UNIVERSITY OF
COPENHAGEN

The Choice of Normalization Directly Affects Feature Selection in Regularized Regression

DSTS's Two-Day Meeting, Autumn 2024

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This Talk

Problem and Motivation

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Feature normalization has large effects in regularized regression (lasso, ridge) but there is no research on this.

Results

- Class balance has a normalization-dependent impact on the model.
- In mixed data, choice of normalization implictly weighs features' importances.

Figure 1: 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:

$$\boldsymbol{\beta}^* = \arg\min_{\beta \in \mathbb{R}^p} \left(\frac{1}{2} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|_2^2 + \underbrace{\lambda_1 \|\boldsymbol{\beta}\|_1}_{\text{lasso}} + \underbrace{\frac{\lambda_2}{2} \|\boldsymbol{\beta}\|_2^2}_{\text{ridge}} \right)$$

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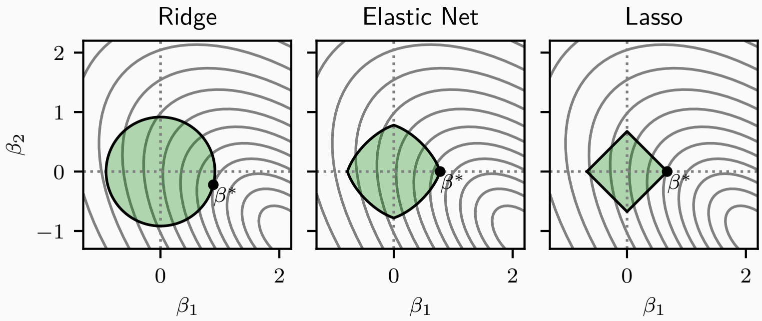


Figure 2: Elastic net is a combination of the lasso and ridge.

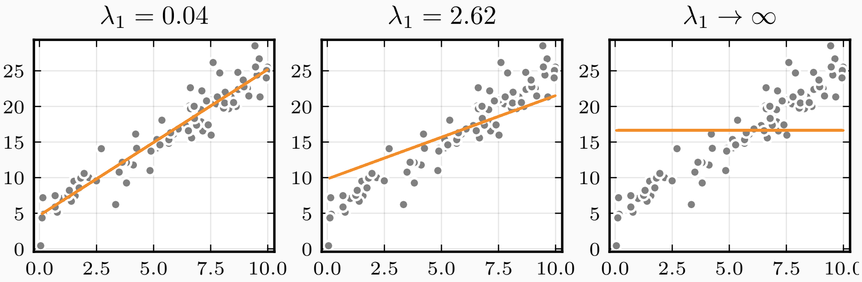
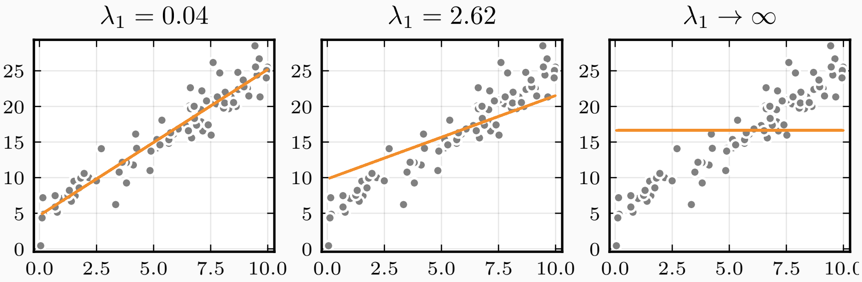


Figure 3: Regularization for a simple linear regression problem

Regularization



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- Uniqueness when $p \gg n$
- To overcome overfitting

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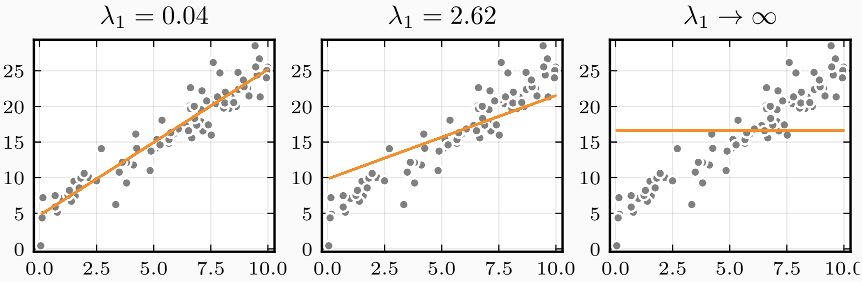

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Why Sparsity? (Lasso)

- Interpretability
- The sparsity bet

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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**.

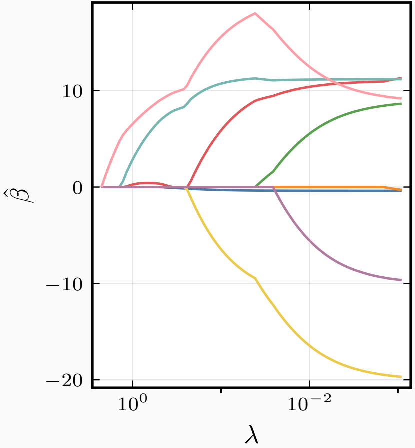

Figure 4: The elastic net path

Sensitivity to Scale

Lasso and ridge penalties are **norms**—feature scales matter!

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Example

Assume

$$\boldsymbol{X} \sim \mathrm{Normal}\left(\begin{bmatrix}0\\0\end{bmatrix}, \begin{bmatrix}4 & 0\\0 & 1\end{bmatrix}\right), \qquad \boldsymbol{\beta}^* = \begin{bmatrix}\frac{1}{2}\\1\end{bmatrix}.$$

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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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- After fitting, we transform the coefficients back to their original scale via

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

where $\hat{\beta}_j^{(n)}$ is a coefficient from the normalized problem.

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

Normalization	Centering (c_j)	Scaling (s_j)
Standardization	$\bar{x}_j = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$	$\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2}$
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 and Aims

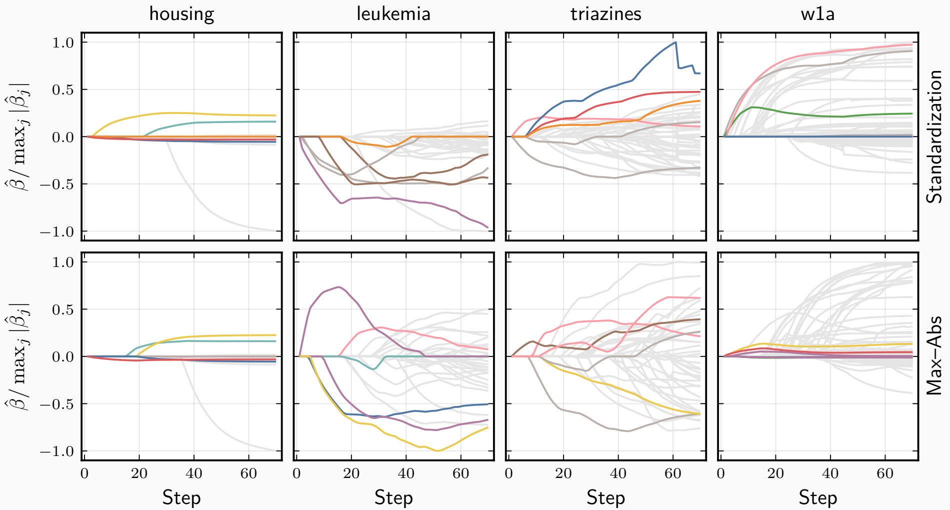

Figure 5: Normalization matters. Lasso paths under two different types of normalization (standardization and max–abs normalization). The union of the first ten features selected in any of the settings are colored.

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Aims

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

Results

Orthogonal Features

There is no explicit solution to the elastic net problem in general (unless $\lambda_1 = 0$).

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But if we assume that the features are orthogonal, that is

$$\tilde{\boldsymbol{X}}^\intercal \tilde{\boldsymbol{X}} = \operatorname{diag}(\tilde{\boldsymbol{x}}_1^\intercal \tilde{\boldsymbol{x}}_1, \dots, \tilde{\boldsymbol{x}}_p^\intercal \tilde{\boldsymbol{x}}_p),$$

then there is:[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

$$\mathrm{S}_\lambda(z) = \operatorname{sign}(z)\max(|z| - \lambda, 0).$$

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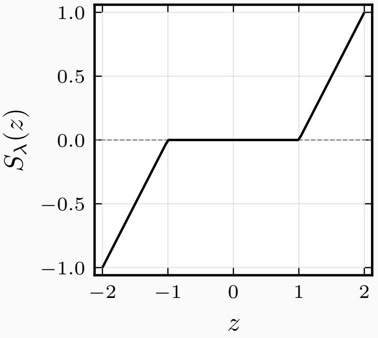

Figure 6: Soft thresholding

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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. Normally-distributed with mean zero and finite variance σ_ε^2, we have

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

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

Bias

The expected value of the soft-thresholding estimator is

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

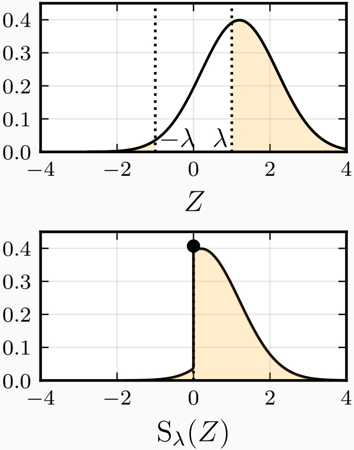

Figure 7: Distributions of Z and its value after soft-thresholding.

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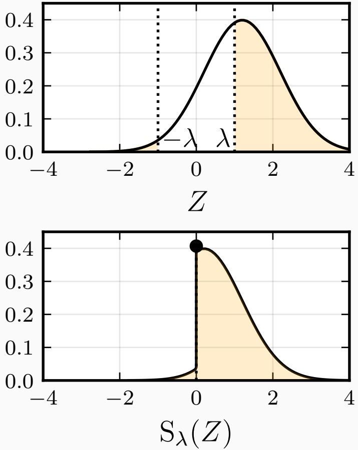
The bias of $\hat{\beta}_j$ is

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

where $d_j = s_j\,(\tilde{\boldsymbol{x}}_j^\intercal \tilde{\boldsymbol{x}}_j + \lambda_2)$.



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Variance

The variance of the soft-thresholding estimator is

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

and consequently the variance of the elastic net estimator is

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

Binary Features

Recall that

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

and assume 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

$$\|\tilde{\boldsymbol{x}}_j\|_2^2 = \frac{n(q - q^2)}{s_j^2},$$

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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 for Binary Features

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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which we will rely on for the rest of the talk.

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  which we will rely on for the rest of the talk.
- Indicates there might be no (simple) s_j that will work for the elastic net.

Probability of Selection

Since $\boldsymbol{X}$ is fixed and $\boldsymbol{\varepsilon}$ is normal, we can compute the probability of selection:

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

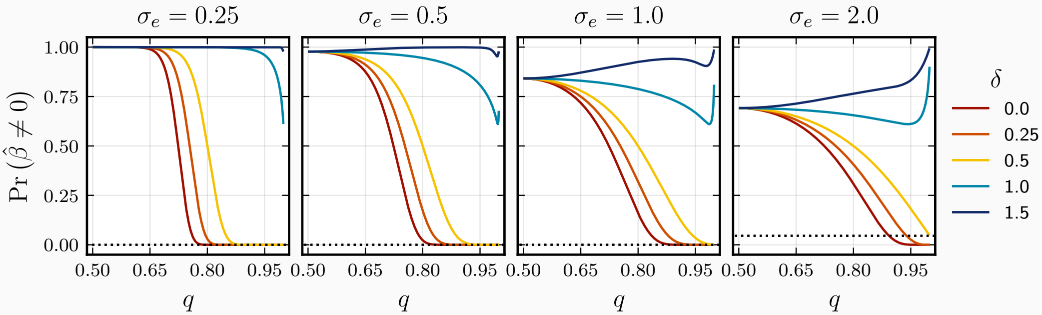

Figure 8: Probability that the elastic net selects a feature across different noise levels (σ_ε), types of normalization (δ), and class balance (q). The dashed line is asymptotic behavior for $\delta = 1/2$. Scaling used is $s_j \propto (q - q^2)^\delta$.

Implications

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Subgroup Data

Results become dependent on data colection.

Collecting more data with different class balances influences the results (since class balances change).

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

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

Asymptotic Results for Bias and Variance

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and

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

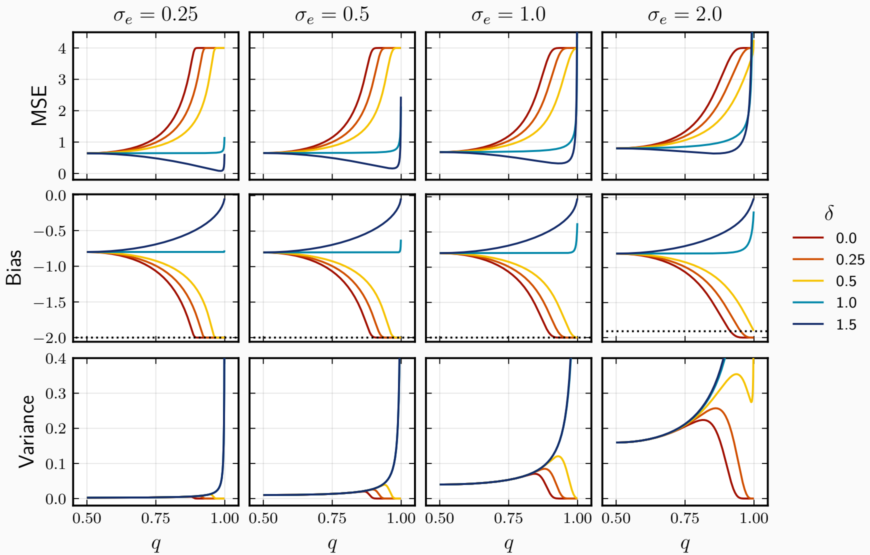
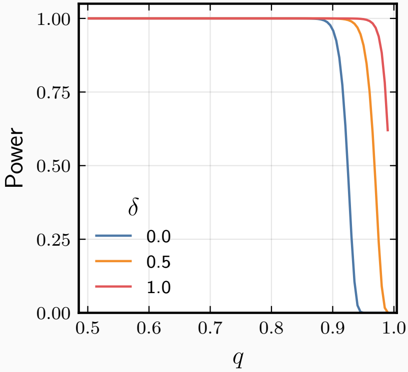
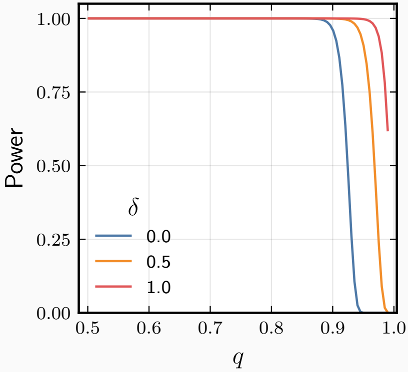


Figure 9: A bias variance tradeoff. Bias, variance, and mean-squared error for a one-dimensional lasso problem. Theoretical result for orthogonal features. Dotted line is asymptotic result or $\delta = 1/2$. Scaling used is $s_j \propto (q - q^2)^{\delta}$.



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

Figure 10: Multiple features: 10 true signals and varying q and p. Mean squared error (MSE), false discovery rate (FDR), and power



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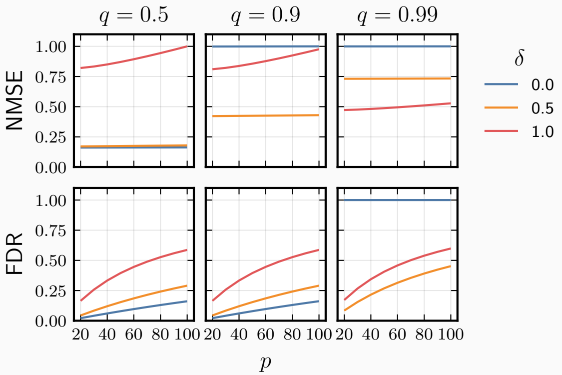

(b) False discovery rate (FDR) and normalized mean-squared error (NMSE).

Figure 10: Multiple features: 10 true signals and varying q and p. Mean squared error (MSE), false discovery rate (FDR), and power

Mixed Data

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

How to put binary features and normal features on the "same" scale?

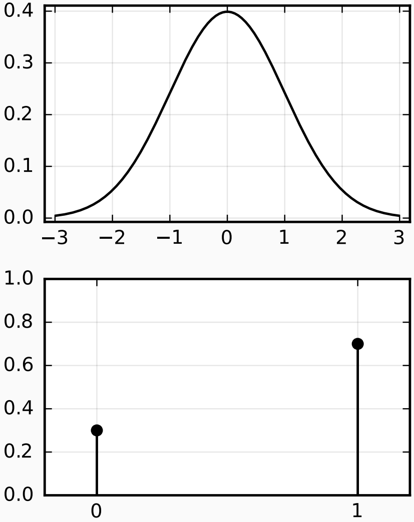

Figure 11: How do we match these?

Mixed Data

Our Definition of Comparability

The effects of a binary feature and a normally distributed feature are comparable if a flip in the binary feature has the same effect as a two-standard deviation change in the normal feature (Gelman 2008).

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Examples

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 $\beta_2^* = 0.25$.

Choice of Scaling in Mixed Data

For the two-standard deviation notion of comparability to hold, we need to modify our scaling factor s_j.

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As before, we assume that $\boldsymbol{x}_1$ is binary and $X_2 \sim \mathrm{Normal}(\mu, 1/2)$, $\beta_1^* = \beta_2^* = 1$ so that they have *comparable* effects. Also assume we standardize $\boldsymbol{x}_2$.

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 choice for the elastic net case.

Experiments

Binary Features (Decreasing q)

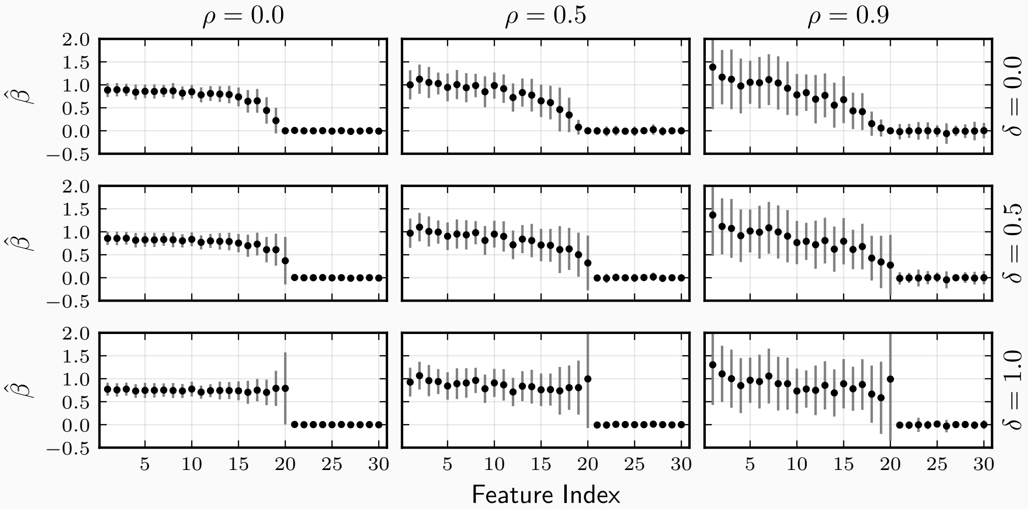

Figure 12: Lasso estimates for first 30 coefficients. First 20 features are true signals with a geometrically decreasing class balance from 0.5 to 0.99. ρ is a measure of autocorrelation.

Binary Features (Signal-to-Noise Ratio)

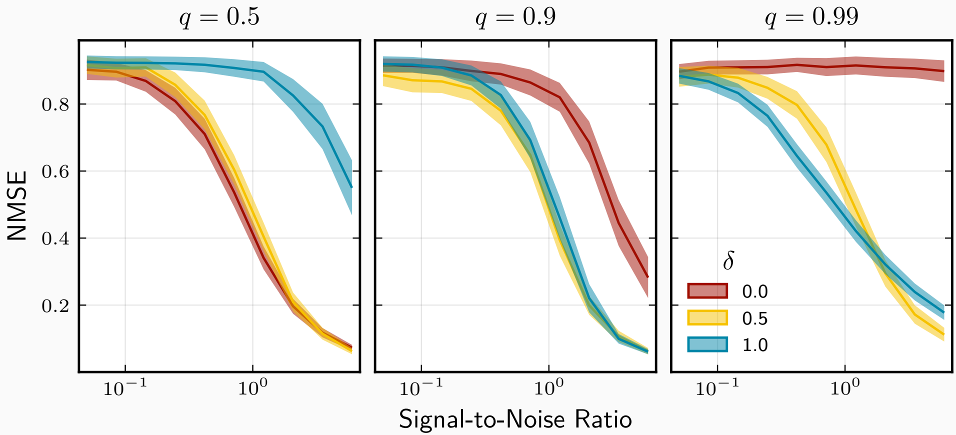

Figure 13: Normalized mean-squared test set error (NMSE).

Mixed Data

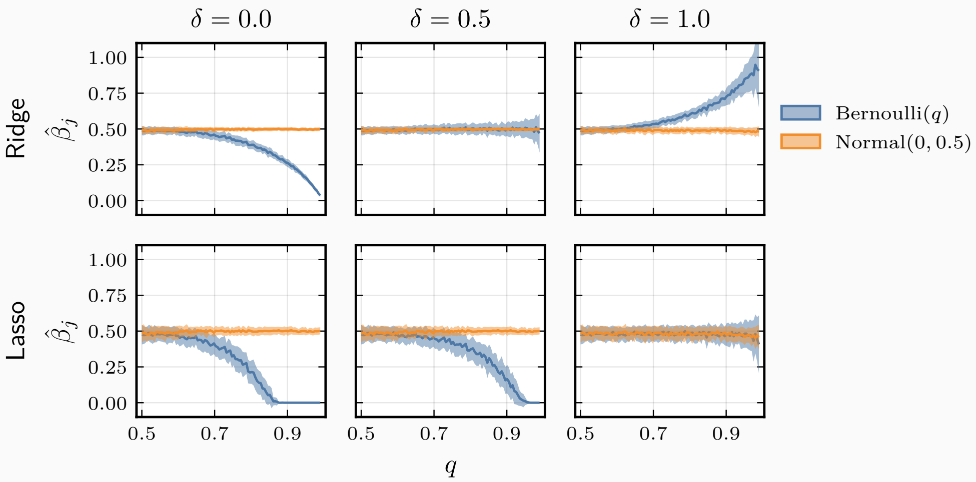

Figure 14: Comparison between lasso and ridge estimators for features generated to resemble features from various distributions.

Hyperparameter Optimization

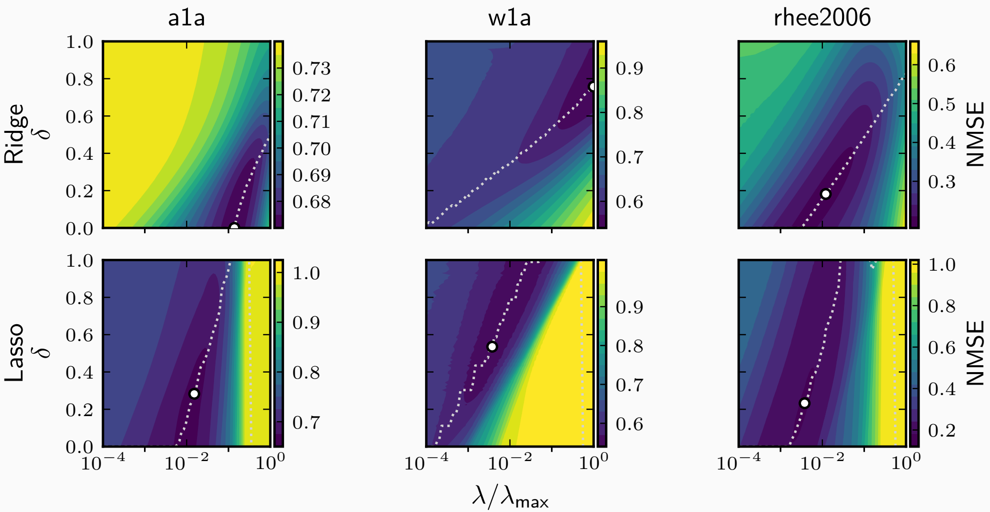

Figure 15: Contour plots of hold-out (validation set) error across a grid of δ and λ values for the lasso and ridge.

Summary

Conclusions

- Class balance plays a crucial role when using regularized regression on binary data.
- As far as we know the first paper to investigate the interplay between normalization and regularization
- New scaling approach to deal with class-imbalanced binary features
- Discussion and suggestions for dealing with mixed data

Summary

Conclusions

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- As far as we know the first paper to investigate the interplay between normalization and regularization
- New scaling approach to deal with class-imbalanced binary features
- Discussion and suggestions for dealing with mixed data

Limitations

- So far only theoretical results for limited cases:
  - Fixed data ($\boldsymbol{X}$), normal noise
  - Orthogonal features
  - Normal and binary features

Thank you!

- 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.
- Gelman, Andrew (July 10, 2008). "Scaling Regression Inputs by Dividing by Two Standard Deviations". In: *Statistics in Medicine* 27.15, pp. 2865–2873. ISSN: 02776715, 10970258. DOI: 10.1002/sim.3107. URL: https://onlinelibrary.wiley.com/doi/10.1002/sim.3107 (visited on 09/27/2023).
- Tibshirani, Robert et al. (Mar. 2012). "Strong Rules for Discarding Predictors in Lasso-Type Problems". In: *Journal of the Royal Statistical Society. Series B: Statistical Methodology* 74.2, pp. 245–266. ISSN: 1369-7412. DOI: 10/c4bb85. URL: https://iths.pure.elsevier.com/en/publications/strong-rules-for-discarding-predictors-in-lasso-type-problems (visited on 03/16/2018).

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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.

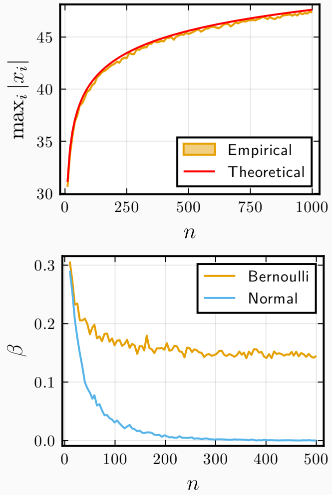

Figure 16: Effects of maximum absolute value scaling.

Hyperparameter Optimization (Support and NMSE)

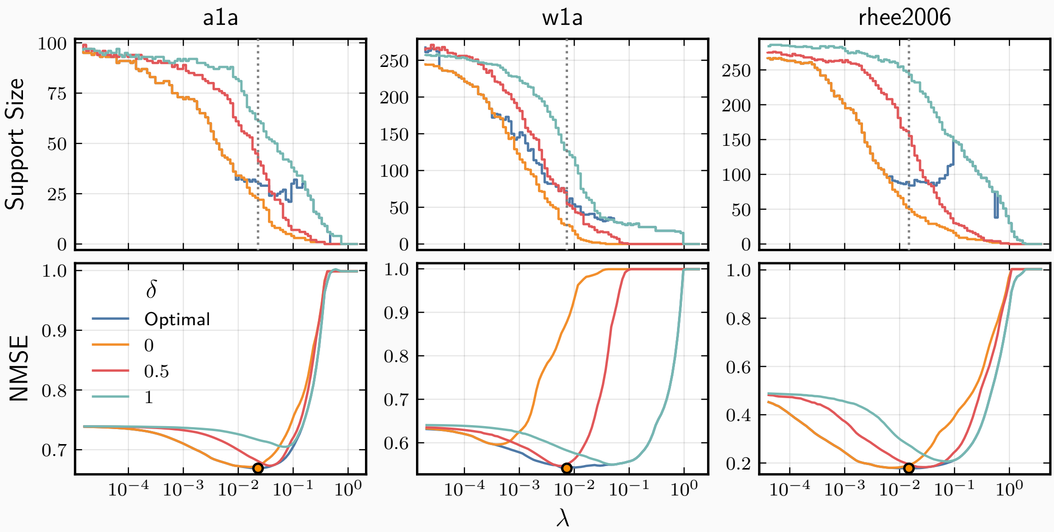

Figure 17: Support and NMSE of the lasso for different values of δ and λ.

Background on the Elastic Net

- Proposed by Zou and Hastie (2005).

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- Lasso (ℓ_1) part:
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- Ridge (ℓ_2) part
  - Mitigates lasso issue in correlated data
  - Better predictive performance when true signal is non-sparse