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Master Thesis

Regularization of Ill-posed Statistical Inverse Problems

A data driven method for choosing 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 in [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 to 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.

Contents

1 Inverse Problems

In this section 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 section 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 the 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 major 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 uses Bayesian statistics. The 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 inverse formulation of the inverse problem to the non-Bayesian one is connected via Tikhonov regularization. In the additive independent normal noise setting, the posterior distribution is normal. Gaussian distributions are completely characterized by their mean and variance. Computing the mean is of the posterior distribution is show to be equivalent to computing the minimum of Tikhonov regulation with ℓ_2 penalty. [11] and [2]

Another 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 numerical 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 that the functional no longer decreased monotonically. Therefore convergence to a minimum is not guaranteed.

1.4 Goals

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 overviews some examples, and how they are related to the functional analytical setting. Chapter 5 is really the first main purpose of this thesis where 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 numerical solve the resulting minimization problem derived in chapter 5. We show that these converge to a critical point of 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 of where the thesis could go next 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 these problems 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 can be greater than 0. In this case the solution may not exist and/or may not be unique.*
3. *if $n > m$, and $rank(A) = m$, then the system of equations is overdetermined. So no solution can exist, if $y \notin Range(A)$.*
4. *if $n < m$, and $rank(A) = n$, 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 and v_i 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 invertable. 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 $A \in \mathbb{R}^{n\times n}$ with $rank(A) = r \leq \min\{n, m\}$. Then using SVD of A the Moore-Penrose pseudo is defined as*

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

where U_r, V_r, Σ_r the first r non-zero eigenvalues.

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 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

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

where $x' \in ker(A)$. Since $n < m$, the $ker(A) = span(v_n + 1, ..., v + m)$. So $x' = Vc$ with $V = [v_n + 1, ..., v + m]$. so the minimum norm solution is when $x' = 0$, 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

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

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. So the solution is not continuous. So 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 that 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 it's bias and variance. For x_{LS}, the bias is zero but the variance can be so high that the solution is still ill-posed as we have seen. To lower the variance we can introduce a biased estimator. Ideally we would and up with a lower MSE over all. One way to avoid dividing by large singular values to regularize the $\sigma_i' s$ by with some regularization function $\mathcal{R}_\alpha$, with regularisation parameter α. The regularization solution is then

Definition 2.6.

$$x_\alpha = V_k \mathcal{R}_\alpha(\sigma_k) U_k^* y \tag{7}$$

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

Possible regularization functions are threasholding functions, such as TVSD, or shifting functions such as Tikhonov regularization.

Definition 2.7. *The Tikhonov regularization solution is*

$$x_\alpha = \sum_{i=1}^{r} \frac{\sigma_i \langle x_i, y \rangle}{\sigma_i^2 + \alpha} v_i \tag{8}$$

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

In the above we modify 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 $\frac{\sigma_i \langle x_i, y \rangle}{\sigma_i^2 + \alpha}$ is relatively unchanged. 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 $A^\dagger$ pseudo inverse. Let $\hat{x}_\alpha = A_\alpha^\dagger y^\delta$ the regularized solution with $A_\alpha^\dagger$ 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 a good 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 measure of how close this estimator is to the truth 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*

$$\mathcal{R}_\lambda(x) = ||Ax - y||^2 + \lambda||x||^2 \tag{9}$$

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

To find the estimate for $\bar{x}$ 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: $\min_{x \in \mathbb{R}^m} (||Ax - y||_2^2 + \lambda||Lx||)$. This can also be written as some constrained optimization problem.
2. The solution is $x_e^\lambda = (A^*A + \lambda L^*L)^{-1}A^*y$. Note that if there is no noise in the model, so we need no regularization, then we get back the least-squares solution.

We will denote the functional $\min_{x \in \mathbb{R}^m} (||Ax - y||_2^2 + \lambda||Lx||)$ 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

$$x_\alpha = (A^*A + \alpha L)^{-1}A^*y = V(\Sigma_r^2 + \alpha L)^{-1}\Sigma_U^* y \tag{10}$$

If the regularization guarantees stability, and $ker\ A \cap ker\ L = \{0\}$, then (12) is a well-posed problem. The estimate x_e^λ, depends on fixed λ, so we must 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 via

1. a-prior rules knowing the noise level
2. Discrepancy principle
3. L-curve
4. Cross validation [2]

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

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-prior rule, a posterior rule, and a heuristic rule, but we now introduce a more data driven rule, that being choosing α via cross validation. Later on we will see that there is a connection between this rule, and the Bayesian method we describe in this thesis. We would like to somehow choose λ from the data alone. We also want that as $\sigma \to 0$ $\lambda \to 0$ so $\hat{x}$ converges to x_{LS} should it exist. To do this we will use Bayesian statistics, and frame (3) in the Bayesian framework. With certain choices, we will see that the Bayesian interpretation of (3), is closely related to the Tikhonov regularization we described above.

Finally we remark that

$$\mathcal{R}_{\lambda}(x) = ||Ax - y||^2 + \lambda||x||^2 \tag{11}$$

for $\lambda \in (0, \infty)$ can be written as [14]

$$\mathcal{R}_{\lambda}(x) = (1-\lambda)||Ax - y||^2 + \lambda||x||^2 \tag{12}$$

for $\lambda \in (0, 1)$ where here we see that that regularization parameter can be seen as balancing the fit versus the smoothing. At the end points 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, and why indeed when λ is minimized we have also balanced the fit versus the smoothing.

3 Statistical 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 section we recap the definitions of certain distributions as characterized by their probability density functions. We also review some algebra rules for the 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 measure. 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 define 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 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 $\in$L$^1(\mathbb{R}^n)$ is the unique is 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 as defined about then such a 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 Some statistics 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. *Multivariate normal distribution A random variable $X \sim \mathcal{N}(\mu, \sigma^2)$ if its probability density function is give by*

$$f_X(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}(x-\mu)^2/\sigma^2} \tag{13}$$

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 random $n-$ 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*

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

for parameters $\mu \in \mathbb{R}^n$ and $\Sigma \in \mathbb{R}^{n\times n}$ symmetric positive definite matrix.

Proof. See Aard van der Vaart chapter 2 lemma 2.3 dictaat. [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 $A \in \mathbb{R}^{m\times m}$ 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 $Z \sim \mathcal{N}(0, I)$ and $X \sim \mathcal{N}(\mu, \Sigma)$ then we can write X as and $X = \mu + \Sigma^{1/2}Z$.*

Remark 3.3. *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 matrix symmetric X of dimension $p \times p$. In which 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 determinate of M and $tr(M)$ is the trace. For X a random variable 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 section we introduce statistical inverse problems, derive Bayes formula in this setting, give a few classic examples, and show the connection to the functional analytic inverse problems We will now consider y, x, e to be random variables and A as some fixed carefully chosen operator. The model (2) can then we written as

$$Y = A(X, E) \tag{15}$$

where X, Y, E are random vectors defined on the probability space $\Omega = \Omega_1 \times \Omega_2$ such that $X : \Omega_1 \to \mathbb{R}^m$, $Y : \Omega_2 \to \mathbb{R}^n$, and $E : \Omega \to \mathbb{R}^n$. We want to learn the relationship between X, Y, E, that is determine their conditional probability distributions. We can relate X after making observations of Y using Bayes formula. First note again some notation. As in the non-random case Y is the observed/measured data, with $Y = y$ the realization of Y, X is the unknown parameter again with $X = x$ the realization of X, and E is still 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 (15) as

$$Y = AX + E \tag{16}$$

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. 1) we can obtain point estimates by computing the most likely value for X which we will describe later, and compute the uncertainty of this estimate by calculating the spread of the posterior distribution. 2) If the distribution is Gaussian, then the MAP estimate connects the non-Bayesian Tikhonov regularization setting to the Bayesian setting.

4.1 Bayes Formula

On key aspect of Bayesian statistics is that we formulate prior knowledge or assumptions of certain parameters in our model. In this setting what we can observe are realizations of Y, and we assume that we have prior knowledge/assumptions of X. Mainly which values of X are occurring and at what frequency. To express this prior knowledge 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 here to get the desired likelihood and resulting Tikhonov regularization. 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 will tells us how X is depending on Y.

Theorem 4.1. *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 $Y = y$, where 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 which is the setting of this paper. But using the formulation in remark (4.1), we can generalize Bayes theorem to the infinite dimensional case using Gaussian measure. The do this in [11][2].*

Before we move further, we go through two classical examples which can be found in [11].

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

$$y = Ax + e$$

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 $A \in R^n - \{0\}$. 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

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

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

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

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 uncertain 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.

Remark 4.3.

It is now natural to ask what well-posedness 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 distributions. 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*

$$x_{MAP} = \max_{\mathbb{R}^m}\pi(x \mid y) \tag{17}$$

To compute 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*

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

To compute this point estimator is an integration problem, which can be very difficult in high dimensional settings.

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*

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

To compute this is a root finding problem.

4.2 Connection to Tikhonov Regularization

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

$$E \sim \mathcal{N}(0, \alpha I) \tag{18}$$
$$X \sim \mathcal{N}(0, \beta\Sigma) \tag{19}$$

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

$$\pi(x, \alpha, \beta) \propto \alpha/2||Ax-y||^2 - \beta/2||Lx||^2 + m/2log(\alpha) + n/2log(\beta) \tag{20}$$

and the potential is

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

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

$$\mu = (\alpha A^*A + \beta L^*L)^{-1}\alpha A^*y \tag{22}$$
$$\Sigma = (\alpha A^*A + \beta L^*L)^{-1} \tag{23}$$

We can further write

$$\mu = (A^*A + \beta/\alpha L^*L)^{-1}\alpha A^*y \tag{24}$$
$$\tag{25}$$

We see that $\mu = \hat{x}_\lambda$ in (10) where from the above formulation of μ, we see that the regularization parameter λ is equal to β/α. So to compute λ 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

$$\min_x \ ||Ax-y||^2 + \beta/\alpha||Lx||^2 - m/2log(\alpha) - n/2log(\beta) \tag{26}$$

5 Bayesian Regularization

In the previous section, 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 parameter $\bar{x}$, while simultaneously estimating the precision parameter of the noise, α, and precision parameter of the underlying parameter x, β.

5.1 Empirical Bayesian Method

Our first method is to use empirical Bayesian method that would allow us to determine α and β from the data only. To do this we minimize the objective function over all three parameters.

$$(x_{MAP}, \alpha_{MAP}, \beta_{MAP}) = \min_{x,\alpha,\beta} \mathcal{J}(x, \alpha, \beta) \tag{27}$$

$$= \min_{x,\alpha,\beta} \alpha/2||Ax - y||^2 + \beta/2||Lx||^2 - m/2log(\alpha) - n/2log(\beta) \tag{28}$$

We propose that

$$(1)\ \mathbb{E}||A\widehat{x}(\widehat{\alpha}, \widehat{\beta}) - y||_2^2 = n\sigma^2 \qquad (2)\ \lim_{\sigma^2 \to 0} \beta/\alpha \to 0 \tag{29}$$

If (1) holds, then we can consistently estimate the noise level as noise 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

We now check that this minimization problem is well-posed.

Claim 5.1. *The empirical Bayesian method is ill-posed.*

Proof. We wish to

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

Suppose that A is invertible. Recall that $y = Ax + e$. Then $||Ax - y|| = 0$, and minimizing $\mathcal{J}$ occurs when $\alpha \to \infty$ and $\beta \to 0$. If $\alpha \to \infty$, and $\beta \to 0$, no regularization occurs as $\lambda = 0$ 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*

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

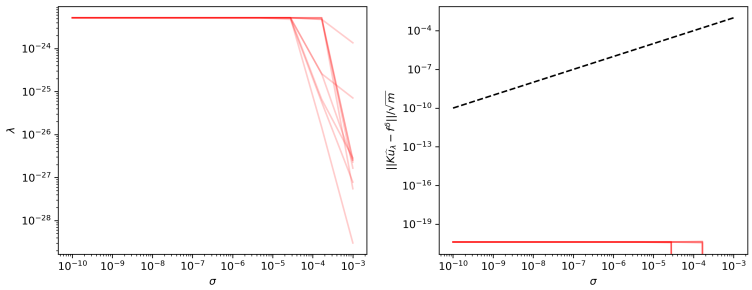


Figure 1: Convergence and consistency of Empirical Bayesian method for $\sigma \in [1e-10, 1e-3]$

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 1. The problem is then that minimization occurs at the bound 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 invertable leading to a 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, and the estimate for residuals was consistent. In [7] they prose that to turn the empirical Bayesian method into a well-posed problem, we need to place 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. In this setting they prove that J a minimum to exists.

Suppose we now add the following hyper priors on the precision parameters

$$\alpha \sim Gamma(a_0, b_0) \tag{30}$$
$$\beta \sim Gamma(a_1, b_1) \tag{31}$$

Then the posterior becomes

$$p(x, \alpha, \beta \mid y) \propto \rho(Ax - y \mid \alpha) \times \pi(\alpha)\pi(x \mid \beta) \times \pi(\beta) \tag{32}$$
$$\propto \alpha^{n/2} e^{-\alpha/2||Ax-y||^2} \alpha^{a_0 - 1} e^{-b_0 \alpha} \beta^{n/2} e^{-\beta/2||Lx||^2} \beta^{a_1 - 1} e^{-b_1 \beta} \tag{33}$$

The resulting minimization problem is

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

Note that if we let $a_0, a_1 = 1$ and $b_0, b_1 = 0$ the we recover the objective function given no hyper priors.

5.4 Well-posedness

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 goes to zero, the method converges to the minimum norm solution. To do this they they use the optimal solutions which we recall below. The partial derivatives are and resulting closed form solutions are useful in tool in the remaining sections. The partial derivatives are

$$\partial/\partial x(J(x,\alpha,\beta)) = (A^*A + \beta/\alpha L^*L)x - A^*y \tag{34}$$
$$\partial/\partial\alpha J(x,\alpha,\beta) = 1/2||Ax-y||^2 - (n/2+a_0-1)/\alpha + b_0 \tag{35}$$
$$\partial/\partial\beta J(x,\alpha,\beta) = 1/2||Lx||^2 - (n/2+a_1-1)/\beta + b_1 \tag{36}$$

so then the optimal solutions are

$$x = (A^*A + \beta/\alpha L^*L)^{-1}A^*y \tag{37}$$
$$\alpha = \frac{(n/2+a_0-1)}{1/2||Ax-y||^2 + b_0} \tag{38}$$
$$\beta = \frac{(n/2+a_1-1)}{1/2||Lx||^2 + b_1} \tag{39}$$

We now state one intermediate lemma proven by Jin and Zou and then restate the main theorem (Theorem 2.3 in [7]). These two theorems prove that (1) and (2) in 29 holds. We brief prove the main theorem in the case $L = I$, in which case we can use singular value decomposition.

Lemma 5.1. *(Lemma 2.2 [7])*

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

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

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

Proof. □

6 Numerical Methods

In this section we propose three different iterative methods to numerically solve $\min_{x,\alpha,\beta} \mathcal{J}(x,\alpha,\beta)$. Suppose that we have some function $f(x,y,z)$ and we want to find the minimum of this function. All critical points are then found when $\frac{\partial f}{\partial x} = 0, \frac{\partial f}{\partial y} = 0$, and $\frac{\partial f}{\partial z} = 0$. Suppose f is strictly convex then any local minimum on a convex set is a global minimum and in fact this minimum is unique. A common method to numerically solve for minimum of f is coordinate descent, where we used the fact that in the parameter of interested we are guaranteed to move downward by strict convexity. We can then do coordinate descent to find the minimum.

Example 6.1. *Suppose we would like to minimize*

$$f(x,y) = (x-y)^2$$

The function is minimized along the line $x = y$. We could have also solved this numerically by first noting that $f(x) = x^2 - 2y'x$ and $f(y) = y^2 - 2yx'$ are convex functions with first derivatives equal to $x - y'$ and $y - x'$. Suppose we start at the point $(1,0)$. And suppose that first we want to minimize along x. Then

$$y = argmin_x f(x,0) = argmin_x x^2 = 0$$

Then

$$x = argmin_y f(0,y) = y^2 = 0$$

So the minimum is at $(0,0)$ which is on the line $x = y$.

Now recall that we have computed the partial derivatives to $\mathcal{J}(x,\alpha,\beta)$ in (36) and computed the critical points as (39). However our function is only bi-(strictly) convex. But we can still implement a similar algorithm to coordinate descent by splitting $\mathcal{J}$ into its two strictly convex parts, and do alternating minimization. The following method was proposed by [7] and we use it as a benchmark to compared to the other two algorithms.

6.1 Method 1

In this method the estimates are found by simultaneous minimize over all three parameters. That is we

$$\min_{x,\alpha,\beta} \mathcal{J}(x,\alpha,\beta) \tag{40}$$

This is done by 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 (39) to the partial derivatives.

$$\begin{aligned} x(\beta/\alpha) &= (A^*A + \beta/\alpha L^*L)^{-1}A^*y \\ \alpha(x) &= \frac{(n/2 + a_0 - 1)}{1/2||Ax - y||^2 + b_0} \\ \beta(x) &= \frac{(n/2 + a_1 - 1)}{1/2||Lx||^2 + b_1} \end{aligned}$$

For fixed a_0, b_0, a_1, b_01, these defined 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).

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 indeed the case when we assume normal prior on x, and Gamma priors on α, β, where by we could recover the Tikhonov regularization with L^2 penalty on x. We now propose two additional methods where we assume we do not have 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 lead to different penalties.

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

6.2 Method 2

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

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

So the inner minimization fixes x at the Tikhonov estimate for some given initial values of α, β. So want we really want to do is

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

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 the joint minimization problem 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). We now prove the same convergence theorems for algorithm 2. 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 $x_1, x_2 \in \mathcal{X}$*

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

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

L is then called the Lipschitz constant of f.

Remark 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 $f : \mathcal{X} \to \mathcal{Y}$. Suppose that f is $L-$Lipschitz continuous. 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 $\mathcal{X}^o$. 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

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

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

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

So $\mathcal{J}$ is monotonically decreasing and bounded below by theorem (**??**) so we have the $\mathcal{J}$ 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 $\epsilon \geq 0$. 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

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 $b_0, b_1 \neq 0$. Similarly as in method two 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

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

. And take one step along the gradient there by finding the next best guess for x given α, β

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

where i denotes where we are in the iteration. So to solve the joint minimization problem start with an initial x, then minimize over α, β by computing their optimal solutions, then iterative solve for $\widehat{x}$ and update α, β. The resulting algorithm is given in Algorithm (3). We now prove the same convergence theorems

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

for algorithm 3.

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

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

So $\mathcal{J}$ is monotonically decreasing and bounded below by theorem (**??**) so we have the $\mathcal{J}$ 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 $\epsilon \geq 0$. Set $\mu = \epsilon / L^2$.

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

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 section we show the results of a particular example we used to test our implementation in python. The inverse problem we are interested in is recovering $sin(x)$ with $x \in [-4\pi, 4\pi]$. We observe

$$y = A(sin(x)) + \epsilon \tag{41}$$

where

$$Af(t) = \int_0^1 \frac{f(y)}{((1 + (t - y)^2)^3/2)} dy \tag{42}$$

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 an m system of equations with n variables which is well defined as the number of columns of A equals the number of rows of $sin(x)$. We observe y with random Gaussian noise center at 0, and variance σ. In our experiments we let $n = m = 200$, and the noise be distributed $\mathcal{N}(0, 0.1)$.

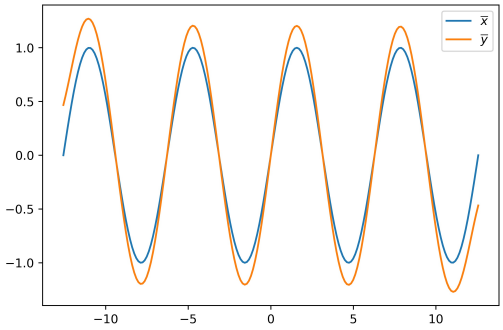


Figure 2: Ground Truth $\bar{x}$, where $\bar{y} = A\bar{x}$

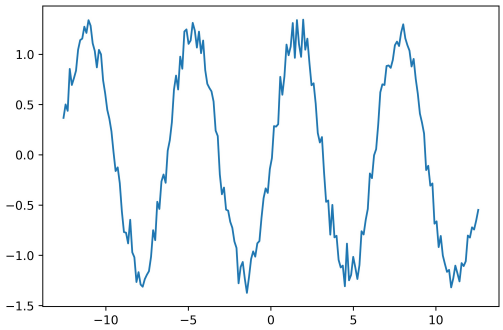


Figure 3: Noisy observation with noise level $\mathcal{N}(0, 0.1)$

7.2 Ill-posedness

In this section we looked at the ill-posedness of finding the least squares estimate. The conditioning number of A is $4887979232 \approx 10^{9.689} >> 1$ which is much larger than 1. A is ill-conditioned so the direct inverse problem of inverting the matrix A is ill-posed. We further plot the decay of the singular values of A. We can see that the eigenvalues quickly decay to zero. Now we examine the Picard condition. Where we see that the Picard condition is not met (5), so in fact the 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 (6). We see that this solution has high variance and does not accurately recover $\bar{x}$. We note that a majority of the variance is around the peaks.

7.3 Regularization

Since the problem of recovering $\bar{x}$ by simply inverting A is an ill-posed we instead solve the well-posed problem using regularization. The resulting well-

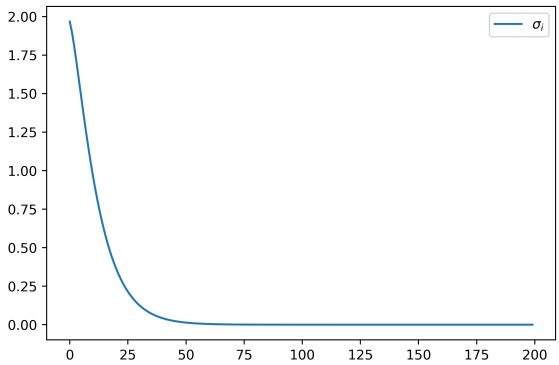


Figure 4: Decay of Singular Values of A

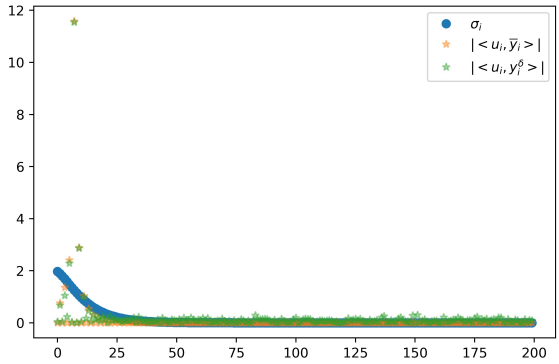


Figure 5: Picard Condition

posed problem is

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

We numerical solve this by the three proposed methods in section 6.1. The stopping condition is the first order condition

$$||\partial_x \mathcal{J}||_2^2 + ||\partial_\alpha \mathcal{J}||_2^2 + ||\partial_\beta \mathcal{J}||_2^2 < tol$$

If the stopping condition is met, then we say that the algorithm has converged. The parameters were set to Recall that $\mathcal{J}(x,\alpha,\beta)$ is convex in α,β. Below we fix x and plot the contour plots. We see that the contour lines are slight 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

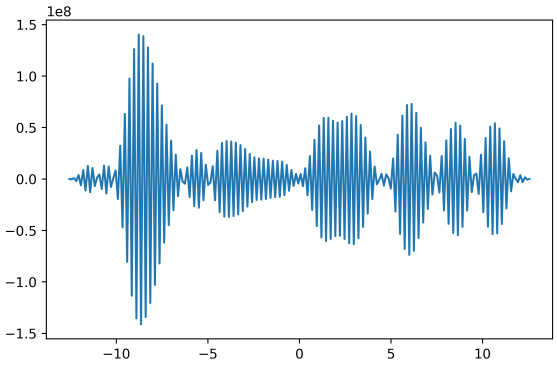


Figure 6: Least Squares solution

tol	$1e-5$
max iter	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

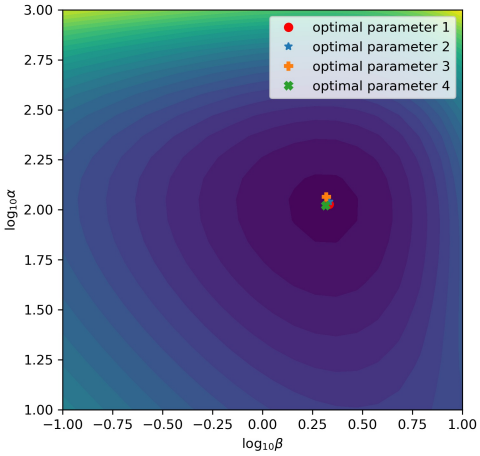


Figure 7: Contour plots of $J(\widehat{x}(\alpha,\beta),\alpha,\beta) = z$. Optimal parameter found by all four algorithms.

setting, we can see these contour plots as highest posterior density confidence intervals for α, β given fixed x. Below 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. In figure (8) we plot the path of the objective function over all iterations that the algorithms ran. We hope to see that they are monotonically decreasing. This is indeed the case in algorithms 1 and 4. However this is not the case in 2 and 3. In algorithm 1 and 4, the objective function converged in less than 10 iterations, and we can see in the left hand plot in figure (8) that after 3 iterations the graph at $\mathcal{J}$ is flat. Algorithm 2 and 3 also converged but much slower. These both converged in under 10,000 iterations. We can also see that the slop 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 pretty continuous path to the minimum, and again in algorithm 3 something strange is happening as we can see there is a small jump to the left. In [7], they prove that for the alternating algorithm (algorithm 1) that for any initial λ_0, the sequence of $\{\lambda_i\}$ generated by the alternating algorithm is monotonic. Moreover they prove that $\{\alpha\}_i, \{\beta\}_i$ is converging 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 minus the first initial guess for β the sequence of $\{\alpha_i, \beta_i, \lambda_i\}$ is monotonic. In figure (11) we again plot the $\widehat{\alpha}, \widehat{\beta}, \widehat{x}$, 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 monotonic,

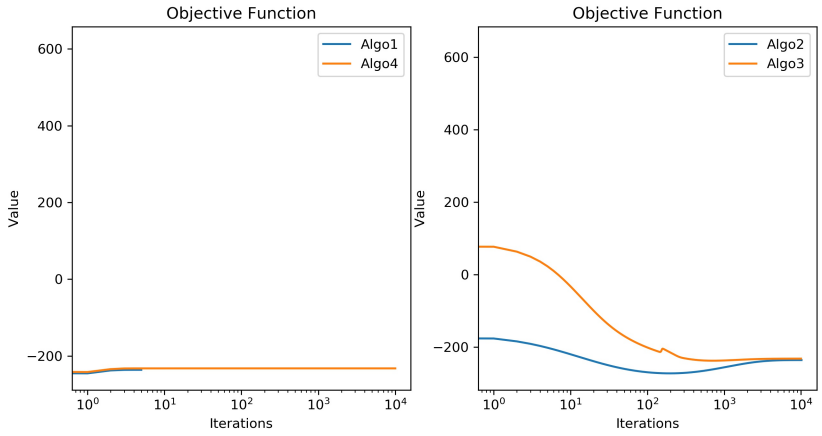
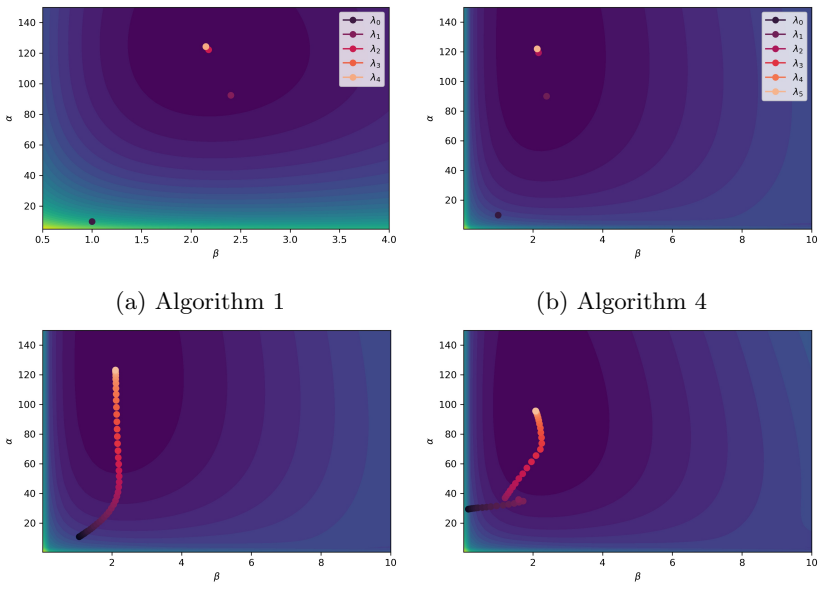


Figure 8: Plot of Objective function over all iterations. On left we plot results from Algorithm 1 and 4. On the right we plot the results of Algorithm 2 and 3.



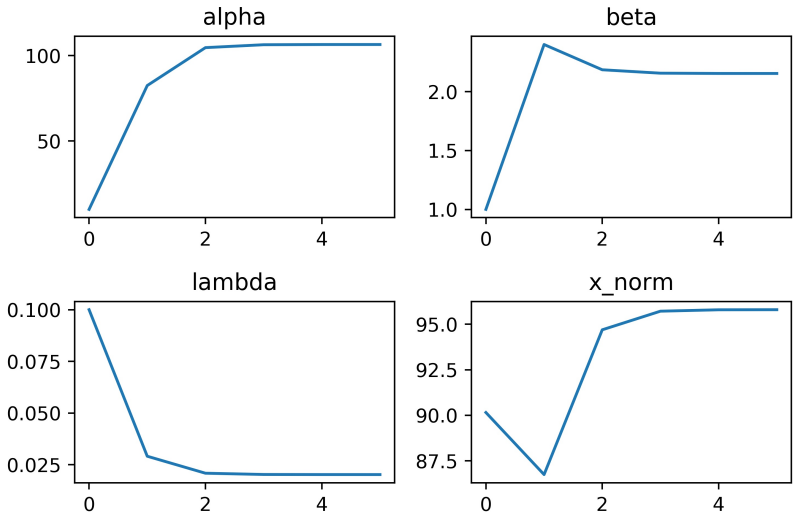
(a) Algorithm 1

(b) Algorithm 4

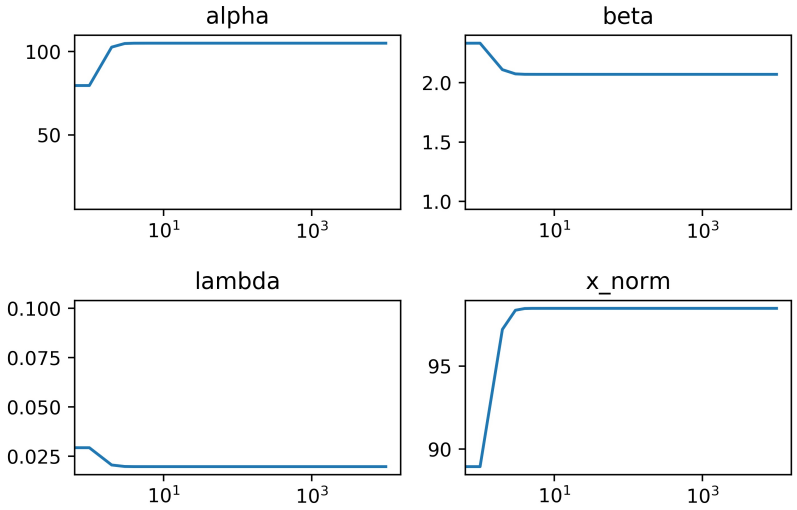
(c) Algorithm 2

(d) Algorithm 3

Figure 9: Plots of Optimal Parameter at Each Iteration

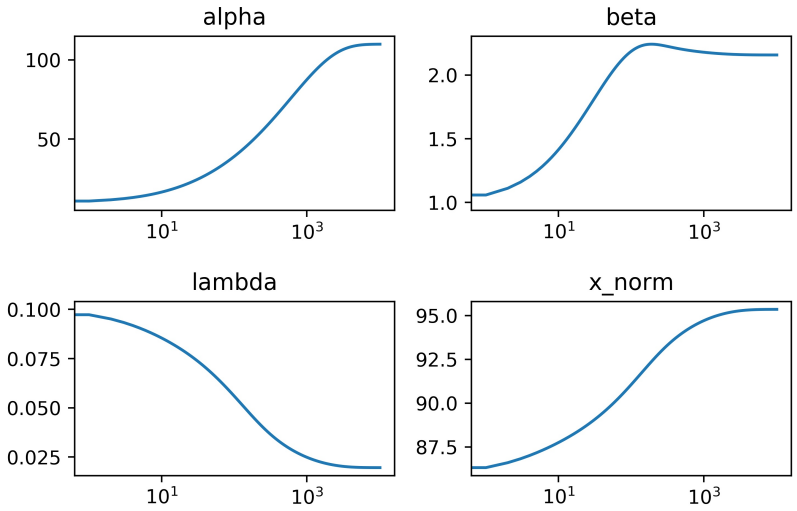


(a) Algorithm 1

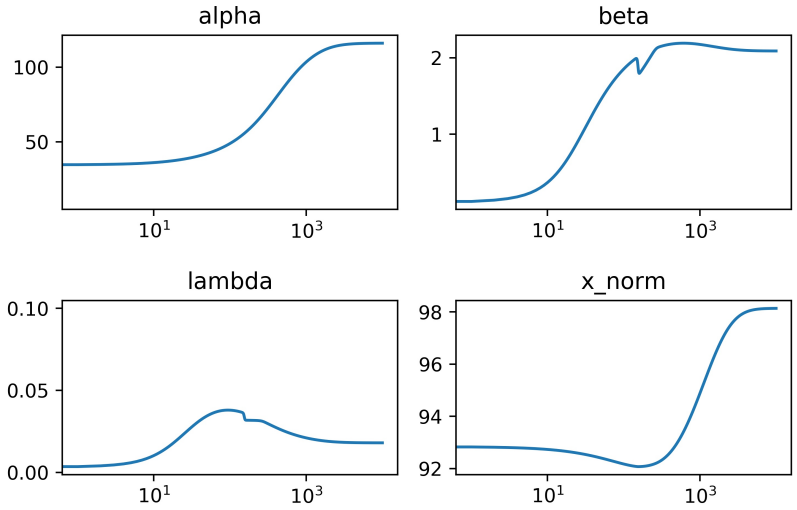


(b) Algorithm 4

Figure 10: Convergence of estimators Algorithm 1 and 4



(a) Algorithm 2



(b) Algorithm 3

Figure 11: Convergence of estimators Algorithm 2 and 3

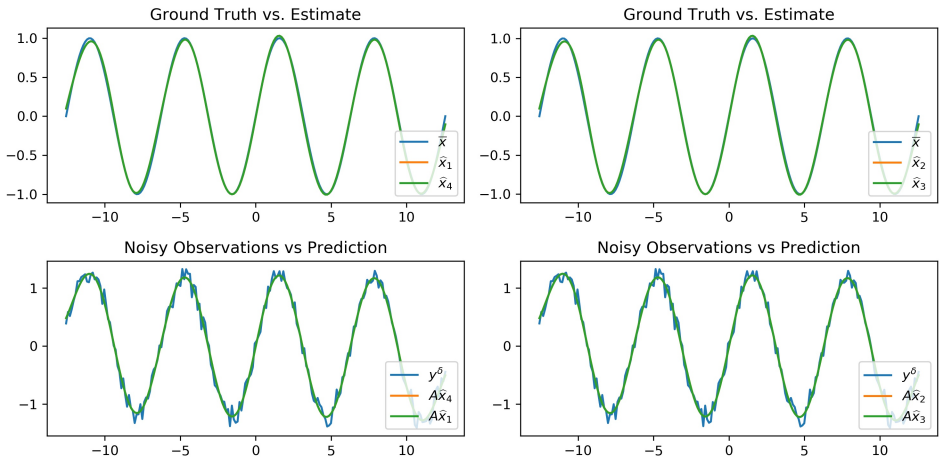


Figure 12: Top plots are of $\widehat{x}$ found by each algorithm versus the ground truth $\bar{x}$. Bottom plots compare the noisy observations versus $A\widehat{x}$ for each Algorithm. On the left we compare Algorithm 1 and 4, and on the right we compare Algorithm 2 and 3.

	$\boldsymbol{\alpha}$	$\boldsymbol{\beta}$	$\boldsymbol{\lambda}$	$\boldsymbol{\mathcal{J}}(x, \alpha, \beta)$	$\boldsymbol{\|\|\bar{x} - \widehat{x}\|\|_2^2}$	**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

However $\{\beta\}_i$ is not. In the bottom plots of figure (11) we see a strange kink that was also seen in figure (d) of (9). We are unsure why this is so.

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

7.4 Convergence and Consistency

In the this section we examine consistency and convergence of Algorithm 1, since this was the only one that converged and converged relatively quickly. We proposed that

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

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

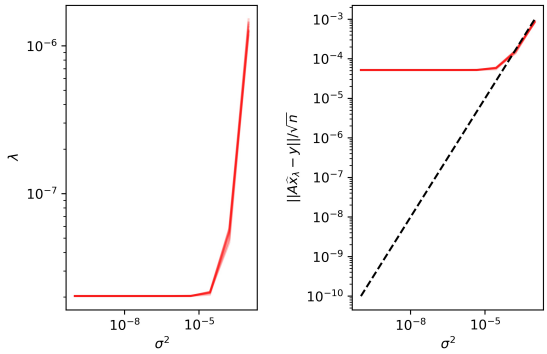


Figure 13: Regularization vs noise and Estimate of residuals vs noise

tion. We also see the effects of bounding β/α in the plot (fig 13) on the right hand side where at some level of noise Algorithm 1 slightly over estimates the noise level as it is bounded away from zero.

7.5 Sensitivity

In this section we examine the sensitive of algorithm 1, to values of the hyper priors. This was already explored in [7], but we make an additional observation that in for certain values of hyper parameters the objective function increased to a critical point rather than decreased to the minimum.

$b_0 = b_1$	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 $b_0 = b_1$

$a_0 = a_1$	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 $a_0 = a_1$

Varying b_0, b_1 the variance parameters to the hyper priors does not seem to effect convergence. We see that too large $b_0 = b_1$ leads to over regularization, but for $b_0 = b_1 < 1e-4$ we see little change. It is strange that in the first two cases $\mathcal{J}$ is minimized at a high positive value [figs 14, 15]. It does seem to be the case that $a_0 = a_1$ can be chosen more freely,([7] pages 16-18), in that small or large values lead to similar regularization and convergence. However the again large values for $a_0 = a_1$ lead to a high value positive of $\mathcal{J}$ at the critical point. See appendix for plots of the objective function and the comparison between $\bar{x}$ vs $\widehat{x}$ and y^δ vs $\widehat{Ax}$.

8 Conclusions

We have shown that under the assumption that the data is coming from a normal distribution and the noise is addition normal computing the MAP estimates of the posterior distribution $p(x, \alpha, \beta \mid y)$ is equivalent to $\min_{x,\alpha,\beta} \mathcal{J}(x, \alpha, \beta)$. Solving the minimization problems allows us to simultaneously estimate the underlying parameter x, the regularization parameter λ, and the noise level. We have developed and implement numerical methods to solve the functional $\mathcal{J}$, in the case that no closed form solution exists for x, and α, β, as well as show their convergence to a minimum. We have shown that in the simple case, these algorithms work relatively well suggesting that using a gradient methods in place of the close form solution should work, as would be necessary in the case of non-smooth priors. We looked again at the effects of the hyper prior on the alternating algorithm from [7], and see that in fact they play important role. For some choice of the hyper priors the functional no longer decreases, so convergence to a minimum is not guarantee. We have seen that for some choice of hyper priors the functional actually increases. Perhaps this is because a saddle point exists or for some hyper priors $\mathcal{J}$ is no longer convex. Additionally while developing methods 2 and 3, we saw that step size played an important role in the convergence. From the theory we know that this step size depends on the Lipschitz continuity. In our implementation, we used an ad-hoc fixed step size in method 3. The step size in method 3 is a weighted step size that accounts for the different scales of α, β, as well as the differing steepness in each direction

respectively.

Further research would be

- Analyze the role of the hyper priors and develop a method to choose them without the knowledge noise level or variance of the underlying parameter.
- Extend the parameter choice method to settings to the non-normal setting such as non smooth and spare priors and larger scale settings where $n >> 200$.
- Adjusted algorithms 2 and 3 to be able to solve the resulting functional.
- Develop and implement an adaptive step size for faster convergence.

9 Appendix

9.1 Sensitivity Plots

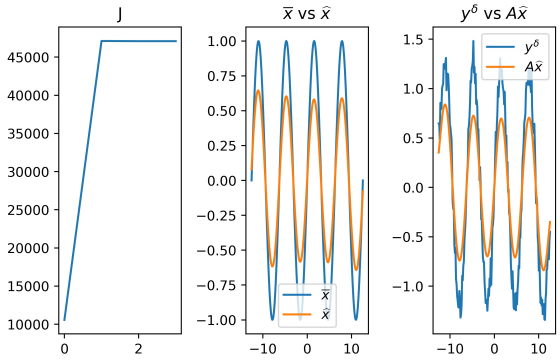


Figure 14: Results when $b_0 = b_1 = 1e4$

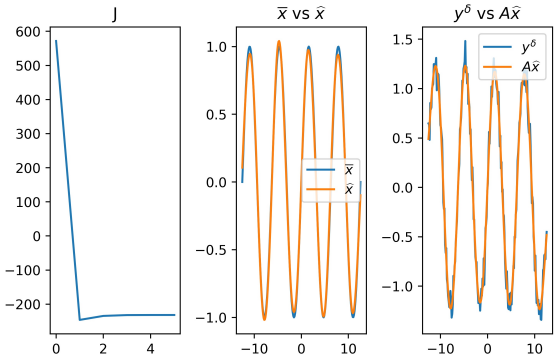


Figure 15: Results when $b_0 = b_1 = 1e-8$

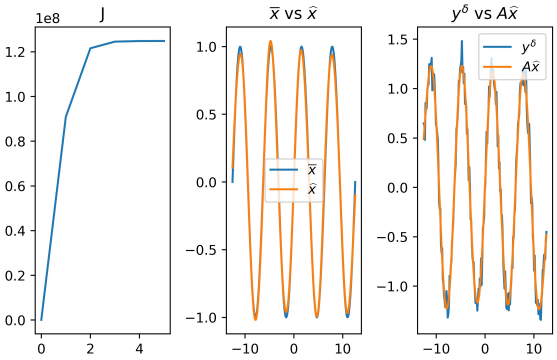


Figure 16: Results when $a_0 = a_1 = 1e4$

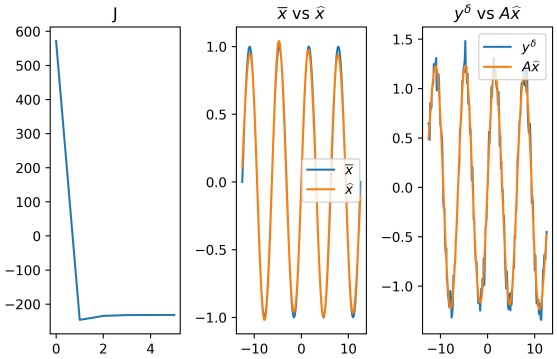


Figure 17: Results when $a_0 = a_1 = 1e-8$

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