Unit 2

Regularized regression: lasso, ridge and elastic net

Linear regression models and least squares

- The linear regression model has the form

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j,$$

  with input vector $X^T = (X_1, \ldots, X_p)$.
- The linear model assumes that $\mathrm{E}(Y|X)$ is linear or that the linear model is a reasonable approximation.
- The variables X_j can come from different sources:
  - quantitative inputs;
  - transformations of quantitative inputs;
  - basis expansions;
  - numeric or “dummy” coding of levels of qualitative inputs;
  - interactions between variables.

Linear regression models and least squares / 2

- The model is linear in the (unknown) parameters $\beta = (\beta_0, \beta_1, \ldots, \beta_p)$.
- Least squares estimation determines β by minimizing the residual sum of squares:

$$\begin{aligned} \text{RSS}(\beta) &= \sum_{i=1}^{N} (y_i - f(\boldsymbol{x}_i))^2 \\ &= \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2. \end{aligned}$$

  In matrix notation:

$$\text{RSS}(\beta) = (\boldsymbol{y} - \boldsymbol{X}\beta)^T (\boldsymbol{y} - \boldsymbol{X}\beta).$$

Linear regression models and least squares / 3

- Differentiating with respect to β gives:

$$\frac{\partial \text{RSS}}{\partial \beta} = -2\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{X}\beta),$$
$$\frac{\partial^2 \text{RSS}}{\partial \beta \partial \beta^T} = 2\boldsymbol{X}^T\boldsymbol{X}.$$

- Assuming that $\boldsymbol{X}$ has full column rank, $\boldsymbol{X}^T\boldsymbol{X}$ is positive definite and the unique solution is given by

$$\hat{\beta} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}.$$

Linear regression models and least squares / 4

- The predicted values are given by

$$\hat{\boldsymbol{y}} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} = \boldsymbol{H}\boldsymbol{y},$$

  with $\boldsymbol{H}$ the "hat"-matrix which orthogonally projects into the subspace spanned by the columns of $\boldsymbol{X}$.
- If $\boldsymbol{X}^T\boldsymbol{X}$ is singular, β is not uniquely determined, but the fitted values $\hat{\boldsymbol{y}}$ are.

Linear regression models and least squares / 5

- Assume

$$\boldsymbol{y} = \boldsymbol{X}\beta + \epsilon,$$

  with

  1. $\mathrm{E}(\epsilon) = 0$
  2. $\mathrm{Var}(\epsilon) = \sigma^2 \boldsymbol{I}$
  3. $\boldsymbol{X}$ deterministic with full column rank.

- Then:
  - The Gauss-Markov Theorem gives that the least squares estimator $\hat{\beta}$ is the best linear unbiased estimator (BLUE).
  - The variance of the estimator is:

$$\mathrm{Var}(\hat{\beta}) = \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}.$$

Linear regression models and least squares / 6

- Typically the variance σ^2 is estimated by

$$\hat{\sigma}^2 = \frac{1}{N-p-1}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2,$$

  to obtain an unbiased estimate.

- Adding the assumption:

  4. $\epsilon \sim N(0, \sigma^2 \boldsymbol{I})$

  gives

$$\hat{\beta} \sim N(\beta, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}),$$
$$(N-p-1)\hat{\sigma}^2 \sim \sigma^2\chi^2_{N-p-1},$$

  and $\hat{\beta}$ and $\hat{\sigma}^2$ are statistically independent.

Linear regression models and least squares / 7

- The t test statistic for the hypothesis test $\beta_j = 0$ is given by

$$t_j = \frac{\hat{\beta}_j}{\hat{\sigma}\sqrt{v_j}},$$

with v_j the jth diagonal element of $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$. Under the Gaussian assumption and the null hypothesis $\beta_j = 0$ t_j follows a t distribution with $N - p - 1$ degrees of freedom.

- This can also be used to construct $(1 - 2\alpha)$ confidence intervals for β_j by:

$$(\hat{\beta}_j - t_{N-p-1}^{(1-\alpha)}\sqrt{v_j}\hat{\sigma}, \hat{\beta}_j + t_{N-p-1}^{(1-\alpha)}\sqrt{v_j}\hat{\sigma}),$$

with $t_{N-p-1}^{(1-\alpha)}$ the $1 - \alpha$ quantile of the t distribution with $N - p - 1$ degrees of freedom.

Linear regression models and least squares / 8

- To compare two nested models, one calculates

$$F = \frac{(\text{RSS}_0 - \text{RSS}_1)/(p_1 - p_0)}{\text{RSS}_1/(N - p_1 - 1)},$$

with

  - RSS_1 being the residual sum-of-squares for the least squares fit of the bigger model with $p_1 + 1$ parameters, and
  - RSS_0 the same for the nested smaller model with $p_0 + 1$ parameters, having $p_1 - p_0$ parameters constrained to be zero.

Under the Gaussian assumption and that the smaller model is correct, the F statistic follows an F-distribution with $p_1 - p_0$ and $N - p_1 - 1$ degrees of freedom.

Estimation in R

The function for fitting a linear regression model in R is:

- The formula specifies the dependent variable as well as how the model matrix is created from the independent variables.
- Least squares estimation is performed using QR method.
- Regression coefficient estimates are identical to maximum likelihood estimates assuming that ϵ is normally distributed:

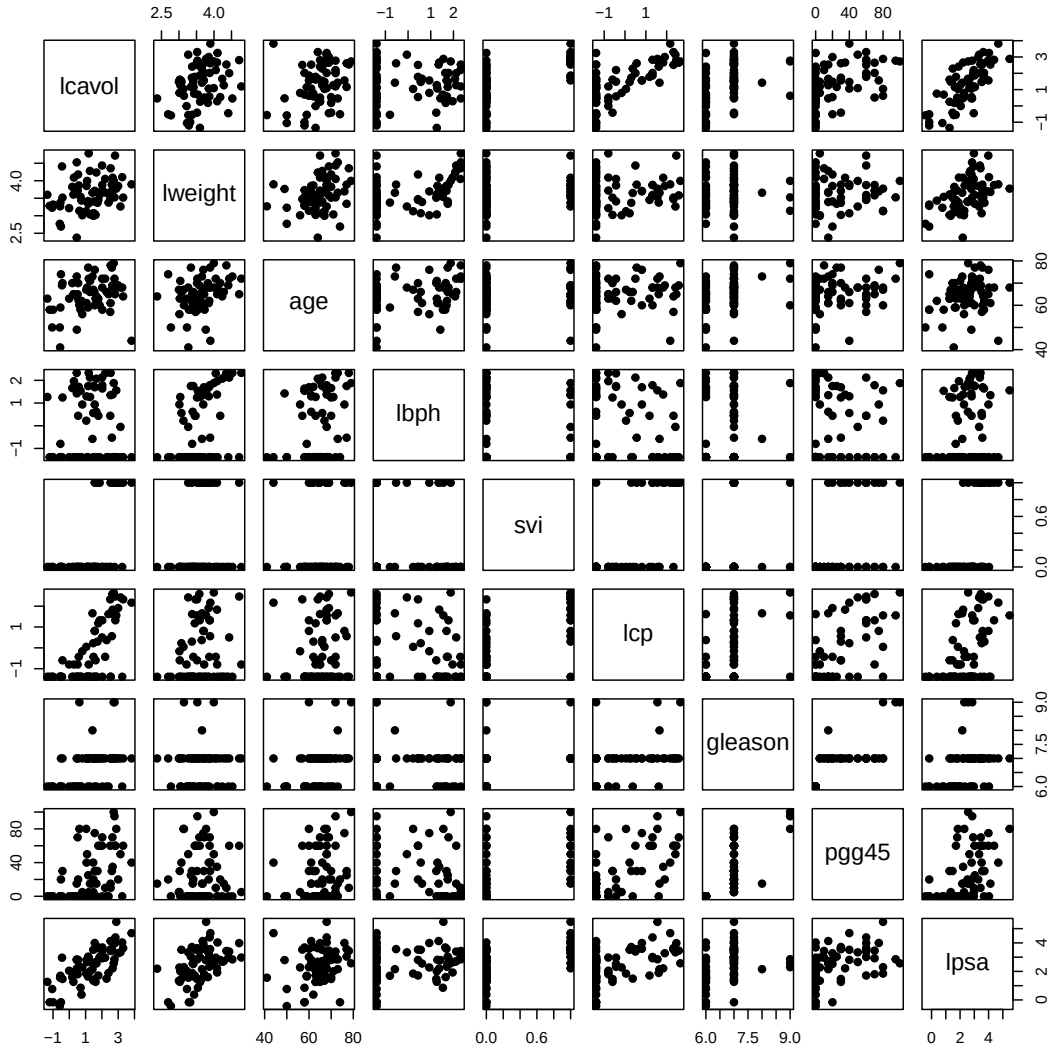
$$\epsilon \sim N(0, \sigma^2 \boldsymbol{I})$$

  Inference performed (e.g., using `summary()`) is based on this assumption.

Example: Prostate Cancer

- Data set provided in the R package **ElemStatLearn**.
- Use only the 67 observations from the training data set.
- The dependent variable is `lpsa`, the level of a prostate-specific antigen.
- The independent variables are clinical measures.
- There is a substantial amount of correlation between the clinical measures.
- The independent variables are standardized before fitting the linear model.

Example: Prostate Cancer / 2



Example: Prostate Cancer / 3

```
             Estimate Std. Error t value Pr(>|t|)
(Intercept)      2.45       0.09   28.18   <2e-16 ***
lcavol           0.72       0.13    5.37   <2e-16 ***
lweight          0.29       0.11    2.75     0.01 **
age             -0.14       0.10   -1.40     0.17
lbph             0.21       0.10    2.06     0.04 *
svi              0.31       0.13    2.47     0.02 *
lcp             -0.29       0.15   -1.87     0.07 .
gleason         -0.02       0.14   -0.15     0.88
pgg45            0.28       0.16    1.74     0.09 .
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘
```

Example: Prostate Cancer / 4

- Dropping the insignificant variables (`age`, `lcp`, `gleason`, `pgg45`) and comparing the two models using the F-test gives:

```
Analysis of Variance Table

Model 1: lpsa ~ (lcavol + lweight + age + lbph + svi + lcp +
    pgg45) - age - lcp - gleason - pgg45
Model 2: lpsa ~ lcavol + lweight + age + lbph + svi + lcp +
    pgg45
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     62 32.815
2     58 29.426  4    3.3886 1.6698 0.1693
```

- Prediction performance on the test dataset measured by the MSE:

```
base model   full model subset model
     1.057        0.521        0.456
```

Model / subset selection

- There are two reasons why least squares estimates are not satisfactory:
  - *Prediction accuracy*: Shrinking or setting coefficients zero might induce bias, but may improve prediction accuracy due to reduced variance.
  - *Interpretation*: Determining a small subset of predictors exhibiting the strongest effects allows to more easily discern important regressors.

Model / subset selection / 2

Strategies for choosing a subset:

- Best subset selection: possible for up to $p = 30$ or 40 using the efficient *leaps and bounds* procedure (Furnival and Wilson, 1974). Available for example in package **leaps** in R.
- Forward- and backward-stepwise selection: seek a good path through subsets of different size.
  - Forward selection starts with the intercept model and iteratively adds predictors which improve the model fit most.
  - Backward selection starts with the full model and iteratively removes the predictor which has the least impact on the fit.
  - Variables are iteratively added or removed. In each step the least squares coefficient estimates are determined for the current *active set*.

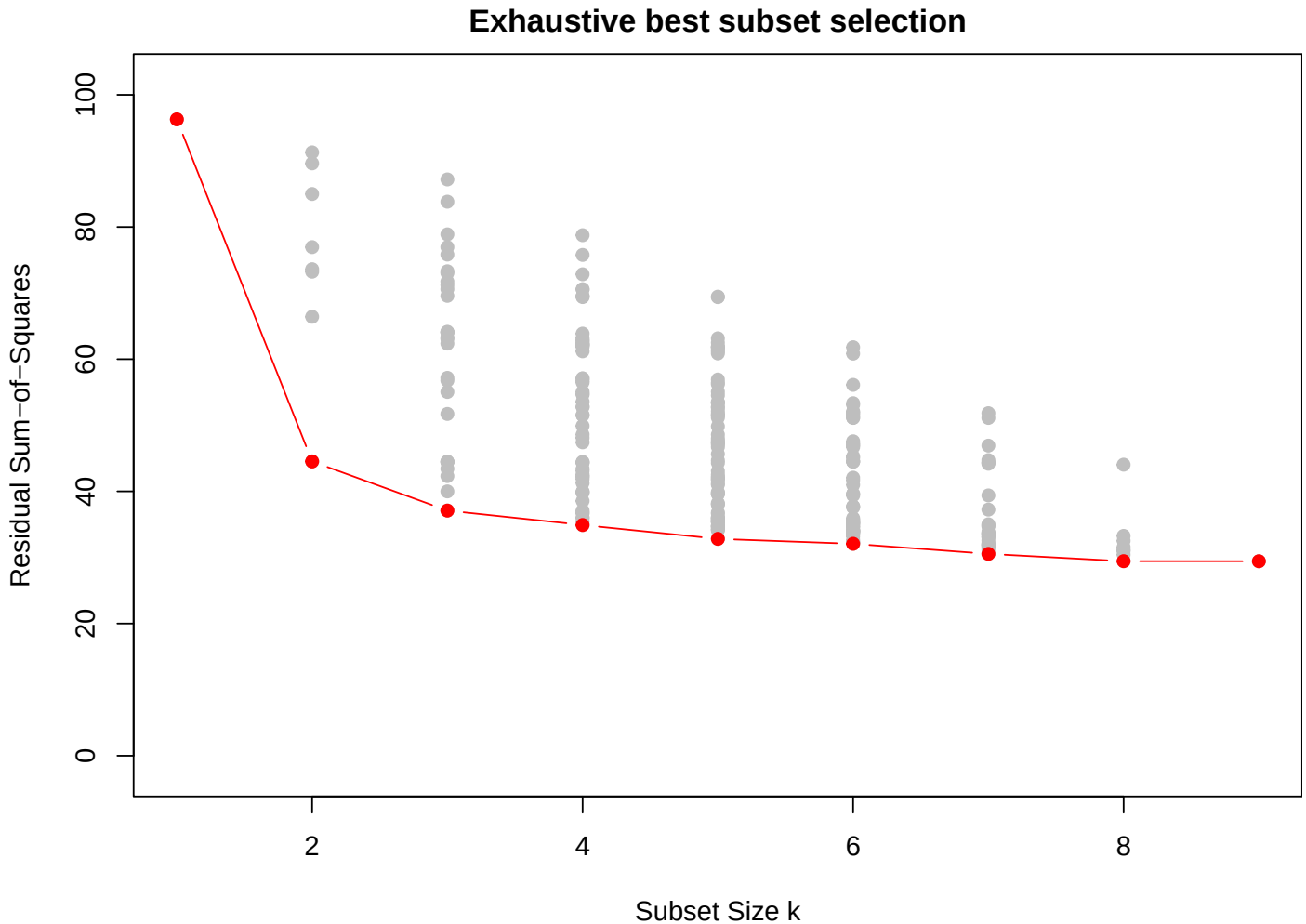
Model / subset selection / 3

- Forward-stagewise regression:
  - In each step the variable is selected which has the largest absolute correlation with the current residual.
  - The simple linear regression coefficient for this variable and the current residual is determined.
  - The coefficients of all other variables remain unchanged.
  - More than p steps necessary to arrive at the full least squares solution.

Model / subset selection / 4

- Least angle regression (LAR):
  - Iterative procedure where one variable is added in each step to the *active set*.
  - Starting at each step the variables in the active set
    - have the same absolute correlation with the current residual,
    - have a higher absolute correlation than the variables not in the active set.
  - The coefficients of the variables in the active set are updated
    - keeping the correlation to the residuals tied,
    - until another variable (not in the active set) has the same correlation with the residuals.
  - This variable is then added to the active set.
  - This process eventually also gives the full least squares solution.

Example: Prostate Cancer



Shrinkage methods

- Shrinkage methods add a complexity parameter which allows to gradually change between a simple model (e.g., intercept only) to a complex model (e.g., the least squares fit of all variables).
- In general the optimization criterion is modified by adding a penalty.
- Examples:
  - Best subset selection
  - Ridge
  - Lasso (least absolute shrinkage and selection operator)
  - Elastic net

Best subset selection

- Regression with best subset selection obtains the estimates by adding a penalty in dependence of the L_0 norm of the regression coefficients:

$$\hat{\beta}^{\text{BSS}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \|\beta_{\setminus 0}\|_0 \right\},$$

  with the L_0 norm being equal to the number of non-zero elements in a vector and with $\lambda \geq 0$ the complexity parameter.
- An equivalent problem formulation is:

$$\hat{\beta}^{\text{BSS}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 \right\},$$

$$\text{subject to } \|\beta_{\setminus 0}\|_0 \leq t,$$

  with a one-to-one correspondence between t and λ.

Ridge

- Ridge regression obtains the estimates by adding a penalty in dependence of the squared Euclidean length of the regression coefficients:

$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right\},$$

  with $\lambda \geq 0$ the complexity parameter:
  - $\lambda = 0$: least squares fit.
  - $\lambda = \infty$: only a constant function β_0 fit.

Ridge / 2

- An equivalent problem formulation is:

$$\hat{\beta}^{\text{ridge}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 \right\},$$

$$\text{subject to } \sum_{j=1}^{p} \beta_j^2 \leq t,$$

  with a one-to-one correspondence between t and λ.
- The intercept β_0 is not penalized to ensure that the solutions do not depend on the origin for Y.
- Ridge regression alleviates the problem of poorly identified coefficients in case of multicollinearity.
- Ridge regression is not equivariant under scaling of the inputs.
  $\Rightarrow$ Normally inputs are standardized before estimation.

Ridge / 3

- The Ridge criterion can also be written as

$$\text{RSS}(\beta) = (\boldsymbol{y} - \boldsymbol{X}\beta)^T(\boldsymbol{y} - \boldsymbol{X}\beta) + \lambda\beta^T\beta,$$

with solution

$$\hat{\beta}^{\text{ridge}} = (\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y},$$

where $\boldsymbol{I}$ is the $p \times p$ identity matrix.

Ridge: Shrinkage effects

- For orthonormal inputs:

$$\hat{\beta}^{\text{ridge}} = \frac{\hat{\beta}}{1 + \lambda}.$$

- Otherwise use the singular value decomposition

$$\boldsymbol{X} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T,$$

with

  - $\boldsymbol{U}$ a $N \times p$ orthogonal matrix,
  - $\boldsymbol{V}$ a $p \times p$ orthogonal matrix,
  - $\boldsymbol{D}$ a $p \times p$ diagonal matrix with $d_1 \geq d_2 \geq \ldots d_p \geq 0$.

Ridge: Shrinkage effects / 2

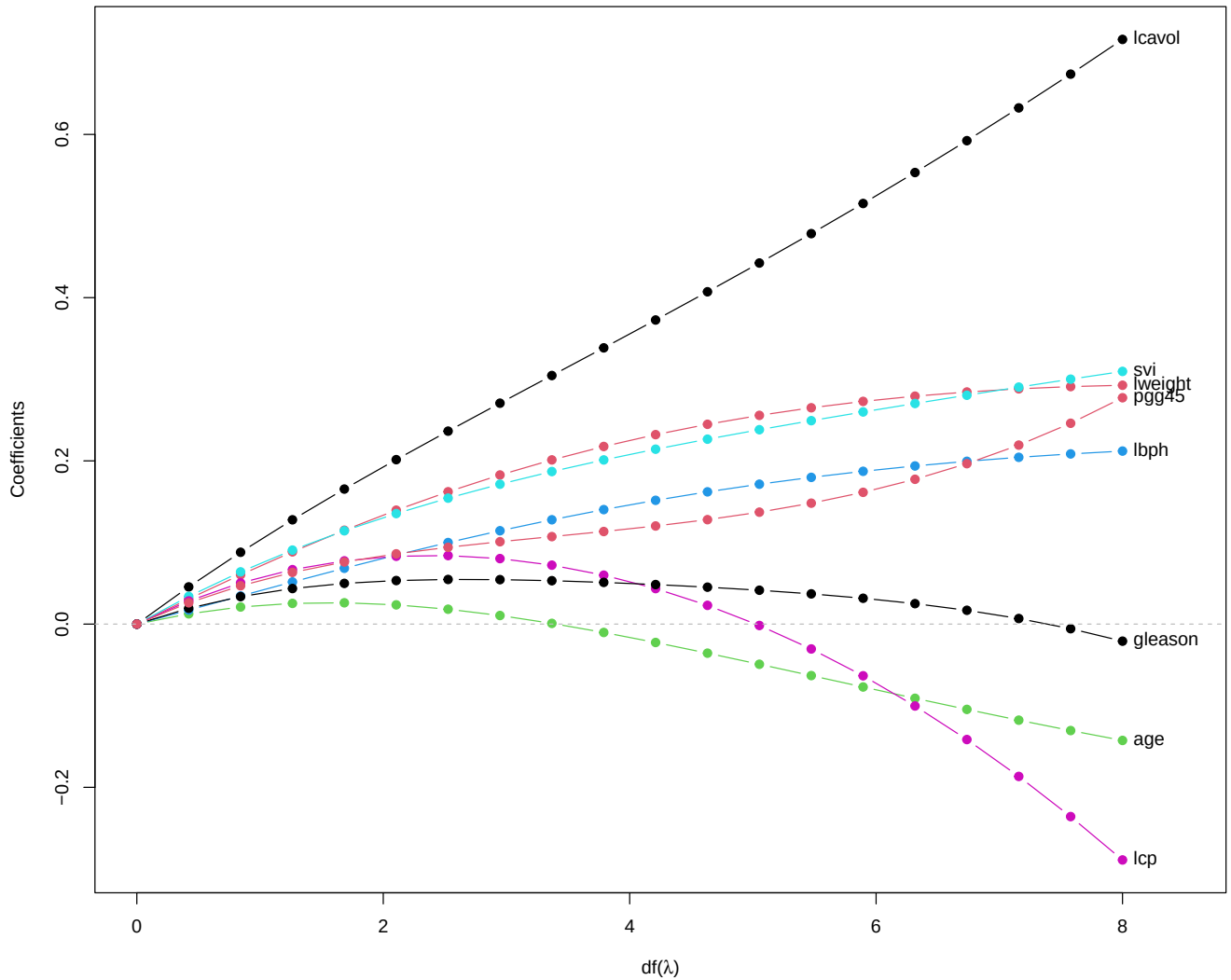
- This gives

$$\begin{aligned} \boldsymbol{X}\hat{\beta}^{\text{ridge}} &= \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ &= \boldsymbol{U}\boldsymbol{D}(\boldsymbol{D}^2 + \lambda\boldsymbol{I})^{-1}\boldsymbol{D}\boldsymbol{U}^T\boldsymbol{y}. \end{aligned}$$

- Ridge regression
  - projects $\boldsymbol{y}$ onto the principal components and
  - shrinks the coefficients of the low-variance components more than the high-variance components.
- The *effective degrees of freedom* are given by

$$\begin{aligned} \text{df}(\lambda) &= \text{tr}(\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})^{-1}\boldsymbol{X}^T] = \text{tr}(\boldsymbol{H}_\lambda) \\ &= \sum_{j=1}^{p} \frac{d_j^2}{d_j^2 + \lambda}. \end{aligned}$$

Example: Prostate Cancer



Lasso

- The lasso estimate is defined by:

$$\hat{\beta}^{\text{lasso}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 \right\},$$

$$\text{subject to } \sum_{j=1}^{p} |\beta_j| \leq t.$$

- The equivalent *Lagrangian form* is given by:

$$\hat{\beta}^{\text{lasso}} = \arg\min_{\beta} \left\{ \frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}.$$

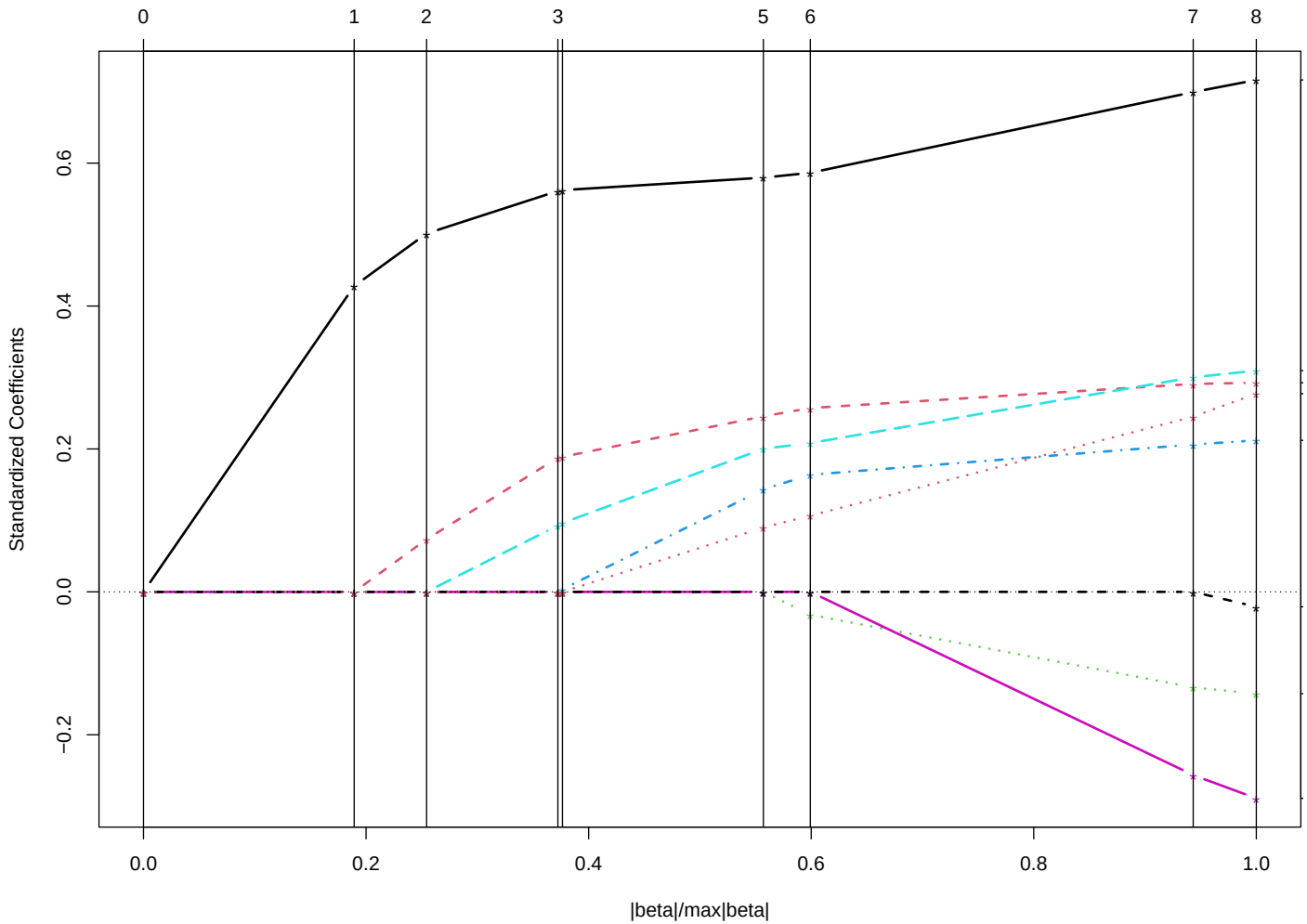
Lasso / 2

- The lasso essentially replaces the L_2 ridge penalty with the L_1 penalty.
- If t is sufficiently small, some of the coefficients will be exactly zero.
- If t is larger than $t_0 = \sum_{j=1}^{p} |\hat{\beta}_j|$, then the lasso estimates are the OLS estimates $\hat{\beta}_j$. If $t = t_0/2$, the lasso estimates are shrunken by 50% on average.
- A standardized penalty parameter is given by

$$s = \frac{t}{\sum_{j=1}^{p} |\hat{\beta}_j|},$$

  with $s \in [0, 1]$.
- Lasso regression is not equivariant under scaling of the inputs.
  $\Rightarrow$ Normally inputs are standardized before estimation.

Example: Prostate Cancer



Elastic net

The following optimization problem is solved in elastic net regression

$$\hat{\beta}_{\text{enet}} = \arg\min_{\beta} \left\{ \|\boldsymbol{y} - \boldsymbol{X}\beta\|_2^2 + \lambda(\alpha\|\beta_{[-0]}\|_2^2 + (1-\alpha)\|\beta_{[-0]}\|_1) \right\}$$

$$= \arg\min_{\beta} \left\{ \sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \left(\sum_{j=1}^{p} \alpha\beta_j^2 + (1-\alpha)|\beta_j| \right) \right\}$$

- The parameter $\lambda \geq 0$ is a complexity parameter, that controls the amount of shrinkage. The parameter $\alpha \in [0, 1]$ determines the compromise between Ridge and LASSO penalty.
- The intercept β_0 is not shrunken.
- The elastic net solutions are not equivariant under scaling of the regressors.
  $\Rightarrow$ One normally standardizes the regressors before analysis.

Comparison

For an orthonormal input matrix $\boldsymbol{X}$:

- Best subset (size M), L_0 loss:

$$\hat{\beta}_j \mathbb{1}_{\text{rank}(|\hat{\beta}_j|) \leq M}$$

- Lasso, L_1 loss:

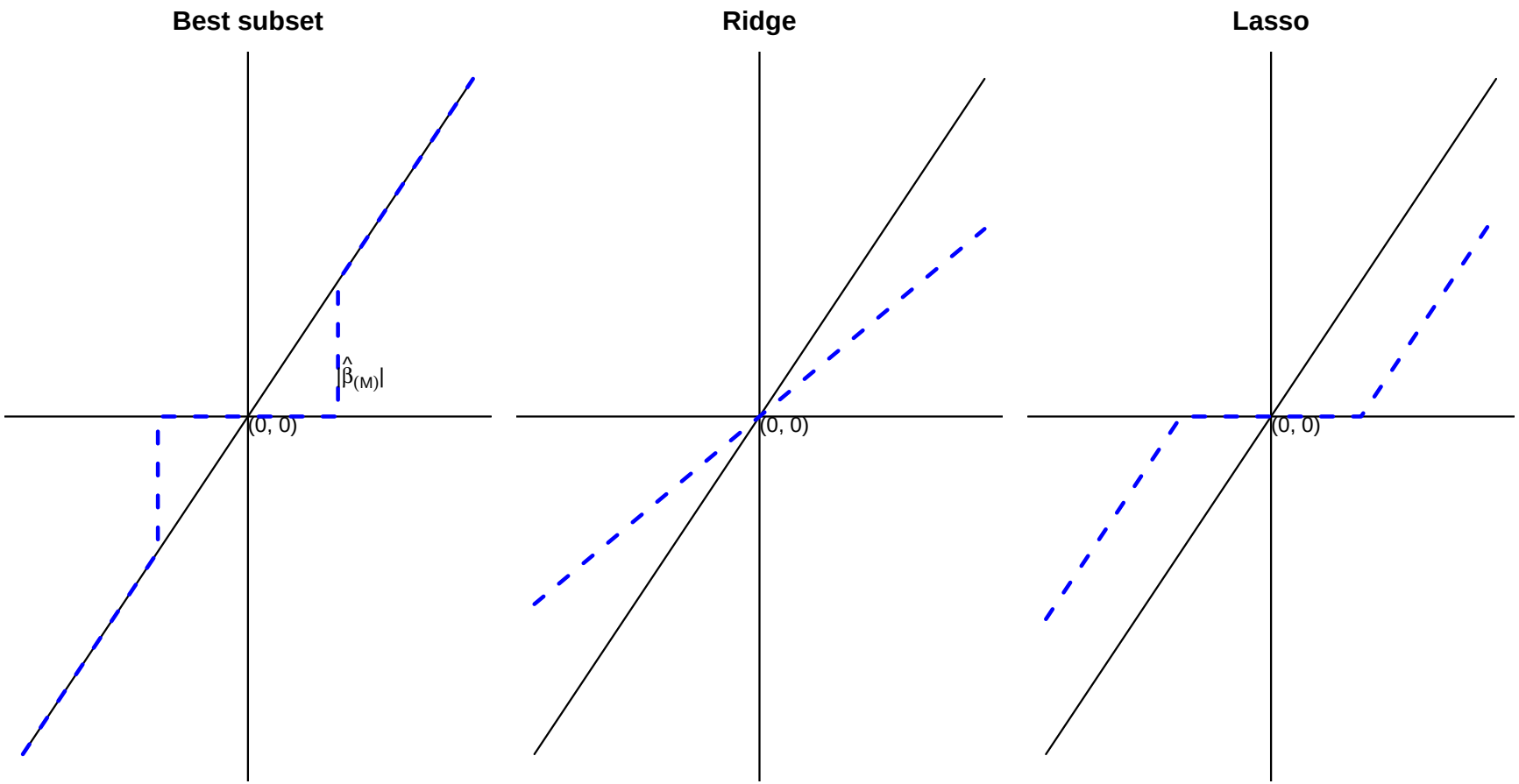
$$\text{sign}(\hat{\beta}_j)(|\hat{\beta}_j| - \lambda)_+$$

- Ridge, L_2 loss:

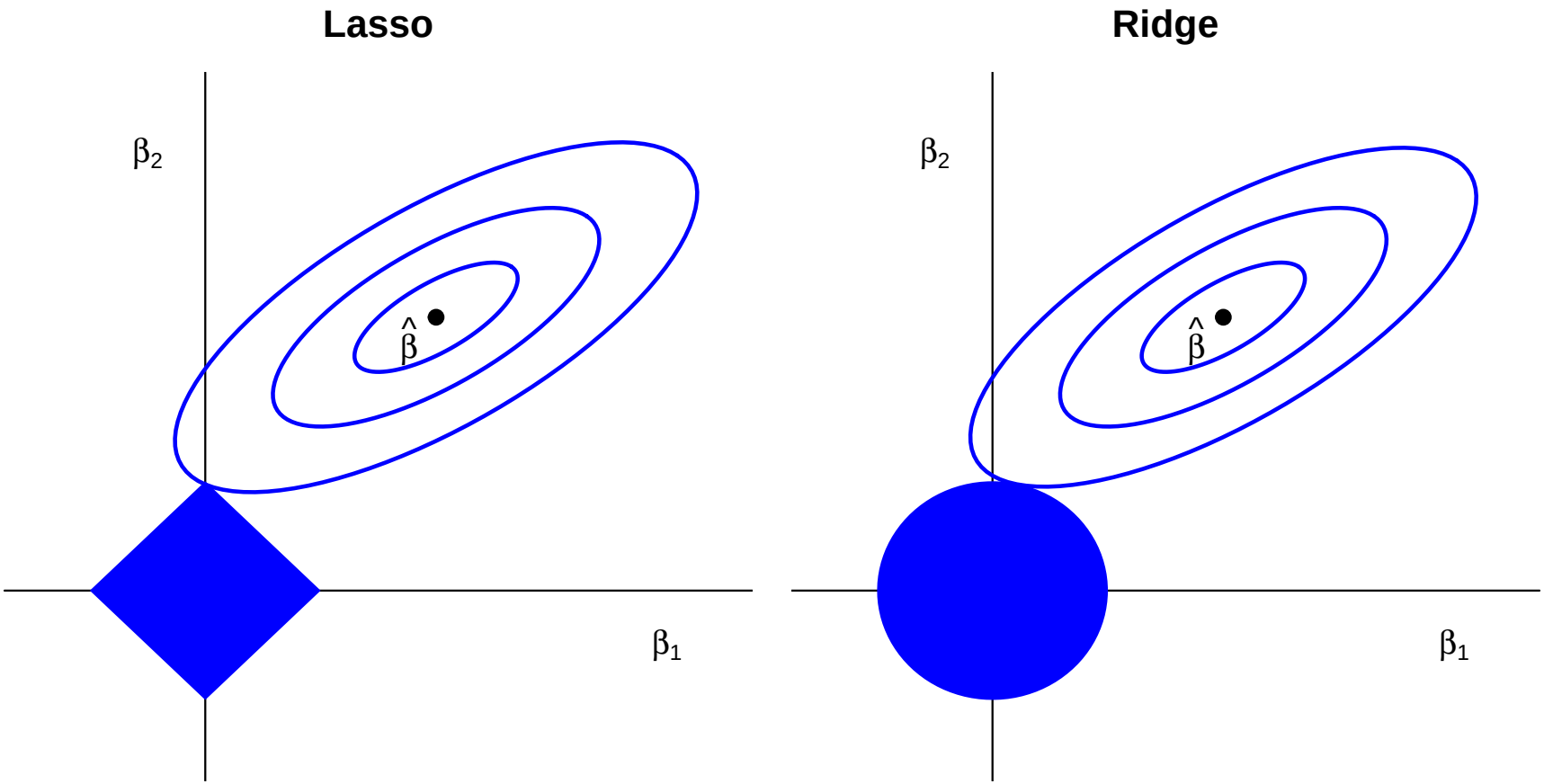
$$\hat{\beta}_j \frac{1}{1 + \lambda}$$

with $\hat{\beta}_j$ the OLS estimator.

Comparison / 2



Comparison / 3



Comparison / 4

- The lasso and ridge regression can be generalized to:

$$\tilde{\beta} = \arg\min_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|^q \right\},$$

with $q \geq 1$.

Comparison / 5

- Elastic net:

$$\hat{\beta}^{\text{elastic net}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} (\alpha\beta_j^2 + (1-\alpha)|\beta_j|) \right\},$$

with $\alpha \in [0, 1]$.

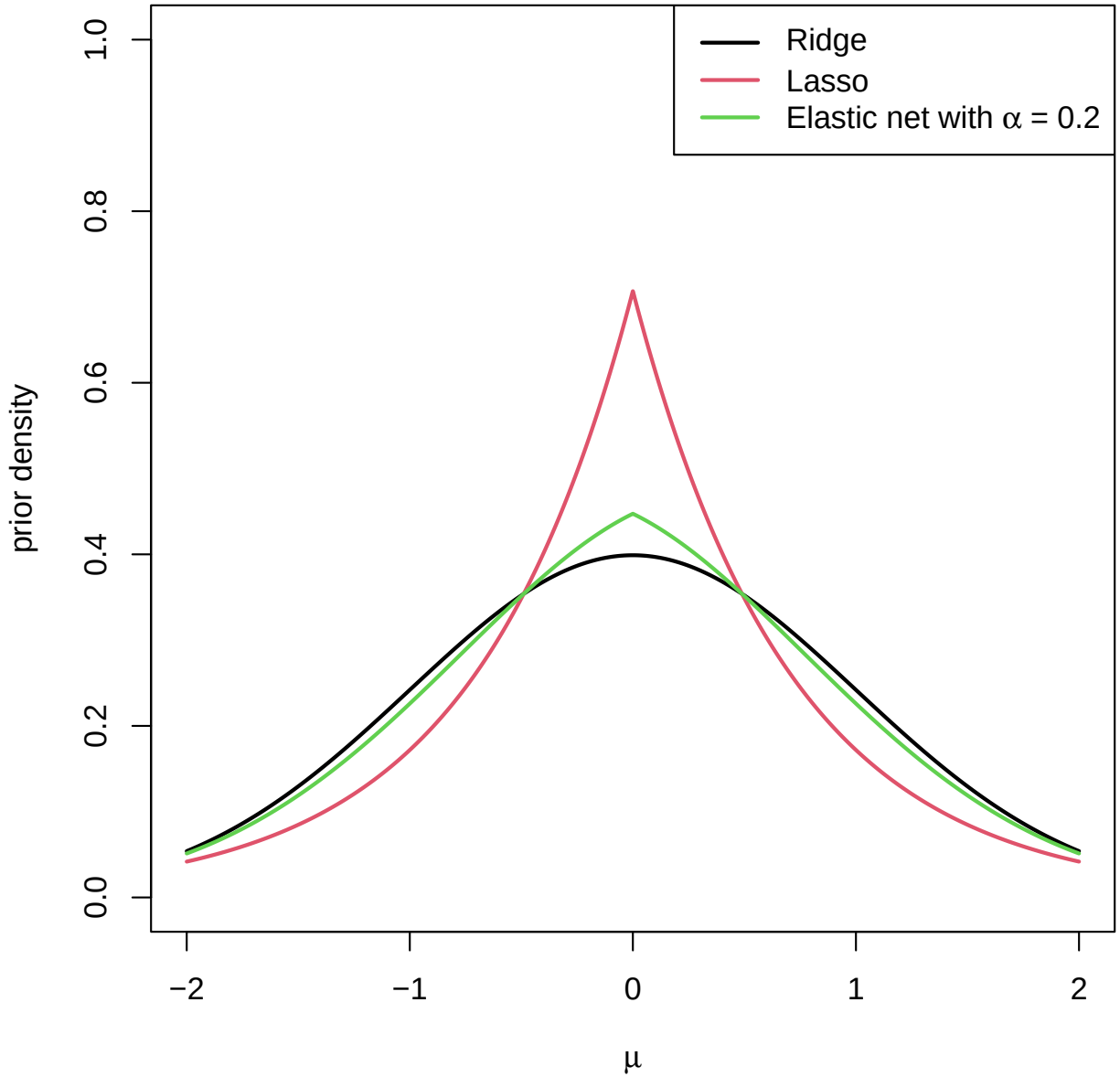
  - Represents a compromise between lasso and ridge.
  - Selects variables like the lasso, and shrinks together the coefficients of correlated predictors like ridge.
  - Has computational advantages over the L_q penalties.

Relation to Bayesian estimation

- Bayesian estimation determines the posterior distribution of a parameter given
  - prior beliefs and
  - observed data

  by combining the prior distribution of the parameter with the likelihood function.
- All penalized approaches can be seen as determining the maximum a-posteriori estimates of the parameters using different prior distributions. E.g., the following priors for:
  - Ridge: normal distribution.
  - Lasso: double-exponential or Laplace distribution.

Relation to Bayesian estimation / 2



Shrinkage methods: Estimation

- Best subset selection:
  - Use of an efficient branch and bound algorithm to avoid enumeration of all subsets.
  - Exploits that in linear regression it holds for the residual sum of squares (RSS) that

$$\text{RSS}(A) \leq \text{RSS}(B),$$

    where A is any set of independent variables and B is a subset of A.

Shrinkage methods: Estimation / 2

- Ridge:
  - Regression coefficient estimates are available in closed form for a given λ.
- Lasso:
  - If λ decreases the coefficient values change in a piecewise linear fashion. The slope only changes if coefficients leave or enter the set of active coefficients.
  - The entire path for all λ values can be determined in a computationally efficient way.
    $\Rightarrow$ See least angle regression (LAR).
  - Pathwise coordinate optimization.
  - Convex optimization problem (as ridge regression).

LAR and lasso

- Assume the input features are standardized.
- For the active set $\mathcal{A}_k$ at step k in LAR it holds:

$$\boldsymbol{x}_j^T(\boldsymbol{y} - \boldsymbol{X}\beta) = \gamma \cdot s_j,$$

for all $j \in \mathcal{A}_k$ and with

- β the current coefficient estimates,
- $s_j \in \{-1, 1\}$,
- γ the common value.

LAR and lasso / 2

- The lasso criterion corresponds to

$$R(\beta) = \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{X}\beta\|_2^2 + \lambda\|\beta\|_1.$$

- If $\mathcal{B}$ is the active set of variables for a given value of λ, $R(\beta)$ is differentiable for these variables and the stationarity conditions need to hold:

$$\boldsymbol{x}_j^T(\boldsymbol{y} - \boldsymbol{X}\beta) = \lambda \cdot \text{sign}(\beta_j),$$

  for all $j \in \mathcal{B}$.
- The LAR and lasso criteria are identical if the sign of β_j matches the sign of the inner product.
  $\Rightarrow$ LAR and lasso start to differ when an active coefficient passes through zero.
  $\Rightarrow$ For the lasso the variable is excluded from the active set.

LAR and lasso / 3

- For the non-active variables the stationarity conditions require

$$|\boldsymbol{x}_k^T(\boldsymbol{y} - \boldsymbol{X}\beta)| \leq \gamma$$

for $k \notin \mathcal{A}$ and

$$|\boldsymbol{x}_k^T(\boldsymbol{y} - \boldsymbol{X}\beta)| \leq \lambda$$

for $k \notin \mathcal{B}$.

Algorithm: Least angle regression

1. Standardize the predictors to have mean zero and unit norm. Start with the residual $\boldsymbol{r} = \boldsymbol{y} - \bar{\boldsymbol{y}}$ and $\beta_1, \ldots, \beta_p = 0$.
2. Find the predictor $\boldsymbol{x}_j$ most correlated with $\boldsymbol{r}$.
3. Move β_j from 0 towards its least squares (LS) coefficient $\langle \boldsymbol{x}_j, \boldsymbol{r} \rangle$, until some other competitor $\boldsymbol{x}_k$ has as much correlation with the current residual as does $\boldsymbol{x}_j$.
4. Move β_j and β_k in the direction defined by their joint LS coefficient of the current residual on $(\boldsymbol{x}_j, \boldsymbol{x}_k)$, until some other competitor $\boldsymbol{x}_l$ has as much correlation with the current residual.
5. Continue in this way until all p predictors have been entered. After $\min(N - 1, p)$ steps, we arrive at the full LS solution.

Lasso modification:

4a. If a non-zero coefficient hits zero, drop its variable from the active set of variables and recompute the current joint LS direction.

Pathwise coordinate optimization

- An alternate approach to the lars algorithm for computing the lasso solution.
- Fix the penalty parameter λ in the Lagrangian form

$$\hat{\beta}^{\text{lasso}} = \arg\min_{\beta} \left\{ \frac{1}{2} \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right\}.$$

- Optimize successively over each parameter, holding the other parameters fixed at their current values.
- This algorithm can be used to efficiently calculate the lasso solutions at a grid of values of λ. One starts with the largest value of λ.
- This algorithm can also be modified to be used with the elastic net.

Pathwise coordinate optimization: Algorithm

- Suppose all predictors are standardized to have mean zero and unit norm and the response also has mean zero.
- The current estimate for β_k at penalty parameter λ is denoted by $\tilde{\beta}_k(\lambda)$.
- The function to optimize can be written as:

$$R(\tilde{\beta}(\lambda), \beta_j) = \frac{1}{2} \sum_{i=1}^{N} \left(y_i - \sum_{k \neq j} x_{ik} \tilde{\beta}_k(\lambda) - x_{ij} \beta_j \right)^2 + \lambda \sum_{k \neq j} |\tilde{\beta}_k(\lambda)| + \lambda |\beta_j|.$$

Pathwise coordinate optimization: Algorithm / 2

- This has an explicit solution with respect to β_j:

$$\tilde{\beta}_j(\lambda) = S\left(\sum_{i=1}^{N} x_{ij}(y_i - \sum_{k \neq j} x_{ik}\tilde{\beta}_k(\lambda)), \lambda\right),$$

  with

$$S(t, \lambda) = \text{sign}(t)(|t| - \lambda)_+$$

  is the soft-thresholding operator.

- Repeatedly iterating over the covariates results in the lasso estimate.

Degrees of freedom

$$\text{df}(\hat{\boldsymbol{y}}) = \frac{1}{\sigma^2} \sum_{i=1}^{N} \text{Cov}(\hat{y}_i, y_i).$$

- For linear regression with k fixed predictors this gives: $\text{df}(\hat{\boldsymbol{y}}) = k$.
- For ridge regression: $\text{df}(\hat{\boldsymbol{y}}) = \text{tr}(\boldsymbol{H}_\lambda)$.
- For LAR after the kth step: $\text{df}(\hat{\boldsymbol{y}}) = k$.
- For lasso $\text{df}(\hat{\boldsymbol{y}})$ approximately equals the number of predictors in the model.
- For best subset selection if k variables are selected: $\text{df}(\hat{\boldsymbol{y}}) \geq k$.

Extensions

- Grouped Lasso:
  - For categorical variables the Lasso penalizes the individual dummy variables and selects them without taking into account that they belong to the same categorical variable.
  - Impose a penalty on the norm of the subvector of regression coefficients for the same categorical variable.
- Other penalties: e.g.,
  - SCAD (smoothly clipped absolute deviation) to achieve that larger coefficients are shrunken less.