

# Ridge regression and mixed models

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## Ridge in a nutshell

- **penalized** models: instead of minimizing  $SSQ = \sum ((y - \mathbf{X}\beta)_i)^2$ , minimize  $SSQ + \lambda ||\beta||_2$  (ridge)
- or  $+ ||\beta||_1$  (lasso)
- optimize *bias-variance tradeoff*
- equivalent to imposing iid Gaussian priors on each element of  $\beta$
- lasso (and elastic net, which is a convex combination of L2 and L1 penalties) are popular because they **induce sparsity**
  - *likelihood surfaces* are non-convex with cusps at zero
  - optimization with non-convex surfaces is a nuisance because it makes the basic optimization problem nonlinear; we need to use a different algorithm (coordinate descent/soft thresholding); can't use *only* linear algebra
- can generalize from penalized LM to penalized GLM

## Andrew Gelman on variable selection

Variable selection (that is, setting some coefficients to be exactly zero) can be useful for various reasons, including: \* It's a simple form of regularization. \* It can reduce costs in future data collection. Variable selection can be fine as a means to an end. Problems can arise if it's taken too seriously, for example as an attempt to discover a purported parsimonious true model.

## Choosing penalty strength

- typically by *cross-validation*
- leave-one-out (LOOCV) vs *k*-fold

## Practical points

- Predictors **must** be standardized
- Intercept should usually be unpenalized
- Avoid **data leakage**
  - don't include variables that are 'future' indicators of the outcome (e.g. see [here](#))
  - full pipeline must be cross-validated (i.e. don't do data-dependent variable selection *before* cross-validating, or use the full data set to select a pipeline)
  - cross-validation must account for structure in the data
  - **either** ensure that residuals are *conditionally* independent
  - **or** take account of grouping structures in the data (block bootstrap, spatial stratification, etc. Wenger and Olden (2012))

## Ridge vs lasso

- In practice people just try both (or elastic net)
- Conjecture: whether ridge or lasso is a better *predictive* model in a particular case depends on the *effect size spectrum*

## Ridge by data augmentation

- set

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

- and  $\mathbf{y}^* = (\mathbf{y} \ 0)$
- so that  $\mathbf{B}^\top \mathbf{B} = \mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}$  and the residual sum of squares is unchanged

## Inference

- inference from penalized models is really hard
- classical CIs for ridge are **identical** to OLS (Obenchain 1977) > ridge techniques do not generally yield new 'normal theory statistical inferences: in particular, ridge does not necessarily produce shifted' confidence regions.
- **no free lunch** (i.e., no true narrowing of CIs/decreased uncertainty without additional assumptions)
- post-selection inference is a big deal but requires very strong assumptions (asymptotic, 'gap')
- prediction intervals are often neglected (conformal prediction, jackknife+ (Barber et al. 2021)): [MAPIE](#)

## Practical

- `glmnet` is very good
- `ridge`, `lmridge`, ... (`library(sos); findFn("{ridge regression}")1`)
- need to give `y` and `X` directly (although see [glmnetUtils package](#))

## Tangent: how do I know if an R package is any good?

- how old is it/how many releases has it had?
- is it actively developed?
- does the documentation give literature citations?
- does it have reverse dependencies?
- what is its ranking on CRAN? `packageRank::packageRank("lmridge")` (80th percentile)

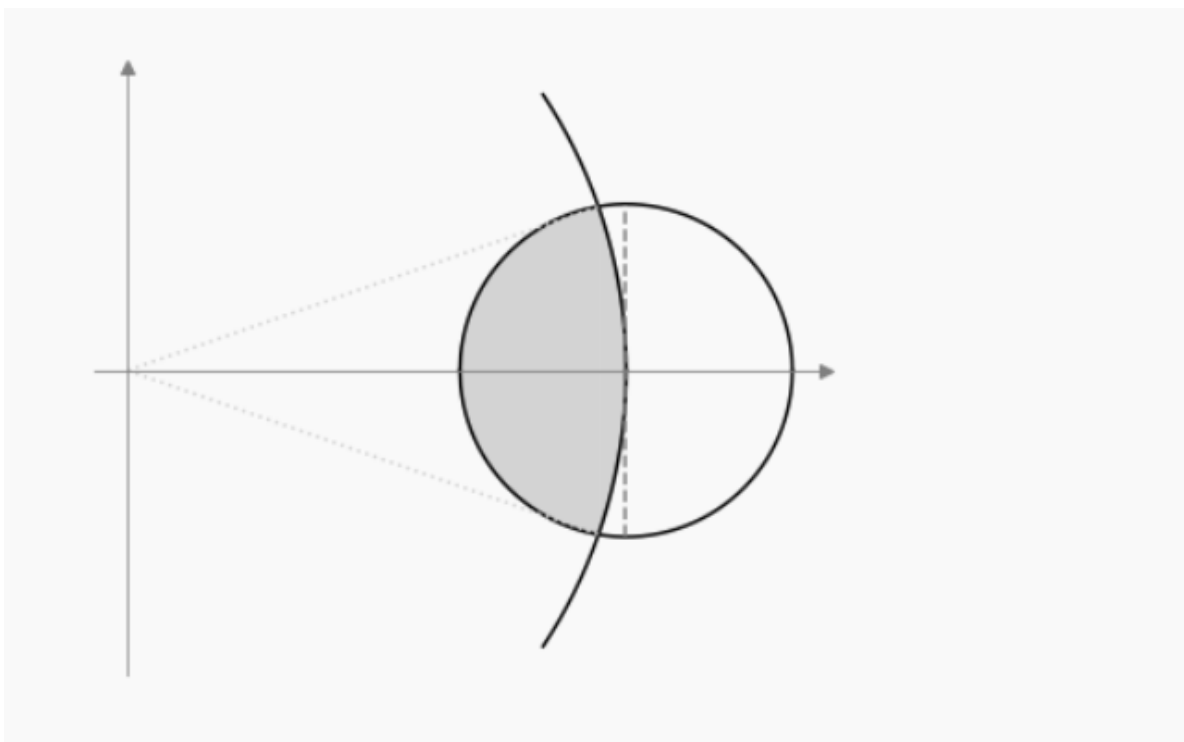
## James-Stein estimators

- more formally, why is ridge better?
- based on a single observation,  $\mathbf{y}$ , of a *multivariate* response with dimension  $m \geq 3$ , shrinking the value (usually toward zero) is a better estimate of the mean than the value itself (!)

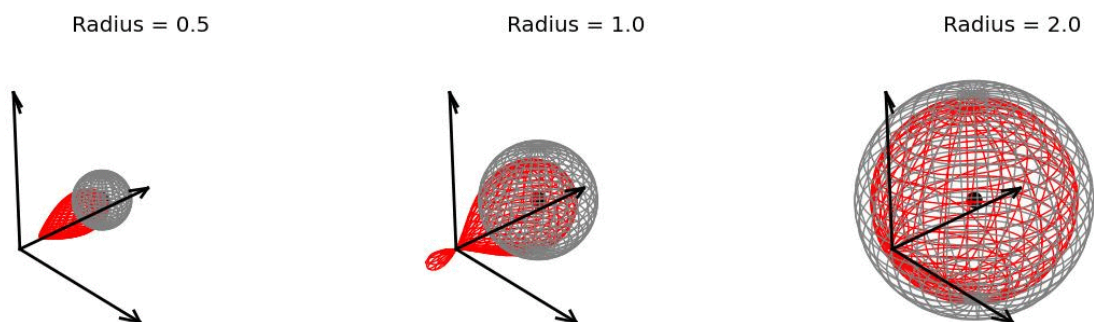
$$\hat{\mu}(X_1, \dots, X_n) = \left(1 - \frac{(p-2)\sigma^2/n}{\|\bar{X}_n\|^2}\right) \bar{X}_n$$

- (connected to recurrence of random walks in  $d \leq 2$ , non-recurrence in  $d \geq 3$  ...)
- “paradox”: the quantities in the vector don’t have to have anything to do with each other (and, we can shrink to any point, not necessarily zero ...)

From Antognini (2021):



From Harris (2013):



- van Houwelingen (2001) gives a very nice explanation/transition from James-Stein to penalized regression etc.

### From ridge to mixed models

i.e. treat this as an *empirical Bayesian* problem (we estimate the  $\beta$  values, but do not put a prior on  $\sigma^2$  or a hyperprior on  $\sigma_g^2 (= 1/\lambda)$ )

From van Houwelingen (2001) (ultimately from Efron and Morris 1972):

If we use a prior with  $\mu_i \sim N(\mu, \tau^2)$  (assuming residual variance is 1 wlog), then

$$E(\mu_i | X_i) = \mu + \frac{\tau^2}{\tau^2 + 1}(X_i - \mu)$$
$$var(\mu_i | X_i) = \frac{\tau^2}{\tau^2 + 1}$$

But we still have to estimate  $\tau$  (or  $\tau^2/(\tau^2 + 1)$ ) from the data).

### **MVN version**

We can be much more general:

$$\mathbf{y} \sim \text{Normal}(\mathbf{X}\beta, \sigma^2)$$
$$\beta \sim \text{MVN}(\mathbf{0}, \sigma_g^2 \mathbf{I})$$

### **Back to 1D**

The simplest case (described in an R formula as  $y \sim 1 + (1|g)$ ) is a model with a population-level intercept  $\beta_0$  and group-level deviations from the population mean  $b_i$ .

This case, and more complex cases, can be written as

$$y_i \sim \text{Normal}((\mathbf{X}\beta + \mathbf{Z}\mathbf{b})_i, \sigma_r^2)$$
$$\mathbf{b} \sim \text{MVN}(\mathbf{0}, \Sigma(\theta))$$

where  $\theta$  is a vector of parameters that defines the covariance matrix  $\Sigma$ .

## How do we estimate this?

- can use EM algorithm (e.g. see [here](#), or the [lmm package](#))
- Or by linear algebra. For LMMs, we do a more complicated version of *data augmentation*.
- given a value for the random-effects variance, we can calculate the log-likelihood in one step (see
- large, sparse matrix computation
- has to be done *repeatedly*
- most efficient if we analyze the matrix and permute to optimize structure (Bates et al. 2015)
- then we need to do some kind of search over the space of variances
- derivatives are available in particular special cases

## The general case

Given a model of the form

$$y_i \sim \text{Normal}((\mathbf{X}\beta + \mathbf{Z}\mathbf{b})_i, \sigma_r^2)$$
$$\mathbf{b} \sim \text{MVN}(\mathbf{0}, \Sigma(\theta))$$

- How do we specify and set up  $\mathbf{Z}$ ?
- How do we specify and set up  $\Sigma$ ?

## constructing the random-effects model matrix

- specify as  $(\tau | g)$ ;  $\tau$  is the *term* and  $g$  is the *grouping factor*
- for intercepts, just the indicator matrix
- for more complex models (random slopes), take the *Khatri-Rao* product of the model matrix of the term with the indicator matrix of  $g$
- concatenate multiple random effects terms into a single  $\mathbf{Z}$  matrix

## constructing the covariance matrix

- blockwise
- what's the best way to parameterize a positive-(semi)definite matrix? (Pinheiro and Bates 1996)
- Cholesky decomposition with
- scaled or unscaled?
- Cholesky or log-Cholesky scale?

- separating correlation and SD vectors: [glmmTMB](#):

$$\Sigma = D^{-1/2} L L^{\top} D^{-1/2}, \quad D = \text{diag}(L L^{\top})$$

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