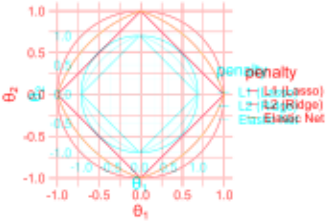
Introduction to Machine Learning

Regularization

Elastic Net and regularized GLMs



Learning goals

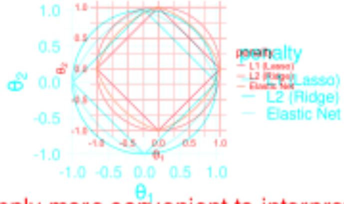
- Compromise between L1 and L2
- Regularized logistic regression

ELASTIC NET AS L1/L2 COMBO

▸ Zou and Hastie 2005

$$\mathcal{R}_{\text{elnet}}(\boldsymbol{\theta}) = \sum_{i=1}^{n}(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 + \lambda_1 \|\boldsymbol{\theta}\|_1 + \lambda_2 \|\boldsymbol{\theta}\|_2^2$$

$$= \sum_{i=1}^{n}(y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 + \lambda\left((1-\alpha)\|\boldsymbol{\theta}\|_1 + \alpha\|\boldsymbol{\theta}\|_2^2\right),\ \alpha = \frac{\lambda_2}{\lambda_1 + \lambda_2}, \lambda = \lambda_1 + \lambda_2$$



- 2nd formula is simply more convenient to interpret hyperpars; λ controls how much we penalize, α sets the "L2-portion"
- Correlated features tend to be either selected or zeroed out together
- Selection of more than n features possible for $p > n$

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SIMULATED EXAMPLE

5-fold CV with $n_{train} = 100$ and 20 repetitions with $n_{test} = 10000$ for setups:

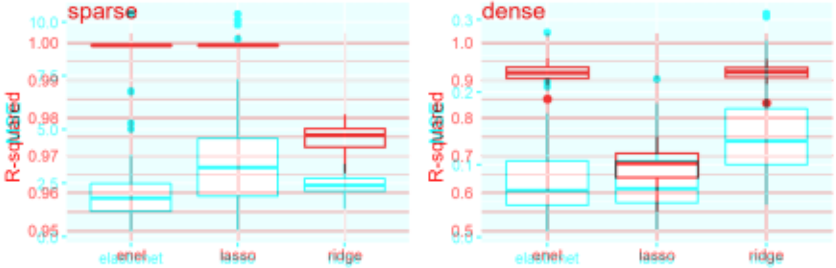
$y = \mathbf{x}^T\theta + \epsilon; \quad \epsilon \sim N(0, 0.1^2); \quad \mathbf{x} \sim N(0, \Sigma); \quad \Sigma_{k,l} = 0.8^{|k-l|}$:

Lasso better for sparse features:

$$\theta = (\underbrace{1, \ldots, 1}_{5}, \underbrace{0, \ldots, 0}_{495})$$

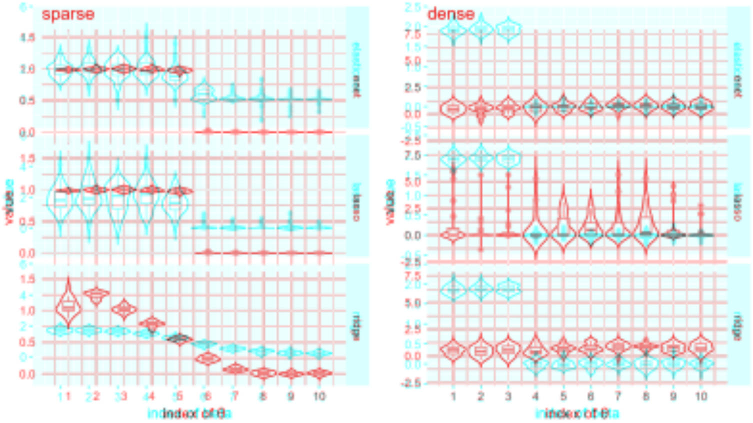
Ridge better for dense features:

$$\theta = (\underbrace{1, \ldots, 1, 1, \ldots, 1}_{500})$$



$\Longrightarrow$ elastic net handles both cases well

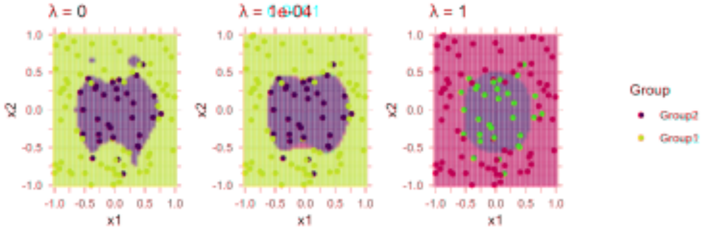
SIMULATED EXAMPLE / 2



- LHS: ridge estimates of noise features hover around 0 while lasso/e-net produce 0s.
- RHS: ridge cannot perform variable selection compared to lasso/e-net.
- Lasso more frequently ignores relevant features than e-net (longer tails in violin plot).

REGULARIZED LOGISTIC REGRESSION

- Penalties can be added very flexibly to any model based on ERM
- E.g.: $L1$- or $L2$-penalized logistic regression for high-dim. spaces and feature selection
- Now: LR with polynomial features for x_1, x_2 up to degree 7 and L2 penalty on 2D "circle data" below



- $\lambda = 0$: LR without penalty seems to overfit
- $\lambda = 0.0001$: We get better
- $\lambda = 1$: Fit looks pretty good