

Concentration Reversals in Ridge Regression

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Abstract

Ridge regression is often the method of choice in ill-conditioned systems. A canonical form identifies regions in the parameter space where Ordinary Least Squares (*OLS*) is problematic. A curious but unrecognized property of ridge solutions emerges: Under spherical errors with or without moments, the relative concentrations of the canonical estimators reverse as the ridge scalar evolves, the estimators least concentrated under *OLS* being most concentrated under ridge regression, and conversely.

Key words: Ill-conditioned systems, least squares, ridge regression, concentration efficiency

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1. Introduction

A full-rank model $\{\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}\}$ yields *OLS* solutions $\widehat{\boldsymbol{\beta}}_L$, unbiased with minimal dispersion $V(\widehat{\boldsymbol{\beta}}_L) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ under conventional errors. Near-dependency among columns of \mathbf{X} , as ill-conditioning, “causes crucial elements of $\mathbf{X}'\mathbf{X}$ to be large and unstable,” $\widehat{\boldsymbol{\beta}}_L$ to be “very sensitive to small changes in \mathbf{X} ” with “inflated variances” Belsley (1986), p. 119. Remedies in wide usage include *ridge estimators* as solutions of $\{(\mathbf{X}'\mathbf{X} + k\mathbf{I}_p)\widehat{\boldsymbol{\beta}}_{Rk} = \mathbf{X}'\mathbf{Y}; k \geq 0\}$; see (Hoerl, 1962; Hoerl, 1964; Hoerl and Kennard, 1970) and a considerable

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further literature. A canonical form is $\{\mathbf{Y} = \mathbf{P}\mathbf{D}_\xi\boldsymbol{\theta} + \boldsymbol{\epsilon}\}$, where $\mathbf{P}'\mathbf{P} = \mathbf{I}_p$; $\mathbf{D}_\xi = \text{Diag}(\xi_1, \dots, \xi_p)$, ordered as $\{\xi_1 \geq \xi_2 \geq \dots \geq \xi_p\}$; and $\boldsymbol{\theta} = \mathbf{Q}'\boldsymbol{\beta}$, with \mathbf{Q} orthogonal. The *OLS* solutions $\hat{\boldsymbol{\theta}}_L = [\hat{\theta}_{L1}, \dots, \hat{\theta}_{Lp}]'$ identify “linear combinations of parameters about which the data at hand are most/least informative” (Thisted, 1987), since their variances $\{\sigma^2/\xi_1^2 \leq \sigma^2/\xi_2^2 \leq \dots \leq \sigma^2/\xi_p^2\}$ escalate for values of ξ_i^2 near zero, a mark of ill-conditioning. In consequence, as gauged by variances through Chebychev’s inequality, elements of $[\hat{\theta}_{L1}, \dots, \hat{\theta}_{Lp}]$ are successively less concentrated in probability about their means. It is germane in practice to ask whether this ordering is preserved as k evolves in ridge regression. To the contrary, we demonstrate under spherical errors that the canonical estimators reverse in peakedness as in Birnbaum (1948), with or without moments. An outline follows.

Notation and supporting materials are collected in Section 2. Section 3 sets forth the principal findings, to include conditions for reversal in concentration of ridge solutions as k evolves, and elementary but illuminating examples. Section 4 revisits a case study given elsewhere, and Section 5 offers a brief summary.

2. Preliminaries

2.1. Notation

Designate Euclidean p -space as \mathbb{R}^p , and its positive orthant as \mathbb{R}_+^p ; matrices and vectors are set in bold type; the transpose, inverse, and trace of \mathbf{A} are \mathbf{A}' , \mathbf{A}^{-1} , and $\text{tr}(\mathbf{A})$; special arrays are the identity \mathbf{I}_p and the diagonal matrix $\mathbf{D}_\mathbf{a} = \mathbf{D}(a_i) = \text{Diag}(a_1, \dots, a_p)$. Let \mathbf{X} , of order $(n \times p)$, have rank $p < n$; its *singular decomposition* is $\mathbf{X} = \mathbf{P}\mathbf{D}_\xi\mathbf{Q}'$, where $\mathbf{D}_\xi = \text{Diag}(\xi_1, \dots, \xi_p)$ comprise its ordered *singular values* $\{\xi_1 \geq \xi_2 \geq \dots \geq \xi_p > 0\}$; and the columns of $\mathbf{P} = [\mathbf{p}_1, \dots, \mathbf{p}_p]$ and of $\mathbf{Q} = [\mathbf{q}_1, \dots, \mathbf{q}_p]$ are the *left-* and *right-singular vectors* of \mathbf{X} , such that $\mathbf{P}'\mathbf{P} = \mathbf{I}_p$ and \mathbf{Q} is orthogonal. This in turn supports the canonical form $\{\mathbf{Y} = \mathbf{P}\mathbf{D}_\xi\boldsymbol{\theta} + \boldsymbol{\epsilon}\}$ for the model $\{\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}\}$ of Section 1, with $(\mathbf{Y}, \boldsymbol{\epsilon}) \in \mathbb{R}^n$, \mathbf{X} of order $(n \times p)$, and $(\boldsymbol{\beta}, \boldsymbol{\theta}) \in \mathbb{R}^p$. In particular, the

canonical ridge equations are $\{(D_\xi^2 + kI_p)\hat{\theta}_{Rk} = D_\xi P'Y; k \geq 0\}$, with $\hat{\theta}_{Rk} = [\hat{\theta}_{Rk}^1, \dots, \hat{\theta}_{Rk}^p]'$.

2.2. Stochastic Concepts

The expectation, dispersion, and law of distribution of $\mathbf{Z} \in \mathbb{R}^p$ are $E(\mathbf{Z})$, $V(\mathbf{Z})$, and $\mathcal{L}(\mathbf{Z})$; moreover, $F_Z(\mathbf{z})$ and $g_Z(\mathbf{t})$ designate its cumulative distribution (*cdf*) and characteristic (*chf*) functions. Following Birnbaum (1948), a probability measure μ on \mathbb{R}^1 is said to be *more peaked* about a than is ν about b on \mathbb{R}^1 , if their translates are ordered as $\mu_a([-c, c]) \geq \nu_b([-c, c])$ for every $c \geq 0$, where $\mu_a([u, v]) = \mu([u - a, v - a])$. Designate this ordering as $\mu \succeq_B \nu$, choosing a and b in context. Further denote by Γ the *order-determining class* on \mathbb{R}^1 , *i.e.*, functions that are even, continuous, and increasing on $[0, \infty)$. The following essential result is from Jensen and Foutz (1989).

Lemma 1. *Let $\{F((x - \theta)/\sigma); (\theta, \sigma) \in \mathbb{R}^1 \times \mathbb{R}_+^1\}$ be a location-scale family of cdfs on \mathbb{R}^1 , each symmetric about θ , and let (μ, ν) be probability measures on \mathbb{R}^1 .*

(i) *For fixed θ , the scale family $\{F((x - \theta)/\sigma); \sigma \in \mathbb{R}_+^1\}$ decreases monotonically in peakedness about θ as σ increases.*

(ii) *The ordering $\mu \succeq_B \nu$ holds if and only if*

$$\int_{-\infty}^{\infty} \gamma(x) d\mu_a(x) \leq \int_{-\infty}^{\infty} \gamma(y) d\nu_b(y) \quad (2.1)$$

for every function $\gamma \in \Gamma$ for which both expectations are defined.

Symmetric errors for $\{\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}\}$, not necessarily having moments, arise in practical circumstances to be noted. Specifically, suppose the error *chf* is $g(\mathbf{t}) = \phi(\sigma^2 \mathbf{t}'\mathbf{t})$ defined on $[0, \infty)$. Then the error distribution $\mathcal{L}(\boldsymbol{\epsilon})$ is called *spherical* on \mathbb{R}^n , to be designated as $\mathcal{L}(\boldsymbol{\epsilon}) = \mathcal{S}_n(\mathbf{0}, \sigma^2 \mathbf{I}_n)$, centered at $\mathbf{0} \in \mathbb{R}^n$ with $\sigma^2 \mathbf{I}_n$ as scale parameters. Examples of note include spherical Cauchy and Gaussian errors in \mathbb{R}^n . Elementary properties of *chfs* imply that $g_Y(\mathbf{t}) = e^{i\mathbf{t}'\mathbf{X}} \phi(\mathbf{t}'\mathbf{t})$ at $\sigma^2 = 1.0$ and, under the affine transformation $\{\mathbf{Y} \rightarrow \mathbf{Z} = \mathbf{A}'\mathbf{Y} + \mathbf{b}\}$ with $\mathbf{A}(n \times k)$ and $\mathbf{b} \in \mathbb{R}^k$, that $g_Z(\mathbf{s}) = e^{i\mathbf{s}'(\mathbf{A}'\mathbf{X} + \mathbf{b})} \phi(\mathbf{s}'\mathbf{A}'\mathbf{A}\mathbf{s})$. The

resulting distribution, having elliptical contours and centered at $\mathbf{A}'\mathbf{X}\boldsymbol{\beta} + \mathbf{b}$, is designated as $\mathcal{L}(\mathbf{Z}) = \mathcal{S}_k(\mathbf{A}'\mathbf{X}\boldsymbol{\beta} + \mathbf{b}, \mathbf{A}'\mathbf{A})$. We return to these error structures subsequently.

3. The Principal Findings

3.1. Ridge Reversals

At issue are concentrations in probability of elements of $\hat{\boldsymbol{\theta}}$ for estimating $\boldsymbol{\theta} \in \mathbb{R}^p$. Under second moments the ordered variances

$$\{\text{Var}(\hat{\theta}_{L1}) \leq \text{Var}(\hat{\theta}_{L2}) \leq \dots \leq \text{Var}(\hat{\theta}_{Lp})\}, \quad (3.1)$$

together with Chebychev inequalities, suffice to order $\{\hat{\theta}_{L1}, \hat{\theta}_{L2}, \dots, \hat{\theta}_{Lp}\}$ from most to least concentrated about their means, as noted earlier. Since the ridge solutions $\hat{\boldsymbol{\theta}}_{Rk}$ are *OLS* at $k = 0$, we seek to determine whether this ordering persists among $\{\hat{\theta}_{Rk}^1, \hat{\theta}_{Rk}^2, \dots, \hat{\theta}_{Rk}^p\}$ as k evolves. Although second moments conform to conventional Gauss–Markov theory, instead we take the error distribution to be *spherical*, with or without moments, *i.e.*, $\mathcal{L}(\boldsymbol{\epsilon}) = \mathcal{S}_n(\mathbf{0}, \sigma^2 \mathbf{I}_n)$, $g(\mathbf{t}) = \phi(\sigma^2 \mathbf{t}'\mathbf{t})$, and $\mathcal{L}(\mathbf{Y}) = \mathcal{S}_n(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n)$, with $(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n)$ as location and scale parameters. On occasion it suffices to take $\sigma^2 = 1.0$. It is shown in Jensen (1997) that elements of $\hat{\boldsymbol{\beta}}_L$ (i) are *median-unbiased* through symmetry, (ii) are *unbiased in mean* under first moments, and (iii) are *modal-unbiased* under unimodal errors. Noting that $\{\hat{\theta}_{L1}, \hat{\theta}_{L2}, \dots, \hat{\theta}_{Lp}\}$ typically differ in location, as do $\{\hat{\theta}_{Rk}^1, \hat{\theta}_{Rk}^2, \dots, \hat{\theta}_{Rk}^p\}$, we proceed to compare the Birnbaum (1948) peakedness about their respective centering parameters. Details follow, where $\{\mathbf{Y} = \mathbf{P}\mathbf{D}_\xi \boldsymbol{\theta} + \boldsymbol{\epsilon}\}$ and $\{\mathbf{U} = \mathbf{P}'\mathbf{Y}\}$ give the reduced form $\{\mathbf{U} = \mathbf{D}_\xi \boldsymbol{\theta} + \mathbf{P}'\boldsymbol{\epsilon}\}$, together with $g_Y(\mathbf{t}) = e^{i\mathbf{t}'\mathbf{P}\mathbf{D}_\xi} \phi(\mathbf{t}'\mathbf{t})$ and $g_U(\mathbf{r}) = e^{i\mathbf{r}'\mathbf{D}_\xi} \phi(\mathbf{r}'\mathbf{r})$, with $\mathbf{r} \in \mathbb{R}^p$. The pivotal *chfs* for $\hat{\boldsymbol{\theta}}_{Rk}$ are

$$\{g_{Rk}^-(\mathbf{s}) = e^{i\mathbf{s}'\mathbf{D}(\xi_i^2/(\xi_i^2+k))} \phi(\mathbf{s}'\mathbf{D}(\xi_i^2/(\xi_i^2+k)^2)\mathbf{s}); k \geq 0\}, \quad (3.2)$$

where $\mathbf{D}(\omega_i) = \text{Diag}(\omega_1, \dots, \omega_p)$; $g_{Rk}^-(\mathbf{s})$ follows at $k = 0$; and under second moments, $\{\hat{\theta}_{Rk}^1, \hat{\theta}_{Rk}^2, \dots, \hat{\theta}_{Rk}^p\}$ are mutually uncorrelated in view of their diagonal second-moment matrix. Moreover, on setting in succession all elements of

\mathbf{s} but one to zero, we deduce that the marginal *chfs* are

$$\{g_{\hat{\theta}_{Rk}^j}(s_j) = e^{is_j\xi_j^2\theta_j/(\xi_j^2+k)}\phi(s_j^2\xi_j^2/(\xi_j^2+k)^2); 1 \leq j \leq p\}. \quad (3.3)$$

Subsequently designate $C_e(\hat{\theta}_{Rk}^j) = \xi_j^2\theta_j/(\xi_j^2+k)$ and $S_c(\hat{\theta}_{Rk}^j) = \xi_j^2/(\xi_j^2+k)^2$ as their respective location and scale parameters where, owing to symmetry, $C_e(\hat{\theta}_{Rk}^j)$ serves as the *center of symmetry* or the *centering parameter* of the corresponding marginal distribution.

We next examine the pair-wise ordering $\mu \succeq_B \nu$ among $\{\hat{\theta}_{L1}, \hat{\theta}_{L2}, \dots, \hat{\theta}_{Lp}\}$, and its evolution with k among $\{\hat{\theta}_{Rk}^1, \hat{\theta}_{Rk}^2, \dots, \hat{\theta}_{Rk}^p\}$, all such comparisons to be taken as peakedness about the respective centers of symmetry.

Theorem 1. Consider ridge solutions in $\{(\mathbf{D}_\xi^2+k\mathbf{I}_p)\hat{\boldsymbol{\theta}}_{Rk} = \mathbf{D}_\xi\mathbf{U}; k \geq 0\}$ under spherical errors having scale parameters $\{S_c(\hat{\theta}_{Rk}^j) = \xi_j^2/(\xi_j^2+k)^2; 1 \leq j \leq p\}$ such that $\{\xi_1^2 \geq \xi_2^2 \geq \dots \geq \xi_p^2 > 0\}$.

(i) OLS solutions are ordered in peakedness as $\{\mathcal{L}(\hat{\theta}_{L1}) \succeq_B \mathcal{L}(\hat{\theta}_{L2}) \succeq_B \dots \succeq_B \mathcal{L}(\hat{\theta}_{Lp})\}$.

(ii) Ridge solutions reverse in peakedness from OLS, i.e., $\mathcal{L}(\hat{\theta}_R^j(k)) \succeq_B \mathcal{L}(\hat{\theta}_R^i(k))$ for $j > i$, if and only if $k > \xi_i\xi_j$.

(iii) Ridge solutions preserve the order of OLS for $k \leq \min\{\xi_i\xi_j\}$.

(iv) Complete reversal $\{\mathcal{L}(\hat{\theta}_{Rk}^p) \succeq_B \dots \succeq_B \mathcal{L}(\hat{\theta}_{Rk}^1)\}$ occurs at $k > \max\{\xi_i\xi_j\}$.

(v) Let $(\hat{\theta}_1, \hat{\theta}_2)$ be any such scalar estimators centered at (θ_1, θ_2) , under spherical errors having finite moments $E(\epsilon_i^{2r})$, such that $\mathcal{L}(\hat{\theta}_1) \succeq_B \mathcal{L}(\hat{\theta}_2)$. Then even moments are ordered as

$$\{E(\hat{\theta}_1 - \theta_1)^{2j} \leq E(\hat{\theta}_2 - \theta_2)^{2j}; 1 \leq j \leq r\};$$

odd moments $\{E(\hat{\theta} - \theta)^{2r-1}; 1 \leq j \leq r\}$ vanish for both; and absolute moments satisfy

$$\{E|\hat{\theta}_1 - \theta_1|^{2r-1} \leq E|\hat{\theta}_2 - \theta_2|^{2r-1}; 1 \leq j \leq r\}.$$

Proof. For a typical $\hat{\tau}_j = [\hat{\theta}_j - C_e(\hat{\theta}_j)]$ at issue here, all marginal distributions have *chfs* of the type $g_{\hat{\tau}_j}(s_j) = \phi(\omega_j s_j^2)$. These all belong to the same scale family, determined by $\phi(\cdot)$, symmetric about $0 \in \mathbb{R}^1$ since $\phi(s^2)$ is an even

function. Conclusion (i) follows on successive applications of Lemma 1(i), since $\{\omega_1 \leq \omega_2 \leq \dots \leq \omega_p\}$ with $\{\omega_j = 1/\xi_j^2; 1 \leq j \leq p\}$. To continue, for $i < j$ and $\xi_i^2 > \xi_j^2$, it suffices to compute the difference $S_c(\hat{\theta}_R^i(k)) - S_c(\hat{\theta}_R^j(k))$ in scale parameters as

$$\frac{\xi_i^2}{(\xi_i^2 + k)^2} - \frac{\xi_j^2}{(\xi_j^2 + k)^2} = \frac{\xi_i^2(\xi_j^2 + k)^2 - \xi_j^2(\xi_i^2 + k)^2}{(\xi_i^2 + k)^2(\xi_j^2 + k)^2}. \quad (3.4)$$

The numerator is $\xi_i^2\xi_j^4 - \xi_i^4\xi_j^2 + k^2(\xi_i^2 - \xi_j^2)$ which, on letting $\xi_i^2 = \xi_j^2 + \delta$ with $\delta > 0$, becomes

$$(\xi_j^2 + \delta)\xi_j^4 - (\xi_j^2 + \delta)^2\xi_j^2 + k^2(\xi_j^2 + \delta - \xi_j^2) = \delta[k^2 - \xi_j^2(\xi_j^2 + \delta)]. \quad (3.5)$$

The latter is positive, so that $S_c(\hat{\theta}_R^i(k)) > S_c(\hat{\theta}_R^j(k))$ and $\mathcal{L}(\hat{\theta}_R^j(k)) \succeq_B \mathcal{L}(\hat{\theta}_R^i(k))$, if and only if $k^2 > \xi_i^2\xi_j^2$, as asserted in conclusion (ii). Conclusions (iii) and (iv) follow on repeated applications of (ii). Conclusion (v) follows from Lemma 1(ii) on noting that all central and absolute central moments, as listed, belong to the order-determining class Γ of Lemma 1. All odd central moments vanish by symmetry. \square

Remark 1. The ordering \succeq_B substantially transcends the variance ordering of *OLS* as in (3.1). Specifically, under first moments Theorem 1(v) implies the L^1 ordering $E(|\hat{\theta}_1 - C_e(\hat{\theta}_1)|) < E(|\hat{\theta}_2 - C_e(\hat{\theta}_2)|)$ when $\omega_1 < \omega_2$, as well as the L^2 ordering $E[\hat{\theta}_1 - C_e(\hat{\theta}_1)]^2 < E[\hat{\theta}_2 - C_e(\hat{\theta}_2)]^2$ under second moments.

Remark 2. Under third moments the quantity $E(|\hat{\theta}_1 - C_e(\hat{\theta}_1)|^3)$ figures prominently in central limit theory, in constructing Berry–Esseen bounds on rates of convergence. Smaller values ensure tighter bounds.

Remark 3. Spherical Student t error distributions on ν degrees of freedom trace to Zellner (1976), but with no apparent contact with ridge regression. Nonetheless, it is remarkable that the canonical estimators exhibit the peakedness orderings of Theorem 1(i)–(iv), even for spherical Cauchy errors at $\nu = 1$ having heavy tails devoid of first moments.

3.2. Example

To illustrate, suppose that $p = 3$; $\boldsymbol{\beta} = [\beta_1, \beta_2, \beta_3]'$; and $\mathbf{X}'\mathbf{X}$, its inverse $(\mathbf{X}'\mathbf{X})^{-1}$, and the matrix \mathbf{Q} are given in succession by

$$\begin{bmatrix} 2.97 & 0 & 0 \\ 0 & 0.015 & 0.005 \\ 0 & 0.005 & 0.015 \end{bmatrix}, \begin{bmatrix} \frac{1}{2.97} & 0 & 0 \\ 0 & 75.00 & -25.00 \\ 0 & -25.00 & 75.00 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}. \quad (3.6)$$

The spectral decomposition $\mathbf{X}'\mathbf{X} = \mathbf{Q}\mathbf{D}_\xi^2\mathbf{Q}'$ gives $\mathbf{D}_\xi^2 = \text{Diag}(2.97, 0.02, 0.01)$ and \mathbf{Q} as displayed. The canonical form $\boldsymbol{\theta} = \mathbf{Q}'\boldsymbol{\beta}$ specifies $\theta_1 = \beta_1$, $\theta_2 = (\beta_2 + \beta_3)/\sqrt{2}$, and $\theta_3 = (\beta_2 - \beta_3)/\sqrt{2}$. Moreover, $\text{V}(\hat{\boldsymbol{\theta}}_L) = \text{Diag}(0.336700, 50, 100)$ under second moments, and the condition number $c_1(\mathbf{X}'\mathbf{X}) = \xi_1^2/\xi_3^2 = 297.0$ is the ratio, $\text{Var}(\hat{\theta}_3)/\text{Var}(\hat{\theta}_1)$, of variances of the least to the most precisely estimated linear functions.

If instead we take $\mathcal{L}(\boldsymbol{\epsilon}) = \mathcal{S}_n(\mathbf{0}, \mathbf{I}_n)$, we may track the comparative peakedness of the estimators *via* Theorem 1. Observe that $k = 0.25 > \xi_1\xi_2 = 0.243721 > \xi_1\xi_3 = 0.172337 > \xi_2\xi_3 = 0.014142$. The scale matrix for ridge estimators at $k = 0.25$ is now $S_c(\hat{\boldsymbol{\theta}}_{Rk}) = \text{Diag}(0.286447, 0.274348, 0.147929)$. Progressing from $k = 0$ for *OLS*, to $k = 0.25$ for ridge, has seen a complete reversal in peakedness for estimating $\boldsymbol{\theta} = [\theta_1, \theta_2, \theta_3]'$. In particular, $\hat{\theta}_3$, least precise under *OLS* for the contrast $\theta_3 = (\beta_2 - \beta_3)/\sqrt{2}$, now has greatest peakedness at approximately half the scale parameters of $\hat{\theta}_1$ and $\hat{\theta}_2$, all as ridge estimators at $k = 0.25$. On the other hand, Theorem 1(iii) assures that no reversals in peakedness might occur among ridge estimates for $k \leq 0.014142$.

4. Case Studies

4.1. The Setting

As reported in Myers (1990), the Hospital Manpower Data consist of records at $n = 17$ U.S. Naval Hospitals, to include: Monthly man-hours (Y); Average daily patient load (X_1); Monthly X-ray exposures (X_2); Monthly

occupied bed days (X_3); Eligible population in the area \div 1000 (X_4); and Average length of patients' stay in days (X_5). The working model is

$$\{Y_i = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4 + \beta_5 X_5 + \epsilon_i; 1 \leq i \leq 17\}. \quad (4.1)$$

Following conventional usage, we center and scale to $\{\mathbf{Y} = \mathbf{Z}\boldsymbol{\beta} + \boldsymbol{\epsilon}\}$ with $\mathbf{Z}'\mathbf{Z}$ in correlation form, our focus being the rates of change $\boldsymbol{\beta} = [\beta_1, \beta_2, \beta_3, \beta_4, \beta_5]'$. The data are given in Table 3.8 of Myers (1990), pp.132–133, and computations reported here utilize PROC IML of the SAS Programming System. The data are remarkably ill-conditioned: Singular values of \mathbf{Z} are $\mathbf{D}_\xi = \text{Diag}(2.048687, 0.816997, 0.307625, 0.201771, 0.007347)$, and the condition number is $c_1(\mathbf{Z}'\mathbf{Z}) = 77,754.86$.

4.2. Ridge Regression

A striking diversity in choices for k has evolved, reflecting the problem as less than well-posed, often with profound differences among the solutions.

Table 1: Choices for k in the Hospital Manpower Data corresponding to conventional criteria DF_k , GCV_k , C_k , $PRESS_k$, and HKB_k .

Name	DF_k	GCV_k	C_k	$PRESS_k$	HKB_k
Value for k	0.0004	0.004787	0.0050	0.2300	0.616964

Selected choices in wide usage are identified in Table 1, together with their values for the Hospital Manpower Data. These encompass $DF_k = \text{tr}(\mathbf{H}_k) = \sum_{i=1}^p \xi_i^2 / (\xi_i^2 + k)$ with $\mathbf{H}_k = [\mathbf{Z}(\mathbf{Z}'\mathbf{Z} + k\mathbf{I}_p)^{-1}\mathbf{Z}']$; $PRESS_k = \sum_{i=1}^n e_{(i,\lambda)}^2$ as the cross-validation statistic of Allen (1974); $GCV_k = SS_{Res,k} / [n - (1 + \text{tr}(\mathbf{H}_k))]^2$, a rotation-invariant analog called *Generalized Cross Validation* in Golub et al. (1979); $C_k = [(SS_{Res,k} / \hat{\sigma}^2) - n + 2 + 2\text{tr}(\mathbf{H}_k)]$ to achieve a variance-bias trade-off (Mallows, 1973); and $HKB_k = \hat{\sigma}^2 / \hat{\boldsymbol{\beta}}_L' \hat{\boldsymbol{\beta}}_L$ as in Hoerl et al. (1975) from simulation studies. Here $SS_{Res,k}$ is the residual sum of squares using ridge regression; $\hat{\sigma}^2$ is the OLS residual mean square; and $\{e_{(i,\lambda)}^2\}$ are the

PRESS residuals from ridge regression. For further details see Myers (1990), pp. 392–411, including numerical values for DF_k , C_k , and $PRESS_k$ as reported here. The ridge parameter k can be estimated by different methods. For more details on the estimation of k , we refer to Kibria (2003) and Muniz and Kibria (2009), among others.

These choices carry hidden consequences regarding the concentration reversals of Theorem 1. Table 2 displays threshold values as products $\{\xi_i\xi_j; i < j\}$.

Table 2: Products $\{\xi_i\xi_j; i < j\}$ for elements of $\mathbf{D}_\xi = \text{Diag}(\xi_1, \dots, \xi_5)$ as singular values for \mathbf{Z} in the Hospital Manpower Data.

ξ_i	$\xi_2=0.816997$	$\xi_3=0.307625$	$\xi_4=0.201771$	$\xi_5=0.007347$
$\xi_1=2.048687$	1.673771	0.630228	0.413365	0.015052
$\xi_2=0.816997$		0.251329	0.164846	0.006003
$\xi_3=0.307625$			0.062070	0.002260
$\xi_4=0.201771$				0.001482

From the matrix $\mathbf{Q} = [\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4, \mathbf{q}_5]$, it is clear that $\theta_1 = \mathbf{q}'_1\boldsymbol{\beta}$ resembles a scaled average of $\{\beta_1, \beta_2, \beta_3, \beta_4, \beta_5\}$, since $\mathbf{q}'_1 = [0.485286, 0.453235, 0.484977, 0.460969, 0.333737]$. At the other extremity, $\theta_5 = \mathbf{q}'_5\boldsymbol{\beta}$, with $\mathbf{q}'_5 = [-0.719480, -0.001160, 0.694081, 0.023436, 0.006780]$, is a near linear contrast between $\{\beta_1, \beta_2\}$ and $\{\beta_3, \beta_4, \beta_5\}$, since the inner product $\mathbf{1}'_5\mathbf{q}_5 = 0.003657$ is approximately zero.

As noted, the *OLS* estimates $\{\hat{\theta}_{L1}, \hat{\theta}_{L2}, \hat{\theta}_{L3}, \hat{\theta}_{L4}, \hat{\theta}_{L5}\}$ exhibit successively diminished precision, as do concentrations of ridge estimates for $k \leq 0.001482$ from Theorem 1(iii). Since $GCV_k = 0.004787$ and $C_k = 0.0050$ exceed both thresholds $\xi_3\xi_5 = 0.002260$ and $\xi_4\xi_5 = 0.001482$, we find that ridge solutions for those choices of k now estimate the near contrast $\theta_5 = \mathbf{q}'_5\boldsymbol{\beta}$, with concentration greater than of $\{\hat{\theta}_{Rk}^3, \hat{\theta}_{Rk}^4\}$. Similarly, since $PRESS_k = 0.2300$ exceeds all of $\{\xi_1\xi_5 = 0.015052, \xi_2\xi_5 = 0.006003, \xi_2\xi_4 = 0.164846, \xi_3\xi_4 = 0.062070, \xi_3\xi_5 = 0.002260, \xi_4\xi_5 = 0.001482\}$, we may assert that the ridge estimate $\hat{\theta}_{Rk}^5$ at $k = 0.2300$ now is most concentrated, with scale parameter smaller than for

$\{\hat{\theta}_{Rk}^1, \hat{\theta}_{Rk}^2, \hat{\theta}_{Rk}^3, \hat{\theta}_{Rk}^4\}$, and that $\hat{\theta}_{Rk}^4$ is more concentrated than $\{\hat{\theta}_{Rk}^2, \hat{\theta}_{Rk}^3\}$, no further reversals being apparent. If instead the choice were $HKB_k = 0.616964$, then the only non-reversals in peakedness, in comparison with both *OLS* and with ridge estimators at $k \leq 0.001482$, are between $(\hat{\theta}_{Rk}^1, \hat{\theta}_{Rk}^2)$ and $(\hat{\theta}_{Rk}^1, \hat{\theta}_{Rk}^3)$. All such reversals emerge as unintended consequences of the widely divergent values for k as derived from various *ad hoc* desiderata.

Observe that the foregoing phenomena could have been discovered numerically, apart from σ^2 , on evaluating $V(\hat{\theta}_{Rk})$ under second moments, equivalently $S_c(\hat{\theta}_{Rk})$ under spherical errors, for cases of note. The advantage of Theorem 1 is that it supports inequality assertions for $\{k > \xi_i \xi_j\}$ generally, and for $\{k \leq \min\{\xi_i \xi_j\}\}$ and $\{k > \max\{\xi_i \xi_j\}\}$ in particular, as in the preceding examples. We see such reversals as unanticipated and heretofore undiscovered consequences of ridge regression as initially formulated.

5. Conclusions

In summary, further insight is offered regarding the use of ridge regression in ill-conditioned models. This study begins with successive concentration orderings of *OLS* estimators for the canonical parameters. The ordering continues to hold for ridge solutions as k evolves, up to a threshold value given in Theorem 1(iii). Exceeding this, individual ridge estimators encounter reversals in their comparative concentrations as k evolves, up to another threshold value in Theorem 1(iv), beyond which complete reversal obtains. Specifically, for k sufficiently large, the estimator least concentrated at the outset, achieves greatest concentration in comparison with other estimators at that k . Knowledge of these facts could be useful in choosing k so as to enhance the comparative performance for selected parameters of singular interest to an investigation.

Ridge regression continues in wide usage, prominently now in calibration studies in the chemical engineering and related literature. See (Frank and Friedman, 1993; Geladi, 2002; Kalivas, 2005; Sundberg, 1999) for recent surveys. Here we have emphasized spherical error models not necessarily having moments, together with the peakedness ordering of Birnbaum (1948). These

encompass spherical Student t distributions on ν degrees of freedom as in Zellner (1976), to include heavy-tailed Cauchy errors at $\nu = 1$ devoid of moments. Connections to calibration problems are found in Jensen and Ramirez (2009), where it is seen that linearly calibrated data, subject to errors of calibration, may arise as ratios of Gaussian variables, thus having Cauchy distributions.

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