# Lecture 10: Regularised regression (cont'd)

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# Regularisation in classification

# Recall: Regularised Discriminant Analysis (RDA)

Given training samples $(i_l, \mathbf{x}_l)$, quadratic DA models

$$p(\mathbf{x}|i) = N(\mathbf{x}|\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i) \quad \text{and} \quad p(i) = \pi_i$$

Estimates $\widehat{\boldsymbol{\mu}}_i$, $\widehat{\boldsymbol{\Sigma}}_i$ and $\widehat{\pi}_i$ are straight-forward to find,...

...but evaluating the normal density requires inversion of $\widehat{\boldsymbol{\Sigma}}_i$. If it is (near-)singular, this can lead to **numerical instability**.

**Regularisation can help here:**

- Use $\widehat{\boldsymbol{\Sigma}}_i = \widehat{\boldsymbol{\Sigma}}_i^{\mathrm{QDA}} + \lambda \widehat{\boldsymbol{\Sigma}}^{\mathrm{LDA}}$ for $\lambda > 0$
- Use LDA (i.e. $\boldsymbol{\Sigma}_i = \boldsymbol{\Sigma}$) and $\widehat{\boldsymbol{\Sigma}} = \widehat{\boldsymbol{\Sigma}}^{\mathrm{LDA}} + \lambda \boldsymbol{\Delta}$ for $\lambda > 0$ and a diagonal matrix $\boldsymbol{\Delta}$

# Recall: Naive Bayes LDA

Naive Bayes LDA means that we assume that $\widehat{\boldsymbol{\Sigma}} = \widehat{\boldsymbol{\Delta}}$ for a diagonal matrix $\widehat{\boldsymbol{\Delta}}$. The diagonal elements are estimated as

$$\widehat{\Delta}^{(j,j)} = \frac{1}{n-K} \sum_{i=1}^{K} \sum_{i_l = i} (\mathbf{x}_l^{(j)} - \widehat{\boldsymbol{\mu}}_i^{(j)})^2$$

which is the **pooled within-class variance**.

Classification is performed by predicting the class with the maximal **discriminant function** value

$$\begin{aligned} \delta_i(\mathbf{x}) &= -\frac{1}{2}(\mathbf{x} - \widehat{\boldsymbol{\mu}}_i)^\top \widehat{\boldsymbol{\Delta}}^{-1} (\mathbf{x} - \widehat{\boldsymbol{\mu}}_i) + \log(\widehat{\pi}_i) \\ &= -\frac{1}{2} \left\| \widehat{\boldsymbol{\Delta}}^{-1/2} (\mathbf{x} - \widehat{\boldsymbol{\mu}}_i) \right\|_2^2 + \log(\widehat{\pi}_i) \end{aligned}$$

where $\left(\widehat{\boldsymbol{\Delta}}^{-1/2}\right)^{(i,i)} = 1 \big/ \sqrt{\widehat{\boldsymbol{\Delta}}^{(i,i)}}$.

## Shrunken centroids (I)

In high-dimensional problems ($p > n$), centroids will

- contain noise
- be hard to interpret when all variables are active

As in regression, we would like to perform **variable selection** and **reduce noise**.

**Recall:** The class centroids solve

$$\widehat{\boldsymbol{\mu}}_i = \frac{1}{n_i} \sum_{i_l = i} \mathbf{x}_l = \arg\min_{\mathbf{v}} \frac{1}{2} \sum_{i_l = i} ||\mathbf{x}_l - \mathbf{v}||_2^2$$

**Idea:** Can we perform variable selection through $\ell_1$-/lasso-style regularisation? How can we account for varying variance in features and stabilise against noise?

# Shrunken centroids (II)

**Nearest shrunken centroids** performs variable selection and stabilises centroid estimates by solving

$$\bar{\boldsymbol{\mu}}_i = \arg\min_{\mathbf{v}} \frac{1}{2} \sum_{i_l = i} \|(\widehat{\boldsymbol{\Delta}} + s_0 \mathbf{I}_p)^{-1/2}(\mathbf{x}_l - \mathbf{v})\|_2^2 + \lambda n_i m_i \|\mathbf{v} - \widehat{\boldsymbol{\mu}}_T\|_1$$

where $s_0 = \mathrm{median}(\widehat{\boldsymbol{\Delta}}^{(1,1)}, \dots, \widehat{\boldsymbol{\Delta}}^{(p,p)})$, $m_i = \sqrt{\frac{1}{n_i} - \frac{1}{n}}$ and $\widehat{\boldsymbol{\mu}}_T = \frac{1}{n} \sum_l \mathbf{x}_l$.

- Penalises distance of class centroid to the overall centroid $\boldsymbol{\mu}_T$
- $\widehat{\boldsymbol{\Delta}} + s_0 \mathbf{I}_p$ is the diagonal regularised within-class covariance matrix. Features that are highly variable across samples are scaled down (**interpretability**)
- $n_i m_i$ scales $\lambda$ in case of unequal class sizes

# Shrunken centroids (III)

The solution for component $j$ can be derived as

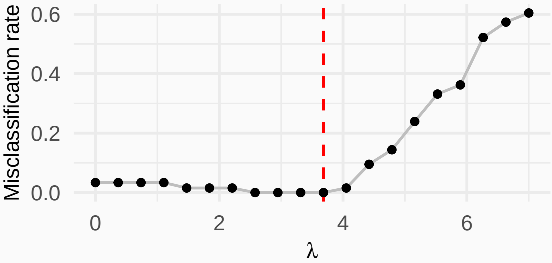
$$\overline{\boldsymbol{\mu}}_i^{(j)} = \widehat{\boldsymbol{\mu}}_T^{(j)} + m_i(\widehat{\boldsymbol{\Delta}}^{(j,j)} + s_0)\,\mathrm{ST}\left(\mathbf{t}_i^{(j)}, \lambda\right) \quad \text{where} \quad \mathbf{t}_i^{(j)} = \frac{\widehat{\boldsymbol{\mu}}_i^{(j)} - \widehat{\boldsymbol{\mu}}_T^{(j)}}{m_i(\widehat{\boldsymbol{\Delta}}^{(j,j)} + s_0)}.$$

**Note:** $\lambda$ is a tuning parameter and has to be determined through e.g. cross-validation.

- Typically, misclassification rate improves first with increasing $\lambda$ and declines for too high values
- The larger $\lambda$ the more components will be equal to the respective component of the overall centroid.

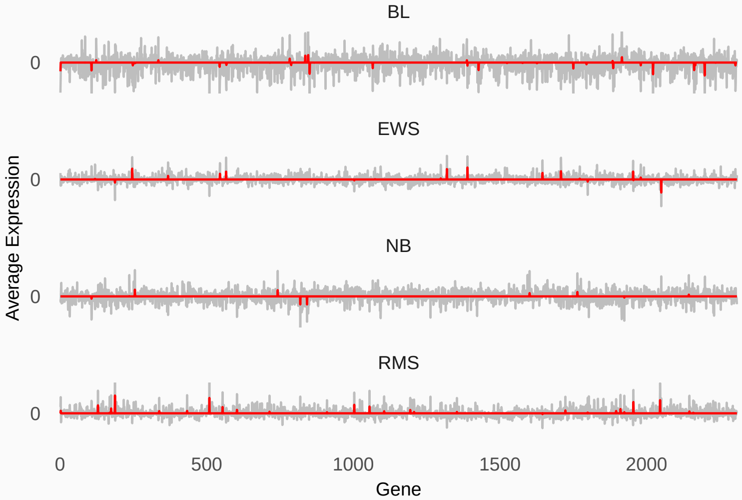
# Application of nearest shrunken centroids (I)

A gene expression data set with $n = 63$ and $p = 2308$. There are four classes (cancer subtypes) with $n_{\mathrm{BL}} = 8$, $n_{\mathrm{EWS}} = 23$, $n_{\mathrm{NB}} = 12$, and $n_{\mathrm{RMS}} = 20$.




5-fold cross-validation curve and largest $\lambda$ that leads to minimal misclassification rate

# Application of nearest shrunken centroids (II)




Grey lines show the original centroids and red lines show the shrunken centroids

# Extensions of the lasso

## The lasso and groups of highly correlated variables

- The lasso does not handle groups of highly correlated variables well.
- **Example:** Two groups of highly correlated variables, e.g.

$$\mathbf{X} \sim N(\mathbf{0}, \mathbf{\Sigma}) \quad \text{where} \quad \mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{\Sigma}_1 \end{pmatrix} \in \mathbb{R}^{200\times 200},$$

  where

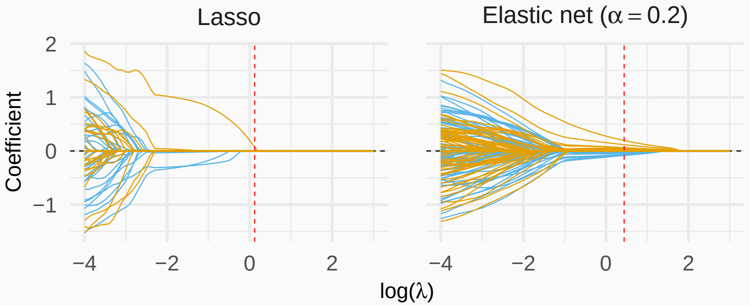
$$\mathbf{\Sigma}_1 \in \mathbb{R}^{100\times 100}, \quad \mathbf{\Sigma}_1^{(i,i)} = 1.04 \quad \text{and} \quad \mathbf{\Sigma}_1^{(i,j)} = 1, \quad i \neq j.$$

  The response is generated for $n = 100$ samples as

$$\mathbf{y} = \mathbf{x}_1 - \mathbf{x}_{102} + \boldsymbol{\varepsilon} \quad \text{where} \quad \boldsymbol{\varepsilon} \sim N(\mathbf{0}, 4\mathbf{I}_p).$$

- **Expectation:** Since the predictors in each group are strongly correlated, all could be considered equally as predictors.
- **Possible caveat:** The lasso makes a sparsity assumption and tries to set as many coefficients to zero as possible.

# The lasso and groups of highly correlated variables in practice




- At optimal $\lambda$ the lasso selects 5 non-zero coefficients 0 of which were in the true coefficient vector.
  - Very precise but 'wrong' estimates.
- An alternative algorithm, the **elastic net** estimates 19 non-zero coefficients. (11 in the 1st group and 8 in the 2nd group, group-wise close coefficients)
  - 'Shares' responsibility among correlated variables

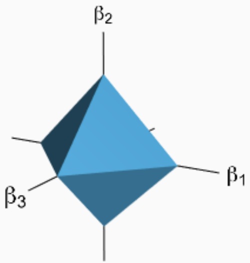
# The elastic net (I)

The **elastic net** solves the problem

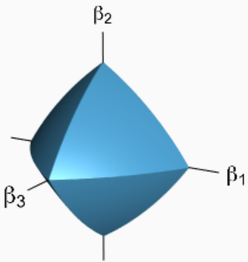
$$\arg\min_{\boldsymbol{\beta}} \frac{1}{2}||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda\left(\frac{1-\alpha}{2}||\boldsymbol{\beta}||_2^2 + \alpha||\boldsymbol{\beta}||_1\right)$$

striking a balance between lasso (**variable selection**) and ridge regression (**grouping of variables**)

Lasso




Elastic net (α = 0.7)



# Notes on the elastic net (II)

- The solution can be found through **cyclic coordinate descent**
- $\alpha$ is an additional tuning parameter that should be determined by cross-validation
- The lasso and ridge regression are special cases of the elastic net ($\alpha = 1$ and $\alpha = 0$, respectively).

## Explicitly adding groups to the lasso

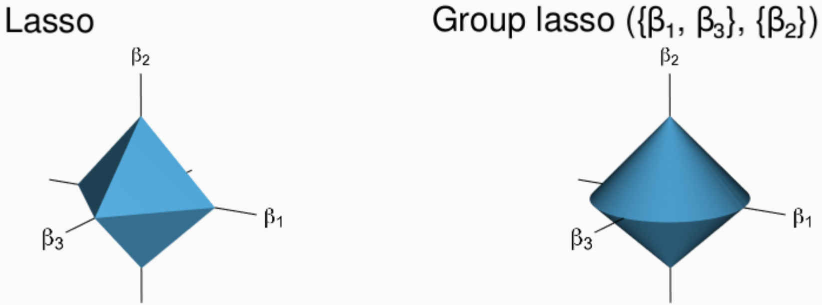
- The lasso in it's original formulation considers each variable separately
- Groups in data can form through e.g.
  - Correlation
  - Categorical variables in dummy encoding
  - Domain-knowledge (e.g. genes in the same signal pathway, signals that only appear in groups in a compressed sensing problem,...)
- Ideally the whole group is either present or not
- The elastic net can find groups, but only does so for highly correlated variables and without external influence. Sometimes more control is necessary.

# The group lasso (I)

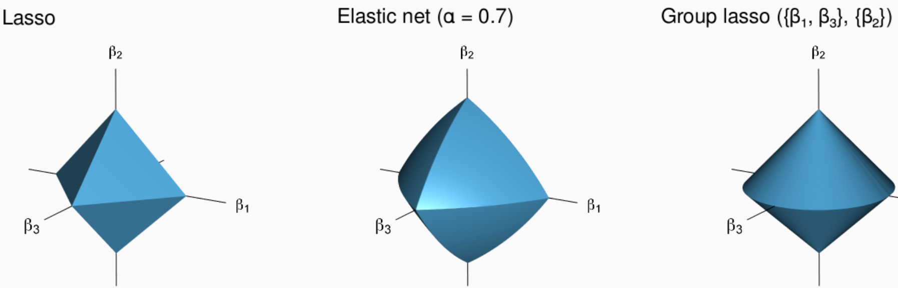
The **group lasso** solves the problem

$$\underset{\boldsymbol{\beta}}{\arg\min}\, \frac{1}{2}||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda \sum_{k=1}^{K} ||\mathbf{B}_k||_2$$

where $\mathbf{B}_k$ is a vector of coefficients $\beta_i$ for the $k$-th group. Note that $||\beta_i||_2 = |\beta_i|$ for singleton groups.



# Comparison: Lasso, elastic net and group lasso




- The lasso sets variables exactly to zero either on a corner or along an edge.
- The elastic net similarly sets variables exactly to zero on a corner or along an edge. The curved edges encourage remaining coefficients to be closer together.
- The group lasso has actual information about groups of variables. It encourages whole groups to be zero or non-zero with similar coefficients.

# Penalisation in GLMs

Penalisation can also be used in generalised linear models (GLMs), e.g. to perform **sparse logistic regression**.

Given $p(y|\boldsymbol{\beta}, \mathbf{x})$ the log-likelihood of the model is

$$\mathcal{L}(\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}) = \sum_{l=1}^{n} \log(p(y_l|\boldsymbol{\beta}, \mathbf{x}_l))$$

Instead of penalising the minimisation of the residual sum of squares (RSS), the **minimisation of the negative log-likelihood is penalized**, i.e.

$$\arg\min_{\boldsymbol{\beta}} -\mathcal{L}(\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}) + \lambda||\boldsymbol{\beta}||_1$$

**Note:** If $p(y|\boldsymbol{\beta}, \mathbf{x})$ is Gaussian and the linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ is assumed, this is equivalent to the lasso.

## Sparse logistic regression

**Recall:** For logistic regression with $i_l \in \{0, 1\}$ it holds that

$$p(1|\boldsymbol{\beta}, \mathbf{x}) = \frac{\exp(\mathbf{x}^\top \boldsymbol{\beta})}{1 + \exp(\mathbf{x}^\top \boldsymbol{\beta})} \quad \text{and} \quad p(0|\boldsymbol{\beta}, \mathbf{x}) = \frac{1}{1 + \exp(\mathbf{x}^\top \boldsymbol{\beta})}$$

and the penalised minimisation problem becomes

$$\arg\min_{\boldsymbol{\beta}} - \sum_{l=1}^{n} \left( i_l \mathbf{x}_l^\top \boldsymbol{\beta} - \log\left(1 + \exp(\mathbf{x}^\top \boldsymbol{\beta})\right)\right) + \lambda ||\boldsymbol{\beta}||_1$$

- The minimisation problem is still convex, but non-linear in $\boldsymbol{\beta}$. Iterative quadratic approximations combined with coordinate descent can be used to solve this problem.
- Another way to perform sparse classification (like e.g. nearest shrunken centroids)

# Sparse multi-class logistic regression

In multi-class logistic regression with $i_l \in \{1, \ldots, K\}$, there is a matrix of coefficients $\mathbf{B} \in \mathbb{R}^{p\times(K-1)}$ and it holds for $i = 1, \ldots, K-1$ that

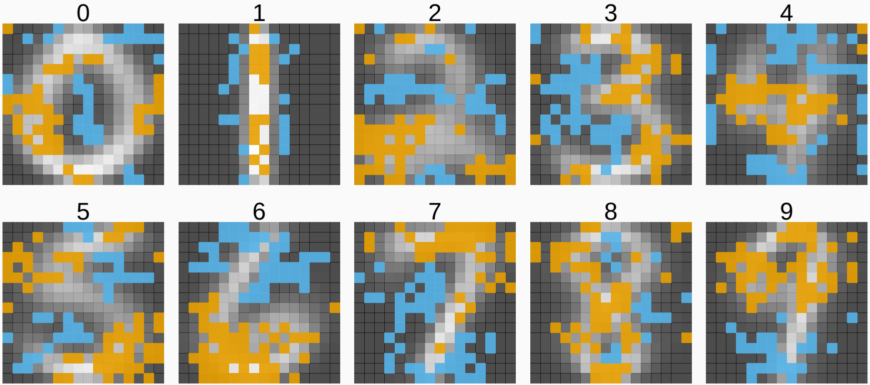
$$p(i|\mathbf{B}, \mathbf{x}) = \frac{\exp(\mathbf{x}^\top \boldsymbol{\beta}_i)}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{x}^\top \boldsymbol{\beta}_j)} \quad \text{and} \quad p(K|\mathbf{B}, \mathbf{x}) = \frac{1}{1 + \sum_{j=1}^{K-1} \exp(\mathbf{x}^\top \boldsymbol{\beta}_j)}$$

- As in two-class case, the absolute value of each entry in $\mathbf{B}$ can be penalised.
- Another possibility is to use the group lasso on all coefficients for one variable, i.e. penalise with $\|\mathbf{B}_{j\cdot}\|_2$ for $j = 1, \ldots, p$.

# Example for sparse multi-class logistic regression

**MNIST-derived zip code digits** ($n = 7291$, $p = 256$)

Sparse multi-class logistic regression was applied to the whole data set and the penalisation parameter was selected by 10-fold CV.




Orange tiles show positive coefficients and blue tiles show negative coefficients. Class averages are shown in the background.

# Take-home message

- Penalisation methods are not only restricted to regression, also applicable to classification
- Sparsity is a very important concept when interpretability of models is important
- Many extensions to the lasso exist, which make it more suitable for a variety of different situations