# MATH 567: Mathematical Techniques in Data Science
# Penalizing the coefficients

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# Shrinkage methods

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- Problem: difficult to solve (combinatorial optimization). Cannot be solved efficiently for a large number of variables.

# Shrinkage methods (cont.)

Relaxations of the previous approach:

2. Ridge regression/Tikhonov regularization:

$$\hat{\beta}^{\text{ridge}} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \left( \|y - X\beta\|_2^2 + \lambda \sum_{i=1}^{p} \beta_i^2 \right).$$

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- Penalty is a smooth function.
- Easy to solve (solution can be written in closed form).
- Generally does not set any coefficient to zero (no model selection).
- Can be used to "regularize" a rank deficient problem ($n < p$).

# Ridge regression: closed form solution

We have

$$\frac{\partial}{\partial \beta}\left(\|y - X\beta\|_2^2 + \lambda \sum_{i=1}^{p} \beta_i^2\right) = 2(X^T X\beta - X^T y) + 2\lambda\beta$$
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- When $\lambda = 0$ and $n > p$, we recover the usual least squares solution.
- Makes rigorous "adding a multiple of the identity" to $X^T X$.

# The Lasso

3. The Lasso (Least Absolute Shrinkage and Selection Operator):

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- Can be seen as a convex relaxation of the $\hat{\beta}^0$ problem.
- No closed form solution, but can solved efficiently using convex optimization methods.
- Performs well in practice.
- Very popular. Active area of research.

# Important model selection property

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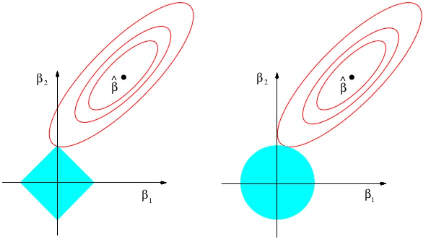


**FIGURE 3.11.** *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

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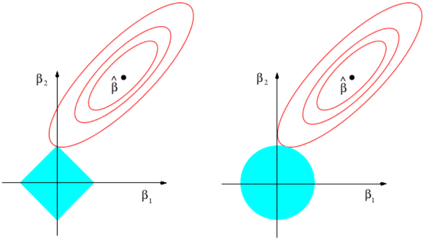


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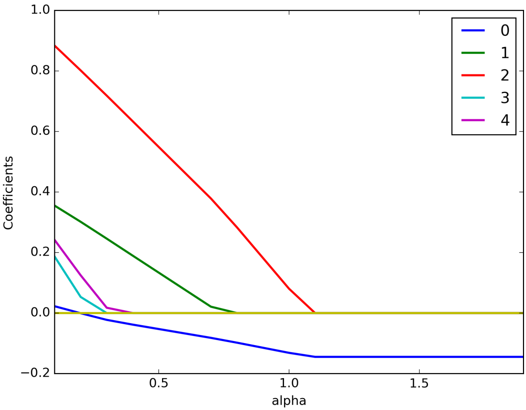
- Solutions are the intersection of the ellipses with the $\|\cdot\|_1$ or $\|\cdot\|_2$ balls. Corners of the $\|\cdot\|_1$ have zero coefficients.
- Likely to “hit” corners. Thus, the solution usually has many zeros.

**Note:** We usually do not penalize the intercept (variable "0" on the figure).



# Elastic net


Elastic net (Zou and Hastie, 2005)

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- Downside: Two parameters to choose instead of one (can increase the computational burden quite a lot in large experiments).

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**$K$-fold cross-validation:**

Split data into $K$ equal (or almost equal) parts/folds at random.
**for** each parameter $\lambda_i$ **do**
  **for** $j = 1, \ldots, K$ **do**
    Fit model on data with fold $j$ removed.
    Test model on remaining fold $\rightarrow$ $j$-th test error.
  **end for**
  Compute average test errors for parameter $\lambda_i$.
**end for**
Pick parameter with smallest average error.

# K-fold CV

More precisely,

- Split data into $K$ folds $F_1, \ldots, F_K$.

| 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|
| Train | Train | Validation | Train | Train |

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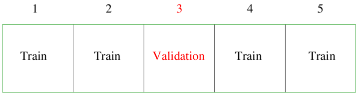


- Let $L(y, \hat{y})$ be a *loss function*. For example, $L(y, \hat{y}) = \|y - \hat{y}\|_2^2 = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$.

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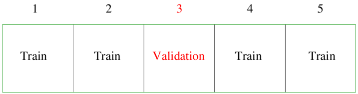


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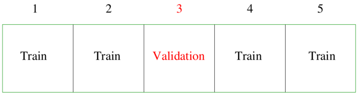


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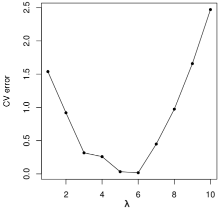
$$CV(\lambda) := \frac{1}{n} \sum_{k=1}^{n} \sum_{i \in F_k} L(y_i, f_\lambda^{-i}(\mathbf{x}_i))$$



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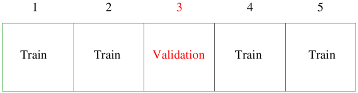


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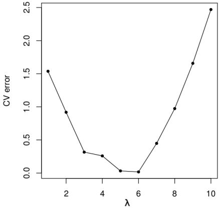


- Pick $\lambda$ among a *relevant* set of parameters

$$\hat{\lambda} = \underset{\lambda \in \{\lambda_1, \ldots, \lambda_m\}}{\operatorname{argmin}} CV(\lambda)$$

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- Typically: $50\%$ train, $25\%$ validate, $25\%$ test.
- Test data is "kept in a vault", i.e., not used for fitting or choosing the model.
- Other methods (e.g. AIC, BIC, etc.) can be used when working with very little data.

# Summary of the regression methods seen so far

1. Ordinary least squares (OLS)
    - Minimizes sum of squares.
    - Solution not unique when $n < p$.
    - Estimate unstable when the predictors are collinear.
    - Generally does not lead to best prediction error.

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    - Minimizes sum of squares.
    - Solution not unique when $n < p$.
    - Estimate unstable when the predictors are collinear.
    - Generally does not lead to best prediction error.
2. Ridge regression ($\ell_2$ penalty)
    - Regularized solution.
    - Estimator exists and is stable, even when $n < p$.
    - Easy to compute (add multiple of identity to $X^T X$).
    - Coefficients not set to zero (no model selection).

# Summary of the regression methods seen so far (cont.)

3. Subset selection methods (best subset, stepwise and stagewise approaches)
   - Generally leads to a favorable bias-variance trade-off.
   - Model selection. Leads to models that are easier to interpret and work with.
   - Can be computationally intensive (e.g. best subset can only be computed for small $p$)
   - Some of the approaches are greedy/less-rigorous.

# Summary of the regression methods seen so far (cont.)

3. Subset selection methods (best subset, stepwise and stagewise approaches)
   - Generally leads to a favorable bias-variance trade-off.
   - Model selection. Leads to models that are easier to interpret and work with.
   - Can be computationally intensive (e.g. best subset can only be computed for small $p$)
   - Some of the approaches are greedy/less-rigorous.
4. Lasso ($\ell_1$ penalty)
   - Shrinks and sets to zero the coefficients (shrinkage + model selection).
   - Generally leads to a favorable bias-variance trade-off.
   - Model selection. Leads to models that are easier to interpret and work with.
   - Can be efficiently computed.
   - Supporting theory. Active area of research.