Degree Project

A general L-curve technique for ill-conditioned inverse problems based on the Cramer-Rao lower bound

Author: Simrah Farooqi & Sruthi Kattuparambil Sreenivasan
Supervisor: Sven Nordebo
 Examiner: Sven Erik Sandström
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Abstract

This project is associated with statistical methods to find the unknown parameters of a model. It is the statistical investigation of the algorithm with respect to accuracy (the Cramer-Rao bound and L-curve technique) and optimization of the algorithmic parameters. This project aims to estimate the true temperature (final temperature) of a certain liquid in a container by using initial measurements (readings) from a temperature probe with a known time constant. Basically, the final temperature of the liquid was estimated, before the probe reached its final reading. The probe obeys a simple first-order differential equation model. Based on the model of the probe and the measurement data the estimate was calculated of the ‘true’ temperature in the container by using a maximum likelihood approach to parameter estimation. The initial temperature was also investigated. Modelling, analysis, calculations, and simulations of this problem were explored.

Keywords: Temperature estimation, Maximum likelihood estimation (MLE), Cramer-Rao Lower bound (CRLB), Fisher information, L-curve analysis.
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Simrah Farooqi and Sruthi Kattuparambil Sreenivasan
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1 Introduction

Many electrical and signal processing systems are built on estimation theory. This theory is employed in a wide range of applications, from voice processing to radar, because it is useful in estimating the needed information from the received data. These systems use parameter estimation to extract the unknown parameter $\theta$ from a given N-point data set [1]. Parameter estimation offers methods for effectively using data to estimate constants that exist in mathematical models [1], [2]. This project also uses parameter estimation as its basis for calculation.

This work focuses on numerically investigating (estimating) the true temperature of a liquid in a container based on measurements (readings) from a temperature probe with a given time constant. Basically, a thermal probe is dipped into the container which measures the temperature of the liquid, but the initial and final temperatures of the probe are unknown and the temperature of the probe changes over time. The probe is too slow to measure the temperature of the liquid immediately. The Maximum Likelihood Estimator (MLE) is used to estimate the true temperature of the liquid for fast response. The MLE is a popular approach for parameter estimation [3]. Further, in this paper, the MLE for the final and the initial temperatures will be derived and discussed. The Cramer Rao bound (CRB) is used for the accuracy which will also be discussed and derived in detail for these temperatures. Based on the CRB, investigations on L-curve are made for the suitable set of measurement points. Theoretical development along with the simulation part of the system will be considered and the result be examined and investigated at the end. More discussion follows the overview of the setup.

The probe obeys a simple first-order differential equation. The first-order differential equation of the probe is given by,

$$\frac{dT}{dt} = a(T_f - T)$$

which can also be written as,
\[
\frac{dT}{dt} + aT = aT_f
\]

(1)

where \(a\) is known or assumed physical constant and \(\tau = \frac{1}{a}\) is the time constant of the temperature probe. Here, \(T\) is the temperature of the probe as a function of time \(t\) and \(T_f\) is the temperature of the liquid (also the final temperature of the probe when \(T_f\) is a constant). According to the given differential equation, the concept of temperature tracking can be plotted as shown below where \(T_0\) denotes the initial temperature of the probe.

![Figure 1: Temperature tracking](image)

The Maximum Likelihood Estimator is used as the tool to calculate the estimate for the true or final temperature of the liquid container. Consider we have random samples, \(x_1, x_2, x_3, x_4, \ldots, x_n\), of the time dependent temperature \(T\), whose probability distribution depends on some unknown parameter \(\theta\), where two unknown parameters are considered, \(T_f\) and \(T_0\). Then the equation for the estimator can be written in the matrix form,

\[
x = H\theta + \omega
\]

In the matrix form, a model \(x\) is created with the unknown parameters.

White (uncorrelated) Gaussian noise \(\omega\) is added to the estimation to simulate the data.
2 Theoretical framework/
Methodological approach

The basic methodology of this thesis is that a maximum likelihood estimator is designed to calculate our required parameters and in doing so it is considered that this problem is an ill-conditioned inverse problem but a well-posed problem. The problem is then regularized with respect to the size of the measurement aperture. By employing a generic technique an L-curve was obtained by plotting the Cramer-Rao lower bound of the estimated parameters with respect to the measurement aperture.

When faced with an inverse problem, we deduce the cause from the observed (estimated) effect. This relationship between the effect and the cause is usually ill-conditioned meaning that the recovered estimate is very noise-sensitive, even a small measurement uncertainty results in a large uncertainty in the knowledge of the quantity to be estimated [4].

To gain a better understanding of this project, we must first examine some fundamental concepts outlined in the following sections.

2.1 Basic setup

In this problem, it is assumed that we have a physical process with measurable parameters, that is, the probe's temperature reading, i.e., $T_1, T_2, T_3, \ldots, T_n$ and is well-defined by a physical model with parameters that we are trying to estimate that is the initial temperature $T_0$ and the final temperature $T_f$ of the probe. The physical model itself (here a differential equation $\frac{dT}{dt} + aT = aT_f$ and the time constant of the probe i.e., $\tau = \frac{1}{a}$) is assumed to be given. The liquid's container is regarded as being "very large," and its temperature doesn't vary noticeably over time (its time constant is quite large). It is therefore regarded as being constant. The probe (the thermometer) is seen as being "small," and it has a time constant that is
comparatively extremely small to the liquid’s time constant, which may be on the order of hours, days, etc., and is reasonably detectable in a few seconds.

2.2 Description of MLE

Maximum Likelihood Estimation (MLE) is used in the process to estimate the parameters $T_0$ and $T_f$. It is a statistical technique for determining the characteristics of a probability distribution that best characterize the data set being studied. The basic principle of MLE is to find the parameter values that maximize the likelihood of the given data, presuming that the observed data were created by the specified distribution. Given the measurement vector $x$, the Maximum Likelihood (ML) estimate $\hat{\theta}_{ML}(x)$ is the parameter vector $\theta$ that maximizes the likelihood function [5].

$$\hat{\theta}_{ML}(x) = \arg \max_\theta p(x|\theta)$$

Or $\hat{\theta}_{ML}(x) = \arg \max_\theta \ln p(x|\theta)$

For larger samples, MLE delivers unbiased findings. This means that the estimator will typically produce the accurate value of the unknown parameter [5]. Generally, the parameter values are anywhere between $a < \theta < b$. According to the unbiasedness, the estimator will always produce the average genuine value of theta. So mathematically the estimator is unbiased if,

$$E(\hat{\theta}) = \theta \quad a < \theta < b$$

Further, in the next section, we will analytically derive the MLE for this project.

2.3 Description of time aperture

It is also assumed that this inverse problem is well-posed as per Hadamard's definition which states that the problem should have a unique solution and the solution's behavior changes continuously with the initial conditions [6]. So, our estimated parameters are unique and depend continuously on the
initial conditions. It is further assumed that measuring data is collected over a finite "aperture" (Δ) specified on the measurement domain and that as the aperture's size decreases toward zero, the inverse issue becomes progressively ill-conditioned and even singular. Based on the temperature $T$ at time $t_n$ the time aperture can be defined by the following equation:

$$t_n = t_c + \frac{n - 1}{N - 1} \Delta$$

where Δ is considered as the time aperture. Here, N is the number of samples and $n= 1, N$. This means that in our canonical example, the time aperture consists of the measurement interval of the temperature probe.

An extremely advantageous situation, in this case, is that we may assume that the time constant of the probe is known, meaning that it can be measured (or modeled) a priori with extremely high accuracy. This creates the ideal environment for formulating an estimation issue using a physical model of the probe and certain statistical presumptions on the measurement noise of the probe.

### 2.4 Usage of CRLB and Fisher Information

In this problem, we have applied the Cramer-Rao lower bound CRB for estimating $T_f$ as a function of time aperture $\Delta$. The Cramer-Rao Lower Bound (CRLB) provides a lower estimate of the variance of the unbiased estimator. It claims that any unbiased estimator's precision is only limited by the Fisher information, or the Fisher information's reciprocal provides a lower bound on its variance [7].

We want to estimate $\theta$ parameter, from N measurement of samples. The variance of any unbiased estimator $\hat{\theta}$ of $\theta$ is then bounded by the reciprocal of the Fisher information. The Cramer-Rao theorem states the following under assumption and other regularity conditions,
\[ \text{Var}(\theta) \geq \frac{1}{I(\theta)} \]

I(\theta) represent the Fisher Information that is the measure of our knowledge about the sample's distribution. Fisher information is a statistical term that quantifies the amount of knowledge regarding an unknown parameter in a statistical model that may be found in an observed dataset. The Fisher information formula is given by,

\[ I(\theta) = E\left\{ \frac{\partial}{\partial \theta} \ln p(x|\theta) \frac{\partial}{\partial \theta^T} \ln p(x|\theta) \right\} \]

and the Cramer-Rao bound formula is given by,

\[ C_\theta = E\{ (\hat{\theta}(x) - \theta) (\hat{\theta}(x) - \theta)^T \} \geq I^{-1}(\theta) \]

where \( \ln p(x|\theta) \) is the log-likelihood function [7]. Simply stated, the CRLB indicates the minimal amount of uncertainty that may be expected when estimating a parameter using the Fisher information. The fisher information and corresponding Cramer Rao lower bound for this project are calculated further in the succeeding section.

2.5 The L-curve Analysis

Fundamentally, this problem is ill-conditioned for short measurement time intervals. To maintain good accuracy on the estimated temperature of the liquid this problem is then regularized by doing the L-curve analysis on the corresponding Cramer Rao lower bound.

The L-curve criterion is a graphical method used to choose parameters in regularization algorithms such as Tikhonov and truncated singular value decomposition (principal component regression). The primary objective of these regularization techniques is to stabilize the solution by integrating more details. Regularization is necessary when solving inverse problems and when we plot the acquired estimation error against some regularization parameter value, we observe a very noticeable L-shaped curve with a distinct 'knee'
where the problem becomes practically insolvable. The L-curve is a user-friendly graphical tool that displays the tradeoff between the size of a regularized solution, and it’s fit to given data, as the regularization parameter changes. The aim of this criterion is to strike a balance between two variables plotted on a logarithmic scale [8].

Further, the regularization and L-curve technique is discussed in little detail to understand it better. Suppose that the ill-posed inverse problem’s solution is denoted by \( \tilde{x} \) which is a regularized least squares function of a particular kind.

\[
\tilde{x} = \arg \min \left\{ ||Ax - b||^2 + \lambda R(x) \right\}
\]

where for a given \( x \), \( Ax-b \) represents the difference between the experimental data \( b \) and the reconstructed data \( Ax \). \( R(x) \) is the regularized term that responds to the noise of \( b \) and it usually includes some previous information on the solution, and \( \lambda \) is an actual regularization parameter that must be chosen by the user. It is to be noted that if the regularization of the solution is too large then it will not fit the given data properly and the residual \( ||Ax - b||^2 \) will be large too. However, the fit will be good, but the solution will be heavily influenced by the contributions from the data errors if insufficient regularization is applied so \( R(x) \) will be too big.

These two values \( (||Ax - b||^2, \lambda R(x)) \) can be plotted against one another naturally as a curve. i.e., the L-curve and parameterized by regularization parameter \( \lambda \). The corner of the L-curve is the point with maximum curvature, where the residual error and solution norms are balanced [8]. Following figure shows an example of the L-curve obtained by plotting Cramer Rao bound with respect to measurement aperture \( \Delta \).
Hence, for an ill-posed inverse problem without a regularization, the problem may become infeasible to solve, but with a regularization beyond a critical point (the ’knee’) the problem solution all in a sudden becomes very stable.

In this thesis, we will demonstrate that a similar behavior will be observed if an ill-conditioned (but well-posed) inverse problem is regularized with respect to the size of the measurement aperture. We will employ the L-curve technique obtained by plotting the Cramer-Rao lower bound of the estimated parameters with respect to the measurement aperture. The method is demonstrated using the temperature probing problem as described previously. This method is also predicted to be applicable to many other different problem formulations because the method formulated is generic rather than specific.

3 Analytical Methodology

3.1 Initial Value Problem to solve the differential equation of the probe

Consider a temperature probe inserted into a large liquid container at time \( t=0 \). Let the temperature of the probe at time \( t=0 \) as \( T_0 \) and the liquid in the
container has a temperature of $T_f$. The rate of change of temperature with respect to time can be represented as,

$$\frac{dT}{dt} = aT_f - aT$$

where, $T_f$ is constant, $a$ is a physical constant given by $a = \frac{1}{\tau}$, where $\tau$ is the time constant.

![Basic concept of temperature probe inside the liquid container](image)

Figure 3: Basic concept of temperature probe inside the liquid container

The homogeneous solution of the problem can be derived as below since $T_f$ is a constant,

$$\frac{dT}{dt} + aT = 0,$$

which implies that,

$$\frac{dT}{dt} = -aT \Rightarrow \int_1^T dT = \int -a dt \Rightarrow$$

$$\ln T = -at + C \Rightarrow T = Ae^{-at}$$

the homogenous solution can be written as,

$$T_h(t) = Ae^{-at} \quad (2)$$

where $A$ is the constant coefficient.
Estimation problem:

Consider \( \frac{dT}{dx} + aT = aT_f \) and \( T(t_1) = T_1 \)

\[ \Rightarrow T(t) = T_1 e^{-at} + T_f(1 - e^{-a(t-t_1)}) \]

\[ = (T_0 e^{-at_1} + T_f (1 - e^{-at_1}) \gamma^{-a(t-t_1)} + T_f (1 - e^{-a(t-t_1)}) \]

\[ = T_0 e^{-at} + T_f (1 - e^{-at}) \]

The statistical model for the estimation problem for simulation can be represented as,

\[ x(t_n) = T_1 e^{-a(t_n-t_1)} + T_f (1 - e^{-a(t_n-t_1)}w_n \]

where \( w_n \) is the white Gaussian noise to simulate the data and it can be represented as \( E(w_nw_m) = \sigma^2 \delta_{nm} \) (Explained in detail in Chapter 2).

\[ t_n = t_1 + \frac{n-1}{N-1} \Delta \]

where \( n \) is the sample index, \( n=1,2,3,....,N \)

\[ t_n - t_1 = \frac{n-1}{N-1} \Delta \] \[ = \frac{m \Delta}{N-1} \] \[ [5] \]

where \( m = n-1= 0,1,2,....,N-1. \)

### 3.1.1 Temperature tracking

Consider the statistical model, \( x(t_n) = T_1 e^{-a(t_n-t_1)} + T_f (1 - e^{-a(t_n-t_1)} + w_n \)

In matrix notation
\[
\begin{bmatrix}
    x(t_1) \\
    \vdots \\
    x(t_N)
\end{bmatrix} =
\begin{bmatrix}
    e^{-a(t_1-t_1)} & 1 - e^{-a(t_1-t_1)} \\
    \vdots & \vdots \\
    e^{-a(t_N-t_1)} & 1 - e^{-a(t_N-t_1)}
\end{bmatrix}
\begin{bmatrix}
    T_1 \\
    \vdots \\
    T_f
\end{bmatrix} +
\begin{bmatrix}
    W_1 \\
    \vdots \\
    W_N
\end{bmatrix}
\]

which is in the form of \( x = H\theta + w \) representing the statistical model.

The estimator operator is,
\[
\hat{\theta}_{ml}(x) = (H^TH)^{-1}H^T x = \begin{bmatrix}
    \hat{T}_1 \\
    \vdots \\
    \hat{T}_f
\end{bmatrix}
\]

From the definition of the Fisher Information Matrix in the previous chapter, the Fisher Information Matrix is, \( I(\theta) = \frac{1}{\sigma^2}H^TH \). From the Fisher Information matrix, the Cramer Rao Lower Bound for the estimator can be written as,
\[
\text{CRB} = I^{-1}(\theta) = \sigma^2(H^TH)^{-1}
\]

which implies the following error covariance for the estimator,
\[
E\{(\hat{T}_f - T_f)^2\} \geq I^{-1}(\theta)
\]

Considering the column vector elements for the H matrix for \( n=1, 2, \ldots, N \) and \( m=0, 1, \ldots, N-1 \),
\[
H = \begin{bmatrix}
    e^{-a(t_N-t_1)} & 1 - e^{-a(t_N-t_1)}
\end{bmatrix}
\]

Substituting for \( n \) in terms of \( m \), \( t_N - t_1 = \frac{m\Delta}{N-1} \) gives,
\[
H = \begin{bmatrix}
    e^{-a\frac{m\Delta}{N-1}} & 1 - e^{-a\frac{m\Delta}{N-1}}
\end{bmatrix}
\]

Now, the Fisher Information is given by \( I = H^TH \)
\[
= \begin{bmatrix}
    \sum_{m=0}^{N-1} e^{-2a\frac{m\Delta}{N-1}} & \sum_{m=0}^{N-1} e^{-a\frac{m\Delta}{N-1}}(1 - e^{-a\frac{m\Delta}{N-1}}) \\
    \sum_{m=0}^{N-1} e^{-a\frac{m\Delta}{N-1}}(1 - e^{-a\frac{m\Delta}{N-1}}) & \sum_{m=0}^{N-1} (1 - e^{-a\frac{m\Delta}{N-1}})^2
\end{bmatrix}
\]
\[
A = \sum_{m=0}^{N-1} e^{-\frac{a m \Delta}{N-1}} \left( e^{-\frac{m \Delta}{N-1}} - 1 \right), \quad B = \sum_{m=0}^{N-1} e^{-\frac{m \Delta}{N-1}} \left( e^{-\frac{a m \Delta}{N-1}} - 1 \right) \quad \text{and substituting} \quad \sum_{m=0}^{N-1} \left( e^{-\frac{m \Delta}{N-1}} - 1 \right) + e^{-\frac{2a m \Delta}{N-1}} = N - 2B + A.
\]

3.1.2 Accuracy optimization of Temperature tracking

Cramer Rao Lower Bound and Fisher Information matrix helps to improve the accuracy of the temperature tracking. From the above substitutions, the Fisher Information Matrix can be represented as follows,

\[
I = \begin{bmatrix} A & B - A \\ B - A & N - 2B + A \end{bmatrix} = \begin{bmatrix} a & b \\ b & c \end{bmatrix}
\]

Cramer Rao Lower Bound for the temperature tracking is the inverse of the Fisher matrix and it can be represented as follows,

\[
I^{-1} = \frac{1}{ac-b^2} \begin{bmatrix} c & -b \\ -b & a \end{bmatrix}
\]

since it is a 2×2 matrix it can be solved as for A and B,

\[
\text{CRB}(T_f) = [I^{-1}]_{22} = \frac{a}{ac-b^2} = \frac{A}{A(N-2B+A)-(B-A)^2}
\]

\[
= \frac{A}{A(N-2B+A)-(B^2-2AB+A^2)} = \frac{A}{A(N-2B+A)B^2+2AB-A^2}
\]

\[
= \frac{1}{N-2B+A-A^{-1}B^2+2B-A} = \frac{1}{N-A^{-1}B^2}
\]

\[
A = \frac{1-e^{-\frac{2a \Delta N}{N-1}}}{1-e^{-\frac{2a \Delta}{N-1}}}, \quad B = \frac{1-e^{-\frac{a \Delta N}{N-1}}}{1-e^{-\frac{a \Delta}{N-1}}}
\]

\[
\lim_{\Delta \to 0} A = 1, \quad \lim_{\Delta \to 0} B = 1 \quad \Rightarrow \quad \lim_{\Delta \to 0} \text{CRB}(T_f) = \frac{1}{N} \quad [5]
\]
With noise $\sigma \neq 1$ we have

$$\text{CRB}\left(T_f\right) = \sigma^2 \frac{1}{N - \frac{B^2}{\Delta}} \quad \text{and} \quad \lim_{\Delta \to \infty} \text{CRB}\left(T_f\right) = \frac{\sigma^2}{N}$$

4 Algorithm analysis and coding

Based on the exponential temperature relaxation model with added noise, there are two parameters to estimate, the initial temperature $T_0$ at sample time $t=0$ and the final temp $T_f$ (at time $t = \infty$). First, the initial model is set up for the simulation. The values given to different parameters in the model are arbitrary, we can set up any values according to our choice which is suitable for calculations. The algorithm and MATLAB coding is based on the calculations done before in the analytical analysis and are as follows.

- The time constant is taken as $\text{tau}$ of the temperature probe is 5 sec.
- $a$ is set as the model parameter calculated as the reciprocal of tau.
- $T_0$ is represented as the initial temperature of the probe.
- $T_f$ is the final temperature of the probe, which is assumed to be the same as the ambient liquid.
- $t$ is the time axis for plotting, ranging from 0 to 90 with a step size of 0.1.
- The modeled temperature without noise is designed using the equation:

$$T = T_0 + (T_f - T_0) \times (1 - e^{-at})$$

This algorithm will create a simulation that will display the actual temperature of the liquid. Then we will further compute the estimated parameters whose values should be closer to these actual parameters. The results and observations of the simulation will be discussed and displayed in the upcoming section of this thesis. Following is the MATLAB coding to create a simulation.
After that, we created two MATLAB scripts to implement the temperature tracking. We will discuss the first one further. The estimate is based on measurements taken at \( N \) uniformly spaced sample times, \( t_1 \) through \( t_N \), with a time aperture of \( \Delta t = t_N - t_1 \). The algorithm and coding are as below.

- We have set the value of \( N \) to 10, representing the number of samples for estimation.
- To begin sampling, set the start time, \( t_1 \), to 0.
- \( \Delta t \), the time aperture for sampling is set, as 2.
- To calculate the stop time for sampling, we need to add \( t_1 \) and \( \Delta t \) together. The result of this addition will be the value of \( t_N \). Generate \( N \) equally spaced sampling times between \( t_1 \) and \( t_N \) using the \texttt{linspace} function and store them in the variable \( t_s \).
- To reshape "ts" into a column vector, we need to modify its dimensions.
- Set the standard deviation of the measurement noise, denoted by \( \sigma \), to 0.1.
- Generate \( N \) samples of zero-mean white Gaussian noise with standard deviation \( \sigma \) and store them in the variable \( w \).
- Simulate the measured temperature with noise at each time point in \( t_s \) using the equation shown below,

\[
x = T_0 + (T_f - T_0) \times (1 - e^{-\frac{t}{\tau}}) + w,
\]
After generating this data, we will generate the matrix \( H \) and then apply the maximum likelihood estimate as calculated in the numerical calculations to find the unknown parameters. The algorithm and coding are as below.

Calculate matrix \( H \):

- Assign a value range of 0 to \( N-1 \) to \( m \).
- Create a column vector from \( m \).
- Use the formula as derived before to calculate the matrix \( H \).

Estimate the parameters:

- Apply the formula as derived before to determine the maximum likelihood estimate of the parameters.
- Extract the estimated final temperature \( \hat{T}_f \) from the maximum likelihood estimate vector.
- Extract the estimated value of initial temperature \( T_1 \) from the maximum likelihood estimate vector.

Plot the estimated values,

- Plot the true temperature value which will be a solid line.
- Plot the measured temperature values \( N \) number of times at specific time instances.
- Plot the estimated final temperature ($T_{f\text{hat}}$) at the corresponding time point ($t_N$).
- Plot the estimated value of $T_1$ ($T_{1\text{hat}}$) at the corresponding time point $t_1$.
- Plot a dashed line at the temperature value $T_f$ for reference.
- Set the x-axis for time ($t$) and y-axis for temperature ($T$).
- Set the title and legends according to the need.

Now, further, we will do the Cramer-Rao bound analysis for the estimated final temperature over time aperture. The Algorithm will explain it further followed by the MATLAB coding:

To calculate the CRB we will first calculate the Fisher information matrix:

- Compute the Fisher information matrix, $I$ using the formula: $I = H' * H / (\sigma^2)$, where $H$ is the matrix defined earlier.

Calculate the Cramer-Rao bound:

- Compute the inverse of the $I$ matrix to get the CRB matrix using the formula: $\text{CRB} = \text{inv}(I)$.
- Extract the Cramer-Rao bound for estimating $T_f$ from the CRB matrix: $\text{CRBT}_f = \text{CRB} (2,2)$. 

```matlab
Estimation of parameters
m=0:N-1;
m=m(:);
H=[exp(-a*m*ap/(N-1)) 1-exp(-a*m*ap/(N-1))];
theta_hat=inv(H'*H)*H'*x;
T_hat=theta_hat(2);
T1_hat=theta_hat(1);
figure(1)
plot estimated values
plot(t,T,'b-')
hold on
plot(tN,T_hat,'k*')
plot(t1,T1_hat,'g*')
plot([0 100],T_f*[1 1],'-')
hold off
axis([0 100 18 100])
xlabel('time t(s)')
ylabel('temperature T(\degree C)')
title('Modeled temperature')
legend('true temp','measured temp','Tfhat (estimate)','T1hat (estimate)')
```
Now to do the L curve analysis we will calculate CRBTF as a loop over time axis \( t_N \)

- Make a range of time aperture values with a specific step size.
- Create an empty vector to store the Cramer-Rao bound values.
- Create a loop and iterate over each value in time aperture.
- Recalculate the matrix \( H \) using the updated \( \text{ap} \) value.
- Recalculate the Fisher information matrix \( I \), using the updated \( H \) matrix.
- Recalculate the inverse of the Fisher information matrix to get CRB.
- Extract the Cramer-Rao bound for estimating \( T_f \) from the CRB matrix and store it in the corresponding index of \( \text{CRBTFvec} \).
- Then make a figure of the above and label it accordingly.

\[
\%
\text{Cramer-Rao bound analysis}
\]
\[
\text{I}=H'^{\ast}H/\left(\text{sigma}^2\right);
\]
\[
\text{CRB}=\text{inv}(\text{I});
\]
\[
\text{CRBTF}=\text{CRB}(2,2);
\]
\[
\text{CRBTFvec} = \text{sigma}^2/\text{N}
\]

\[
\%
\text{Calculate CRBTF as a loop over } t_N
\]
\[
\text{apvec}=0.1:0.1:10; \% \text{time aperture for sampling}
\]
\[
\text{CRBTFvec}=\text{zeros}(1,\text{length(apvec)});
\]
\[
\text{for ind}=1:\text{length(apvec)}
\]
\[
\text{ap}=\text{apvec}(\text{ind}); \% \text{time aperture}
\]
\[
H=\text{exp}\left(-\text{a}*\text{ap}/\left(\text{N}-1\right)\right)\text{ exp}\left(-\text{a}*\text{ap}/\left(\text{N}-1\right)\right);
\]
\[
\text{I}=H'^{\ast}H/\left(\text{sigma}^2\right); \% \text{Fisher information matrix}
\]
\[
\text{CRB}=\text{inv}(\text{I}); \% \text{Inverse of Fisher information matrix}
\]
\[
\text{CRBTFvec}(\text{ind})=\text{CRB}(2,2); \% \text{Cramer-Rao bound for estimating } T_f
\]
\[
\text{end}
\]
\[
\text{figure}(2)
\]
\[
\text{plot}(\text{apvec},\text{CRBTFvec})
\]
\[
\text{axis([0 10 -1 30])}
\]
\[
\text{title('Cramer-Rao bound for estimating } T_f \text{ (L-curve)')}
\]
\[
\text{xlabel('ap (time aperture)')}
\]
\[
\text{ylabel('CRB(Tf)')}
\]
\[
\text{grid on}
\]

The other MATLAB script performs the identical computations, but to illustrate how the estimation might go over time, it increases the values of the estimation start time \( t_1 \) and end time \( t_N = t_1 + \text{ap} \). The coding is given below:
% Temperature tracking algorithm and analysis

% Loop over start time t1
t1vec=0:0.1:20;
for index=1:length(t1vec)
    t1=t1vec(index); % start time for sampling

% Model set-up for simulation
tau=5; % time constant of temperature probe
a=1/tau; % model parameter
T0=20; % initial temperature of the probe
Tf=80; % final temperature of the probe (same as ambient liquid)
t=0:0.1:90; % time axis for plot
% modeled temperature for 'true' parameters without noise
T=T0+(Tf-T0)’*(1-exp(-a*t));
N=5; % number of samples for estimation
% generate random data
t1=0; % start time for sampling
ap=5; % time aperture for sampling
Nt=1+ap; % stop time for sampling
tns=linspace(t1,tN,Nt); % sampling times
t=ts(:,1); % make ts column vector
sigma=0.1; % standard deviation of noise
w=sigma*randn(N,1); % measurement noise (zero-mean white Gaussian noise with standard deviation sigma)

% Simulated (measured) Temperature with noise at time ts
x=T0+(Tf-T0)’*(1-exp(-a*t1))+w;
% end of data simulation

% Estimation of parameters
m=0:N-1;
m(:,1);
H=[exp(-a*m*ap/(N-1)) 1-exp(-a*m*ap/(N-1))];
thetaHat=inv(H’*H)*H’*x; % maximum Likelihood estimate
Tthat=thetaHat(2); % Estimated final temperature (Tfhat)
T1=thetaHat(1); % Estimated value of T1
% Plot estimated values
figure(1)
plot(t,T,'b-')
hold on
plot(tns,x,'r*')
plot(tN,Tthat,'k*')
plot(t1,T1,'g*')
plot([0 100],Tf*[1 1],'-')
hold off
axis([0 100 10 100])
xlabel('time t(s)')
ylabel('temperature T(°C)')
title('Modeled temperature')
Fortunately, as mentioned earlier, the estimation error (CRB(Tf)) is independent of t1, which is quite interesting. The results and observations will be discussed in the next section.

5 Results and Observations

From the simulation results of the above coding the following observations can be derived.

5.1 Result

In the first script the estimate is based on

Tau=5 seconds
N=10 samples
ap=2 seconds (time aperture)
t1=0

The result can be seen below in the MATLAB plots.
Figure 4: Plot showing the result of temperature estimation algorithm

In the results and observations, the red circles represent the N number of samples which are taken over the time $t_1$ to $t_N$. The time axis for plots is set to 0-90 secs and the time constant of the probe is set to $\tau=5$ secs. The figure shows the modelled noiseless (true) temperature curve going from $T_0=20^\circ$ C to $T_f=80^\circ$ C that is the blue solid line. The estimated value of $T_f$, $T_{\text{hat}}$ is seen as a black star. From the graphical results we can see that the estimated value of final temperature is nearly equal to the actual temperature i.e., $80^\circ$ C. We can also observe the estimated initial temperature as green star i.e., nearly equal to the actual initial temperature $20^\circ$ C. The command window also shows the results. Further observations are also done in the next section.

$T_{\text{hat}} =$

80.5627

>> $T_{\text{ihat}}$

$T_{\text{ihat}} =$

19.9566
In the second MATLAB plot we can see the corresponding Cramer-Rao lower bound CRB(Tf) for estimating Tf as a function of time aperture ap.

![Cramer-Rao bound for estimating Tf (L-curve)](image)

**Figure 5**: L-curve analysis for the estimation problem

The most interesting aspect of this problem analysis is to see the very distinct 'L-shaped' curve of the CRB(Tf) as a function of time aperture ap shown in figure. We can see a very distinct 'knee' at about 0.5 secs. This means that the estimation error will increase very fast for time apertures ap less than 0.5 secs, and the error will decrease very slowly for time apertures ap greater than 0.5 secs.

The value of CRBTF can be observed as

```
CRB_Tf =
0.0626
```

```
an =
1.0000e-03
```
5.2 Observations

5.2.1 Change in the estimation curve with change in the time aperture ‘ap’

In the temperature tracking problem, it is assumed that the measurement data is collected within a limited 'aperture' (ap) that is defined on the measurement domain. As the aperture value grows, the estimation time significantly increases, leading to algorithm efficiency due to prolonged measurement time. As the aperture value decreases, the inverse problem gets more ill-conditioned and may even become singular as the aperture size approaches zero. In the example shown, the aperture refers to the specific range of measurements taken by the temperature probe.

In summary, the most interesting aspect of this discovery is the analysis conducted using the 'L-cure'. It provides guidance on selecting the time aperture 'ap'. For instance, when we execute the code with the assignment of ap=0.2 instead of 0.5, we can clearly witness the significant degradation of the estimate. In this application, we aim to minimize the time aperture to get a rapid estimator. However, we must avoid making it excessively small, since this would result in an ill-conditioned problem, leading to significant estimate errors.

![Figure 6: Plot showing the degradation estimate when time aperture is reduced](image)

Figure 6: Plot showing the degradation estimate when time aperture is reduced
5.2.2 Behaviour of L-curve according to ‘tau’

When the corner of the L-curve is closer to 0, it often suggests that the model exhibits a higher degree of bias towards simplicity or underfitting. Put simply, the model might not be able to accurately represent the complexities found in the data. This can lead to decreased model performance and less capacity to properly depict the fundamental patterns in the data. Under such circumstances, it may be imperative to contemplate augmenting the intricacy of the model or fine-tuning the regularization parameters to enhance the model's conformity to the data. The below example shows the results from the estimation algorithm with tau changed to 2 instead of 5.

Figure 7: Temperature estimation with tau changed to 2

Figure 8: Behaviour of L-curve with tau = 2
5.2.3 Proportional change in Estimation error with respect to N

Another observation that can be inferred from the simulation results is the variation in the number of samples (N). As the number of samples increases, the estimate error decreases. The decline in the CRB curve is negatively correlated with N. A CRB value close to 0 suggests that the estimated parameters of a statistical model have a minimal variance. The CRB represents the minimum possible variance of an unbiased estimator for a parameter in a statistical model. When CRB approaches 0, it indicates that the predicted parameters are extremely accurate and have very little uncertainty.

![Figure 9: Estimation error when number of samples, N=5](image1)

![Figure 10: More accurate estimation when number of samples, N=50](image2)
A low CRB score indicates that the estimated parameter values are dependable and have a significant level of certainty. Precise parameter estimate is vital in domains such as signal processing, estimation theory, and parameter estimation, making it very advantageous. Nevertheless, it is crucial to acknowledge that the CRB is a theoretical limit and may not consistently mirror the practical performance of an estimator in real-life situations.

### 5.2.4 Effect of standard deviation (σ) on the L-curve

A statistical measure used to quantify the degree of variation or dispersion in a group of data points is called the standard deviation of noise. It denotes the average deviation of individual data points from the mean or expected value in the environment of noise. Greater variability or unpredictability in the data is indicated by a higher standard deviation, whereas less variability and a more predictable pattern are suggested by a smaller standard deviation.

In the original simulation, the value of sigma (σ) is chosen to be 0.1 to keep the required noise level for the estimation problem. If the value of sigma is increased to 0.5 or 1.0 then, the corner of CRB curve shifts away from the zero value. This indicates that the problem becomes ill conditioned because of the increased noise addition to the estimation. If the value of sigma is decreased instead of increasing, there will be no L-curve present, as the Fisher information is inversely proportional to $\sigma^2$ (variance). In general, a low variation in the properties of the L-curve indicates a problem that is well-constrained, with a distinct optimal regularisation parameter that effectively balances the accuracy and smoothness of the solution.
Within the framework of Fisher information, the term "variance" denotes the quantification of the extent or dispersion of the distribution of the estimated parameter. The Fisher information variance precisely measures the level of ambiguity or precision involved in predicting the unknown value. A smaller variance signifies that the estimator is more exact and yields more dependable estimates, whereas a bigger variance implies increased uncertainty and reduced precision in the estimation process. To summarise, the variability in Fisher information indicates the degree of certainty one can have in the calculated value based on the given data.

Figure 11: Estimation error when \( \sigma = 0.5 \)

Figure 12: Shifting of L-curve away from zero when \( \sigma = 0.5 \)
5.2.5 Temperature change
The simulation can be used for estimating temperature ranging from high to low and from low to high. The same code can be implemented for both purposes. The algorithm will automatically adapt to the requirement. Below figure shows how a cold temperature of -10°C is estimated using the algorithm. The final temperature and initial value temperature are changed.

![Figure 13: Estimation of cold temperature (-10 °C) from initial value temperature of 60 °C](image)

6 Practical implication
In many fields, monitoring temperature is a crucial operation that necessitates very accurate and effective measurements. This project can also be used for different applications.

6.1 In chemical industry
The major implication on which this project is considered at first is that if there is some industrial process where we wish to measure the temperature of various bulk constituents, such as liquids (chemicals) in containers, etc. It is assumed that these containers may be quite large in numbers flowing in a stream on some kind of production line. For practical technical reasons, we do not have the possibility to keep a thermometer in every container. Hence, we wish to employ a single thermometer probe to take samples of the
temperature on each of the containers as they are passing through the production line. Now, we have a requirement of measurement speed, say one measurement per second, at the same time the time constant of the probe is rather long, say in the order of 10-60 seconds. The relatively long time constant of the probe could be for technical reasons, such as a protective arrangement for hostile chemical environments, etc. A very positive circumstance here is that we can assume the time constant of the probe, i.e., it can be measured (or modelled) a priori with very high accuracy. Then together with some statistical assumptions about the measurement noise of the probe and the physical model of the probe, we have built a perfect setup to solve this estimation problem. So, by our established method we can calculate the temperatures of the bulk of liquid containers in a shorter period.

6.2 In Glass manufacturing
Accurate temperature measurement is essential for effectively controlling and enhancing production operations in the glass manufacturing sector. To adhere to the regulations, it is crucial to meticulously monitor the temperature of both the glass and apparatus, owing to the stringent quality criteria. Old techniques of temperature measurements were using infra-red techniques and using temperature probes [9], which are of less accuracy. Our technology enables efficient measurement and monitoring of the temperature during glass manufacturing, hence enhancing the speed of the production process. While estimating temperature rise in two different glass melting furnaces to compare the efficiency of different melting furnaces [10].

6.3 In the production of Renewable energy
Efficient energy production from renewable sources relies on accurate temperature measurement. Measuring and regulating temperatures are critical factors for renewable energy sources like geothermal sources, windmills, water turbines, biomass combustion equipment, solar heating pumps, and so on. This project can be integrated with the production of renewable energy to make the temperature sensing part quicker. For example, in a thermal power
plant to operate efficiently, the superheater steam temperature is a crucial and significant characteristic that needs to be continuously monitored and controlled. A superheater is one crucial part of the steam generation system in a thermal power plant. Its main function is to raise the boiler's steam output temperature. Additionally, it aids in regulating the pressure and temperature of the steam that is fed to the turbine. By doing this, the turbine's power generation is maximized, and it runs within the parameters of its design [11]. But if the temperature of the steam fluctuates then it can damage the superheater and hence the efficiency of the entire plant is compromised. A popular method in power plant operations is to estimate the superheater steam temperature using regression models. In this scenario, the desired output is the superheater steam temperature, and regression models estimate it using historical data and a variety of input variable [12]. The temperature of the superheater steam can likewise be estimated in this situation through our project.

6.4 In the oil withdrawal

Oil mining is a crucial process. The knowledge of underground temperature plays a great role in this process. Both the wellbore's integrity and the surrounding rock formations are impacted by the temperature below ground. The reservoir and wellbore integrity may be harmed by thermal stress brought on by extremely high temperatures. Subsurface temperature management and monitoring by operators is necessary to prevent these risks and guarantee the long-term viability of oil mining activities [13].

The design and functionality of numerous pieces of equipment used in oil mining, including pumps, pipelines, and heat exchangers, depend heavily on the temperature below the surface. A thorough understanding of temperature conditions aid’s in the selection of suitable materials and the design of effective systems that are resistant to certain thermal conditions

Drilling activities are impacted by the underground temperature. Several issues might arise in high temperatures, including viscous drilling fluid,
limited equipment, and possible formation damage. Planning drill operations and choosing the right drilling techniques are aided by keeping an eye on the temperature below the surface. For example, the temperature can become too high while drilling deeper into the ground without pausing, the drill can become too hot and break. So, by our statistical method, we can ensure safety and efficiency. This project can give an accurate measurement of the final underground temperature and can be integrated with different mining projects.

7 Conclusion

In this thesis, we successfully estimated the unknown parameters of the model which was developed. This paper proposes an estimation model for the tracking of temperature of large liquid containers more quickly and unbiasedly with better accuracy. From the study, it is understood that both CRLB and MLE can be used for the estimation of the temperature of the liquid in large containers with precisions high enough to be used for applications like the comparison of temperatures of different containers.

We collected some initial data from the probe over a few points in time and then placed it in our designed estimator to obtain the final estimated temperature of the liquid before the probe reached its final temperature. This final estimated temperature comes out to be exactly near the real value of the final temperature obtained by the probe later. Same way we also estimated the initial temperature of the liquid. In the process, we learned that this problem is an ill-conditioned inverse problem. It was also a well-posed problem. But we regularize it to the size of the measurement aperture. Then for accuracy, we used the Cramer Rao lower bound, and we investigated and analyzed the L curve obtained by plotting the Cramer Rao bound. First, we derived the differential equations and then developed the maximum likelihood estimator and other factors like the Fisher information matrix analytically, then we worked on it in MATLAB to obtain the results in graphical form. Some investigations were also done on the results as
mentioned in the observation section. In conclusion, we can say that this project is canonical, and, in the future, we can integrate it with different projects in which we have to estimate the temperature parameters rapidly and with precision.

**Reference**


