Statistical Learning with Sparsity

Generalizations of loss functions and lasso panelties

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Lasso: recap

Least Absolute Shrinkage and Selection Operator (lasso)

Recall that the lasso estimate is defined by

$$\hat{\beta}^{\text{lasso}}(\lambda) = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \left\{ \frac{1}{2N} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_1 \right\},$$

where $\lambda \geq 0$ is a tuning parameter that controls the amount of shrinkage.

For the red part of the objective function, we can generalize the square loss to other loss functions:

- Negative log-likelihood for GLMs
- Negative log-partial-likelihood for Cox models
- Hinge loss for SVM

For the blue part of the objective function, we can generalize the lasso penalty to other penalties:

- Elastic net
- Group lasso
- Fused lasso

Part I

- Negative log-likelihood for GLMs
- Negative log-partial-likelihood for Cox models
- Hinge loss for SVM

Binary response variable

- For simplicity, we can still use the linear model for a binary outcome
- Linear probability model $y_i = x_i^{\mathrm{T}} \beta + \varepsilon_i, \quad E(\varepsilon_i \mid x_i) = 0$

$$P(y_i = 1 \mid x_i) = E(y_i \mid x_i) = x_i^{\mathrm{T}} \beta.$$

- Easy interpretation

$$\frac{\partial P(y_i = 1 \mid x_i)}{\partial x_{ij}} = \beta_j$$

However, there are two defects:

- Heteroskedasticity $\quad \mathrm{Var}(y_i \mid x_i) = x_i^{\mathrm{T}} \beta \left(1 - x_i^{\mathrm{T}} \beta\right).$
- Not natural for binary outcome because probability is bounded between zero and one.

Link functions

We can use a monotone transformation to force the linear predictor to lie within the interval $[0, 1]$:

$$P(y_i = 1 | x_i) = g(x_i^{\mathrm{T}} \beta).$$

Here, the inverse of g is called the **link function**.
There are some canonical choices of g:

- Logit link: $g(t) = \frac{e^t}{1+e^t} = \frac{1}{1+e^{-t}}$, c.f. standard logistic distribution
- Probit link: $g(t) = \Phi(t)$, c.f. standard normal distribution
- Complementary log-log link: $g(t) = 1 - e^{-e^t}$, c.f. standard log-Weibull distribution
- Cauchit link: $g(t) = \frac{1}{\pi} \arctan(t) + \frac{1}{2}$, c.f. standard Cauchy distribution

Negative log-likelihood

Now we consider minimize negative log-likelihood with a penalty:

$$\underset{\beta_0,\beta}{\text{minimize}}\left\{-\frac{1}{N}\mathcal{L}\left(\beta_0,\beta;\boldsymbol{y},\boldsymbol{X}\right)+\lambda\|\beta\|\right\}$$

where the type of norm is specified in the problem. We consider the linear model as an example of GLM. Assuming $Y|X=x\sim\mathcal{N}(\mu(x),\sigma^2)$. Then:

$$\mathcal{L}\left(\beta_0,\beta;\boldsymbol{y},\boldsymbol{X}\right)=-\sum_{i=1}^{N}\frac{(y_i-\beta_0-\beta x_i)^2}{2\sigma^2}+c=-\frac{\|\boldsymbol{y}-\beta_0-\beta\boldsymbol{X}\|_2^2}{2\sigma^2 N}+c$$

where c is a constant that does not depend on β_0 and β.
Hence, negative log-likelihood is equivalent to the square error loss in this case.

Remarks on negative log-likelihood

Why? Under regular conditions, the Fisher information matrix is positive definite, so the negative log-likelihood is a convex function of the parameter.

An example for classification

Suppose we take $Y_i \in \{+1, -1\}$, namely, $P(Y_i = 1) = \pi_i, P(Y_i = -1) = 1 - \pi_i$, and

$$\mathrm{logit}(\pi_i) = \beta_0 + \beta_1^T x_i, i = 1, ..., n.$$

Then the likelihood function is

$$\mathcal{L}(\pi | y_1, ..., y_n) = \prod_{i=1}^{n} \frac{1}{1 + \left(\frac{1-\pi_i}{\pi_i}\right)^{y_i}}.$$

After some trivial algebras, we can get the following negative log-likelihood function with a penalty:

$$\frac{1}{N} \sum_{i=1}^{N} \log\left(1 + e^{-y_i\left(\beta_0 + \beta^\top x_i\right)}\right) + \lambda \|\beta\|_1.$$

Here, $y_i\left(\beta_0 + \beta^\top x_i\right)$ can be interpreted as the **margin** of the i-th observation, for which positive values indicate correct classification and negative values indicate incorrect classification.

Case study: document classification

- The 20 Newsgroups data set is a collection of approximately 20,000 newsgroup documents, partitioned (nearly) evenly across 20 different newsgroups. It was originally collected by Ken Lang, for his **Newsweeder: Learning to filter netnews** paper, though he does not explicitly mention this collection. The 20 newsgroups collection has become a popular data set for experiments in text applications of machine learning techniques, such as **text classification** and **text clustering**.
- Koh, Kim, Boyd (2007) analysis the data set by logistic regression interior point method.
- Freidman, Hastie, Tibshirani (2010) use this data to illustrate their `glmnet` via coordinate descent.
- A team at Renmin U and Tsinghua U (2022) developed a Bayesian method for classification and summerization, their work published on Journal of Machine Learning Research.

Case study: document classification

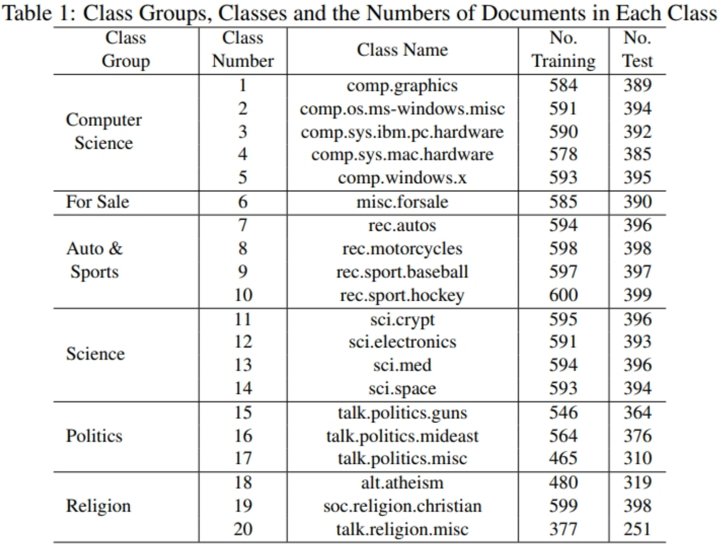


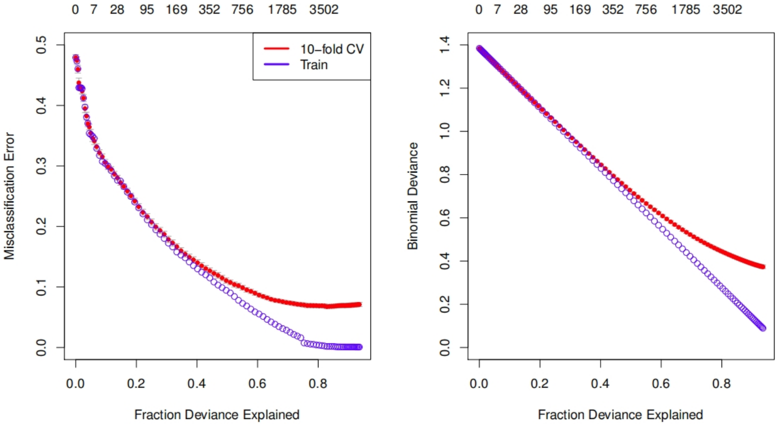
Table 1: Class Groups, Classes and the Numbers of Documents in Each Class

Class Group	Class Number	Class Name	No. Training	No. Test
Computer Science	1	comp.graphics	584	389
	2	comp.os.ms-windows.misc	591	394
	3	comp.sys.ibm.pc.hardware	590	392
	4	comp.sys.mac.hardware	578	385
	5	comp.windows.x	593	395
For Sale	6	misc.forsale	585	390
Auto & Sports	7	rec.autos	594	396
	8	rec.motorcycles	598	398
	9	rec.sport.baseball	597	397
	10	rec.sport.hockey	600	399
Science	11	sci.crypt	595	396
	12	sci.electronics	591	393
	13	sci.med	594	396
	14	sci.space	593	394
Politics	15	talk.politics.guns	546	364
	16	talk.politics.mideast	564	376
	17	talk.politics.misc	465	310
Religion	18	alt.atheism	480	319
	19	soc.religion.christian	599	398
	20	talk.religion.misc	377	251

Case study: document classification

- We have $N = 11314$ documents that we want to classify into two different groups ($Y \in \{-1, +1\}$).
- The features are defined as the set of **trigrams** (with some restrictions). In NLP, trigrams mean a sequence of three adjacent elements from a string of tokens. We have $p = 777811$ features in total.
- Each document contains an average of 425 nonzero features. So this is a sparse problem.
- We want to perform ℓ_1 regularized logistic regression.

Case study: document classification



You can see that overfitting occurs when λ is too small, or equivalently, fraction deviance explained is too large, namely, the model is too "saturated".

Case study: document classification

The **fraction deviance explained** $\left(D^2_\lambda\right)$ is then defined by:

$$D^2_\lambda = \frac{\mathrm{Dev}_{\mathrm{null}} - \mathrm{Dev}_\lambda}{\mathrm{Dev}_{\mathrm{null}}}$$

$$R^2 = \frac{\mathrm{SS}_{\mathrm{tot}} - \mathrm{SS}_{\mathrm{res}}}{SS_{\mathrm{tot}}}$$

Deviance: (Dev_λ) is defined as minus twice the difference in the log-likelihood for a model fit with parameter λ and the "saturated model"(having $\hat{y} = y_i$).

Remarks on GOF statistics

It also reminds me conditional MSE in Guorong Dai's setup:

$$\frac{\mathbb{E}\{(Y - g(U))^2 | S = s\}}{\mathbb{E}\{(Y - d(X))^2 | S = s\}}.$$

So when we comparing two models, a natural choice is to find a proper ratio of the "errors" of two models.

Multiple outcomes

Setting

$Y \in \{1, ..., K\}$ for $K > 2$ classes. There are two natural ways for reduction to binary classification in general:

- OvO (One versus One): all $\binom{K}{2}$ pairs of classes samples are used to fit $\binom{K}{2}$ binary classifiers, then the predicted class is the one which is predicted the most.
- OvA (One versus All): treat all other classes as a single negative class.

Drawbacks

- OvO: **computationally exhaustive** and cases where same amount of votes for more classes.
- OvA: **imbalance** amounts positive and negative observations.

Multinomial distribution

- Suppose we have nomial variable: a categorical variable that does not have intrinsic ordering or ranking, e.g., gender, colors, marital status, race, blood types
- Multinomial distribution

$$y \sim \text{ Multinomial } \{1; (\pi_1, \ldots, \pi_K)\}, \quad \sum_{k=1}^{K} \pi_k = 1$$

  y takes values in $\{1, ..., K\}$ with probability $P(y = k) = \pi_k$.
- We want to model y_i based on covariates x_i.

$$y_i \mid x_i \sim \text{ Multinomial } [1; \{\pi_1(x_i), \ldots, \pi_K(x_i)\}],$$

$$\sum_{k=1}^{K} \pi_k(x_i) = 1 \text{ for all } x_i.$$

$$\pi_{y_i}(x_i) = \prod_{k=1}^{K} \{\pi_k(x_i) \text{ if } y_i = k\} = \prod_{k=1}^{K} \{\pi_k(x_i)\}^{1(y_i=k)}.$$

Multinomial logistic / Softmax regression

- View category K as the reference level, we model the ratios of the probabilities of category k and K

$$\log \frac{\pi_k(x_i)}{\pi_K(x_i)} = x_i^{\mathrm{T}} \beta_k \quad (k = 1, \ldots, K - 1)$$

$$\pi_k(x_i) = \pi_K(x_i)\, e^{x_i^{\mathrm{T}} \beta_k}$$

- Denote $\beta_K = 0$,

$$\begin{aligned} \sum_{k=1}^{K} \pi_k(x_i) = 1 &\Longrightarrow \pi_K(x_i) \sum_{k=1}^{K} e^{x_i^{\mathrm{T}} \beta_k} = 1 \\ &\Longrightarrow \pi_K(x_i) = 1 / \sum_{k=1}^{K} e^{x_i^{\mathrm{T}} \beta_k} \\ &\Longrightarrow \pi_k(x_i) = \frac{e^{x_i^{\mathrm{T}} \beta_k}}{\sum_{l=1}^{K} e^{x_i^{\mathrm{T}} \beta_l}} \end{aligned}$$

Multinomial logistic with penalty

Instead of traditional multinomial logistic regression, we can consider the following over specified version:

$$\Pr(Y = k \mid X = x) = \frac{e^{\beta_{0k} + \beta_k^T x}}{\sum_{\ell=1}^{K} e^{\beta_{0\ell} + \beta_\ell^T x}}.$$

- we regularize the coefficients, and the regularized solutions are not equivariant under base changes,
- the regularization automatically eliminates the redundancy.
- The penalty term is $\lambda \sum_{k=1}^{K} \|\beta_k\|_1$.

Multinomial logistic with penalty

The negative log-likelihood function is

$$-\frac{1}{N}\sum_{i=1}^{N}\log\Pr\left(Y=y_i\mid x_i;\{\beta_{0k},\beta_k\}_{k=1}^{K}\right)$$

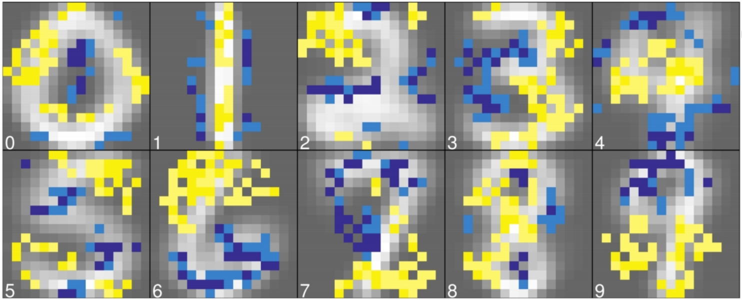
Denote by $\mathbf{R}$ the $N\times K$ indicator response matrix with elements $r_{ik}=\mathbb{I}\left(y_i=k\right)$. Then we can write the log-likelihood in the more explicit form

$$\frac{1}{N}\sum_{i=1}^{N}w_i\left[\sum_{k=1}^{K}r_{ik}\left(\beta_{0k}+\beta_k^T x_i\right)-\log\left\{\sum_{k=1}^{K}e^{\beta_{0k}+\beta_k^T x_i}\right\}\right]$$

- The weights w_i are used to adjust the contribution of each observation to the likelihood, $w_i=1/N$ by default.
- $\{\beta_{kj}+c_j\}_{k=1}^{K}$ and $\{\beta_{kj}\}_{k=1}^{K}$ produce the same likelihood, then the criterion to resolve the choice of c_j is the penalty term.

$$c_j=\arg\min_{c\in\mathbb{R}}\left\{\sum_{k=1}^{K}\left|\tilde{\beta}_{kj}-c\right|\right\}$$

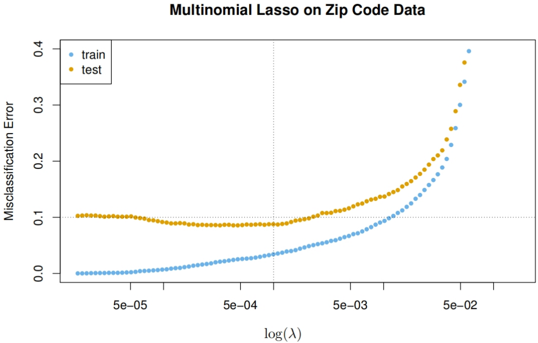
Case study: Handwritten digits



- Handwritten Digit Recognition with a Back-Propagation Network is published in 1989.
- LeNet-5: The first part includes two convolutional layers and two pooling layers which are placed alternatively. The second part consists of three fully connected layers.

Case study: Handwritten digits

- We have $N = 7921$ gray-scale images of $p = 256$ pixels representing handwritten digits from 0 yo 9, namely, $Y \in \{0, ..., 9\}$.
- Each one of the p features represents the intensity in a $[0, 1]$-scale of the corresponding pixel (0 black, 1 white).
- We can fit a 10-classes lasso multinomial model.
- Deep networks indeed have better performance.



Count outcomes

- A random variable y is Poisson (λ) if its probability mass function is

$$P(y=k)=e^{-\lambda}\frac{\lambda^k}{k!}, \quad (k=0,1,2,\ldots)$$

- If $y \sim \text{Poisson}(\lambda)$, then $\mathbb{E}(y)=\text{Var}(y)=\lambda$.
- If $y_1,\ldots,y_K$ are mutually independent with $y_k \sim \text{Poisson}\left(\lambda_k\right)$

$$y_1+\cdots+y_K \sim \text{Poisson}(\lambda),$$

$$(y_1,\ldots,y_K) \mid y_1+\cdots+y_K=n \sim \text{Multinomial}\left(n,(\lambda_1/\lambda,\ldots,\lambda_K/\lambda)\right),$$

where $\lambda=\lambda_1+\cdots+\lambda_K$.

Some extensions of Poisson distribution

- The Poisson distribution restricts that the mean must be the same as the variance. It cannot capture the feature of **over-dispersed data** with variance larger than the mean.
- Negative binomial distribution: a scale-mixture of Poisson.

$$P(y = k) = \frac{\Gamma(k+\theta)}{\Gamma(k+1)\Gamma(\theta)} \left(\frac{\theta}{\mu+\theta}\right)^{\theta} \left(\frac{\mu}{\mu+\theta}\right)^{k}, \quad (k = 0, 1, 2, \ldots)$$

  with $\mathbb{E}(y) = \mu$ and $\mathrm{Var}(y) = \mu + \mu^2/\theta$.

- Zero-inflated Poisson: a mixture of Poisson and point mass at zero.

$$P(y = k) = \begin{cases} p + (1-p)e^{-\lambda}, & \text{if } k = 0 \\ (1-p)e^{-\lambda}\frac{\lambda^k}{k!}, & \text{if } k = 1, 2, \ldots \end{cases}$$

$$\mathbb{E}(y) = (1-p)\lambda \text{ and } \mathrm{Var}(y) = (1-p)\lambda(1+p\lambda)$$

Poisson regression model / log-linear model

- $$\begin{cases} y_i \mid x_i & \sim \mathrm{Poisson}\left(\lambda_i\right), \\ \lambda_i & = \lambda\left(x_i, \beta\right) = e^{\beta_0 + x_i^{\mathrm{T}} \beta}. \end{cases}$$
  $$E\left(y_i \mid x_i\right) = \mathrm{var}\left(y_i \mid x_i\right) = e^{\beta_0 + x_i^{\mathrm{T}} \beta}.$$
- This model is also called log-linear model
  $$\log \mathbb{E}\left(y_i \mid x_i\right) = \beta_0 + x_i^{\mathrm{T}} \beta$$
- Interpretation: conditional log mean ratio
  $$\log \frac{\mathbb{E}\left(y_i \mid \ldots, x_{ij} + 1, \ldots\right)}{\mathbb{E}\left(y_i \mid \ldots, x_{ij}, \ldots\right)} = \beta_j$$

Poisson regression with penalty

- Likelihood:

$$L(\beta) = \prod_{i=1}^{n} e^{-\lambda_i} \frac{\lambda_i^{y_i}}{y_i!} \propto \prod_{i=1}^{n} e^{-\lambda_i} \lambda_i^{y_i}$$

$$\log L(\beta) = \sum_{i=1}^{n} (-\lambda_i + y_i \log \lambda_i) = \sum_{i=1}^{n} \left(-e^{\beta_0 + x_i^{\mathrm{T}} \beta} + y_i(\beta_0 + x_i^{\mathrm{T}} \beta) \right).$$

- The penalty term is $\lambda \|\beta\|_1$.

$$-\frac{1}{N} \sum_{i=1}^{N} \left\{ y_i \left(\beta_0 + \beta^\top x_i \right) - e^{\beta_0 + \beta^\top x_i} \right\} + \lambda \|\beta\|_1$$

Poisson regression for rates modeling

- If observation windows have different lengths T_i, then

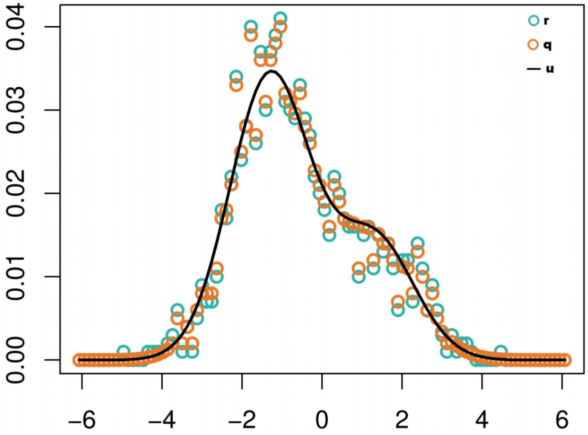
  $$\mathbb{E}\left[y_i \mid X_i = x_i\right] = T_i \mu\left(x_i\right)$$

  where $\mu\left(x_i\right)$ rate per unit time interval.
- 6 months vs yearly visit to doctor has $T = 6$.
- $$\log \mathbb{E}[Y \mid X = x, T] = \underbrace{\log T}_{\text{“offset”}} + \beta_0 + \beta^\top x$$
- The terms $\log T_i$ for each observation require no fitting, and are called an offset (偏移量).

Case study: distribution smoothing

- N count variables $\{y_k\}_{k=1}^N$ coming from a N-cell multinomial distribution.
- $\boldsymbol{r} = \{r_k\}_{k=1}^N = \left\{y_k / \sum_{k=1}^N y_k\right\}_{k=1}^N$ vector of proportions.
- Issue: $\boldsymbol{r}$ could be sparse. Want to regularize it toward a more stable distribution $\boldsymbol{u} = \{u_k\}_{k=1}^N$.
- $$\underset{\boldsymbol{q}\in\mathbb{R}^N, q_k \geq 0}{\text{minimize}} \quad \underbrace{\sum_{k=1}^N q_k \log\left(\frac{q_k}{u_k}\right)}_{\text{Kullback-Leibler divergence}} \quad \text{such that } \|\boldsymbol{q}-\boldsymbol{r}\|_\infty \leq \delta, \sum_{k=1}^N q_k = 1$$
- We want a distribution $\boldsymbol{q}$ which is approximately equal to our observed proportions but at the same time as close as possible to a nominal distribution $\boldsymbol{u}$.

Case study: distribution smoothing



Case study: distribution smoothing

Why this problems falls in Poisson model framework?

- The previous minimization problem $\underset{\boldsymbol{q}\in\mathbb{R}^N, q_k\geq 0}{\text{minimize}} \sum_{k=1}^N q_k \log\left(\frac{q_k}{u_k}\right)$ such that $\|\boldsymbol{q}-\boldsymbol{r}\|_\infty \leq \delta, \sum_{k=1}^N q_k = 1$ has Lagrange dual

$$\underset{\beta_0,\boldsymbol{\alpha}}{\text{maximize}} \left\{ \sum_{k=1}^N r_k \left[\log u_k + \beta_0 + \alpha_k - u_k e^{\beta_0+\alpha_k}\right] - \delta\|\boldsymbol{\alpha}\|_1 \right\}$$

- This is equivalent to fitting a Poisson model with offset $\log u_k$, individual parameter α_k and design matrix $X = \mathbb{I}_{N\times N}$.

Time-to-event data

- Survival analysis in biostatistics
    - Outcome denotes the Survival time or the time to the recurrent of the disease
- Duration analysis in econometrics
    - Outcome denotes the weeks unemployed or days until the next arrest after being released from incarceration
- Time-to-event-data
    - Non-negative
    - May be censored, resulting in inadequate tail information

Survival function

- Medical studies interested in time to death T of sick patients, usually characterized by the **survival function** $S(t) := \mathbb{P}(T > t)$, the probability of surviving beyond a certain time t.
- Some patients drop out the study or die because of unrelated causes: we call this situation a **censoring time** C.
- $Y := \min(C, T)$ is the **observed outcome variable**, together with an indicator $\delta := \mathbb{I}_{\{Y=T\}}$ of whether the patient died correctly (because of the studied illness).

Hazard function and Cox model

- **Hazard function**: Instantaneous probability of death at time t, given survival up till t.

  $$h(t) = \lim_{\delta \to 0} \frac{\mathbb{P}(Y \in \{t, t+\delta\} \mid Y \geq t)}{\delta} = \frac{f(t)}{S(t)}$$

  where $f(t)$ density of T.

- **Cox's model** treats special cases of hazard functions:

  $$h(t|x) = h_0(t) e^{\beta^\top x}$$

  where x represents e.g. gene expressions and $h_0(t)$ is **baseline hazard**: hazard for one individual with $x = 0$.

The hazard of hazard ratio (Hernán, 2010)

- Treatment Z_i and time-to-event outcome Y_i.
- Hazard: the event rate at time t conditional on survival until time t or later
$$\lim_{\Delta t \to 0} \frac{P(t \leq Y < t + \Delta t | Y \geq t)}{\Delta t}.$$
- Survival analysis assumes models for hazard, e.g., Cox models, additive hazard models, etc.
- Hazard ratio between the treatment and control compares
$$\lim_{\Delta t \to 0} \frac{P(t \leq Y(1) < t + \Delta t | Y(1) \geq t)}{\Delta t}, \quad \lim_{\Delta t \to 0} \frac{P(t \leq Y(0) < t + \Delta t | Y(0) \geq t)}{\Delta t}$$
which compares the populations $\{i : Y_i(1) \geq t\}$ and $\{i : Y_i(0) \geq t\}$.
- Hazard ratio has a built-in selection bias.

Risk sets and partial likelihood

- Go back to the Cox model.

$$h(t|x) = h_0(t)e^{\beta^\top x}.$$

- Denote by $R_i := \{j \mid y_j \geq y_i\}$ the risk set of subject i (individuals which are still in the study when subject i dies).
- The partial likelihood of subject i is given by

$$\frac{h\left(y_i|x_i\right)}{\sum_{j\in R_i} h\left(y_j|x_j\right)} = \frac{e^{\beta^\top x_i}}{\sum_{j\in R_i} e^{\beta^\top x_j}}$$

Note that baseline hazard h_0 has no effect here.

Cox model with penalty

The log-partial-Likelihood is

$$\mathcal{L}(\beta; \boldsymbol{x}, \boldsymbol{\delta}) = \underbrace{\sum_{\{i:\delta_i=1\}}}_{\text{died "correctly"}} \log\left[\frac{e^{\beta^\top x_i}}{\sum_{j\in R_i} e^{\beta^\top x_j}}\right]$$

with corresponding ℓ_1-penalized CPH problem:

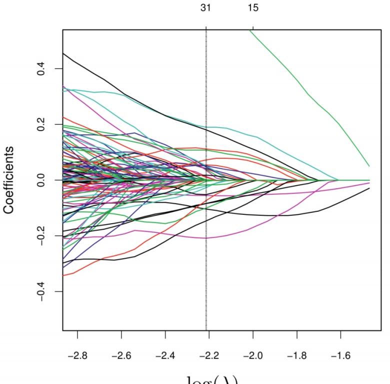
$$\underset{\beta}{\text{minimize}} \left\{ - \sum_{\{i:\delta_i=1\}} \log\left[\frac{e^{\beta^\top x_i}}{\sum_{j\in R_i} e^{\beta^\top x_j}}\right] + \lambda\|\beta\|_1 \right\}$$

Case study: lymphoma data

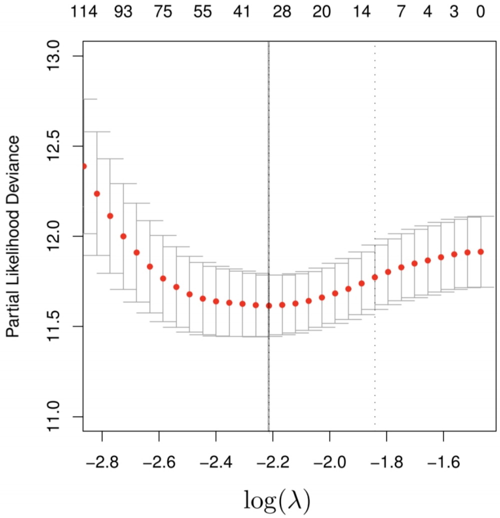
- We want to estimate the hazard function S for $N = 240$ Lymphoma patients with $p = 7399$ variables measuring gene expressions. 102 of these samples are right censored, i.e.

$$Y = \min(T, C) = C$$

- They use the ℓ_1-penalized CPH problem to find $\hat{\beta}(\lambda_{\min})$.



Case study: lymphoma data



Pre-validation

- The Cox model is a semi-parametric model, and the proportional hazard assumption is crucial.
- The proportional hazard assumption is not always satisfied, and the Cox model may not be the best choice.
- Pre-validation is a method to check the proportional hazard assumption.
- The idea is to split the data into two parts, and fit the Cox model to each part separately.
- If the proportional hazard assumption holds, the estimated coefficients should be similar.

Kaplan-Meier estimator

We use the Kaplan-Meier estimator of survivor function $S(t)$: let $\hat{\eta}(x) := \hat{\beta}\left(\lambda_{\min}\right)^{\top} x$, then

$$\widehat{S}(t) = \prod_{i: y_i \leq t} \left(1 - \frac{e^{\hat{\eta}(x_i)}}{\sum_{j \in R_i} e^{\hat{\eta}(x_j)}}\right)$$

is an estimate of $S(t)$. We use these in the following plot.
In computing the score $\hat{\eta}\left(x_i\right)^{(k)}$ for the observations in fold k, we use the coefficient vector $\widehat{\beta}^{(-k)}$ computed with those observations omitted. Doing this for all K folds, we obtain the "pre-validated" dataset $\left\{\left(\hat{\eta}\left(x_i\right)^{(k)}, y_i, \delta_i\right)\right\}_{i=1}^{N}$.

Case study: lymphoma data

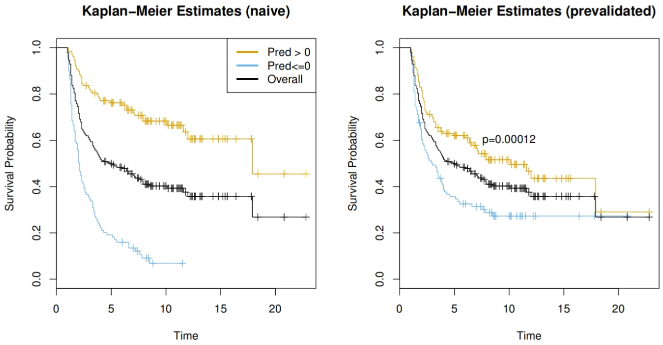
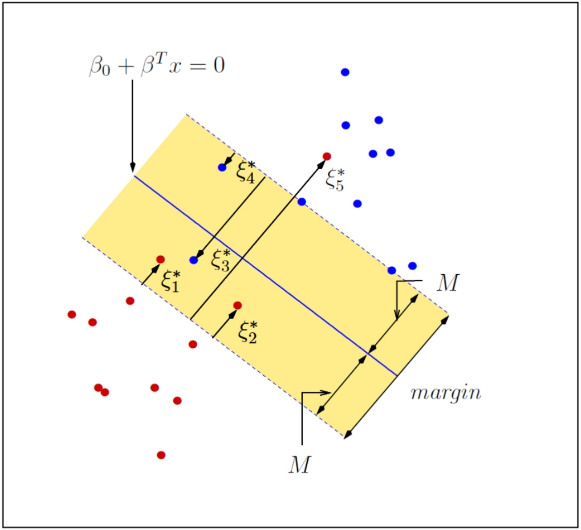


Figure 3.7 *The black curves are the Kaplan–Meier estimates of $S(t)$ for the Lymphoma data. In the left plot, we segment the data based on the* predictions *from the Cox proportional hazards lasso model, selected by cross-validation. Although the tuning parameter is chosen by cross-validation, the predictions are based on the full training set, and are overly optimistic. The right panel uses* prevalidation *to build a prediction on the entire dataset, with this training-set bias removed. Although the separation is not as strong, it is still significant. The spikes indicate censoring times. The p-value in the right panel comes from the log-rank test.*

Support vector machine



SVM: A toy model

- Suppose we have a classification rule : $\{x : f(x) = \beta_0 + x^T\beta\}$, here $x = (x_1, x_2)^T \in \mathbb{R}^2$.
- Consider the following lines:

$$\begin{aligned} l_1 &: \beta_0 + \beta_1 x_1 + \beta_2 x_2 = 1, \\ l_{-1} &: \beta_0 + \beta_1 x_1 + \beta_2 x_2 = -1 \\ l_0 &: \beta_0 + \beta_1 x_1 + \beta_2 x_2 = 0. \end{aligned}$$

- Then, by geometry,

$$d(l_0, l_1) = d(l_0, l_{-1}) = \frac{1}{\sqrt{\beta_1^2 + \beta_2^2}} = \frac{1}{\|\beta\|_2}.$$

- So if the dataset is linear separable, by setting the closest point x_i to the classification boundary l_0 as $f(x_i) = 1$, we have $\exists \beta_0, \beta$ such that

$$f(x_i) = \begin{cases} \geq +1, & \text{if } y_i = +1, \\ \leq -1, & \text{if } y_i = -1. \end{cases}$$

SVM geometric interpretation

Consider the Boundary $B = \{x \in \mathbb{R}^p \mid f(x) = 0\}$, where

$$f(x) = \beta_0 + \beta^\top x$$

Then the distance between the boundary and the point x_0 is

$$\mathrm{dist}\,(x_0, B) = \inf_{z \in B} \|z - x_0\|_2 = \frac{|f(x_0)|}{\|\beta\|_2}$$

So we find that the optimal separating plane $f^*(x) = 0$ has margin

$$M_2^* = \max_{\beta_0, \beta} \left\{ \min_{i \in \{1, \dots, n\}} \frac{y_i f(x_i, \beta_0, \beta)}{\|\beta\|_2} \right\}$$

SVM with slack variable ξ_i

- We allow some points to be misclassified, and introduce a slack variable $\xi = (\xi_1, ..., \xi_n), \xi_i \geq 0$ for each observation.
- $y_i(\beta_0 + x_i^T\beta)$ represents the "distance" of x_i to the classification boundary.
- Foundamentally, we want $y_i(\beta_0 + x_i^T\beta) \geq M$,
- But we allow some points to be misclassified, so we relax the constraint to $y_i(\beta_0 + x_i^T\beta) \geq M(1 - \xi_i)$.
- $\sum_{i=1}^N \xi_i \leq C$ will introduce a bias-variance trade-off:
  - $C = 0$: hard margin SVM, no misclassification allowed,
  - C large: wide margin, introduce large bias and low variance in classification,
  - C small: narrow margin, introduce small bias and high variance in classification.

Optimization problem of SVM

- Denote M as half width of the yellow part in the illustrator as the **margin** of the classifier.
- Objective:

$$\max_{\beta_0, \beta, \{\xi_i\}_{i=1}^N} M$$

- Constraints: $y_i \underbrace{\left(\beta_0 + \beta^\top x_i\right)}_{f(x_i, \beta_0, \beta)} \geq M\left(1 - \xi_i\right), \forall i.$

  $\xi_i \geq 0 \forall i, \sum_{i=1}^N \xi_i \leq C, \|\beta\|_2 = 1.$

- Note that by the constraints, we have

$$\xi_i \geq 1 - y_i f\left(x_i, \beta_0, \beta\right), \quad \xi_i \geq 0.$$

  so $\sum_{i=1}^N \xi_i \geq \sum_{i=1}^N [1 - y_i(\beta_0 + \beta^T x_i)]_+$.

Optimization problem of SVM

- By writing the Lagrangian equivalent of the original minimization problem (SVM), we get:

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ \frac{1}{N} \sum_{i=1}^{N} [1 - y_i f(x; \beta_0, \beta)]_+ + \lambda \|\beta\|_2^2 \right\}$$

  Decreasing λ corresponds to decreasing C and $f(x_i; \beta_0, \beta) = \beta_0 + \beta^T x_i$.

- Hinge loss $[1 - y_i f(x; \beta_0, \beta)]_+$ is zero when if x_i lies on the correct side of the margin. For data on the wrong side of the margin, the function's value is proportional to the distance from the margin.
- ℓ_1 penalized version:

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ \frac{1}{N} \sum_{i=1}^{N} [1 - y_i f(x_i; \beta_0, \beta)]_+ + \lambda \|\beta\|_1 \right\}.$$

RKHS and kernel trick

Kernel

Let $\mathcal{X}$ be a non-empty set. A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a kernel if there exists an $\mathbb{R}$-Hilbert space and a map $\phi : \mathcal{X} \to \mathcal{H}$ such that $\forall x, x' \in \mathcal{X}$,

$$k\left(x, x'\right) := \langle \phi(x), \phi\left(x'\right) \rangle_{\mathcal{H}}.$$

RKHS

Let $\mathcal{H}$ be a Hilbert space of $\mathbb{R}$-valued functions defined on a non-empty set $\mathcal{X}$. A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a reproducing kernel of $\mathcal{H}$, and $\mathcal{H}$ is a reproducing kernel Hilbert space, if k satisfies

- $\forall x \in \mathcal{X}, \quad k(\cdot, x) \in \mathcal{H}$,
- $\forall x \in \mathcal{X}, \forall f \in \mathcal{H}, \langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$ (the reproducing property).

Examples of kernels

- If $K(x, y) = (\langle x, y\rangle + c)^2 = (x_1y_1 + x_2y_2 + c)^2 = \langle \Phi(x), \Phi(y)\rangle$, then $\Phi(x) = (x_1, x_2, \sqrt{2c}x_1, \sqrt{2c}x_2, c)^T$.
- There are many other kernels,
  - Polynomial kernel: $K(x, y) = (\langle x, y\rangle + c)^d$,
  - Gaussian kernel: $K(x, y) = \exp(-\|x - y\|^2/2\sigma^2)$,
  - Laplacian kernel: $K(x, y) = \exp(-\|x - y\|/\sigma)$,
  - Sigmoid kernel: $K(x, y) = \tanh(\kappa\langle x, y\rangle + \theta)$.
- The linear SVM can be generalized using a kernel to create nonlinear boundaries.
- $\|\beta\|_2 \rightsquigarrow \|\beta\|_{\mathcal{H}_K}$.

SVM vs logistic regression

- Penalized logistic:

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \underbrace{\log\left(1 + e^{-y_i f(x_i,\beta_0,\beta)}\right)}_{\text{logistic loss}} + \lambda \|\beta\| \right\}$$

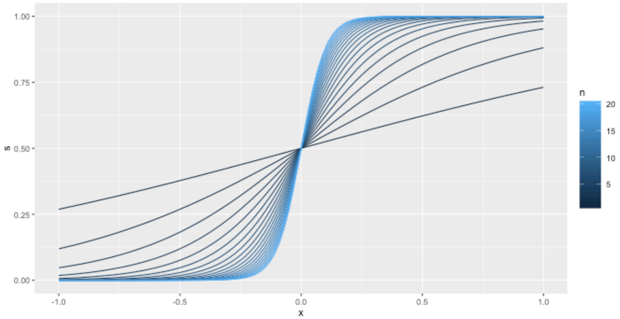
- Penalized svm:

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \underbrace{[1 - y_i f(x;\beta_0,\beta)]_+}_{\text{hinge loss}} + \lambda \|\beta\| \right\}$$

- Data is separable: there exists a hyperplane that separates the two cases. In this cases logistic regression has a problem:

$$P(Y = 1 \mid X = x) = \frac{e^{\beta_0 + \beta^\top x}}{1 + e^{\beta_0 + \beta^\top x}}$$

Problem of logistic regression



Problem: When $p \gg N$, the points are almost always separable.

Relationship between SVM and logistic regression

Consider the problem

$$\underset{\beta_0,\beta}{\text{minimize}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \log\left(1 + e^{-y_i f(x_i,\beta_0,\beta)}\right) + \lambda \|\beta\|_2^2 \right\}$$

Let $\left(\tilde{\beta}_0(\lambda), \tilde{\beta}(\lambda)\right)$ be the solution, then (Rosset et al. 2004) showed that

$$M_2^* = \lim_{\lambda \to 0} \left\{ \min_{i \in \{1,\dots,N\}} \frac{y_i f\left(x_i, \tilde{\beta}_0(\lambda), \tilde{\beta}(\lambda)\right)}{\|\tilde{\beta}(\lambda)\|_2} \right\}$$

So for $\lambda \to 0$ we have that the ℓ_2-regularized logistic regression corresponds to the SVM solution.

Relationship between SVM and logistic regression

In particular, if $\left(\breve{\beta}_0, \breve{\beta}\right)$ solve the SVM problem for $C = 0$, then we have that:

$$\lim_{\lambda \to 0} \frac{\tilde{\beta}(\lambda)}{\|\tilde{\beta}(\lambda)\|_2} = \breve{\beta}$$

Note that the division by the ℓ_2 norm of $\tilde{\beta}(\lambda)$ makes sure that the solution on the SVM problem does not blow up.

- As $\lambda \to 0$, logistic regression and SVM solutions coincide.
- SVM leads to a more stable numerical method for computing the solution in this region.
- Logistic regression is more useful in the sparser part of the solution path.

Part II

- Elastic net
- Group lasso / overlap group lasso
- Fused lasso

Case study: comparison of lasso and elastic net on highly correlated variables

1. 2 sets of 3 variables, pairwise correlations around 0.97 in each group
2. sample size: $N = 100$,
3. data are simulated as follows:

$$
\begin{aligned}
&Z_1, Z_2 \sim N(0,1) \quad \text{independent} \\
&Y = 3Z_1 - 1.5Z_2 + 2\epsilon, \quad \epsilon \sim N(0,1) \\
&X_j(j = 1,2,3) = Z_1 + \xi/5, \quad \xi_j \sim N(0,1) \\
&X_j(j = 4,5,6) = Z_2 + \xi/5, \quad \xi_j \sim N(0,1)
\end{aligned}
$$

Case study: comparison of lasso and elastic net on highly correlated variables

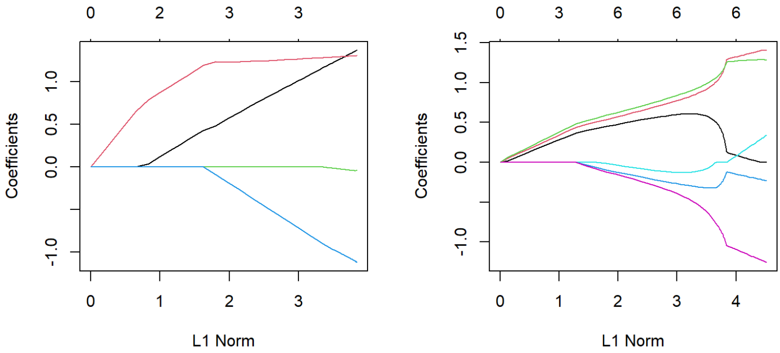
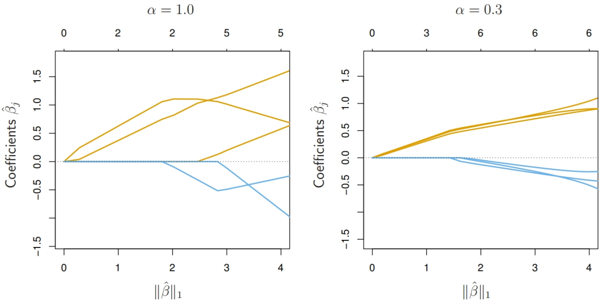


图: The lasso estimates ($\alpha = 1$), as shown in the left panel, exhibit somewhat erratic behavior as the regularization parameter λ is varied. In the right panel, the elastic net with $(\alpha = 0.3)$ includes all the variables, and the correlated groups are pulled together.

Case study: comparison of lasso and elastic net on highly correlated variables



- lasso estimates exhibit erratic behavior as λ varies: one variable is excluded and the correlations among variables are not clear.
- elastic net includes all variables and correlated groups are pulled together, sharing values approximately equally.
- the difference between my plot and the book's plot is due to the random seed.

Elastic net

Recap, the elastic net problem is defined as

$$\underset{(\beta_0,\beta)\in\mathbb{R}\times\mathbb{R}^p}{\text{minimize}}\left\{\frac{1}{2}\sum_{i=1}^{N}\left(y_i-\beta_0-x_i^T\beta\right)^2+\lambda\left[\frac{1}{2}(1-\alpha)\|\beta\|_2^2+\alpha\|\beta\|_1\right]\right\}$$

- Denote R as the objective function of elastic net, then for $\beta_j > 0$,

$$\begin{aligned}\frac{\partial R}{\partial\beta_j} &= \frac{1}{N}\sum_{i=1}^{N}\left(y_i-\beta_0-\boldsymbol{x_j}^\top\boldsymbol{\beta}\right)(-x_{ij})+\lambda\left[(1-\alpha)\beta_j+\alpha\,\mathrm{sgn}\,(\beta_j)\right]\\ &= \frac{1}{N}\sum_{i=1}^{N}(\underbrace{y_i-\beta_0-\sum_{k\neq j}x_{ik}\beta_k}_{=r_{ij}}-x_{ij\beta_j})\,(-x_{ij})+\ldots\\ &= -\frac{1}{N}\sum_{i=1}^{N}r_{ij}x_{ij}+\frac{1}{N}\sum_{i=1}^{N}x_{ij}^2\beta_j+\lambda\left[(1-\alpha)\beta_j+\alpha\,\mathrm{sgn}\,(\beta_j)\right].\end{aligned}$$

Elastic net

- Setting the derivatives to zero yields

$$\left[\frac{1}{N}\sum_{i=1}^{N} x_{ij}^2 + \lambda(1-\alpha)\right]\beta_j + \alpha\lambda\,\mathrm{sgn}(\beta) = \frac{1}{N}\sum_{i=1}^{N} r_{ij}x_{ij}$$

  As we did in lasso case, here coordinate descent have a close form update for each β_j.

$$\widehat{\beta}_j = \frac{\mathcal{S}_{\lambda\alpha}\left(\sum_{i=1}^{N} r_{ij}x_{ij}\right)}{\sum_{i=1}^{N} x_{ij}^2 + \lambda(1-\alpha)},$$

  where $r_{ij} = y_i - \tilde{\beta}_0 - \sum_{k\neq j} x_{ik}\hat{\beta}_k$ and $\mathcal{S}_\mu(z) := \mathrm{sign}(z)(z-\mu)_+$.
- In practice, group structure may not be as evident as the previous ‘ideal’ model, this example does capture the main idea of elastic net.
- By adding ridge penalty to lasso penalty, elastic net automatically controls for strong within-group correlations.

Why does elastic net promote grouping?

Grouping effect (Zou and Hastie, 2005)

Given data $(\boldsymbol{y}, \boldsymbol{X})$ and parameters (λ_1, λ_2), the response $\boldsymbol{y}$ is centered and the predictor $\boldsymbol{X}$ are standardized. Let $\hat{\beta}(\lambda_1, \lambda_2)$ be the naive elastic net estimate. Suppose that $\hat{\beta}_i(\lambda_1, \lambda_2)\hat{\beta}_j(\lambda_1, \lambda_2) > 0$. Then

$$D_{\lambda_1,\lambda_2}(i,j) = \frac{1}{\|\mathbf{y}\|_2}\left|\hat{\beta}_i(\lambda_1, \lambda_2) - \hat{\beta}_j(\lambda_1, \lambda_2)\right| \leq \frac{1}{\lambda_2}\sqrt{2(1-\rho)}$$

where $\rho = \boldsymbol{x}_i^T \boldsymbol{x}_j$, the sample correlation.

The unitless quantity $D_{\lambda_1,\lambda_2}(i,j)$ describes the difference between the coefficient paths of predictors i and j. If $\mathbf{x}_i$ and $\mathbf{x}_j$ are highly correlated, i.e. $\rho \doteq 1$ (if $\rho \doteq -1$ then consider $-\mathbf{x}_j$), theorem 1 says that the difference between the coefficient paths of predictor i and predictor j is almost 0 .

Grouping effect

Consider the overall minimization

$$\min_{\beta} \underbrace{\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|^2 + \lambda_1\|\boldsymbol{\beta}\|_1 + \lambda_2\|\boldsymbol{\beta}\|^2}_{L(\boldsymbol{\beta})}.$$

Then the optimality at β_i and β_j is

$$\begin{cases} \frac{\partial L}{\partial \beta_i} = -2\boldsymbol{x_i}^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) + 2\lambda_2\beta_i + \lambda_1 \operatorname{sgn}(\beta_i) = 0 \\ \frac{\partial L}{\partial \beta_j} = -2\boldsymbol{x_j}^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) + 2\lambda_2\beta_j + \lambda_1 \operatorname{sgn}(\beta_j) = 0 \end{cases}$$

Substracting the two equations, we have

$$2(\boldsymbol{x_j} - \boldsymbol{x_i})^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) + 2\lambda_2(\beta_i - \beta_j) + \lambda_1\left(\underbrace{\operatorname{sgn}(\beta_i) - \operatorname{sgn}(\beta_j)}_{=0,\text{ by assumption}}\right) = 0$$

Grouping effect (cont'd)

By the previous equation, we have

$$(\beta_i - \beta_j) = \frac{1}{\lambda_2} (\boldsymbol{x_i} - \boldsymbol{x_j})^\top (\boldsymbol{y} - \boldsymbol{X\beta})$$

Then, we have

$$(\beta_i - \beta_j)^2 \leq \frac{1}{\lambda_2^2} \|\boldsymbol{x_i} - \boldsymbol{x_j}\|^2 \|\boldsymbol{y} - \boldsymbol{X\beta}\|^2 \quad \text{(by Cauchy)}$$

Then we can bound the inequality by parts. For $\|\boldsymbol{x_i} - \boldsymbol{x_j}\|^2$, by centered dataset, we have $\|\boldsymbol{x_i}\|^2 = 1, i = 1, ..., p$ and $\boldsymbol{x_i^T x_j} = \rho$, so

$$\|\boldsymbol{x_i} - \boldsymbol{x_j}\|^2 = \|\boldsymbol{x_i}\|^2 + \|\boldsymbol{x_j}\|^2 - 2\boldsymbol{x_i^T x_j} = 2(1 - \rho).$$

Grouping effect (cont'd)

For $\|\boldsymbol{y}-\boldsymbol{X}\beta\|^2$, by optimization,

$$\|\boldsymbol{y}-\boldsymbol{X}\hat{\beta}\|_2^2+\lambda_1\|\hat{\boldsymbol{\beta}}\|_1+\lambda_2\|\hat{\boldsymbol{\beta}}\|_2^2=L(\hat{\boldsymbol{\beta}})\leq L(0)=\|\boldsymbol{y}\|_2^2.$$

then,

$$\|\boldsymbol{y}-\boldsymbol{X}\hat{\beta}\|_2^2\leq\|\boldsymbol{y}\|_2^2-\lambda_1\|\hat{\boldsymbol{\beta}}\|_1-\lambda_2\|\hat{\boldsymbol{\beta}}\|_2^2\leq\|\boldsymbol{y}\|_2^2.$$

Combining all the upper bounds, we have

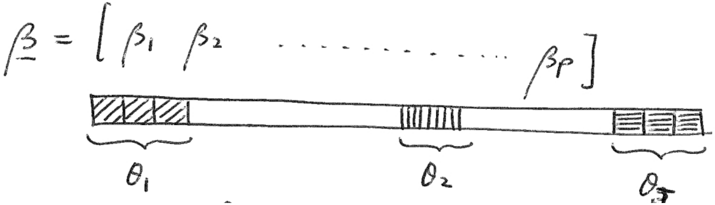
$$|\beta_i-\beta_j|\leqslant\frac{1}{\lambda_2}\sqrt{2(1-p)}\|y\|_2,$$

which completes the proof.

Group lasso

- Groups of covariates be selected into or out of a model together.
- Desirable to have all coefficients within a group become nonzero (or zero) simultaneously.

We use group lasso penalty for such situations.



$\underline{\beta} = [\beta_1 \ \beta_2 \ \ldots\ldots \ \beta_p]$
θ_1
θ_2
θ_J

Group lasso

- Consider linear regression model involving J groups of covariates, where $j = 1, ..., J$.
- Vector $\boldsymbol{Z_j} = (X_{j1}, ..., X_{jp_j})^T \in \mathbb{R}^{p_j}$ represents the covariates in group j.
- Goal: predict real-valued response $Y \in \mathbb{R}$ based on collection of covariates $(Z_1, ..., Z_J)$.
- Linear model $\mathbb{E}(Y|Z)$ takes the form $\theta_0 + \sum_{j=1}^{J} \boldsymbol{Z_j^T}\theta_j$, where $\theta_j \in \mathbb{R}^{p_j}$.

Group lasso

Given a collection of N samples $\{(y_i, z_{i1}, z_{i2}, \ldots, z_{iJ})\}_{i=1}^{N}$ the group lasso solves the convex problem:

$$\underset{\theta_0 \in \mathbb{R}, \theta_j \in \mathbb{R}^{p_j}}{\text{minimize}} \left\{ \frac{1}{2} \sum_{i=1}^{N} \left(y_i - \theta_0 - \sum_{j=1}^{J} z_{ij}^T \theta_j \right)^2 + \lambda \sum_{j=1}^{J} \|\theta_j\|_2 \right\}$$

Where $\|\theta_j\|_2$ is the Euclidean norm.
This is group generalization of the lasso with properties:

- Depending on $\lambda \geq 0$ either the entire vector $\hat{\theta}_j$ will be zero, or all its elements will be nonzero.
- When $p_j = 1, j = 1, ..., J$, then we have $\|\theta_j\|_2 = |\theta_j|$, so reduces to the ordinary lasso.

Lasso vs group lasso

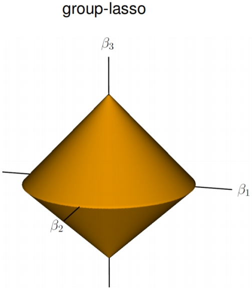
Lasso penalty:

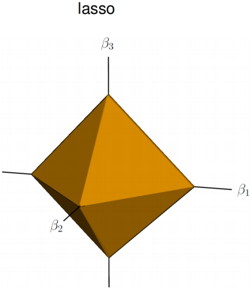
- $|\beta|_1 = \sum_{j=1}^{p} |\beta_j|$,
- $\hat{\beta}$ is sparse.

Group lasso penalty:

- $\boldsymbol{\beta} = (\boldsymbol{\theta_1}, ..., \boldsymbol{\theta_J})$
- By notation abuse, denote $\|\boldsymbol{\beta}\|_{2,1} = \sum_{j=1}^{p} \|\theta\|_2$, denote $\boldsymbol{\theta} = (\|\theta_1\|_1, ..., \|\theta_J\|_2)$.
- $\hat{\boldsymbol{\theta}}$ is sparse.

An unit ball example for group lasso penalty





- Left unit ball can be characterized as $\sqrt{\beta_1^2 + \beta_2^2} + |\beta_3| \leq 1$.
- Right unit ball can be characterized as $|\beta_1| + |\beta_2| + |\beta_3| \leq 1$.

Example: multitask learning

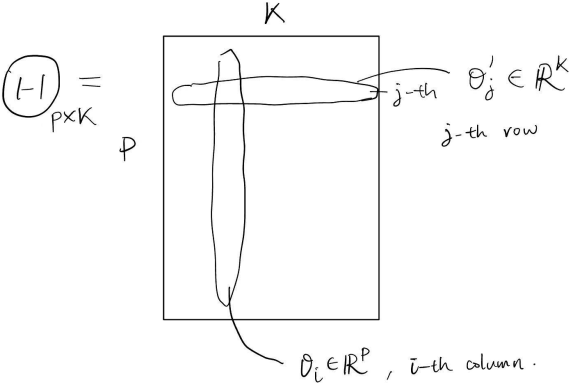
- Multivariate response $\boldsymbol{Y} \in \mathbb{R}^{N \times K}$, predictor matrix $\boldsymbol{X} \in \mathbb{R}^{N \times p}$.
- Matrix of coefficients $\boldsymbol{\Theta} \in \mathbb{R}^{p \times K}$ with, matrix of errors $\boldsymbol{E} \in \mathbb{R}^{N \times K}$.
- $Y \in \mathbb{R}^K$ may be correlated, for example, taking Y as K movies ratings of N users, then the ratings of different movies are correlated.
- Goal: estimate $\boldsymbol{\Theta}$ by minimizing the following objective function:

$$\underset{\boldsymbol{\Theta} \in \mathbb{R}^{p \times K}}{\text{minimize}} \left\{ \frac{1}{2} \|\mathbf{Y} - \mathbf{X}\boldsymbol{\Theta}\|_F^2 + \lambda \left(\sum_{j=1}^{p} \left\| \theta_j' \right\|_2 \right) \right\}$$

where $\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2}$. θ_j' is the jth row of $\boldsymbol{\Theta}$, which means the coefficients of the jth task.

Example: multitask learning

- If we only use $\sum_{j=1}^{p} \sum_{k=1}^{K} \left|\boldsymbol{\Theta}_{jk}\right|$, namely, $\|\boldsymbol{\Theta}\|_1$, then we have no way of controlling group sparsity.
- $\sum_{j=1}^{p} \left\|\theta_j'\right\|_2$ can do group sparsity because once the j^{th} row is actuated, all elements on the row are activated.



$\Theta_{p\times K} =$
K
P
j-th
$\theta_j' \in \mathbb{R}^K$
j-th row
$\theta_i \in \mathbb{R}^p$, i-th column.

Computation for group lasso

We ignore the intercept and rewrite the optimization problem as follows:

$$\min_{(\theta_1,\dots,\theta_j)} \left\{ \frac{1}{2} \left\| \boldsymbol{y} - \sum_{j=1}^{J} \boldsymbol{Z_j \theta_j} \right\|_2^2 + \lambda \sum_{j=1}^{J} \|\boldsymbol{\theta_j}\|_2 \right\}.$$

By taking sub-derivative on the objective function and letting the derivative to be zero, we have the following estimating equation:

$$-\boldsymbol{Z_j}^T \left(\boldsymbol{y} - \sum_{j=1}^{J} \boldsymbol{Z_j} \hat{\theta}_j \right) + \lambda \hat{s}_j = 0,$$

where $\hat{s}_j \in \partial \|\hat{\theta}_j\|_2 = \begin{cases} \frac{\hat{\theta}_j}{\|\theta_j\|_2}, & \text{if } \hat{\theta}_j \neq 0, \\ \text{any } \boldsymbol{v} \text{ s.t. } \|\boldsymbol{v}\|_2 \leq 1, & \text{if } \hat{\theta}_j = 0. \end{cases}$

Computation for group lasso

Denote $\boldsymbol{r_j} = \boldsymbol{y} - \sum_{k \neq j} \boldsymbol{Z_k} \hat{\boldsymbol{\theta}}_{\boldsymbol{k}}$, then the estimating equation gives

$$-\boldsymbol{Z_j}^T \left(\boldsymbol{r_j} - \boldsymbol{Z_j} \hat{\theta}_j \right) + \lambda \hat{s}_j = 0.$$

By coordinate descent lemma, we have

$$\hat{\theta}_j = \begin{cases} \left(\mathbf{Z}_j^T \mathbf{Z}_j + \frac{\lambda}{\|\widehat{\theta}_j\|_2} \mathbf{I} \right)^{-1} \mathbf{Z}_j^T \boldsymbol{r}_j, & \text{if } \|\boldsymbol{Z_j}^T \boldsymbol{r_j}\|_2 \geq \lambda, \\ \mathbf{0}, & \text{otherwise.} \end{cases}$$

This is not a closed form solution, one can use iterative methods to solve the equation, or add some assumptions on $\boldsymbol{Z_j}$, for example, if $\boldsymbol{Z_j}$ is orthogonal, then the solution is closed form.

Sparse group lasso

- When a group is included in a group-lasso fit, all the coefficients in that group are nonzero.
- We want sparsity both with respect to which groups are selected, and which coefficients are nonzero within a group.

An example for group lasso

Genes and proteins often lie in known pathways, an investigator may be more interested in which pathway are related to an outcome than whether particular individual genes are.

An example for sparse group lasso

Although a biological pathway may be implicated in the progression of a particular type of cancer, not all gene in the pathway need be active.

Sparse group lasso

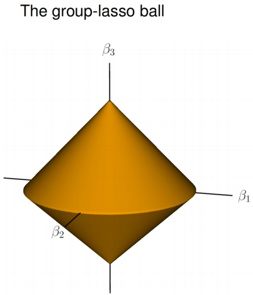
In order to achieve within-group sparsity, augment with additional ℓ_1-penalty, leading to the convex program:

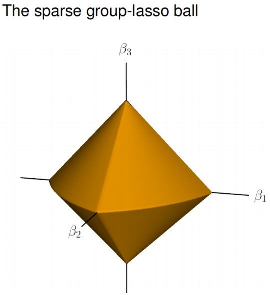
$$\underset{\{\theta_j \in \mathbb{R}^{p_j}\}_{j=1}^{J}}{\text{minimize}} \left\{ \frac{1}{2} \left\| \mathbf{y} - \sum_{j=1}^{J} \mathbf{Z}_j \theta_j \right\|_2^2 + \lambda \sum_{j=1}^{J} \left[(1-\alpha) \|\theta_j\|_2 + \alpha \|\theta_j\|_1 \right] \right\},$$

where $\alpha \in [0, 1]$.

- $\alpha = 0$, reduces to the group lasso.
- $\alpha = 1$, reduces to the lasso.

Sparse group lasso constraint region


The group-lasso ball


The sparse group-lasso ball

- Left unit ball can be characterized as $\sqrt{\beta_1^2 + \beta_2^2} + |\beta_3| \leq 1$.
- Right unit ball can be characterized as $(1-\alpha)\sqrt{\beta_1^2 + \beta_2^2} + \alpha(|\beta_1| + |\beta_2|) + (1-\alpha)|\beta_3| + \alpha|\beta_3| \leq 1$.

Overlap group lasso

- Sometimes variables can belong to more than one group.
- Genes can belong to more than one biological pathway.
- For example, we divide 5 variables into 2 groups,

$$\boldsymbol{Z}_1 = (X_1, X_2, X_3), \quad \boldsymbol{Z}_2 = (X_3, X_4, X_5).$$

  - If we simply replicate variable X_3, then use group lasso, then X_3 will be selected to the model with higher probability.
  - If we simply replicate parameter then use sparese group lasso, then X_3 will be selected to the model only when both two groups are selected.
- So replicate variable is preferred.

Overlap group lasso

- $\nu_j \in \mathbb{R}^p$ is a vector which is zero everywhere except in those positions corresponding to member of the group j.
- $\mathcal{V}_i \subseteq \mathbb{R}^p$ subspace of possible vectors.
- For $X = (X_1, \ldots, X_p)$ the coefficient vector is given by $\beta = \sum_{j=1}^{J} \nu_j$
- The overlap group lasso solves the problem:

$$\text{minimize}_{\nu_j \in \mathcal{V}_j, j=1,\ldots,J} \left\{ \frac{1}{2} \left\| \mathbf{y} - \mathbf{X} \left(\sum_{j=1}^{J} \nu_j \right) \right\|_2^2 + \lambda \sum_{j=1}^{J} \|\nu_j\|_2 \right\}$$

- (Jacob et al., 2009) showed that, the equivalent optimization problem can be put in the form:

$$\underset{\beta \in \mathbb{R}^p}{\text{minimize}} \left\{ \frac{1}{2} \|\mathbf{y} - \mathbf{X}\beta\|_2^2 + \lambda \Omega_{\mathcal{V}}(\beta) \right\}, \quad \Omega_{\mathcal{V}}(\beta) := \inf_{\substack{\nu_j \in \mathcal{V}_j \\ \beta = \sum_{j=1}^{J} \nu_j}} \sum_{j=1}^{J} \|\nu_j\|_2 \, .$$

Additive models

Additive models

Additive models are based on approximating the regression function by sums of the form:

$$f(x) = f(x_1, \ldots, x_J) \approx \sum_{j=1}^{J} f_j(x_j), \quad f_j \in \mathcal{F}_j, \quad j = 1, \ldots, J$$

- $\mathcal{F}_j$ are fixes set of univariate function classes
- Each $\mathcal{F}_j$ assumed to be a subset of $L^2(\mathbb{P}_j)$
- $\mathbb{P}_j$ is the distribution of covariate X_j equipped with squared $L^2(\mathbb{P}_j)$ norm
$$\|f_j\|_2^2 := \mathbb{E}\left[f_j^2(X_j)\right]$$
- Some theoretical results need $\mathcal{F}$ to be the Sobelev class of functions on $[a, b]$. (Buhlmann and van de Geer, 2010)

Additive models

Best additive approximation to regression function $\mathbb{E}(Y \mid X = x)$ solves problem:

$$\underset{f_j \in \mathcal{F}_j j=1,\ldots,J}{\text{minimize}} \, \mathbb{E}\left[\left(Y - \sum_{j=1}^{J} f_j\left(X_j\right)\right)^2\right]$$

The optimal solution $\left(\tilde{f}_1, \ldots, \tilde{f}_J\right)$ is characterized by the **backfitting equations**:

$$\tilde{f}_j\left(x_j\right) = \mathbb{E}\left[Y - \sum_{k \neq j} \tilde{f}_k\left(X_k\right) \mid X_j = x_j\right], \text{ for } j = 1, \ldots, J$$

Sparse additive models (SPAM)

- $\|f_j\|_2 = \sqrt{\mathbb{E}\left[f_j^2\left(X_j\right)\right]}$,
- For $\lambda \geq 0$ type of best sparse approximation:

$$\mathrm{minimize}^{\mathrm{m}}_{f_j \in \mathcal{F}_j = 1,\ldots,J} \left\{ \mathbb{E}\left[\left(Y - \sum_{j \in S} f_j\left(X_j\right)\right)^2\right] + \lambda \sum_{j=1}^{J} \|f_j\|_2 \right\}$$

- SPAM combines ideas from sparse linear modeling and additive nonparametric regression.

Multiple Penalization

- Multiple ways of enforcing sparsity for a nonparametric problem. (SPAM backfitting, COSSO).
- SPAM backfitting base on a combination of ℓ_1-norm: $\|f\|_{N,1} := \sum_{j=1}^{J} \|f_j\|_N$ with $\|f_j\|_N^2 := \frac{1}{N} \sum_{j=1}^{J} f_j^2 \left(x_{ij}\right)$
- COSSO method uses combination of the ℓ_1-norm with the Hilbert norm:

$$\|f\|_{\mathcal{H},1} := \sum_{j=1}^{J} \|f_j\|_{\mathcal{H}}$$

- General family of estimator:

$$\min_{f_j \in \mathcal{H}_j j=1,\dots,J} \left\{ \frac{1}{N} \sum_{i=1}^{N} \left(y_i - \sum_{j=1}^{J} f_j\left(x_{ij}\right) \right)^2 + \lambda_{\mathcal{H}} \sum_{j=1}^{J} \|f_j\|_{\mathcal{H}_j} + \lambda_N \sum_{j=1}^{J} \|f_j\|_N \right\}$$

Fused lasso

The fused LASSO (signal approximator) solves the problem

$$\underset{\theta\in\mathbb{R}^n}{\text{minimize}}\left\{\sum_{i=1}^{n}(Y_i-\theta_i)^2+\lambda_1\sum_{i=1}^{n}|\theta_i|+\lambda_2\sum_{i=2}^{n}|\theta_i-\theta_{i-1}|\right\}.$$

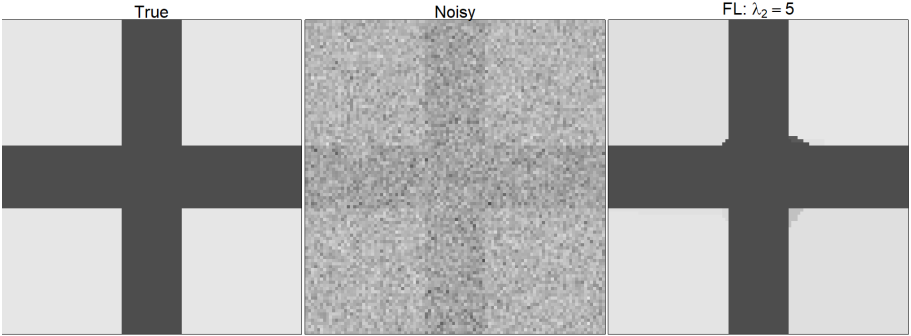
More generally one can use the penalty

$$\lambda_2\sum_{i\sim j}|\theta_i-\theta_j|\,,$$

where $\sim$ is a relation depending on the problem at hand.

- Fused term : $\sum_{i=2}^{n}|\theta_i-\theta_{i-1}|$.
- Lasso term : $\sum_{i=1}^{n}|\theta_i|$.

Case study: total variation denoising



- The idea here is that there exists a ”true” image, but we only see a noisy image, from which we would like to recover the true image.

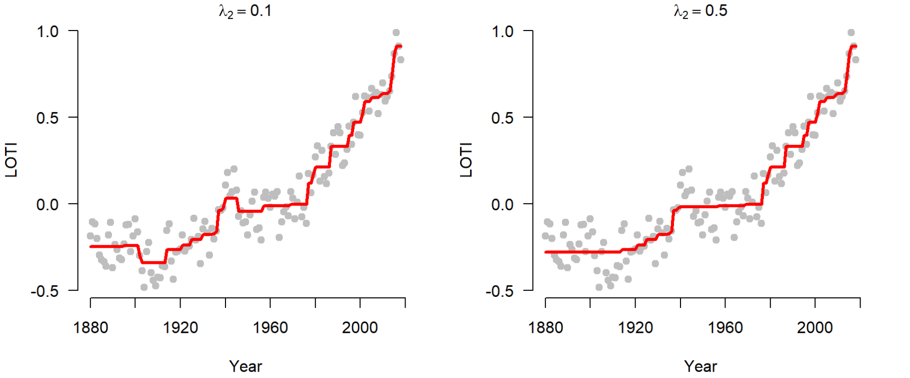
Isotonic regression

- $$\underset{\boldsymbol{\theta}\in\mathbb{R}^N}{\text{minimize}}\left\{\sum_{i=1}^{N}(y_i-\theta_i)^2\right\}\text{ subject to }\theta_1\leq\theta_2\leq\ldots\leq\theta_N$$

- Nearly isotonic regression is a natural relaxation, in which we introduce a regularization parameter $\lambda \geq 0$, and instead solve the penalized problem

$$\underset{\boldsymbol{\theta}\in\mathbb{R}^N}{\text{minimize}}\left\{\frac{1}{2}\sum_{i=1}^{N}(y_i-\theta_i)^2+\lambda\sum_{i=1}^{N-1}(\theta_i-\theta_{i+1})_+\right\}$$

Case study: global warming



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