Bayesian Tikhonov Regularization

A Bayesian Hierarchical Model for Estimating the Regularization Parameters in Tikhonov Regularization

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Abstract

In this thesis we discuss the theory behind the regularizing Tikhonov functional proposed by Jin and Zou [7]. We reimplement their Alternating Iterative Algorithm. The role of the hyper-priors in the Alternating Iterative Algorithm is reexamined, and we find cases in which convergence to a minimum is not guaranteed. Furthermore, their method depends on the existence of the closed form solutions. We, therefore, extend their algorithms by proposing two additional iterative methods that do not depend on the closed form solutions. The convergence of the two methods is proven. We analyze the properties of the two novel methods through a simple simulation study.

Contents

1 Inverse Problems

In this chapter we give a brief introduction and motivation to functional analytic inverse problems. We then give an overview of the research done and summarize the goals of the thesis. At the end of this chapter an outline is provided.

1.1 Introduction

What are inverse problems? To understand what is inverse about inverse problem, we must first define the direct problem. The direct problem models the effects from known causal factors. However, in inverse problems we observe only the effects and want to infer the causes. It is easiest to understand by example.

Example 1.1 (Image Processing)**.** *Suppose we observe an 2-D digital image by convolving the ground truth with some filter and added noise. We can mathematically model this by the discrete model*

$$y_i = \left(\sum_{j \in \mathbb{Z}^2} a_{i,j} x_j \right) + \epsilon_i$$

where y_i is the measured image, x_j are the pixel values the ground truth $i = (i_1, i_2)$ and $j = (j_1, j_2)$ and $a : \mathbb{Z}^2 \times \mathbb{Z}^2 \to \mathbb{R}$ the filter. The continuous model is

$$y(t) = \left(\int_\Omega a(t-y)x(y)dy \right) + \epsilon(t)$$

where $x(y)$ is the image represented as a function, $\Omega \subset \mathbb{R}^2$ is the image domain, and $a : \Omega \times \Omega \to \mathbb{R}$ is the convolution kernel. The inverse problem is then deconvolution.

Another common example of inverse problems is seismic inversion, where again we wish to infer the observable underlying causes from observed measurements on some subsurface. Other applications of inverse problems are in image reconstruction, magnetic resonance imagining, tomography, and heat diffusion. Inverse problems also arise in non-physical situations such as in root finding, matrix inversion, and differentiation.

1.2 Basic Formulation

In inverse problems, the goal is to recover the unknown parameter x from observations y. Suppose that the problem can be modeled as

$$y = Ax \tag{1}$$

where $y \in \mathcal{Y}$ is the observed/measured data, $x \in \mathcal{X}$ is the unknown parameter, and $A : \mathcal{X} \to \mathcal{Y}$ is the forward linear operator that describes how x relates to y. We assume there exists some ground truth $\bar{x} \in \mathcal{X}$ such that (1) holds, and that

the forward problem linking x to y is well-defined. We typically observe only noisy measurements of the $\bar{x}$, so really our model should be

$$y = A(x, e) \tag{2}$$

Solving for x in this model is not possible. For example if A is not invertible. This is an example of ill-posedness. A formal definition of well-posedness is give in section 2.1. It is assumed throughout this paper that e is some additive noise. Therefore, we can write

$$y = Ax + e \tag{3}$$

Below we return to the example of convolution as an inverse problem that arises in imagining and signal processing. This demonstrates that finding a solution to (3) is not trivial.

Example 1.2. *(DeConvolution [1])*

Let $\mathcal{X} = \mathcal{Y} = L^2(\mathbb{R})$ be the space of square integrable functions. Let $A : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ such that

$$(Af)(x) = g \circ f = \int_{\mathbb{R}} g(x-y)f(y)dy$$

Let $g(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$. The Fourier transform of (Af) is

$$\mathcal{F}(Af)(\xi) = \int_{\mathbb{R}} e^{-i\xi x} Af(x)dx = \hat{g}\hat{f}(\xi)$$

If $Af = 0 \implies \hat{f} = 0 \implies f = 0$ so A is injective. So the solution is unique and exists. The solution to $Af = h$ is given by

$$f(x) = \mathcal{F}^{-1}(\hat{g}^{-1}\hat{h})(x)$$

The solution is not well defined for an arbitrary $h \in L^2(\mathbb{R})$. Suppose we observe small errors in h. As $\hat{g}^{-1}$ grows exponentially, h may no longer be in the range of A. So the integral does not converge, and no solution exists.

Inverse problem can be categorized by the forward operator. They are either linear or non-linear. Most inverse problems arising from physical systems are non-linear, but in this thesis we will study the simpler case of discrete finite linear inverse problems.

1.3 Previous Research

The topic of Inverse problems is well studied. A variety of classical examples of inverse problem can be in found in [8] and [6]. These two sources also give a thorough introduction into the topic.

Ill-posedness is a major area of research, as inverse problems are often inherently ill-posed. A common method to over come the ill-posedness is regularization. This is a large area of research that tries to reconstruct good estimates of the causal parameters given the data. Regularization methods have been studied in [6], [3], and, more recently, in [9].

One particular type of regularization is Tikhonov regularization. The regularized solution is a good estimate conditional on the regularization parameter, that balances interpolating the data points versus other desired properties such as smoothness. The choice of regularization parameter is often ad-hoc or assumes we have access to unknown information such as the noise level.

Another related, and rather new area of research in inverse problems is one that uses Bayesian statistics. This research aims to pose the functional analytic model that we have seen previously into a Bayesian framework. The major benefit of this is that we can mathematically incorporate the uncertainty of the model parameters by considering them as random variables defined by (conditional) distributions. An overview of statistical inverse problems can be found in [2], which introduces the finite/discrete setting, and [11] which is focused on the infinite/continuous setting.

The Bayesian formulation of the inverse problem to the functional analytic one is connected via Tikhonov regularization. In the additive independent normal noise model, the posterior distribution is normal. Gaussian distributions are completely characterized by their mean and variance. Computing the mean of the posterior distribution is show to be equivalent to computing the minimum of Tikhonov regulation with ℓ_2 penalty in [11] and [2].

Another complimentary area of research is developing numerical methods, to solve Tikhonov type regularization functionals. In [7], Jin and Zou, study the additive normal noise case in detail, proving convergence and consistency of this estimator as well as proposing and implementing an alternating algorithm to numerically solve the minimization problem. This alternating algorithm relies on the closed form solution to compute the gradient in all directions of the unknown parameters. They prove the convergence of this method to a minimum, without dependence on the parameters of the hyper-prior. We found, however, that for certain parameters of the hyper-prior the functional no longer decreased monotonically. Therefore convergence to a minimum is not guaranteed.

1.4 Research Aims

We have two main goals. They are as follows

- Present a data driven way to choose the regularization parameter in Tikhonov regularization. We will show that this is a well-posed problem. We will also show that the resulting estimate converges to the least squares estimate as the noise level goes to zero.
- Derive numerical methods to solve the minimization problem resulting from regularization of the inverse problem. The first method implemented was proposed by [7]. We extend their work by proposing and implementing

additional algorithms that are suitable for a more general case - a setting where the noise is not normal. We will show that these methods converge to a minimum. We then implement our methods and test them on a simple example. Through this example we will also explore the effect of changing the parameters of the hyper-priors on the convergence of the methods. The implementation can be found on github.[1]

1.5 Outline

The outline to the thesis is as follows. In Chapter 2 we explain one of the key questions in inverse problems. Is the formulated problem of solving for x well-posed? We define what ill-posedness is in a specific setting, and then discus numerous situation in which we encounter ill-posedness. This then naturally leads us to the resolution of ill-posed problems where we explain how we can stabilize the solution through regularization. So far everything until then has been in the non statistical finite dimensional vector space setting, and we transition to the statistical setting in Chapters 3 and 4. Chapter 3 is a brief over view the statistical and probability notation and definitions used to define statistical inverse problems. Then Chapter 4 briefly introduces statistical inverse problems, and gives an overview with some examples, and how they are related to the functional analytical setting. In Chapter 5 we explain how from the Bayesian setting of inverse problems we can have a data driven method to infer the regularization parameters from the observations. We prove that the purely empirical Bayesian method is ill-posed in certain cases, and that a hierarchical model resolves this. Chapters 6 and 7 contain the second major half of this thesis. In this chapter, we design three different numerical algorithms to solve the resulting minimization problem derived in Chapter 5. We show that these converge to a critical point of the regularization functional. Then in Chapter 7 we implement the methods in python, and explain the results. We also look at the models' sensitively to the choice of hyper priors and the convergence and consistency. In Chapter 8, we conclude with a discussion topics for further research and how we can improve on the results seen in Chapter 7.

[1] `https://github.com/Tienstra/BayesianRegularization`

2 Regularization

In Example 1.2 we have seen that solving for x is more than just inverting the forward operator. The above example was an ill-posed problem. Ill-posedness is a common characteristic of inverse problems. To resolve the problem of ill-posedness, we will introduce regularization into the direct inverse problem. The resulting problem will be well-posed and the resulting solution will be regularized.

2.1 Ill-posedness

Hadamard defined a well-posed problem as one that meets all of the following conditions [6]:

Definition 2.1. *A problem is well posed if the following three conditions hold*

1. *Existence: There exists a solution*
2. *Uniqueness: The solution is unique.*
3. *Stability: The solution depends continuously on the observed data.*

Let us return the linear setting. Let $\mathcal{X} = \mathbb{R}^m, \mathcal{Y} = \mathbb{R}^n$, and suppose that we wish to solve the following for x

$$y = Ax$$

Now $y \in \mathbb{R}^n, x \in \mathbb{R}^m, A \in \mathbb{R}^{n \times m}$.

Remark 2.1. *We then consider the following cases:*

1. *If A is a square matrix, and A has full rank, then A is invertible. We then have that $x = A^{-1}y$ is the solution to the above.*
2. *If A is a square matrix and is not full rank then then by the rank-nullity theorem, the dimension of the null space is greater than 0. In this case the solution may not exist and/or may not be unique.*
3. *if $n > m$, and $rank(A) \leq m$, then the system of equations is overdetermined. So no solution can exist, if $y \notin Range(A)$.*
4. *if $n < m$, and $rank(A) \leq n$, then the system of equations is underdetermined, and a solution exist but is not unique.*

So a unique solution exists if and only if $ker(A) = 0$. Then we have that

$$x = A^{-1}y$$

To check if this solution is stable we recall the following two definitions. Since we are in the finite dimensional case, A can be represented by a singular system.

Definition 2.2. *Let $A \in \mathbb{R}^{n\times m}$, then the singular value decomposition of A is a factorization of A,*

$$A = U\Sigma V^*$$

where $U \in \mathbb{R}^{n\times n}$ is an orthogonal matrix, $\Sigma \in \mathbb{R}^{n\times m}$ is a rectangular diagonal matrix with non-negative entries, and $V \in \mathbb{R}^{m\times m}$ is an orthogonal matrix. The diagonal entries of Σ, denoted by σ_i are the singular values of A, and are listed in descending order. That is $\sigma_1 \geq \sigma_2 \geq .... \geq \sigma_m \geq 0$. We sometimes write $U = [u_1, ...u_n]$ and $V = [v_1, ..., v_m]$ where $\{u_i\}_{i=1}^n$ and $\{v_i\}_{i=1}^m$ are orthogonal basis for $\mathbb{R}^n$ and $\mathbb{R}^m$ respectively. The singular system of A is then $\{u_i, v_i, \sigma_i\}_{1\leq i\leq \min(n,m)}$.

and

Definition 2.3. *Let A be an invertible matrix. Let σ_{min} and σ_{max} be the minimum and maximum eigenvalues of A respectively. Then the condition number of A is*

$$\begin{aligned}\kappa(A) &= ||A^{-1}||\ ||A|| \\ &= \frac{\sigma_{max}}{\sigma_{min}}\end{aligned}$$

Example 2.1. *Suppose we would like to solve the following equation for x,*

$$y = Ax$$

Let δy be the error in y. Assume that A is invertible. Then the $A(x + \delta x) = y + \delta y$, so $(x + \delta x) = A^{-1}(y + \delta y) = A^{-1}y + A^{-1}\delta y$. The error in the solution is then $A^{-1}\delta y$. We can compute the ratio of the relative error in the solution compared to the the relative error in y as

$$\frac{||A^{-1}\delta y||}{||\delta y||}\frac{||y||}{||A^{-1}y||}$$

Then we see from the above definition that

$$\begin{aligned}\kappa(A) &= ||A^{-1}||\ ||A|| \\ &= \frac{\sigma_{max}}{\sigma_{min}} \\ &= \max_{\delta y, y\neq 0}\left\{\frac{||A^{-1}\delta y||}{||\delta y||}\frac{||y||}{||A^{-1}y||}\right\} \\ &= \max_{\delta y\neq 0}\left\{\frac{||A^{-1}\delta y||}{||\delta y||}\right\}\max_{y\neq 0}\left\{\frac{||Ay||}{||y||}\right\}\end{aligned}$$

where $||y||$ is the euclidean norm, $||A||$ is the induced matrix norm, and σ_{max}, σ_{min} are the maximum and minimum singular values of A respectively. So then

$$\frac{||x - x_\delta||}{||x||} \leq \kappa(A)\frac{||y - y_\delta||}{||y||}.$$

Example 2.2 (Matrix Inversion [3]). *Let $y \in \mathbb{C}^n, x \in \mathbb{C}^n, A \in \mathbb{C}^{n\times n}$. Assume that A is symmetric positive definite. From the above, we can write*

$$A = \sum_{i=1}^{n} \sigma_i a_i a_i^T$$

where σ_i are the eigenvalues of A ordered such that $\sigma_1 \geq \sigma_2 \geq \ldots > 0$, and eigenvectors $a_i \in \mathbb{R}^n$ where $a_i \perp a_j$ for $i \neq j$. Assume we observe y^δ where $y^\delta = Ax^\delta$. Then we have that

$$x - x^\delta = \sum_{i=1}^{n} \sigma_i^{-1} a_i a_i^T (y - y^\delta).$$

The error between x and the estimate x^δ is

$$\begin{aligned} ||x - x^\delta||_2^2 &= \sum_{i=1}^{n} \sigma_i^{-2} ||a_i||^2 |a_i^T (y - y^\delta)|^2 \\ &\leq \sigma_n^{-2} ||y - y^\delta||_2^2 \\ &\leq \sigma_n^{-1} ||y - y^\delta||_2^2 \\ &\leq \kappa(A)\delta \end{aligned}$$

Let $y = Ax$ and $y^\delta = Ax + e$, such that $||y - y^\delta||_2^2 \leq \delta\kappa$. Suppose that $\kappa(A) \ll \infty$, then the solution depends continuously on the data, as the relative error in x is bounded by the relative error in y times a small constant. On the other hand if $\kappa(A)$ is very large, in which case A is ill-conditioned, then the solution does not depend continuously on the data as a small change in y can result in a large change in x. Since $\kappa(A) = \frac{\sigma_{max}}{\sigma_{min}}$ we see that a large $\kappa(A)$ occurs if σ_{min} is very small. If $\sigma_{min} \to 0$ then $\kappa(A) \to \infty$. So stability is determined by the decay of the singular values of A. To guarantee a stable solution, we need to bound the singular values of A away from zero.

Definition 2.4. *Let $A \in \mathbb{R}^{n\times m}$ with $rank(A) = r \leq \min\{n, m\}$. Then using SVD of A the Moore-Penrose pseudo is defined as*

$$A^\dagger = V_r \Sigma_r^{-1} U_r^* \tag{4}$$

where Σ_r^{-1} the reciprocal of the first r non-zero eigenvalues. That is $\Sigma_r^{-1} = diag(1/\sigma_1, 1/\sigma_2 ..., 1/\sigma_r, ...0...)$

Suppose now $n \geq m$ and $y \notin Range(A)$. Suppose also that A has full rank. The SVD of A is

$$A = U_m \Sigma_m V_m^* \tag{5}$$

Then

$$Ax = U_m U_m^* y$$

since U_m is an orthogonal matrix $U_m U_m^*$ projects y onto the range of A. The solution is then given by

$$\hat{x} = V_m \Sigma_m^{-1} U_m^* y = A^\dagger y$$

Claim 2.1. *The least squares solution to $y = Ax$ is given by*

$$x_{LS} := \min_x ||Ax - y||_2^2 \equiv V_m \Sigma_m U_m^* y \equiv A^\dagger y \tag{6}$$

where $A = U_m \Sigma_m V_m^*$ is the singular value decomposition of the matrix operator A, $U_m = (u_1, ..., u_m), V_m = (v_1, ..., v_m)$, are the m left and right singular vectors and Σ_m is the diagonal matrix with the first m singular values. $A^\dagger$ is the Moore-Penrose pseudo inverse of A.

Suppose now that $n < m$, and A has full rank. The solution exists but is not unique. The solution we would like then is the minimum norm solution. In this case the solution is given by

$$x = x' + \sum_{i=1}^{n} \frac{\langle u_i, y \rangle}{\sigma_i} v_i$$

where $x' \in ker(A)$. Since $n < m$, the $ker(A) = span(v_n + 1, ..., v + m)$. So $x' = Vc$ with $V = [v_n + 1, ..., v + m]$. The solution has minimum norm in case of $x' = 0$, and the solution does not contribute to the $ker(A)$. So the minimum norm solution is

$$\hat{x} = V_n \Sigma_n^{-1} U_n^* y = A^\dagger y$$

Is the least squares or minimum norm solution stable? Using the SVD of the pseudo inverse of A we get that

$$\hat{x} = \sum_{i=1}^{r} \frac{\langle u_i, y \rangle}{\sigma_i} v_i \tag{7}$$

where $r = \min(m, n)$. We see that the continuity of $\hat{x}$ is depending on the singular values σ_i. If σ_i is small, then $\langle u_i, y \rangle$ can be large, amplifying the $v_i^t h$ component of y. So it is possible that $v_i^t h$ with small singular values exaggerate the noise of y. The solution is not continuous. When is the solution stable?

Definition 2.5. *For $y = Ax$, y satisfies the Picard condition if the Fourier coefficients $\langle u_i, y \rangle$ as derived above decay faster than σ_i, the singular values defined above. That is*

$$\sum_{i=1}^{r} \left| \frac{\langle u_i, y \rangle}{\sigma_i} \right|^2 < \infty$$

2.2 Stabilization

Recall that we can decompose the mean square error of an estimator into the bias and variance parts. For x_{LS}, the bias is zero but the variance can be so high that the solution is ill-posed as we have seen. To lower the variance we can introduce a biased estimator. Ideally, we would end up with a lower MSE over all. The high variance came from division by very small singular values. One way to avoid dividing by small singular values is to regularize the $\sigma_i's$ with some regularization functional $\mathcal{R}_\alpha$, where regularisation parameter α. The regularized solution is then

Definition 2.6.

$$x_\alpha = V_k \mathcal{R}_\alpha(\sigma_k) U_k^* y \tag{8}$$

where $\mathcal{R}_\alpha$ is the regularizing functional depending on regularization parameter α.

Possible regularization functionals are threshold functions, such as Truncated Singular value composition, which cuts off small singular values based on the regularization parameter; or shifting functions such as Tikhonov regularization. In this thesis we are interested in Tikhonov type regularization.

Definition 2.7. *The Tikhonov regularization solution is*

$$x_\alpha = \sum_{i=1}^{r} \frac{\sigma_i \langle x_i, y \rangle}{\sigma_i^2 + \alpha} v_i \tag{9}$$

such that $\mathcal{R}_\alpha(\sigma) = \sigma/(\sigma^2 + \alpha)$, and α is the regularization parameter.

In the above we modify the pseudo inverse by adding some weight to the singular values. The denominator is then bounded by α even if $\sigma \to 0$. When $\sigma_i \gg \alpha$ the ratio $\frac{\sigma_i \langle x_i, y \rangle}{\sigma_i^2 + \alpha} \approx \frac{\sigma_i \langle x_i, y \rangle}{\sigma_i^2}$. In the case where $\sigma_i \ll \alpha$, the ratio is decreased, thus overall decreasing the variance $\hat{x}$. The consequence of this is that resulting estimator x_α will be a biased. We can compare the difference between the non-regularized solution $\hat{x}$ and the regularized solutions x_α. This difference displays the bias-variance trade.

Definition 2.8. *Let $\hat{x} = A^\dagger y$, the non-regularized solution, with the $A^\dagger$ the pseudo inverse. Let $\hat{x}_\alpha = A_\alpha^\dagger y^\delta$, the regularized solution with $A_\alpha^\dagger$, the regularized pseudo inverse.*

$$||\hat{x} - x_\alpha|| \leq ||(A^\dagger - A_\alpha^\dagger) y|| + ||A^\dagger (y - y^\delta)||$$

The bias is measured as $||(A^\dagger - A_\alpha^\dagger) y||$ and variance is measured as $||A^\dagger (y - y^\delta)||$.

When $\alpha \to 0$, $A^\dagger = A_\alpha^\dagger \implies ||(A^\dagger - A_\alpha^\dagger)|| = 0$. Now that we have an estimator we would like know how good this estimator is. To do this we can compute the mean squared error as

Definition 2.9. *Let $x = Ay$ be the true parameter. Let $x_\alpha = A_\alpha^\dagger y^\delta$ be the regularized solution. The mean squared error of this estimator is given by*

$$||x - x_\alpha|| \leq ||x - A_\alpha^\dagger y|| + ||A_\alpha^\dagger (y - y^\delta)||$$

2.3 Tikhonov Regularization Revisited

Above we defined everything in terms of SVD. But there is a variational formulation of Tikhonov regularization that turns solving for x into an optimization problem.

Definition 2.10. *Let $\lambda > 0$ be a a fixed constant. The Tikhonov regularized solution x_λ to (3) $x_\lambda \in \mathcal{X}$ is the minimum of the the functional*

$$\mathcal{R}_\lambda(x) = ||Ax - y||^2 + \lambda||x||^2 \tag{10}$$

assuming that such a minimizer exists. $\mathcal{R}_\lambda(x) : \mathcal{X} \to \mathcal{Y}$ and λ is called the regularization parameter.

Estimating $\bar{x}$ is now an optimization problem, where we want to minimize $\mathcal{R}_\lambda(x)$ for some fixed λ. We get the following scheme

1. Minimize: $(||Ax - y||_2^2 + \lambda||Lx||)$.
2. The solution is $x_\lambda = (A^*A + \lambda L^*L)^{-1}A^*y$. Note that if there is no noise in the model, we need no regularization. So then, we should recover the least-squares solution.

We will denote the functional $||Ax-y||_2^2+\lambda||Lx||$ by $\mathcal{J}(x)$, which consist of two portions, the data fidelity term $||Ax - y||_2^2$, and the regularization term $||x||_2^2$. We can check that the problem of minimizing $\mathcal{R}_\lambda(x)$ for a given λ is well-posed problem, by checking that

1. For fixed λ, $\mathcal{R}_\lambda(x)$ is well defined
2. For fixed λ, $\mathcal{R}_\lambda(x)$ is continuous in $\mathcal{Y}$.
3. We can select λ such that if $y \to A(\bar{x})$, then $\mathcal{R}_\lambda(x) \to \bar{x}$.

In this setting, we can check well-posedness by looking at the SVD of the regularized solution. We can find the solution to the minimization problem by writing down the normal equation. We get that

$$x_\alpha = (A^*A + \alpha L)^{-1}A^*y = V(\Sigma_r^2 + \alpha L)^{-1}\Sigma_U^* y \tag{11}$$

If the regularization guarantees stability, and $ker\ A \cap ker\ L = \{0\}$, then (13) is a well-posed problem. The estimate x_e^λ, depends on fixed λ, so we need some method to choose λ such that the solution to the optimization problem is continuous (condition 3 in the above). Common methods to choose λ are the following which we define below,

1. a-prior rules knowing the noise level
2. Discrepancy principle
3. L-curve

4. Cross validation [2]

Definition 2.11. *Assume we know the noise level, and denote the noise level by e. We can then a-prior choose $\alpha(e)$, the regularization parameter now depending on e. This is called an a-prior rule. This is called convergent if and only if*

$$\lim_{e\to 0} \alpha(e) = 0$$
$$\lim_{e\to 0} e||A^{\dagger}_{\alpha(e)}|| = 0$$

Claim 2.2. *If the $\alpha(e)$ as defined above is convergent then the total error $||A^{\dagger}y_e A^{\dagger}y||_2^2 \to 0$ as $e \to 0$. So we have consistency.*

Definition 2.12. *The discrepancy principle chooses α a-posterior depending on both y_e and e, such that*

$$||AA^{\dagger}y_e - y_e||_2^2 \leq \eta e$$

for $\eta > 1$ fixed. If $y_e \in ker(A^{\dagger})$ then no such α can exist.

Definition 2.13. *The L-curve method chooses α heuristically via a minimization problem*

$$\min_{\alpha>0} ||A^{\dagger}_{\alpha}||_2^2 ||AA^{\dagger}_{\alpha}y_e - y_e||_2^2$$

the optimal α should lie at the corner of the curve $||A^{\dagger}_{\alpha}||_2^2||AA^{\dagger}_{\alpha}y_e - y_e||_2^2$. We do not have consistency with this choice of α.

So far we have seen a a-priori rule, a-posterior rule, and a heuristic rule, but we now introduce data driven method using the bayesian framework for inverse problems. We want that as $\sigma \to 0$ $\lambda \to 0$, so $\hat{x}$ converges to x_{LS} should it exist.

Finally we remark that

$$\mathcal{R}_{\lambda}(x) = ||Ax - y||^2 + \lambda||x||^2 \tag{12}$$

for $\lambda \in (0, \infty)$ can be written as

$$\mathcal{R}_{\lambda}(x) = (1-\lambda)||Ax - y||^2 + \lambda||x||^2 \tag{13}$$

for $\lambda \in (0, 1)$ [14]. Here we see that that regularization parameter can be seen as balancing the data fit versus smoothing in the case that we penalize the second derivative of x. When $\lambda = 0$ we get interpolation of the data points, and when $\lambda = 1$ we get over-smoothing. In the rest of this thesis we explicitly define how to choose λ from the data using a Bayesian framework for inverse problems.

[2] An example of choosing the regularization parameter in ridge regression can be found in [14]

3 Statistics and Probability

Below we review some measure theoretic probability facts and definitions that are necessary for defining Bayes formula for inverse problems. In the second chapter, we recap the definitions of certain distributions as characterized by their probability density functions. We also review some algebra rules for multivariate normally distributed vectors.

3.1 Probability Theory

Recall that a probability space consists of a sample space Ω, a $\sigma-$algebra $\mathcal{F}$, and a probability measure $\mathbb{P}$. In this thesis we consider only $\sigma-$finite measures. So, measures that are countable unions of finite measure measurable sets. Particularly we use the $\sigma-$ finite Lebesgue measure on $\mathbb{R}^n$. We denote a measurable space as $(X, \mathcal{B}(X))$ where X is some (metric) space and $\mathcal{B}(X)$ is the borel $\sigma-$algebra. In the case that $X = \mathbb{R}$ we know that $\mathcal{B}(X)$ is generated by the open intervals $(a, b]$ for $a, b \in \mathbb{R}$. We can extend this to $\mathbb{R}^n$. Also recall that the random variable,f, is a measurable map $f : \Sigma \to X$ and induces a probability measure X.

Definition 3.1. *Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and $(X, \mathcal{B}(X))$ a measurable space. Then the measure μ induced by the random variable $f : \Omega \to X$ is defined as*

$$\mu(A) = \mathbb{P}(f^{-1}(A)) = \{\omega \in \Omega \mid f(\omega) \in A\}, A \in \mathcal{B}(X)$$

where μ is the distribution f. We denote this as $f \sim \mu$.

Definition 3.2. *Let μ and ν be measures on a measure space (x, Σ). Then we have the following*

1. *If $\nu(A) = 0 \implies \mu(A) = 0$ for all $A \in \Sigma$, then μ is dominated by ν and we say that μ is absolutely continuous with respect to ν. We denote this as $\mu \ll \nu$*
2. *If $\mu \ll \nu$ and $\nu \ll \mu$ then μ and ν are equivalent.*
3. *Let A and $B \in \mathcal{B}(X)$ be disjoint sets such that $A \cup B = \mathcal{B}(X)$ and $\mu(A) = 0$ while $\nu(B) = 0$, then μ and ν are mutually singular. We denote this as $\mu \perp \nu$.*

We will now state the Radon–Nikodym theorem which we can use to relate random variables to their probability density functions, as well as proving that the conditional posterior distribution is a solution to the Bayesian inverse problem when Bayes rule holds.

Theorem 3.1. *Let (X, Σ) be a measurable space. Then let μ and ν be $\sigma-$finite measures defined on this space. Suppose also that $\nu \ll \mu$. Then there exists a*

unique up to a $\mu-$null set Σ measurable function $f : X \to [0, \infty)$ such that for all $A \subset X$,

$$\nu(A) = \int_A f d\mu$$

We call f the Radon–Nikodym derivative and denote it as $\frac{d\nu}{d\mu}$.

In the case that the measure space is $(\mathbb{R}^n, \mathcal{B}(\mathbb{R}^n))$ for some finite n, and $X \sim \nu$ and $\mu = leb(\cdot)$, then by the Radon–Nikodym theorem, $f \in \mathcal{L}^1(\mathbb{R}^n)$ is the unique probability density function for $X \sim \nu$.

What follows is a few definitions to define conditional distributions. With these we can precisely write down the posterior distribution as a conditional distribution.

Definition 3.3. *Let $\mathcal{G} \subset \mathcal{F}$ be a sub$-\sigma-$algebra. Let y be a $\mathcal{G}$ measurable function. We call $y : \Omega \to X$ a conditional expectation of a random variable $f : \Omega \to X$ with respect to $\mathcal{G}$ if*

$$\int_{\mathcal{G}} f d\mathbb{P} = \int_{\mathcal{G}} y d\mathbb{P}$$

Definition 3.4. *Let $\mathcal{G} \subset \mathcal{F}$ be a sub$-\sigma-$algebra. The condition probability of $B \in \mathcal{B}(X)$, given $\mathcal{G}$ is*

$$\mathbb{P}(B \mid \mathcal{G}) = \mathbb{E}(1_B \mid \mathcal{G})$$

Definition 3.5. *Let $(\mu(\cdot, \omega))_{\omega \in \Omega}$ be a family of probability distributions on $(X, \mathcal{B}(X))$. Then $(\mu(\cdot, \omega))_{\omega \in \Omega}$ is a regular conditional distribution of f given $\mathcal{G} \subset \mathcal{F}$ if*

$$\mu(B, \cdot) = \mathbb{E}(1_B(f) \mid \mathcal{G}) \ a.s.$$

for all $B \in \mathcal{B}(X)$. If f is defined as above then such a regular conditional distribution exists.

Remark 3.1. *Let $\mathcal{G} = \sigma(y)$ be the sub-$\sigma-$algebra generated by the observations $y = AX + e$ in the Bayesian setting. If we let π_{post} denote the posterior distribution and π_{prior} denote the prior distribution on x, then we have that*

$$\pi_{post}(B, y(\omega) = \mathbb{E}(1_B(x) \mid \sigma(y))(\omega)$$

for $B \in \mathcal{B}(X)$. So then

$$\pi_{post}(B, y) = \pi_{prior}(B \mid y).$$

3.2 A Few Statistical Definitions

We denote random variables by capital letters. For example X, Y, E. Denote realization of these random variables by the corresponding lower case letter for example $Y = y$, y is one realization of Y.

Definition 3.6. *A random variable $X \sim \mathcal{N}(\mu, \sigma^2)$ is normally distributed if its probability density function is give by*

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(x-\mu)^2/\sigma^2} \tag{14}$$

for $\mu \in \mathbb{R}$ and $\sigma > 0$.

Now let $\mu \in \mathbb{R}^n$ and $\Sigma \in \mathbb{R}^{n\times n}$ a non-negative symmetric matrix. Then we can define $X \sim \mathcal{N}(\mu, \Sigma)$ for X a $n-$ dimensional random vector.

Definition 3.7. *A random vector $X \sim \mathcal{N}(\mu, \Sigma)$ if and only if its probability density function is given by*

$$f_X(x) = \frac{1}{(2\pi)^{n/2}\sqrt{|\Sigma|}} e^{-\frac{1}{2}}(x-\mu)^T\Sigma^T(x-\mu) \tag{15}$$

for parameters $\mu \in \mathbb{R}^n$ and $\Sigma \in \mathbb{R}^{n\times n}$ symmetric positive definite matrix, and $|\Sigma|$ is the determinate of Σ. See [12].

Theorem 3.2. *If $c \in \mathbb{R}^n$ and X is an $n-$dimensional random vector such that $X \sim \mathcal{N}(\mu, \Sigma)$. Then $c + X \sim \mathcal{N}(c + \mu, \sigma)$.*

Theorem 3.3. *If X is an $n-$dimensional random vector such that $X \sim \mathcal{N}(\mu, \Sigma)$, and $A \in \mathbb{R}^{m\times n}$ a fixed matrix with rank $m \leq n$, then $AX \sim \mathcal{N}(A\mu, A\Sigma A^T)$ is an m dimensional normally distributed random vector with mean $A\mu$ and covariance $A\Sigma A^T$.*

Remark 3.2. *If $X \sim \mathcal{N}(\mu, \Sigma)$ is an $n-$dimensional random vector such that each X_i is independent from X_j for $i \neq j$, then Σ is a diagonal matrix with the variance of each X_i on the diagonal.*

Definition 3.8. *Let $\alpha > 0$, the the Gamma function $\Gamma(\alpha) = \int_0^\infty y^{\alpha-1}e^{-y}dy$. A random variable X is Gamma distributed with parameters $\alpha, \beta > 0$ if the pdf is characterized by*

$$f_X(x) = \frac{1}{\beta^\alpha\Gamma(\alpha)} x^{\alpha-1}e^{-x/\beta}, x > 0.$$

We denote this as $X \sim Gamma(\alpha, \beta)$. [13]

We can extend this definition to a random symmetric matrix X of dimension $p \times p$. In which case we have the Wishart distribution.

Definition 3.9. *Let M be a $p \times p$ positive definite matrix. Then the multivariate Gamma function Γ_p for a given α is define as*

$$\Gamma_p(M) = \pi^{p(p-1)/4} \prod_{j=1}^{p} \Gamma\left(\frac{n}{2} - \frac{j-1}{2}\right)$$

here $|M|$ is the determinant of M and $tr(M)$ is the trace. For X a random vector then, X is Gamma distributed if the pdf is characterized by

$$f_X(x) = \frac{|x|^{(n-p-1)/2} e^{-tr(M^{-1}x)/2}}{2^{\frac{np}{2}} |M|^{n/2} \Gamma_p(\frac{n}{2})}$$

where $n > p - 1$ is the degrees of freedom.

4 Statistical Inverse Problems

In this chapter we introduce statistical inverse problems, derive Bayes formula in this setting, give a few classical examples, and show the connection to the functional analytic inverse problems. We will now consider y, x, e to be random variables and A some fixed operator. The model (2) can then rewritten as

$$Y = A(X, E) \tag{16}$$

where X, Y, E are random vectors defined on the probability space $\Omega = \Omega_1 \times \Omega_2$ such that $X : \Omega_1 \to \mathbb{R}^m$, and $Y : \Omega_2 \to \mathbb{R}^n$. We want to learn the relationship between X, Y, E, that is, determine their conditional probability distributions. We can relate X to Y after making observations of Y using Bayes formula. First note again some notation. As in the non-random case, Y is the observed data, with $Y = y$ the realization of Y. The unknown parameter is X, where $X = x$ is the realization of X, and E models the noise. We will now consider this noise to be additive and Y, X, E to be random vectors in $\mathbb{R}^n, \mathbb{R}^m$ and $\mathbb{R}^n$ respectively. We then rewrite (16) as

$$Y = AX + E \tag{17}$$

The solution to the above problem is a conditional posterior distribution for X given $Y = y$. Two things are gained from posing the inverse problem in the Bayesian setting. We can obtain point estimates by computing the most likely value for X which we will see later connects the statistical inverse problem to the Tikhonov regularized one in Chapter 2. Furthermore, we can compute the uncertainty of this estimate by calculating the spread of the posterior distribution.

4.1 Bayes Formula

A key aspect of Bayesian statistics is that we formally include prior knowledge or assumptions of the parameters into the model. In this setting, what we can observe are realizations of Y, and what we assume is that we have prior assumptions for X. Mainly, which values of X are occurring and at what frequency. To formally model this prior assumption, we place a prior distribution on X. We denote this by F_X with density π_X. We also assume that $E \sim F_E$ with density π_E and that E is independent of X. We will see later that independence is important. With these assumption we can find the likelihood $Y \mid X$ for $X = x$.

Claim 4.1. *The likelihood* $L(Y = y \mid X = x) = \pi_E(y - Ax)$.

Proof. [8] Since we assume that $X \perp E$, the distribution of E conditioned on $X = x$ is unaffected. That is

$$\mu_E(B \mid x) = \mathbb{P}(E \in B) = \int_B \pi_E(e)de$$

where $B \in \mathcal{B}(\mathbb{R}^n)$. If we condition Y on $X = x$, then $Y = A(X) + E$ is distributed like E, with shift $A(x)$. □

Lemma 4.1. *$(X, Y) \in \mathbb{R}^m \times \mathbb{R}^n$ is a random variable with Lebesgue density $\pi(x, y) = \pi_E(y - Ax)\pi_X(x)$*

We now formulate Bayes theorem which tells us how X is depending on Y.

Theorem 4.1 (Bayes Formula)**.** *Assume that the $m(y) = \int_{\mathbb{R}}^n \pi_E(y-Ax)\pi_X(x)dx > 0$. This is called the normalizing constant. Then $Y = y \mid X = x$ is a random variable with Lebesgue density*

$$\pi(x, y) \overset{(rem3.1)}{=} \pi_X(x \mid y) = \frac{1}{m(y)}\pi_E(y - Ax)\pi_X(x)$$

Definition 4.1. *Recall that $\pi_E(y - Ax)$ is the likelihood of $Y = y$ given $X = x$. Let $\phi(y; x) = -log(\pi_E(y - Ax))$. Then $\phi(y; x)$ is called the potential function. note that this is the negative log-likelihood.*

Remark 4.1. *Let Π and Π^X be measures on $\mathbb{R}^m$ with densities π and π_X respectively. Then from the above theorem we have*

$$\frac{d\Pi^X}{d\Pi}(x) = \frac{1}{m(y)} exp\left(-\phi(x; y)\right)$$
$$m(y) = \int_{\mathbb{R}}^m exp\left(-\phi(x; y)\right) d\Pi(x)$$

so we can reformulate Bayes theorem as

$$\frac{1}{\pi_X}(x)\pi_E(y - Ax)(x \mid y) = \frac{1}{m(y)}\pi_X(y \mid x)$$

The result is that the posterior distribution is absolutely continuous with respect to the prior, and the Radon-Nikodym derivative is proportional to the likelihood.

We now have a formula to find the conditional probability for $X = x$ given our measurements $Y = y$. We saw that the conditional posterior distribution is a product of the likelihood and the prior on X.

Remark 4.2. *So far we have formulated the Radon-Nikodym theorem with respect the finite dimensional case. But using the formulation in remark (4.1), we can generalize Bayes theorem to the infinite dimensional case using a Gaussian measure. We will not cover this in this thesis as we are interested in the finite discrete setting. To see the exact details we refer the reader to [11][2].*

Before we move further, we go through two classical examples [3].

Example 4.1. *Let $x \in \mathbb{R}$, $y \in \mathbb{R}^n$ for $n \geq 1$, and let $A \in \mathbb{R}^n - \{0\}$. Define the observations as*

$$y = Ax + e$$

[3] These examples are found in many sources but we refer to [11].

where $e \sim \mathcal{N}(0, \delta^2 I)$. By Bayes theorem the conditional posterior distributing is then

$$\pi(x \mid y) \propto exp\left(-\frac{1}{\delta^2}||Ax - y||_2^2 - \frac{1}{2}|x|^2\right)$$

The posterior is Normal and is completely characterized by its mean and covariance. The inner equation of exponential is quadratic. We can complete the square and compute the mean and variance, μ and Σ^2 as

$$\mu = \frac{\langle A, y\rangle}{\delta^2 + ||A||_2^2} \qquad and\ \Sigma^2 = \frac{\delta^2}{\delta^2 + ||A||^2}$$

We propose that as $\delta \to 0$, μ will converge to $\frac{\langle A,y\rangle}{||A||_2^2}$ (consistency) and that the covariance will converge to 0 (convergence). Indeed by the definition of μ and Σ we can easily see that as $\delta \to 0$, we have convergence and consistency.

Example 4.2. *Let $x \in \mathbb{R}^n$ with $n \geq 2$, and let $y \in \mathbb{R}$. Let $A \in \mathbb{R}^n - \{0\}$. Again the observations are*

$$y = Ax + e$$

where $e \sim \mathcal{N}(0, \delta^2 I)$. Assume that $x \sim \mathcal{N}(0, \Delta^2 I)$ By Bayes theorem the conditional posterior distributing is then

$$\pi(x \mid y) \propto exp\left(-\frac{1}{\delta^2}|\langle A, y\rangle - y|^2 - \frac{1}{2}\langle x, \Delta^{-1}x\rangle\right)$$

Again by completing the square we have that

$$\mu = \frac{x\Delta A}{\delta^2 + \langle A, \Delta A\rangle} \qquad and\ \Sigma^2 = \Delta - \frac{(\Delta A)(\Delta A)^*}{\delta^2 + \langle A, \Delta A\rangle}$$

Then again we check what happens when the noise level goes to zero.

$$\lim_{\delta\to 0}\mu = \frac{x\Delta A}{\langle A, \Delta A\rangle} \qquad and\ \lim_{\delta\to 0}\Sigma^2 = \Delta - \frac{(\Delta A)(\Delta A)^*}{\langle A, \Delta A\rangle}$$

Then the $\langle \mu, A\rangle = \bar{x}$, the ground truth, and $\Sigma^2 A = 0$. So as $\delta \to 0$, uncertainty about $\hat{x}$ goes to zero in the direction of A. There is uncertainty in the directions not aligned with A. So in the underdetermined case the prior plays a role even as noise the goes to zero. In the overdetermined case, the prior plays no role as the noise goes to zero.

It is now natural to ask what is the definition of well-posedness in the statistical setting. The solution is no longer a point estimator, but rather an entire distribution. Roughly, well-posedness is the same definition we saw in the functional analytic case. We can still check if the solution exists, if it is unique, and if it is stable. While this is interesting area of research, it is beyond the scope of this thesis, but has been studied in papers [11][1].

The solution to the statistical inverse problem is a conditional distribution. We would now like to analyze this distribution. Already if $n > 2$ we cannot graph the posterior distribution. Common methods to explore the (higher dimensional) posterior distribution are either computing point estimators such as those defined below, or by MCMC sampling methods such as Gibs Sampling. In the finite dimensional functional analytic setting the solution was a vector, and we can produce such an estimate by computing point estimators of the resulting posterior distribution.

Definition 4.2. *The maximum a posterior estimator of x is found by maximizing the posterior distribution if the maximum exists. That is*

$$x_{MAP} = \max_{\mathbb{R}^m} \pi(x \mid y) \tag{18}$$

The computation of this point estimator is an optimization problem. Another point estimator is the conditional mean estimator defined as

Definition 4.3. *The conditional mean estimator of x given y is*

$$x_{CM} = \mathbb{E}(x \mid y) = \int_{R^m} x \ \pi_X(x \mid y) dx$$

The computation of this point estimator is an integration problem, which can be very difficult in high dimensional settings. When the posterior distribution is symmetric and unimodal, the MAP estimate and the conditional mean estimate are equivalent.

We can also compute spread estimators by computing Bayesian Credible sets. These are defined as follows:

Definition 4.4. *Let $\alpha \in (0, 1)$, then a $1 - \alpha$ level credible set C_α is given by*

$$\Pi(C_\alpha \mid y) = \int_{C_\alpha} \pi_X(x \mid y) dx = 1 - \alpha$$

The computation of this is a root finding problem.

4.2 Connection to Tikhonov Regularization

Now that we have seen some examples, we will explain under which conditions we can return to the Tikhonov regularization. We will consider the independent Gaussian noise model with a normal prior. Suppose that we model the noise E as additive Gaussian noise with each e_i i.i.d and independent of X. Suppose also that we assume X is Gaussian, and that X is smooth. We formally write this as

$$E \sim \mathcal{N}(0, \alpha I) \tag{19}$$
$$X \sim \mathcal{N}(0, \beta \Sigma) \tag{20}$$

for fixed α, β, Σ. Note that here α, β are precision parameters. Using Bayes formula we find that posterior distribution of $X = x \mid Y = y$ to be proportional to

$$\pi(x, \alpha, \beta) \propto \alpha/2||Ax - y||^2 - \beta/2||Lx||^2 + m/2log(\alpha) + n/2log(\beta) \tag{21}$$

where $ker(A) \cap ker(L) = \{0\}$, $rank(L) = m$, and the potential, which is the negative log-likelihood, is

$$\mathcal{J}(x, \alpha, \beta)) = \alpha/2||Ax - y||^2 + \beta/2||Lx||^2 - m/2log(\alpha) - n/2log(\beta) \tag{22}$$

The resulting posterior distribution x is Gaussian with mean μ and variance Σ. A Gaussian distribution is completely characterized by its mean and variance. For these parameters we compute the MAP estimate of $\pi(x \mid \alpha, \beta)$. We have that

$$\mu = (\alpha A^* A + \beta L^* L)^{-1} \alpha A^* y \tag{23}$$

$$\Sigma = (\alpha A^* A + \beta L^* L)^{-1} \tag{24}$$

We can further write

$$\mu = (A^* A + \beta/\alpha L^* L)^{-1} \alpha A^* y \tag{25}$$

$$\tag{26}$$

We see that $\mu = \hat{x}_\lambda$ in (11) where, from the above formulation of μ, we see that the regularization parameter λ is equal to β/α. The computation of λ thus requires estimating the precision parameters. To find the MAP estimates we compute the minimum of the potential function. We can now easily see that computing the MAP estimate is equivalent to computing the Tikhonov solution given by

$$\min_x \ ||Ax - y||^2 + \beta/\alpha||Lx||^2 - m/2log(\alpha) - n/2log(\beta) \tag{27}$$

5 Bayesian Regularization

In the previous chapter, we have seen that in the independent additive Gaussian noise model computing the MAP estimate is equivalent to computing the Tikhonov regularized solution. We can find the MAP estimate by minimizing the objective function $J(x, \alpha, \beta)$ over all parameters. The result is that we find estimates for the underlying ground truth $\bar{x}$, while simultaneously estimating the precision parameters α, β of the noise and of $\bar{x}$ respectively.

5.1 Empirical Bayesian Method

Our first proposed method is an empirical Bayesian method that would allow us to determine α and β. The parameters of the priors are not set a-priori, but are thus estimated from data. To do this we minimize the objective function over all three parameters. Let $A, L \in \mathbb{R}^{n \times m}$, such that $ker(A) \cap ker(L) = \{0\}$. Suppose also that $Rank(L) = m$, then

$$(x_{MAP}, \alpha_{MAP}, \beta_{MAP}) = \min_{x,\alpha,\beta} \mathcal{J}(x, \alpha, \beta) \tag{28}$$

$$= \min_{x,\alpha,\beta} \alpha/2||Ax - y||^2 + \beta/2||Lx||^2 - m/2log(\alpha) - n/2log(\beta) \tag{29}$$

We model the noise as Gaussian with mean zero. We call the noise level the variance of the noise, which we will sometimes denote by σ^2. As the mean is zero if $\sigma^2 \to 0$, then there is no noise in the model. We say that the noise level goes to zero. We propose that

$$(1)\ \mathbb{E}||A\widehat{x}(\widehat{\alpha}, \widehat{\beta}) - y||_2^2 = n\sigma^2 \qquad (2)\ \lim_{\sigma^2 \to 0} \beta/\alpha \to 0 \tag{30}$$

If (1) holds, then we can consistently estimate the noise level as the noise level converges to zero. If (2) holds then as the noise level converges to zero, the regularization converges to zero, and the estimate for x converges to the least squares estimate.

5.2 Well-posedness, Consistency, and Convergence

We will now show that the empirical Bayesian method is not well-posed.

Claim 5.1. *The empirical Bayesian method is ill-posed. Moreover (1) and (2) do not hold in general.*

Proof. We want to find

$$(\widehat{x}, \widehat{\alpha}, \widehat{\beta}) = \min_{x,\alpha,\beta} \alpha/2||Ax - y||^2 + \beta/2||Lx||^2 - m/2log(\alpha) - n/2log(\beta)$$

Suppose that A is invertible and ill-conditioned. Recall that $y = Ax + e$. Then $||A\widehat{x} - y|| = 0$, and minimizing $\mathcal{J}$ happens when $\alpha \to \infty$ and $\beta \to 0$. Recall

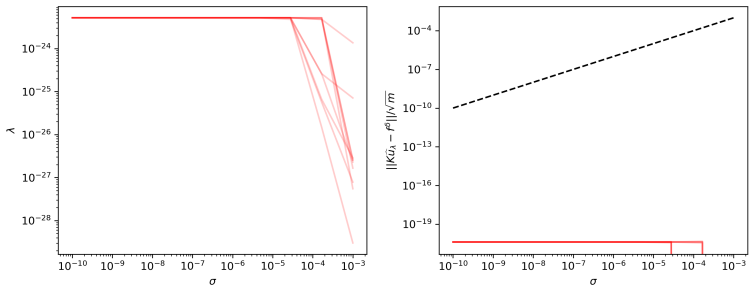


Figure 1: Here we plot the convergence and consistency of Empirical Bayesian method for each $\sigma \in [1e{-}10, 1e{-}3]$. On the left hand side, we plot regularization parameter found given σ. We want to see that as the noise level decrease, the regularization decreases with it. We see however that this is not the case. On the right hand side we plot the residuals versus the noise level. The dashed line represents $||Ax - y||_2^2 = n\sigma^2$. However, we see this is not the case, as the red lines are very far off.We repeat the two simulation above, ten times, and plot the results. The results are represented by the red lines.

that $\lambda = \beta/\alpha$. If $\alpha \to \infty$, and $\beta \to 0$, no regularization occurs as $\lambda \to 0$. The bias goes to zero, but the variance is high. If $\beta \to 0$ then $\widehat{x}$ goes to the zero vector. So the method is not well-posed exactly when $A^{-1}x = y$. □

Example 5.1. *Let $A = I_n$ the identity matrix. This is invertible. Let*

$$y = Asin(x) + e$$

for $x \in [-4\pi, 4\pi]$, $e \sim \mathcal{N}(0, \sigma^2)$. We want that

$$\lim_{\sigma \to 0} \beta/\alpha = 0$$
$$\mathbb{E}||Ax - y||_2^2 = n\sigma^2$$

We expect however that $\beta/\alpha = \lambda \to 0$ regardless of the σ.

We see that this is indeed the case in Figure (1). The problem is then that the minimum occurs at the extreme values for α, β, which we have seen results in ill-posedness.

5.3 Hierarchical Bayesian Method

We have seen that the empirical Bayesian method of regularization is not a well-posed problem. Failure occurred exactly when A is invertible, leading to the solution $A^{-1}y = \hat{x}$, so that $\alpha \to \infty$ and $\beta \to 0$. It did not hold in general, that if the noise level went to zero, the regularization went to zero at the same rate. The estimate for residuals was not always consistent. In [7] they prose that to turn the empirical Bayesian method into a well-posed problem, we need to place

hyper-priors on the precision parameters α and β. Since we assume a Gaussian prior on X and E the natural (conjugate) hyper-priors are Gamma distributions. The resulting functional is called the augmented Tikhonov functional. In [7], Jin and Zou prove that at least one minimum exists, and that the augmented Tikhonov functional converges monotonically to a minimum.

We now reconstruct the augmented Tikhonov functional. Suppose we place the following hyper priors on the precision parameters

$$\alpha \sim Gamma(a_0, b_0) \tag{31}$$
$$\beta \sim Gamma(a_1, b_1) \tag{32}$$

Then the posterior becomes

$$p(x, \alpha, \beta \mid y) \propto \rho(Ax - y \mid \alpha) \times \pi(\alpha)\pi(x \mid \beta) \times \pi(\beta) \tag{33}$$
$$\propto \alpha^{n/2} e^{-\alpha/2||Ax-y||^2} \alpha^{a_0-1} e^{-b_0\alpha} \beta^{n/2} e^{-\beta/2||Lx||^2} \beta^{a_1-1} e^{-b_1\beta} \tag{34}$$

The resulting potential function i.e. the augmented Tikhonov functional is

$$\mathcal{J}(x, \alpha, \beta) = \alpha/2||Ax - y||^2 - (n/2 + a_0 - 1)log(\alpha) + b_0\alpha + \beta/2||Lx||^2 - (n/2 + a_1 - 1)log(\beta) + b_1\beta$$

The resulting minimization problem is

$$\min_{x,\alpha,\beta} \mathcal{J}(x, \alpha, \beta) = \alpha/2||Ax - y||^2 - (n/2 + a_0 - 1)log(\alpha) + b_0\alpha + \beta/2||Lx||^2 - (n/2 + a_1 - 1)log(\beta) + b_1\beta$$

Notice that if we let $a_0, a_1 = 1$ and $b_0, b_1 \to 0$ then we recover the objective function given no hyper-priors.

5.4 Well-posedness, Consistency, and Convergence

In the paper by Jin and Zou [7], they prove that the hierarchical Bayesian method, is well-posed. They also prove that the method can estimate the noise level and that as the noise level goes to zero, the method converges to the minimum norm solution.

We now state two main lemmas (Lemma 2.2 and 2.6 in [7]) and one main theorem (Theorem 2.3 in [7]). Together Lemma 5.1 and Theorem 5.1 prove conditions (1) and (2) in (30). We refer the reader to the paper for the proofs.

We first set some notation from the paper. Let $\lambda = \beta/\alpha$. Recall that $E \sim \mathcal{N}(0, \alpha I)$, where α was the precision parameter. Let σ_0^2 be the true variance of E. We have that

$$\alpha_\lambda = \frac{(n/2 + a_0 - 1)}{1/2||Ax(\lambda) - y||^2 + b_0}$$

and that $\frac{1}{\alpha_\lambda}$ is the estimate for σ_0^2. Denote the estimate of σ_0^2 as $\sigma^2(\lambda) := \frac{1}{\alpha_\lambda}$ so then

$$\sigma^2(\lambda) = \frac{||Ax(\lambda) - y||^2 + 2b_0}{n + 2a_0 - 2}$$

Now let $A \in \mathbb{R}^{n\times m}$, $L \in \mathbb{R}^{p\times m}$, where $m \gg n \gg p$. Then the generalized singular value decomposition of the matrix pair (A, L) can be written as

$$A = U \begin{pmatrix} \Sigma & 0 \\ 0 & I_{n-p} \end{pmatrix} X^{-1}, \qquad L = V(M0_{p\times(n-p)})X^{-1} \tag{35}$$

where $U \in \mathbb{R}^{m\times n}, V \in \mathbb{R}^{p\times p}, X \in \mathbb{R}^{n\times n}$, are orthogonal matrices. $\Sigma \in \mathbb{R}^{n\times n}, M \in \mathbb{R}^{p\times p}$ are rectangular diagonal matrices with non-negative entries. The diagonal entries of Σ, denoted by σ_i are the singular values of A, and are listed in ascending order. The diagonal entries of M, denoted by μ_i are listed in descending order. We also define $\gamma_i = \sigma_i/\mu_i$, where σ_i, and μ_i are as above. We call γ_i the generalized singular values of (A, L). Furthermore, we normalize σ_i and μ_i such that $\sigma_i^2 + \mu_i^2 = 1$.

Lemma 5.1. *Denote the Fourier coefficients of $\bar{x}$, the ground truth parameter, by $\bar{f}_i = \langle u_i, \bar{x}\rangle$ for $i \in \{1, ..., n\}$. Then we have that*

$$\mathbb{E}||A\hat{x}_\lambda - x||^2 = \sum_{i=1}^{p} \frac{\lambda^2 \bar{f}_i}{(\lambda + \gamma_i^2)^2} + ||P_U^\perp \bar{x}||^2 + \left[(m-n)\sum_{i=1}^{p} \frac{\lambda^2}{\lambda + \gamma_i^2}\right]\sigma_0^2$$

where $P_U^\perp = I_m - UU^*$, is the orthogonal projection onto the complement of U.

It is also shown in the paper by Jin and Zou, that estimate $\sigma^2(\lambda)$ is "relatively independent of the regularisation parameter [...] and of order σ_0^2" ([7] p. 9). We denote this by $c_E\sigma_0^2$.

Lemma 5.2. *Assume that η is a random vector such that $|\eta_i| \le c_E\sigma_0^2$ for $i \in \{1, ..., n\}$. Then there exist two constants $c_{r,0}$ and $c_{r,1}$ depending on $n/2 + a_1 - 1$ such that*

$$c_{r,0}\sigma_0^2 \le \lambda^* \le c_{r,1}\sigma_0^2$$

where $\lambda^* = \beta^*/\alpha^*$, and (x^*, α^*, β^*) is a minimum of $\mathcal{J}$.

Theorem 5.1. *Let σ_0^2 denote the variance. Assume that the random variable η_i is such that $|\eta_i| \le c_E\sigma_0^2$ for $i = 1, ..., n$. Fix b_1 and let $\frac{n}{2} + a_1 - 1 \sim \sigma_0^d$ for $0 < d < 2$. Then*

$$\lim_{\sigma_0^2 \to 0} ||\hat{x}_\lambda - x_{LS}||_2^2 = 0$$

that is, as the variance goes to zero, the regularization should also go to zero.

The key tool of the proofs of the Lemma 5.1 and the Theorem 5.1 is writing out $\hat{x}_\lambda$ and x_{LS} as a summation using the generalized singular value decomposition. In the case where $L = I$, we can replace the equations in (35) by the singular value decomposition from (9) and (7) respectively.

6 Numerical Methods

In this chapter we propose three different iterative methods to numerically find $\min_{x,\alpha,\beta} \mathcal{J}(x,\alpha,\beta)$. We begin by computing the partial derivatives which are given below

$$\partial/\partial x(J(x,\alpha,\beta)) = (A^*A + \beta/\alpha L^*L)x - A^*y \tag{36}$$

$$\partial/\partial \alpha J(x,\alpha,\beta) = 1/2||Ax-y||^2 - (n/2 + a_0 - 1)/\alpha + b_0 \tag{37}$$

$$\partial/\partial \beta J(x,\alpha,\beta) = 1/2||Lx||^2 - (n/2 + a_1 - 1)/\beta + b_1 \tag{38}$$

By setting the partial derivatives to zero, we define a set of normal equations. The optimal solutions are the roots of the of the normal equations, which we compute below

$$x = (A^*A + \beta/\alpha L^*L)^{-1}A^*y \tag{39}$$

$$\alpha = \frac{(n/2 + a_0 - 1)}{1/2||Ax-y||^2 + b_0} \tag{40}$$

$$\beta = \frac{(n/2 + a_1 - 1)}{1/2||Lx||^2 + b_1} \tag{41}$$

As our function is only bi-convex, we cannot simply implement coordinate descent over all three parameters, x, α, β. We can still implement a similar algorithm to coordinate descent by splitting $\mathcal{J}$ into the two strictly convex parts, and do an alternating minimization. This method was proposed by ([7]). Below we rederive it.

6.1 Method 1: Alternating Algorithm in the Case of Closed Form Solutions

In this method the estimates are found by simultaneously minimizing over all three parameters. We want to find

$$\min_{x,\alpha,\beta} \mathcal{J}(x,\alpha,\beta) \tag{42}$$

This is done by an alternating method, where at each iteration we define either a normal equation for x or a normal equation for α, β. The next best guess for x, respectively α, β is then the root of the normal equation. Recall that these roots are the optimal solutions (41) to the partial derivatives. So the estimates are given by

$$x(\beta/\alpha) = (A^*A + \beta/\alpha L^*L)^{-1}A^*y$$

$$\alpha(x) = \frac{(n/2 + a_0 - 1)}{1/2||Ax-y||^2 + b_0}$$

$$\beta(x) = \frac{(n/2 + a_1 - 1)}{1/2||Lx||^2 + b_1}$$

For fixed a_0, b_0, a_1, b_1, these define closed form solutions for x, α, β. Suppose, then, that we start with some initial values α_0, β_0. Then using the optimal solution for x, we can define an estimate

$$\begin{aligned} x_0 &= x(\beta_0/\alpha_0) \\ &= (A^*A + \beta_0/\alpha_0 L^*L)^{-1} A^*y \end{aligned}$$

Notice that this is the normal Tikhonov regularized solution with regularization parameter β_0/α_0. To find the next estimates for α, β we compute

$$\begin{aligned} \alpha_1 &= \alpha(x_0) \\ &= \frac{(n/2 + a_0 - 1)}{1/2||Ax_0 - y||^2 + b_0} \\ \beta_1 &= \beta(x_0) \\ &= \frac{(n/2 + a_1 - 1)}{1/2||Lx_0||^2 + b_1} \end{aligned}$$

We can repeatedly alternate between minimizing over x versus minimizing over α, β until some stopping criterion is met. The resulting algorithm is given in Algorithm (1), where I is the maximum number of iterations, and ϵ is the tolerance level. These definitions will be the same for the additional algorithms.

Algorithm 1 Alternating Algorithm

Require: $I, x_0, \alpha_0, \beta_0, \epsilon \geq 0$

Require: $a_0, b_0, a_1, b_1 > 0$

$i \leftarrow 1$

$g \leftarrow ||\nabla \mathcal{J}(x_0, \alpha_0, \beta_0)||_2^2$

while $i \leq I$ & $g < \epsilon$ **do**

$x_i \leftarrow (A^*A + \beta_{i-1}/\alpha_{i-1} L^*L)^{-1} A^*y$

$\alpha_i \leftarrow \frac{(n/2+a_0-1)}{1/2||Ax_i - y||^2 + b_0}$

$\beta_i \leftarrow \frac{(n/2+a_1-1)}{1/2||Lx_i||^2 + b_1}$

$g \leftarrow ||\nabla \mathcal{J}(x_i, \alpha_i, \beta_i)||_2^2$

$i \leftarrow i + 1$

end while

In [7] the following two theorems are proven for Algorithm 1.

Theorem 6.1. *(Theorem 3.1 in [7]) Let $\{x_i, \alpha_i, \beta_i\}_{i \in I}$ be the sequence of estimators generated by Algorithm 1. Then the sequence $\{\mathcal{J}(x_i, \alpha_i, \beta_i)\}_{i \in I}$ converges monotonically.*

Theorem 6.2. *(Theorem 3.2 in [7]) Let $\{x_i, \alpha_i, \beta_i\}_{i \in I}$ be the sequence of estimators generated by Algorithm 1, then this sequence converges to a critical point of $\mathcal{J}(x, \alpha, \beta)$.*

This method works when we can compute the partial derivatives of x, α, β, and have closed form solutions. This is the case when the model is an additive normal noise model with independent normal prior on X, and Gamma priors on α, β. The result is the Tikhonov regularization with ℓ^2 penalty on x. We now propose two additional methods, for which we do not need to assume existence of the closed form solutions. This way we can still numerically solve $\min_{x,\alpha,\beta} \mathcal{J}(x, \alpha, \beta)$ in case where different prior assumptions result in different penalties.

6.2 Method 2: Gradient Descent in α, β

Suppose now that we do not have closed form solutions for α, β. Define

$$\mathcal{J}_1(\alpha, \beta) = \mathcal{J}(\alpha, \beta; x) = \alpha/2||A\widehat{x}(\alpha, \beta) - y||^2 - (n/2 + a_0 - 1)log(\alpha) + b_0\alpha + \beta/2||L\widehat{x}(\alpha, \beta)||^2 - (n/2 + a_1 - 1)log(\beta) + b_1\beta$$

for fixed $\widehat{x}(\alpha, \beta)$. First, supposing that α, β, are fixed we can then minimize $\mathcal{J}$ with

$$x \overset{set}{=} (A^*A + \beta/\alpha L^*L)^{-1}A^*y.$$

So the inner minimization fixes x at the Tikhonov estimate for some given initial values of α, β. We now want to find

$$\min_{\alpha,\beta} \left[\min_x \mathcal{J}(x, \alpha, \beta)\right]$$

The inner minimization can be done using the closed form solution of x, but to minimize over α, β we must use gradient descent. That is

$$\alpha_{i+1} = \alpha_i - \mu\partial_\alpha \mathcal{J}_1(\alpha_i, \beta_i)$$
$$\beta_{i+t} = \beta_i - \mu\partial_\beta \mathcal{J}_1(\alpha_i, \beta_i)$$

Thus to solve this joint minimization problem we start with an initial α, β, compute $x(\beta/\alpha)$, then solve for $\widehat{\alpha}, \widehat{\beta}$ by taking one step along the gradient in the direction α, β. The resulting algorithm is given in Algorithm (2). Note that we chose different steps sizes for α and β to account for the different scales.

We now prove convergence of Algorithm 2 to a minimum of $\mathcal{J}(x, \alpha, \beta)$. First recall the following theorems:

Definition 6.1. *Let $(\mathcal{X}, ||\cdot||_\mathcal{X})$ and $(\mathcal{Y}, ||\cdot||_\mathcal{Y})$ be metric space with distance metrics $||\cdot||_\mathcal{X}$ and $||\cdot||_\mathcal{Y}$ respectively. Let $f : \mathcal{X} \to \mathcal{Y}$. Then f is Lipschitz continuous if there exists a $K \in \mathbb{R}$ with $K \geq 0$ such that for all $x_1, x_2 \in \mathcal{X}$*

$$||f(x_1) - f(x_2)||_\mathcal{Y} \leq L||x_1 - x_2||_\mathcal{X}$$

L is then called the Lipschitz constant of f.

Algorithm 2 Gradient Descent in α, β

Require: $x_0, \alpha_0, \beta_0, \epsilon > 0$

Require: $a_0, b_0, a_1, b_1 > 0$

Require: $I > \mathcal{O}(1/\epsilon)$

$i \leftarrow 1$

$g \leftarrow ||\nabla \mathcal{J}(x_0, \alpha_0, \beta_0)||_2^2$

while $i \leq I$ & $g < \epsilon$ **do**

$x_i \leftarrow (A^*A + \beta_{i-1}/\alpha_{i-1} L^*L)^{-1} A^*y$

$L_\alpha \leftarrow \frac{1}{2}||Ax_i - y||_2 - (n/2 + a_0 - 1) + b_0$

$L_\beta \leftarrow \frac{1}{2}||Lx_i||_2 - (n/2 + a_1 - 1) + b_1$

$\mu_\alpha \leftarrow \epsilon / L_\alpha^2$

$\mu_\beta \leftarrow \epsilon / L_\beta^2$

$\alpha_i \leftarrow \alpha_{i-1} - \mu_\alpha \partial_\alpha \mathcal{J}_1(\alpha_{i-1}, \beta_{i-1})$

$\beta_i \leftarrow \beta_{i-1} - \mu_\beta \partial_\alpha \mathcal{J}_1(\alpha_{i-1}, \beta_{i-1})$

$g \leftarrow ||\nabla \mathcal{J}(x_i, \alpha_i, \beta_i)||_2^2$

$i \leftarrow i + 1$

end while

Remark 6.1. *Then for all $x_1, x_2 \in \mathcal{X}$*

$$\frac{||f(x_1) - f(x_2)||_{\mathcal{Y}}}{||x_1 - x_2||_{\mathcal{X}}} \leq L$$

Remark 6.2. *Let $\mathcal{X}, \mathcal{Y}, f$ be defined as in the previous remark. Suppose that $\mathcal{X}$ is closed and that f is differentiable on $\mathcal{X}^o$. Then by the mean value theorem,*

$$\frac{f(x_1) - f(x_2)}{x_1 - x_2} \leq f'(z)$$

for all $x_1 < z < x_2 \in \mathcal{X}^o$. This implies that we can find L such that $||f'(z)||_{\mathcal{Y}} < L$.

Theorem 6.3. *Let $\{x_i, \alpha_i, \beta_i\}_{i \in I}$ be the sequence of estimators generated by Algorithm 2. Then the sequence $\{\mathcal{J}(x_i, \alpha_i, \beta_i)\}_{i \in I}$ converges monotonically.*

Proof. For fixed a_0, b_0, a_1, b_1, recall that we defined

$$\mathcal{J}_1(\alpha, \beta) = \mathcal{J}(\widehat{x}, \alpha, \beta) = \min_x \mathcal{J}(x, \alpha, \beta)$$

So then

$$x_{i+1} = \operatorname*{argmin}_x \mathcal{J}(x_i, \alpha, \beta)$$

$$\begin{pmatrix} \alpha_{i+1} \\ \beta_{i+1} \end{pmatrix} = \begin{pmatrix} \alpha_i - \mu \partial_\alpha \mathcal{J}_1(\alpha_i, \beta_i; x_{i+1}) \\ \beta_i - \mu \partial_\beta \mathcal{J}_1(\alpha_i, \beta_i; x_{i+1}) \end{pmatrix}$$

Fix a_0, b_0, a_1, b_1 such that $\mathcal{J}_1(\alpha, \beta)$ and $\mathcal{J}_2(x)$ are convex. Let L be such that $||\nabla \mathcal{J}_1(\alpha, \beta)||_2 < L$ and $\epsilon > 0$. Set $\mu = \epsilon / L^2$. Then

$$\mathcal{J}_1(\alpha_{i+1}, \beta_{i+1}; x_{i+1}) \leq \mathcal{J}_1(\alpha_i, \beta_i; x_{i+1})$$

This implies that

$$\mathcal{J}(x_{i+1}, \alpha_{i+1}, \beta_{i+1}) \leq \mathcal{J}(x_{i+1}, \alpha_i, \beta_i) \leq \mathcal{J}(x_i, \alpha_i, \beta_i).$$

Then $\mathcal{J}$ is monotonically decreasing and bounded below (Theorem 2.1 in [7]). Consequentially, we have that $\mathcal{J}$ converges. □

Theorem 6.4. *Let $\{x_i, \alpha_i, \beta_i\}_{i \in I}$ be the sequence of estimators generated by Algorithm 2, then this sequence converges to a critical point $\{x_*, \alpha_*, \beta_*\}$ of $\mathcal{J}(x, \alpha, \beta)$.*

Proof. Fix a_0, b_0, a_1, b_1 such that $\mathcal{J}_1(\alpha, \beta)$ and $\mathcal{J}_2(x)$ are convex. Let L be such that $||\nabla \mathcal{J}_1(\alpha, \beta)||_2 < L$ and $\epsilon > 0$. Set $\mu = \epsilon / L^2$.

$$J_2(\alpha_i, \beta_i) \to J_2(\alpha_*, \beta_*)$$

Recall that $\widehat{x_i}(\alpha_{i-1}, \beta_{i-1}) = (A^*A + \beta_{i-1}/\alpha_{i-1} L^* L)^{-1} A^* y$. Then

$$\mathcal{J}_2(\alpha_i, \beta_i; \widehat{x}(\alpha_i, \beta_i)) \to \mathcal{J}_2(\alpha_*, \beta_*; \widehat{x}(\alpha_*, \beta_*)) = \mathcal{J}(x_*, \alpha_*, \beta_*)$$

□

6.3 Method 3: Gradient Descent in x

Suppose now that we do not have a closed form solution for x. Then define

$$\mathcal{J}_2(x) = \mathcal{J}(x; \widehat{\alpha}(x), \widehat{\beta}(x)) = \widehat{\alpha}(x) ||Ax - y||_2^2 + \widehat{\beta}(x) ||Lx||_2^2$$

for fixed $\widehat{\alpha}(x), \widehat{\beta}(x)$ and constants a_0, b_0, a_1, b_1 such that $a_0, a_1 \neq 1$ and $b_0, b_1 \neq 0$. Similar to method 2 we compute estimates for x by taking one step along the gradient of $\mathcal{J}$ in the direction of x. Our minimization problem is then

$$\min_x \left[\min_{\alpha, \beta} \mathcal{J}(x, \alpha, \beta) \right]$$

The inner minimization can be solve by using the closed form solution for α, β given some fixed x. For the outer minimization we need to use a gradient method. To do this we compute

$$\nabla_x \mathcal{J}_2(x) = (A^*A + \beta(x)/\alpha(x) L^* L) y - A^*.$$

Next, take one step along the gradient thereby finding the next best guess for x given α, β

$$x_{i+1} = x_i - \mu \nabla_x \mathcal{J}_2(x_i)$$

Algorithm 3 Gradient Descent in x

Require: $x_0, \alpha_0, \beta_0, \epsilon > 0$

Require: $a_0, b_0, a_1, b_1 > 0$

Require: $I > \mathcal{O}(1/\epsilon)$

$i \leftarrow 1$

$g \leftarrow ||\nabla \mathcal{J}(x_0, \alpha_0, \beta_0)||_2^2$

while $i \leq I$ & $g < \epsilon$ **do**

$\alpha_i \leftarrow \frac{(n/2+a_0-1)}{1/2||Ax_{i-1}-y||^2+b_0}$

$\beta_i \leftarrow \frac{(n/2+a_1-1)}{1/2||Lx_{i-1}||^2+b_1}$.

$L \leftarrow ||A^*A + \beta_{i-1}/\alpha_{i-1}L^*L||_2$

$\mu \leftarrow \epsilon/L^2$

$x_i \leftarrow x_{i-1} - \mu\nabla\mathcal{J}_2(x_{i-1})$

$g \leftarrow ||\nabla \mathcal{J}(x_i, \alpha_i, \beta_i)||_2^2$

$i \leftarrow i + 1$

end while

where i denotes the iteration. To solve this joint minimization problem we start with an initial x, then minimize over α, β by computing their optimal solutions. Then iteratively solve for $\widehat{x}$ and update α, β. The resulting algorithm is given in Algorithm (3). We now prove convergence of Algorithm 3 to a minimum of $\mathcal{J}(x, \alpha, \beta)$.

Theorem 6.5. *Let $\{x_i, \alpha_i, \beta_i\}_{i\in I}$ be the sequence of estimators generated by Algorithm 3. Then the sequence $\{\mathcal{J}(x_i, \alpha_i, \beta_i)\}_{i\in I}$ converges monotonically.*

Proof. For fixed a_0, b_0, a_1, b_1, recall that we defined

$$\mathcal{J}_2(x) = \mathcal{J}(x, \widehat{\alpha}, \widehat{\beta}) = \min_{\alpha,\beta} \mathcal{J}(x, \alpha, \beta)$$

So then

$$(\alpha_{i+1}, \beta_{i+1}) = \operatorname*{argmin}_{\alpha,\beta} \mathcal{J}(x_i, \alpha, \beta)$$
$$x_{i+1} = x_i - \mu\nabla\mathcal{J}_2(x_i; \alpha_{i+1}, \beta_{i+1})$$

Fix a_0, b_0, a_1, b_1 such that $\mathcal{J}_1(\alpha, \beta)$ and $\mathcal{J}_2(x)$ are convex. Let L be such that $||\partial\mathcal{J}_2(x)||_2 < L$ and $\epsilon > 0$. Set $\mu = \epsilon/L^2$. Then

$$\mathcal{J}_2(x_{i+1}; \alpha_{i+1}, \beta_{i+1}) \leq \mathcal{J}_2(x_i; \alpha_{i+1}, \beta_{i+1})$$

This implies that

$$\mathcal{J}(x_{i+1}, \alpha_{i+1}, \beta_{i+1}) \leq \mathcal{J}(x_i, \alpha_{i+1}, \beta_{i+1}) \leq \mathcal{J}(x_i, \alpha_i, \beta_i).$$

Then $\mathcal{J}$ is monotonically decreasing and bounded below (Theorem 2.1 in [7]). Consequentially, we have that $\mathcal{J}$ converges. □

Theorem 6.6. *Let $\{x_i, \alpha_i, \beta_i\}_{i \in I}$ be the sequence of estimators generated by Algorithm 3, then this sequence converges to a critical point of $\mathcal{J}(x, \alpha, \beta)$.*

Proof. Fix a_0, b_0, a_1, b_1 such that $\mathcal{J}_1(\alpha, \beta)$ and $\mathcal{J}_2(x)$ are convex. Let L be such that $||\partial \mathcal{J}_1(\alpha, \beta)||_2 < L$ and $\epsilon > 0$. Set $\mu = \epsilon / L^2$. Then

$$J_1(x_i) \to J_1(x_*)$$

Recall that

$$\widehat{\alpha_i}(x_{i-1}) = \frac{(n/2 + a_0 - 1)}{1/2||Ax_{i-1} - y||^2 + b_0}$$
$$\widehat{\beta_i}(x_{i-1}) = \frac{(n/2 + a_1 - 1)}{1/2||Lx_{i-1}||^2 + b_1}$$

Then

$$\mathcal{J}_1(x_i; \widehat{\alpha_i}(x_{i-1}), \widehat{\beta_i}(x_{i-1})) \to \mathcal{J}_1(x_*; \widehat{\alpha_i}(x_*), \widehat{\beta_i}(x_*)) = \mathcal{J}(x_*, \alpha_*, \beta_*)$$

□

7 Implementation

7.1 Example

In this chapter we show the results of a particular example we use to test our implementation in Python. The inverse problem we are interested in is to recover $sin(x)$ with $x \in [-4\pi, 4\pi]$. We observe

$$y = A(sin(x)) + \epsilon \tag{43}$$

where

$$Af(t) = \int_0^1 \frac{f(y)}{((1 + (t - y)^2)^3/2)} dy \tag{44}$$

for our implementation we discretize the the interval $[-4\pi, 4\pi]$ into n evenly spaced points, and discretize A by letting the step size be equal to m. The resulting forward problem $A(sin(x))$ is a system of equations with m equations and n variables which is well defined if the number of columns of A equals the number of rows of $sin(x)$. We set $n = m = 200$. We observe y with additive random Gaussian noise centered at 0, and variance $\sigma^2 = 0.1$. We set L to be the discretized second order differential operator that imposes smoothness on X. We have that $ker(A) \cap ker(L) = \{0\}$, so a unique solution exists. In Figure (2) we plot $\bar{x}$, the ground truth parameter we wish to recover, and $\bar{y} = A\bar{x}$.

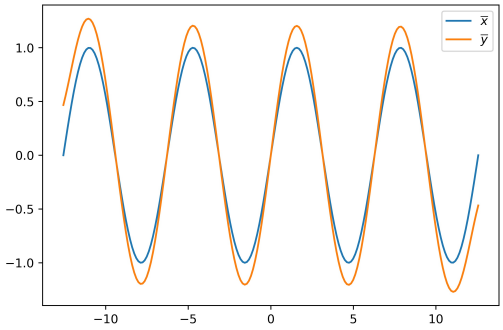


Figure 2: Plot of the ground truth $\bar{x}$, and the non-noisy observations where $\bar{y} = A\bar{x}$. In this case the observational operator, A, does not have much effect.

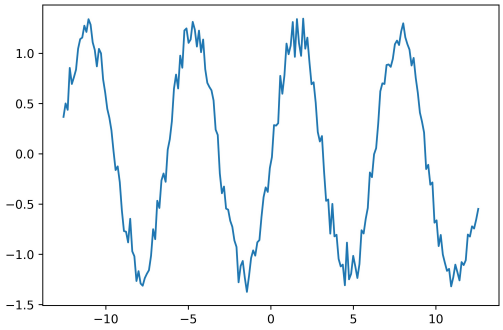


Figure 3: Plot of noisy observation with noise level $\sigma_0^2 = 0.1$.

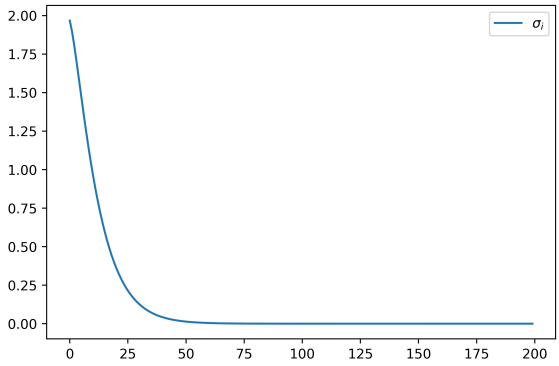


Figure 4: Plot of the decay of Singular Values of A. We see that many of the singular values are close to zero.

7.2 Ill-posedness

In this section, we look at the ill-posedness of the least squares estimator. The conditioning number of A is $4887979232 \approx 10^{9.689}$ which is much larger than 1. Therefore, A is ill-conditioned. In Figure (4), we plot the decay of the singular values of A. We can see that the eigenvalues quickly decay to zero. We now examine the Picard condition, where we see that the Picard condition is not met as seen in Figure (5). Thus, the direct inverse problem is ill-posed. If we were to ignore the ill-posedness and directly invert A, which we can do since A is full rank and $det(A) \neq 0$, the resulting solution is the least squares solution which we plot below in Figure (6). We see that this solution has high variance and does not accurately recover $\bar{x}$.

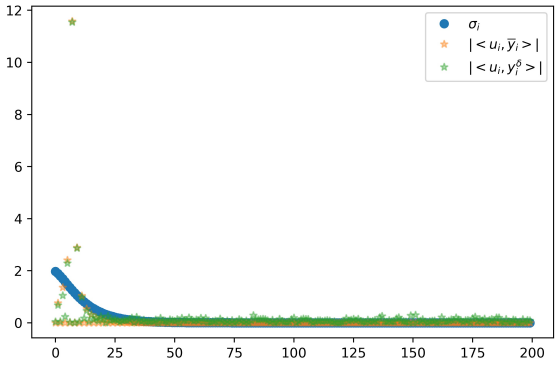


Figure 5: Plot of the Picard Condition.

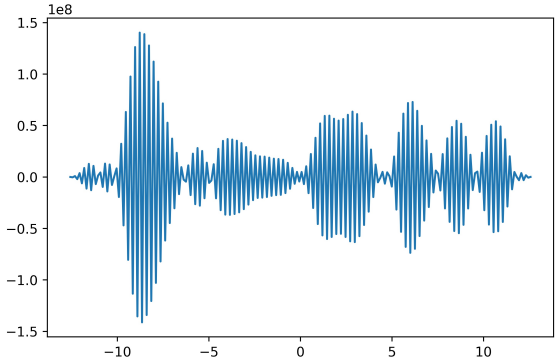


Figure 6: Plot of $A^{-1}y = x$, the least squares solution, which we see does not closely resemble the ground truth $\bar{x}$.

tol (ϵ)	$1e-5$
max iter (I)	100,000
n	200
$\boldsymbol{\alpha_{initial}}$	10
$\boldsymbol{\beta_{initial}}$	1
$\boldsymbol{x_{initial}}$	$\kappa = \frac{\|\|A*y^{\delta}\|\|_2^2}{\|\|AA^*y^{\delta}\|\|_2^2}, x = \kappa A^* y^{\delta}$
$\boldsymbol{a_0 = a_1}$	$1 + 1e-6$
$\boldsymbol{b_0 = b_1}$	$1e-6$

Table 1: Initial parameters

7.3 Regularization

Since the problem of recovering $\bar{x}$ by simply inverting A is ill-posed, we can use Tikhonov regularization with ℓ_2 penalty. We justify this choice of penalty as we can see in Figure (2), that $\bar{x}$ is smooth. The resulting problem is

$$\min_{x,\alpha,\beta} \mathcal{J}(x,\alpha,\beta) = \ell(x,\alpha,\beta \mid y) = \alpha/2||Ax-y||^2 - (n/2+a_0-1)log(\alpha)+b_0\alpha+ \\ \beta/2||Lx||^2 - (n/2+a_1-1)log(\beta)+b_1\beta$$

and is well-posed as we have seen in the previous sections. We numerically solve this by the three proposed methods we proposed in section 6.1. The stopping condition is the first order condition

$$||\partial_x \mathcal{J}||_2^2 + ||\partial_\alpha \mathcal{J}||_2^2 + ||\partial_\beta \mathcal{J}||_2^2 \leq \epsilon$$

If the stopping condition is met, then we say that the algorithm has converged. The parameters were set to the initial values in Table (4).

Recall that $\mathcal{J}(x,\alpha,\beta)$ is convex in α,β. In Figure (7) we fix x and plot the contour plots. We see that the contour lines are slightly non-circular. The gradient is steeper in β than it is in α. The red dot approximates the minimum of $\mathcal{J}(\widehat{x}(\alpha,\beta),\alpha,\beta)$. Finally, taking advantage of the Bayesian framework, we can see these contour plots as highest posterior density confidence intervals for α,β fixed x.

In Figure (8), we plot the results of running all 3 algorithms. We ran a fourth algorithm that was a modification of method 1, where we replaced the closed form solution to x in method 1, with that of a gradient method implemented from python.

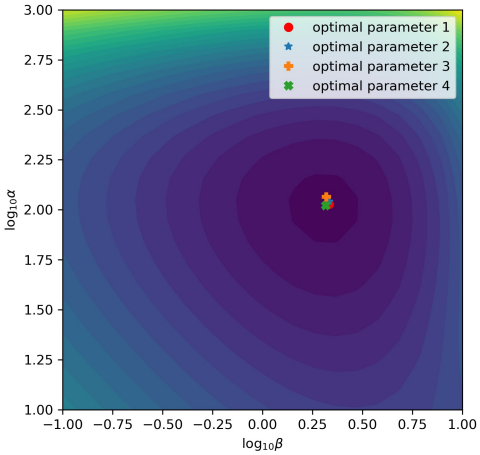


Figure 7: Contour plots of $J(\widehat{x}(\alpha,\beta),\alpha,\beta) = z$. We also plot the estimated optimal parameter, $\widehat{\lambda}_*$, as found by all four algorithms.

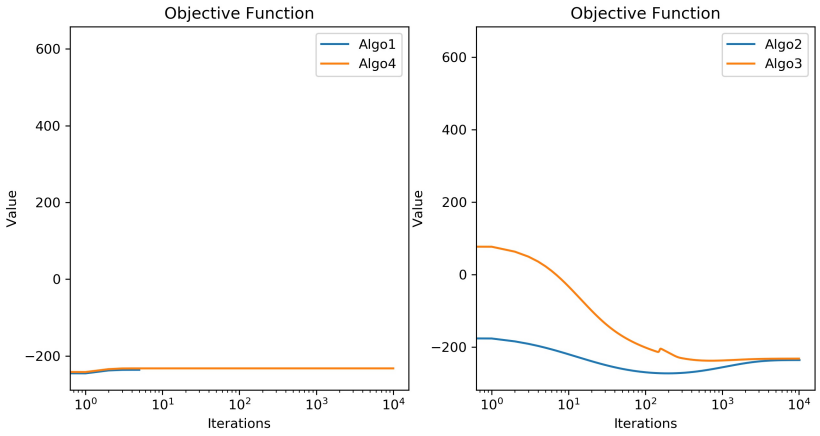
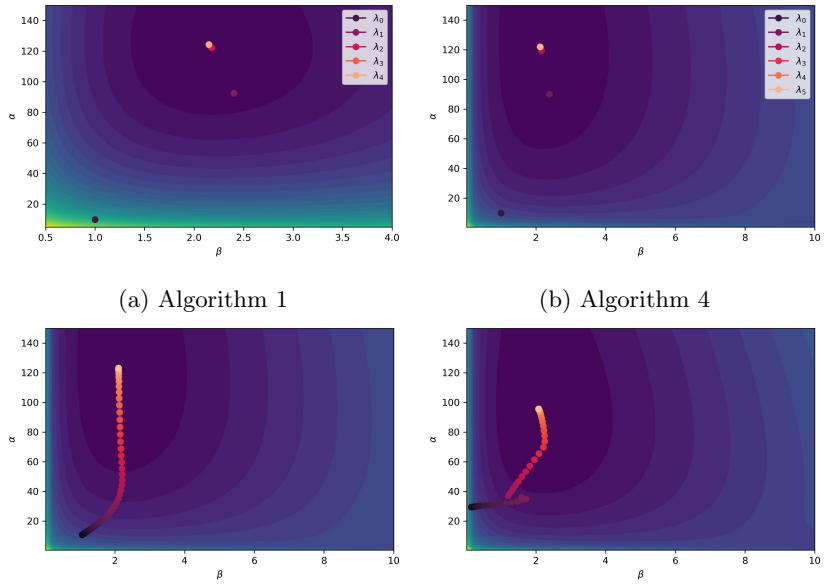


Figure 8: Plot of Objective function over all iterations. On left we plot results from Algorithm 1 and 4. On the right we plot the results of Algorithm 2 and 3.



(a) Algorithm 1

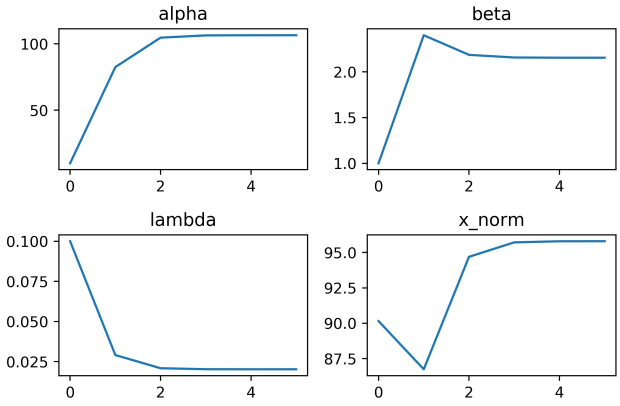
(b) Algorithm 4

(c) Algorithm 2

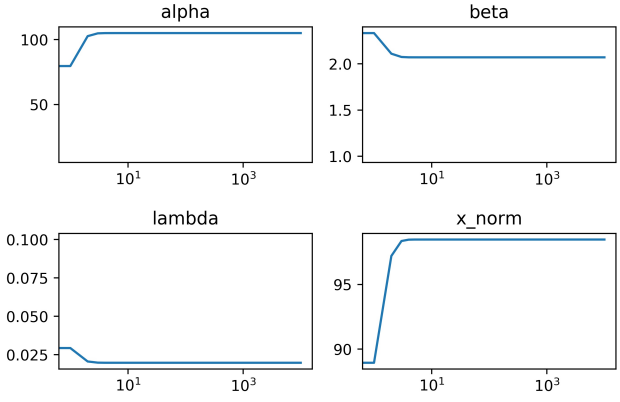
(d) Algorithm 3

Figure 9: Plots of regularization parameter over the iterations run, where λ_i is the regularization parameter at iteration i.

In Figure (8) we plot the path of the objective function over all iterations that the algorithms ran. We want that they are monotonically decreasing. This is indeed the case in Algorithms 1 and 4. However, this is not the case in Algorithms 2 and 3. In Algorithm 1 and 4, the objective function converged in less than 10 iterations. We can see in the left hand plot in figure (8) that after 3 iterations the graph of $\mathcal{J}$ is very flat. Algorithm 2 and 3 also converged but at a much slower rate. These two algorithms converged in under 10,000 iterations. We can also see that the slope of $\mathcal{J}$ in Algorithm 1 and 4 is very steep in comparison to that of Algorithm 2 and 3. The slope of $\mathcal{J}$ is steeper in Algorithm 2, than in Algorithm 3. In Figure (9), we plot the optimal parameter found at each iteration. We see that in Algorithm 1 and 4, we jump very quickly to the minimum. In Algorithm 2 we have a relatively continuous path to the minimum. However in Algorithm 3, we see there is a small jump to the left. Further exploration would be needed to explain this result. In [7], they prove that for the Alternating Algorithm, for any initial λ_0, the sequence of $\{\lambda_i\}$ generated by the Alternating Algorithm is monotonic. Moreover, they prove that $\{\alpha\}_i, \{\beta\}_i$ converges monotonically to critical points α_*, β_*. In Figure (10), we plot the $\widehat{\alpha}, \widehat{\beta}, \widehat{x}$, and $\widehat{\lambda}$ over all iterations for Algorithms 1 and 4. We see that besides the initial guess for β the sequence of $\{\alpha_i, \beta_i, \lambda_i\}$ is monotonic. In Figure (11) we again plot the estimates $\widehat{\alpha}, \widehat{\beta}, \widehat{x}$, and $\widehat{\lambda}$ over all iterations for Algorithms 2 and 3. We see that in Algorithm 2, the sequence of $\{\alpha_i, \lambda_i\}$ is

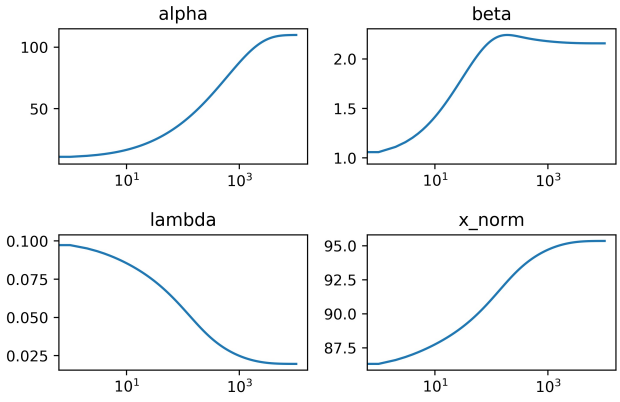


(a) Algorithm 1

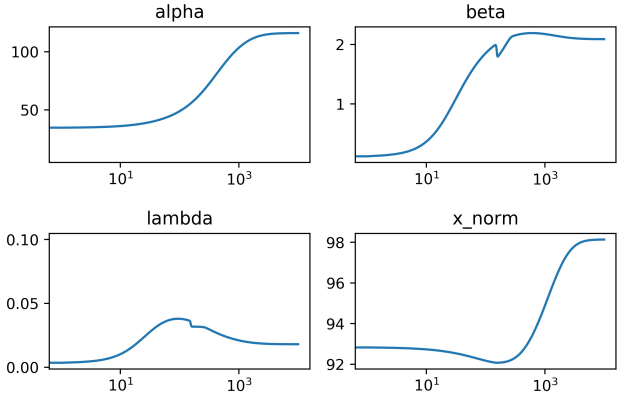


(b) Algorithm 4

Figure 10: Convergence plots of the estimators computed in Algorithm 1 and 4 over all iterations run.



(a) Algorithm 2



(b) Algorithm 3

Figure 11: Convergence plots of the estimators computed in Algorithm 2 and 3 over all iterations run.

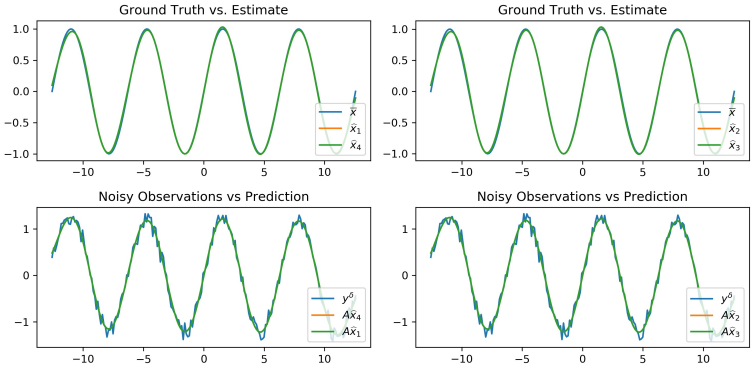


Figure 12: The top two plots show the estimator $\widehat{x}$ found by each algorithm versus the ground truth $\bar{x}$.The bottom two plots compare the noisy observations versus $A\widehat{x}$ for each algorithm. On the left column we compare Algorithm 1 and 4, and on the right column we compare Algorithm 2 and 3.

monotonic. However $\{\beta\}_i$ is not. In the bottom plots of Figure (11), we see the jump that was also seen in figure (d) of Figure (9).

In the upper plots of Figure 12, we see that all estimates of $\bar{x}$ are close to the ground truth, and even hard to distinguish from each other. We also see that each estimate has much lower variance than that of the least squares estimate (Fig. 6). In Table (2) we summarize the results. Overall Algorithms 1,2, and 4 found roughly the same regularization parameter. Algorithm 4 found a higher regularization parameter and resulted in a lower error.

	$\boldsymbol{\alpha}$	$\boldsymbol{\beta}$	$\boldsymbol{\lambda}$	$\boldsymbol{\mathcal{J}}(x,\alpha,\beta)$	$\boldsymbol{\|\|\bar{x}-\widehat{x}\|\|_2^2}$	**niter**
Algo1	122.06212	2.13766	0.01751	-233.60244	0.18775	4
Algo2	117.01666	2.15817	0.01844	-235.73951	0.18871	6598
Algo3	107.86797	2.14434	0.01988	-235.74297	0.20619	6302
Algo4	88.73767	2.12964	0.02400	-234.66994	0.18082	4

Table 2: Results of All Four Algorithms. Here we compare the computed minimizers $(\widehat{x}_*, \widehat{\alpha}_*, \widehat{\beta}_*)$ of the functional $\mathcal{J}$.

7.4 Convergence and Consistency

In this section we examine consistency and convergence of Algorithm 1. Recall, that we proposed that

$$\mathbb{E}||A\widehat{x}(\widehat{\alpha},\widehat{\beta})-y||_2^2 = n\sigma^2 \qquad\qquad \lim_{\sigma^2\to 0}\beta/\alpha \to 0$$

We see that as the noise level of the model goes to zero, so does the regular-

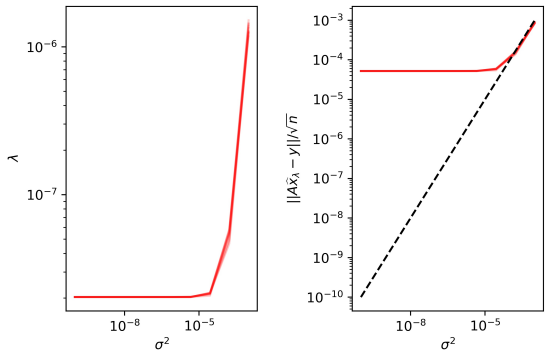


Figure 13: On the left hand side we plot of the level of regularization as noise level decreases. On the right hand side we plot of the estimate of residuals as noise level decreases.

ization. We also see the effects of bounding β/α on the right hand side in the Figure 13 where at small level of noise Algorithm 1 slightly over estimates the noise level as it is bounded from below and away from zero.

7.5 Sensitivity

In this section we reexamine the sensitivity of the Alternating Algorithm from [7]. We found that for certain values of the hyper parameters the objective function increased rather than decreased to the minimum. See Figures (14, 15) in appendix. Because of this, is not guaranteed that they converged to a minimum.

We see that varying b_0, b_1 does seem to affect convergence. We see that too large $b_0 = b_1$ led to relatively large λ. For $b_0 = b_1 < 1e-4$ we see little change. On the other hand, it does seem to be the case that $a_0 = a_1$ can be chosen more freely, ([7] pages 16-18), i.e. small or large values lead to similar regularization and convergence. See appendix for plots of the objective function. In certain extreme cases for b_0, b_1, a_0, a_1 the objective function increased. We also see that for extreme values of b_0, b_1 the algorithm did not find the estimate with low error.

$b_0 = b_1$	α	β	λ	$\mathcal{J}(x, \alpha, \beta)$	$\|\|\overline{x} - \widehat{x}\|\|_2^2$	niter
$1e4$	0.010 0	0.010 0	0.999 5	47086.284332	15.344035	3
$1e2$	0.896 7	0.843 4	0.940 5	156.021743	14.264391	7
$1e1$	45.548 7	2.173 5	0.047 7	-259.513647	0.246932	4
$1e-2$	87.911 3	2.130 3	0.024 2	-235.477913	0.181100	4
$1e-4$	88.729 5	2.129 6	0.024 0	-234.678019	0.180828	4
$1e-6$	88.737 7	2.129 6	0.024 0	-234.669902	0.180825	4
$1e-8$	88.737 8	2.129 6	0.024 0	-234.669821	0.180825	4

Table 3: Results of varying hyper priors $b_0 = b_1$, $a_0 = a_1 = 1 + 1e - 6$

$a_0 = a_1$	α	β	λ	$\mathcal{J}(x, \alpha, \beta)$	$\|\|\overline{x} - \widehat{x}\|\|_2^2$	niter
$1e4$	9 206.617 7	216.801 7	0.023 5	9.200286e+07	0.1785	4
$1e2$	182.309 3	4.293 1	0.023 5	1.762785e+04	0.1785	4
$1e1$	92.066 2	2.168 0	0.023 5	-1.472485e+02	0.1785	4
$1e-2$	91.163 7	2.146 8	0.023 5	-2.348479e+02	0.1785	4
$1e-4$	91.154 7	2.146 6	0.023 5	-2.357148e+02	0.1785	4
$1e-6$	91.154 6	2.146 6	0.023 5	-2.357235e+02	0.1785	4
$1e-8$	91.154 6	2.146 6	0.023 5	-2.357236e+02	0.1785	4

Table 4: Results of varying hyper priors $a_0 = a_1$, $b_0 = b_1 = 1e - 6$

8 Conclusions

We showed that under the additive independent Gaussian noise model, with the assumption that X is smooth, computing the MAP estimates of the posterior distribution $p(x, \alpha, \beta \mid y)$ is equivalent to minimizing the functional $\mathcal{J}(x, \alpha, \beta)$. By solving the minimization problem, we can simultaneously estimate the underlying parameter x, the regularization parameter λ, and the noise level.

We have developed and implemented numerical methods to compute the estimates, $\widehat{x}$ and $\widehat{\lambda}$, in the case that no closed form solution exists for x, or for α, β. Furthermore, we showed their convergence to a minimum of $\mathcal{J}(x, \alpha, \beta)$. We have shown in a simple simulation, that these algorithms work well, suggesting that using a gradient method in the place of root finding should work. Additionally, while implementing Method 2, we saw that step size played an important role in the convergence. We used an ad-hoc fixed step size in Method 2. The step size in Method 2 is a weighted step size that accounts for the different scales of α, β.

We reexamined the influence of the hyper-prior on the Alternating Algorithm from [7], and saw that in fact, they play an important role in the convergence. For some choices of hyper-priors the functional no longer decreased monotonically. Thus, the convergence to a minimum was no longer guarantee. We saw that for some choice of hyper-priors the functional actually increased (see plots in appendix). Perhaps this is because a saddle point exists or for some hyper-priors $\mathcal{J}$ is no longer convex.

However, we were not able to investigate all details of the proposed methods. Further research should be done in the following topics:

- Analyzing the role of the hyper-priors and develop a method to choose them without knowledge of the noise level or the variance of the underlying parameter.
- Extending Method 2 and 3 to the non-normal setting such as non-smooth and sparse priors, as well as large scale settings where $n \gg 200$.
- Developing and implementing an adaptive step size for faster convergence of Method 2 and 3.

9 Appendix

9.1 Sensitivity Plots

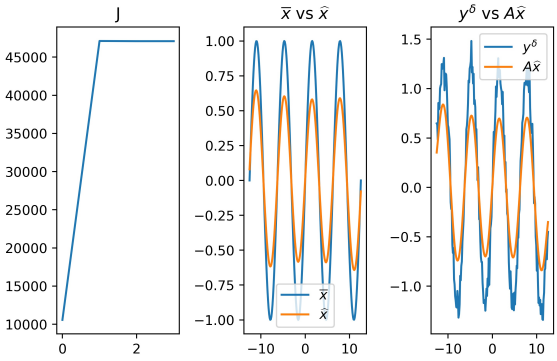


Figure 14: Results when $b_0 = b_1 = 1e4$

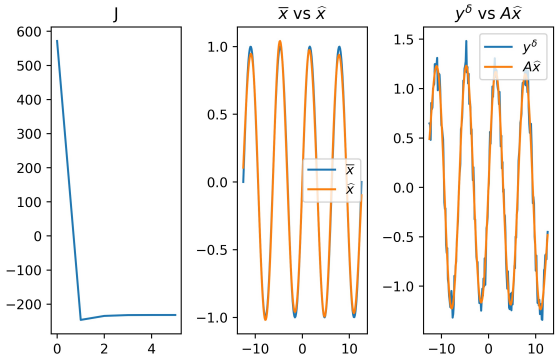


Figure 15: Results when $b_0 = b_1 = 1e - 8$

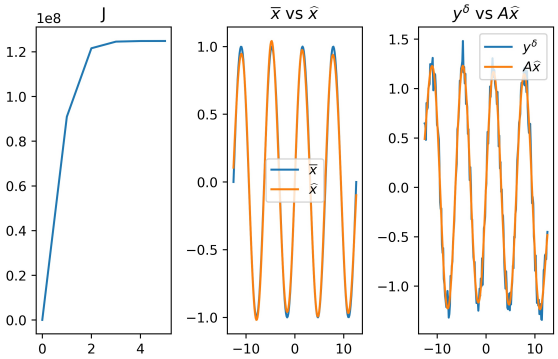


Figure 16: Results when $a_0 = a_1 = 1e4$

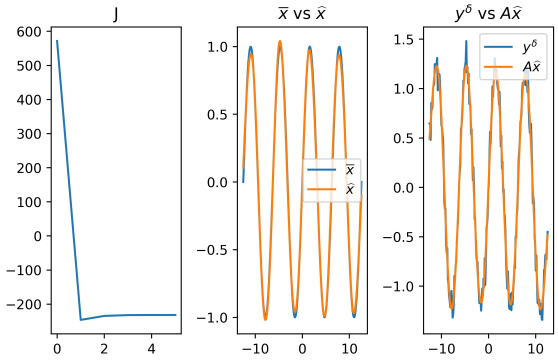


Figure 17: Results when $a_0 = a_1 = 1e - 8$

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