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arXiv:1809.00249v1 [math.NA] 1 Sep 2018

CONVERGENCE OF REGULARIZATION PARAMETERS FOR SOLUTIONS USING THE FILTERED TRUNCATED SINGULAR VALUE DECOMPOSITION

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Abstract. The truncated singular value decomposition (TSVD) may be used to find the solution of the linear discrete ill-posed problem $A\mathbf{x} \approx \mathbf{b}$ using Tikhonov regularization. Regularization parameter α^2 balances between the sizes of the fit to data functional $\|A\mathbf{x} - \mathbf{b}\|_2^2$ and the regularization term $\|\mathbf{x}\|_2^2$. Minimization of the unbiased predictive risk estimation (UPRE) function is one suggested method to find α when the noise $\boldsymbol{\eta}$ in the measurements $\mathbf{b}$ is assumed to be normally distributed with white noise variance σ^2. We show that α_k, the regularization parameter for the solution obtained using the TSVD with k terms, converges with k, when estimated using the UPRE function. For the analysis it is sufficient to assume that the discrete Picard condition is satisfied for exact data but that noise contaminates the measured data coefficients s_i for some ℓ, $E(s_i^2) = \sigma^2$ for $i > \ell$, and that the problem is mildly, moderately or severely ill-posed. The relevance of the noise assumptions in terms of the decay rate of the model is investigated and provides a lower bound on α in terms of the noise level and the decay rate of the singular values. Supporting results are contrasted with those obtained using the method of generalized cross validation that is another often suggested method for estimating α. An algorithm to efficiently determine α_k, which also finds the optimal k, is presented and simulations for two-dimensional examples verify the theoretical analysis and the effectiveness of the algorithm for increasing noise levels.

1. Introduction

We consider the the solution of $A\mathbf{x} \approx \mathbf{b}$, or $A\mathbf{x} \approx \mathbf{b}_{\text{true}} + \boldsymbol{\eta} = \mathbf{b}$ for noise (measurement error) $\boldsymbol{\eta}$, where $A \in \mathcal{R}^{m\times n}$ is ill-conditioned, and the system of equations arises from the discretization of an ill-posed inverse problem that may be over or under determined. The general Tikhonov regularized linear least squares problem

$$\mathbf{x}^* = \arg\min_{\mathbf{x}} \{\|A\mathbf{x} - \mathbf{b}\|_{W_\mathbf{b}}^2 + \|D(\mathbf{x} - \mathbf{x}_0)\|_{W_\mathbf{x}}^2\}, \tag{1}$$

is a well-accepted approach for finding the solution $\mathbf{x}$. Here $\mathbf{x}_0$ is given prior information, $W_\mathbf{b}$ and $W_\mathbf{x}$ are weighting matrices on the data fidelity and regularization terms, resp., D is an optional regularization operator, and we use the weighted norm $\|\mathbf{x}\|_W^2 := \mathbf{x}^T W \mathbf{x}$. Often D is imposed as a spatial differential operator, controlling the size of the derivative(s) of $\mathbf{x}$, but then (1) can be brought into standard form in which D is replaced by I,[1, 13]. Further, it is immediate that the equation can be rewritten in terms of a new variable $\mathbf{y} = \mathbf{x} - \mathbf{x}_0$ when $\mathbf{x}_0 \neq 0$. With statistical information on the error, e.g. $\boldsymbol{\eta} \sim \mathcal{N}(0, C_\mathbf{b})$,

Date: September 5, 2018.

implying Gaussian, mean 0 with covariance matrix $C_{\mathbf{b}}$, $W_{\mathbf{b}} = C_{\mathbf{b}}^{-1}$ can be used to whiten the noise.

While solutions of (1) under the noted assumptions have been extensively studied, e.g. [10, 13, 14, 27] there is still much discussion concerning the selection of α even for the single parameter case, $W_{\mathbf{x}} = \alpha^2 I$. Suggested techniques include, among others, using the Morozov discrepancy principle (MDP) which assumes that the solution should be found within some prescribed χ^2 noise estimate [19], balance of the terms in (1) using the L-curve [13], and minimization of the generalized cross validation (GCV) function [6] or of the statistically motivated Unbiased Predictive Risk Estimator (UPRE) [27]. Although the Singular Value Decomposition (SVD) for A, [7], given by $A = U\Sigma V^T$, does not provide a practical approach for solving (1) for large scale problems, it is a useful tool for understanding the solutions of (1) as a function of the regularization parameter α and for writing down the relevant expressions for finding α. Here we examine how the regularization parameter converges as a function of the number of terms, k, in the SVD, when α is found using the UPRE.

Having noted that it is not practical to use the SVD for large scale problems, the convergence analysis will still be relevant for realistic problems. For example, one may only have a limited number of terms of the SVD available, called a partial SVD in [5], or only an approximation to the associated dominant subspaces defined by the first few columns of U and V. The approach complements the analysis in [21] which required very specifically that the matrix A is derived from a square integrable kernel in order to show convergence of the regularization parameter with the number of terms k in the partial SVD. Analysis presented in [22] also discussed the relationship of the regularization parameter obtained when using the LSQR Krylov method for large scale problems. More recently, the determination of α from the partial SVD for use with the GCV was discussed in [5]. There it was demonstrated that information about a partial SVD can be useful for determining bounds on the GCV function which can then be used to find α iteratively. Further, extensive discussion on regularization methods is provided in [5], and in the literature [13, 14, 27], and is thus not repeated here. In contrast to the direction of the results in [5] our new work specifically addresses the convergence with the number of dominant terms of the partial SVD, here called the truncated SVD (TSVD), and leads to a lower bound on α found using the UPRE. This is then relevant for large scale problems for which an approximation of the TSVD is available, with convergence dependent on the degree of ill-posedness of the specific problem, and the noise level in the data.

Throughout we use the SVD $A = U\Sigma V^T$, [7], with columns $\mathbf{u}_i$ and $\mathbf{v}_i$ of orthonormal U and V respectively, and where the singular values σ_i of A are ordered on the principal diagonal of Σ, from largest to smallest. We assume that the matrix A has effective numerical rank r; $\sigma_r > 0$, and σ_i, $i > r$ is effectively zero as determined by the machine precision. We discuss the solution of (1) with $\mathbf{x}_0 = 0$, $D = I$, $W_{\mathbf{x}} = \alpha^2 I$, and $W_{\mathbf{b}} = I$, assuming $\boldsymbol{\eta} \sim \mathcal{N}(0, \sigma^2 I)$. Then, in terms of the SVD components, the solution of (1) is given by

$$\mathbf{x}^* = \sum_{i=1}^{r} \frac{\sigma_i^2}{\sigma_i^2 + \alpha^2} \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i = \sum_{i=1}^{r} \gamma_i(\alpha) \frac{\mathbf{u}_i^T \mathbf{b}}{\sigma_i} \mathbf{v}_i, \quad \gamma_i(\alpha) = \frac{\sigma_i^2}{(\sigma_i^2 + \alpha^2)}. \tag{2}$$

Here we denote the filter function by $\gamma_i(\alpha)$ and note that the solution in terms of the TSVD with k components, $A_k = U_k \Sigma_k V_k^T$, is then immediately obtained by replacing r by k. Further, the optimal choice for α for a given parameter estimation method when using A_k or A in (2), respectively, is denoted by α_k, respectively, $\alpha^* = \alpha_r$.

Overview of main contributions. In this work we present a theoretical convergence result for finding α_k using the UPRE parameter estimator. The results employ assumptions on the degree of ill-posed of the underlying model and on the noise level in the data. Thus, we briefly review how both the degree of ill-posedness and the noise level impact the choice for A_k to use in finding $\mathbf{x}$, and show that the noise level is far more restrictive in determining k than is the actual numerical rank of the problem. This analysis is presented on the standard model for estimating the degree of ill-posedness of a problem [15]. We also use these results to show that the simple $1D$ problems from [12] generally require a very small k for reasonable levels of noise, but are also then useful for illustrating how α_k quickly converges to α^* with k for UPRE and GCV estimators for α_k. The convergence of α_k is also illustrated for mildly to moderately ill-posed two dimensional imaging deblurring problems from the Restore Tools package [20]. The theory presented in Section 3 then leads to Theorems 3.1 and 3.2 which verify that α_k found using the UPRE estimator does indeed converge to α^* for $\alpha_k^2 > \sigma_{\ell+1}^2/(1-\sigma_{\ell+1}^2)$, under the assumption of a unique minimum of the UPRE function. These results lead to an efficient approach for finding the optimal converged regularization parameter, α^*, as well as the optimal number of terms k_{opt} to use from the TSVD. This is implemented in Algorithm 1 and presented results for image deblurring verify its practicality.

The paper is organized as follows: In Section 2 we present background motivating results based on assumptions on the degree of ill-posedness of the problem in Section 2.1, a discussion of numerical rank in Section 2.2, how noise enters into the problem in Section 2.3 and the estimation of the regularization parameter in Section 2.4. The theoretical results providing our main contributions are presented in Section 3. A practical algorithm for estimating α^*, and hence also k_{opt}, is presented in Section 4 with simulations verifying the analysis and the algorithm for two dimensional cases. Conclusions and future extensions are provided in Section 5.

2. Motivating Results

2.1. **Degree of Ill-Posedness.** As in [15, Definition 2.42], and subsequently adopted in [13], for the analysis we assume specific decay rates for the singular values dependent on whether the problem is mildly, moderately or severely ill-posed. Suppose that ζ is an arbitrary constant, then the decay rates are given by

$$\sigma_i = \begin{cases} \zeta i^{-\tau} & \frac{1}{2} \leq \tau \leq 1 \quad \text{mild ill conditioning} \\ \zeta i^{-\tau} & \tau > 1 \quad \text{moderate ill conditioning,} \\ \zeta \tau^{-i} & \tau > 1 \quad \text{severe ill conditioning.} \end{cases} \tag{3}$$

Here τ is a problem dependent parameter and it is assumed that the decay rates hold on average for sufficiently large i. For ease, and without loss of generality, we pick the constant

Table 1. Number of significant singular values r for precision $\epsilon = 10^{-15}$ as a function of τ. i.e. r is the numerical rank of the problem.

	τ	1.25	1.50	1.75	2.00	2.50	3.00	4.00	5.00	6.00
Moderate	r	1e+12	1e+10	4e+8	3e+7	1e+6	1e+5	5623	1000	316
Severe	r	155	86	62	50	38	32	25	22	20

ζ in (3) so that $\sigma_1 = 1$ in all cases. Equivalently we use

$$\sigma_i = \begin{cases} i^{-\tau} & \frac{1}{2} \le \tau \le 1 \quad \text{mild ill conditioning,} \\ i^{-\tau} & \tau > 1 \quad \text{moderate ill conditioning,} \\ \tau^{1-i} & \tau > 1 \quad \text{severe ill conditioning,} \end{cases} \tag{4}$$

and note the recurrences

$$\sigma_{\ell+1} = \sigma_\ell \begin{cases} (\frac{\ell}{\ell+1})^\tau & \text{mild or moderate ill conditioning,} \\ \tau^{-1} & \text{severe ill conditioning.} \end{cases}$$

2.2. **Numerical Rank.** The precision of the calculations, as determined by the machine epsilon ϵ, is relevant in terms of the number of singular values that are significant in the calculation. This is dependent on the decay rate parameters of the singular values. We define the effective rank by $r = \text{argmax}\{i : \sigma_i > \epsilon\sigma_1\}$.

Proposition 2.1. *Assuming the scaling of the singular values as given by* (4)*, the effective numerical rank r is bounded by*

$$r < \begin{cases} \epsilon^{-1/\tau} & \textit{mild / moderate decay,} \\ 1 - \frac{\log \epsilon}{\log \tau} & \textit{severe decay,} \end{cases} \tag{5}$$

where ϵ is the machine epsilon.

Proof. Using (4) and normalization $\sigma_1 = 1$, it is immediate that we obtain (5) from

$$\begin{aligned} &\text{mild / moderate:} && r^{-\tau} > \epsilon \text{ implies } r < \epsilon^{-1/\tau} \\ &\text{severe :} && \tau^{1-r} > \epsilon \text{ implies } r < 1 - \tfrac{\log \epsilon}{\log \tau}. \end{aligned}$$

□

Estimates for numerical rank dependent on the decay rates, are given in Table 1 for moderate and severe decay. It is immediate that r is very small for cases of severe decay. Hence, for any problem exhibiting this severe decay Table 1 suggests the maximum number of terms that one would use for the TSVD regardless of the size of the problem. Equivalently, with estimates of τ and ϵ one may use (5) to determine the maximum number of terms for the TSVD, the maximum effective numerical rank of the problem. These results are further illustrated in Figure 1 in which we plot the singular values of test problems from the Regularization toolbox, [12] contrasted with singular values generated using (5) for choices shown in the legend. The simulated choices are chosen to illustrate the dependence on the decay rate and to provide examples roughly approximating the cases in [12]. The same scales and normalizations are used in all cases. The plots show that standard

one dimensional test cases are primarily severely ill-posed, and thus, according to Table 1, guaranteed to have numerically very few accurate terms in the TSVD used for the solution (2). Indeed the number of terms that can be used practically is largely independent on the discretization of the problem, the results in Table 1 do not involve n in the calculation, and as an example we show in Figure 1c the singular value distributions for the same cases and on the same scales as in Figure 1a but using $n = 256$. This verifies that there is little to be gained by the use of those problems with severe decay, as presented in [21], to validate convergence of techniques with increasing problem size. The dominant features are always represented by very few terms of the TSVD for cases with severe decay rates of the singular values.

(a) Toolbox $n = 128$ [12] (b) Modeled decay rates (c) Toolbox $n = 256$ [12]

Figure 1. The singular value distribution for $n = 128$ for noted examples from [12], normalized to $\sigma_1 = 1$ in Figure 1a. For each of the toolbox examples it is possible to contrast with a simulated case for a specific decay rate by illustrating (4) for severe, moderate or mild decay choices of τ, as appropriate, given in Figure 1b. To show the independence of n, decay for $n = 256$ for the same examples from [12] is also shown in Figure 1c.

2.3. **Noise Contamination.** We now turn to the consideration of the noise in the coefficients $s_i = \mathbf{u}_i^T \mathbf{b}$ of the data and the impact on the potential resolution in the solution, as also discussed in [13, 4.8.1]. Assume that there exists ℓ such that $E(s_i^2) = \sigma^2$, where we use $E(\cdot)$ to denote expected value, for all $i > \ell$ and that on average the absolute values of the exact coefficients decay faster than the singular values. For the exact coefficients we suppose then

$$(s_i^2)_{\text{true}} \leq \sigma_i^{2(1+\nu)} \quad \text{for} \quad 0 < \nu < 1 \tag{6}$$

and the discrete Picard condition is satisfied, [13, Theorem 4.5.1]. Equivalently, the coefficients decay at least faster than the singular values in order that the discrete Picard condition is satisfied, [11]. Suppose that

$$\sigma_{\ell+1}^2 < \sigma_{\ell+1}^{1+\nu} < \sigma < \sigma_\ell^{1+\nu} < \sigma_\ell,$$

Table 2. For different noise levels σ the size of ℓ for given τ and with $\delta = \nu = 0.5$. Entries calculated with rounding using (7).

τ	1.25	1.50	1.75	2.00	2.50	3.00	4.00	5.00	6.00
σ	Moderate decay								
1e−1	3	2	2	2	1	1	1	1	1
1e−2	11	7	5	4	3	2	2	1	1
1e−4	135	59	33	21	11	7	4	3	2
1e−8	18478	3593	1115	464	135	59	21	11	7
σ	Severe decay								
1e−1	7	4	3	3	2	2	2	1	1
1e−2	14	8	6	5	4	3	3	2	2
1e−4	28	16	11	9	7	6	5	4	4
1e−8	56	31	22	18	14	12	9	8	7

and that definition (4) holds as a function of i for a non integer index $\ell + \delta$.

Proposition 2.2. *Let $\sigma = \sigma_{\ell+\delta}^{1+\nu}$ for $0 < \delta < 1$ and $0 < \nu < 1$, then the s_i are dominated by noise for $i > \ell$ where*

$$\ell \approx \begin{cases} \sigma^{-1/(\tau(1+\nu))} - \delta & \textit{mild / moderate decay,} \\ (1-\delta) - \frac{\log \sigma}{(\nu+1)\log \tau}. & \textit{severe decay.} \end{cases} \tag{7}$$

Proof. As in the proof of Proposition 2.1 we solve for ℓ dependent on the decay rate with respect to the upper bound in (7). This gives

$$\begin{aligned} &\text{mild / moderate:} && (\ell+\delta)^{-\tau(1+\nu)} = \sigma \text{ implies } \ell = \sigma^{-1/(\tau(1+\nu))} - \delta, \\ &\text{severe :} && \tau^{(1-(\ell+\delta))(1+\nu)} = \sigma \text{ implies } \ell = (1-\delta) - \frac{\log \sigma}{(\nu+1)\log \tau}. \end{aligned}$$

□

Estimates using $\delta = \nu = 0.5$ are indicated in Table 2 showing that the number of terms is relatively small even for moderate decay of the singular values for acceptable noise estimates σ. Contrasting with Table 1 we see that the number of coefficients that can be distinguished from the noise is generally less than the numerical rank of the problem for relevant noise levels and machine precision. This limits the number of the terms of the TSVD to use. In particular, suppose that α has to be found to filter the dominant noise terms with index $i \geq \ell$, then coefficients with $i \gg \ell$ will be further damped because the filter factors given in (2), decrease as a function of i. These terms then become insignificant in terms of the expansion for the solution.

2.4. **Regularization Parameter Estimation.** We deduce from Tables 1 and 2 that the number of terms of the TSVD used for the solution of the regularized problem may strongly influence the choice for α. Specifically the number of terms of the TSVD, k, to use should be less than the numerical rank, $k < r$, and is dependent on the noise level in the data.

We are interested in investigating the choice of α when obtained using the UPRE, but for contrast we also give the GCV function needed for the simulations. Ignoring constant terms in the UPRE that do not impact the location of the minimum, and introducing $\phi_i(\alpha) = 1 - \gamma_i(\alpha) = \alpha^2/(\sigma_i^2 + \alpha^2)$, these are given by

$$(8) \quad U_k(\alpha) = \sum_{i=1}^{k} (1-\gamma_i(\alpha))^2 (\mathbf{u}_i^T \mathbf{b})^2 + 2\sigma^2 \sum_{i=1}^{k} \gamma_i(\alpha) = \sum_{i=1}^{k} \phi_i^2(\alpha) s_i^2 + 2\sigma^2 \sum_{i=1}^{k} \gamma_i(\alpha)$$

$$(9) \quad G_k(\alpha) = \frac{\sum_{i=1}^{m} (1-\gamma_i(\alpha))^2 (\mathbf{u}_i^T \mathbf{b})^2}{\left(\sum_{i=1}^{m} (1-\gamma_i(\alpha))\right)^2} = \frac{\sum_{i=1}^{k} \phi_i^2(\alpha) s_i^2 + \sum_{i=k+1}^{m} s_i^2}{\left((m-k) + \sum_{i=1}^{k} \phi_i(\alpha)\right)^2}.$$

Here the subscript $k \leq r$ indicates that these are expressions obtained using the TSVD, see e.g. [22, Appendix B] for derivations of the UPRE and GCV functions for arbitrary pairs (m, n), also using the notation that $\gamma_i = 0$, $i > k$. Replacing k by r gives the standard functions for the full SVD. Further, we do not need all terms of the SVD to calculate the numerator in (9). Using $\|\mathbf{b}\|_2^2 = \|U^T \mathbf{b}\|_2^2$ we can use

$$\sum_{i=k+1}^{m} (\mathbf{u}_i^T \mathbf{b})^2 = \|\mathbf{b}\|_2^2 - \sum_{i=1}^{k} (\mathbf{u}_i^T \mathbf{b})^2 = \|\mathbf{b}\|_2^2 - \sum_{i=1}^{k} s_i^2.$$

To illustrate the movement of α_k when found using these functions we illustrate an example of a problem that is only moderately ill-posed ($\tau \approx 1.5$), showing the results of calculating the UPRE and GCV functions for data with noise variance $\sigma^2 \approx 1\text{e}{-4}$ and $\sigma^2 \approx 1\text{e}{-2}$ for the problem `deriv2`. The data and solution $\mathbf{x}_{\text{true}}$ are normalized so that $\|\mathbf{b}_{\text{true}}\|_2 = 1$. Consistent with the decay rate assumptions the singular values are normalized by σ_1, requiring additional normalization of $\mathbf{b}_{\text{true}}$ by σ_1. Then noise contaminated data are generated as $\mathbf{b} = \mathbf{b}_{\text{true}} + \boldsymbol{\eta}$ for $\boldsymbol{\eta} \sim \mathcal{N}(0, \sigma^2 I)$, for noise level σ. In these examples, the optimal value α_k is obtained by first locating the minimum of the relevant function evaluated for σ_i, $1 \leq i \leq k$, giving an estimate α_{est}, and then using `fminbnd` of Matlab to find the minimum within the interval $[.01\alpha_{\text{est}}, 100\alpha_{\text{est}}]$. We pick this specific example in Figure 2 to highlight the discussion as applied to a problem which is not severely ill-posed. We also give the same information in Figure 3 for the severely ill-posed problem `gravity` ($\tau \approx 1.5$), see Figure 1a. To gain further insight the Picard plot, plots of σ_i, $|\mathbf{u}_i^T \mathbf{b}|$ and the ratio $|\mathbf{u}_i^T \mathbf{b}|/\sigma_i$, is given in each case in Figures 2b and 2d for `deriv2` and in Figures 3b and 3d for `gravity`. The solutions are contaminated very quickly for small k, corresponding to fast convergence of $\{\alpha_k\}$ with k.

It is trivial to show the convergence behavior of $\{\alpha_k\}$ for additional one dimensional examples from the Regularization Toolbox, [12]. We therefore turn immediately to two dimensional cases, based on examples `Grain` and `Satellite` from the Restore Tools package [20], but for feasibility of the SVD computations we use problem sizes 64×64 and 128×128. To use the tools in [20] for the blurring of the images we use the point spread function (PSF) provided, and downsample to a new coarser PSF. The function `KronApprox` is used to generate the approximation of the PSF and then the first term of the approximation is

(a) α_k convergence. (b) Picard Plot (c) α_k convergence. (d) Picard Plot

Figure 2. Example `deriv2` from [12] showing the convergence of $\{\alpha_k\}$ for UPRE and GCV functions for TSVD sizes of $1:25$ as compared to the decay of the singular values, for the original problem of size 128 and the associated Picard plot for the data. In Figures 2a-2b, and Figures 2c-2d, the noise variances are $\sigma^2 \approx 1\text{e}{-4}$ and $\sigma^2 \approx 1\text{e}{-2}$, respectively.

(a) α_k convergence. (b) Picard Plot (c) α_k convergence. (d) Picard Plot

Figure 3. Example `gravity` from [12] showing the convergence of $\{\alpha_k\}$ for UPRE and GCV functions for TSVD sizes of $1:25$ as compared to the decay of the singular values, for the original problem of size 128 and the associated Picard plot for the data. In Figures 3a-3b, and Figures 3c-3d, the noise variances are $\sigma^2 \approx 1\text{e}{-4}$ and $\sigma^2 \approx 1\text{e}{-2}$, respectively.

extracted to provide the system used in these simulations. The regularization parameter is calculated using both UPRE and GCV functions for TSVD approximations of sizes $k = 10$, 15, 20, 50, 100, 200, 250, 500, 1000, 1500, 2000, 4000, and 8000 for the problem of size 128×128, and examined for noise levels with $\sigma = .1, .05$, and $.01$. From the Picard plots shown in Figures 4-5 it is apparent that these two problems are only mildly ill-posed and thus it is realistic to take TSVD approximations with k of a moderate size. Indeed, applying nonlinear data fitting for the singular values using (4) for mild/moderate decay yields $\tau \approx .5$ and 1.5 for `Grain` and `Satellite` respectively, with the estimate of τ dependent on the

range used in the data fit. The results shown in Figures 6a-6d, demonstrate the convergence of the regularization parameter with increasing k, even for problems that are not severely ill-posed, and also motivate the theoretical study of convergence in Section 3.

(a) Noise: $\sigma \approx .1$ (b) Noise: $\sigma \approx .5$ (c) Noise: $\sigma \approx .01$

Figure 4. The Picard plots for the `Grain` data of size 64×64 with noise levels using $\sigma \approx .1, .05$, and $.01$.

(a) Noise: $\sigma \approx .1$ (b) Noise: $\sigma \approx .05$ (c) Noise: $\sigma \approx .01$

Figure 5. The Picard plots for the `Satellite` data of size 64×64 with noise levels using $\sigma \approx .1, .05$, and $.01$.

3. Theoretical Results

We aim to find effective practical bounds on the regularization parameter α when found using the UPRE function. Observe first that we would not expect the regularization parameter to be larger than σ_1, otherwise all filter factors are less than $1/2$. Indeed imposing $\alpha = \sigma_1$ would lead to over smoothed solutions, and all of the dominant singular value components (the components without noise contamination) would be represented

(a) Convergence of α_k for `Grain` size 64×64.

(b) Convergence of α_k for `Satellite` size 64×64.

(c) Convergence of α_k for `Grain` size 128×128.

(d) Convergence of α_k for `Satellite` size 128×128.

Figure 6. The convergence of $\{\alpha_k\}$ for the `Grain` and `Satellite` data of size 64×64 and 128×128 with noise levels for $\sigma \approx .1, .05$, and $.01$ (10%, 5%, and 1% noise) using both UPRE and GCV estimators.

in the solution with filtering e.g [14, Sections 4.4, 4.7]. In particular, the norm of the covariance matrix for the truncated filtered Tikhonov solution, the *a posteriori* covariance of the solution, is approximately bounded by $\sigma^2/(4\alpha^2)$ which suggests smooth solutions for large α. In contrast, the approximate bound for the *a posteriori* covariance when using the TSVD with k terms without filtering is given by σ^2/σ_k^2 [14, Sections 4.4.2,

4.4]. Thus the filtered TSVD solution will be smoother than the TSVD solution when $\alpha > \sigma_k$: increasing α reduces the covariance but provides more smoothing. Practically it is reasonable to impose the upper bound $\alpha_{\max} \leq \sigma_1 = 1$ for α. To limit the noise that can enter the solution it is also desirable to find the lower bound $\alpha_{\min}$. Solutions obtained for $\alpha \in [\alpha_{\min}, \alpha_{\max}]$, dependent on the spectrum of A, should be sufficiently filtered but retain relatively unfiltered dominant components of the solution. We proceed to determine $\alpha_{\min}$ and to give a convergence analysis for α_k as the number of terms in the TSVD is increased.

3.1. **Convergence of $\{\alpha_k\}$ calculated using UPRE.** Denote the UPRE function (8) for the rank r problem by $U(\alpha) = U_r(\alpha)$ and the optimal α for the filtered TSVD solution with k components on the given interval as

$$\alpha_k = \operatorname{argmin}_{\alpha \in [\alpha_{\min}, \alpha_{\max}]} U_k(\alpha). \tag{10}$$

Ideally it would be helpful to find an interval $[\alpha_{\min}, \alpha_{\max}]$ in which $U_k(\alpha)$ is strongly convex, but we have not been able to show this in general. Instead, in the following we show that a useful estimate of $\alpha_{\min}$ can be found.

For ease of notation within proofs we use ϕ_i and γ_i to indicate $\phi_i(\alpha)$ and $\gamma_i(\alpha)$, respectively, and denote differentiation of a function $f(\alpha)$ with respect to α as f'.

Proposition 3.1.

$$\frac{\partial U_k}{\partial \alpha} = \frac{4}{\alpha}\left(\sum_{i=1}^{k} s_i^2 \phi_i^2(\alpha)\gamma_i(\alpha) - \sigma^2 \sum_{i=1}^{k} \phi_i(\alpha)\gamma_i(\alpha)\right), \tag{11}$$

$$\begin{aligned} \frac{\partial^2 U_k}{\partial \alpha^2} &= -\frac{1}{\alpha}\frac{\partial U_k}{\partial \alpha} + \frac{8}{\alpha^2}\left(\sum_{i=1}^{k} s_i^2 \phi_i^2(\alpha)\gamma_i(\alpha)(2\gamma_i(\alpha) - \phi_i(\alpha)) - \right. \\ &\qquad \left. \sigma^2 \sum_{i=1}^{k} \phi_i(\alpha)\gamma_i(\alpha)(\gamma_i(\alpha) - \phi_i(\alpha))\right). \end{aligned} \tag{12}$$

Proof. We use

$$\gamma_i' = -\frac{2\alpha\sigma_i^2}{(\sigma_i^2 + \alpha^2)^2} = -\frac{2}{\alpha}\phi_i\gamma_i = -\phi_i' < 0.$$

Directly differentiating $U_k(\alpha)$ gives (11)

$$U_k' = \sum_{i=1}^{k} s_i^2 2\phi_i\phi_i' + 2\sigma^2 \sum_{i=1}^{k} \gamma_i' = \frac{4}{\alpha}\left(\sum_{i=1}^{k} s_i^2 \phi_i^2 \gamma_i - \sigma^2 \sum_{i=1}^{k} \gamma_i \phi_i\right).$$

Likewise for the second derivative

$$U_k'' = -\frac{1}{\alpha}U_k' + \frac{4}{\alpha}\left(\sum_{i=1}^{k} s_i^2(2\phi_i\phi_i'\gamma_i + \phi_i^2\gamma_i') - \sigma^2 \sum_{i=1}^{k}(\phi_i'\gamma_i + \phi_i\gamma_i')\right), \tag{13}$$

giving (12) after substitution for the derivatives. □

Proposition 3.2. *Suppose that* $0 < \bar{\alpha} < \frac{\sigma_k}{\sqrt{2}}$ *is a stationary point for* $U_k(\alpha)$*, for any* $1 \le k \le r$*. Then* $\bar{\alpha}$ *is a unique minimum for* $U_k(\alpha)$ *on the interval* $0 < \bar{\alpha} < \frac{\sigma_k}{\sqrt{2}}$*.*

Proof. Removing the first term in (13), identically zero at $\alpha = \bar{\alpha}$ by assumption that $\bar{\alpha}$ is a stationary point, gives

$$\begin{aligned}\frac{\partial^2 U_k}{\partial \alpha^2}(\bar{\alpha}) &= \frac{8}{\bar{\alpha}^2}\left(\sum_{i=1}^{k} s_i^2\phi_i^2(\bar{\alpha})\gamma_i(\bar{\alpha})(2\gamma_i(\bar{\alpha}) - \phi_i(\bar{\alpha})) - \sigma^2\sum_{i=1}^{k}\phi_i(\bar{\alpha})\gamma_i(\bar{\alpha})(\gamma_i(\bar{\alpha}) - \phi_i(\bar{\alpha}))\right)\\ &= \frac{8}{\bar{\alpha}^2}\left(\sum_{i=1}^{k} s_i^2\phi_i^2(\bar{\alpha})\gamma_i(\bar{\alpha})(2 - 3\phi_i(\bar{\alpha})) - \sigma^2\sum_{i=1}^{k}\phi_i(\bar{\alpha})\gamma_i(\bar{\alpha})(1 - 2\phi_i(\bar{\alpha}))\right).\end{aligned}$$

Now we substitute for $\sum_{i=1}^{k} s_i^2\phi_i^2(\bar{\alpha})\gamma_i(\bar{\alpha}) = \sigma^2\sum_{i=1}^{k}\gamma_i(\bar{\alpha})\phi_i(\bar{\alpha})$ using (11) at $\bar{\alpha}$ and note all terms are positive for $1 - 3\phi_i(\bar{\alpha}) > 0$, $i = 1 : k$. But ϕ_i is increasing with i due to the ordering of the σ_i. Thus $1 - 3\phi_i(\bar{\alpha}) \ge 1 - 3\phi_k(\bar{\alpha}) > 0$ for $\bar{\alpha} < \sigma_k/\sqrt{2}$ and $U_k''(\bar{\alpha}) > 0$. This result is true for any stationary point $\bar{\alpha}$ on the interval. Hence $U_k(\bar{\alpha})$ is a minimum for $U_k(\alpha)$ and it is only possible to have a maximum at $\alpha = 0$, the end point of the given interval, but the end point is explicitly excluded from consideration. There are therefore no other stationary points within the interval and the minimum is unique. □

Remark 3.1. *Although a minimum must exist in* $[0, \sigma_k/\sqrt{2}]$ *because* $U_k(\alpha)$ *is a continuous function on a compact set, this result does not show that a minimum exists in* $(0, \sigma_k/\sqrt{2})$ *.*

The next steps in the analysis rely on a number of assumptions about the model and the data, and we recall the normalization $\sigma_1 = 1$.

Assumption 1 (Decay Rate)**.** *The measured coefficients decay according to* $s_i^2 = \sigma_i^{2(1+\nu)} > \sigma^2$ *for* $0 < \nu < 1$*,* $1 \le i \le \ell$*, i.e. the dominant measured coefficients follow the decay rate of the exact coefficients.*

Assumption 2 (Noise in Coefficients)**.** *There exists* ℓ *such that* $E(s_i^2) = \sigma^2$ *for all* $i > \ell$*, i.e. that the coefficients* s_i *are noise dominated for* $i > \ell$*.*

For the remaining results we distinguish between the terms in the UPRE function that are, and are not, contaminated by noise.

Proposition 3.3. *Suppose Assumption 2, then for* $r > k + 1 > \ell$

$$E\left(\frac{\partial U_r}{\partial \alpha}\right) < \cdots < E\left(\frac{\partial U_{k+1}}{\partial \alpha}\right) \quad < \quad E\left(\frac{\partial U_k}{\partial \alpha}\right) < \frac{\partial U_\ell}{\partial \alpha} \ \forall\ \alpha, \tag{14}$$

$$E\left(\frac{\partial^2 U_r}{\partial \alpha^2}\right) > \cdots > E\left(\frac{\partial^2 U_{k+1}}{\partial \alpha^2}\right) \quad > \quad E\left(\frac{\partial^2 U_k}{\partial \alpha^2}\right) > \frac{\partial^2 U_\ell}{\partial \alpha^2} \ \textit{if}\ \alpha > \frac{\sigma_{\ell+1}}{\sqrt{5}} \tag{15}$$

$$\left\{\begin{array}{c} E(\frac{\partial^2 U_r}{\partial \alpha^2}) \\ \textit{for}\ \alpha < \frac{\sigma_r}{\sqrt{5}} \end{array}\right\} < \cdots < \left\{\begin{array}{c} E(\frac{\partial^2 U_{k+1}}{\partial \alpha^2}) \\ \textit{for}\ \alpha < \frac{\sigma_{k+1}}{\sqrt{5}} \end{array}\right\} \quad < \quad \left\{\begin{array}{c} E(\frac{\partial^2 U_k}{\partial \alpha^2}) \\ \textit{for}\ \alpha < \frac{\sigma_k}{\sqrt{5}} \end{array}\right\} < \frac{\partial^2 U_\ell}{\partial \alpha^2}. \tag{16}$$

Proof. We note that the expectation operator is linear and when a is not a random variable $E(a) = a$. Applying these properties first to (11) yields

$$\begin{aligned} E(U_k') &= E\left(U_\ell' + \frac{4}{\alpha}\sum_{i=\ell+1}^{k} \phi_i\gamma_i(s_i^2\phi_i - \sigma^2)\right) \\ &\approx U_\ell' + \frac{4\sigma^2}{\alpha}\sum_{i=\ell+1}^{k} \phi_i\gamma_i(\phi_i - 1) < U_\ell'. \end{aligned}$$

In particular, in expectation each term for $i > \ell$ is negative and recursively both inequalities in (14) apply. Applying the expectation operator now to (12) gives

$$\begin{aligned} E(U_k'') &\approx \frac{\partial^2 U_\ell''}{\partial\alpha^2} + \frac{4\sigma^2}{\alpha^2}\left(\sum_{i=\ell+1}^{k} \phi_i\gamma_i(1-\phi_i) + 2\left(\phi_i^2\gamma_i(2\gamma_i - \phi_i) - \phi_i\gamma_i(\gamma_i - \phi_i)\right)\right) \\ &= U_\ell'' + \frac{4\sigma^2}{\alpha^2}\left(\sum_{i=\ell+1}^{k} \phi_i\gamma_i\left(1 - \phi_i + 2\left(\phi_i(2\gamma_i - \phi_i) - (\gamma_i - \phi_i)\right)\right)\right) \\ &= U_\ell'' + \frac{4\sigma^2}{\alpha^2}\left(\sum_{i=\ell+1}^{k} \phi_i\gamma_i\left(1 - \phi_i + 2\left(\phi_i(2 - 3\phi_i) - (1 - 2\phi_i)\right)\right)\right) \\ &= U_\ell'' + \frac{4\sigma^2}{\alpha^2}\left(\sum_{i=\ell+1}^{k} \phi_i\gamma_i\left(-6\phi_i^2 + 7\phi_i - 1\right)\right). \end{aligned}$$

The sign of the second term depends on the sign of $-6\phi_i^2 + 7\phi_i - 1$ which is increasing from -1 as a function of $\phi \le 1$. Hence

$$-6\phi_i^2 + 7\phi_i - 1 \begin{cases} \ge -6\phi_{\ell+1}^2 + 7\phi_{\ell+1} - 1 & = \frac{\sigma_{\ell+1}^2(5\alpha^2 - \sigma_{\ell+1}^2)}{(\alpha^2+\sigma_{\ell+1}^2)^2} & > 0 \quad \text{if } \alpha > \frac{\sigma_{\ell+1}}{\sqrt{5}} \\ \le -6\phi_k^2 + 7\phi_k - 1 & = \frac{\sigma_k^2(5\alpha^2 - \sigma_k^2)}{(\alpha^2+\sigma_k^2)^2} & < 0 \quad \text{if } \alpha < \frac{\sigma_k}{\sqrt{5}}. \end{cases}$$

Again, in expectation, terms for $i > \ell$ are all positive when $\alpha \ge \frac{\sigma_{\ell+1}}{\sqrt{5}}$ and the nested inequalities in (15) apply. The requirement that the ith term is necessarily positive becomes more severe as i increases, yielding the additional nested inequalities with conditions on α given in (16). □

Corollary 3.1. *Suppose Assumption 2, and that for $\alpha_\ell > \frac{\sigma_{\ell+1}}{\sqrt{5}}$, $U_\ell(\alpha_\ell)$ is a minimum for $U_\ell(\alpha)$. Then for $\ell < k \le r$, $U_k(\alpha)$ is concave up decreasing at α_ℓ,*

$$E\left(\frac{\partial U_k(\alpha_\ell)}{\partial\alpha}\right) < 0 \quad \textit{and} \quad E\left(\frac{\partial^2 U_k(\alpha_\ell)}{\partial\alpha^2}\right) > 0.$$

Proof. If $U_\ell(\alpha_\ell)$ is a minimum, then $U_\ell'(\alpha_\ell) = 0$ and $U_\ell''(\alpha_\ell) > 0$ and the inequalities follow immediately from (14) and (15). □

Corollary 3.2. *Suppose Assumption 2. If a stationary point $\alpha_r < \sigma_r/\sqrt{5}$ exists there are no stationary points of $U_k(\alpha)$ for $\alpha \in (\sigma_r/\sqrt{5}, \sigma_k/\sqrt{2})$.*

Proof. Suppose that $\alpha_r \in [0, \sigma_r/\sqrt{5})$. The existence of α_r in this interval does not contradict Proposition 3.2 since $\sigma_r/\sqrt{5} < \sigma_r/\sqrt{2}$. By assumption, $U_r'(\alpha_r) = 0$ and $U_r''(\alpha_r) > 0$. Thus by (14) and (16) $U_k'(\alpha_r) > 0$ and $U_k''(\alpha_r) > 0$, and $U_k(\alpha)$, $\ell \le k \le r-1$ is concave up increasing at α_r. Therefore, by continuity, $U_k(\alpha)$ cannot reach a minimum for $\alpha_r < \alpha_k < \sigma_k/\sqrt{2}$ without first passing through a stationary point which is a maximum. But by Proposition 3.2 there is no maximum of $U_k(\alpha)$ to the left of $\sigma_k/\sqrt{2}$ and thus there is also no minimum for $\alpha_r < \alpha < \sigma_k/\sqrt{2}$. In particular $U_k(\alpha)$ has no stationary point for $\sigma_r/\sqrt{5} \le \alpha \le \sigma_k/\sqrt{2}$. □

Remark 3.2. *We have shown through Corollary 3.2 that if $U_r(\alpha_r)$ is a minimum for $U_r(\alpha)$ and $\alpha_r < \sigma_r/\sqrt{5}$ then $U_k(\alpha_k)$ can only be a minimum for $U_k(\alpha)$ if either $\alpha_k \le \alpha_r \le \sigma_r/\sqrt{5}$ or $\alpha_k > \sigma_k/\sqrt{2}$, i.e. we may require $\alpha_k > \sigma_k/\sqrt{2}$ under the assumption that we seek $\alpha_r > \sigma_r$. This applies for all k with $1 \le \ell \le k \le r-1$.*

Although this result does provide a refined lower bound for α_k, it is dependent on k and decreasing with k, which is not helpful when k gets large, as needed for finding α^*, i.e. this bound would suggest that α^* needs to be found using the pessimistic lower bound $\sigma_r/\sqrt{2}$. We investigate now whether these lower bounds on α are indeed realistic by looking for bounds on the UPRE functions $U_k(\alpha)$.

Proposition 3.4. *Suppose Assumptions 1 and 2, then lower and upper bounds on $U_k(\alpha)$ and its derivatives are given by $\mathcal{L}_k(\alpha)$ and $\mathcal{U}_k(\alpha)$ and their derivatives, respectively, where*

(17)
$$0 < \mathcal{L}_k(\alpha) = G(\alpha) + F_k(\alpha) < E(U_k(\alpha)) < H(\alpha) + F_k(\alpha) = \mathcal{U}_k(\alpha)$$

(18) $$\mathcal{L}_k'(\alpha) = G'(\alpha) + F_k'(\alpha) < E(U_k'(\alpha)) < H'(\alpha) + F_k'(\alpha) = \mathcal{U}_k'(\alpha),$$

(19) $$\mathcal{L}_k''(\alpha) = G''(\alpha) + F_k''(\alpha) < E(U_k''(\alpha)) < H''(\alpha) + F_k''(\alpha) = \mathcal{U}_k''(\alpha), \text{ for } \alpha \le \sigma_\ell \text{ but}$$
$$\mathcal{U}_k''(\alpha) = H''(\alpha) + F_k''(\alpha) < E(U_k''(\alpha)) < G''(\alpha) + F_k''(\alpha) = \mathcal{L}_k''(\alpha), \text{ for } \alpha > 1.$$

Here $G(\alpha)$ and $H(\alpha)$ are independent of k, while $F_k(\alpha)$ very clearly depends on the k terms in the sums as given by

(20) $$G(\alpha) = \alpha^4 \sum_{i=1}^{\ell} \gamma_i^2, \; H(\alpha) = \alpha^2 \sum_{i=1}^{\ell} \phi_i \gamma_i, \text{ and}$$

(21) $$F_k(\alpha) = \sigma^2 \left((k-\ell) + 2\sum_{i=1}^{\ell} \gamma_i + \sum_{i=\ell+1}^{k} \gamma_i^2 \right).$$

Proof. By (6) due to Assumption 1 for $i \le \ell$

(22) $$\sigma_i^4 < \sigma_i^{2(1+\nu)} = s_i^2 < \sigma_i^2.$$

Thus

(23) $$\alpha^4 \gamma_i^2 = \sigma_i^4 \phi_i^2 < \phi_i^2(\alpha) s_i^2 < \sigma_i^2 \phi_i^2 = \alpha^2 \phi_i \gamma_i.$$

Now from (8)

$$E(U_k(\alpha)) \;=\; \sum_{i=1}^{\ell}\phi_i^2 s_i^2 + \sigma^2(2\sum_{i=1}^{k}\gamma_i(\alpha) + \sum_{i=\ell+1}^{k}\phi_i^2) = \sum_{i=1}^{\ell}\phi_i^2 s_i^2 + F_k(\alpha),$$

may be bounded using (22). This yields immediately (17) with the noted definitions for G, H and F_k, as given in (20)-(21).

To show (18) introduce $D_i(\alpha) > 0$, $i = 1, 2$, given by

$$\begin{aligned} D_1(\alpha) &= E(U_k(\alpha)) - (G(\alpha) + F_k(\alpha)) = \sum_{i=1}^{\ell}(\phi_i^2 s_i^2 - \alpha^4\gamma_i^2) \\ D_2(\alpha) &= (H(\alpha) + F_k(\alpha)) - E(U_k(\alpha)) = \sum_{i=1}^{\ell}(\alpha^2\phi_i\gamma_i - \phi_i^2 s_i^2). \end{aligned}$$

Then D_i are independent of k and

$$\begin{aligned} D_1'(\alpha) &= \sum_{i=1}^{\ell}\left(\frac{2}{\alpha}(2\phi_i^2\gamma_i s_i^2 + 2\alpha^4\gamma_i^2\phi_i) - 4\alpha^3\gamma_i^2\right) = \frac{4}{\alpha}\sum_{i=1}^{\ell}(\phi_i^2\gamma_i s_i^2 - \alpha^4\gamma_i^3) \text{ and} \\ D_2'(\alpha) &= \sum_{i=1}^{\ell}(2\alpha\phi_i\gamma_i + \frac{2}{\alpha}(\alpha^2\phi_i\gamma_i(1-2\phi_i) - 2\phi_i^2\gamma_i s_i^2)) = \frac{4}{\alpha}\sum_{i=1}^{\ell}(\alpha^2\phi_i\gamma_i^2 - s_i^2\phi_i^2\gamma_i). \end{aligned}$$

But now again applying Assumption 1 we have

$$\alpha^4\gamma_i^3 = \sigma_i^4\phi_i^2\gamma_i < s_i^2\phi_i^2\gamma_i < \sigma_i^2\phi_i^2\gamma_i = \alpha^2\phi_i\gamma_i^2. \tag{24}$$

Therefore $D_i'(\alpha) > 0$, $i = 1, 2$ and we immediately obtain (18).

The second derivative result follows similarly using

$$\begin{aligned} D_1''(\alpha) &= \frac{12}{\alpha^2}\sum_{i=1}^{\ell}\gamma_i(1-2\phi_i)(s_i^2\phi_i^2 - \alpha^4\gamma_i^2) > 0 \\ D_2''(\alpha) &= \frac{12}{\alpha^2}\sum_{i=1}^{\ell}\phi_i\gamma_i(1-2\phi_i)(\gamma_i\alpha^2 - s_i^2\phi_i) > 0, \end{aligned}$$

where in each case we apply (24) and note $1 - 2\phi_i \geq 0$, for $1 \leq i \leq \ell$ and $\alpha \leq \sigma_\ell$. This then immediately gives the reverse inequalities for $\alpha > 1$. □

From (20)-(21) we see that we may write G, H and F_k in terms of sums $S_p(i_1, i_2) = \sum_{i=i_1}^{i_2}\gamma_i^p$ for $p = 1$ and $p = 2$ by writing $\phi_i\gamma_i = \gamma_i - \gamma_i^2$. Hence

$$G(\alpha) = \alpha^4 S_2(1,\ell),\; H(\alpha) = \alpha^2(S_1(1,\ell) - S_2(1,\ell)) \quad \text{and}$$
$$F_k(\alpha) = \sigma^2(k - \ell + 2S_1(1,\ell) + S_2(\ell+1,k)).$$

Thus for $U_\ell(\alpha)$ we have the bounding functions by Proposition 3.3

$$\begin{aligned}\mathcal{L}_\ell(\alpha) &= G(\alpha) + F_\ell(\alpha) = \alpha^4 S_2 + 2\sigma^2 S_1 \\ \mathcal{U}_\ell(\alpha) &= H(\alpha) + F_\ell(\alpha) = \alpha^2(S_1 - S_2) + 2\sigma^2 S_1,\end{aligned}$$

where the sums all range from 1 to ℓ. Moreover, also by Proposition 3.3, $\mathcal{L}'_\ell(\alpha) < U_\ell(\alpha) < \mathcal{U}'_\ell(\alpha)$ where

$$\begin{aligned}\mathcal{L}'_\ell(\alpha) &= 4\alpha^3 S_2 + \alpha^4 S'_2 + 2\sigma^2 S'_1 = 4\alpha^3(S_2 + S_3 - S_2) + \frac{4\sigma^2}{\alpha}(S_2 - S_1) \\ &= \frac{4}{\alpha}(\alpha^4 S_3 + \sigma^2(S_2 - S_1)) \\ \mathcal{U}'_\ell(\alpha) &= 2\alpha(S_1 - S_2) + \alpha^2(S'_1 - S'_2) + 2\sigma^2 S'_1 \\ &= 2\alpha(S_1 - S_2) + 2\alpha(S_2 - S_1 - 2(S_3 - S_2)) + \frac{4}{\alpha}\sigma^2(S_2 - S_1) \\ &= \frac{4}{\alpha}(\alpha^2(S_2 - S_3) + \sigma^2(S_2 - S_1)),\end{aligned}$$

and we used $\gamma'_i = -\frac{2}{\alpha}\gamma_i\phi_i = \frac{2}{\alpha}(\gamma_i^2 - \gamma_i)$ and $(\gamma_i^2)' = -\frac{4}{\alpha}\gamma_i^2\phi_i = \frac{4}{\alpha}(\gamma_i^3 - \gamma_i^2)$.

Proposition 3.5. *Suppose Assumption 1, then necessarily $U'_\ell(\alpha) < 0$ for $\alpha^2 < \sigma_{\ell+1}^2/(1 - \sigma_{\ell+1}^2)$. Hence $\alpha_\ell^2 > \sigma_{\ell+1}^2/(1 - \sigma_{\ell+1}^2)$.*

Proof. If the upper bound has a negative slope, $\mathcal{U}'_\ell(\alpha) < 0$ for some α, then $U'_\ell(\alpha) < 0$ also. Immediately $\mathcal{U}'_\ell(\alpha) < 0$ for $\alpha^2(S_2 - S_3) + \sigma^2(S_2 - S_1) < 0$, and for $U'_\ell(\alpha) < 0$ it is sufficient that for $1 \le i \le \ell$

$$0 \;>\; \alpha^2(\gamma_i^2 - \gamma_i^3) + \sigma^2(\gamma_i^2 - \gamma_i) = \gamma_i(\alpha^2\gamma_i(1 - \gamma_i) + \sigma^2(\gamma_i - 1)) = \gamma_i\phi_i(\alpha^2\gamma_i - \sigma^2),$$

and we need $(\alpha^2\gamma_i - \sigma^2) < 0$, or $\alpha^2\sigma_i^2 - \sigma^2(\alpha^2 + \sigma_i^2) < 0$. Now, for $i \le \ell$, $\sigma_i^2 \ge \sigma_\ell^2 > \sigma^2$ and we obtain $\alpha^2 < \min(\frac{\sigma^2\sigma_i^2}{\sigma_i^2 - \sigma^2})$ for all $1 \le i \le \ell$. But $x^2/(x^2 - a^2)$ is decreasing with x for $x^2 > a^2$, hence we need $\alpha^2 < \sigma^2/(1 - \sigma^2)$. For $\sigma_{\ell+1}^2 < \sigma^2 < \sigma_\ell^2$ and using $x^2/(1 - x^2)$ which is increasing with $x \in (0, 1)$ we obtain $\alpha^2 < \sigma_{\ell+1}^2/(1 - \sigma_{\ell+1}^2)$. Hence we must have $\alpha_\ell^2 > \sigma_{\ell+1}^2/(1 - \sigma_{\ell+1}^2)$. □

We now extend the analysis to obtain a lower bound on α_k for all $k > \ell$.

Theorem 3.1. *Suppose Assumptions 1 and 2, and that $U_k(\alpha_k)$ is a minimum for $U_k(\alpha)$, then $\alpha_k > \alpha_\ell > \sigma_{\ell+1}/\sqrt{1 - \sigma_{\ell+1}^2} = \alpha_{\min}$ for $k \ge \ell$.*

Proof. First suppose the contrary and that $\alpha_k \le \sigma_{\ell+1}/\sqrt{1 - \sigma_{\ell+1}^2}$. Then $U'_k(\alpha_k) = 0$ and by (14) $U'_\ell(\alpha_k) > 0$. But by Proposition 3.5 $U'_\ell(\alpha) < 0$ for $\alpha \le \sigma_{\ell+1}/\sqrt{1 - \sigma_{\ell+1}^2}$ and we have a contradiction yielding $\alpha_k > \sigma_{\ell+1}/\sqrt{1 - \sigma_{\ell+1}^2} = \alpha_{\min}$, $k \ge \ell$. It remains to determine whether it is possible to have $\sigma_{\ell+1}/\sqrt{1 - \sigma_{\ell+1}^2} < \alpha_k < \alpha_\ell$ where α_ℓ is the first minimum

point of $U_\ell(\alpha)$ to the right of $\alpha_{\min}$. Again we proceed by contradiction and suppose that $\alpha_k \in [\alpha_{\min}, \alpha_\ell]$ exists. Then we have the following:

(1) By (14) $E(U_k')(\alpha_\ell) < U_\ell'(\alpha_\ell) = 0$, and by (15), noting $\alpha > \sigma_{\ell+1}/\sqrt{5}$, $E(U_k'')(\alpha_\ell) > U_\ell''(\alpha_\ell) > 0$. Hence $U_k(\alpha)$ is concave up with negative slope at α_ℓ.

(2) At the minimum critical point $\alpha_k < \alpha_\ell$, $U_k'(\alpha_k) = 0$. Thus there must also be a second critical point which is a maximum for some $\bar{\alpha}$ in the interval $\alpha_k < \bar{\alpha} < \alpha_\ell$, for which $U_k'(\bar{\alpha}) = 0$ and $U_k''(\bar{\alpha}) < 0$.

(3) At $\bar{\alpha}$ we then have by (14) that $U_\ell'(\bar{\alpha}) > 0$. Hence $U_\ell(\alpha)$ is increasing at $\bar{\alpha} < \alpha_\ell$ but is decreasing at $\alpha_{\min} < \bar{\alpha}$, i. e. $U_\ell'(\alpha)$ changes sign for some α in the interval $[\alpha_{\min}, \bar{\alpha}]$. But by continuity then $U_\ell(\alpha)$ has at least one minimum on this interval. By assumption, however, α_ℓ is the first minimum point of $U_\ell(\alpha)$ to the right of $\alpha_{\min}$ and we have arrived at a contradiction.

□

We have now obtained a tight lower bound on α_k to go along with the generous upper bound

$$\alpha_{\min} = \frac{\sigma_{\ell+1}}{\sqrt{1-\sigma_{\ell+1}^2}} < \alpha_k \le 1 \quad \ell \le k \le r. \tag{25}$$

It remains to discuss the convergence of $\{\alpha_k\}$ to α^* with increasing k. We note that one approach would be to show that the $U_k(\alpha)$ are convex for $\alpha > \sigma_\ell$, but the sign result in (19) only immediately applies for $\alpha > 1$, hence investigating the sign requires a more refined bound for each interval $\alpha \in [\sigma_i, \sigma_{i-1}]$ for $i \le \ell$. Instead we obtain the following result, which relies on the uniqueness of α_k.

Theorem 3.2. *Suppose Assumptions 1, 2 and that α^* and each α_k, $k > \ell$ are unique within the given interval $\sigma_{\ell+1}/\sqrt{1-\sigma_{\ell+1}^2} < \alpha < 1$. Then, the sequence $\{\alpha_k\}_{k>\ell}$ is on the average increasing with $\lim_{k\to r} E(\alpha_k) = E(\alpha^*)$ and $\{U_k(\alpha_k)\}$ is increasing.*

Proof. It is immediate from (8) that $U_k(\alpha) \ge U_\ell(\alpha)$ for any $k > \ell$ and any α, and that $U_{k+1}(\alpha) \ge U_k(\alpha)$. Thus the $\{U_k(\alpha)\}$ is an increasing set of functions with $k > \ell$. By (14) of Proposition 3.3 we also have $E(\frac{\partial U_{k+1}(\alpha)}{\partial \alpha}) < E(\frac{\partial U_k(\alpha)}{\partial \alpha}) < \frac{\partial U_\ell(\alpha)}{\partial \alpha}$, and $\{E(\frac{\partial U_k(\alpha)}{\partial \alpha})\}$ is a decreasing set of functions for $k > \ell$. In particular $E(\frac{\partial U_{k+1}(\alpha_\ell)}{\partial \alpha}) < E(\frac{\partial U_k(\alpha_\ell)}{\partial \alpha}) < 0$. Moreover, by Corollary 3.1 and (15) of Proposition 3.3, when $\alpha_\ell > \sigma_{\ell+1}/\sqrt{5}$ the expected second derivatives at α_ℓ are positive and increasing with k so that the first derivative increases to 0 more quickly for larger k. Thus, not only do we have $E(\alpha_k) > \alpha_\ell > \alpha_{\min}$ for all k, we also have that $\{E(\alpha_k)\}$ converges from below to $E(\alpha^*)$. □

Corollary 3.3 (Faster Decay Rate of the Coefficients)**.** *Suppose that the coefficients s_i decay at the rate $s_i^2 = \sigma_i^{2(\rho+\nu)}$ for integer $\rho > 1$. Then the results of Theorems 3.1-3.2 still hold.*

Proof. This holds by modifying the inequality (6) for the faster decay rate yielding

$$K_i \sigma_i^4 < \sigma_i^{2(\rho+\nu)} = s_i^2 < \sigma_i^2 K_i, \quad K_i = \sigma_i^{2(\rho-1)}.$$

Thus the coefficients are bounded as in (23) but with scale factor K_i

$$\alpha^4\gamma_i^2 K_i = \sigma_i^4\phi_i^2 K_i \quad < \quad \phi_i^2(\alpha)s_i^2 < K_i\sigma_i^2\phi_i^2 = K_i\alpha^2\phi_i\gamma_i.$$

Using this relation all the results presented in Proposition 3.4 still hold with $H(\alpha)$ and $G(\alpha)$ replaced by

$$G_\rho(\alpha) = \alpha^4\sum_{i=1}^{\ell} K_i\gamma_i^2, \quad \text{and} \quad H_\rho(\alpha) = \alpha^2\sum_{i=1}^{\ell} K_i\phi_i\gamma_i.$$

Then again redefining the summations S_p to now depend on the coefficients with K_i, for H_ρ and G_ρ, following Proposition 3.5 yields the condition

$$\gamma_i\phi_i(\alpha^2 K_i\gamma_i - \sigma^2) < 0$$

for $U_\ell'(\alpha) < 0$. Continuing the argument as in the proof of Proposition 3.5 still yields the lower bound $\alpha_\ell^2 > \sigma_{\ell+1}^2/(1-\sigma_{\ell+1}^2)$. But this is all that is required for Theorems 3.1-3.2 and hence the results follow without modification. □

Remark 3.3. *This result shows that given a TSVD which sufficiently conquers the dominant terms of the SVD expansion, including sufficient terms that are noise-contaminated, α_k will be an increasingly good approximation for α^*. Moreover, including additional terms in the expansion will have limited impact on the solution, because $\alpha^* > \alpha_\ell$ and filter factor $\gamma_i(\alpha^*)$ is decreasing with i. In particular, $\gamma_i(\alpha^*) < \gamma_i(\alpha_\ell) < \gamma_{\ell+1}(\alpha_\ell) < \gamma_{\ell+1}(\sigma_{\ell+1}) = \frac{1}{2}$, for $i > \ell+1$ and $\alpha_\ell > \sigma_{\ell+1}$.*

Remark 3.4. *Although the main result of this paper effectively relies on an assumption that the UPRE functions have unique minima within the obtained bounds, $\alpha_{\min} < \alpha_k < 1$, proving that the minima are indeed unique seems to require using the discrete summations occurring in $U_k(\alpha)$ as approximations to continuous integrals. This approach is very technical, not very general, being dependent on the decay rate parameter τ, and serves only to tighten the lower bound for α. We therefore chose not to present results along this direction, relying on the computational results that are supportive of the unique identification of a minimum within these realistic bounds.*

Remark 3.5. *The results given depend on the assumption that summations with s_i^2 for terms with $i > \ell$ may be approximated in terms of the noise variance. For $r-\ell$ small relative to r, this assumption breaks down. As $r-\ell$ increases the assumptions become more reliable and less impacted by outlier data for s_i^2. Still the main convergence theorem holds only with respect to this analysis and we cannot expect that $\{\alpha_k\}$ will always converge monotonically to α^* in practice. With sufficient safeguarding, as noted in the algorithm presented in Section 4, it is reasonable to expect that α^* is quickly and accurately identified.*

Remark 3.6 (Posterior Covariance)**.** *We have shown $\{\alpha_k\}$ increases with k. Thus the approximate a posteriori covariance of the filtered TSVD solution $\sigma^2/(4\alpha^2)$ decreases with k, to $\sigma^2/(4(\alpha^*)^2)$. Thus in trading off the minimization of the risk by using the UPRE to find the optimal α, the method naturally finds a solution which has increasing smoothness with increasing k, thus limiting the impact of the possibly non-smooth components of the*

solution corresponding to small singular values that would contaminate the unfiltered TSVD solution.

4. Practical Application

The convergence theory for $\{\alpha_k\} \to \alpha_r$ as $k \to r$ presented in Section 3 motivates the construction of an algorithm to automatically determine an optimal index k_{opt} and associated regularization parameter $\alpha_{k_{\text{opt}}}$. The algorithm is presented and discussed in Section 4.1 and verified for $2D$ test problems in Section 4.2. These results also corroborate the convergence theory presented in Section 3.

4.1. **Algorithm.** We propose an algorithm that works by iteratively minimizing (8) on the TSVD subspace of size $k \leq r$ until a set of convergence criteria are met. These convergence criteria rest on the observation that the relative change, $c_k = |(\alpha_k - \alpha_{k+1})|/\alpha_k > 0$, between successive parameter estimates, α_k and α_{k+1}, decreases as k increases towards r. If during the iterative procedure there exists a k such that it is reasonably believed that $\alpha_k^* \approx \alpha_i$ for all $i > k$, the algorithm terminates, producing k_{opt} and $\alpha_{k_{\text{opt}}}$. A pseudo-code implementation is given as Algorithm 1.

Algorithm 1: Truncated UPRE Parameter Estimation

Input: SVD or TSVD; initial index k_0; maximum k, $k_{\max}$; step size Δ_k; relative tolerance δ; window length w; optional estimate for ℓ

Output: Converged parameter $\alpha_{k_{\text{opt}}}$; convergence index k_{opt}; relative mean change $\hat{c}_{iw}$;

$k \longleftarrow k_0$; $\hat{c}_{iw} \longleftarrow \inf$
Initialize $\alpha_{\min}$ according to (25) using ℓ if provided, otherwise using k
$\alpha(0) \longleftarrow \arg\min_\alpha U_k(\alpha)$ over interval $[\alpha_{\min}, 1]$
while $(\hat{c}_{iw} > \delta$ **and** $k < k_{\max})$ **or** $(\alpha(i) = \alpha_{\min})$ **do**
  $i \longleftarrow i + 1$; $k \longleftarrow k + \Delta_k$
  If ℓ not provided, update $\alpha_{\min}$ according to (25) using k
  $\alpha(i) \longleftarrow \arg\min_\alpha U_k(\alpha)$ over interval $[\alpha_{\min}, 1]$
  $c(i) = (|\alpha(i) - \alpha(i-1)|)/\alpha(i)$
  if $i \geq w$ **then**
    $\hat{c}_{iw} \longleftarrow \texttt{mean}(c(i), c(i-1), \ldots, c(i-w+1))$
  end
end
return $k = k_{\text{opt}}$, $\alpha(i) = \alpha_{k_{\text{opt}}}$, $\hat{c}_{iw}$

Algorithm 1 takes as input a full or TSVD as well as a number of required and optional parameters which we now discuss. For large scale problems it is not necessary, and is even discouraged, to compute α_k for all $k \leq k_{\text{opt}}$. For moderately or mildly ill-posed problems, and for problems with high signal to noise ratios in which the expected k_{opt} is likely to be large relative to the problem size, it is recommended to start

the algorithm at some $k_0 \neq 1$ and to increment k by some $\Delta_k \neq 1$, yielding the sequence $\{k(i) : k_0, k_0 + \Delta_k, k_0 + 2\Delta_k, \dots k_0 + i\Delta_k\}$. The algorithm computes the sequence $\{\alpha_{k_0}, \alpha_{k_0+\Delta_k}, \alpha_{k_0+2\Delta_k}, \alpha_{k_0+3\Delta_k}, \dots\}$, each solving (10) for the given index, until either $k_0 + i\Delta_k \geq k_{\max}$ or until α_k has converged, where k_0, Δ_k, and $k_{\max}$ are provided by the user. For each $k_0 + i\Delta_k$ the relative change in α is computed as $c_i = |\alpha_{k_0+i\Delta_k} - \alpha_{k_0+(i-1)\Delta_k}|/\alpha_{k_0+i\Delta_k}$. While convergence can be determined by the condition $c_i < \delta$, for some user provided tolerance δ, it is observed that higher confidence in convergence can be achieved by requiring $\hat{c}_{iw} < \delta$ where $\hat{c}_{iw}$ is the mean calculated over the window of size w, i.e. over $\{c_i, c_{i+1}, \dots, c_{i+w}\}$. This protects against the possibility of stopping the parameter search early due to the condition that $c_i < \delta$, while at the same time $c_j \geq \delta$ for some $j > i$. Due to the impact of noise on calculating the parameter α_k it is entirely possible that relative changes between successive estimates of α_k may be either extremely small or large. Comparing $\hat{c}_{iw}$ to δ enables a broader view of the convergence of α_k, and the moving window average smooths out the natural variation in c_i. To summarize then, the required input to the proposed algorithm is a full or TSVD, a starting index k_0, a step size between successive estimates Δ_k, an upper-bound $k_{\max}$ dependent on the severity of the problem and the noise level, a tolerance δ, and a width w over which the moving average of relative changes in successive estimates of α is computed.

The results of Theorem 3.1 are incorporated into Algorithm 1 with the inclusion of an optional parameter ℓ specifying an estimate for the index at which noise dominates the coefficients. If a Picard plot is available ℓ can be estimated visually, otherwise an approach relying on Picard parameter estimates similar to that used by [24] and [16] can be used. If an estimate for ℓ is available, $\alpha_{\min}$ is calculated according to (25), and α_k is found using $\alpha_{\min} = \sigma_\ell/\sqrt{1-\sigma_\ell^2}$ and $\alpha_{\max} = 1$ in (10). Otherwise, the looser bound $\sigma_k/\sqrt{1-\sigma_k^2}$ is used in (10). In either case if the lower bound is achieved then the theory indicates that noise has not yet dominated and the algorithm is allowed to continue. Thus, in the case where $k < k_{\max}$, necessary conditions for the termination of Algorithm 1 are $\hat{c}_{iw} < \delta$ and α_k should be greater than the specified $\alpha_{\min}$.

4.2. **Verification of the Algorithm and Theory.** We now present the evaluation of Algorithm 1 on the test problem `Satellite` of size 128×128 with noise levels 10%, 5%, 1%, and 100 noise instances generated for each noise level. These results are representative of applying Algorithm 1 to other $2D$ test cases. A moving window of size $w = 5$ in computing $\hat{c}_{iw}$ with relative tolerance of $\delta = 1\text{e}{-3}$ was found to work well for each noise level, but may need to be adapted to the severity of the ill-posedness of the problem. Recorded in each run are the converged $\alpha_{k_{\text{opt}}}$, the size of the TSVD subspace k_{opt} to be used, and the relative reconstruction error (RRE) of the solution obtained by using $\alpha_{k_{\text{opt}}}$ for the regularized TSVD solution.

Figure 7. Box plots showing the index k_{opt} produced by Algorithm 1 for problem `Satellite` computed from 100 runs for noise levels 1%, 5%, and 10%. The number of terms k in the TSVD that provide useful information decreases as the noise level increases.

(a) Noise level = 1% (b) Noise level = 5% (c) Noise level = 10%

Figure 8. Box plots comparing parameter estimates $\alpha_{k_{\text{opt}}}$ with α^* for problem `Satellite` computed from 100 runs for noise levels 1%, 5%, and 10%. For each noise level, the estimate $\alpha_{k_{\text{opt}}}$ produced by Algorithm 1 is an excellent approximation to α^*, demonstrating that terms in the TSVD for $k > k_{\text{opt}}$ do not heavily impact the value of α^*. Note that the limits on the $y-$axes vary across subplots to better visualize the parameter distributions across noise levels.

Figure 7 is a box plot[1] showing the spread of k_{opt} values for the 100 noise instances run for each noise level, where in each case $k_{\text{opt}} \ll r = 16384$. Figure 8 is a box plot comparing

[1]A box plot is a visual representation of summary statistics for a given sample. Horizontal lines of each plotted box represent the 75%, 50% (median), and 25% quantiles, with outliers plotted as individual crosses or points.

(a) Noise level = 1% (b) Noise level = 5% (c) Noise level = 10%

Figure 9. Line plots showing the calculated estimates for $\{\alpha_k\}$ with increasing number of terms k in the TSVD. The results are given for problem `Satellite` for noise levels 1%, 5%, and 10%, for 10 random noise instances at the specified noise level. The resulting point $(k_{\text{opt}}, \alpha_{k_{\text{opt}}})$ produced by Algorithm 1 is displayed as a cyan triangle. Note that the limits on the $y-$axes vary across subplots to better visualize the convergence across noise levels.

the $\alpha_{k_{\text{opt}}}$ returned by the algorithm, and α^* obtained by minimizing the UPRE on the full space. These figures together reaffirm that the optimal regularization parameter found by UPRE is largely determined by a relatively small number of terms in the TSVD, and less impacted by the tail of the coefficients dominated by noise. The estimation of $\{\alpha_k\}$ with increasing number of terms in the TSVD is depicted in Figure 9 for the first 10 runs of each noise level, where the point of convergence $(k_{\text{opt}}, \alpha_{k_{\text{opt}}})$ is represented as a cyan triangle. In should be noted that the estimated lower bound $\alpha_{\min}$ was not used, and α was minimized over the interval $(0, 1)$ using `fminbnd`. A tolerance of $\delta = 1\text{e}{-3}$ was found to produce a value for $\alpha_{k_{\text{opt}}}$ just prior to the point where $\{\alpha_k\}$ began to stabilize. A smaller δ will necessarily increase k_{opt}, but with negligible changes in $\alpha_{k_{\text{opt}}}$. In these simulations averaged over all 100 runs, $\alpha_{k_{\text{opt}}}$ was within 1.16%, 1.47%, and 2.47% of α^* for noise levels 1%, 5%, and 10% respectively using fewer than 3% of the SVD components.

In terms of RRE, the regularized TUPRE using a subspace of size k_{opt} with parameter $\alpha_{k_{\text{opt}}}$ obtained by Algorithm 1 generally provided a better solution than obtained using full UPRE for each noise level. Figures 10 and 11 show box plots and histograms respectively of the RRE comparing the regularized TSVD and the full UPRE solution. Over all noise levels, the median and mean reconstruction error of 100 noise instances is lower in the regularized TSVD solution. Similar to the Picard parameter approaches of [24], Algorithm 1 identifies an index k_{opt} for which coefficients s_k are dominated by noise for $k > k_{\text{opt}}$. Our approach, however, does not rely on performing statistical tests on the coefficients, but

instead examines the stabilization of α_k as k increases. Once α_k has stabilized, adding additional noise dominated terms in the solution delivers no benefit. Furthermore, if a TSVD with $k_{\max}$ terms has been calculated, then either α_k converges for $k < k_{\max}$ or we know that the optimal choice k_{opt} is greater than $k_{\max}$, and that $\hat{c}_{iw}$ provides some estimate for whether $k_{\text{opt}} >> k_{\max}$ or whether the given TSVD can be assumed to be sufficient in providing a good estimate for the solution $\mathbf{x}$.

(a) Noise level = 1% (b) Noise level = 5% (c) Noise level = 10%

Figure 10. Box plots of RRE comparing solutions using truncated UPRE with parameter $\alpha_{k_{\text{opt}}}$ and solutions using full UPRE with parameter α^* for problem `Satellite` computed from 100 runs for noise levels 1%, 5%, and 10%. Regularization parameter α_{kopt} obtained by UPRE on a TSVD generally has lower error, as evident from Truncated UPRE plots being vertically shifted downwards relative to full UPRE boxplots. Note that the limits on the $y-$axes vary across subplots to better visualize the spread of the distributions across noise levels.

In these simulations ℓ is not known precisely but was estimated by visual inspection of the Picard coefficients, as well as by comparing the distributions of the noise contaminated and noise free coefficients. This approach for estimating ℓ is not possible in general as the noise free coefficients are unknown in practice, this method of estimating ℓ was employed for the purpose of validating the results of Theorem 3.1. An estimate for the lower bound $\alpha_{\min}$ obtained from (25) is depicted as the red dashed curve in Figure 12, with $\{\alpha_k\}$ plotted in black. It can be seen that $\alpha_{\min}$ serves as a tight lower bound for the converged parameter $\alpha_{k_{\text{opt}}}$, and while not as tight, a lower bound of $\sigma_k/\sqrt{1-\sigma_k^2}$ can be used effectively in cases where an estimate of ℓ is not available.

In summary, given a TSVD or SVD, an optional estimate of ℓ, and suitable parameters determined by the ill-posedness of the problem, Algorithm 1 is able to effectively determine a regularization parameter $\alpha_{k_{\text{opt}}}$ obtained by UPRE minimization over the TSVD subspace

(a) Noise level = 1% (b) Noise level = 5% (c) Noise level = 10%

Figure 11. Histograms of RRE comparing solutions using $\alpha_{k_{\text{opt}}}$ and solutions using α^* for problem `Satellite` computed from 100 runs for each noise level 1%, 5%, and 10%. Regularization parameter $\alpha_{k_{\text{opt}}}$ obtained by UPRE on a TSVD generally has lower error, as evident from the truncated histograms having peaks shifted to the left relative to the full UPRE.

of size k_{opt}, such that the regularized truncated solution $\mathbf{x}$ has consistently lower RRE than the full UPRE solution.

5. Conclusions

We have demonstrated that the regularization parameter obtained using the UPRE estimator converges with increasing number of terms k used from the TSVD for the solution. If using a severely ill-posed problem the convergence occurs very quickly independent of the size of the problem due to the fast contamination of data coefficients by practical levels of noise.

Practically-relevant problems are often, however, only moderately or mildly ill-posed, e. g. [2, 9, 25, 26], and it is therefore important to accurately and efficiently find both k_{opt} and $\alpha_{k_{\text{opt}}}$. Theoretical results have been presented that demonstrate the convergence of the regularization parameter α_k with k, increasing from below to α^*, the optimal value for the full SVD. The posterior covariance thus decreases with k, leveling at approximately $\sigma^2/(4(\alpha^*)^2)$. In trading off the minimization of the risk by using the UPRE to find α^*, the method naturally finds a solution which has increasing smoothness with increasing k. An effective and practical algorithm that implements the theory has also been provided, and validated for 2D image deblurring. These results expand on recent research on the characterization of the regularization parameter as closely dependent on the size of the singular subspace represented in the solution, [5, 21, 22]. As there is a resurgence of interest in using a TSVD solution for the solution of ill-posed problems due to increased feasibility of finding a good approximation of a dominant singular subspace using techniques from

(a) Noise 1% (b) Noise 5% (c) Noise 10%

Figure 12. Line plots showing the convergence of $\{\alpha_k\}$ for problem `Satellite` for noise levels 1%, 5%, and 10%. In each subplot, α^* is plotted in black for 10 random noise instances at the specified noise level. The dotted blue curve represents the lower bound in (25) as a function of k, with the red dashed line representing the lower bound according to Theorem 3.1 and dependent on ℓ for a single run.

randomization, e.g. [3, 4, 8, 17, 18, 23], the results are more broadly relevant for more efficient estimates of the TSVD. We note that this work is limited by its assumption of standard Tikhonov regularization with the TSVD, and thus it is of future interest to study the feasibility of extending these results in the context of smoothing regularizers.

Acknowledgements

Rosemary Renaut acknowledges the support of NSF grant DMS 1418377: "Novel Regularization for Joint Inversion of Nonlinear Problems".

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