{X}^T\mathbf{y}$
- $\partial_{\mathbf{w}} E(\mathbf{w}) = \mathbf{w} - \mathbf{X}^T\mathbf{y} + \lambda(\partial|w_0| \times \cdots \times \partial|w_p|)$
- $\mathbf{0} \in \partial_{\mathbf{w}} E(\hat{\mathbf{w}}^{lasso})$ implies $0 \in \hat{w}_i^{lasso} - \hat{w}_i^{OLS} + \lambda\partial|\hat{w}_i^{lasso}|$
- If $\hat{w}_i^{lasso} > 0$, $\partial|\hat{w}_i^{lasso}| = \{1\}$, and $\hat{w}_i^{lasso} = \hat{w}_i^{OLS} - \lambda$ with $\hat{w}_i^{OLS} > \lambda$
- If $\hat{w}_i^{lasso} < 0$, $\partial|\hat{w}_i^{lasso}| = \{-1\}$, and $\hat{w}_i^{lasso} = \hat{w}_i^{OLS} + \lambda$ with $\hat{w}_i^{OLS} < -\lambda$
- If $\hat{w}_i^{lasso} = 0$, $\partial|\hat{w}_i^{lasso}| = [-1, 1]$, and $\hat{w}_i^{OLS} \in [-\lambda, \lambda]$
- In summary, $\hat{w}_i^{lasso} = (|\hat{w}_i^{OLS}| - \lambda)_+ \mathrm{sign}(\hat{w}_i^{OLS})$

Shrinkage and Selection Property of LASSO

$\hat{w}_i^{lasso} = (|\hat{w}_i^{OLS}| - \lambda)_+ \mathrm{sign}(\hat{w}_i^{OLS})$ is called soft thresholding of $\hat{w}_i^{OLS}$, where $(a)_+ = \max(a, 0)$ is the positive part of a



Maximum A Posteriori (MAP) Estimation

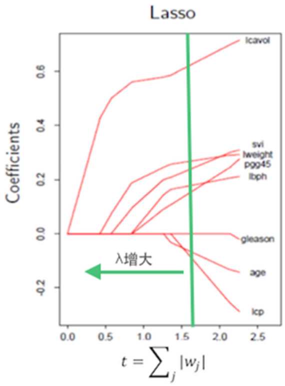
- Given θ, the conditional distribution of $\mathbf{y}$ is $\mathrm{P}(\mathbf{y}|\theta)$
- In addition, assume the parameter θ has a prior distribution $\mathrm{P}(\theta)$
- The posterior distribution of θ given the data $\mathbf{y}$ is $\mathrm{P}(\theta|\mathbf{y}) \propto \mathrm{P}(\mathbf{y}|\theta)\mathrm{P}(\theta)$
- MAP choose the point of maximal posterior probability :

$$\hat{\theta}^{MAP} = \arg\max_{\theta} \mathrm{P}(\theta|\mathbf{y}) = \arg\max_{\theta} \big(\log \mathrm{P}(\mathbf{y}|\theta) + \log \mathrm{P}(\theta) \big)$$

- If $\theta = \mathbf{w}$, and we choose the log-prior proportional to $\lambda\|\mathbf{w}\|_2^2$ (i.e., the normal prior $\mathcal{N}(0, \frac{\sigma^2}{\lambda}\mathbf{I})$), we recover the ridge regression
- If the log-prior is proportional to $\lambda\|\mathbf{w}\|_1$, i.e., the prior is the tensor product of Laplace (or double exponential) distribution Laplace$(0, \frac{2\sigma^2}{\lambda})$
- Different log-prior lead to different penalties (regularization), but this is not the case in general : some penalties may not be the logarithms of probability distributions, some other penalties depend on the data (prior is independent of the data)

LASSO Path

- When λ varies, the values of the coefficients form paths (regularization paths)
- The paths are piecewise linear with the same change points, may cross the x-axis many times
- In practice, choose λ by cross-validation



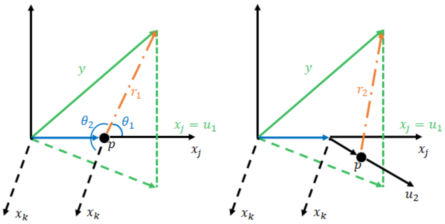
Hyper-parameter Tuning

- Regularization : $\min\limits_{f \in F} \frac{1}{n} \sum\limits_{i=1}^{n} L(y_i, f(\mathbf{x}_i)) + \lambda J(f)$
- In linear regression, $L(y, f) = (y - f)^2$, $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$, $f \in F \Leftrightarrow \mathbf{w} \in \mathbf{R}^{p+1}$
- Model complexity : $J(f) = \begin{cases} \|\mathbf{w}\|_2^2, & \text{Ridge regression} \\ \|\mathbf{w}\|_1, & \text{Lasso regression} \end{cases}$
- Cross-validation (CV) : training set = training subset + validation subset
  - Simple CV : randomly split once into two subsets
  - K-fold CV : randomly split the data into K disjoint subsets **with the same size**, treat the union of $K - 1$ subsets as training set, the other one as validation set, do this repeatedly and select the best λ with smallest validation error : $CV(\hat{f}, \lambda) = \frac{1}{N} \sum\limits_{i=1}^{N} L(y_i, \hat{f}^{-\kappa(i)}(x_i, \lambda))$, where $\kappa : \{1, \ldots, N\} \to \{1, \ldots, K\}$ is a partition index map
  - Leave-one-out CV : $K = n$ in the previous case

1	2	3	4	5
Train	Train	Validation	Train	Train

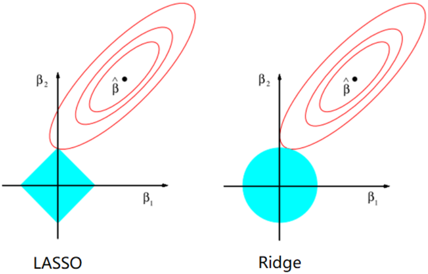
LARS (Optional) : (by Hastie and Efron) a Package for Solving LASSO

1. Start with all coefficients w_i equal to zero
2. Find the predictor x_i most correlated with y
3. Increase the coefficient w_i in the direction of the sign of its correlation with y. Take residuals $r = y - \hat{y}$ along the way. Stop when some other predictor x_k has as much correlation with r as x_i has
4. Increase (w_i, w_k) in their joint least squares direction, until some other predictor x_m has as much correlation with the residual r
5. Continue until all predictors are in the model



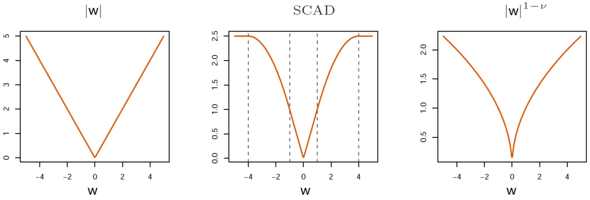
Other Solvers

- "glmnet" by Friedman, Hastie and Tibshirani, implemented by coordinate descent, can be used in linear regression, logistic regression, etc., with LASSO (l_1), ridge (l_2) and elastic net ($l_1 + l_2$) regularization terms
- Why LASSO seeks the sparse solution in comparison with ridge ?



Related Regularization Models

- Elastic net : $\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda_1 \|\mathbf{w}\|_2^2 + \lambda_2 \|\mathbf{w}\|_1$
- Group LASSO : $\hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \sum_{g=1}^{G} \lambda_g \|\mathbf{w}_g\|_2$, where $\mathbf{w} = (\mathbf{w}_1, \ldots, \mathbf{w}_G)$ is the group partition of $\mathbf{w}$
- Dantzig Selector : $\min_{\mathbf{w}} \|\mathbf{w}\|_1$, subject to $\|\mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{w})\|_\infty \leqslant \mu$
- Smoothly clipped absolute deviation (SCAD) penalty by Fan and Li (2005) : replace the penalty $\lambda \sum_{i=0}^{p} |w_i|$ by $\sum_{i=0}^{p} J_a(w_i, \lambda)$, where $J_a(x, \lambda)$ satisfies (for $a \geqslant 2$) : $\frac{\mathrm{d}J_a}{\mathrm{d}x} = \lambda \mathrm{sign}(x) \Big(I(|x| \leqslant \lambda) + \frac{(a\lambda - |x|)_+}{(a-1)\lambda} I(|x| > \lambda) \Big)$
- Adaptive LASSO : weighted penalty $\sum_{i=0}^{p} \mu_i |w_i|$ where $\mu_i = \frac{1}{|\hat{w}_i^{OLS}|^\nu}$ with $\nu > 0$, as an approximation to $|w_i|^{1-\nu}$, non-convex penalty



Outlines

Errors and R^2

- Mean absolute error (MAE) : $MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$
- Mean square error (MSE) : $MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$
- Root mean square error (RMSE) :
  $RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$
- Coefficient of Determination R^2 : $R^2 := 1 - \frac{SS_{res}}{SS_{tot}}$, where
  $SS_{tot} = \sum_{i=1}^{n}(y_i - \bar{y})^2$ is the total sum of squares, and
  $SS_{res} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ is the residual sum of squares ;
  $R^2 \in [0,1]$ (might be negative) ; the larger the R^2, the smaller the ratio of SS_{res} to SS_{tot}, thus the better the model

Adjusted Coefficient of Determination

- Adjusted coefficient of determination : $R^2_{adj} = 1 - \frac{(1-R^2)(n-1)}{n-p-1}$
- n is the number of samples, p is the dimensionality (or the number of attributes)
- The larger the R^2_{adj} value, the better performance the model
- When adding important variables into the model, R^2_{adj} gets larger and SS_{res} is reduced
- When adding unimportant variables into the model, R^2_{adj} may gets smaller and SS_{res} may increase
- In fact, one can show that $1 - R^2_{adj} = \frac{\hat{\sigma}^2}{S^2}$, where $\hat{\sigma}^2 = \frac{1}{n-p-1}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ and $S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2$ with $(n-p-1)\frac{\hat{\sigma}^2}{\sigma^2} \sim \chi^2_{n-p-1}$ and $(n-1)\frac{S^2}{\sigma^2} \sim \chi^2_{n-1}$ if $\mathbf{w} = \mathbf{0}$.

Outlines

References

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- T. Hastie, R. Tibshirani, and J. Friedman, The Elements of Statistical Learning : Data mining, Inference, and Prediction, 2nd Edition, 2009