

# Chapter 2 (week 2)

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## “God is in every leaf of every tree”

- From Andrew Gelman ([blog](#))
- “No problem is too small or too trivial if we really do something about it.” (Dyson (2005) quoting Richard Feynman)
- (an excuse for going down rabbit holes?)

Dyson, Freeman. 2005. “Wise Man.” *New York Review of Books*, October. <https://www.nybooks.com/articles/2005/10/20/wise-man/>.

## feature selection

- *feature*  $\approx$  a column of the model matrix
- termwise selection, e.g.
  - all columns associated with a categorical variable
  - all columns of a basis expansion (polynomial etc.) of a continuous variable
- columnwise selection
  - fine for prediction
  - silly for inference?
- selection maintaining the **principle of marginality** (Venables 1998) (i.e., don’t drop lower-order effects from a model containing interactions)
- ¿ a way to **merge categories** on the fly (based on rarity, correlation, predictive ability)?

Venables, W. N. 1998. “Exegeses on Linear Models.” In. 1998 International S-PLUS User Conference. Washington, DC. <http://www.stats.ox.ac.uk/pub/MASS3/Exegeses.pdf>.

## why select?

- save memory
- save “flops” (floating-point operations)
- optimize bias-variance tradeoff

- optimize data collection
- parsimonious/simple explanations (e.g. `rms::fastbw` in R)

## why select (2)?

- save memory: OK
- save flops, optimize B-V
  - which is best: soft (ridge), semi-soft (lasso/SCAD), hard (stepwise/subset) penalization?

## selection: filters, wrappers, embedded methods

Jović, Brkić, and Bogunović (2015)

- **filters**: standalone recipes
  - e.g. minimum-redundancy maximum relevance (mrMR) (Peng, Long, and Ding 2005)
    - \* similar to stepwise forward, but no estimation done (compute mutual information)
    - \* **greedy**
  - general, low-cost
- **wrappers**: applied around specific methods
  - e.g. stepwise regression
  - general, evaluates prediction
- **embedded methods**: integrate estimation and selection
  - e.g. lasso etc.
  - most efficient? can combine shrinkage and selection

Jović, A., K. Brkić, and N. Bogunović. 2015. “A Review of Feature Selection Methods with Applications.” In *38th International Convention on Information and Communication Technology, Electronics and Microelectronics (MIPRO)*, 1200–1205. <https://doi.org/10.1109/MIPRO.2015.7160458>.

Peng, Hanchuan, Fuhui Long, and C. Ding. 2005. “Feature Selection Based on Mutual Information Criteria of Max-Dependency, Max-Relevance, and Min-Redundancy.” *IEEE Transactions on Pattern Analysis and Machine Intelligence* 27 (8): 1226–38. <https://doi.org/10.1109/TPAMI.2005.159>.

## stepwise abuse

- stepwise regression for **prediction** may be fine (Murtaugh 2009)
  - selection based on AIC etc. more sensible than with p-values

Murtaugh, Paul A. 2009. “Performance of Several Variable-Selection Methods Applied to Real Ecological Data.” *Ecology Letters* 12 (10): 1061–68. <https://doi.org/10.1111/j.1461-0248.2009.01361.x>.

- note  $\Delta AIC \propto p$  – value, if using columnwise/1-df steps
  - \*  $\Delta \log(L) \leftrightarrow \Delta AIC = 0 \leftrightarrow p = 0.16$
  - \* leave-one-out cross-validation (LOOCV) asymptotically equiv. to AIC (Stone (1977); but see [CV](#))
- for **inference**, terrible if done naively (but see Blanchet, Legendre, and Borcard (2008))
  - see [CrossValidated](#)
  - unstable, biased estimates; overconfident inference (“snooping”)
- ESL: stepwise as a jumping-off point/comparator for different

Stone, M. 1977. “An Asymptotic Equivalence of Choice of Model by Cross-Validation and Akaike’s Criterion.” *J. Royal Stat. Soc. B* 39 (1): 44–47. <https://www.jstor.org/stable/2984877>.

Blanchet, F. Guillaume, Pierre Legendre, and Daniel Borcard. 2008. “Forward Selection of Explanatory Variables.” *Ecology* 89 (9): 2623–32. <https://doi.org/10.1890/07-0986.1>.

## POLLS

- did you learn to do stepwise regression in a class? Were you warned about its limitations?
- have you used stepwise regression? were you aware of its limitations at the time?
- have you used SR “in real life”? for prediction or inference?

## contrasts for categorical variables

- expanding categorical variables to dummy variables
- automatically handled by `model.matrix()` in R (`StatsModels.jl:modelmatrix` in Julia)

```
library(palmerpenguins)
library(tidyverse)
library(faux)
set.seed(101)
pp <- penguins[sample(nrow(penguins)), c("species", "island")] ## scramble
head(model.matrix(~species+island, pp))
```

	(Intercept)	speciesChinstrap	speciesGentoo	islandDream	islandTorgersen
1	1	1	0	1	0
2	1	1	0	1	0
3	1	0	0	1	0
4	1	0	1	0	0
5	1	1	0	1	0
6	1	1	0	1	0

```
## faux makes nicer factors!
## rename variables/**idempotent** operations: f(f(x)) = f(x) x
pp2 <- mutate(pp, across(where(is.factor), contr_code_treatment))
head(model.matrix(~species+island, pp2))
```

	(Intercept)	species.Chinstrap-Adelie	species.Gentoo-Adelie
1	1	1	0
2	1	1	0
3	1	0	0
4	1	0	1
5	1	1	0
6	1	1	0

	island.Dream-Biscoe	island.Torgersen-Biscoe
1	1	0
2	1	0
3	1	0
4	0	0
5	1	0
6	1	0

```
colnames(model.matrix(~species*island, pp2))
```

```
[1] "(Intercept)"
[2] "species.Chinstrap-Adelie"
[3] "species.Gentoo-Adelie"
[4] "island.Dream-Biscoe"
[5] "island.Torgersen-Biscoe"
[6] "species.Chinstrap-Adelie:island.Dream-Biscoe"
[7] "species.Gentoo-Adelie:island.Dream-Biscoe"
```

```
[8] "species.Chinstrap-Adelie:island.Torgersen-Biscoe"
[9] "species.Gentoo-Adelie:island.Torgersen-Biscoe"
```

- identifiability constraints: leave out one category
  - post-hoc evaluation (e.g. `emmeans` R pkg)
  - penalized methods

## regression, again

- hat matrix ( $\mathbf{H} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$ ) as *projection matrix* from  $\mathbf{R}^N$  to  $\mathbf{R}^p$ 
  - (what if we first transformed  $\mathbf{X}$  to be orthonormal?)
- **non-full-rank** case ( $\text{rank}(\mathbf{X}) < p$ )
  - non-unique solutions
  - may break our linear algebra, depending on what we use

```
X <- matrix(c(1:3, 2*(1:3)), ncol = 2)
y <- 1:3
Matrix::rankMatrix(X)
```

```
[1] 1
attr(,"method")
[1] "tolNorm2"
attr(,"useGrad")
[1] FALSE
attr(,"tol")
[1] 6.661338e-16
```

```
try(solve(X %*% t(X)))
```

```
Error in solve.default(X %*% t(X)) :
Lapack routine dgesv: system is exactly singular: U[2,2] = 0
```

```
try(qr.solve(qr(X),y))
```

Error in qr.solve(qr(X), y) : singular matrix 'a' in solve

```
lm.fit(X, y)$coefficients
```

```
x1 x2
1 NA
```

**Q:** how would we do this with SVD (`svd`), or Cholesky decomposition (`chol`)?

**side note: Bessel's correction**

- ESL gives  $\hat{\sigma}^2 = \frac{1}{N-p-1} \cdot \text{RSS}$ 
  - **note**  $p$  doesn't include the constant term/intercept column
- note unbiased estimate of the residual variance
- MLE would give  $\text{RSS}/N$
- unbiased estimate of resid std. error divides by  $N - 1.5$ ; minimum MSE (for Normal distribution) divides by  $N + 1$  (!)
- bias is scale-dependent ( $E(f(x)) \neq f(E(x))$  in general) and might not matter as much as you think

**prostate cancer example**

- data exploration: `pairs(., gap = 0)` (can be extended with `panel` function); `corrplot::corrplot.mixed(., lower="number", upper = "ellipse"); GGally::ggpairs()`. Can use `faraway::prostate`.

```
## a bit of data exploration
pp <- (prostate
```

```

|> mutate(across(
  where(~length(unique(.))<=4),
  factor))
)
ggpairs(pp)
corrplot::corrplot.mixed(cor(prostate),
  lower = 'number', upper = 'ellipse')

```

## train/test error

- hardly worth it for simple regression problems (measures like adjusted  $R^2$  and AIC(c) give reasonable estimates of out-of-sample error)

## Gauss-Markov theorem

- simple
- applicable as long as data are independent and homoscedastic (iid is stronger)
- MVUE (minimum-variance *unbiased* estimator)
- but **not** necessarily minimum MSE!

## regression by orthogonalization (3.2.3)

- build up regression by successive orthogonalization
  - regress  $\mathbf{x}_j$  on residuals of all previous columns ( $\mathbf{z}_0, \mathbf{z}_1, \dots, \mathbf{z}_j$ ) to get coefficients  $\hat{\gamma}_{\ell j}$ , residual  $\mathbf{z}_j$ .
  - regress  $\mathbf{y}$  on  $\mathbf{z}_p$  to get  $\hat{\beta}_p$
  - order???
- Gram-Schmidt orthogonalization (successive projection)
- if  $\mathbf{Z}$  is the residual columns and  $\Gamma$  is the (upper-triangular) matrix of  $\gamma_{\ell j}$ , then  $\mathbf{X} = \mathbf{Z}\Gamma$
- if  $\mathbf{D} = \text{Diag}(\|\mathbf{z}_j\|)$
- and  $\mathbf{X} = \mathbf{Z}\mathbf{D}^{-1}\mathbf{D}\Gamma = \mathbf{Q}\mathbf{R}$  with  $\mathbf{Q}$  orthonormal,  $\mathbf{R}$  upper triangular
- $\rightarrow$  standard decomposition!



## multiple outputs

- somewhat niche problem ...
- changing  $\mathbf{y}$  to  $\mathbf{Y}$ ,  $\beta$  to  $\mathbf{B}$ , the algebra mostly stays the same
- separate coefficients for each problem
- if homoscedastic, no need to consider correlation of observations!

## return to subset/stepwise selection

- still not sure it's worth it
- can update efficiently based on QR decomp
- forward-stagewise: **less** efficient
- **digression**: inefficiency as a virtue
  - improve bias-var tradeoff by *worsening* fit
  - early stopping, dropout, etc. etc.

## shrinkage methods

### ridge

- L2 penalty on coefficients
- predictors must be normalized! (scale of  $\beta_j$  depends on scale of  $x_j$ )
- equivalence between penalty ( $+\lambda \sum \beta^2$ ) and constraint ( $\sum \beta^2 \leq t$ )  
("one-to-one correspondence" between  $\lambda$  and  $t$ , but not simple!)
- add  $\lambda \mathbf{I}$  in the normal equations
- works for non-full-rank problems

### Bayesian analogue

- analogous to setting iid Gaussian prior on individual  $\beta$  parameters

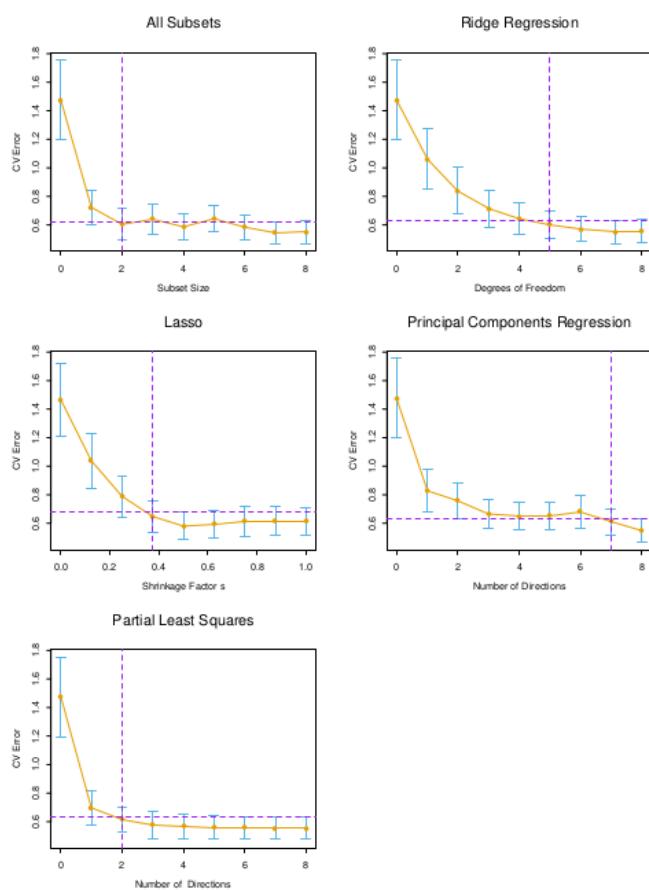


Figure 1: ESL fig 3.7

- $\log\text{-posterior} = \log\text{-likelihood} + \log\text{-prior} \propto \sigma^2\text{RSS} + \lambda \sum \beta^2$
- MAP (maximum *a posteriori*) estimate, **not** “proper” Bayesian est (mode, not mean, of posterior)

## solving ridge by QR

- note that we can solve ridge regression by introducing *pseudo-observations* (*data augmentation*)
- set

$$\mathbf{B} = \begin{pmatrix} \mathbf{X}^\top \mathbf{X} \\ \sqrt{\lambda} \mathbf{I} \end{pmatrix}$$

- and  $\mathbf{y}^* = (\mathbf{y} \ 0)$
- and solving  $(\mathbf{B}^\top \mathbf{B})\beta = \mathbf{B}^\top \mathbf{y}^*$  by QR decomposition (Atlas 2013)
- $\ll$  a trick for solving for successive  $\lambda$  values faster ... ?

Atlas. 2013. “QR Factorization for Ridge Regression.” *Mathematics Stack Exchange*. <https://math.stackexchange.com/questions/299481/qr-factorization-for-ridge-regression>.

## singular value decomposition

- if  $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$  then
 
$$\begin{aligned} \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} &= \mathbf{U}\mathbf{D}\mathbf{V}^\top (\mathbf{V}\mathbf{D}\mathbf{U}^\top \cdot \mathbf{U}\mathbf{D}\mathbf{V}^\top)^{-1} \mathbf{V}\mathbf{D}\mathbf{U}^\top \mathbf{y} \\ &= \mathbf{U}\mathbf{D}\mathbf{V}^\top (\mathbf{V}\mathbf{D}^2\mathbf{V}^\top)^{-1} \mathbf{V}\mathbf{D}\mathbf{U}^\top \mathbf{y} \\ &= \mathbf{U}\mathbf{U}^\top \mathbf{y} \end{aligned}$$
- and ridge translates to  $\sum \mathbf{u}_j \frac{d_j^2}{d_j^2 + \lambda} \mathbf{u}_j^\top \mathbf{y}$
- i.e. **shrinking the  $j^{\text{th}}$  principal component** by  $\frac{d_j^2}{d_j^2 + \lambda}$
- (if inputs are orthonormal all coefficients are shrunk equally)

## effective df

- this also shows that effective df = trace of hat matrix =  $\sum \frac{d_j^2}{d_j^2 + \lambda}$
- see also Hastie (2020)

Hastie, Trevor. 2020. “Ridge Regularization: An Essential Concept in Data Science.” *Technometrics* 62 (4): 426–33. <https://doi.org/10.1080/00401706.2020.1791959>.

## ridge projection

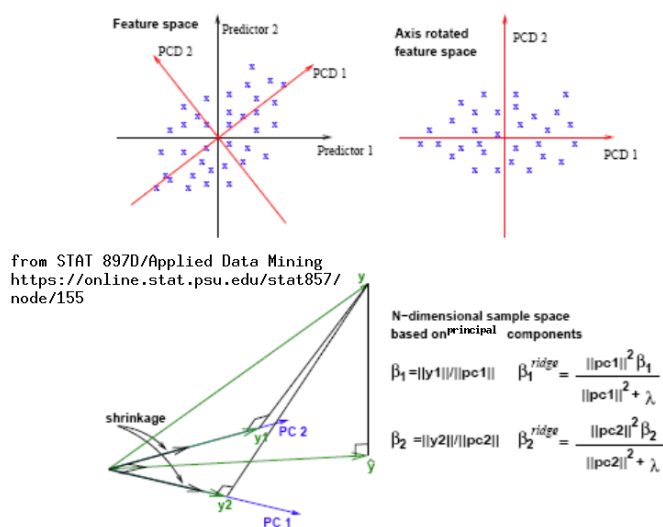


Figure 2: The Geometric interpretation of principal components and shrinkage by ridge regression.

## lasso

- L1 regularization
- **sparsity-inducing**
- least-angle regression (LARS): nice, but superseded (also, doesn't work for GLMs)
- `glmnet` et al. use cyclic/pathwise coordinate descent (Friedman, Hastie, and Tibshirani 2010) (also in [Julia analogue](#))
  - plus “warm-start” algorithm

## pathwise coordinate descent

- ESL § 3.8.6
- $\tilde{\beta}_k(\lambda)$  is **current** estimate of  $\beta_k(\lambda)$ . Then

Friedman, Jerome, Trevor Hastie, and Rob Tibshirani. 2010. “Regularization Paths for Generalized Linear Models via Coordinate Descent.” *Journal of Statistical Software* 33 (1): 1–22. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2929880/>.

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

- i.e. univariate lasso on  $j$  with  $k$  parameters fixed
- or lasso on *partial residual*  $(y_i - \tilde{y}_i^{(j)}) = y_i - \sum_{k \neq j} \tilde{\beta}_k(\lambda)$
- **solution:**

$$\tilde{\beta}_j(\lambda) \leftarrow S \left( \sum_{i=1}^N x_{ij} (y_i - \tilde{y}_i^{(j)}), \lambda \right)$$

- where  $S(t, \lambda) = \text{sign}(t)(|t| - \lambda)$
- can't do all  $\lambda$  automatically, but **warm start** algorithm works quickly
  - start with large  $\lambda$  such that all coefficients  $\rightarrow 0$
  - reduce in small steps, using values from previous  $\lambda$  to initialize
- how much worse does this get for other loss functions (e.g. GLMs)?

## other penalties

- could use  $L_p$  penalization with  $1 < p < 2$  (equivalent to a *generalized normal* or *exponential power* prior:  $\propto \exp(-|(x - \mu)/s|^p)$  (**gnorm** package)
- **elastic-net** (penalty  $\propto \alpha \sum \beta^2 + (1 - \alpha) \sum |\beta|$ )
  - computationally nicer and sparsity-inducing

## ridge vs lasso vs best-subset vs elastic net

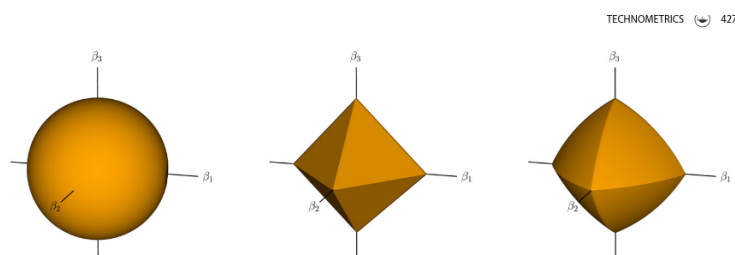


Figure 1. Constraint balls for ridge, lasso, and elastic-net regularization. The sharp edges and corners of the latter two allow for variable selection as well as shrinkage.

## and more penalties

- fit unrestricted (linear regression or other) model on lasso-selected variables (why??) (Zhao, Witten, and Shojaie 2021)
- **relaxed lasso**: re-fit lasso on selected variables (why??)
- **smoothly clipped absolute deviation** (SCAD):  $\lambda|\beta| \rightarrow J_a(\beta, \lambda)$ , with

$$\frac{dJ_a(\beta, \lambda)}{d\beta} = \lambda \cdot \text{sign}(\beta) \left[ I(|\beta| \leq \lambda) + \frac{(a\lambda - |\beta|)_+}{(a-1)\lambda} I(|\beta| > \lambda) \right]$$

for  $a \geq 2$

- **adaptive lasso**  $\approx |\beta|^{1-\nu}$

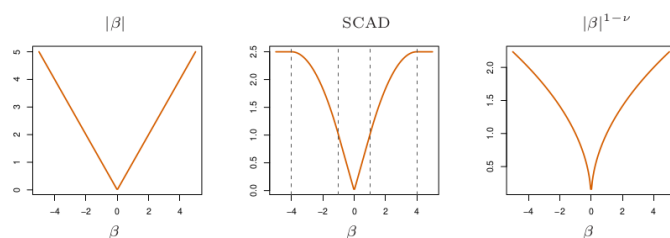


FIGURE 3.20. The lasso and two alternative non-convex penalties designed to penalize large coefficients less. For SCAD we use  $\lambda = 1$  and  $a = 4$ , and  $\nu = \frac{1}{2}$  in the last panel.

## grouped lasso

- ESL § 3.8.4; Yuan and Lin (2006)

Zhao, Sen, Daniela Witten, and Ali Shojaie. 2021. “In Defense of the In-defensible: A Very Naïve Approach to High-Dimensional Inference.” *Statistical Science* 36 (4): 562–77. <https://doi.org/10.1214/20-STS815>.

Yuan, Ming, and Yi Lin. 2006. “Model Selection and Estimation in Regression with Grouped Variables.” *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 68 (1): 49–67. <https://doi.org/10.1111/j.1467-9868.2005.00532.x>.

- lasso on groups of parameters: compute  $\|\beta_\ell\|_2$  by group ( $\beta_\ell$  is the sub-vector of parameters in group  $\ell$ , of length  $p_\ell$ )
- RSS criterion plus penalty

$$\lambda \sum_{\ell=1}^L \sqrt{p_\ell} \|\beta_\ell\|_2$$

\* reduces to lasso if every parameter is in a separate group  
 ( $\|c\|_2 = |c|$  if  $c$  is a scalar) \* ESL: “encourages sparsity at both the group and individual levels” \*  $\wr$ ridge-like within groups, lasso-like between groups

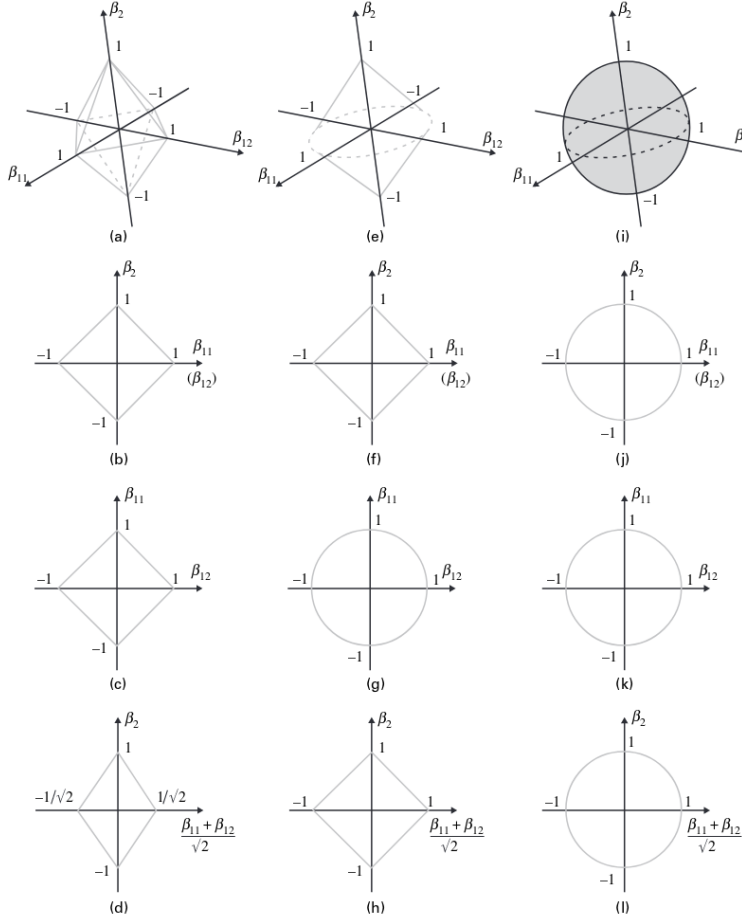


Fig. 1. (a)–(d)  $l_1$ -penalty, (e)–(h) group lasso penalty and (i)–(l)  $l_2$ -penalty

- `¿has someone written a formula-to-groupedlasso interface?`
- **sparse grouped lasso**: like elastic net (convex combination) but for regular lasso + grouped lasso

## finding packages

```
a1 <- available.packages()
grep("lasso", rownames(a1), ignore.case = TRUE, value = TRUE)
```

[1] "abglasso"	"ALassoSurvIC"	"BayesianGLasso"
[4] "biglasso"	"bolasso"	"BTdecayLasso"
[7] "BTLasso"	"CARlasso"	"CDLasso"
[10] "cglasso"	"clogitLasso"	"covglasso"
[13] "CVglasso"	"DIFlasso"	"DLASSO"
[16] "DWLasso"	"elasso"	"extlasso"
[19] "gamlss.lasso"	"genlasso"	"gglasso"
[22] "glamlasso"	"glasso"	"glassoFast"
[25] "glmLasso"	"GPCMLasso"	"grplasso"
[28] "grplassocat"	"hglasso"	"higlasso"
[31] "ipflasso"	"islasso"	"LassoBacktracking"
[34] "LassoGEE"	"LassoNet"	"lassopv"
[37] "lassoshooting"	"LassoSIR"	"lglasso"
[40] "mglasso"	"MSGlasso"	"MWLasso"
[43] "nnlasso"	"PabonLasso"	"PACLasso"
[46] "palasso"	"pcLasso"	"PCLassoReg"
[49] "ppmlasso"	"prioritylasso"	"sealasso"
[52] "sglasso"	"slasso"	"smoothedLasso"
[55] "SSLASSO"	"SummaryLasso"	"Tlasso"
[58] "vennLasso"	"VSOLassoBag"	

- also see `sos` package

## arm-waving

- optimization: scaling/robustness vs speed
- how do we decide on a 'best' model?



- run everything and compare on a test set? (Do we need another level of nested cross-validation?)
- appropriate metrics: fit quality? fit quality/time or within a time threshold?
- interpretability?
- analogue of [no free lunch theorem](#): “any two optimization algorithms are equivalent when their performance is averaged across all possible problems” (Wolpert and Macready 1997; Giraud-Carrier and Provost 2005)

Wolpert, D. H., and W. G. Macready. 1997. “No Free Lunch Theorems for Optimization.” *IEEE Transactions on Evolutionary Computation* 1 (1): 67–82. <https://doi.org/10.1109/4235.585893>.

Giraud-Carrier, Christophe, and Foster Provost. 2005. “Toward a Justification of Meta-Learning: Is the No Free Lunch Theorem a Show-Stopper?” *Proceedings of the ICML-2005 Workshop on Meta-Learning*, January.