Identification

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1 Introduction

We aim to identify unknown parameters in an open two-level quantum system. The system's density matrix $\rho(t)$ evolves according to the following Lindblad master equation:

$$\begin{cases} \dot{\rho}(t) = -i[H,\rho] + \gamma_1 \left(\sigma^+ \rho \sigma^- - \frac{1}{2}\{\sigma^-\sigma^+, \rho\}\right) + \gamma_2 \left(Z\rho Z - \rho\right), \\ \rho(0) = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \end{cases}$$

Definitions and Notation

- X, Y, Z are the Pauli matrices.
- $H = \frac{\omega}{2} Z + \frac{u\kappa}{2} X$ is the Hamiltonian.
- $\sigma^+ = \frac{1}{2}(X + iY), \quad \sigma^- = \frac{1}{2}(X - iY)$ are the raising and lowering operators.
- $\omega, \kappa, \gamma_1, \gamma_2, u$ are the unknown parameters to be identified.

Physical Meaning of Parameters

(To be completed)
Brief explanations of the physical significance of each parameter!.

Solving the Lindblad Equation

Since $\rho(t)$ is a Hermitian, trace-one matrix, it belongs to the Bloch ball, a subset of $\mathbb{R}^3$. There exists an isomorphism between the space of density matrices $\mathcal{D}$ and $\mathbb{R}^3$ via the Pauli basis representation:

$$\rho(t) = \frac{1}{2}\left(I + x(t)X + y(t)Y + z(t)Z\right),$$

where $(x(t), y(t), z(t)) \in \mathbb{R}^3$ is the Bloch vector.
Differentiating with respect to time:

$$\dot{\rho}(t) = \frac{1}{2}\left(\dot{x}(t)X + \dot{y}(t)Y + \dot{z}(t)Z\right).$$

Our goal is to transform the master equation into the standard form:

$$\dot{v}(t) = Mv(t) + b,$$

where $v(t) = \begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix}$, M is a 3×3 real matrix, and $b \in \mathbb{R}^3$. This is done by expressing each term of $\dot{\rho}(t)$ in the Pauli basis.

We decomposed the Lindblad operator into four parts:

1.Hamiltonian Evolution

$$-i[H,\rho] = \frac{-\omega y}{2}\cdot X + \frac{(\omega x - u\kappa z)}{2}\cdot Y + \frac{u\kappa y}{2}\cdot Z$$

2. The Term: $\sigma^+\rho\sigma^-$

$$\sigma^+\rho\sigma^- = \frac{(1-z)}{4}\cdot I + \frac{(1-z)}{4}\cdot Z$$

3. Anticommutator Term

$$\frac{1}{2}\left\{\sigma^-\sigma^+,\rho\right\} = \frac{1}{4}((1-z)\cdot I + x\cdot X + y\cdot Y + (z-1)\cdot Z)$$

4. Dephasing Term

$$Z\rho Z - \rho = -x\cdot X - y\cdot Y$$

Combining these results we obtain the following linear differential equation:

$$\begin{cases} \dot{v}(t) = \begin{pmatrix} -\frac{1}{2}\gamma_1 - 2\gamma_2 & -\omega & 0 \\ \omega & -\frac{1}{2}\gamma_1 - 2\gamma_2 & -u\kappa \\ 0 & uk & -\gamma_1 \end{pmatrix}\cdot\begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \gamma_1 \end{pmatrix} \\ v(0) = (0 \quad 0 \quad -1)^T \end{cases}$$

the general solution is given by :

$$v(t) = e^{Mt}v(0) + \int_0^t e^{M(t-s)}b\,ds,$$

where $v(t) \in \mathbb{R}^3$ is the Bloch vector, $M \in \mathbb{R}^{3\times 3}$ is a real matrix derived from the Lindblad equation in the Pauli basis, and $b \in \mathbb{R}^3$ is a constant vector.

Explicit Solution Strategy

Since diagonalizing M directly is not straightforward—due to the large number of unknown parameters and the complexity of solving the characteristic polynomial analytically, we'll consider two scenarios depending on the value of the control parameter u:

Two Cases for the Control Parameter u

1. **Case** $u = 0$**:**
   In this situation, the dynamics simplify significantly, making the system easier to analyze. We can derive an explicit solution and estimate parameters like $\omega, \gamma_1, \gamma_2$, leaving only κ unknown. Once these parameters have been successfully identified, determining the remaining unknown κ becomes a straightforward task, especially when reintroducing the control input u.

2. **Case** $u \neq 0$**:**
   We employ a numerical optimization technique based on gradient descent to estimate all parameters, including κ. The optimization is performed by minimizing the least squares error between the measured output $\tilde{y}_i$ and the simulated output $y(t_i)$:

   $$\arg min_\theta \sum_{i=0}^{n} \left\|y(t_i) - \tilde{y}_i\right\|^2,$$

   where $\theta = (\omega, \kappa, \gamma_1, \gamma_2)$ are the parameters to be identified.

[1] Xue, S., Wu, R., Li, D., & Jiang, M. (2021). **A gradient algorithm for Hamiltonian identification of open quantum systems.** *arXiv preprint arXiv:2102.06006.*

Identifying the Parameters

In this approach we identify parameters independently by choosing a specific time of measure and controls after analyzing the explicit solution for the dynamical system.

Identifying γ_1

By imposing a null control term, we can identify γ_1. In this case the linear differential equation becomes:

$$\begin{cases} \dot{v}(t) = \begin{pmatrix} -\frac{1}{2}\gamma_1 - 2\gamma_2 & -\omega & 0 \\ \omega & -\frac{1}{2}\gamma_1 - 2\gamma_2 & 0 \\ 0 & 0 & -\gamma_1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \gamma_1 \end{pmatrix}, \\ v(0) = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} \end{cases}$$

We observe that the system matrix M is block-diagonal:

$$M = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}, \quad \text{with} \quad A = \begin{pmatrix} -\frac{1}{2}\gamma_1 - 2\gamma_2 & -\omega \\ \omega & -\frac{1}{2}\gamma_1 - 2\gamma_2 \end{pmatrix}, \quad B = \begin{pmatrix} -\gamma_1 \end{pmatrix}.$$

Exponentiating M is straighforward and given by :

$$\exp(M) = \begin{pmatrix} \exp(A) & 0 \\ 0 & \exp(B) \end{pmatrix}$$

Since $A = (-\frac{1}{2}\gamma_1 - 2\gamma_2)I_2 + r$ where r is a symetric matrix (infitisimal rotation near the origin) then :

$$\exp(At) = \begin{pmatrix} e^{(-\frac{1}{2}\gamma_1 - 2\gamma_2)t} & 0 \\ 0 & e^{(-\frac{1}{2}\gamma_1 - 2\gamma_2)t} \end{pmatrix} \cdot \begin{pmatrix} \cos(\omega t) & -\sin(\omega t) \\ \sin(\omega t) & \cos(\omega t) \end{pmatrix}$$

we obtain :

$$\exp(Mt) = \begin{pmatrix} e^{(-\frac{1}{2}\gamma_1 - 2\gamma_2)t}.\cos(\omega t) & -e^{(-\frac{1}{2}\gamma_1 - 2\gamma_2)t}.\sin(\omega t) & 0 \\ e^{(-\frac{1}{2}\gamma_1 - 2\gamma_2)t}\sin(\omega t) & e^{(-\frac{1}{2}\gamma_1 - 2\gamma_2)t}\cos(\omega t) & 0 \\ 0 & 0 & e^{-\gamma_1 t} \end{pmatrix}$$

General Solution the general solution is given by :

$$v(t) = \exp(Mt) \cdot v_0 + \int_0^t \exp(M(t-s)) \cdot b \, ds = \begin{pmatrix} 0 \\ 0 \\ 1 - 2e^{-\gamma_1 t} \end{pmatrix}$$

the expected value of observing the excited state E_1 is given by :

$$\mathrm{Tr}(E_1\rho(t)) = \mathrm{Tr}\left(\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} 1 + z(t) & x(t) - iy(t) \\ x(t) + iy(t) & 1 - z(t) \end{pmatrix} \right) = \boxed{\frac{1}{2}(1 - z(t))} = e^{-\gamma_1 t}$$

setting at time t_1 :

$$e^{-\gamma_1 t_1} = \frac{s}{n}$$

we can solve for γ_1
An estimation for γ_1 is given then by :

$$\gamma_1 \sim \frac{-\log(\frac{s}{n})}{t_1}$$

Error Analysis for the Estimation To evaluate the quality of our estimator $\hat{\gamma}_1$, we compute several statistical indicators:

1. Bias

We define the bias of the estimator as:

$$\text{Bias}(\hat{\gamma}_1) = \mathbb{E}[\hat{\gamma}_1] - \gamma_1$$

Let $\hat{p} = \frac{s}{n}$ be the empirical success rate, where $s \sim \text{Binomial}(n, p)$ and $p = e^{-4\gamma_1 t_1}$. Since $\mathbb{E}[\hat{p}] = p$, and using the approximation $\mathbb{E}[\log(\hat{p})] \approx \log(\mathbb{E}[\hat{p}]) = \log(p)$ we get:

$$\mathbb{E}[\hat{\gamma}_1] \approx \frac{-\log(p)}{t_1} = \gamma_1$$

So the bias is approximately:

$$\text{Bias}(\hat{\gamma}_1) \approx 0$$

2. Variance

To compute the variance, we use a second-order Taylor expansion of the function $f(\hat{p}) = -\frac{\log(\hat{p})}{4t_1}$ around p:

$$\text{Var}(\hat{\gamma}_1) \approx \left(\frac{f'(p)}{t_1}\right)^2 \text{Var}(\hat{p}) = \left(\frac{1}{t_1 p}\right)^2 \cdot \frac{p(1-p)}{n} = \frac{1-p}{t_1^2 pn}$$

3. Standard Deviation

The standard deviation is simply the square root of the variance:

$$\text{SD}(\hat{\gamma}_1) = \sqrt{\text{Var}(\hat{\gamma}_1)} = \sqrt{\frac{1-p}{t_1^2 pn}}$$

4. Mean Squared Error (MSE)

Since the bias is approximately zero, the MSE reduces to the variance:

$$\text{MSE}(\hat{\gamma}_1) = \text{Var}(\hat{\gamma}_1) + \text{Bias}(\hat{\gamma}_1)^2 \approx \text{Var}(\hat{\gamma}_1) = \frac{1-p}{t_1^2 pn}$$

This shows that the quality of the estimator improves as n increases, with the error decreasing asymptotically as $\mathcal{O}\left(\frac{1}{n}\right)$.

Remark: The case $u = 0$ does not allow us to identify all the parameters of the system. Regardless of the initial state, the expected value of the observable E_1 always reduces to the expression:

$$\mathbb{E}[E_1] = \frac{1}{2}(1 - z(t)),$$

which only depends on the parameter γ_1. Hence, the other parameters such as ω, κ, γ_2 remain unidentifiable in this scenario.

From this point onward, we assume that γ_1 has been estimated using the $u = 0$ case. We now proceed to study the case $u \neq 0$, which will allow us to identify the remaining unknown parameters.

$$\text{Tr}(E_1 \rho(t_1)) = \frac{s}{n}$$

we use **the Elimination Algorithm** developped in the previous project to identify the right parameter

Identifying κ

To identify κ we're going to make some hypothesis, find a solution from these hypothesis and then generalize and see if the method we used can be applied for the general case. When we suppose that $\gamma_1 = 4\gamma_2$ some intersting happen : the linear differential equation becomes :

$$\begin{cases} \dot{v}(t) = \begin{pmatrix} -\gamma_1 & -\omega & 0 \\ \omega & -\gamma_1 & -u\kappa \\ 0 & u\kappa & -\gamma_1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \gamma_1 \end{pmatrix} \\ v(0) = (0 \quad 0 \quad -1)^T \end{cases} \tag{S}$$

This way we can explicit the solution since the exponential is easy to calculate. Consider the matrix:

$$M = \begin{pmatrix} -4\gamma_2 & -\omega & 0 \\ \omega & -4\gamma_2 & -u\kappa \\ 0 & u\kappa & -4\gamma_2 \end{pmatrix}$$

We can decompose this matrix as:

$$M = A + N, \quad \text{where} \quad N = \begin{pmatrix} 0 & -\omega & 0 \\ \omega & 0 & -u\kappa \\ 0 & u\kappa & 0 \end{pmatrix} \text{ and } A = \begin{pmatrix} -4\gamma_2 & -\omega & 0 \\ \omega & -4\gamma_2 & -u\kappa \\ 0 & u\kappa & -4\gamma_2 \end{pmatrix}$$

This decomposition is useful because the matrix A commutes with N. Therefore:

$$\exp(Mt) = \exp(At + Nt) = \exp(At) \cdot \exp(Nt)$$

The matrix N is skew-symmetric, and thus $N \in \mathfrak{so}(3)$, the Lie algebra of the rotation group SO(3). Its exponential $\exp(Nt) \in \mathrm{SO}(3)$, i.e., a rotation matrix.

We use the isomorphism between $\mathfrak{so}(3)$ and $\mathbb{R}^3$, defined by:

$$[a] = \begin{pmatrix} 0 & -a_3 & a_2 \\ a_3 & 0 & -a_1 \\ -a_2 & a_1 & 0 \end{pmatrix} \longleftrightarrow a = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

In our case, the skew-symmetric matrix N corresponds to the vector:

$$n = \Omega \cdot \begin{pmatrix} \frac{u\kappa}{\Omega} \\ 0 \\ \frac{\omega}{\Omega} \end{pmatrix}, \quad \text{with norm} \quad \Omega = \sqrt{\omega^2 + (u\kappa)^2}$$

Rodrigues' Formula for the Exponential

The exponential of a skew-symmetric matrix $[n]$ is given by Rodrigues' formula (for a unit vector n):

$$\exp(\theta[n]) = Id + \sin(\theta).[n] + (1 - \cos(\theta)).[n]^2$$

Using this, we compute $\exp(Nt)$:

$$\exp(Nt) = \begin{pmatrix} \frac{\omega^2(\cos(\Omega t) - 1)}{\Omega^2} + 1 & \frac{-\omega \sin(\Omega t)}{\Omega} & \frac{\omega u\kappa(1 - \cos(\Omega t))}{\Omega^2} \\ \frac{\omega \sin(\Omega t)}{\Omega} & \cos(\Omega t) & \frac{-u\kappa \sin(\Omega t)}{\Omega} \\ \frac{\omega u\kappa(1 - \cos(\Omega t))}{\Omega^2} & \frac{u\kappa \sin(\Omega t)}{\Omega} & \frac{(u\kappa)^2(\cos(\Omega t) - 1)}{\Omega^2} + 1 \end{pmatrix}$$

Final Result

For simplicity reasons we

$$\begin{aligned} x(t) &= \frac{e^{-\gamma t}\, u\kappa\omega}{\Omega^2(\gamma^2 + \Omega^2)} \Big(-2\gamma^2 + (-2 + e^{\gamma t})\Omega^2 + (2\gamma^2 + \Omega^2)\cos(t\Omega) - \gamma\Omega \sin(t\Omega) \Big) \\ y(t) &= \frac{e^{-\gamma t}\, u\kappa}{\Omega(\gamma^2 + \Omega^2)} \Big(-e^{\gamma t}\gamma\Omega + \gamma\Omega\cos(t\Omega) + (2\gamma^2 + \Omega^2)\sin(t\Omega) \Big) \\ z(t) &= \frac{e^{-\gamma t}}{\Omega^2(\gamma^2 + \Omega^2)} \Big[(-2 + e^{\gamma t})\Omega^2(\gamma^2 + \Omega^2) + u^2\kappa^2 \left(2\gamma^2 - (-2 + e^{\gamma t})\Omega^2\right) \\ &\qquad + u^2\kappa^2 \left(-(2\gamma^2 + \Omega^2)\cos(t\Omega) + \gamma\Omega \sin(t\Omega) \right) \Big] \end{aligned}$$

The expected value of observing the excited state E_1 is related to $z(t)$ by the formula:

$$\mathbb{E}[E_1] = \frac{1}{2}\left(1 - z(t)\right)$$

The trick is to choose the control parameters and measurement time wisely to simplify the expression.

Asymptotic Regime: $u \to \infty$ and $t = \frac{1}{u}$

We now analyze the behavior of $z(t)$ under the scaling:

$$t = \frac{1}{u}, \quad u \to \infty$$

In this regime, we have:

$$\Omega = \sqrt{u^2\kappa^2 + \omega^2} = u\kappa\sqrt{1 + \frac{\omega^2}{u^2\kappa^2}} = u\kappa\left(1 + \frac{1}{2}\cdot\frac{\omega^2}{u^2\kappa^2} + \wr(\frac{1}{u^2})\right) = u\kappa + \mathcal{O}\left(\frac{1}{u}\right)$$

Thus:

$$t\Omega = \kappa + \mathcal{O}\left(\frac{1}{u}\right)$$

We can now expand the trigonometric terms:

$$\begin{aligned}
\cos(t\Omega) &= \cos(\kappa) + \mathcal{O}\left(\frac{1}{u}\right), \\
\sin(t\Omega) &= \sin(\kappa) + \mathcal{O}\left(\frac{1}{u}\right), \\
e^{-\gamma t} &= 1 - \frac{\gamma}{u} + \mathcal{O}\left(\frac{1}{u^2}\right), \\
e^{\gamma t} &= 1 + \frac{\gamma}{u} + \mathcal{O}\left(\frac{1}{u^2}\right)
\end{aligned}$$

Plugging all these into the expression for $z(t)$, and simplifying all terms, we find:

$$z(t) \xrightarrow[u\to\infty]{t=1/u} -\cos(\kappa)$$

Thus, the expected value of observing the excited state E_1 simplifies to:

$$\mathbb{E}[E_1] = \frac{1}{2}\left(1 - z(t)\right) \xrightarrow[u\to\infty]{} \frac{1}{2}(1 + \cos(\kappa))$$

This result shows that by tuning κ, we can control the population probability of the excited state E_1, even in the limit of strong control $u \to \infty$.

Identifying κ in Practice

1. Fix a large control amplitude u.
2. Choose the measurement time as $t_1 = \frac{1}{u}$.
3. Repeat the experiment a sufficient number of times and record the number of times the system is observed in the excited state.
4. Use the empirical estimate to approximate:

   $$\frac{1}{2}(1 + \cos(\kappa)) = \frac{s}{n},$$

   where s is the number of excited state observations and n is the total number of measurements.
5. Solve for κ using the inverse cosine:

   $$\kappa = \arccos\left(\frac{2s}{n} - 1\right) + z\pi, \quad \text{where } z \in \mathbb{Z}.$$

6. Apply the **Elimination Algorithm** to determine the correct value of κ among the possible candidates.

General case This method is useful because even if we generalize ($\gamma_1 \neq \gamma_2$) we still can apply the same trick but first we need to prove this Lemma

Lemma 1.1. Let $M \in \mathbb{C}^{n\times n}$ and $b \in \mathbb{C}^n$. Then the following identity holds:

$$\int_0^t e^{(t-s)M} \cdot b \, ds = M^{-1}(e^{tM} - I) \cdot b$$

Proof. Define the functions:

$$\Phi(t) = M^{-1}(e^{tM} - I) \cdot b, \quad \Psi(t) = \int_0^t e^{(t-s)M} \cdot b \, ds$$

We compute the derivatives:

$$\frac{d}{dt}\Phi(t) = M^{-1} \cdot Me^{tM} \cdot b = e^{tM} \cdot b$$

we can write :

$$\dot{\Phi}(t) = M\Phi + b$$

and by the Fundamental Theorem of Calculus:

$$\frac{d}{dt}\Psi(t) = e^{(t-t)M} \cdot b + \int_0^t \frac{d}{dt}e^{(t-s)M} \cdot b \, ds = I \cdot b + M \cdot \int_0^t e^{(t-s)M} \cdot b \, ds = e^{tM} \cdot b$$

we can write :

$$\dot{\Psi}(t) = M\Psi + b$$

Therefore, both $\Phi(t)$ and $\Psi(t)$ satisfy the same differential equation:

$$\dot{f}(t) = e^{tM} \cdot b$$

with the same initial condition $\Phi(0) = \Psi(0) = 0$. By uniqueness of solutions to linear ODEs, we conclude:

$$\Phi(t) = \Psi(t)$$

□

Using this Lemma we want to find an equivalent for $v(t)$ when $u \xrightarrow{t=\frac{1}{u}} \infty$. the general solution becomes :

$$v(t) = e^{M\frac{1}{u}}v(0) + \int_0^{\frac{1}{u}} e^{M(\frac{1}{u}-s)}b \, ds,$$

the first term is equivalent when $u \to \infty$ to :

$$\frac{1}{u}M = \begin{pmatrix} \frac{-\frac{1}{2}\gamma_1 - 2\gamma_2}{u} & \frac{-\omega}{u} & 0 \\ \frac{-\omega}{u} & \frac{-\frac{1}{2}\gamma_1 - 2\gamma_2}{u} & -\kappa \\ 0 & k & \frac{-\gamma_1}{u} \end{pmatrix} \xrightarrow{u\to\infty} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\kappa \\ 0 & \kappa & 0 \end{pmatrix} \quad \textbf{(skew-symmetric matrix)}$$

which yields :

$$e^{M\frac{1}{u}}v(0) \xrightarrow{u\to\infty} \begin{pmatrix} 0 \\ \sin(\kappa) \\ -\cos(\kappa) \end{pmatrix}$$

For the second term, we apply the lemma with $t = \frac{1}{u}$, obtaining:

$$\int_0^{\frac{1}{u}} e^{M(\frac{1}{u}-s)}b, ds = M^{-1}(e^{\frac{1}{u}M} - I)b.$$

Expanding the exponential in a Taylor series gives:

$$e^{\frac{1}{u}M} - I = \frac{1}{u}M + \frac{1}{2u^2}M^2 + \cdots,$$

so that:

$$M^{-1}(e^{\frac{1}{u}M} - I) = \frac{1}{u}I + \frac{1}{2u^2}M + \cdots.$$

From this, we deduce the following asymptotic behavior:

$$\int_0^{\frac{1}{u}} e^{M(\frac{1}{u}-s)}b, ds = \frac{1}{u}b + o\left(\frac{1}{u}\right) \quad \text{as } u \to \infty.$$

Conclusion In the general case, if we choose a sufficiently large control term and set the measurement time to be inversely proportional to u, we can extract information about the parameter κ. Indeed, we observe that:

$$\mathbb{E}[E_1] = \frac{1}{2}\left(1 - z(t)\right) \xrightarrow[u\to\infty]{t=\frac{1}{u}} \frac{1}{2}\left(1 + \cos(\kappa)\right),$$

which allows for the identification of κ from the asymptotic behavior of the observable $z(t)$ as $u \to \infty$.

Identifying ω

Rotation of the Initial State In this method, we apply a quantum gate to the initial state of the qubit before allowing it to evolve under the system dynamics. This gate corresponds to a rotation around the X-axis and is represented by the unitary operator:

$$U = e^{i\frac{\pi}{4}X}$$

Lemma 1.2. Under this transformation, the Pauli matrices transform as follows:

$$\begin{cases} U^\dagger X U = X \\ U^\dagger Y U = Z \\ U^\dagger Z U = -Y \end{cases}$$

Under this rotated frame, the Bloch vector dynamics are governed by the following system of differential equations:

$$\begin{cases} \dot{v}(t) = \begin{pmatrix} -\frac{1}{2}\gamma_1 - 2\gamma_2 & -\omega & 0 \\ \omega & -\frac{1}{2}\gamma_1 - 2\gamma_2 & -u\kappa \\ 0 & u\kappa & -\gamma_1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \gamma_1 \end{pmatrix} \\ v(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \end{cases} \tag{S}$$

Assuming $u = 0$, the system simplifies to a block-diagonal matrix:

$$M = \begin{pmatrix} -\frac{1}{2}\gamma_1 - 2\gamma_2 & -\omega & 0 \\ \omega & -\frac{1}{2}\gamma_1 - 2\gamma_2 & 0 \\ 0 & 0 & -\gamma_1 \end{pmatrix}, \quad b = \begin{pmatrix} 0 \\ 0 \\ \gamma_1 \end{pmatrix}$$

The matrix exponential $\exp(Mt)$ can be computed explicitly:

$$\exp(Mt) = \begin{pmatrix} e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\cos(\omega t) & -e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\sin(\omega t) & 0 \\ e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\sin(\omega t) & e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\cos(\omega t) & 0 \\ 0 & 0 & e^{-\gamma_1 t} \end{pmatrix}$$

From this, the general solution of the linear system is:

$$v(t) = \exp(Mt)\, v(0) + \int_0^t \exp(M(t-s))\, b\, ds = \begin{pmatrix} -e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\sin(\omega t) \\ e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\cos(\omega t) \\ 1 - e^{-\gamma_1 t} \end{pmatrix}$$

Returning to the original (lab) frame by applying the inverse rotation around the X-axis yields:

$$v_x(t) = \begin{pmatrix} -e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\sin(\omega t) \\ e^{-\gamma_1 t} - 1 \\ e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\cos(\omega t) \end{pmatrix}$$

Using this method, once the frequency ω is identified, the parameter γ_2 can be directly inferred. Furthermore, the probability of measuring the excited state at time t is given by:

$$\mathrm{Tr}(E_1\rho(t)) = \frac{1}{2}(1 - z(t)) = \frac{1}{2}\left(1 - e^{-t(\frac{1}{2}\gamma_1 + 2\gamma_2)}\cos(\omega t)\right)$$

Assuming γ_1 is known, both ω and γ_2 can be identified by solving a nonlinear least squares optimization problem that minimizes the mean square error between the theoretical prediction and observed data.

Initial Guess by Approximation Around 0 Around $t = 0$, the expected probability of finding the system in the excited state is given by:

$$P(t) = \frac{1}{2}\left(1 - e^{-t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right)}\cos(\omega t)\right)$$

We can approximate this expression using a second-order Taylor expansion around $t = 0$. First, we expand the exponential and cosine functions:

$$e^{-t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right)} = 1 - t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right) + \frac{1}{2}t^2\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right)^2 + o(t^2)$$

$$\cos(\omega t) = 1 - \frac{1}{2}\omega^2 t^2 + o(t^2)$$

Multiplying the two approximations:

$$\begin{aligned} e^{-t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right)}\cos(\omega t) &= \left(1 - t\left(\frac{1}{2}\gamma_1 + 2\gamma_2 + o(t^2)\right)\right)\left(1 - \frac{1}{2}\omega^2 t^2 + o(t^2)\right) \\ &= 1 - t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right) - \frac{1}{2}\omega^2 t^2 + t^2\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right)\frac{1}{2}\omega^2 + o(t^2) \\ &= 1 - t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right) + \frac{1}{2}t^2\omega^2\left(\frac{1}{2}\gamma_1 + 2\gamma_2 - 1\right) \end{aligned}$$

Hence, the approximated probability becomes:

$$\begin{aligned} \mathbb{P}(t) &= \frac{1}{2}\left(1 - \left[1 - t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right) - \frac{1}{2}\omega^2 t^2 + \frac{1}{2}t^2\omega^2\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right)\right]\right) \\ &= \frac{1}{2}\left(t\left(\frac{1}{2}\gamma_1 + 2\gamma_2\right) + \frac{1}{2}\omega^2 t^2\left(1 - \left(\frac{1}{2}\gamma_1 + 2\gamma_2\right)\right)\right) \end{aligned}$$

This gives a second-order approximation of the probability near $t = 0$, which can be used to extract rough estimates of ω and γ_2 if γ_1 is known.

Solving these two equations provides an initial guess for ω and γ_2, which can be used as a starting point in the optimization procedure.

Case $u \neq 0$

In this case, deriving an explicit solution for the Lindblad equation $\rho(t)$ becomes significantly more complex. Consequently, directly identifying the system parameters from the analytical solution is not practical.

To address this, we will follow these four steps:

Step 1: Reformulate the Identification Problem as an Optimization Problem

We transform the parameter estimation task into a minimization problem by defining a cost function that quantifies the mismatch between model predictions and observed data.

Step 2: Define a Suitable Loss Function

We introduce a loss function, typically a squared-error norm, that measures the discrepancy between the observed measurements and the simulated outputs of the quantum system.

Step 3: Optimize Measurement Times t_k

To enhance the identifiability of the parameters, we select measurement times t_k so that the loss function has the steepest descent (the times that gives the smallest variance). (Ludovic's idea.)

Step 4: Choose and implement a gradient-based optimization Algorithm

Finally, we implement a gradient-descent algorithm to minimize the loss function and iteratively update the parameter estimates.(choose any optimization algo)

Step 1 : Optimization problem

Let's recall that the solution to the Lindblad equation $\rho(t)$ can be expressed in the Pauli basis as:

$$\rho(t) = \frac{1}{2}\left(I_2 + x(t)X + y(t)Y + z(t)Z\right),$$

where $(x(t), y(t), z(t)) \in \mathbb{R}^3$ evolves according to the differential equation system previously derived.

We consider the observable $E_1 = |1\rangle\langle 1|$, which corresponds to the excited state of a qubit. The probability of measuring the system in this state at time t_k is given by:

$$p_{t_k} = \begin{cases} \mathrm{Tr}(E_1\rho(t_k)) & \textbf{(Theoretical probability)} \\ \dfrac{s}{n} = \dfrac{\#\text{successes}}{\#\text{measurements}} & \textbf{(Empirical probability)} \end{cases}$$

In theory, both probabilities should match at every measurement time. This motivates the introduction of function $\eta : \mathbb{R}^5 \to \mathbb{R}$, parameterized by the system parameters $(\omega, \kappa, u, \gamma_1, \gamma_2)$, such that:

$$\eta(\omega, \kappa, \gamma_1, \gamma_2 \mid t_k, u_k) = \mathrm{Tr}(E_1\rho(t_k)).$$

Let L denote the loss function quantifying the discrepancy between theoretical and empirical probabilities. The parameter identification problem thus becomes the following optimization problem:

$$\underset{\omega,\kappa,u,\gamma_1,\gamma_2}{\arg\min}\ L(\omega, \kappa, u, \gamma_1, \gamma_2).$$

Step 2 : Loss function

We propose using the Mean Squared Error (MSE) between the theoretical probabilities and observed frequencies as our loss function:

$$L = \frac{1}{n}\sum_{k=1}^{n}\left(\mathrm{Tr}(E_1\rho(t_k)) - \frac{s_k}{n_k}\right)^2,$$

where $\frac{s_k}{n_k}$ is the observed frequency at time t_k but it's open for discussion with the team.

Step 3: Optimize Measurement Times t_k

As suggested in the referenced paper, a simple and common strategy is to choose equally spaced measurement times in the interval $[0, t_f]$:

$$t_k = \frac{kt_f}{n}, \quad \text{for } k = 0, 1, \ldots, n.$$

but it is still open to discussion with the team.

Sensitivity Analysis

Critical Times and Controls

To better understand the behavior of the function

$$J : (t, u) \mapsto J(t, u) = \frac{1}{2}(1 - z(t)),$$

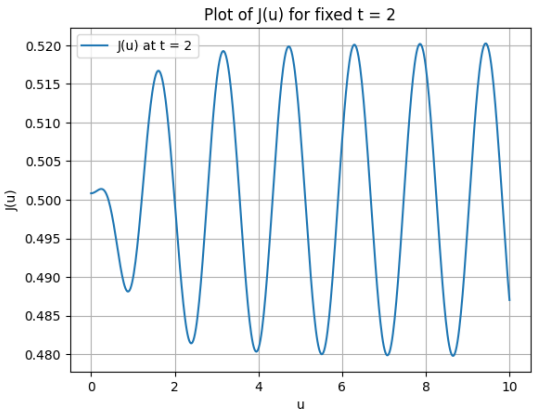
and to identify optimal values (t_k, u_k) that minimize or maximize J, we proceed in two steps:

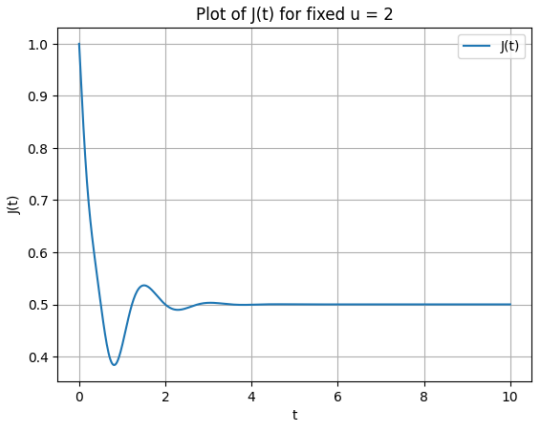
- First, we fix the time t and study the variation of J as a function of the control parameter u.
- Then, we fix u and analyze J as a function of time t.

For both graphs, we use the following parameter values:

- $\omega = 1$
- $\kappa = 2$
- $\gamma_1 = 0.3$

The resulting plots are shown below:





The graph($J(t)$)seems logical since for large t the system tends to stabilize in a mixed state that corresponds to maximum entropy (center of the Bloch ball)

Interpretation of the Graphs (to be discussed with the team)

Choice of the measurement time t

- Since the function $J(t)$ stabilizes around 0.5 as t increases, we suggest taking the measurements right after the system is initialized. This helps avoid maximum entropy and identical measurement outcomes.
- We propose restricting all measurements to the interval $t \in [0, 2]$, and taking as many measurements as possible within this range to gather more data.

Choice of the control parameter u

- The graph of J as a function of u shows oscillatory behavior around 0.5 with an approximate period of 2. This suggests that optimal values of u lie within intervals of the form $[2k, 2(k+1)]$ for some integer k.
- On the graph, we can distinguish three relevant types of u values:
  - values for which $p = 0.5$,
  - values for which $p > 0.5$, and
  - values for which $p < 0.5$.

  We want to avoid control values u that lead to $J \approx 0.5$, as they lead to not very useful information. Both u values yielding $p > 0.5$ and $p < 0.5$ are informative. We will be taking u that maximizes J.

Sensitivity analysis

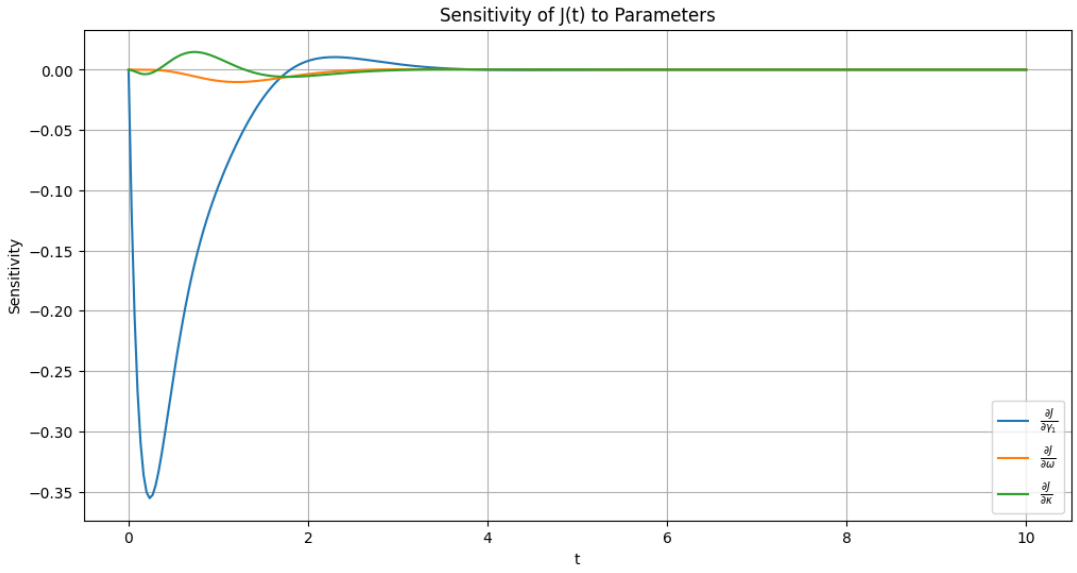
After discussing what optimal values for t and u should be, we will perform sensitivity analysis to see how small changes in the parameters can affect the loss function defined before. This analysis involves evaluating the gradient of the loss function $L(\gamma_1, \omega, \kappa)$, which is given by:

$$\frac{\partial L}{\partial \theta} = \frac{2}{n} \sum_{i=0}^{n} (J(\theta | t_i, u_i) - \frac{s_i}{n_i}) \cdot \frac{\partial J(\theta)}{\partial \theta}$$

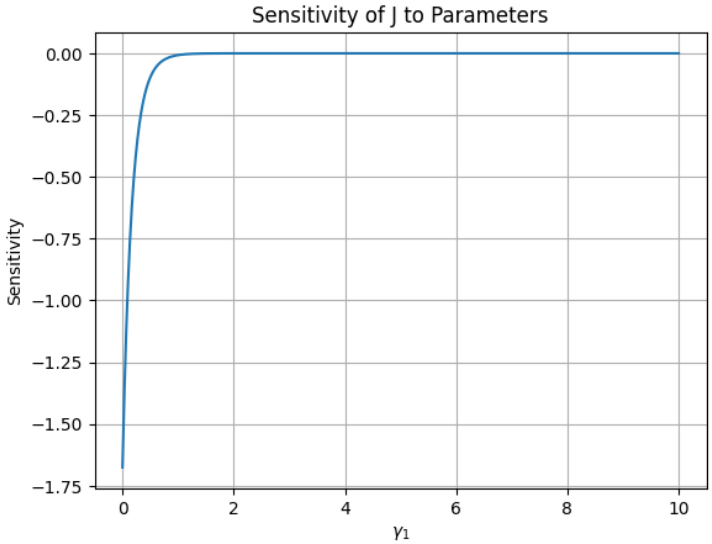
By studying the gradient of J, we can compute the gradient of L.

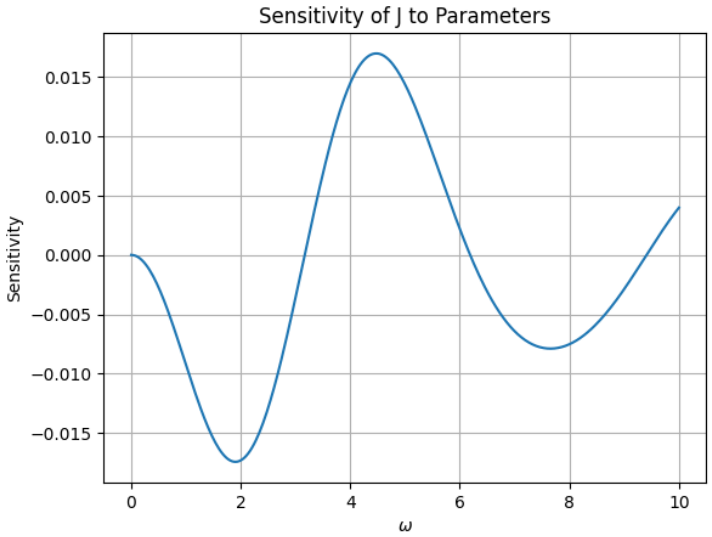
Due to the complexity of the analytic expressions for the partial derivatives $\frac{\partial J}{\partial \gamma_1}$, $\frac{\partial J}{\partial \omega}$, and $\frac{\partial J}{\partial \kappa}$, we will use Automatic Differentiation in Python to compute these gradients and generate plots to analyze the regions where the gradient is highly sensitive to each parameter.

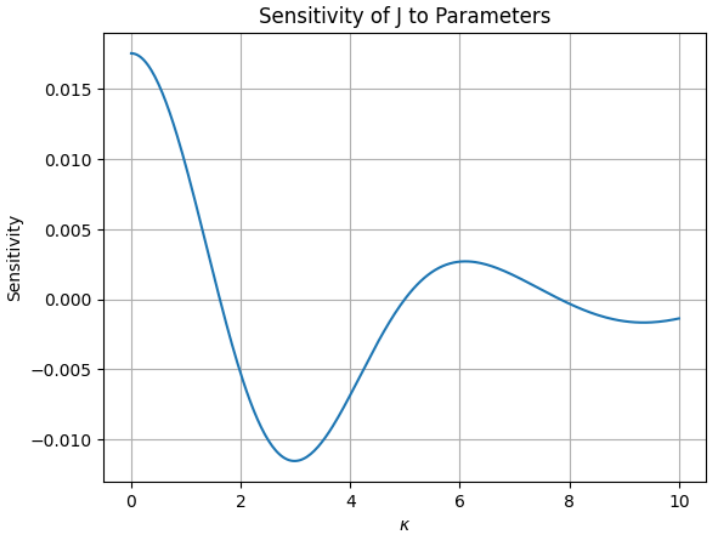
This graph shows how sensitive the gradient of J over time for fixed (γ_1, ω, κ) :



Now the sensitivity for variable parameter :


Sensitivity of J to Parameters
Sensitivity
0.00
−0.25
−0.50
−0.75
−1.00
−1.25
−1.50
−1.75
0
2
4
6
8
10
γ_1


Sensitivity of J to Parameters
Sensitivity
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
0
2
4
6
8
10
ω


Sensitivity of J to Parameters
Sensitivity
0.015
0.010
0.005
0.000
−0.005
−0.010
0
2
4
6
8
10
κ