Normalization for Class-Imbalanced Binary Features in Regularized Regression

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Presentation

- PhD student at Lund University (supervised by Jonas Wallin). As of September, post doc at Copenhagen University.
- Work so far: mostly computational optimization and algorithms for speeding up sparse regression.

This Talk

Topic

Normalization (scaling) of binary features in regularized regression

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Notes

- Not yet published (and partly work-in-progress)
- Joint work with Jonas Wallin

Overview

Preliminaries

General Setup

- Data consists of a fixed matrix of features $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ and a response vector $\boldsymbol{y} \in \mathbb{R}^n$.
- $\boldsymbol{y}$ comes from a linear model, that is,

$$y_i = \beta_0^* + \boldsymbol{x}_i^\intercal \boldsymbol{\beta}^* + \varepsilon_i \quad \text{for} \quad i \in 1, \ldots, n,$$

  where $\boldsymbol{\beta}^*$ is the vector of *true* coefficients.
- ε_i is the measurement noise, generated from some random variable

The Elastic Net

Linear regression plus a combination of the ℓ_1 and ℓ_2 penalties:

$$(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) = \underset{\beta_0 \in \mathbb{R}, \beta \in \mathbb{R}^p}{\arg\min} \left(\frac{1}{2} \|\boldsymbol{y} - \beta_0 - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \lambda_1 \|\boldsymbol{\beta}\|_1 + \frac{\lambda_2}{2} \|\boldsymbol{\beta}\|_2^2 \right).$$

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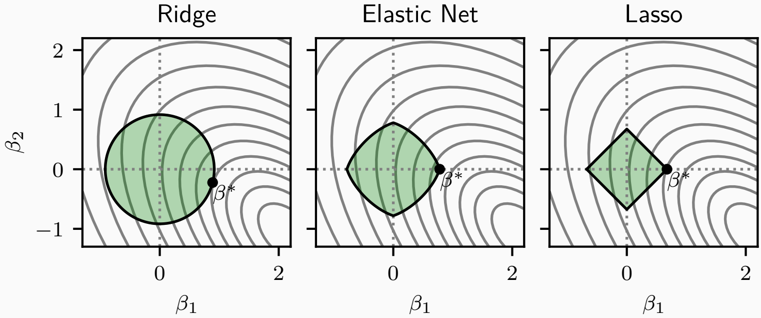

Figure 1: The elastic net penalty is a combination of the lasso and ridge penalties. Here shown as a constrained problem.

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- Common parametrization:

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  with $\alpha \in [0, 1]$.
- For each α, solve the elastic net over a sequence of λ: the **elastic net path**.

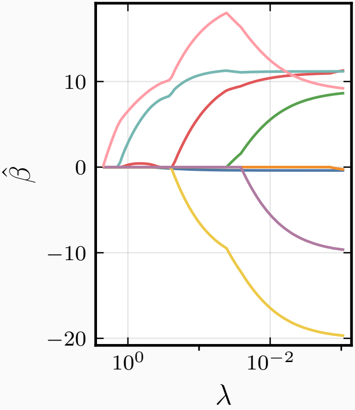

Figure 2: The elastic net path

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  - Mitigates lasso issue in correlated data
  - Better predictive performance when true signal is non-sparse
- Very efficient solvers for the full path (coordinate descent)

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Example

Assume

$$\boldsymbol{X} \sim \mathrm{Normal}\left(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}2 & 0\\0 & 1\end{bmatrix}\right), \qquad \boldsymbol{\beta}^* = \begin{bmatrix}\frac{1}{2}\\1\end{bmatrix}.$$

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Model	$\hat{\boldsymbol{\beta}}$	$\hat{\boldsymbol{\beta}}_{\text{std}}$
OLS	$\begin{bmatrix}0.50 & 1.00\end{bmatrix}^\intercal$	$\begin{bmatrix}1.00 & 1.00\end{bmatrix}^\intercal$
Lasso	$\begin{bmatrix}0.38 & 0.50\end{bmatrix}^\intercal$	$\begin{bmatrix}0.74 & 0.50\end{bmatrix}^\intercal$
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Large scale means less penalization because the size of β_j can be smaller for an equivalent effect (on $\boldsymbol{y}$).

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- Usage of key terms ambiguous in literature.
- After fitting, we transform the coefficients back to their original scale via

$$\hat{\beta}_j = \frac{\hat{\beta}_j^{(n)}}{s_j} \quad \text{for} \quad j = 1, 2, \dots, p.$$

Table 1: Common ways to normalize $\boldsymbol{X}$

Normalization	Centering (c_j)	Scaling (s_j)
Standardization	$\frac{1}{n}\sum_{i=1}^{n} x_{ij}$	$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2}$
Min–Max	$\min_i(x_{ij})$	$\max_i(x_{ij}) - \min_i(x_{ij})$
Unit Vector (L2)	0	$\sqrt{\sum_{i=1}^{n} x_{ij}^2}$
Max–Abs	0	$\max_i(\lvert x_{ij}\rvert)$
Adaptive Lasso	0	β_j^{OLS}

Motivation

The Type of Normalization Matters

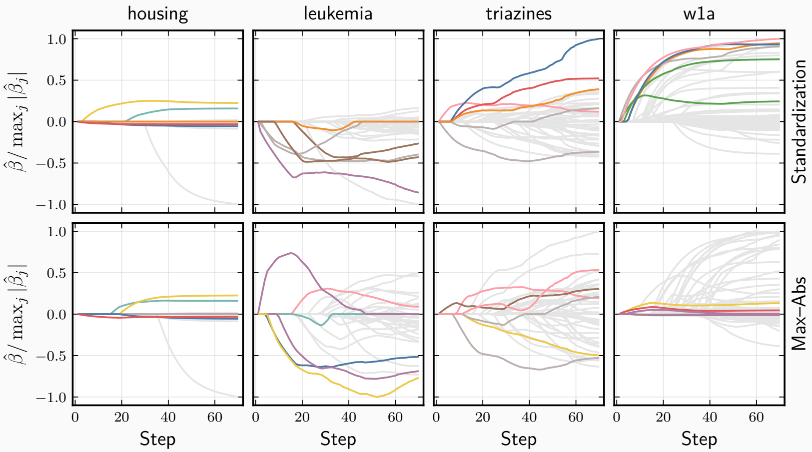

Figure 3: Lasso paths under two different types of normalization (standardization and max–abs normalization). The union of the first ten features selected in any of the schemes are colored.

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- Everyone agrees that you need to normalize (for most data), but how to do so is not discussed and often motivated by being "standard".
- Documentation for popular machine learning packages advocate different normalization strategies when data is sparse.
- Consensus for approximately normal features but little discussion on binary features and choice seems domain-specific. (Statisticians standardize, machine learning people scale to $[0, 1]$ or $[-1, 1]$.)

Aims

We focus on the following aspects of normalization in the context of the elastic net:

- Binary features, particularly with respect to the class balance thereof
- A mix of binary and normally distributed features
- Interactions

Results

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then there is an explicit solution to the elastic net problem[1]:

$$\hat{\beta}_j = \frac{\mathrm{S}_{\lambda_1}\left(\tilde{\boldsymbol{x}}_j^\intercal \boldsymbol{y}\right)}{s_j\left(\tilde{\boldsymbol{x}}_j^\intercal \tilde{\boldsymbol{x}}_j + \lambda_2\right)},$$

where

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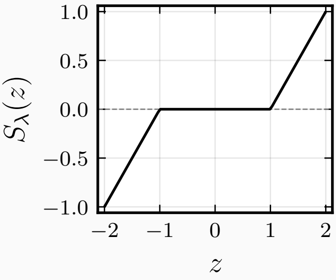

Figure 4: Soft thresholding

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Bias and Variance of the Elastic Net Estimator

The goal is computing the expected value of the elastic net estimator,

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since we treat $\boldsymbol{X}$ as fixed.

Letting $Z = \tilde{\boldsymbol{x}}^\intercal \boldsymbol{y}$ and assuming that ε_i is i.i.d. with mean zero and finite variance σ_ε^2, we have

$$\begin{aligned}
\operatorname{E} Z = \mu &= \operatorname{E}\left(\tilde{\boldsymbol{x}}_j^\intercal(\boldsymbol{x}_j\beta_j + \boldsymbol{\varepsilon})\right) = \tilde{\boldsymbol{x}}_j^\intercal \boldsymbol{x}_j \beta_j,\\
\operatorname{Var} Z = \sigma^2 &= \operatorname{Var}\left(\tilde{\boldsymbol{x}}_j^\intercal \boldsymbol{\varepsilon}\right) = \sigma_\varepsilon^2 \|\tilde{\boldsymbol{x}}_j\|_2^2.
\end{aligned}$$

Next, will will turn to $\operatorname{E} \operatorname{S}_{\lambda_1}(Z)$.

Bias of Soft-Thresholding

The expected value of the soft-thresholding estimator is

$$
\begin{aligned}
&\operatorname{E} \operatorname{S}_\lambda(Z) \\
&= \int_{-\infty}^{\infty} \operatorname{S}_\lambda(z) f_Z(z) \,\mathrm{d}z \\
&= \int_{-\infty}^{-\lambda} (z+\lambda) f_Z(z) \,\mathrm{d}z \\
&\quad + \int_{\lambda}^{\infty} (z-\lambda) f_Z(z) \,\mathrm{d}z.
\end{aligned}
$$

And so the bias of $\hat{\beta}_j$ is

$$\operatorname{E} \hat{\beta}_j - \beta_j^* = \frac{1}{d_j} \operatorname{E} \operatorname{S}_\lambda(Z) - \beta_j^*.$$

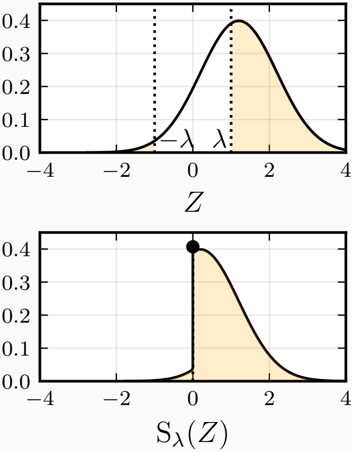

Figure 5: Distributions of Z and the its value after soft-thresholding.

Variance of Soft-Thresholding

The variance of the soft-thresholding estimator is

$$\operatorname{Var} S_\lambda(Z) = \int_{-\infty}^{-\lambda} (z+\lambda)^2 f_Z(z)\,\mathrm{d}z + \int_{\lambda}^{\infty} (z-\lambda)^2 f_Z(z)\,\mathrm{d}z - \left(\operatorname{E} \mathrm{S}_\lambda(Z)\right)^2$$

and consequently the variance of the elastic net estimator is therefore

$$\operatorname{Var} \hat{\beta}_j = \frac{1}{d_j^2} \operatorname{Var} \mathrm{S}_\lambda(Z).$$

Normally Distributed Noise

We now assume that $\varepsilon_i \sim \mathrm{Normal}\left(0, \sigma_\varepsilon^2\right)$, which means that

$$Z \sim \mathrm{Normal}\left(\tilde{\boldsymbol{x}}_j^\intercal \boldsymbol{x}_j \beta_j, \sigma_\varepsilon^2 \|\tilde{\boldsymbol{x}}_j\|_2^2\right).$$

Let $\theta = -\mu - \lambda_1$ and $\gamma = \mu - \lambda_1$. Then the expected value of soft-thresholding of Z is

$$\begin{aligned}
\mathrm{E}\,\mathrm{S}_{\lambda_1}(Z) &= \int_{-\infty}^{\frac{\theta}{\sigma}} (\sigma u - \theta)\,\phi(u)\,\mathrm{d}u + \int_{-\frac{\gamma}{\sigma}}^{\infty} (\sigma u + \gamma)\,\phi(u)\,\mathrm{d}u \\
&= -\theta\,\Phi\left(\frac{\theta}{\sigma}\right) - \sigma\,\phi\left(\frac{\theta}{\sigma}\right) + \gamma\,\Phi\left(\frac{\gamma}{\sigma}\right) + \sigma\,\phi\left(\frac{\gamma}{\sigma}\right)
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where $\phi(u)$ and $\Phi(u)$ are the pdf and cdf of the standard normal distribution, respectively.

Similar, but more complicated, expression can be derived for $\operatorname{Var} \operatorname{S}_{\lambda_1}(Z)$.

Binary Features

Let's say we have a binary feature $\boldsymbol{x}_j$, such that $x_{ij} \in \{0, 1\}$. Let $q \in [0, 1]$ be the class balance of this feature, that is: $q = \bar{\boldsymbol{x}}_j$.

In this case, we observe that

$$\tilde{\boldsymbol{x}}_j^\intercal \tilde{\boldsymbol{x}}_j = \frac{1}{s_j^2}(\boldsymbol{x}_j - \mathbf{1}c_j)^\intercal(\boldsymbol{x}_j - \mathbf{1}c_j) = \frac{1}{s_j^2}(nq - 2nq^2 + nq^2) = \frac{n(q - q^2)}{s_j^2},$$

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And consequently

$$\mu = \frac{\beta_j^* n(q - q^2)}{s_j}, \qquad \sigma^2 = \frac{\sigma_\varepsilon^2 n(q - q^2)}{s_j^2}, \qquad d_j = \frac{n(q - q^2)}{s_j} + \lambda_2 s_j.$$

Noiseless Case

In the noiseless case, we have

$$\hat{\beta}_j = \frac{\mathrm{S}_{\lambda_1}(\tilde{\boldsymbol{x}}^\intercal \boldsymbol{y})}{s_j\left(\tilde{\boldsymbol{x}}_j^\intercal \tilde{\boldsymbol{x}}_j + \lambda_2\right)} = \frac{\mathrm{S}_{\lambda_1}\left(\frac{\beta_j^* n(q-q^2)}{s_j}\right)}{s_j\left(\frac{n(q-q^2)}{s_j^2} + \lambda_2\right)}.$$

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- To remove the effect of q, an intuitive setting would be $s_j = q - q^2$ (the variance of $\boldsymbol{x}_j$) in the case of the lasso and $s_j = \sqrt{q - q^2}$ (the standard deviation of $\boldsymbol{x}_j$) in the case of the ridge.

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- Indicates there might be no (simple) s_j that will work for the elastic net.

Probability of Selection

Since $\boldsymbol{X}$ is fixed and ε is normal, it is straightforward to compute the probability of selection:

$$\Pr(\hat{\beta}_j \neq 0) = \Phi\left(\frac{\mu - \lambda_1}{\sigma}\right) + \Phi\left(\frac{-\mu - \lambda_1}{\sigma}\right).$$

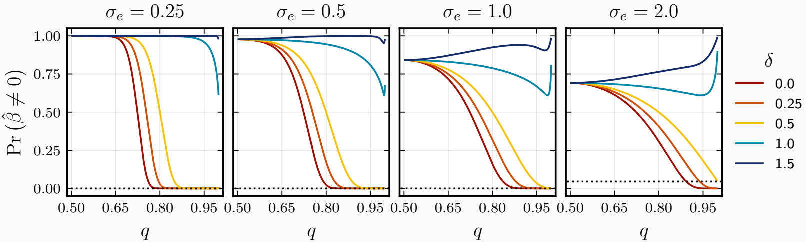


Figure 6: Probability that the elastic net selects a feature across different noise levels (σ_ε), types of normalization (δ), and class balance (q). The dashed line is asymptotic behavior for $\delta = 1/2$.

Asymptotic Results for Bias and Variance

Theorem

If $\boldsymbol{x}_j$ is a binary feature with class balance $q \in (0,1)$ and $\lambda_1, \lambda_2 \in (0, \infty)$, $\sigma_\varepsilon > 0$, and $s_j = (q - q^2)^\delta$, $\delta \geq 0$, then

$$\lim_{q \to 1^+} \mathrm{E}\, \hat{\beta}_j = \begin{cases} 0 & \textit{if } 0 \leq \delta < \frac{1}{2}, \\ \frac{2n\beta_j^*}{n+\lambda_2}\, \Phi\left(-\frac{\lambda_1}{\sigma_\varepsilon \sqrt{n}}\right) & \textit{if } \delta = \frac{1}{2}, \\ \beta_j^* & \textit{if } \delta \geq \frac{1}{2}. \end{cases}$$

Asymptotic Results for Bias and Variance

Theorem

If $\boldsymbol{x}_j$ is a binary feature with class balance $q \in (0,1)$ and $\lambda_1, \lambda_2 \in (0,\infty)$, $\sigma_\varepsilon > 0$, and $s_j = (q - q^2)^\delta$, $\delta \geq 0$, then

$$\lim_{q \to 1^+} \operatorname{E} \hat{\beta}_j = \begin{cases} 0 & \text{if } 0 \leq \delta < \frac{1}{2}, \\ \frac{2n\beta_j^*}{n+\lambda_2} \, \Phi\left(-\frac{\lambda_1}{\sigma_\varepsilon \sqrt{n}}\right) & \text{if } \delta = \frac{1}{2}, \\ \beta_j^* & \text{if } \delta \geq \frac{1}{2}. \end{cases}$$

and

$$\lim_{q \to 1^+} \operatorname{Var} \hat{\beta}_j = \begin{cases} 0 & \text{if } 0 \leq \delta < \frac{1}{2}, \\ \infty & \text{if } \delta \geq \frac{1}{2}. \end{cases}$$

A Bias–Variance Tradeoff

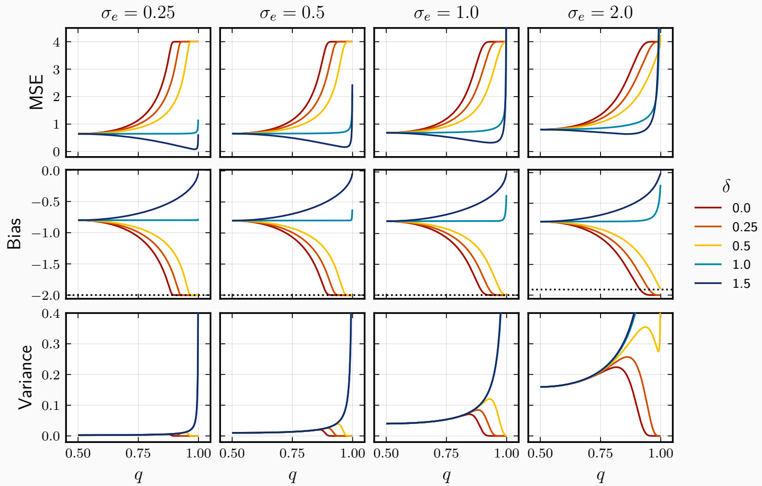
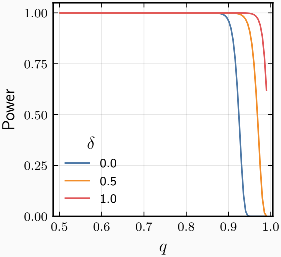


Figure 7: Bias, variance, and mean-squared error for a one-dimensional lasso problem. Theoretical result for orthogonal features. Dotted line is asymptotic result or $\delta = 1/2$.

Multiple Features: Power, FDR, and NMSE

Lasso example with 10 true signals and varying q and p.



(a) Power in the sense of detecting all the true signals. Constant p.

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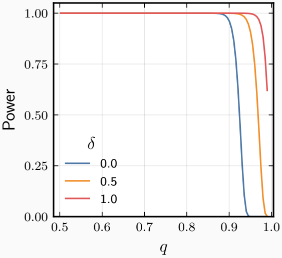

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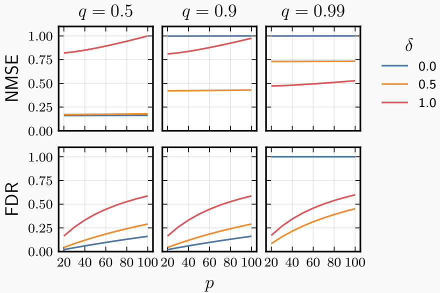

(b) False discovery rate (FDR) and normalized mean-squared error (NMSE).

Figure 8: Mean squared error (MSE), false discovery rate (FDR), and power.

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So far: all binary features. What about mixing binary and continuous (normal) features?

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Assume entries in $\boldsymbol{x}_1$ are binary and $\boldsymbol{x}_2$ come from a random variable X_2. The effects are comparable in the following cases:

- $X_2 \sim \mathrm{Normal}(\mu, 1/2)$, $\beta_1^* = 1$, and $\beta_2^* = 1$.
- $X_2 \sim \mathrm{Normal}(\mu, 2)$, $\beta_1^* = 1$, and $\beta_2^* = 0.25$.

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Additional Scaling

To account for this, we need to invoke additional scaling.

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We want $\hat{\beta}_1 = \hat{\beta}_2$. That is,

$$\underbrace{\frac{\mathrm{S}_{\lambda_1}\left(\frac{n(q-q^2)}{s_j}\right)}{s_1\left(\frac{n(q-q^2)}{s_1^2} + \lambda_2\right)}}_{\hat{\beta}_1} = \underbrace{\frac{\mathrm{S}_{\lambda_1}\left(\frac{n}{2}\right)}{\frac{1}{2}\left(n + \lambda_2\right)}}_{\hat{\beta}_2}.$$

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The choice $s_1 = (2(q - q^2))^\delta$ works when classes are balanced ($q = 0.5$). But no clear chocie for the elastic net case.

Experiments

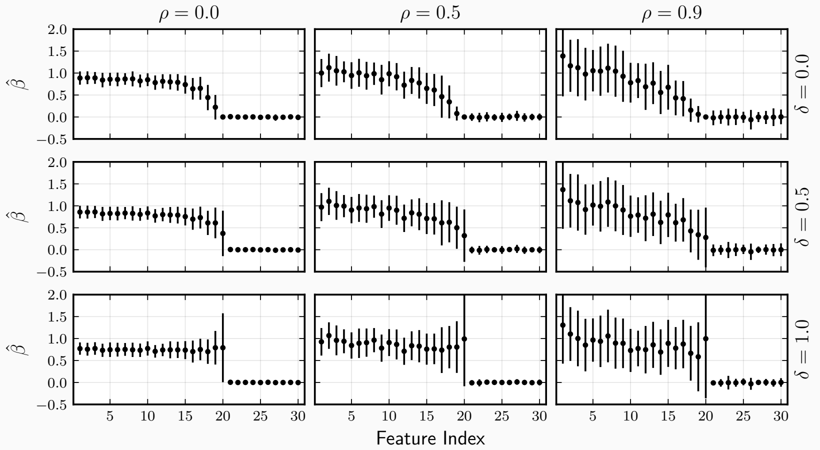

Figure 9: Lasso estimates for first 30 coefficients. First 20 features are true signals with a geometrically decreasing class balance from 0.5 to 0.99.

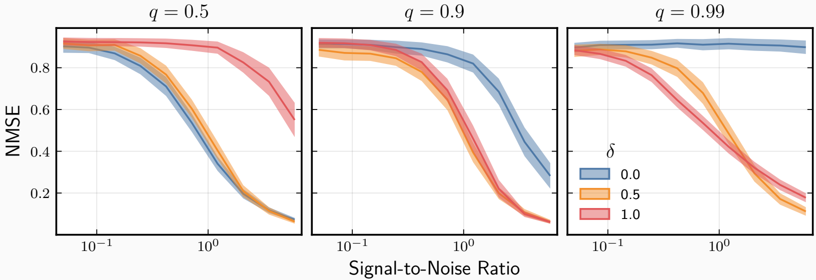

Figure 10: Normalized mean-squared test set error (NMSE).

Mixed Data

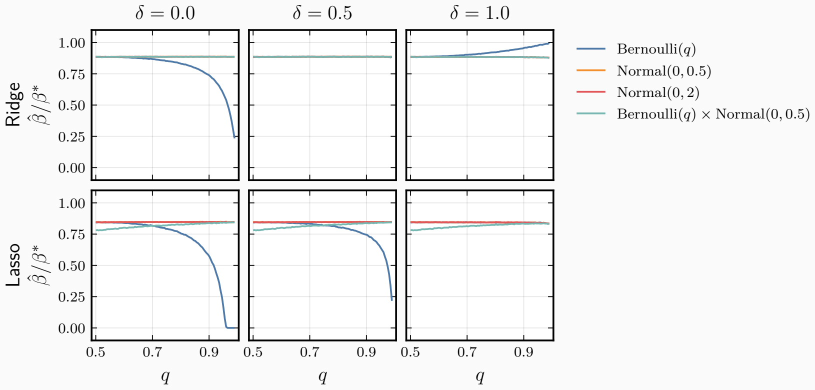

Figure 11: Comparison between lasso and ridge estimators for features generated to resemble features from various distributions.

Hyperparameter Optimization

Idea: The choice of δ affects the model, so let's optimize over it.

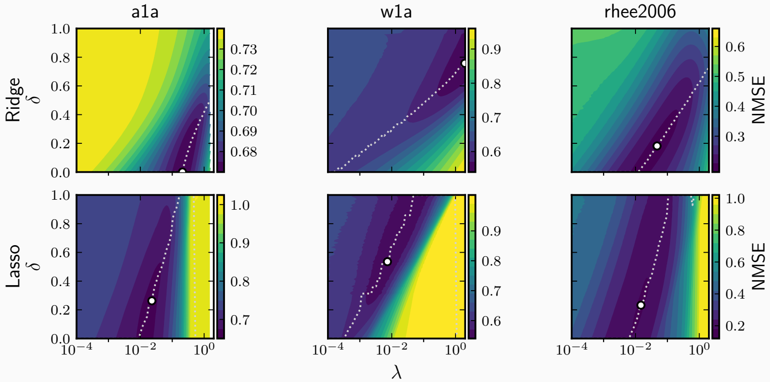

Figure 12: Contour plots of hold-out (validation set) error across a grid of δ and λ values for the lasso and ridge.

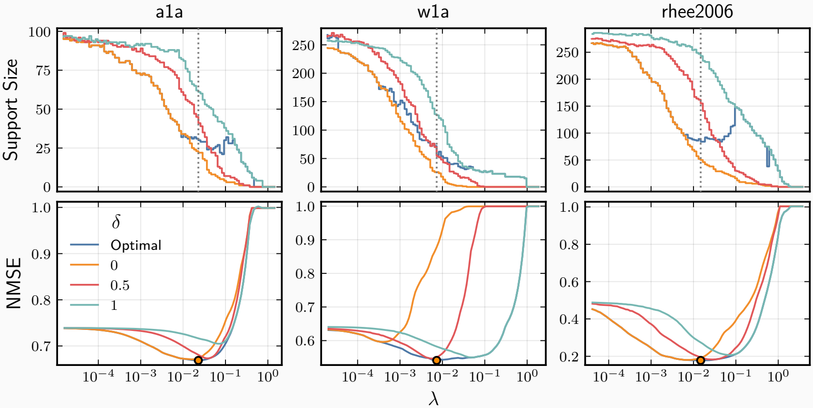

Figure 13: Support and NMSE of the lasso for different values of δ and λ.

Interaction Effects

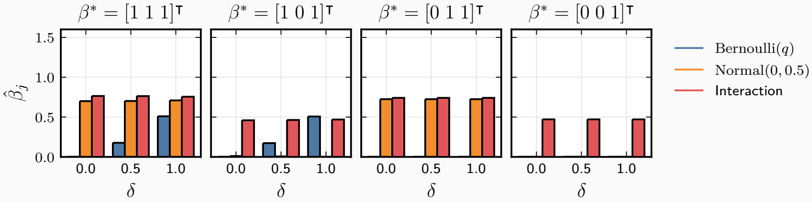

Figure 14: The effect of different normalization strategies for mixed data with interactions.

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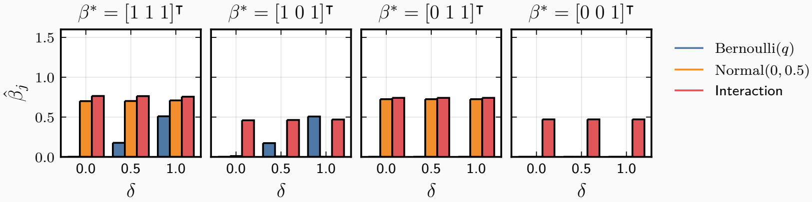

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Open Questions

- How to deal with features with different locations?
- Should the interaction features be normalized conditionally?

Conclusions

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- Class balance plays a crucial role for binary features.
- Effect depends on penalty
- Normalization mediates this effect at the cost of increased variance.
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Future Research

- Random $\boldsymbol{X}$
- Theory for $\boldsymbol{X}$ with correlation structure
- Non-Gaussian continuous features
- Other loss functions (GLMs, hinge loss, neural networks)
- Other penalties (group lasso, SCAD, MCP, SLOPE)

Thank you!

References i

El Ghaoui, Laurent, Vivian Viallon, and Tarek Rabbani (Sept. 21, 2010). *Safe Feature Elimination in Sparse Supervised Learning*. Technical report UCB/EECS-2010-126. Berkeley: EECS Department, University of California. URL: http://www.eecs.berkeley.edu/Pubs/TechRpts/2010/EECS-2010-126.html.

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Zou, Hui and Trevor Hastie (2005). “Regularization and Variable Selection via the Elastic Net”. In: *Journal of the Royal Statistical Society. Series B (Statistical Methodology)* 67.2, pp. 301–320. ISSN: 1369-7412. URL: www.jstor.org/stable/3647580 (visited on 03/12/2018).

Extras

Max–Abs Scaling of Continuous Features

- Min–max normalization is sometimes used in continuous data
- Very sensitive to outliers
- But also depend on sample size!
- In other words, results in model validation with varying sample sizes can yield very strange results.

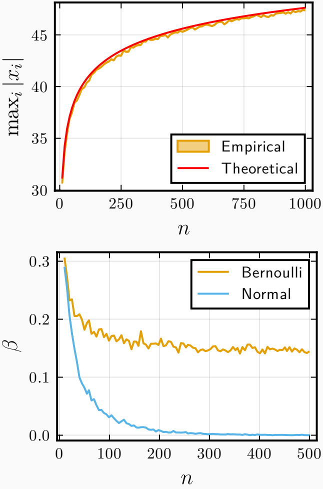

Figure 15: Effects of maximum absolute value scaling.