Maximum Likelihood Ridge Regression

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Abstract

My first paper exclusively about “ridge regression” was published in Technometrics and chosen for invited presentation at the 1975 Joint Statistical Meetings in Atlanta. Unfortunately, that paper contained a wide range of assorted details and results. Luckily, Gary McDonald’s published discussion of that paper focused primarily on my use of Maximum Likelihood estimation under normal distribution-theory. In this review of some results from all four of my ridge publications between 1975 and 2022, I highlight the Maximum Likelihood findings that appear to be most important in practical application of shrinkage in regression.

Hoerl(1962) wrote “A maximum likelihood solution for the ridge analysis has not yet been theoretically derived.” This paper is dedicated to Arthur E. Hoerl (1921-1994) and Robert W. Kennard (1923-2011) in memory of their pioneering spirits.

1 Introduction

The “Ordinary Least Squares” (OLS) estimator of the \( \beta \)-coefficient vector in linear regression is \( \hat{\beta}^o = (X'X)^+X'y \), where the superscript + denotes the Moore–Penrose pseudo-inverse of \( X'X \). This OLS estimator is unquestionably the most “well-known” estimator that achieves “maximum likelihood” under normal distribution-theory. In fact, Rao (1973), Section 4g, pages 264–265, states...
that $\hat{\beta}^o$ is the “BLUE” or “Best Linear Unbiased” estimator for linear models with independent and homoscedastic error-terms because it achieves minimum MSE risk under those assumptions.

Surprisingly, the “Main Difficulty” with OLS in practical applications of linear regression is that it is unbiased: $E(\hat{\beta}^o) = \beta$. Unbiasedness implies that the variances of and the covariances between $\hat{\beta}^o$—estimates can be quite large when the $X$—matrix of predictors has $p \geq 2$ columns that are highly inter-correlated (ill-conditioned). See Figure (1) on page −3— for a simulated illustration of this with $p = 2$ coefficients.

The well-known ridge estimators of Hoerl and Kennard (1970a,b) use a single (scalar) parameter, $k$, commonly characterized as being a “small positive numerical constant” that is added to each diagonal element of the $X'X$—matrix before it is inverted: $\hat{\beta}(k) = (X'X + kI)^{-1}X'y$. These $\hat{\beta}(k)$ estimators are biased when $k > 0$, but the normal distribution-theory “likelihood” of these estimators to be optimally biased had not been quantified before the publication of Obenchain(1975).

Every “generalized” ridge regression shrinkage “path” starts at $\hat{\beta}^o$, the OLS Best estimator. Since the terminus of the shrinkage path is (usually) taken to be $\hat{\beta} = 0$, and the overall length of the shrinkage path is always finite, it is somewhat unfortunate that Hoerl and Kennard’s $k$—parameter must approach $+\infty$ to actually approach this terminus. My (1975–1977) generalized ridge estimators used two strictly finite parameters, $q$ and $m$, to determine both the $q$—Shape or “curvature” of a “shrinkage path” $[-5 \leq q \leq +5]$ as well as the $m$—Extent of shrinkage $[0 \leq m \leq p]$ along that path.

Gunst (2000, p. 62) wrote: “Although ridge regression is widely used in the application of regression methods today, it remains as controversial as when it was first introduced.” Many early proposals for choosing the $k$—factor appear to have been based mainly upon heuristics. In his discussion of Obenchain (1975), McDonald (1975) echoed the “likelihood” remark of Hoerl (1962) about why shrinkage heuristics or Cross-Validation or Bootstrapping methods were commonly used to determine the $k$—factor.

While my first three ridge publications (1975, 1977, 1978) provided a sound, theoretical “likelihood” foundation for shrinkage, they focused on “parsimonious” 2—parameter paths that typically miss the global maximum likelihood $\beta$—estimator when the “centered” $X$—matrix has rank $> 2$. My fourth ridge publication, Obenchain (2022a), proposed an Efficient Shrinkage Path which usually applies a different $\delta$—factor to each “uncorrelated component” of the OLS estimator, $\hat{\beta}^o$. This $p$—Parameter path consists of two-piece linear functions that first connect each (unbiased) OLS
Figure 1: This figure from Obenchain (2022a) displays Kernel Density estimates for a pair of bootstrap distributions for two $\hat{\beta}$-coefficients. True coefficients $\beta_1 = 2.3382$ and $\beta_2 = -1.7809$ were used to generate $n = 500$ observations on a $y$-variable with errors that were I.I.D. Normal with mean 0 and $\sigma^2 = 18$. In the top plot, note that the distribution of OLS estimates definitely appears to be unbiased but has high variability. In the bottom plot, the corresponding distribution of GRR estimates most likely to be optimally biased is much less variable and achieves lower overall MSE risk.
coefficient estimate to it’s optimally biased estimate, and then heads directly for the shrinkage terminus.

This (unpublished) paper outlines and updates the technical material needed by researchers to understand the details of my published work on shrinkage in regression and, hopefully, to make genuinely “new” contributions to regression methodology and/or software development.

1.1 Multiple Regression Notation and Standardization

The usual model for multiple linear regression is written as

$$ E(y|X) = 1\mu + X\beta \text{ and } Var(y|X) = \sigma^2 I, $$

where $y$ is a $n \times 1$ vector of observed response values, $X$ is a $n \times p$ matrix of non-constant coordinates for $p$ predictor variables, 1 is a $n \times 1$ vector of ones, $\mu$ is an unknown intercept, and $\beta$ is a $p \times 1$ vector of unknown regression coefficients. Note that the $X$—matrix is assumed given, while the $y$—vector of response outcomes is assumed to be (conditionally) stochastic in the sense that it consists of uncorrelated observations with constant unknown variance, $\sigma^2$.

In this paper, the $y$—vector and the columns of the $X$—matrix are assumed to have been “centered” by subtracting off column means; thus, $1'y = 0$ and $1'X = 0'$. We also assume that the centered $X$—matrix has full column rank, $p \leq (n-1)$, so that the OLS estimator of the $\beta$—vector is well-defined and uniquely determined. Note that this centering allows model (1) to be written more succinctly as $E(y|X) = X\beta$ and $Var(y|X) = \sigma^2(I - 11'/n)$, where the $\mu$ intercept term from equation (1) will be implicitly estimated by $\bar{y} - \bar{x}'\hat{\beta}$. A key advantage of this centering is that the $\hat{\mu}$ estimate will then adjust appropriately in response to any changes in $\hat{\beta}$—estimates. Specifically, the fitted regression hyperplane will always pass through $y = \bar{y}$ at $x = \bar{x}$.

Finally, we remark that a regression model can truly be “ill-conditioned” only when $p > 1$. However, shrinkage can still reduce the MSE risk of a scalar $\hat{\beta}$ estimate. The YonX() function in the RXshrink R-package, Obenchain (2022b), provides Trace displays and other pedagogical graphics for this (simple) $p = 1$ special-case.
1.2 Principal Axis Rotation to Uncorrelated Components

The singular value decomposition of regressors is $X = H \Lambda^{1/2} G'$, where $H$ is the $n \times p$ semi-orthogonal matrix of principal coordinates of $X$, $\Lambda$ is the $p \times p$ diagonal matrix of eigenvalues of $X'X = G G'$, and $G$ is the $p \times p$ orthogonal matrix of principal axis direction cosines. Note that $1' H = 0'$ because $1' X = 0'$. Furthermore, $G' G$ and $H' H$ are $p \times p$ identity matrices. Principal axes are assumed here to be ordered such that the eigenvalues, $\lambda_1 \geq \cdots \geq \lambda_p > 0$, of the regressor inner products matrix are non-increasing.

The ordinary least-squares (OLS) estimator, $\hat{\beta}^o$, of $\beta$ in equation (1) is not uniquely determined when $\text{rank}(X) < p$, so we adopt the convention here that

$$\hat{\beta}^o \equiv X^+ y = Gc,$$

where $X^+$ is the (unique) Moore-Penrose inverse of $X$, and $c$ denotes the $p \times 1$ vector containing the (sample) uncorrelated components of $\hat{\beta}^o$, given by

$$c \equiv \Lambda^{-1/2} H' y = (y' y)^{1/2} \Lambda^{-1/2} \rho .$$

In this third equation, $\rho = H' y / \sqrt{y' y}$ denotes the computed $p \times 1$ vector of observed principal correlations between $y$ and the columns of $H$. Since these principal-correlation estimates will appear in many equations below, I apologize for any ambiguity caused by using a Greek letter (without a “hat”) to denote them!

Note that $E[c|X] = G' \beta \equiv \gamma$, which is the $p \times 1$ vector of unknown true components of $\beta$, and that $\text{Var}[c|X] = \sigma^2 \Lambda^{-1}$, which is a diagonal $p \times p$ matrix.

The F-ratio for testing $\gamma_i = 0$ is then

$$F_i = \frac{c_i^2}{s^2/\lambda_i} = \frac{(n - p - 1) \cdot \rho_i^2}{(1 - R^2)}. $$

In equation (4), $R^2$ is the familiar R-squared “Coefficient of Determination” that can also be written as the sum-of-squares of observed principal correlations: $R^2 = \rho_1^2 + \cdots + \rho_p^2$. Note also that $(n - p - 1)$ is the number of “degrees-of-freedom for error”, and that $s^2 = y'(I - HH') y / (n - p - 1) = (y' y) \cdot (1 - R^2) / (n - p - 1)$ is the unbiased estimator of $\sigma^2$ under normal distribution-theory.
Note further that equation (4) illustrates that the statistical significance of the uncorrelated components depends only upon their corresponding principal correlations. On the other hand, equation (3) shows that

\[ c_i = \rho_i \cdot \sqrt{\frac{y'y}{\lambda_i}}. \]  

**Key Insight** from equation (5): An uncorrelated component can be relatively large, numerically, simply because its corresponding eigenvalue, \( \lambda_i \), is relatively small, even when its sample principal correlation, \( \rho_i \), is not relatively large. This “ill-conditioning” occurs when correlations between \( X \)-variables cause the centered \( X'X \) matrix to have a wide range of unequal eigenvalues. Furthermore, components with relatively small eigenvalues necessarily have relatively large variance, \( V[c_i|X] = \sigma^2/\lambda_i \), and thus are primary candidates for generalized ridge shrinkage.

Finally, Generalized Ridge Regression (GRR) estimators are of the form

\[ \hat{\beta}(\Delta) \equiv G\Delta c, \]  

where \( \Delta \) is a \( p \times p \) diagonal matrix containing \( p \) “shrinkage” \( \delta_i \)-factors such that \( 0 \leq \delta_i \leq 1 \) and are ideally known constants given the \( X \)-matrix of “standardized” predictor co-ordinates.

Equation (6) shows that Generalized Ridge Regression may possibly best be viewed as the “shrinkage” version of Principal Components Regression, Massy(1965), where each individual \( \delta_i \)-factor is taken to be either 1 or 0.

### 1.3 Optimal Shrinkage Factors

To apply normal-theory maximum likelihood to shrinkage estimation, we will need a definition for the \( \Delta \) factors that make \( \hat{\beta}(\Delta) = G\Delta c \) the minimum MSE, linear estimator of \( \beta \). We start by computing the risk of \( \delta_i \times c_i \) as an estimator of the \( i \)-th true component \( \gamma_i \):

\[ MSE(\delta_i c_i) = E[(\delta_i c_i - \gamma_i)^2] = E\{[\delta_i(c_i - \gamma_i) - (1 - \delta_i)\gamma_i]^2\}. \]  

Under the assumption that \( \delta_i \) is nonstochastic given \( X \), this risk expression can first be rewritten as

\[ MSE(\delta_i c_i) = \delta_i^2 E[(c_i - \gamma_i)^2] - 2\delta_i(1 - \delta_i)E(c_i - \gamma_i) + (1 - \delta_i)^2\gamma_i^2, \]  

where \( \delta_i \) is nonstochastic given \( X \).
Figure 2: When the “standardized” $X$–matrix is of rank $p = 2$, the $b^* = \hat{\beta}^0 = Gc$ decomposition of equations (2) and (3) becomes $\hat{\beta}^0 = g_1c_1 + g_2c_2$ where $g_1$ and $g_2$ are the columns of $G$. This principal axis rotation (or reflection) orients the edges of the rectangle displayed above. It contains all shrinkage estimators of the form $\hat{\beta}(\Delta) = G\Delta c = g_1\delta_1c_1 + g_2\delta_2c_2$ where $0 \leq \delta_1, \delta_2 \leq 1$. 
and then simplified, using \( E(c_i) = \gamma_i \) and \( V(c_i) = \sigma^2/\lambda_i \), to yield:

\[
MSE(\delta_i c_i) = \delta_i^2 \sigma^2/\lambda_i + (1 - \delta_i)^2 \gamma_i^2. \tag{9}
\]

Next, we compute the partial derivatives of MSE risk with respect to changes in the \( i \)-th shrinkage factor:

\[
\frac{\partial MSE(\delta_i c_i)}{\partial \delta_i} = 2\delta_i \sigma^2/\lambda_i - 2(1 - \delta_i)\gamma_i^2, \quad \text{and} \tag{10}
\]

\[
\frac{\partial^2 MSE(\delta_i c_i)}{\partial \delta_i^2} = 2\sigma^2/\lambda_i + 2\gamma_i^2. \tag{11}
\]

Since the second derivative will be strictly positive whenever \( \sigma > 0 \), the solution of \( \partial MSE/\partial \delta_i = 0 \) corresponds to minimum risk. This solution will be denoted by \( \delta_i = \delta_i^{MSE} \), where \( \delta_i^{MSE} \) can be written in at least three equivalent ways:

\[
\delta_i^{MSE} \equiv \gamma_i^2/\frac{\gamma_i^2}{\gamma_i^2 + (\sigma^2/\lambda_i)} = \frac{\lambda_i}{\lambda_i + (\sigma^2/\gamma_i^2)} = \frac{\varphi_i^2}{\varphi_i^2 + 1}, \tag{12}
\]

where \( \varphi_i^2 = \gamma_i^2 \lambda_i/\sigma^2 \) is the (unknown) noncentrality of the F-ratio for testing \( \gamma_i = 0 \), equation (4). In fact, \( n \cdot F_i/(n-r-1) \) is the maximum likelihood estimator of the \( \varphi_i^2 \) noncentrality parameter under normal distribution-theory.

Note that \( 0 \leq \delta_i^{MSE} \leq 1 \). Furthermore, \( \delta_i^{MSE} = 0 \) only when \( \gamma_i = 0 \) or in the limit as \( \sigma^2 \) increases to \(+\infty\). Similarly, \( \delta_i^{MSE} = 1 \) only when \( \sigma^2 = 0 \) or in the limit as \( |\gamma_i| \) increases to \(+\infty\).

Substituting \( \delta_i^{MSE} \) into equation (7) and simplifying, we have shown that

\[
MSE(\delta_i c_i) \geq \delta_i^{MSE} \cdot (\sigma^2/\lambda_i) \tag{13}
\]

for all non-stochastic shrinkage factors \( 0 \leq \delta_i \leq 1 \), with equality only when \( \delta_i = \delta_i^{MSE} \).

One never really knows when a non-stochastic choice for \( \delta_i \) is equal to \( \delta_i^{MSE} \); after all, \( \delta_i^{MSE} c_i = c_i/[1+(\sigma^2/\lambda_i \gamma_i^2)] \) is a non-estimator of \( \gamma_i \) because its \( (\sigma^2/\gamma_i^2) \) factor is unknown. The OLS estimator, \( c_i \), is the unique minimax estimator of \( \gamma_i \) under normal distribution-theory; its risk, \( MSE(c_i) = \sigma^2/\lambda_i \), is constant for all values of \( \gamma_i \).

Obenchain(1978) considered alternative definitions for MSE optimal shrinkage but ultimately concluded that (12) is the most reasonable definition overall.
2 Likelihood in Shrinkage Estimation

Equation (12) can be inverted to yield

\[ \frac{\gamma_i^2}{\sigma^2} = \frac{\delta_{i \text{MSE}}}{\lambda_i(1 - \delta_{i \text{MSE}})} \]  

Equation (14) quantifies the KEY relationships used in Obenchain (1975) to define the normal distribution-theory likelihood that any given set of \( p \) shrinkage \( \delta \)-factors achieves overall minimum MSE-risk.

Specifically, the likelihood that any given set of numerical shrinkage \( \delta \)-factors within the half-open interval \( [0 \leq \delta_i < 1) \) are MSE-optimal is defined to equal the likelihood that \( \gamma_i \) is \( \pm \sigma^{**}\delta_i/\lambda_i(1 - \delta_i)^{1/2} \) ...where this likelihood has been maximized by choice of the \( \sigma^{**} \) estimate of \( \sigma \) and by choice of the positive and negative signs.

The \( j^{th} \)-component of the resulting ML shrinkage-estimator under normal-theory is:

\[ \hat{\gamma}_j^{\text{ML}} = \hat{\delta}_j^{\text{MSE}}c_j = \left( \frac{n\hat{\rho}_j^2}{n\hat{\rho}_j^2 + (1 - R^2)} \right) \left( \hat{\rho}_j \sqrt{\frac{y'y}{\lambda_j}} \right) \]  

where \( y'y = (n - 1) \) when the response vector has been standardized. Each component, \( \hat{\gamma}_j^{\text{ML}} \), of this ML estimator is a rational function of all \( p \) principal correlation estimators, \( \hat{\rho}_1, \ldots, \hat{\rho}_p \). Note that the numerator consists of a single term cubic in \( \hat{\rho}_j \), while the denominator is quadratic in all of the principal correlation estimators. In other words, this ML estimator is clearly not a linear function of the response \( y \)-vector.

Since linear models use conditional distribution-theory where the \( X \)-matrix is considered given, rather than subject to random variation, the \( H \) and \( G \) matrices as well as all functions of the eigenvalues of the \( X \)-matrix are also given constants. The \( \hat{\gamma}_j^{\text{ML}} \) estimators of equation (15) are thus given functions of \( y \) multiplied by \( \sqrt{y'y/\lambda_j} \). In particular, note that the normal-theory conditional distributions of the \( \hat{\rho}_j \)-estimators are not those of correlation coefficients.

Unfortunately, the \( \hat{\beta}(\Delta) \) estimate most likely to be \( \hat{\beta}^{\text{MSE}} \) will not always achieve smaller Summed MSE than OLS. After all, equation (15) shows that \( \hat{\beta}(\Delta) \) is a non-linear function of the \( y \)-vector.

The “efficient path” of Obenchain (2022a) consists of \( p \) two-piece linear functions, each having a single interior knot at the \( \hat{\beta} \)-estimator with Maximum Likelihood of achieving minimum MSE risk under normal distribution-theory. This new “path” is efficient in the senses that it is the shortest
path and, at least when \( p > 2 \), essentially the only known shrinkage path that always contains the \( \hat{\beta} \)–vector that is most likely to be optimally biased. Functions in R-packages freely distributed via CRAN perform the calculations and produce graphics that illustrate optimal shrinkage. These new concepts and visualization tools provide invaluable data-analytic insights and improved self-confidence to applied researchers and data scientists fitting linear models to data.

Computations and Trace displays for the efficient GRR path (plus other graphics) were first implemented in Version 2.0 of the \textit{RXshrink} R-package, Obenchain (2022b).

Each GRR Trace typically displays estimates of \( p \) quantities that change as shrinkage occurs. The “coef” Trace shows how fitted linear-model \( \hat{\beta} \)–estimates change with shrinkage. The “rmse” Trace displays corresponding estimates of relative mean-squared-error given by dividing each diagonal element of the MSE-matrix by the OLS-estimate of \( \sigma^2 \). When shrinkage becomes excessive, the “infd” Trace displays direction-cosine estimates of the \textit{inferior-direction} in \( p \)–dimensional \( X \)–space along which over-shrunken coefficients have higher MSE risk than their corresponding OLS estimates, Obenchain (1978).

The two final types of Trace diagnostics, called “spat” and “exev”, are somewhat different; they refer to the \( p \geq 2 \) rotated axes defining the \textit{principal-coordinates} of the centered and rescaled \( X \)–predictors rather than to any single regression \( \hat{\beta} \)–coefficient estimator. The additional restriction that \( p \leq (n - 4) \) then assures that \( p \times p \) matrices of unbiased estimates of MSE risk exist, Obenchain (1978, eq. (3.4)). However, to assure that plotted relative risk values are at least as large as their relative variances, a \textit{correct-range} estimate of relative MSE risk is displayed when the unbiased estimate would be misleading.

While the above conventions have placed all \( X \)–information about the form and extent of any \textit{ill-conditioning} into a convenient canonical-form, these conventions have done nothing to predetermine the relative importance of individual \( x \)–variables in models that predict \( y \)–outcomes. That information, as well as information on the many effects of deliberate shrinkage, may well be best and most-clearly revealed via visual examination of Trace diagnostic plots.

### 3 Quantifying Extent of Shrinkage

A measure of the extent of shrinkage applied by equation (3) is given by

\[
m \equiv p - \delta_1 - \cdots - \delta_p = \text{rank}(X) - \text{trace}(\Delta). \tag{16}
\]
This scalar, called the *multicollinearity allowance*, Obenchain (1977), is always $\geq 0$ and $\leq p = \text{Rank of the } X$–matrix.

**Five KEY Advantages of using $m$–Scaling on “Ridge TRACE” Diagnostic Plots**

- **GENERALITY**: Any sort of Shrinkage PATH can be displayed in a plot with $m$ on its horizontal axis.

- **Rank DEFICIENCY**: A vertical (dashed) line can be drawn on a TRACE display at the $m$–Extent most likely to represent the amount of $\delta$–factor shrinkage *most likely to achieve minimum MSE risk*. When this $m$–value is strictly positive, it quantifies an approximate “rank deficiency” in the given $X$–matrix due to ill-conditioning (partial redundancy among columns). For examples, see the four TRACEs in Figure 4 on page 15.

- **FINITE Width and Height**: All “static” 2–dimensional plots have these restrictions, and $m \leq p$ is clearly finite.

- **STABLE Relative Magnitudes**: Shrunken regression coefficients and other estimates with *perfectly stable relative magnitudes* form “straight lines” when plotted on TRACEs using $m$–scaling.

- **Bayesian Posterior Precision**: For any given value of $m$, the average value of all $p$ shrinkage $\delta$–factors is $(p - m)/p$, which is also the proportion of Bayesian posterior precision due to *sample information* ...rather than due to *prior information*. This proportion thus decreases linearly as $m$ increases from 0 to $p$.

In the TRACE plot proposed by Hoerl and Kennard (1970a,b), their $k$–factor starts at 0 but must end abruptly at some finite $k$–max value specified by the user. Essentially, their shrinkage terminus must be the $(0,\ldots,0)$ vector containing $p$ zeros, and $k$–max is apparently chosen via trial-and-error.

Use of $m$–scaling on the horizontal axis of Trace Diagnostic plots also suggests using simplified notation, $\hat{\beta}_m$, to denote individual $\hat{\beta}(\Delta)$ estimators in equation (6). The OLS solution ($\hat{\beta}^o$) which occurs at the beginning ($m = 0$) of each GRR shrinkage-path would then be denoted by $\hat{\beta}_0$. Similarly, $\hat{\beta}_p \equiv 0$ occurs at the shrinkage terminus, $m = p$. 
Figure 3: Again, when the “standardized” $X$–matrix is of rank $p = 2$, the above plot shows paths of four different $q$–Shapes. Two issues strike me as intuitively clear from this graphic. First, 2-parameter paths with $q < -1$ or $q > +2$ would be needed to come closer to the upper and lower “corners”, respectively, of the displayed shrinkage-factor rectangle. Secondly, more parameters than just $k$ and $q$ are clearly needed when $p \geq 3$ to come anywhere close to overall-optimal shrinkage, defined as $\delta_j \equiv \delta_j^{MSE}$ for $j = 1, ..., p$.

4 Two-Parameter Shrinkage Paths

Obenchain (1975) proposed restricted GRR Shrinkage Paths of the general form:

$$\delta_j = \frac{\lambda_j}{(\lambda_j + k \times \lambda_j^q)} = \frac{1}{1 + k \times \lambda_j^{q-1}} . \quad (17)$$

for $j = 1, ..., p$, where $k$ and $q$ are scalars such that $0 < k < +\infty$ and $-5 \leq q \leq +5$. Goldstein and Smith (1974), equation (13), considered almost equivalent paths except that their parameter $m = 1 - q$ was assumed to be an integer.

The two well known special cases of equation (17) are (i) $q = 0$ for the “ordinary” path of Hoerl and Kennerd (1970a,b) and (ii) $q = +1$ for Mayer-Willke (1973) “uniform” shrinkage, $\hat{\beta}(\delta \cdot I) = \delta \cdot \hat{\beta}^o$. 

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4.1 Restricted Maximum Likelihood Shrinkage

Note that equation (12) is easily solved to express the unknowns ($\gamma$ and $\sigma^2$) as functions of the known eigenvalues ($\lambda_1, \cdots, \lambda_r$) and of the MSE optimal shrinkage factors ($\delta^*_1, \cdots, \delta^*_r$); this expression is

$$\gamma_i = \pm \sigma \sqrt{\delta^*_i / (1 - \delta^*_i)} / [\lambda_i (1 - \delta^*_i)].$$

If an estimator within the restricted, 2-parameter shrinkage factor family $\delta_i = 1 / (1 + k \lambda^q_i)$ of equation (17) were MSE optimal, equation (18) would then become

$$\gamma_i = \pm \sigma / \sqrt{k \lambda^q_i}.$$  

Letting $\nu^2$ denote the common, unknown value of $\gamma_i^2 \lambda^q_i = \cdots = \gamma_r^2 \lambda^q_r = \sigma^2 / k$ within our restricted 2-parameter search for MSE optimal shrinkage factors, the normal-theory likelihood that $\sigma^2$ and $\gamma$ are of this highly restricted form for any given values of $k$ (or $m$) and $q$ is $L(\gamma, \sigma) = (2\pi \sigma^2)^{-n/2} e^{-u^2/2\sigma^2}$ when $1'y = 0$ and $1'X = 0'$. The quadratic form in the exponential term of $L(\gamma, \sigma)$ is then

$$u^2 = (y - X\beta)'(y - X\beta)$$

$$= y'y - 2\sqrt{y'y} \cdot \nu \cdot \sum |\rho_i| \lambda^{(1-q)/2} + \nu^2 \cdot \sum \lambda^{(1-q)}$$

because $y'X\beta = y'H\Lambda^{1/2}C'\beta = \sqrt{y'y} \cdot \rho' \Lambda^{1/2} \gamma$ and $\gamma_i = \pm \nu \lambda_i^{-q/2}$ under the restriction. Note, in particular, that the numerical sign of each $\gamma_i$ has been taken to agree with its principal correlation, $\rho_i$, in equation (20); these sign choices make the middle term of (20) as negative as possible and reduce the quadratic form when $\nu > 0$ and $p = \text{rank}(X)$ is at least 1.

Once maximized by choice of a positive value of $\nu$, the $L(\gamma, \sigma)$ likelihood implied by equation (20) is, by definition, the likelihood that a given $k$ (or $m$–Extent) and $q$–Shape of shrinkage yield MSE optimal $\delta$–factors.

Since the second derivative, $\partial^2[u^2]/\partial \nu^2 = 2 \cdot \sum \lambda_i^{(1-q)}$, is strictly positive, the minimum of the $u^2$ quadratic form is achieved at $\partial[u^2]/\partial \nu = 0$, which is $\nu = \sqrt{y'y} \cdot \sum |\rho_j| \lambda_j^{(1-q)/2} / \sum \lambda_j^{(1-q)} > 0$ when $r = \text{rank}(X)$ is at least 1. The corresponding minimum $u^2$ is thus $u^2 = y'y \cdot [1 - R^2 CRL^2(q)]$, Obenchain(1975b), for $R^2$ of (4) where the curlicue function is

$$CRL(q) = \frac{\sum |\rho_j| \lambda_j^{(1-q)/2}}{\sqrt{\sum \rho_j^2 \sum \lambda_j^{(1-q)}}}.$$
Note that $CRL(q)$ is the Cosine of the angle between the R-vector of absolute values of the principal correlations $[\rho$ of equation (3)] and the L-vector of predictor eigenvalues raised to the power $(1-q)/2$.

### 4.2 Optimal Choice of Path $q-$Shape

Our crucial next step is to minimize the minus-two-log-likelihood of $n \cdot \ln(2\pi \sigma^2) + \hat{u}^2/\sigma^2$ given $q$ by choice of a conditional estimate of $\sigma^2$, where $n$ is the number of observations. Differentiating as usual, we find that the best choice for $\hat{\sigma}^2$ is the minimum $\hat{u}^2$ divided by $n$. More importantly, the corresponding MSE optimal $k-$factor, Obenchain(1981), can be written as

$$\hat{k} = \hat{k}(q) = \hat{\sigma}^2/\hat{\rho}^2 = \left[ \sum \lambda_j^{(1-q)} \right] \cdot \frac{[1 - R^2 \cdot CRL^2(q)]}{n \cdot R^2 \cdot CRL^2(q)}.$$ (22)

The final step is then to further minimize the $\hat{u}^2$ quadratic form (maximize the likelihood) by maximizing $CRL(q)$ over choice of alternative $q-$Shapes for the shrinkage path. While there is no known closed form solution here, simple linear searches are fast within $-5 \leq q \leq +5$.

Note that the arguments used here do not, technically, assume that each $\sigma^2/\gamma_i^2$ actually is equal to $k\lambda_i^q$. Rather, we are simply asking: “Which choice of $k$ and $q$ make it most likely that the unknown $\sigma^2/\gamma_i^2$ are of this $k\lambda_i^q$ form under normal distribution-theory?” The corresponding minus-twice-log-likelihood-ratio for the maximum likelihood 2-parameter solution relative to the unrestricted solution of (12) is

$$\chi^2(q) = n \cdot \ln\left\{ 1 + \frac{R^2[1 - CRL^2(q)]}{(1 - R^2)} \right\}.$$ (23)

This large sample chi-squared test of the 2-parameter restriction has $(r-2)$ degrees-of-freedom when $\chi^2(q)$ has been minimized by choice of $q-$Shape and $r = \text{rank}(X) \geq 3$. A sufficiently large $\chi^2(q)$ then suggests that the 2-parameter family of (17) is too restrictive (smooth) to contain the overall MSE optimal shrinkage $\delta-$factors.

The qm.ridge() function in the RXshrink R-package of Obenchain(2022b) searches, by default, over only integer and half-integer $q-$Shapes between $q_{\text{min}} = -5$ and $q_{\text{max}} = +5$. The limit as $q$ approaches $+\infty$ is optimal for the Gibbons(1981) “unfavorable” case where the true $\beta$ vector is parallel to the eigenvector with smallest eigenvalue, $\lambda_p$. Shrinkage to $m = p-1$ ($\delta_1 = \cdots = \delta_{p-1} = 0$) then reduces all components of $\hat{\beta}^o$ orthogonal to the true $\beta$ to zero! This is essentially an extreme form of Massy(1965) “type (b)” principal components regression.
Figure 4: These are Efficient 4-parameter and QM 2-parameter TRACE displays for the shrunken $\beta$-coefficients and their corresponding “Relative” MSE-error estimates for the “haldport” dataset included in the RXshrink R-package. The vertical dashed-lines indicating Maximum Likelihood of Minimal MSE Risk occur at $m = 1.85$ in the two top panels and at $m = 2.12$ in the bottom panels. Note that the relative magnitudes of ML estimates (especially the solid-black and dashed-red coefficients) are quite different between these two Paths.
Figure 5: Negative Log Likelihood Ratio curves for two different shrinkage-paths on the “haldport” dataset. The solid black curve shows how the $-2 \log$ Likelihood-Ratio under Normal-theory drops all of the way to 0 at $m = 1.85$ for the “Efficient” 4–parameter path. The solid blue curve depicts the corresponding L-R for the 2–parameter path of “best” $q – \text{Shape} = -5$ on the default search grid. This $-2\log(LR)$ reaches a minimum of 26.4 at $m \approx 2.12$. Since the upper 99%–point of a $\chi^2$–variate with 2 degrees-of-freedom is only 9.21. Thus, the “best” 2–parameter fit is actually significantly different from being MSE Risk-optimal.
Finally, the limit as \( q \) approaches \(-\infty\) contains all Massy(1965) “type (a)” principal components regression solutions. As in the above \( q = +\infty \) case, the shrinkage path travels along a series of edges of the generalized shrinkage hyper-rectangle. My experience is that the \( q = \pm 5 \) paths are frequently adequate to approximate their corresponding \( q = \pm \infty \) limiting cases.

5 Estimation of “Relative” MSE Risk

An unbiased estimate of the “scaled” or “relative” Mean Squared Error matrix, \( MSE(\Delta c)/\sigma^2 \), where \( \Delta \) is a non-stochastic diagonal matrix and \( E(c) = \gamma \), is given by

\[
\hat{T} = \frac{(n-p-3)}{(n-p-1)}(I - \Delta)\Lambda^{-1/2}\tau\tau'\Lambda^{-1/2}(I - \Delta) + \Lambda^{-1}(2\Delta - I), \tag{24}
\]

where \( \tau \) is the column vector of t-statistics corresponding to the \( F \)-ratios of equation (4):

\[
\tau_i = \rho_i\sqrt{\frac{n-p-1}{1-R^2}} \text{ for } 1 \leq i \leq p. \tag{25}
\]

These \( \tau_i \)–estimators first appeared in equation (3.4) of Obenchain (1978) and are used by functions in the RXshrink R–package, Obenchain (2022b), to display the “Relative MSE” Traces on the right-hand side of Figure(4).

When the \( \delta_i \) are known and non-stochastic, the unknown relative risk, \( MSE(\delta_i c_i)/\sigma^2 \), must be \( \geq \delta_i^2/\lambda_i^2 \) due to equation (9). Thus the known scaled variance of \( \delta_i c_i \) is \( \delta_i^2/\lambda_i \), which provides a lower bound for the unknown relative MSE Risk of \( \delta_i c_i \) when \( \delta_i \) is non-stochastic.

6 Simulated MSE Risk Comparisons

The only published simulation results comparing the Maximum Likelihood approach described here with other methods for choosing an extent of shrinkage are those of Gibbons (1981). She generated her “O-method” results before the closed-form expression, (22), for the maximum likelihood \( k \)–factor was developed. Instead, Gibbons maximized \( CRL(q) \) over the range \(-5 \leq q \leq +1 \) and then performed a second search for the optimal shrinkage \( k \)–extent using the “general” likelihood monitoring equations of Obenchain(1975b). Gibbons found that the O-method is superior to the Golub, Heath and Wahba(1979) approach to generalized cross-validation (GHW) when \( R^2 \) exceeds
0.5 and the MSE optimal shrinkage pattern corresponds to $q = -\infty$ (i.e. the true $\beta$ vector lies along the first, major principal axis of regressors.)

The top half of Figure 7 in Gibbons(1981), page 138, is reproduced here as Figure 6. Note in particular that, of the 12 methods simulated, only the O-method consistently reduces MSE risk by at least 50% in these so-called “favorable” cases.

The O-method could not perform well in Gibbon’s “unfavorable” cases because Gibbons never allowed the selected $q-$Shape to exceed +1, which corresponds to uniform shrinkage, $\delta_1 = \cdots = \delta_p = 0$. However, Gibbons did report that this most positive of allowed $q-$Shapes was, indeed, always selected by her “O-method” calculations in all simulations where the true $\beta$ vector lies along the last, minor principal axis of regressors.

The 10 “other” shrinkage estimators that Gibbons was simulating (besides ordinary LS and O) always follow the Hoerl-Kennard path of $q-$Shape = 0. This is a clearly inappropriate overall pattern for shrinkage when the true $\beta$ vector is parallel to the final principal direction of $p-$dimensional $X-$space with smallest, positive singular value. This pathological case is (hopefully) quite rare in practical applications; after all, why focus shrinkage on the final uncorrelated component, $c_p$ of (5), that contains the lone “signal” principal correlation, $\rho_p$, while minimizing shrinkage of the remaining pure “noise” components of the ordinary LS solution? If the O-method had been allowed to select a $q-$Shape much larger than +1, e.g. +5, in these Gibbons “unfavorable” scenarios, it would have truly dominated its 10 competitors on all measures of MSE risk.

The closed form expression, (22), for the maximum likelihood choice of $k-$extent for shrinkage along any path of given $q-$Shape makes it easier to study the MSE risk of O-method estimators using a variety of techniques ...ranging from exact calculations to large sample approximations to numerical integration to Monte-Carlo simulation. The primary challenge in developing risk profiles for maximum likelihood shrinkage estimation lies primarily in handling the high dimensionality of realistic scenarios. Specifically, the extensive array of parameters that could be varied include the relative sizes of true $\gamma$ components, spread in regressor $\lambda$ eigenvalues, size of the error $\sigma^2$ variance, number $p$ of $X-$variables, singular $X-$matrices, number of degrees-of-freedom for error, etc, etc.
Figure 6: Here are some key comparisons from Figure 7 of Gibbons (1981). Note that the O-method is conservative; it never shrinks aggressively enough to reduce MSE risk to less than 20% of LS risk = 1.0. Yet the maximum risk of O-method selections is consistently less than 50% of this LS risk.
7 Summary

Over the last 50 years, computers have helped shape statistical theory as well as its practice. Freely available software can provide computational and visual fast-tracks into the strengths and weaknesses of alternative statistical methods. In fact, R and Python functions are becoming almost indispensable tools for today’s teachers of regression methods as well as for students, applied researchers and data-scientists who use and/or extend these methods.

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