Machine Learning in Bioinformatics

Feature Selection

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Feature selection problem

$$\hat{\theta} = \begin{cases} \arg\min\limits_{\theta} & \|y - X\theta\|_2^2 \\ \text{subject to} & \|\theta\|_0 = m \end{cases} \quad \text{with } \binom{p}{m} \text{ possible subsets}$$

- Required are computationally efficient methods to approximate the feature selection problem
- *Offline methods*: Select features before estimating parameters
- *Online methods*: Features are selected during parameter estimation

Feature selection methods

- Offline methods:
  - Safe and Strong rules
  - Sure independence screening (SIS)
  - Estimation of mutual information
- Online methods:
  - (Orthogonal) matching pursuit
  - Least angle regression (LARS) / Homotopy algorithm
  - Penalty methods

Linear Regression - recap

$$y = X\theta + \epsilon$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(p)} \\ x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(p)} \\ \vdots & \vdots & \ddots & \vdots \\ x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(p)} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

response : $y \in \mathbb{R}^n$

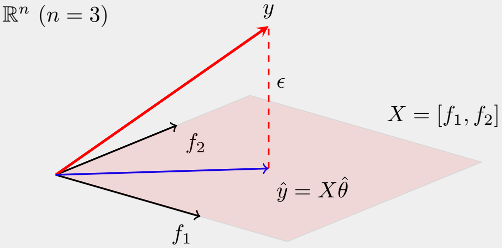
covariates : $X \in \mathbb{R}^{n \times p}$

coefficients : $\theta \in \mathbb{R}^p$

residuals : $\epsilon \in \mathbb{R}^n$

Geometric interpretation of ordinary least squares [Hastie et al., 2009]:

$$\hat{\theta} = \arg\min_{\theta} \|\epsilon\|_2^2$$
$$= \arg\min_{\theta} \|y - X\theta\|_2^2$$



Sure Independence Screening (SIS)

Sure independence screening (SIS)

- Consider the case of ultrahigh-dimensional data, where the number of features p is much larger than the number of observations n
- Specifically, we assume that p is so large that we cannot compute an estimate of θ
- Assuming θ is sparse, we can first select a *promising* subset of q features M_q (called *feature screening*)
- The coefficients θ are estimated based on the subset M_q

Sure independence screening (SIS)

- Consider the solution of rigde regression:

$$\hat{\theta}(\lambda) = (X^\top X + \lambda I)^{-1} X^\top y$$

- For $\lambda \to 0$ we obtain the OLS solution
- For $\lambda \to \infty$ it follows that $\lambda\hat{\theta}(\lambda)$ converges to the componentwise regression estimator

$$\hat{\theta}_k(\lambda) = \tilde{X}^\top y$$

  where $\tilde{X}$ is the data matrix X with normalized columns f_j such that $f_j^\top f_j = 1$
- Traditionally, for very large p we would select λ large in order to decrease the variance of $\hat{\theta}$

- $\tilde{X}^\top y = (f_1^\top y, \ldots, f_p^\top y)$ can be interpreted as the correlation of features f_j with y
- Sure independence screening (SIS) [Fan and Lv, 2008] selects a subset of features

$$\Omega = \left\{ j \,\middle|\, |f_j^\top y| > t \right\} \tag{1}$$

  based on their correlation with y, where t is a threshold such that $|\Omega| = q < p$
- The OLS estimate $\hat{\theta}$ is computed using only the selected features Ω
- All remaining components of $\hat{\theta}$ are set to zero

- The same idea can be applied to more complex models [Fan and Song, 2010], such as logistic regression, where

$$\hat{\theta} = \arg\max_{\theta} \mathrm{pr}_{\theta}(y \mid X)$$

- Select a subset of features

$$\Omega = \left\{ j \;\middle|\; \mathrm{score}(f_j, y) > t \right\} \tag{2}$$

- The score is given by the independent estimate

$$\mathrm{score}(f_j, y) = \arg\max_{\theta_j} \mathrm{pr}_{\theta_j}(y \mid f_j)$$

for all $j = 1, \ldots, p$

Matching Pursuit for Linear Regression

Feature selection problem

$$\hat{\theta} = \begin{cases} \arg\min_{\theta} & \|y - X\theta\|_2^2 \\ \text{subject to} & \|\theta\|_0 = m \end{cases} \quad \text{with } \binom{p}{m} \text{ possible subsets}$$

Feature selection problem

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Matching Pursuit

Greedy approximation to feature selection problem.

Feature selection problem

$$\hat{\theta} = \begin{cases} \underset{\theta}{\arg\min} & \|y - X\theta\|_2^2 \\ \text{subject to} & \|\theta\|_0 = m \end{cases} \quad \text{with } \binom{p}{m} \text{ possible subsets}$$

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Greedy approximation to feature selection problem.

If we must represent y with only one feature, which one should we take?

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Matching Pursuit

Greedy approximation to feature selection problem.

If we must represent y with only one feature, which one should we take?

$$j_1 = \arg\min_{j} \left\|y - f_j \hat{\theta}_j\right\|_2^2, \quad \text{where} \quad \hat{\theta}_j = \arg\min_{\theta_j} \|y - f_j \theta_j\|_2^2$$

Matching Pursuit for linear regression

$$j_1 = \arg\min_{j} \left\| y - f_j \hat{\theta}_j \right\|_2^2 , \quad \text{where} \quad \hat{\theta}_j = \arg\min_{\theta_j} \left\| y - f_j \theta_j \right\|_2^2$$

$$
\begin{aligned}
j_1 &= \arg\min_j \left\| y - f_j \hat{\theta}_j \right\|_2^2 , \quad \text{where} \quad \hat{\theta}_j = \arg\min_{\theta_j} \left\| y - f_j \theta_j \right\|_2^2 \\
&= \arg\max_j \frac{(f_j^\top y)^2}{f_j^\top f_j} \\
&= \arg\max_j \left| f_j^\top y \right|
\end{aligned}
$$

[assuming normalized data, i.e. $f_j^\top f_j = 1$]

$\Rightarrow$ select feature j with maximal scalar projection of y onto f_j

Matching Pursuit for linear regression

$$\begin{aligned}\epsilon &= y - X\theta \\ &= \underbrace{\underbrace{\underbrace{y}_{r_0} - f_{j_1}\theta_{j_1}}_{r_1} - f_{j_2}\theta_{j_2}}_{r_2} - \ldots - f_{j_p}\theta_{j_p}\end{aligned}$$

$$\begin{aligned}j_1 &= \arg\min_j \left\|y - f_j\hat{\theta}_j\right\|_2^2 \qquad = \arg\min_j \left\|r_0 - f_j\hat{\theta}_j\right\|_2^2 \\ &= \arg\max_j \left|f_j^\top r_0\right|\end{aligned}$$

Matching Pursuit for linear regression

$$\begin{aligned}\epsilon &= y - X\theta \\ &= \underbrace{\underbrace{\underbrace{y}_{r_0} - f_{j_1}\theta_{j_1}}_{r_1} - f_{j_2}\theta_{j_2}}_{r_2} - \dots - f_{j_p}\theta_{j_p}\end{aligned}$$

$$\begin{aligned}j_1 &= \arg\min_j \left\| y - f_j\hat{\theta}_j \right\|_2^2 && = \arg\min_j \left\| r_0 - f_j\hat{\theta}_j \right\|_2^2 \\ &= \arg\max_j \left| f_j^\top r_0 \right| \\ j_2 &= \arg\min_j \left\| y - f_{j_1}\hat{\theta}_{j_1} - f_j\hat{\theta}_j \right\|_2^2 && = \arg\min_j \left\| r_1 - f_j\hat{\theta}_j \right\|_2^2 \\ &= \arg\max_j \left| f_j^\top r_1 \right|\end{aligned}$$

Matching pusuit (MP) [Tropp et al., 2007]

The MP feature selection rule is given by

$$j_k = \arg\max_j \left| f_j^\top r_{k-1} \right| \qquad k = 1, \ldots, m$$

where r_k are the residuals at step k:

$$\begin{aligned} \epsilon &= y - X\theta \\ &= \underbrace{\underbrace{\underbrace{y}_{r_0} - f_{j_1}\theta_{j_1}}_{r_1} - f_{j_2}\theta_{j_2}}_{r_2} - \ldots - f_{j_p}\theta_{j_p} \end{aligned}$$

Orthogonal Matching Pursuit

Orthogonal Matching Pursuit: Re-estimate parameters after every iteration.

After every iteration t, update all θ_{Ω_t} entries, where $\Omega_t = \{j_1, j_2, \ldots, j_t\}$, i.e. compute

$$\theta_{\Omega_t} = \arg\min_{\theta} \|y_{\Omega_t} - X_{\Omega_t}\theta\|_2^2 \ .$$

This update changes the residuals

$$r_t = y - f_{j_1}\theta_{j_1} - f_{j_2}\theta_{j_2} - \cdots - f_{j_t}\theta_{j_t}$$

used in the next iteration of the algorithm.

Matching Pursuit for Logistic Regression

$$\begin{bmatrix} \mathrm{pr}_\theta(y_1 = 1) \\ \mathrm{pr}_\theta(y_2 = 1) \\ \vdots \\ \mathrm{pr}_\theta(y_n = 1) \end{bmatrix} = \sigma \left(\begin{bmatrix} x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(p)} \\ x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(p)} \\ \vdots & \vdots & \ddots & \vdots \\ x_n^{(1)} & x_n^{(2)} & \dots & x_n^{(p)} \end{bmatrix} \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{bmatrix} \right)$$

class labels : $y \in \{0, 1\}^n$

covariates : $X \in \mathbb{R}^{n \times p}$

coefficients : $\theta \in \mathbb{R}^p$

Parameter estimation for logistic regression:

$$\begin{aligned}\hat{\theta} &= \arg\max_{\theta} \mathrm{pr}_{\theta}(y) \approx \arg\min_{\theta} \|y - \sigma(X\theta)\|_2^2 \quad \text{[but not convex]} \\ &= \arg\max_{\theta} \sum_{i=1}^{n} \log \mathrm{pr}_{\theta}(y_i) \\ &= \arg\max_{\theta} \sum_{i=1}^{n} \{y_i \log \sigma(x_i\theta) + (1 - y_i) \log(-x_i\theta)\} \\ &= \arg\max_{\theta} \sum_{i=1}^{n} \log \sigma(\tilde{y}_i x_i \theta)\,,\end{aligned}$$

where $\tilde{y}_i = 2y_i - 1 \in \{-1, 1\}$

Pseudo-residuals

$$
\begin{aligned}
r_k &= y - \sigma(f_{j_1}\theta_{j_1} + f_{j_2}\theta_{j_2} + \cdots + f_{j_k}\theta_{j_k}) \\
X^\top r_p &= \nabla \log \mathrm{pr}_\theta(y)
\end{aligned}
$$

Pseudo-residuals

$$r_k = y - \sigma(f_{j_1}\theta_{j_1} + f_{j_2}\theta_{j_2} + \cdots + f_{j_k}\theta_{j_k})$$
$$X^\top r_p = \nabla \log \mathrm{pr}_\theta(y)$$

$$\begin{aligned} j_1 &= \arg\min_j \left\| y - \sigma(f_j\hat{\theta}_j) \right\|_2^2 \\ &\approx \arg\max_j \left| f_j^\top r_0 \right| \end{aligned}$$

Pseudo-residuals

$$r_k = y - \sigma(f_{j_1}\theta_{j_1} + f_{j_2}\theta_{j_2} + \cdots + f_{j_k}\theta_{j_k})$$
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j_1 &= \arg\min_j \left\| y - \sigma(f_j\hat{\theta}_j) \right\|_2^2 \\
&\approx \arg\max_j \left| f_j^\top r_0 \right| \\
j_2 &= \arg\min_j \left\| y - \sigma(f_{j_1}\hat{\theta}_{j_1} - f_j\hat{\theta}_j) \right\|_2^2 \\
&\approx \arg\max_j \left| f_j^\top r_1 \right|
\end{aligned}
$$

Matching pursuit feature selection rule [Lozano et al., 2011]

Assuming normalized data, i.e. $f_j^\top f_j = 1$, the OMP rule is given by

$$j_k = \arg\max_j \left| f_j^\top r_{k-1} \right|$$

where r_k are the kth pseudo-residuals

$$\begin{aligned} r_k &= y - \sigma(f_{j_1}\theta_{j_1} + f_{j_2}\theta_{j_2} + \cdots + f_{j_k}\theta_{j_k}) \\ X^\top r_p &= \nabla \log \mathrm{pr}_\theta(y) \end{aligned}$$

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OMP Performance

Greedy strategy causes poor performance of Orthogonal Matching Pursuit in practice

Least Angle Regression (LARS)

Least Angle Regression (LARS)

- Consider ℓ_1-penalized linear regression (LASSO) where

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

- There exists a regularization strength $\lambda = \lambda_{\max}$ for which all estimated coefficients are zero
- Least Angle Regression (LARS) [Efron et al., 2004] is a method to efficiently compute $\hat{\theta}(\lambda)$ for all $0 \leq \lambda \leq \lambda_{\max}$
- LARS computes breakpoints λ_k at which individual coefficients $\hat{\theta}_j(\lambda_k) \in \mathbb{R}$ change its value from
  - zero to non-zero, or from
  - non-zero to zero
- Between breakpoints the values of coefficients can be linearly interpolated

Least Angle Regression (LARS)

- Remember that the OLS solution $\hat{\theta}(0)$ for $\lambda = 0$ requires that

$$\nabla_\theta \|y - X\theta\|_2^2 = 2X^\top(y - X\theta) = 0$$

- For $\lambda > 0$ the solution requires

$$X^\top(y - X\theta) \in \frac{\lambda}{2}\partial \|\theta\|_1$$

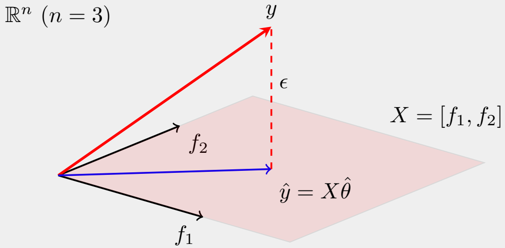
where $\partial \|\theta\|_1$ is the subgradient with respect to θ

- We define

$$c(\theta) = X^\top(y - X\theta)$$

which is interpreted as the correlation of features $X = [f_1, f_2, \dots, f_p]$ with the residuals $\epsilon = y - X\theta$

- The correlation $\hat{c}(\lambda) = c(\hat{\theta}(\lambda))$ varies with λ as follows:
  - $\hat{c}(\lambda) = c_{\max}$ for $\lambda = \lambda_{\max}$
  - $\hat{c}(\lambda) = 0$ for $\lambda = 0$



Least Angle Regression (LARS)

- LARS maintains a set of active features $\Omega \subset \{1, \ldots, p\}$ all equally correlated with the residuals $y - X\hat{\theta}(\lambda)$ for the current estimate $\hat{\theta}(\lambda)$
- Let $X_\Omega = (f_j)_{j \in \Omega}$ denote the covariate matrix and $\theta_\Omega = (\theta_j)_{j \in \Omega}$ the coefficients restricted to the features in the active set Ω
- In each iteration, the coefficients θ are updated

$$\theta \leftarrow \theta + \gamma^* v \,,$$

where γ^* is the amount by which the correlation $c_\Omega(\theta)$ is reduced and $v \in \mathbb{R}^p$ defines the direction and relative size of the update

- The vector v is selected so that for features in Ω the difference in correlation $c_\Omega(\theta) - c_\Omega(\theta + \gamma v)$ shrinks uniformly towards zero with rate γ, i.e.

$$c_\Omega\ (\theta) - c_\Omega\ (\theta + \gamma v) = \gamma \operatorname{sign} c_\Omega(\theta)\,, \quad \text{while}$$
$$c_{\Omega^c}(\theta) - c_{\Omega^c}(\theta + \gamma v) = 0\,.$$

- Both conditions can be combined into

$$c(\theta) - c(\theta + \gamma v) = \gamma \operatorname{sign} c(\theta)\,,$$

since $\operatorname{sign} c_{\Omega^c}(\theta) = 0$

- It follows that

$$v_\Omega = [X_\Omega^\top X_\Omega]^{-1} \operatorname{sign} c_\Omega(\theta)$$

and $v_{\Omega^c} = 0$

- LARS stop shrinking the correlations whenever:
  - Case 1: A non-active feature becomes equally correlated with the residuals
  - Case 2: A coefficient of an active feature becomes zero[1]
- Case 1: More formally, γ is increased until some feature $j' \in \Omega^c$ outside the active group satisfies

$$
\begin{aligned}
|c_{j'}(\theta + \gamma v)| &= |c_j(\theta + \gamma v)| \\
&= \lambda - \gamma \,,
\end{aligned}
$$

where $j \in \Omega$, and $\lambda = |c_j(\theta)|$ is the absolute correlation of the active features

[1] This case was not part of the initial LARS algorithm but was later on added in order to ensure equivalence with the LASSO (see also Homotopy algorithm [Osborne et al., 2000])

- The solution is given by

$$\gamma^{+} = \min_{j\in\Omega^c}{}^{+} \left\{ \frac{\lambda - c_j(\theta)}{1 - f_j^\top X v}, \frac{\lambda + c_j(\theta)}{1 + f_j^\top X v} \right\} ,$$

  where $\min^{+}$ is the minimum over positive elements and note that $f_j^\top X v = f_j^\top X_\Omega v_\Omega$

- Case 2: The algorithm also removes a feature j from the active set when for some γ

$$\theta_j + \gamma v_j = 0$$

  so that $\gamma^{-} = \min_{j\in\Omega}\{-\theta_j / v_j\}$

- The subsequent breakpoint is given by $\gamma^* = \min\{\gamma^{+}, \gamma^{-}\}$

SAFE and Strong Rules

Penalized regression

$$\omega(\theta) = -\log \mathrm{pr}_\theta(y) \qquad \text{(logistic regression), or}$$
$$\omega(\theta) = \|y - X\theta\|_2^2 \qquad \text{(linear regression)}$$

$$\hat{\theta} = \begin{cases} \arg\min_\theta & \omega(\theta) \\ \text{subject to} & \|\theta\|_1 = \Lambda \end{cases}$$

Basic idea: Select Λ such that $\|\theta\|_0 = m$

Numerical solution of penalized regression

Identify saddle points of Lagrangian

$$\mathcal{L}(\theta, \lambda) = \omega(\theta) + \lambda(\|\theta\|_1 - \Lambda)$$

Numerical solution of penalized regression

Identify saddle points of Lagrangian

$$\mathcal{L}(\theta, \lambda) = \omega(\theta) + \lambda(\|\theta\|_1 - \Lambda)$$

In practice the constraint $\|\theta\|_1 = \Lambda$ is ignored, but λ is chosen such that classification performance is optimal:

Penalized regression in practice

$$\hat{\theta}(\lambda) = \arg\min_{\theta} \omega(\theta) + \lambda \|\theta\|_1$$

SAFE rule: What features can we neglect for a fixed λ?

SAFE Rule for linear regression

SAFE rule: What features can we neglect for a fixed λ?

SAFE rule [Ghaoui et al., 2010, Kim et al., 2007] for ℓ_1-penalized linear regression

jth component of $\hat{\theta}$ must be zero if

$$|f_j^\top y| < \lambda - \|f_j\|_2 \|y\|_2 \frac{\lambda_{\max} - \lambda}{\lambda_{\max}}$$

$$\lambda_{\max} = \max_j |f_j^\top y|$$

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$$\lambda_{\max} = \max_j |f_j^\top y|$$

$$|f_j^\top (y - \underbrace{X\theta}_{\theta=0})| < \lambda - \|f_j\|_2 \|y\|_2 \frac{\lambda_{\max} - \lambda}{\lambda_{\max}}$$

SAFE rule for linear regression: jth component of $\hat{\theta}$ must be zero if

$$|f_j^\top y| < \lambda - \|f_j\|_2 \|y\|_2 \frac{\lambda_{\max} - \lambda}{\lambda_{\max}}$$

$$\lambda_{\max} = \max_j |f_j^\top y|$$

Strong rule for ℓ_1-penalized linear regression [Tibshirani et al., 2012]

Discard jth component if

$$|f_j^\top y| < \lambda - (\lambda_{max} - \lambda) = 2\lambda - \lambda_{max}$$

$$\lambda_{\max} = \max_j |f_j^\top y|$$

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$$\lambda_{\max} = \max_j |f_j^\top y|$$

Remark

Strong rule may drop features that should not be discarded $\Rightarrow$ KKT conditions must be checked, i.e.

$$X^\top(y - X\hat{\theta}) \in \lambda \partial_{\theta=\hat{\theta}} \|\theta\|_1$$

Strong rule for ℓ_1-penalized linear regression [Tibshirani et al., 2012]

Discard jth component if

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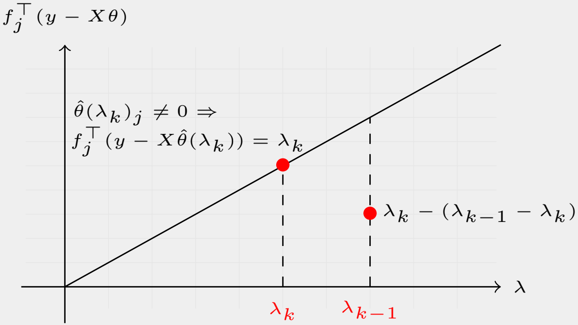
$$\lambda_{\max} = \max_j |f_j^\top y|$$

Strong sequential rule for ℓ_1-penalized linear regression[Tibshirani et al., 2012]

Discard jth feature if

$$|f_j^\top \{y - \sigma(X\hat{\theta}(\lambda_{k-1}))\}| < 2\lambda_k - \lambda_{k-1}$$

Compute $\hat{\theta}(\lambda_k)$ for all $\lambda_1 > \cdots > \lambda_k > \cdots > \lambda_K$



$$\text{Assumption}: |f_j^\top(y - X\hat{\theta}(\lambda_{k-1} - \epsilon)) - f_j^\top(y - X\hat{\theta}(\lambda_{k-1}))| \leq \epsilon$$
$$\Rightarrow |f_j^\top(y - X\hat{\theta}(\lambda_{k-1}))| < 2\lambda_k - \lambda_{k-1}$$

References I

Boyd, S. and Vandenberghe, L. (2004).
Convex optimization.
Cambridge university press.

Defazio, A., Bach, F., and Lacoste-Julien, S. (2014).
Saga: A fast incremental gradient method with support for non-strongly convex composite objectives.
Advances in neural information processing systems, 27.

Efron, B., Hastie, T., Johnstone, I., Tibshirani, R., et al. (2004).
Least angle regression.
The Annals of statistics, 32(2):407–499.

Fan, J. and Lv, J. (2008).
Sure independence screening for ultrahigh dimensional feature space.
Journal of the Royal Statistical Society: Series B (Statistical Methodology), 70(5):849–911.

References II

Fan, J. and Song, R. (2010).
Sure independence screening in generalized linear models with NP-dimensionality.
The Annals of Statistics, 38(6):3567–3604.

Ghaoui, L. E., Viallon, V., and Rabbani, T. (2010).
Safe feature elimination for the lasso and sparse supervised learning problems.
arXiv preprint arXiv:1009.4219.

Hastie, T., Tibshirani, R., and Friedman, J. (2009).
The elements of statistical learning: data mining, inference, and prediction.
Springer Science & Business Media.

Kim, S.-j., Koh, K., Lustig, M., Boyd, S., and Gorinevsky, D. (2007).
An interior-point method for large-scale ℓ1-regularized logistic regression.
In *Journal of Machine learning research*. Citeseer.

References III

Lozano, A., Swirszcz, G., and Abe, N. (2011).
Group orthogonal matching pursuit for logistic regression.
In *Proceedings of the fourteenth international conference on artificial intelligence and statistics*, pages 452–460. JMLR Workshop and Conference Proceedings.

Osborne, M. R., Presnell, B., and Turlach, B. A. (2000).
A new approach to variable selection in least squares problems.
IMA journal of numerical analysis, 20(3):389–403.

Tibshirani, R., Bien, J., Friedman, J., Hastie, T., Simon, N., Taylor, J., and Tibshirani, R. J. (2012).
Strong rules for discarding predictors in lasso-type problems.
Journal of the Royal Statistical Society: Series B (Statistical Methodology), 74(2):245–266.

References IV

Tropp, J., Gilbert, A. C., et al. (2007).
Signal recovery from partial information via orthogonal matching pursuit.
IEEE Trans. Inform. Theory, 53(12):4655–4666.

Derivation of the SAFE Rule for linear regression

$$\hat{\theta} = \arg\min_{\theta} \|y - X\theta\|_2^2 + \lambda \|\theta\|_1$$

Define

$$\beta = y - X\theta$$

Equivalent optimization problem

$$\hat{\theta} = \begin{cases} \arg\min_{\theta} & \beta^\top \beta + \lambda \|\theta\|_1 \\ \text{subject to} & \beta = y - X\theta \end{cases}$$

Derivation of the SAFE Rule for linear regression

Lagrangian

$$\mathcal{L}(\theta,\beta,\nu) = \beta^\top\beta + \lambda\,\|\theta\|_1 + \nu^\top(y - X\theta - \beta)$$

Dual function

$$\inf_{\theta,\beta}\mathcal{L}(\theta,\beta,\nu) = \begin{cases} G(\nu) & \text{if } |f_j^\top\nu| \le \lambda\,,\ j = 1,\ldots,p \\ -\infty & \text{otherwise} \end{cases}$$

where $G(\nu) = -\frac{1}{4}\nu^\top\nu + \nu^\top y$. Lagrange dual

$$\hat{\theta}^* = \begin{cases} \arg\max_{\nu} & G(\nu) \\ \text{subject to} & |f_j^\top\nu| \le \lambda\,,\ j = 1,\ldots,p \end{cases}$$

Derivation of the SAFE Rule for linear regression

Side note: Since the primal problem satisfies Slater's condition, we know that the duality gap $\gamma = \hat{\theta} - \hat{\theta}^*$ is zero, i.e.

$$\hat{\theta} = \hat{\theta}^*$$

For a dual feasible point ν_0, we solve for each $j = 1, \ldots, p$

$$\begin{aligned}\xi_j(\nu_0) &= \begin{cases} \arg\max_{\nu} & |f_j^\top \nu| \\ \text{subject to} & G(\nu) \geq G(\nu_0) \end{cases} \\ &= |f_j^\top y| + \sqrt{(y^\top y - 2G(\nu_0)) f_j^\top f_j}\end{aligned}$$

If $\xi_j(\nu_0) < \lambda$ we know that $\hat{\theta}_j = 0$. A simple dual feasible point is $\nu_0 = y\lambda/\lambda_{max}$. The SAFE rule is obtained from

$$\xi_j(y\lambda/\lambda_{max}) < \lambda$$

Logistic Regression Classifier

SAGA algorithm [Defazio et al., 2014]: select $j \in \{1, \dots, n\}$ at random

$$\vartheta_{j,t+1} = \theta_t$$
$$\vartheta_{i,t+1} = \vartheta_{i,t+1} \text{ for all } i \neq j$$
$$\theta^*_{t+1} = \theta_t - \gamma \left[\nabla \ell_j(\vartheta_{j,t+1}) - \nabla \ell_j(\vartheta_{j,t}) + \frac{1}{n} \sum_{i=1}^{n} \nabla \ell_i(\vartheta_{i,t}) \right]$$
$$\theta_{t+1} = \arg\min_{\theta} \left\{ \lambda \|\theta\|_1 + \frac{1}{2\gamma} \|\theta - \theta^*_{t+1}\|_2^2 \right\}$$