On Optimal and Feasible Regularization in Linear Models in Time Series

Erez Buchweitz,* Shlomo Ahal, Oded Papish, Guy Adini
Istra Research Ltd.

Abstract

We discuss predictive linear modeling in the presence of: (i) stochastic regressors that are not strictly but rather contemporaneously exogenous to the residual noise; (ii) autocorrelation and heteroscedasticity in the regressors and residual noise of unknown structure. The two are prevalent in time series data. In such settings, ordinary least squares (OLS) is often the preferred estimator in practice, due to its guaranteed consistency. However, it demonstrates instability related to distinctive features of the covariates, such as autocorrelation and association with random effects. In this paper, we attempt to mitigate this drawback of OLS using well-informed regularization. We show that given ideal knowledge of the covariance of an estimator, a maximum a-posteriori probability regularized estimator can be devised admitting desirable properties even when the underlying estimator is misspecified. We give particular consideration to ridge regularization, although our method is widely applicable and generalizations are discussed therein. In order for the well-regularized estimator to be employed in practice, we detail a three staged method of estimating the OLS covariance comprising estimation, shrinkage and normalization. The estimated covariance is then used to form a feasible regularized estimator that is both well-adjusted to the data and consistent.

*Corresponding author; erezmb@gmail.com.
1 Introduction

Let $X$ be the $n \times p$ matrix representing $n$ samples of $p$ covariates, and let $y \in \mathbb{R}^n$ be the response vector corresponding to the samples. For simplicity of the discussion we restrict to the case where $X$ is of full column rank, and we treat any vector as a column vector. Suppose the underlying relation between $X$ and $y$ is linear in a strictly exogenous sense, i.e. $y = X\beta + \varepsilon$ where $\beta \in \mathbb{R}^p$ is fixed and the residual noise $\varepsilon \in \mathbb{R}^n$ admits

$$E[\varepsilon | X] = 0.$$  (1)

This setting appears in most theoretical analyses (e.g. [6, 8]), however it is often absurd when facing real-world problems in which $X$ is stochastic. In time series, for example, it is common to include covariates that are correlated with past observations of $\varepsilon$, even such as lags of the response variable itself [6]. Hence, fixing $X$ might determine the value of $\varepsilon$ to a considerable extent, in contradiction with (1). The more modest assumption of contemporaneous exogeneity may be considered,

$$E[\varepsilon | X_{i1}, ..., X_{ip}] = 0$$  (2)

for all $i = 1, ..., n$. Here, the noise is required to be exogenous only to the contemporaneously sampled covariates. This loosens the previous assumption by permitting the covariates to contain information on $\varepsilon$ between observations. Contemporaneous exogeneity (2) entails, along with some further mild assumptions, that $X^T \varepsilon / n$ vanishes as $n \to \infty$. Consequently, the ordinary least squares (OLS) estimator $\hat{\beta} = (X^T X)^{-1} X^T y = \beta + (X^T X)^{-1} X^T \varepsilon$ is a consistent estimator of $\beta$ (see [15]).

Whenever strict exogeneity (1) fails to maintain, we typically encounter autocorrelation (serial correlation) and heteroscedasticity in the response. The efficient estimator for such situations under strict exogeneity is generalized least squares (GLS) [6], which constitutes the maximum likelihood estimator. Suppose $S$ is an $n \times n$ matrix such that $S^T S = \text{Cov}(\varepsilon | X)$, the GLS estimator is given by solving the transformed model

$$SX\beta + S\varepsilon = Sy$$

using OLS. However, when strict exogeneity is not granted, if $S$ is incorrectly specified we are not guaranteed that $SX$ be contemporaneously exogenous to $S\varepsilon$, thus rendering the GLS estimator inconsistent (see [15]). The same issue arises for example with standard mixed effects estimators (see section 2). As result of this, many authors and practitioners refrain from using GLS-based estimators (e.g. [3, 4, 15]), opting instead for the misspecified yet consistent OLS estimator. The popularity of Newey-West-type standard errors [16] in econometrics is a further testament to this.

The presence of autocorrelation (correlation between different samples of the same variable) and random effects are a common feature of time series. In time series the covariates, effects and noise constitute together a process developing in time. If the effects are not evenly realized along time, one is resorted to modeling multiple steps into the future or face compounded misspecification error
Modeling more than one step ahead results in possible overlap and thus autocorrelation in $\varepsilon$. Random effects are another source of autocorrelation and heteroscedasticity of the errors (see section 2). The OLS estimator neglects to take such considerations into account, effectively assuming $\varepsilon$ comprises uncorrelated and homoscedastic observations. While consistent, it bears the caveat in uneven variance.

In section 2, we prove a result relating the OLS variance to the joint covariance structure of $X$ and $\varepsilon$. We then demonstrate that components of $\beta$ corresponding to autocorrelated covariates, or covariates associated with random effects, are susceptible to increased variance. As covariates differ from each other in these meaningful respects, the produced fit might be adversely dominated by high-variance, uncertain elements. This is detrimental to out-of-sample predictive power, in light of the bias-variance decomposition. The problem is furthermore aggravated in that the difficulty in learning heavily autocorrelated or random-effect covariates might in practice deter us from including such covariates in our model, or unwittingly fail if we nevertheless try.

In this paper we attempt to alleviate these concerns by using well-informed regularization. As regularization methods are by and large methods for reducing the variance of the fit, we stand to benefit if we can adjust them to suppress more harshly those elements in the OLS fit that inherently have higher variance. We do not expect even an ideally well-regularized OLS estimator to achieve the predictive power of correctly-specified GLS, indeed whenever GLS is applicable it is preferrable. We will, however, aspire to obtain improved results over OLS with standard ridge, while not risking consistency. The notion of correcting an OLS estimator using its covariance has been popularized for inference purposes in econometric practice, originating from the work of Newey and West [14]. Approaches of obtaining consistent estimators more efficient than OLS without regularization will be discussed elsewhere.

Working on top of an underlying OLS estimator we are guaranteed consistency. We therefore permit ourselves to assume from this point forth the setting of strict exogeneity (1), which is pleasant for analysis. We make in-place adaptations to contemporaneous exogeneity when necessary.

Suppose then, that assumption (1) holds. We study the particular case of the ridge estimator given by

$$\hat{\beta}_\lambda = (X^T X + \lambda X^T X C)^{-1} X^T y$$

(3)

where $C = \text{Cov}(\hat{\beta}|X)$ and $\lambda \geq 0$ (see section 3). The estimator in (3) arises as the informed combination of the OLS estimator with the usual uninformed ridge prior, according to ideal knowledge of the distribution of the OLS estimator upon the data. We show that the estimator in (3) upholds some pleasant and desirable properties that are lost by standard ridge due to misspecification of the covariance $\text{Cov}(\hat{\beta}|X)$, and that it is furthermore the maximum a-posteriori probability estimator given the underlying OLS estimator. The approach employed to obtain the ridge estimator in (3) can be further generalized to include other priors such as lasso, and other estimators beside OLS (see section 4).
In practice, the covariance $C = \text{Cov}(\hat{\beta}|X)$ required for computing the ridge estimator in (3), is not in general known. We therefore suggest to estimate it and use the estimator $\hat{C}$ in place of $C$ in (3), resulting in a feasible ridge estimator that is well-adjusted to the data. Our method for obtaining the covariance estimate $\hat{C}$ comprises three stages: estimation, shrinkage and normalization. In the estimation stage (see section 5), a crude estimate of $\text{Cov}(\hat{\beta}|X)$ is obtained. For this, we draw from the rich literature available on this topic in econometric theory, known as heteroscedasticity and autocorrelation-consistent (HAC) estimation. The covariance estimator is then smoothened and refined in the shrinkage stage (see section 6), presuming it is too volatile to be used for prediction purposes as is. We discuss two shrinkage approaches; a posteriori estimation and principal component analysis (PCA) denoising. The third stage involves a final act of rescaling the covariance estimator to standardize its effect.

We conclude the paper with a simulation study demonstrating our well-adjusted ridge estimator in a number of settings (see section 7).

2 Motivating Examples

In this section we demonstrate the effects of autocorrelation in the covariates and of random effects on the variance of the OLS fit. We first state a general proposition relating the asymptotic variance of the OLS fit to the joint covariance structure of $X$ and $\varepsilon$.

**Proposition 1.** Let $\{X_n\}_{n=1}^\infty$ be a sequence of random variables with zero mean and uniformly bounded fourth moments, and let $\{\varepsilon_n\}_{n=1}^\infty$ be another sequence of random variables with zero mean conditioned upon any finite subset of $\{X_n\}_{n=1}^\infty$ and with finite variances. Denote by $\{\Sigma_n\}_{n=1}^\infty$ the conditional finite-sample noise covariance matrices, i.e. $(\Sigma_n)_{ij} = \text{Cov}(\varepsilon_i, \varepsilon_j|X_1, \ldots, X_n)$ for $i, j = 1, \ldots, n$. Assume that:

1. $(X_1^2 + \ldots + X_n^2)/n \to 1$ in probability, as $n \to \infty$.
2. $\{(\Sigma_n)_{ij}X_iX_j/n\}_{n=1}^\infty$ converges in probability to a constant, as $n \to \infty$.
3. $\{\Sigma_n/n\}_{n=1}^\infty$ are uniformly bounded in operator norm.
4. $\{n(X_1^2 + \ldots + X_n^2)^{-1}\}_{n=1}^\infty$ are uniformly integrable for large enough $n$.

Suppose $y_n = X_n\beta + \varepsilon_n$ for all $n$, where $\beta \in \mathbb{R}$ is fixed, and denote the OLS estimator for the finite sample of size $n$ by $\hat{\beta}_n = (\sum_{i=1}^n X_i^2)^{-1}(\sum_{i=1}^n X_i y_i)$. Then,

$$\lim_{n \to \infty} n \text{Var}(\hat{\beta}_n) = \lim_{n \to \infty} \frac{1}{n} \sum_{i,j=1}^n \text{Cov}(X_i \varepsilon_i, X_j \varepsilon_j).$$

provided that the limit on the right-hand side exists.

The assumptions of proposition 1 are mild and amount to well-behavior of the data as the sample size $n$ increases (see [15]). The proof of the proposition
appears in appendix 9. The proposition readily generalizes to a multivariate setting.

Our first example is that of an autocorrelated covariate. Proposition 1 shows that when the entries \( \varepsilon \) are uncorrelated, autocorrelation in \( X \) does not come into effect. However, when \( \varepsilon \) is autocorrelated, the OLS fit has higher variance the more \( X \) is autocorrelated. Intuitively, an autocorrelated covariate replenishes only every some number of rows. Our data thus effectively contains fewer samples of it, and its fit will be less reliable. Over data containing covariates with varying degrees of autocorrelation, the OLS fit will admit uneven variance. We consider the example of autoregressive \( X \) and \( \varepsilon \).

**Corollary 2.** In the setting of proposition 1, if

\[
\text{Cov}(X_i, X_j) = \pi^{|i-j|}; \quad \text{Cov}(\varepsilon_i, \varepsilon_j|\{X_{n}\}_{n=1}^{\infty}) = \sigma^2 \rho^{|i-j|}
\]

for \( \sigma^2 > 0 \) and \( 0 \leq \pi, \rho < 1 \), then

\[
n \text{Var}(\hat{\beta}_n) \xrightarrow{n \to \infty} \frac{\sigma^2}{1 - \pi \rho} + \frac{\pi}{1 - \pi \rho}.
\]

Fixing \( \rho > 0 \) the autocorrelation coefficient of \( \varepsilon \), we see the OLS variance grows along with \( 0 \leq \pi < 1 \) the autocorrelation coefficient of \( X \). The proof of corollary 2 is given in appendix 9.

We move on to discuss random effects, which reduce to heteroscedasticity in the noise with magnitude aligned to the covariates associated with random-effects. Suppose \( y_i = X_i \beta_i + \varepsilon_i \) for all \( i = 1, \ldots, n \), with \( \beta_1, \ldots, \beta_n \) random such that \( E[\beta_i|X] = \beta \) is constant among all \( i \). An equivalent formulation is

\[
y = X\beta + \eta \quad ; \quad \eta_i = \varepsilon_i + X_i(\beta_i - \beta)
\]

for all \( i = 1, \ldots, n \). We have \( E[\eta|X] = 0 \) so long as \( E[\varepsilon|X] = 0 \), yet the noise variance is dependent on the covariate value. Standard methods for estimating the fixed and random effects in a mixed-effects model, require knowledge of the covariances of the noise and random effects and utilize them in similar way as GLS [1]. They are therefore likewise susceptible to misspecification under contemporaneous exogeneity, and we are resorted to using OLS to estimate the effects.

We now demonstrate that fitting a covariate associated with a random effect is accompanied with increased variance, in a simplistic setting of autoregressive random effect.

**Corollary 3.** Suppose \( y_i = X_i \beta + (\varepsilon_i + X_i b_i) \), where \( \{X_i\}_{i=1}^{\infty} \) are independent and identically distributed with mean zero and variance one, \( \{\varepsilon_i\}_{i=1}^{\infty} \) are independent with mean zero and variance \( \sigma^2 \), and \( \{b_i\}_{i=1}^{\infty} \) have mean zero and covariance \( \text{Cov}(b_i, b_j) = \text{Var}(b_1)\tau^{|i-j|} \). Assume furthermore that \( \{X_i\}_{i=1}^{\infty}, \{\varepsilon_i\}_{i=1}^{\infty}, \text{and } \{b_i\}_{i=1}^{\infty} \) are independent of each other, and that the conditions for proposition 1 are met. Then, in the setting of proposition 1 it holds that

\[
n \text{Var}(\hat{\beta}_n) \xrightarrow{n \to \infty} \frac{\sigma^2}{1 - \pi} + \frac{2\pi}{1 - \tau} \left( \text{Var}(X_1^2) + \frac{\pi}{1 - \pi \rho} \right).
\]
Note that $\mathbb{E}[X_i^4] \geq \mathbb{E}[X_i^2]^2 = 1$ by Jensen's inequality. The OLS variance grows as the variance and autocorrelation of the random effect grow. The proof of corollary 3 is given in appendix 8. To complement corollary 3 we compare to a similar situation in which the variance of the noise is not aligned with the covariate.

**Corollary 4.** Suppose $y_i = X_i \beta + (\varepsilon_i + Z_i b_i)$, where $\{Z_i\}_{i=1}^{\infty}$ are independent with mean zero and variance one, and are furthermore independent of $\{X_i\}_{i=1}^{\infty}$, $\{\varepsilon_i\}_{i=1}^{\infty}$, $\{b_i\}_{i=1}^{\infty}$. Assume that the conditions of corollary 3 otherwise hold. Then,

$$n \mathbb{V}ar(\hat{\beta}_n) \xrightarrow{n \to \infty} \sigma^2 + \mathbb{V}ar(b_1).$$

The proof of corollary 4 is given in appendix 9. This ends our discussion of random effects, henceforth we assume everywhere that $\beta$ is fixed, without stating so explicitly.

### 3 The Ideal Ridge Estimator

We begin with a definition.

**Definition 1.** Suppose $y = X \beta + \varepsilon$ where $\mathbb{E}[\varepsilon|X] = 0$. Denote $C = \text{Cov}(\hat{\beta}|X)$ where $\hat{\beta}$ is the OLS estimator. Then the estimator given by

$$\hat{\beta}_\lambda = \left(X^T X + \lambda X^T X C\right)^{-1} X^T y$$

for some $\lambda \geq 0$ is called an **ideal ridge estimator**.

An ideal ridge estimator is obtained by combining the OLS estimator with the usual uninformed ridge prior, according to ideal knowledge of the OLS covariance. Indeed, if the noise $\varepsilon|X$ is normally distributed then $\hat{\beta}|X \sim \mathcal{N}(\beta, C)$ and conversely

$$\beta|X, \hat{\beta} \sim \mathcal{N}(\hat{\beta}, C). \tag{5}$$

Otherwise, the OLS estimator under mild assumptions still has normal asymptotic distribution [6], also under contemporaneous exogeneity [15], and (5) is condoned anyway. We then combine with an uninformed ridge prior

$$\beta \sim \mathcal{N}(0, \lambda^{-1} I_p) \tag{6}$$

where $I_p$ is the identity $p \times p$ matrix, as a source of information on $\beta$ independent of the data, or equivalently as posterior estimation. The resulting distribution of $\beta$ has density which is given by the product of the individual densities [5] and [6]. In general, if the densities of two normal distributions $Z_1 \sim \mathcal{N}(\mu_1, \Sigma_1)$ and $Z_2 \sim \mathcal{N}(\mu_2, \Sigma_2)$ are multiplied with each other, the product distribution unfolds to be normal by completing the square. Its mean is the average of the individual means weighted inversely by their respective variances,

$$Z = Z_1|Z_1 = Z_2 \sim \mathcal{N}(\mu, \Sigma)$$

$$\mu = (\Sigma_1^{-1} + \Sigma_2^{-1})^{-1}(\Sigma_1^{-1} \mu_1 + \Sigma_2^{-1} \mu_2); \quad \Sigma^{-1} = \Sigma_1^{-1} + \Sigma_2^{-1}.$$
We take as estimator the mode of the combined distribution, given by

\[ \hat{\beta}_\lambda = \left( C^{-1} + \lambda I \right)^{-1} C^{-1} \beta = (X^T X + \lambda X^T X C)^{-1} X^T y \]

which is the ideal ridge estimator as in definition \[1\].

See that as \[ \hat{\beta} = \beta + (X^T X)^{-1} X^T \varepsilon \] and \[ E[\varepsilon|X] = 0 \] we the OLS covariance is given by

\[ C = \text{Cov}(\hat{\beta}|X) = (X^T X)^{-1} X^T \text{Cov}(\varepsilon|X) X (X^T X)^{-1}. \]

Whenever \( \text{Cov}(\varepsilon|X) \) is a scalar matrix it follows that \( \text{Cov}(\hat{\beta}|X) \) is proportional to \( (X^T X)^{-1} \). In this case the underlying OLS estimator is the maximum likelihood estimator, and the ideal ridge estimator \( \hat{\beta}_\lambda \) coincides with the standard ridge estimator \( \hat{\beta}_{\text{ridge}} = (X^T X + \lambda I_p)^{-1} X^T y \). Furthermore, the approach described above to obtain the ideal ridge estimator is identical to maximum a posteriori probability estimation. In general, we do not require that the OLS estimator be correctly specified, in the sense that \( \text{Cov}(\hat{\beta}|X) \) is in fact proportional to \( (X^T X)^{-1} \). This enables us to study the properties of ridge regularization disjointly from its underlying estimator.

Whenever \( \text{Cov}(\varepsilon|X) \) is not scalar, the standard ridge estimator no longer is the maximum a posteriori probability estimator, and it furthermore reneges on some of its appealing properties. For example, the variance of fit \( \text{Var}(X^T \hat{\beta}_{\text{ridge}}|x, X) \) may in fact increase for some new observation \( x \in \mathbb{R}^p \), when adding regularization.

**Proposition 5.** Suppose \( y = X \beta + \varepsilon \) with \( E[\varepsilon|X] = 0 \). Let \( \Lambda \) be a symmetric and positive semidefinite \( p \times p \) matrix, and define

\[ \hat{\beta}_{\Lambda,\lambda} = (X^T X + \lambda X^T X \Lambda)^{-1} X^T y. \]

Then, \( \text{Cov}(\hat{\beta}_{\Lambda,\lambda}|X) \) is monotone decreasing in \( \lambda \geq 0 \) in the sense of positive definite matrices, if and only if

\[ \Lambda C^{-1} + C^{-1} \Lambda \]

is positive semidefinite, where \( C = \text{Cov}(\hat{\beta}|X) \) is the covariance of the OLS estimator \( \hat{\beta} \).

Standard ridge uses \( \Lambda = (X^T X)^{-1} \), whereas ideal ridge uses \( \Lambda = C \), rendering \( \Lambda C^{-1} + C^{-1} \Lambda = 2I_p \). The proof of proposition 5 and related discussion appear in appendix 10. Furthermore, see the ideal ridge estimator can be written as

\[ \hat{\beta}_{\lambda} = (I + \lambda C)^{-1} \hat{\beta}. \]

It follows that harsher regularization is administered wherever the OLS covariance \( C = \text{Cov}(\hat{\beta}|X) \) admits high variance.

What are the boundaries of the expressive power of ridge? Recall that the OLS estimator \( \hat{\beta}(y) = (X^T X)^{-1} X^T y \) projects \( y \) orthogonally onto the column space
of $X$. Therefore, $\hat{\beta}(Py) = \hat{\beta}(y)$ where $P$ is the matrix of orthogonal projection onto the column space of $X$. By \ref{eq:OLS} the same is true for the ideal ridge estimator, $\hat{\beta}_\lambda(Py) = \hat{\beta}_\lambda(y)$.

Thus, $\hat{\beta}_\lambda$ is indifferent to the $(n-p)$-dimensional part of $y$ that is orthogonal to the column space of $X$, and cannot extract any information from it. Apart from this, $\hat{\beta}_\lambda$ is the maximum a posteriori probability estimator assuming ridge prior.

**Proposition 6.** Suppose $y = X\beta + \varepsilon$ such that $\varepsilon|X$ is normally distributed with mean zero. Then the ideal ridge estimator is the maximum a posteriori probability estimator assuming ridge prior, if $y$ is substituted with $\hat{y} = X\hat{\beta}$.

In the above, $\hat{\beta}$ is the OLS estimator. We conclude the section by proving proposition \ref{prop:ridge}. The following lemma will be useful.

**Lemma 7.** Let $X$ be an $n \times p$ matrix of rank $p$, and let $\Sigma$ be an $n \times n$ matrix of rank $p$ such that $P\Sigma P = \Sigma$, where $P = X(X^T X)^{-1}X^T$ is the matrix of orthogonal projection onto the column space of $X$. Then, 

$$(X^T \Sigma X)^{-1} = (X^T X)^{-1}X^T \Sigma^+ X(X^T X)^{-1}$$

where $\Sigma^+$ is the Moore-Penrose pseudo-inverse matrix of $\Sigma$.

**Proof.** To see that one is the inverse of the other, multiply the two 

$$X^T \Sigma X(X^T X)^{-1}X^T \Sigma^+ X(X^T X)^{-1} = X^T P\Sigma P^2 \Sigma^+ X(X^T X)^{-1} = X^T \Sigma \Sigma^+ X(X^T X)^{-1} = X^T PX(X^T X)^{-1} = I.$$

**Proof of proposition \ref{prop:ridge}**. Denote by $P$ the matrix of orthogonal projection onto the column space of $X$, and by an assumption of the proposition we may replace $y$ with $X\hat{\beta} = Py = X\hat{\beta} + P\varepsilon$. We may thus assume without loss of generality that $\varepsilon$ originated from a distribution such that $P\text{Cov}(\varepsilon|X)P = \text{Cov}(P\varepsilon|X) = \text{Cov}(\varepsilon|X)$.

Denote $\Sigma = \text{Cov}(\varepsilon|X)$. The maximum a posteriori probability estimator with ridge prior, also known as generalized least squares (GLS), is given here by 

$$\hat{\beta}_{\text{GLS}} = (X^T \Sigma^+ X + \lambda I)^{-1}X^T \Sigma^+ \hat{y} = (X^T \Sigma^+ X + \lambda I)^{-1}X^T \Sigma^+ X(X^T X)^{-1}X^T y = (X^T X + \lambda X^T X(X^T \Sigma^+ X)^{-1})^{-1}X^T y.$$ 

where $\Sigma^+$ is the Moore-Penrose pseudo-inverse of $\Sigma$. By equation \ref{eq:ridge} succeeded by lemma \ref{lem:ridge}, we have 

$$(X^T \Sigma^+ X)^{-1} = (X^T X)^{-1}X^T \Sigma X(X^T X)^{-1} = \text{Cov}(\hat{\beta}|X)$$

therefore $\hat{\beta}_{\text{GLS}}$ is identical to the ideal ridge estimator by definition.
4 Generalizations to Lasso and Other Estimators

We extend the previously discussed framework to a more general setting.

**Definition 2.** Suppose $X, y$ are sampled and let $\hat{\beta}(X, y)$ be an estimator of some parameter $\beta$. Let $p(\hat{\beta}|X, \beta)$ denote the density of the conditional distribution of $\hat{\beta}$, and let $p(\beta)$ denote the density of some prior distribution of $\beta$. Then the estimator given by

$$\hat{\beta} = \arg\max_{\beta} \left\{ p(\hat{\beta}|X, \beta) \cdot p(\beta) \right\}.$$

is called an *ideally regularized estimator*.

Consider the likelihood of $\beta$ according to the estimator on the data,

$$L(\beta|X, \hat{\beta}) = p(\hat{\beta}|X, \beta).$$

The posterior distribution has density which is the product of the likelihood and prior $p(\beta)$. The ideally regularized estimator is the mode of the posterior density, equivalently obtained by combining the likelihood and prior as two independent sources of information on $\beta$.

Unsurprisingly, the ideally regularized estimator is a maximum a posteriori probability estimator.

**Proposition 8.** The ideally regularized estimator is the maximum a posteriori probability estimator if only $X, \hat{\beta}(X, y)$ are observed.

Since $\hat{\beta}$ is observed but $y$ is not, we cannot discriminate between any $y, y'$ such that $\hat{\beta}(X, y) = \hat{\beta}(X, y')$.

**Proof of proposition** Fix $X$. Denote by $y(\hat{\beta})$ the set of all $y$ such that $\hat{\beta}(X, y) = \hat{\beta}$. As only $y(\hat{\beta})$ is observed, the likelihood function is

$$L(y(\hat{\beta})|X, \beta) = \int_{y(\hat{\beta})} p(y|X, \beta) \cdot dy = p(\hat{\beta}|X, \beta) = L(\beta|X, \hat{\beta})$$

where $p(\hat{\beta}|X, \beta)$ is defined as the push-forward probability distribution. Therefore, maximizing the likelihood $L(y(\hat{\beta})|X, \beta)$ as in maximum a posteriori probability estimation, is equivalent to formulating the ideally regularized estimator by definition.

- If $\hat{\beta}|X \sim N(\beta, C)$, the ideally regularized estimator is equivalent to

$$\hat{\beta} = \arg\min_{\beta} \left\{ (\beta - \hat{\beta})^T C^{-1} (\beta - \hat{\beta}) - 2 \log p(\beta) \right\}. \quad (9)$$

When $\hat{\beta}$ is the OLS estimator and $p(\beta)$ is a ridge prior, the ideally regularized estimator as in (9) coincides with the ideal ridge estimator, as previously defined. For other priors, equation (9) leads to a way of computing the ideally regularized estimator.
Proposition 9. The ideally regularized estimator for $\hat{\beta}$ the OLS estimator and some prior density $p(\beta)$ (such as ridge or lasso prior) is equivalent to solving OLS with prior density $p(\beta)$ over data $\tilde{X}, \tilde{y}$ such that

$$\tilde{X}^T\tilde{X} = C^{-1} ; \quad \tilde{X}^T\tilde{y} = C^{-1}\hat{\beta}.$$ 

Proof. To solve ordinary least squares with prior density $p(\beta)$ is to find $\beta^* = \arg\min_\beta \left\{ (\tilde{y} - \tilde{X}\beta)^T(\tilde{y} - \tilde{X}\beta) - c_1 \log p(\beta) \right\}$ where $c_1 > 0$ is a constant that does not depend on $\beta$. See that $(\tilde{y} - \tilde{X}\beta)^T(\tilde{y} - \tilde{X}\beta) = (\beta - \hat{\beta})^TC^{-1}(\beta - \hat{\beta}) + c_2$ where $c_2$ is a constant that does not depend on $\beta$, possibly vanishing. The proposition is then proven using equation (9).

5 A Feasible and Well-Adjusted Ridge Estimator

The ideal ridge estimator was defined in section 3 by

$$\hat{\beta}_\lambda = (X^TX + \lambda X^T\hat{C}X)^{-1}X^Ty.$$ \hspace{1cm} (10)

In order to use ideal ridge, the OLS covariance $C = \text{Cov}(\hat{\beta}|X)$ must be known. In practice, the OLS covariance is rarely known a-priori, and we suggest to estimate $\text{Cov}(\hat{\beta}|X)$ and use the estimator in place of $C$ in (10).

Definition 3. Let $\hat{C}$ be an estimator of the conditional covariance $\text{Cov}(\hat{\beta}|X)$ of the OLS estimator. Then the estimator given by

$$\hat{\beta}_\lambda = (X^TX + \lambda X^T\hat{C}X)^{-1}X^Ty$$

for $\lambda \geq 0$ is called a well-adjusted ridge estimator.

We disregard the abuse in using the same notation $\hat{\beta}_\lambda$ for the ideal ridge estimator and the well-adjusted ridge estimator. In the next sections we outline a three-staged method of estimating the covariance $\text{Cov}(\hat{\beta}|X)$, comprising estimation, regularization and normalization. In the first, a crude estimate of the covariance matrix is obtained. In the second, the estimate is smoothened and shrunken to obtain a more well-behaved estimate. Finally, the estimate is rescaled to standardize the magnitude of the ridge penalty. We begin with estimation.

Estimation.

Robust estimation of the covariance $\text{Cov}(\hat{\beta}|X)$ of an OLS estimator has been studied in the econometric literature for inference purposes. This is known as heteroscedasticity and autocorrelation consistent (HAC) estimation, originating
from the work of Newey and West [14]. The literature regarding HAC estimators is significant, and we do not contribute here anything substantial to it. Rather, we suggest for our purposes to employ, from the extensive range available, a HAC estimator that will suit the problem at hand. We refer to the introduction of HAC estimators by Zeileis [16] and the references therein. We are particularly fond of the following simple and robust methods that are based on resampling. These are akin to those described by Colin Cameron and Miller [4].

For the purpose of resampling, partition the data into folds \((X_1, y_1), \ldots, (X_\Omega, y_\Omega)\). When resampling dependent data, i.e. when the observations are not independent of each other, the guiding principle is that the folds are to be made roughly independent of each other. Often, dependence between rows diminishes as the rows grow farther apart. This suggests partitioning the data into continuous nonoverlapping blocks. The blocks should be large enough so that dependence on other blocks, which is an issue near the boundaries and less so in the interior, is negligible. Further aspects of resampling dependent data by blocks are discussed in [4, 12].

**Cross validation.**

For each fold \(\omega = 1, \ldots, \Omega\), the OLS estimator \(\hat{\beta}_\omega\) is computed on the combined data of all the folds, apart from the \(\omega\)-th fold \((X_\omega, y_\omega)\). The out-of-sample residual for the \(\omega\)-th fold is then \(\hat{\epsilon}_\omega = y_\omega - X_\omega \hat{\beta}_\omega\). Use the covariance estimator

\[
\hat{C}_{cv} = (X^T X)^{-1} \left( \sum_{\omega=1}^{\Omega} X_\omega^T \hat{\epsilon}_\omega \hat{\epsilon}_\omega^T X_\omega \right) (X^T X)^{-1}
\]

which uses an estimate of \(X^T \text{Cov}(\epsilon|X) X\) appearing in equation (7) based on the out-of-sample residuals. This resembles a HAC estimator, with out-of-sample rather than in-sample residuals, and a Lumley-Heagerty-type kernel [16]. We assumed here that \(\text{Cov}(\epsilon|X) = \mathbb{E} [\epsilon \epsilon^T | X]\), which is invalid under contemporaneous exogeneity. However, the approach described above is still valid in approximation for large samples due to consistency of \(\hat{\beta}\).

**Bootstrap.**

Compute a host of perturbed OLS estimates \(\hat{\beta}^1, \ldots, \hat{\beta}^B\), and use

\[
\hat{C}_{\text{bootstrap}} = \frac{1}{B-1} \sum_{b=1}^{B} (\hat{\beta}^b - \bar{\hat{\beta}})(\hat{\beta}^b - \bar{\hat{\beta}})^T
\]

as the covariance estimator, where \(\bar{\hat{\beta}} = (\hat{\beta}^1 + \ldots + \hat{\beta}^B) / B\). We describe the plain nonparametric plug-in approach [5] for generating the perturbed estimates \(\hat{\beta}^1, \ldots, \hat{\beta}^B\), though other bootstrap schemes have been developed for resampling regression coefficients, and for dependent data (see [11]). We thus let \(\hat{\beta}^b\) denote, for each iteration \(b = 1, \ldots, B\), the OLS estimate computed on the combined data of \(\Omega\) folds sampled randomly from among the available \(\Omega\) folds with replacement.

In practice, we have found that the cross validation and bootstrap methods outlined above tend to yield very similar covariance estimates, as well as several
other HAC estimators we have tested. We reserve the discussion of regularization of the covariance estimator to section 6 and skip directly to the concluding stage of normalization.

Normalization.
Standard ridge is a particular case of well-adjusted ridge, using \( \hat{C} = (X^T X)^{-1} \) as estimator for the covariance \( \text{Cov}(\hat{\beta}|X) \) in the formula
\[
\hat{\beta}_\lambda = (X^T X + \lambda X^T \hat{C})^{-1} X^T y
\]
given in definition 3. However, in the setting to which standard ridge is aimed to be adapted to, we rather have \( \text{Cov}(\hat{\beta}|X) = \sigma^2(X^T X)^{-1} \) where
\[
\sigma^2 = n^{-1} \text{tr} (\text{Cov}(\varepsilon|X)).
\]
Thus, standard ridge scales the parameter \( \lambda \) by absorbing the noise variance \( \sigma^2 \) into it.

In order to make well-adjusted ridge behave more like standard ridge in this respect, we suggest as an optional feature to normalize the penalty matrix \( X^T X \hat{C} \) appearing in (11) by its mean diagonal element. That is, to scale the covariance estimator \( \hat{C} \) by
\[
\hat{C}_{\text{norm}} = \hat{C} \cdot \left( \frac{\text{tr} (X^T X \hat{C})}{p} \right)^{-1}.
\]
In this case the penalty matrix \( X^T X \hat{C}_{\text{norm}} \) has the property
\[
\text{tr} (X^T X \hat{C}_{\text{norm}}) = p
\]
incuring total ridge penalty \( p \), akin to standard ridge which uses \( X^T X \hat{C} = I \).
Thus, the parameter \( \lambda \) is similarly scaled between well-adjusted and standard ridge and the two are comparable on a given data set. A further property of this normalization is being indifferent to rescaling of the covariates in \( X \).

6 Covariance Estimator Shrinkage

We have discussed approaches of directly estimating the \( p \times p \) covariance matrix \( \text{Cov}(\hat{\beta}|X) \). However, these are usually too erratic to be used in prediction as they are, and can be improved using shrinkage methods. To underscore this, we repeat here a simple argument by Ledoit and Wolf [13], showing that a covariance matrix estimator overfits by spreading the eigenvalues.

Lemma 10. Let \( C \) be a \( p \times p \) symmetric and positive definite matrix, and let \( \hat{C} \) be an unbiased, symmetric and positive definite estimator of \( C \). Denote by \( \lambda_1(C), \ldots, \lambda_p(C) \) the eigenvalues of \( C \), arranged in some order, and similarly for \( \hat{C} \). Then,
\[
\mathbb{E} \left[ \sum_{i=1}^{p} \lambda_i(\hat{C}) \right] = \sum_{i=1}^{p} \lambda_i(C) ; \quad \mathbb{E} \left[ \sum_{i=1}^{p} \lambda_i(\hat{C})^2 \right] \geq \sum_{i=1}^{p} \lambda_i(C)^2.
\]
with the latter inequality strict unless \( \hat{C} \) is identically equal to \( C \).
While the average eigenvalue of \( \hat{\mathbf{C}} \) is unbiased, the dispersion of empirical eigenvalues tends to be larger than that of the true covariance. We thus underestimate the variance in some directions and overestimate in others. A proof of lemma 10 adapted from [13] appears in appendix 11. We detail two approaches of shrinking the covariance estimator \( \hat{\mathbf{C}} \); a posteriori estimation and denoising by principal component analysis (PCA).

**A posteriori estimation.**
Suppose we wish to combine the previously obtained estimator \( \hat{\mathbf{C}} \) with another covariance matrix \( \mathbf{\Pi} \) as prior. We suggest to use a convex combination of the two, as alleged by the following proposition.

**Proposition 11.** Suppose \( \mathbf{y} = \mathbf{X}\beta + \mathbf{\varepsilon} \) with \( \mathbb{E}[\mathbf{\varepsilon}|\mathbf{X}] = 0 \). Let \( \hat{\mathbf{C}} \) be an estimator of the covariance \( \text{Cov}(\hat{\beta}|\mathbf{X}) \), and let \( \mathbf{\Pi} \) be a symmetric and positive definite matrix. Then the following methods for combining \( \hat{\mathbf{C}} \) with \( \mathbf{\Pi} \) as prior are equivalent:

1. A convex combination: \((1 - \kappa)\hat{\mathbf{C}} + \kappa\mathbf{\Pi}\) where \(0 \leq \kappa \leq 1\).
2. Assuming a Wishart distribution on \( \hat{\mathbf{C}} \) and an inverse-Wishart prior with natural parameter proportional to \( \mathbf{\Pi} \).
3. Assuming a Wishart distribution on \( \mathbf{X}\hat{\mathbf{C}}\mathbf{X}^T \) as an estimator of \( \text{Cov}(\mathbf{\varepsilon}|\mathbf{X}) \) and an inverse-Wishart prior with natural parameter proportional to \( \mathbf{X}\mathbf{\Pi}\mathbf{X}^T \).
4. A ridge-type prior: \( \arg\min_{\mathbf{\Gamma}} \left\{ \|\hat{\mathbf{C}} - \mathbf{\Gamma}\|^2_F + \lambda\|\mathbf{\Gamma} - \mathbf{\Pi}\|^2_F \right\} \) where \( \lambda = \kappa/(1 - \kappa) \) and \( 0 \leq \kappa \leq 1 \).

The Frobenius norm is given by \( \|\mathbf{\Gamma}\|^2_F = \text{tr}(\mathbf{\Gamma}^T\mathbf{\Gamma}) \). A convex combination of the estimated covariance matrix with a prior appears, e.g. in [13].

**Proof of proposition 11.** The inverse-Wishart distribution is conjugate to the Wishart distribution, and their combination is linear in the parameters \( \hat{\mathbf{C}} \) and \( \mathbf{\Pi} \). This shows equivalence of statements 1 and 2, and furthermore 3 by equation (7). Equivalence of these to statement 4 can be derived by differentiation. \( \square \)

We thus combine the empirical estimate \( \hat{\mathbf{C}} \) with a prior by

\[
\hat{\mathbf{C}}_\kappa = (1 - \kappa)\hat{\mathbf{C}} + \kappa\mathbf{\Pi}
\]  

(12)

where \(0 \leq \kappa \leq 1\). The question remains of which prior covariance \( \mathbf{\Pi} \) to choose. In the absence of an evident a priori candidate, we suggest to use

\[
\mathbf{\Pi} = (\mathbf{X}^T\mathbf{X})^{-1} \frac{\text{tr}(\hat{\mathbf{C}})}{\text{tr}(\mathbf{X}^T\mathbf{X})^{-1}}.
\]  

(13)

This is the standard estimator of OLS covariance, scaled to have trace equal to that of \( \hat{\mathbf{C}} \). When \( \kappa = 1 \), the well-adjusted ridge estimator as in definition 3 degenerates back to the standard ridge estimator, up to rescaling of \( \lambda \). Thus, the parameter \(0 \leq \kappa \leq 1\) serves as both to mitigate the degrees of freedom of the covariance estimator, and to scale between standard ridge and well-adjusted
ridge. The coefficient in (13) is included so that the combination in (12) will not interfere with the scale of the estimator \( \text{tr}(\hat{C}) \), which is presumably unbiased by lemma 10.

**PCA denoising.**

In extreme cases, the \( p \times p \) symmetric matrix \( \text{Cov}(\hat{\beta}_i|X) \) may be too difficult to estimate reasonably. This might lead to a regularized estimator \( \hat{C}_\kappa \) that relies too heavily on the prior \( \Pi \), thus missing the benefit of using a well-adjusted ridge estimator. However, the number of estimated parameters can be reduced to \( p \) if we use the prior matrix \( \Pi \) for denoising \( \hat{C} \) via principal component analysis (PCA).

Indeed, let \( U \) be an orthogonal \( p \times p \) matrix such that \( U^T\Pi U \) is diagonal. Then the columns of \( U \) are an orthogonal basis of eigenvectors of \( \Pi \). Define the orthogonal projection onto the set of eigenvectors of \( \Pi \) by

\[
p_{\Pi}(\hat{C}) = U((U^T\hat{C}U) \circ I)U^T
\]

where \( \circ \) is the Hadamard entry-wise product, \( (A \circ B)_{ij} = A_{ij}B_{ij} \). The projection \( p_{\Pi}(\hat{C}) \) switches \( \hat{C} \) to the basis \( U \), eliminates all off-diagonal entries, then switches back to the original basis. This is in fact an orthogonal projection in the space of matrices; \( p_{\Pi}(C) \) is the closest symmetric matrix to \( C \) which has the same eigenvectors as \( \Pi \), in Frobenius norm. That is,

\[
\arg\min_{\Gamma} \left\{ \|\hat{C} - \Gamma\|_F \mid U^T\Gamma U \text{ is diagonal} \right\} = p_{\Pi}(\hat{C}).
\]

Thus, as an alternative to the regularized estimator (12) we may use

\[
\hat{C}_\kappa = (1 - \kappa) \cdot p_{\Pi}(\hat{C}) + \kappa \Pi
\]

The PCA-denoised covariance \( p_{\Pi}(\hat{C}) \) estimates the variance along the directions of only the \( p \) eigenvectors of \( \Pi \). In practice, we have found in many cases that \( p_{\Pi}(\hat{C}) \) with \( \Pi = (X^TX)^{-1} \) as in (13) retains most of the information contained in the original estimator \( \hat{C} \), at least in the sense of \( \|p_{\Pi}(\hat{C})\|_F \) being the major portion of \( \|\hat{C}\|_F \). This, while sharply reducing the condition number and eigenvalue dispersion of \( \hat{C} \).

We may, however, wish not to eliminate the off-diagonal elements in \( p_{\Pi}(\hat{C}) \) altogether, as they do contain some information. Similar to proposition 11 we may penalize them in ridge-like fashion

\[
\arg\min_{\Gamma} \left\{ \|\hat{C} - \Gamma\|_F^2 + \lambda \sum_{i \neq j} (u_i^T\Gamma u_j)^2 \right\} = (1 - \mu) \hat{C} + \mu \cdot p_{\Pi}(\hat{C})
\]

where \( u_1, \ldots, u_p \) are the columns of \( U \) and \( \mu = \lambda/(1 + \lambda) \). This leads to a regularized estimator which generalizes both previous ones we discussed,

\[
\hat{C}_{\mu, \kappa} = (1 - \kappa)((1 - \mu) \hat{C} + \mu \cdot p_{\Pi}(\hat{C})) + \kappa \Pi
\]

(15)
Here, $\mu$ is the denoising parameter and $\kappa$ scales between well-adjusted and standard ridge. When $\mu = 0$, this is the regularized estimator in (12). When $\mu = 1$, we arrive at the estimator in (14). When $\kappa = 0$ this results in a widely permissive estimator which uses the prior $\Pi$ only for denoising.

**Choosing $\kappa$ and $\mu$.**

In order to choose good values of the parameters $\kappa$ and $\mu$ for a given problem, one may measure how well they predict the covariance matrix out-of-sample over the training data, using resampling. To this end, a metric $d(C, C')$ between covariance matrices is required. Let $\hat{C}$ be the covariance estimate computed on a part of the data, and let $\hat{C}_{\text{out}}$ be computed on an independent part of the data. Then, select

$$\kappa^*, \mu^* = \arg \min_{\kappa, \mu} d(\hat{C}_{\mu, \kappa}, \hat{C}_{\text{out}})$$

over many iterations of the resampling algorithm. The metric $d$ can be any matrix norm, or alternatively, considering that $\hat{C}$ is assumed to be the covariance of a normal distribution, the metric $d$ may use any metric $d'$ over probability distributions

$$d(C, C') = d'(N(\beta, C), N(\beta, C')).$$

### 7 Simulation Study

We describe here the results of two simulation studies examining the performance of the well-adjusted ridge estimator different settings.

In the first study, one of the covariates has significantly higher autocorrelation than the others. Let $y = X\beta + \varepsilon$ where $X$ is an $n \times p$ matrix and $y \in \mathbb{R}^n$. In this study we used $p = 10$ covariates with $n = 2000$ observations. The covariates were sampled independently of each other, from a normal distribution with mean zero and variance one. For each of nine covariates, the observations were sampled independently from the other. The remaining covariate, without loss of generality the first covariate, follows an autoregressive scheme with mean lifetime 10, i.e. $\text{Cov}(X_{i1}, X_{j1}) = \pi^{|i-j|}$ for $\pi = \exp(-1/10)$. The $p$ individual effects $\beta = (\beta_1, ..., \beta_p)$ were sampled independently from each other and independently from the covariates, from a normal distribution with mean zero and variance one. The residual noise $\varepsilon$ was sampled independently from the covariates and effects, from a normal distribution with mean zero and variance $\sigma^2 I_p$, such that $1/\sigma^2$ can be said to be the **signal-to-noise ratio**. The residual noise follows an autoregressive scheme with mean lifetime 10, i.e. $\text{Cov}(\varepsilon_i, \varepsilon_j) = \sigma^2 p \rho^{|i-j|}$ for $\rho = \exp(-1/10)$. We then computed the standard ridge estimator $\hat{\beta}_{\text{ridge}, \lambda} = (X^TX + \lambda I)\hat{X}^Ty$, the well-adjusted ridge estimator $\hat{\beta}_{\text{well-adjusted}, \lambda} = (X^TX + \lambda X^T\hat{C}_{\mu, \kappa})^{-1}X^Ty$ and the ideal ridge estimator $\hat{\beta}_{\text{ideal}, \lambda} = (X^TX + \lambda X^TXC)^{-1}X^Ty$ for various values of $\lambda \geq 0$ and $0 \leq \mu, \kappa \leq 1$. The ideal ridge estimator $\hat{\beta}_{\text{ideal}, \lambda}$ uses the true OLS covariance $C = \text{Cov}(\hat{\beta}_{\text{OLS}}(X))$. The well-adjusted ridge estimator $\hat{\beta}_{\text{well-adjusted}, \lambda}$ uses the covariance estimate $\hat{C}_{\mu, \kappa}$ which was computed using the block-bootstrap approach outlined in section 5 with $B = 2000$ iterations and
Ω = 20 continuous non-overlapping equal-sized blocks. We used shrinkage with \( \mu, \kappa \) as described in section 5 using prior covariance proportional to \((X^T X)^{-1}\).

For each resulting estimator \( \hat{\beta} \) we then computed its squared estimation error \((\hat{\beta}_1 - \beta_1)^2 + \ldots + (\hat{\beta}_p - \beta_p)^2\), e.g. for the zero estimator \( \hat{\beta} = 0 \) we expect squared estimation error of \( p \). Notice that as the columns of \( X \) and independent and have unit variance, the squared estimation error as above is equal to expected out of sample prediction error. We repeated this process \( N = 50000 \) independent times, and we report the average and standard error of squared estimation errors over the \( N \) tries.

We first show the results for \( \sigma^2 = 10 \) (table 1), a low signal-to-noise environment, where regularization is imperative. We report results for OLS, and for standard and well-adjusted ridge with optimal \( \lambda \geq 0 \), selected as the value of \( \lambda \) which gave the lowest squared estimation error averaged over the \( N \) tries.

| method              | \( \mu = 0 \) | \( \mu = 0.2 \) | \( \mu = 0.4 \) | \( \mu = 0.6 \) | \( \mu = 0.8 \) |
|---------------------|----------------|----------------|----------------|----------------|----------------|
| OLS \( \lambda = 0 \) | 0.953          | 0.869          | 0.784          | 0.760          |
| standard ridge      |                | (0.0033)       | (0.0028)       |
| optimal \( \lambda \) |                |                |                |
| well-adjusted ridge | 0.784          | 0.782          | 0.795          | 0.819          | 0.846          |
| optimal \( \lambda \) | (0.0024)       | (0.0024)       | (0.0024)       | (0.0026)       | (0.0027)       |
| ideal ridge         | 0.760          |                |                |                |
| optimal \( \lambda \) | (0.0023)       |

The average (standard error) of squared estimation error over \( N = 50000 \) tries is reported.

Here, using well-adjusted ridge over standard ridge doubles the contribution from using standard ridge over unregularized OLS. This simple setting allows for covariance shrinkage even as light as \( \mu = \kappa = 0 \) with near-optimal result. Recall that well-adjusted ridge with \( \mu = \kappa = 1 \) is identical to standard ridge. In the same experiment, we report the average \( \hat{\beta}_1^2 \) over all repetitions, and show that it diminishes harsher in well-adjusted ridge than other elements of \( \hat{\beta} \) (see table 2).
Table 2: Magnitude of $\hat{\beta}_1$ with autocorrelation, $\sigma^2 = 10$

| method                | $\mu = 0$ | $\mu = 0.2$ | $\mu = 0.4$ | $\mu = 0.6$ | $\mu = 0.8$ |
|-----------------------|-----------|-------------|-------------|-------------|-------------|
|                       | $\kappa = 0$ | $\kappa = 0.2$ | $\kappa = 0.4$ | $\kappa = 0.6$ | $\kappa = 0.8$ |
| OLS $\lambda = 0$    | 1.503     |             |             |             |             |
| standard ridge       |           |             |             |             |             |
| optimal $\lambda$    |           |             |             |             |             |
| well-adjusted ridge  | 1.238     | (9.037)     |             |             |             |
| optimal $\lambda$    |           |             |             |             |             |
| ideal ridge          | 0.694     | 0.808       | 0.931       | 1.053       | 1.160       |
| optimal $\lambda$    | (9.223)   | (9.089)     | (9.026)     | (9.010)     | (9.020)     |

The average of $\hat{\beta}_1^2$ (in parentheses $\hat{\beta}_1^2 + \ldots + \hat{\beta}_p^2, p = 10$) over $N = 50000$ tries is reported.

In a relatively higher signal-to-noise environment, $\sigma^2 = 2$ (table 3), the contribution of well-adjusted ridge is smaller in absolute value, but still retains the relative benefit over using standard ridge.

Table 3: Estimation error with autocorrelation, higher signal-to-noise ($\sigma^2 = 2$)

| method                | $\mu = 0$ | $\mu = 0.2$ | $\mu = 0.4$ | $\mu = 0.6$ | $\mu = 0.8$ |
|-----------------------|-----------|-------------|-------------|-------------|-------------|
|                       | $\kappa = 0$ | $\kappa = 0.2$ | $\kappa = 0.4$ | $\kappa = 0.6$ | $\kappa = 0.8$ |
| OLS $\lambda = 0$    | 0.1907    |             |             |             |             |
| standard ridge       |           |             |             |             |             |
| optimal $\lambda$    |           |             |             |             |             |
| well-adjusted ridge  | 0.1871    | 0.1818      | 0.1828      | 0.1844      | 0.1860      |
| optimal $\lambda$    | (0.0006)  | (0.0006)    | (0.0006)    | (0.0006)    | (0.0006)    |
| ideal ridge          | 0.1805    |             |             |             |             |
| optimal $\lambda$    | (0.0006)  |             |             |             |             |

The average (standard error) of squared estimation error over $N = 50000$ tries is reported.

In the second study, one of the covariates is associated with a random effect. The setting in this study was identical to that of the first study, except in the following respects. There is no autocorrelation in the covariates and response, i.e. $\pi = \rho = 0$. Instead, additional noise is added with magnitude proportional to the first covariate, recall corollary 3 and the discussion preceding it. That is, we have $y = X\beta + \eta$ where $\eta_i = \varepsilon_i + X_i b_i$ for $i = 1, \ldots, n$, and it remains to describe $b_1, \ldots, b_n$. Indeed, $b_1, \ldots, b_n$ were sampled randomly from a normal distribution with mean zero following an autoregressive scheme such that $\text{Cov}(b_i, b_j) = \text{Var}(b_1) \tau^{|i-j|}$, compare with corollary 3. We used $\tau = \exp(-1/100)$ to model a relatively-slowly moving effect, alongside $\text{Var}(b_1) = 5$ and $\sigma^2 = 0.5$, recall $\text{Var}(\varepsilon_1) = \sigma^2 p = 5$, in order for the noise attributed to the random effect to be a discernible part of the total noise $\eta$, recall corollary 3. The results are reported in table 4.
Table 4: Estimation error with random effect

| method               | $\mu = 0$ $\kappa = 0$ | $\mu = 0.2$ $\kappa = 0.2$ | $\mu = 0.4$ $\kappa = 0.4$ | $\mu = 0.6$ $\kappa = 0.6$ | $\mu = 0.8$ $\kappa = 0.8$ |
|----------------------|-------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| OLS $\lambda = 0$   | 0.506 (0.0030)          |                               |                               |                               |                               |
| standard ridge       | 0.483 (0.0027)          |                               |                               |                               |                               |
| ideal ridge          | 0.362 (0.0020)          |                               |                               |                               |                               |
| well-adjusted ridge  | 0.367 (0.0020)          | 0.375 (0.0021)                | 0.396 (0.0021)                | 0.430 (0.0023)                | 0.464 (0.0025)                |
| optimal $\lambda$    |                         |                               |                               |                               |                               |

The average (standard error) of squared estimation error over $N = 50000$ tries is reported.

8 References

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9 Appendix: Proofs for Motivating Examples

In this section we provide proofs for the statements made in section 2.

Proof of proposition 2. Denote \( \hat{\beta} = \hat{\beta}_n \), \( X = (X_1, \ldots, X_n) \) and \( \varepsilon = (\varepsilon_1, \ldots, \varepsilon_n) \), permitting the abuse in disregarding the dimension \( n \). As \( \varepsilon \) has zero mean conditioned upon \( X \) we have

\[
\text{Var}(\hat{\beta}) = n \cdot \mathbb{E} \left[ \frac{X^T \varepsilon \varepsilon^T X}{(X^T X)^2} \right] = \mathbb{E} \left[ \frac{X^T \Sigma_n X / n}{(X^T X / n)^2} \right]. \tag{16}
\]

By the assumptions of the proposition, \( (X^T X / n)^2 \to 1 \) in probability, whereas the numerator \( \{X^T \Sigma_n X / n\}_{n=1}^\infty \) in (16) converges in probability as well and we shall compute the limit. See that

\[
\mathbb{E} \left[ X^T \Sigma_n X \right] = \sum_{i,j=1}^n \mathbb{E} \left[ (\Sigma_n)_{ij} X_i X_j \right] = \sum_{i,j=1}^n \text{Cov}(X_i \varepsilon_i, X_j \varepsilon_j) \tag{17}
\]

and we denote this by \( V_n = \mathbb{E} \left[ X^T \Sigma_n X \right] \). As \( \{X_n\}_{n=1}^\infty \) have uniformly bounded fourth moments, the sequence \( \{X^T X / n\}_{n=1}^\infty \) is uniformly integrable [7]. Since \( \{\Sigma_n\}_{n=1}^\infty \) is uniformly bounded in operator norm there exists \( M > 0 \) such that \( X^T \Sigma_n X \leq M X^T X \), hence the sequence \( \{X^T \Sigma_n X / n\}_{n=1}^\infty \) is uniformly integrable as well. Therefore, by convergence by uniform integrability [7] and by (17), the limit is

\[
\frac{X^T \Sigma_n X}{n} \xrightarrow{p} \lim_{n \to \infty} \mathbb{E} \left[ \frac{X^T X}{n} \right] = \lim_{n \to \infty} \frac{1}{n} V_n.
\]

Consequently, the integrand in (16) converges in probability to

\[
\frac{X^T \Sigma_n X / n}{(X^T X / n)^2} \xrightarrow{p} \lim_{n \to \infty} \frac{1}{n} V_n. \tag{18}
\]

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It remains to apply convergence by uniform integrability again, this time on the variance formula (16) to obtain that the limit variance is the probability limit of the integrand. Indeed, using $M$ as before we have

$$
\frac{X^T \Sigma_n X/n}{(X^T X/n)^2} \leq \frac{M}{X^T X/n}
$$

By assumption \{n(X^T X)^{-1}\}_{n=1}^\infty are uniformly integrable, hence the integrand in (16) constitutes a uniformly integrable sequence as well, and thus by convergence by uniform integrability and by (16) and (18) we obtain

$$
n \text{Var}(\beta) = \mathbb{E} \left[ \frac{X^T \Sigma_n X/n}{(X^T X/n)^2} \right] \longrightarrow \lim_{n \to \infty} \frac{1}{n} V_n
$$

as required. \hfill \square

\textbf{Proof of corollary 2} See that

$$
\text{Cov}(X_i \varepsilon_i, X_j \varepsilon_j) = \mathbb{E}[X_i X_j \varepsilon_i \varepsilon_j] = \mathbb{E}[X_i X_j \mathbb{E}[\varepsilon_i \varepsilon_j | X, X_j]] = \sigma^2 (\pi \rho)^{|i-j|}.
$$

Hence,

$$
\frac{1}{n} \sum_{i,j=1}^n \text{Cov}(X_i \varepsilon_i, X_j \varepsilon_j) = \frac{\sigma^2}{n} \sum_{i,j=1}^n (\pi \rho)^{|i-j|} = \frac{\sigma^2}{n} \sum_{\omega=-n}^n (n - |\omega|)(\pi \rho)^{|\omega|}.
$$

We now show that

$$
\sum_{\omega=-n}^n \left( 1 - \frac{|\omega|}{n} \right) a^{|\omega|} \xrightarrow{n \to \infty} \frac{1+a}{1-a}
$$

for any $0 \leq a < 1$ and this will suffice to prove the corollary. Indeed,

$$
\sum_{\omega=-n}^n a^{|\omega|} = -1 + 2 \sum_{\omega=0}^n a^\omega = -1 + \frac{2(1-a^{n+1})}{1-a} \xrightarrow{n \to \infty} \frac{1+a}{1-a}.
$$

Likewise,

$$
\frac{1}{n} \sum_{\omega=-n}^n |\omega| a^{|\omega|} \leq \frac{2}{n} \sum_{\omega=0}^\infty \omega a^\omega = \frac{2a}{n(1-a)^2} \xrightarrow{n \to \infty} 0.
$$

Combining (20) with (21) we get (19). \hfill \square

\textbf{Proof of corollary 3} By proposition 1

$$
\lim_{n \to \infty} n \text{Var}(\beta_n) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^\infty \text{Cov}(X_i(\varepsilon_i + X_i b_i), X_j(\varepsilon_j + X_j b_j)).
$$

Denote $V_{ij} = \text{Cov}(X_i(\varepsilon_i + X_i b_i), X_j(\varepsilon_j + X_j b_j))$. As all variables have mean zero and as \{b_i\}_{i=1}^\infty, \{X_i\}_{i=1}^\infty, \{\varepsilon_i\}_{i=1}^\infty are independent of each other, we have

\begin{align*}
V_{ij} &= \mathbb{E}[X_i X_j (\varepsilon_i + X_i b_i)(\varepsilon_j + X_j b_j)] \\
&= \mathbb{E}[X_i X_j] \cdot \mathbb{E}[\varepsilon_i \varepsilon_j] + \mathbb{E}[X_i^2 X_j^2] \cdot \mathbb{E}[b_i b_j] \\
&= \delta_{ij} \cdot (\sigma^2 + \mathbb{E}[X_i^2] \cdot \text{Var}(b_i)) + (1 - \delta_{ij}) \cdot \text{Cov}(b_i, b_j)
\end{align*}

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where \( \delta_{ij} \) equals one when \( i = j \) and zero otherwise. As \( \{X_i\}_{i=1}^{\infty} \) are identically distributed we have \( \mathbb{E}[X_i^2] = \mathbb{E}[X_1^2] \) for all \( i = 1, \ldots, n \). Furthermore, \( \text{Cov}(b_i, b_j) = \text{Var}(b_1) \tau^{i|j|} \) and in particular \( \text{Var}(b_i) = \text{Var}(b_1) \). Then, by (22) we get

\[
\lim_{n \to \infty} n \text{Var}(\hat{\beta}_n) = \sigma^2 + \text{Var}(b_1) \left( \mathbb{E}[X_1^2] - 1 + \lim_{n \to \infty} \frac{1}{n} \sum_{i,j=1}^{n} \tau^{i|j|} \right).
\]

In the proof of corollary 2 we computed

\[
\lim_{n \to \infty} \frac{1}{n} \sum_{i,j=1}^{n} \tau^{i|j|} = \frac{1 + \tau}{1 - \tau}
\]

and this concludes the proof of the corollary.

**Proof of corollary 7** By proposition 1

\[
\lim_{n \to \infty} n \text{Var}(\hat{\beta}_n) = \lim_{n \to \infty} \frac{1}{n} \sum_{i,j=1}^{\infty} \text{Cov}(X_i(\varepsilon_i + Z_i b_i), X_j(\varepsilon_j + Z_j b_j)). \quad (23)
\]

Denote \( V_{ij} = \text{Cov}(X_i(\varepsilon_i + X_i b_i), X_j(\varepsilon_j + X_j b_j)) \). As all variables have mean zero and as \( \{b_i\}_{i=1}^{\infty}, \{X_i\}_{i=1}^{\infty}, \{Z_i\}_{i=1}^{\infty}, \{\varepsilon_i\}_{i=1}^{\infty} \) are independent of each other, we have

\[
V_{ij} = \mathbb{E}[X_i X_j (\varepsilon_i + Z_i b_i)(\varepsilon_j + Z_j b_j)]
\]

\[
= \mathbb{E}[X_i X_j] \cdot \mathbb{E}[\varepsilon_i \varepsilon_j] + \mathbb{E}[X_i X_j] \cdot \mathbb{E}[Z_i Z_j] \cdot \mathbb{E}[b_i b_j]
\]

\[
= \delta_{ij} \cdot (\sigma^2 + \text{Var}(b_1)).
\]

where \( \delta_{ij} \) equals one when \( i = j \) and zero otherwise. By (23), the corollary is proven.

**10 Appendix: Monotonicity of Ridge**

We begin by proving proposition 5.

**Proof of proposition 5** See that \( \hat{\beta}_{A,\lambda} = (I + \lambda A)^{-1} \hat{\beta} \) and consequently

\[
\text{Cov}(\hat{\beta}_{A,\lambda}|X) = (I + \lambda A)^{-1} C(I + \lambda A)^{-1}. \quad (24)
\]

The covariance \( \text{Cov}(\hat{\beta}_{A,\lambda}|X) \) is monotone decreasing in \( \lambda \geq 0 \) in the sense of positive definite matrices, if and only if its inverse \( \text{Cov}(\hat{\beta}_{A,\lambda}|X)^{-1} \) is increasing \cite{9}. Inverting, we get

\[
\text{Cov}(\hat{\beta}_{A,\lambda}|X)^{-1} = C^{-1} + \lambda(AC^{-1} + C^{-1}A) + \lambda^2 AC^{-1}A. \quad (25)
\]

The matrix \( \Delta C^{-1}A \) in (25) is symmetric and positive semidefinite. If the matrix \( \Delta C^{-1} + C^{-1}A \) is positive semidefinite as well, then \( \text{Cov}(\hat{\beta}_{A,\lambda}|X)^{-1} \) is monotonely increasing for as \( \lambda \) increases, a positive semidefinite matrix is added. Conversely,

\[
\frac{d}{d\lambda} \bigg|_{\lambda=0} \text{Cov}(\hat{\beta}_{A,\lambda}|X)^{-1} = \Delta C^{-1} + C^{-1}A
\]

therefore when \( \Delta C^{-1} + C^{-1}A \) is not positive semidefinite, \( \text{Cov}(\hat{\beta}_{A,\lambda}|X)^{-1} \) cannot be monotone increasing.
Recall by (7) that
\[ C = C(\Sigma) = (X^TX)^{-1}X^T\Sigma XX^TX)^{-1}. \]
Since \( \Sigma \) is an arbitrary \( n \times n \) symmetric and positive semidefinite matrix, \( C \) can be assumed the form of any \( p \times p \) symmetric and positive semidefinite matrix. Indeed, for a given matrix \( A \) consider \( \Sigma(A) = AXAX^T \) for which \( C(\Sigma(A)) = A \).

The standard ridge estimator uses \( \Lambda = (X^TX)^{-1} \), as it implicitly assumes that the covariance \( C \) of the OLS estimator is proportional to \( (X^TX)^{-1} \). As \( C^{-1} \) is general, the matrix \( \Lambda C^{-1} + C^{-1} \Lambda \) in equation (25) is not in general positive semidefinite, hence \( \text{Cov}(\hat{\beta}_{A,\lambda}|X) \) is not in general decreasing in \( \lambda \). Consider, for example
\[ C^{-1} = \begin{pmatrix} 1 & 1 \\ 1 & 10 \end{pmatrix}; \quad \Lambda = \begin{pmatrix} 1 & -2 \\ -2 & 10 \end{pmatrix}; \quad \Lambda C^{-1} + C^{-1} \Lambda = \begin{pmatrix} -2 & -11 \\ -11 & 196 \end{pmatrix}. \]

See though, that by equation (25) when \( \lambda \) is large enough, \( \text{Cov}(\hat{\beta}_{A,\lambda}|X) \) becomes monotone decreasing regardless of the choice of symmetric \( \Lambda \).

To emphasize the consequence of this, see that by equation (24) we have
\[ \frac{d}{d\lambda} \bigg|_{\lambda=0} \text{Cov}(\hat{\beta}_{A,\lambda}|X) = -\text{tr}(AC + CA). \]
Hence, if \( AC + CA \) is not positive semidefinite then for some \( x \in \mathbb{R}^p \),
\[ \text{Var}(x^T\hat{\beta}_{A,\lambda}|x, X) = x^T\text{Cov}(\hat{\beta}_{A,\lambda}|X)x \]
is increasing when little regularization is added to the unregularized OLS estimator, resulting in an estimator \( \hat{\beta}_{A,\lambda} \) which is both biased and has increased variance compared to the unregularized OLS estimator.

11 Appendix: Overfitting Covariance Matrices

Proof of lemma 10 Assume without loss of generality that \( C \) and \( \hat{C} \) are given in an orthogonal basis in which \( C \) is diagonal. We may thus assume \( \lambda_i(C) = C_{ii} \) for all \( i = 1, \ldots, p \). Now, the sum of eigenvalues is unbiased by linearity. For the sum of squared eigenvalues, let \( V \) be an orthogonal matrix such that \( V^T\hat{C}V \) is diagonal. Then,
\[ \sum_{i=1}^p \lambda_i(\hat{C})^2 = \text{tr}((V^T\hat{C}V)^2) = \text{tr}(\hat{C}^2) = \sum_{i,j=1}^p \hat{C}_{ij}^2 \geq \sum_{i=1}^p \hat{C}_{ii}^2 \]
with the latter inequality strict unless \( \hat{C}_{ij} = C_{ij} = 0 \) for all \( i \neq j \). Hence,
\[ \mathbb{E} \left[ \sum_{i=1}^p \lambda_i(\hat{C})^2 \right] \geq \sum_{i=1}^p \mathbb{E} [\hat{C}_{ii}^2] \geq \sum_{i=1}^p \mathbb{E} [\hat{C}_{ii}]^2 = \sum_{i=1}^p C_{ii}^2 = \sum_{i=1}^p \lambda_i(C)^2 \]
where the latter inequality, given by Jensen’s inequality, is strict unless \( \hat{C}_{ii} \) is identically equal to \( C_{ii} \) for all \( i \).