Ridge regression and mixed models

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Ridge in a nutshell

- **penalized** models: instead of minimizing SSQ $= \sum((\mathbf{y}-\mathbf{X}\beta)_i)^2$, minimize SSQ $+ \lambda||\beta||_2$ (ridge)
- or $+ \lambda||\beta||_1$ (lasso)
- optimize *bias-variance tradeoff*
- equivalent to imposing iid Gaussian priors on each element of β
- 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 harder; we need to use a different algorithm (e.g. coordinate descent with *soft thresholding*, see Friedman, Hastie, and Tibshirani (2010)); can't use pure linear algebra or pure gradient descent/quasi-Newton
- generalizing from penalized LM to penalized GLM isn't too hard

Variable selection

Variable selection has some characteristics in common with multicollinearity and conditional Normality, i.e. that people generally overestimate its importance.

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.

Variable selection is a way of **inducing sparsity** in a model; thus it can also be computationally useful ...

Choosing penalty strength

- in ML/predictive contexts, typically by *cross-validation*
- leave-one-out (LOOCV) vs k-fold: bias/variance tradeoff (James et al. (2013) §5.1.4)
  - small folds (LOO); low bias (sample size $\approx$ total), but lots of overlap (correlation) between training sets, so high variance. Large folds (e.g. 2-fold), *vice versa*

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)
- Whether ridge or lasso is a better *predictive* model in a particular case depends on the *effect size spectrum*
- van Houwelingen (2001):

> The performance of any of these shrinkage estimators depends on the true value of $\mu_1, \ldots, \mu_k$. Simulation studies can never cover all possibilities. For given $\mu_1, \ldots, \mu_k$ that procedure performs best for which the corresponding prior model gives the best fit. Therefore, simulation studies that prove superiority of a particular procedure should always be mistrusted. They only show that the author managed to find some μ-configuration for which his procedures work[s] best. ...

... the LASSO will behave well if the βs look like coming from a double exponential distribution, that is many close to zero and some very big. The classic Ridge Regression will behave better if the histogram of the βs look[s] more normal.

Ridge by data augmentation

- set
$$\mathbf{B} = \begin{pmatrix} \mathbf{X} \\ \sqrt{\lambda}\mathbf{I} \end{pmatrix}$$
- and $\mathbf{y}^* = (\mathbf{y}\ \mathbf{0})$
- so that $\mathbf{B}^\top\mathbf{B} = \mathbf{X}^\top\mathbf{X} + \lambda I$ 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, ridging 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 (see work by Witten, Hastie, others) but requires strong assumptions (asymptotic, magnitude of smallest non-zero β)
- 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}")`)
- need to give `y` and `X` directly as in `[g]lm.fit()` (although see glmnetUtils package)

More on penalization

- also described as *regularization*, *shrinkage* estimator, or as equivalent to imposing a Bayesian prior
- we've already seen it (for dealing with complete separation)
- could use it for forcing negative binomial parameter away from $\theta = \infty$?

- we'll use a different form of penalization later to mitigate *singular* mixed-model fits (variance = 0)

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)

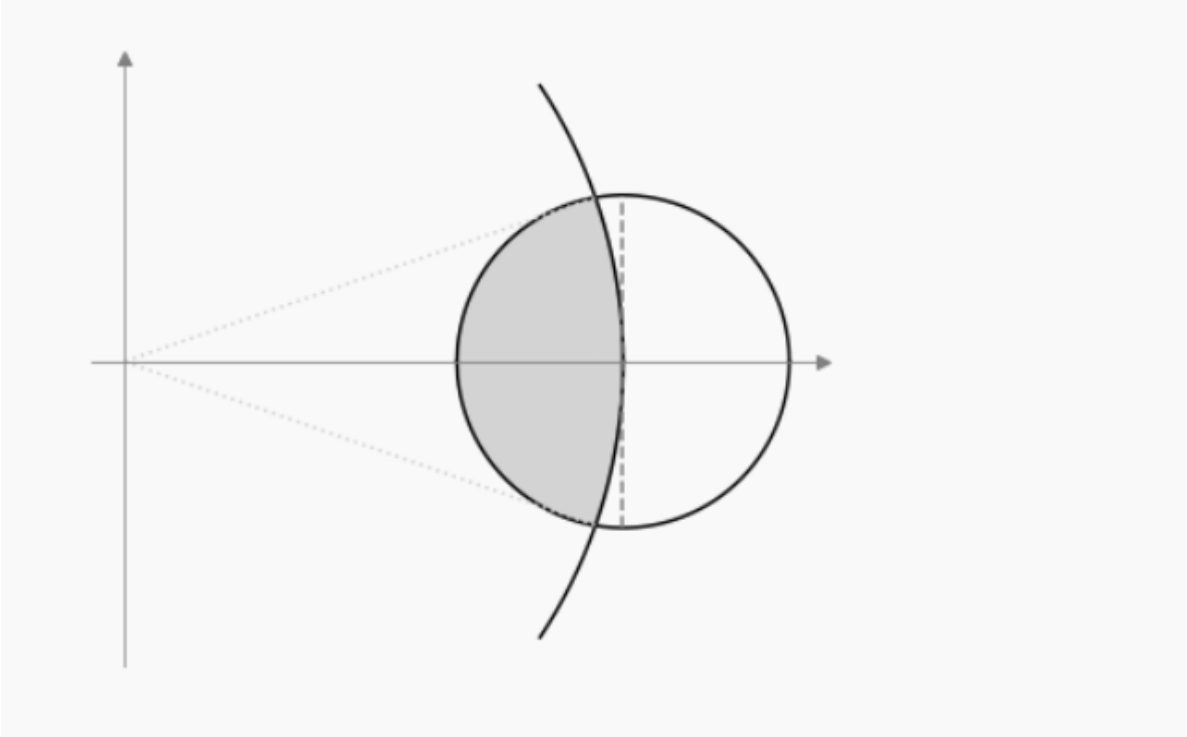
James-Stein estimators

- 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 (lower mean squared error) than the value itself.

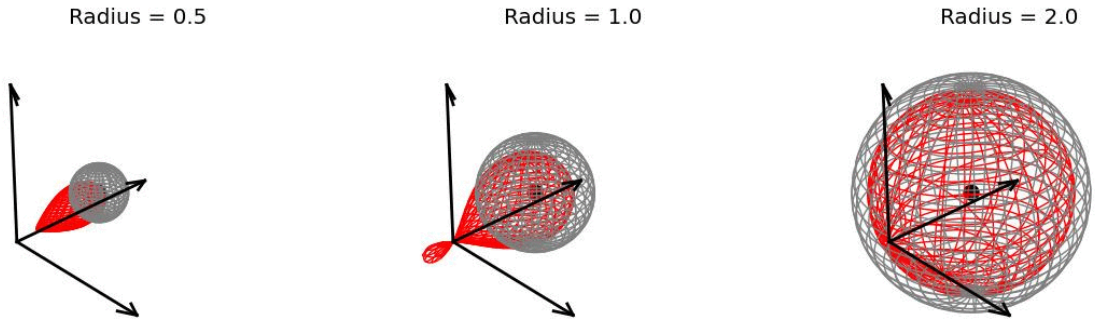
$$\hat{\mu}(X_1, \ldots, X_n) = \max\left(0, \left(1 - \frac{(m-2)\sigma^2/n}{||\bar{X}_n||^2}\right)\right) \bar{X}_n$$

- (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

From Antognini (2021): typical points in a cloud of uncertainty are farther from zero than the mean is



From Harris (2013): effects of J-S shrinkage



- 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 β values, but do not put a prior on σ^2 or a hyperprior on σ_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

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

But we still have to estimate τ (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 ~ 1 + (1|g)`) is a model with a population-level intercept β_0 and group-level deviations from the population mean b_i.

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

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

where θ is a vector of parameters that defines the covariance matrix Σ.

How do we estimate this?

- expectation-maximization (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 (Bates et al. 2015)
- 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

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

- How do we specify and set up Z?
- How do we specify and set up Σ?

constructing the random-effects model matrix

- specify as `(t|g)`; `t` 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 `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:
  - scaled or unscaled?
  - Cholesky or log-Cholesky scale?

– separating correlation and SD vectors: glmmTMB:

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

Key references

- Hastie, Tibshirani, and Friedman (2009) for ridge/lasso/elastic net
- Bates et al. (2015) for linear algebra underlying LMMs; incomplete MS on GLMM implementation here
- van Houwelingen (2001) for the connections between James-Stein, ridge and other penalties, and mixed models

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