Quasi-Optimal Entanglement Characterisation in Quantum States

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Introduction

Quantum entanglement serves as a fundamental resource for various quantum information and communication protocols, including quantum teleportation, superdense coding, and quantum error correction. Entangled qubits exhibit the remarkable ability to surpass classical computers with exponential speedup, underscoring their crucial role in universal quantum algorithms. While quantum entanglement is an experimentally well-established phenomenon, its precise and reliable characterization remains an ongoing and challenging problem in the field of quantum science and technology. The challenge involves an optimization task, namely, the minimization of the distance of a given state ρ over a convex subset of all density matrices, which is computationally intensive in conventional approaches. Explicitly, if we denote the set of all disentangled states (density matrices) as $\mathfrak{D}$, which is a convex subset of all density matrices, an entanglement measure can be defined as follows

$$E(\sigma) = \min_{\sigma \in \mathfrak{D}} d(\rho, \sigma).$$

Here, d represents any distance function between two density matrices such that $E(\sigma)$ meets the criteria of entanglement measures [1]. In this project, we focus on a few-qubit system to develop a machine learning algorithm through Bayesian optimization to evaluate some entanglement measures, such as the quantum relative entropy, Bures measure of entanglement, and geometric measure of entanglement [1, 2, 3]. We would also like to generalize this method to analyze entanglement among a large number of qubits.

Since the nature of the optimisation landscape is not known beforehand, we will follow a global optimisation approach, namely Bayesian optimisation [1].

Task

Within the scope of the project, the task will be to formulate the entanglement characterisation problem as a global optimisation problem. We will implement the objective function in Python, and the optimization routines using PyTorch or Tensorflow. We will begin with a (small scale problem, two-qubit system, which would involve optimization of four variables function), and subsequently increase the complexity to address large number of qubits systems.

Required expertise

1. Good understanding of Python programming
2. Basic understanding of machine learning / willingness to learn about machine learning, neural networks and quantum information processing

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PROJECT REPORT

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Abstract

Precisely characterizing quantum entanglement is an important problem for quantum information and communication technologies and is a significant challenge. Despite its well-established experimental basis, the accurate quantification of quantum entanglement involves overcoming substantial computational demands. One approach includes minimizing the distance between a given quantum state and a convex subset of density matrices. Such optimization problems become exceedingly time and resource-consuming as the size and complexity of the quantum system grows. The focus of this work is on developing an innovative machine-learning method using Bayesian optimization. This method is designed to efficiently evaluate entanglement measures, such as the geometric measure of entanglement, particularly in systems with a limited number of qubits. We demonstrate that the proposed approach enhances the accuracy and efficiency of entanglement characterization, potentially positively impacting the field of quantum computing and communication.

1 Introduction

Quantum entanglement, first described by Einstein, Podolsky, and Rosen [1], and later by Schrödinger [2], emerged as a peculiar quantum phenomenon challenging the completeness of quantum theory. Bell's work further illuminated its peculiarities, demonstrating experimentally testable deviations from classical physics [3]. Now recognized as a crucial resource in quantum information theory, entanglement underpins groundbreaking protocols like quantum cryptography [4], teleportation [5], and measurement-based quantum computation [6]. This evolution from a theoretical anomaly to a practical tool illustrates the significant steps made in quantum science and technology.
Despite its experimental validation, the precise and reliable characterization of entanglement remains a challenging and vital area of ongoing research, especially due to the significant role entanglement plays in quantum computing. Entangled qubits are the cornerstone of quantum information processing, providing exponential speedup over classical computers for certain algorithms. The characterization of quantum entanglement not only helps to understand the fundamental aspects of quantum theory but is also crucial for practical implementations of quantum computing.

Entanglement measures are measurable properties that enable the evaluation of the strength and nature of entanglement within a quantum system. The challenge in characterizing entanglement involves an optimization task, the minimization of the distance of a given quantum state ρ over a convex subset of all density matrices that represent disentangled or separable states. This optimization is computationally intensive using conventional approaches due to the high-dimensional nature of the problem and the complex structure of quantum states.
Explicitly, if we denote the set of all disentangled states (density matrices) as D, which is a convex subset of all density matrices, an entanglement measure can be defined as follows:

$$E(\sigma) = \min_{\rho \in D} d(\rho, \sigma).$$

Here, d represents any distance function between two density matrices such that $E(\sigma)$ meets the criteria of entanglement measures. Such criteria requires that the measure is zero for disentangled states and positive for entangled states, invariant under local unitary transformations, and non-increasing under local operations and classical communication (LOCC).
In this project, we focus on a two-qubit system to develop a machine-learning approach through Bayesian optimization. This modern approach is chosen to navigate the complexity of evaluating some entanglement measures efficiently and effectively. Bayesian optimization provides a probabilistic model-based approach for global optimization that is particularly well-suited for optimization problems that are noisy, costly to evaluate or have a large number of parameters, as is often the case in quantum computing applications.
Our objective is to use Bayesian optimization to iteratively update our knowledge of the entanglement landscape and to guide the search for the optimal distance measure in the space of density matrices. By integrating principles from quantum information theory and machine learning, we aim to create a robust tool that can accelerate the characterization of entangled states and thus,

potentially, the development of quantum technologies.
In Section 2, we explore quantum entanglement in multipartite systems, focusing on quantification methods and their mathematical foundations. This part provides the core theoretical concepts for our later computational approaches. The methodology with an explanation of the Bayesian optimization technique and an introduction to our code is given in Section 3. Our result is presented in Section 4 and discussed in Section 5.

2 Exploring Quantum Entanglement

In this section, we explore the fundamental aspects of bipartite entanglement. This discussion forms the foundation for understanding the more complex topic of multipartite entanglement, which is addressed in the subsequent section. The exploration of bipartite entangled states facilitates a comprehensive introduction to the central concepts of entanglement detection.

2.1 Quantum States and Bipartite Systems

In quantum mechanics, physical systems are described by quantum states. 'Bipartite' systems refer to systems composed of two parts (or particles). Entanglement occurs when the quantum states of these two parts become interconnected in such a way that the state of one particle cannot be described independently of the state of the other. This connection persists even if the two particles are separated by large distances. If one measures a property (like spin or polarization) of one particle in an entangled pair, one instantaneously determines the corresponding property of the other particle, regardless of the distance separating them.

2.2 Single-Particle Systems and Hilbert Space

The characterization of a single-particle system in quantum mechanics is essentially described within the Hilbert space framework, represented as $\mathcal{H}$. Within this framework, a state $|\Psi\rangle$ is defined as a unit vector, conforming to the normalization condition $\langle\Psi|\Psi\rangle = 1$. This condition implies that the integrated probability of the particle's presence throughout the space is exactly one, a core principle in quantum theory.
The Hilbert space is further structured by a basis B, which consists of a complete set of state vectors $\{|\Psi_0\rangle, |\Psi_1\rangle, |\Psi_2\rangle, \ldots\}$. These vectors serve as the foundational elements that allow any quantum state $|\Psi\rangle$ to be represented as a linear combination of the basis vectors. Specifically,

$$|\Psi\rangle = \sum_i c_i |\Psi_i\rangle, \tag{1}$$

where the coefficients c_i are constrained by the condition

$$\sum_i |c_i|^2 = 1. \tag{2}$$

This relation ensures the preservation of probability within the quantum system.

2.3 The Qubit and the Bloch Sphere

Introducing the qubit concept, the quantum counterpart to the classical bit, the qubit's Hilbert space has a dimensionality of $\dim(\mathcal{H}) = 2$, equating to $\mathcal{H} \equiv \mathbb{C}^2$. Visualized on the Bloch sphere, a qubit state $|\Psi\rangle$ is represented as

$$|\Psi\rangle = c_0|0\rangle + c_1|1\rangle, \tag{3}$$

with the computational basis states $|0\rangle$ and $|1\rangle$, and coefficients c_0 and c_1 parameterized by angles θ and ϕ. The Bloch sphere is visualized in figure 1.

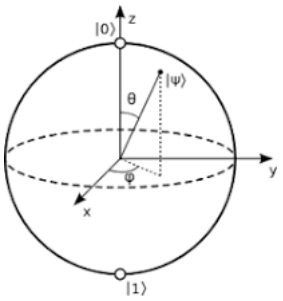

Figure 1: Bloch sphere, a geometrical representation of pure state space of a qubit, the parameters θ and ϕ are interpreted in spherical coordinates [7].

2.4 Seperable state and Entaglement

In quantum mechanics, separable states in multipartite systems are quantum states that can be expressed as a convex combination of product states. Product states, on the other hand, are multipartite quantum states that can be written as a tensor product of states within each individual subsystem. Mathematically, for a bipartite system (two subsystems), a separable state $|\Phi\rangle$ can be expressed as the tensor product of the states of the individual subsystems:

$$|\Phi\rangle = |\Phi_1\rangle \otimes |\Phi_2\rangle \tag{4}$$

Here, $|\Phi_1\rangle$ and $|\Phi_2\rangle$ are the states of the individual subsystems. This concept can be extended to multipartite systems with more than two subsystems.
On the other hand if a composite system consists of two entangled subsystems, the joint state of the system cannot be expressed as a simple tensor product of the individual states of the subsystems. In other words, the entangled state cannot be written as the above equation. Instead, the joint state of the entangled system is described by a more complex superposition of states, and measuring one subsystem instantaneously determines the state of the other, regardless of the distance between them.

2.5 Quantum Entanglement and Multipartite Systems

Quantum entanglement presents a distinctive challenge, particularly when clarifying the interconnections within a multipartite quantum system. By considering a general n-partite pure state

$$|\Psi\rangle = \sum_{p_1 \cdots p_n} \chi_{p_1 p_2 \ldots p_n} |e_{p_1}^{(1)} e_{p_2}^{(2)} \ldots e_{p_n}^{(n)}\rangle \tag{5}$$

the entanglement is quantifiable by the geometric distance or angle between the state $|\Psi\rangle$ and the nearest separable state $|\Phi\rangle$, represented by the norm squared

$$\| |\Psi\rangle - |\Phi\rangle \|^2 . \tag{6}$$

Here, $\Phi = \Phi^{(1)}\Phi^{(2)} \ldots \Phi^{(n)}$ is an arbitrary separable (i.e., Hartree) n-partite pure state, where the index $i = 1, \ldots, n$ labels the parts, and

$$|\Phi^{(i)}\rangle \equiv \sum_{p_i} c_{p_i}^{(i)} |e_{p_i}^{(i)}\rangle. \tag{7}$$

The entanglement eigenvalue Λ is derived by resolving an eigenproblem that minimizes this norm under normalization constraints, indicative of the entanglement level. A greater Λ implies a state nearing separability and thus, is less entangled. For bipartite systems, this constitutes a linear problem akin to the Schmidt decomposition, while for systems with more components, the problem becomes nonlinear, often requiring a numerical solution approach.

2.6 Analytical Determination of Entanglement Eigenvalues in Specific Families of Pure States

The maximum eigenvalue, denoted as $\Lambda_{\max}$, referred to as the entanglement eigenvalue, signifies proximity to the nearest separable state and is equal to the maximum overlap

$$\Lambda_{\max} = \max_{\Phi} \|\langle\Phi|\Psi\rangle\|\,, \tag{8}$$

where $|\Phi\rangle$ is an arbitrary separable pure state.
By adopting $E^2_{\text{sin}} \equiv 1 - \Lambda^2_{\max}$ as our entanglement measure in bipartite applications solving the problem is equivalent to finding the Schmidt decomposition. Where the entanglement eigenvalue is equal to the maximal Schmidt coefficient. For example with a given Schmidt decomposition of some two-qubit pure state for $0 \leq p \leq 1$:

$$|\Psi\rangle = \sqrt{p}|00\rangle + \sqrt{1-p}|11\rangle. \tag{9}$$

We can read off the entanglement eigenvalue:

$$\Lambda_{\max} = \max\{\sqrt{p}, \sqrt{1-p}\}.$$

The entanglement coefficient C for this state is represented by the expression $2\sqrt{p(1-p)}$. So we have:

$$\Lambda^2_{\max} = \frac{1}{2}(1 + \sqrt{1-C^2}) \tag{10}$$

which holds for arbitrary two-qubit pure states.

2.7 2-Qubit System

In this section, we explore the specifics of a 2-Qubit System, which is a fundamental building block in the study of quantum mechanics and quantum computing. We consider a quantum state $|\Psi\rangle$ within a 2-Qubit System. This state is described by a linear combination of base state, represented by complex numbers a, b, c, d. Mathematically, the state is expressed as:

$$|\Psi\rangle = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}, \tag{11}$$

It is subject to a normalization condition, which maintains the fundamental principle of quantum mechanics that the total probability of all possible states must sum to one. This is expressed as:

$$|a|^2 + |b|^2 + |c|^2 + |d|^2 = 1. \tag{12}$$

We define $\Lambda(\Phi)$, which has an important role in determining the entanglement measure of our system and understanding how entanglement varies with different quantum states. This function maps a pair of points on two unit spheres to the real numbers. Mathematically, this is represented as:

$$\Lambda(\Phi) = \langle\Phi|\Psi\rangle = \alpha_1\alpha_2 a + \alpha_1\beta_2 b + \beta_1\alpha_2 c + \beta_1\beta_2 d, \tag{13}$$

The separable two-qubit state can be parametrized as a product of two unit spheres $S^2 \times S^2$ where based on (2.4) we have

$$|\Phi_1\rangle = \cos\left(\frac{\theta_1}{2}\right)|0\rangle + e^{i\phi_1} \cdot \sin\left(\frac{\theta_1}{2}\right)|1\rangle \tag{14}$$

$$|\Phi_2\rangle = \cos\left(\frac{\theta_2}{2}\right)|0\rangle + e^{i\phi_2} \cdot \sin\left(\frac{\theta_2}{2}\right)|1\rangle \tag{15}$$

The variables θ_i ranging from 0 to π and ϕ_i ranging from 0 to 2π to the real numbers $\mathbb{R}$.
The key to quantifying entanglement lies in identifying the global maximum of $\Lambda(\Phi)$. This maximum value indicates the highest degree of entanglement achievable under given conditions. To find this maximum, we must perform an optimization procedure over the domain of the spherical coordinates (θ_i, ϕ_i). These coordinates represent points on the unit spheres S^2, and their optimal combination leads to the maximum entanglement measure. By quantifying entanglement accurately, we can better understand the behavior of quantum systems and improve the design of quantum algorithms and quantum communication protocols.
In this project, we solve the optimisation problem given in (8) for a family of Ψ computationally. We use the Bayesian Optimisation method [8] to find the maximum, calculate the entanglement measure E^2_{sin} defined in section 2.6, and compare it to the analytical solution given in (10).

3 Methodology

In the following chapter, the optimization strategy is described. Furthermore, the implementation is described, which leads to the results in Section 4. A detailed description of the used Python library in which the optimization strategy is implemented is also given.

3.1 Bayesian optimization

Bayesian optimization is a sequential model-based approach which aims to maximize an unknown objective function f:

$$x^* = \arg\max_{x \in X} f(x)$$

where X represents the space of interest and is usually a subset of $\mathbb{R}^d$. However it is versatile enough to be extended to other search spaces such as categorical or conditional inputs. It is assumed, that the unknown function f does not have a simple closed form. The derivatives may be unavaible or computationally expensive to obtain, we rely solely on the evaluation of f at point x. The evaluation can be noisy.

Since $f(x)$ is noisy and/or computationally expensive to evaluate, the goal is to evaluate $f(x)$ at strategically selected points. These points iteratively lead to the global maximum of $f(x)$ by trading off exploration and exploitation. To find a sequence of query points, a so-called acquisition function $a_n : X \to \mathbb{R}$ is designed. The function a_n is relatively cheap to maximize, due to having analytical forms, leading to the next query point.

The model treats the unknown objection function $f(x)$ as a function sampled from a distribution, described initially by a prior, and subsequently updated upon obtaining data (from $f(x)$) to get a posterior distribution. As the sampling process (via the acquisition function) is iterative, the posterior is also updated iteratively.

The process is shown in Algorithm 1.

Algorithm 1 Bayesian Optimisation Method

1: Initial prior belief regarding the potential objective function f
2:
3: **for** 1,2,... **do**
4: maximize acquisition functions to choose the next query point
5: refining the model iteratively as data comes in through Bayesian posterior updates

The query points are chosen by harnessing the uncertainty in the predictive distribution to guide the exploration process. This work considers the expected improvement acquisition function owing its balanced exploitation behavior [8]. Essentially, the acquisition function helps balance the trade-off between exploration and exploitation. The goal is to choose the next point to evaluate in the objective function by considering both the expected improvement in the objective value and the uncertainty associated with that improvement, implying that x_{n+1} is chosen by maximizing a_n. Figure 2 illustrates how the acquisition function is used to choose the next point to evaluate f at. Each iteration shows the maximum of the acquisition function as the next query point.

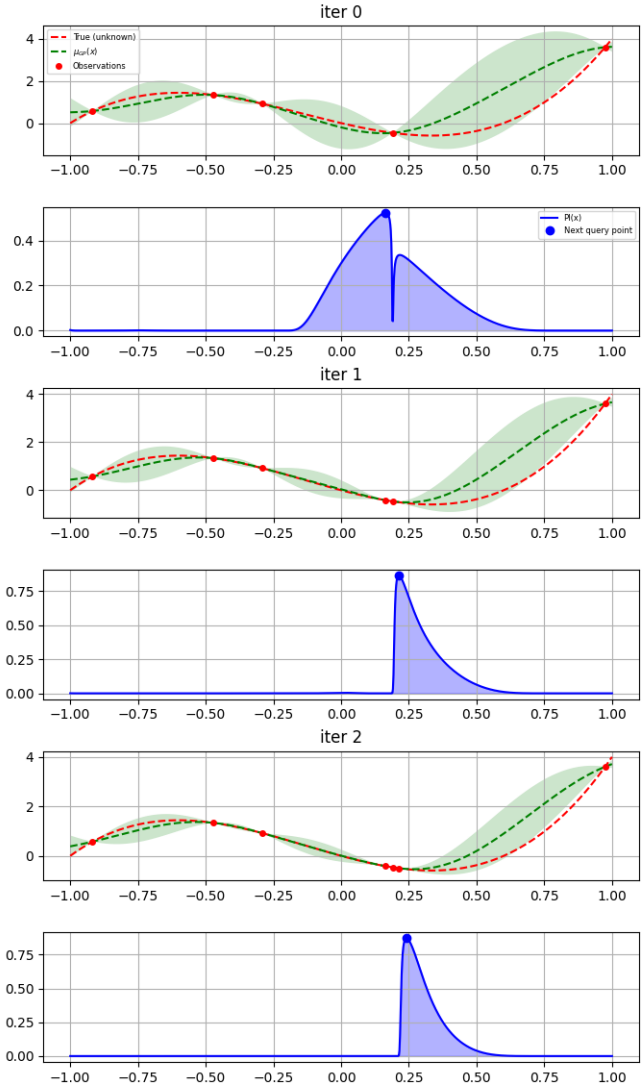

Figure 2: Example of Bayesian Optimization over three iterations. It shows the usually unknown objection function in red and the posterior uncertainty (in green) and mean (green line). In blue the different a_n values are shown, with the maximum labeled. The maximum indicates the new observation point.

There are different functions, that can be used as acquisition functions a_n, which are separated according to three strategies [8]. The probability of improvement or expected improvement are examples of an improvement-based policy. Another option is to use optimistic policies such as upper confidence bound. One can also use information-based policies such as Thompson sampling or entropy search.

These models can be parametric or non-parametric. In the case of this project, the focus lies on non-parametric models. To build the surrogate model, one can use many approaches, such as polynomial interpolation, neural networks, support vector machines, and random forests. In this project, we use Gaussian processes.

3.1.1 Gaussian Processes

The Gaussian Process approach uses the kernel trick to construct a Bayesian non-parametric regression model [8].
A Gaussian process (GP) is a stochastic process that corresponds to the collection of random variables such that the joint distribution of every finite subset of those random variables is multivariate Gaussian [9].
A GP is fully characterized by a mean $\mu(x)$ function and a covariance function $k(x, x')$ (kernel). The mean function represents the average behavior of the process, while the covariance function captures the relationships and dependencies between different input points. The model is built on the assumptions:

$$f|X \sim \mathcal{N}(m, K) \tag{16}$$

$$y|f, \sigma^2 \sim \mathcal{N}(f, \sigma^2 I) \tag{17}$$

M is mean vector with $m_i := \mu_0(x_i)$ and K is covariance matrix with $K_{i,j} := k(x_i, x_j)$ [8]. It is assumed, that one is dealing with a Gaussian distribution, in which uncertainties are updated via the data points. One can see the Gaussian Process in Figure 2 depicted by the green uncertainties and the mean prediction (dotted green line).
GP's predictive power is maximized by selecting the right covariance/kernel and the appropriate hyperparameters associated with the corresponding kernel since they influence the smoothness, periodicity, and other properties of the functions sampled from the GP. Common kernels include the radial basis function (RBF) and the Matérn kernel [8].

3.2 Libraries

Scikit-learn [10] is a machine learning library for Python. It provides tools for data analysis and modeling, including a wide array of machine learning algorithms for tasks such as classification, regression, clustering, and dimensionality reduction. The main library we will use is built on Scikit-Learn, which is Scikit-Optimize and specifically the function gp_minimize [11].

Scikit-Optimize, or skopt, is an efficient library which is designed to minimize or maximize expensive and noisy black-box functions. It implements several methods for sequential model-based optimization.

In gp_minimize, Bayesian optimization is implemented. The function is approximated by a Gaussian process, the kernel built between the parameters. Hyperparameter are the following:

- Number of calls
- Number of initial points
- The acquisition function is to be used

3.3 Structure and implementation of code

The core parts of our algorithms are as follows:

1. To begin with, the points generated are sampled from a spherical surface. In order to achieve this we generate two lists *phi* and *theta* which contain our polar and azimouthian coordinates. In the current implementation we have discretized the space into 2000 points.

2. After the sampling is performed we construct our α and β using the following equations.

$$\alpha_1 = \cos\left(\frac{\theta_1}{2}\right)$$
$$\alpha_2 = \cos\left(\frac{\theta_2}{2}\right)$$
$$\beta_1 = e^{i\phi_1} \cdot \sin\left(\frac{\theta_1}{2}\right)$$
$$\beta_2 = e^{i\phi_2} \cdot \sin\left(\frac{\theta_2}{2}\right)$$

3. The black box function which is to be optimized takes as input a list of 4 numbers ranging between 0 and 2000 signifying the index locations of the *phi* and *theta* lists. Then it proceeds to calculate the inner product of Φ and the given Ψ. Utilizing the optimization method `gp_minimize`, designed to determine the minimum value of a function, we negate the result to effectively find the maximum.

4. In the optimization process, by using the `space` variable in order to create continuous search space for four variables, denoted as x_1, x_2, x_3, and x_4. These variables are constrained within the range $[0,\ N-1]$, where N is a predefined constant representing the number of points we have decided to discretize the spherical space. In this case the number is 2000.

   Next, we employ the `gp_minimize` function to perform the optimization. The hyperparameters configuration includes the choice of acquisition function where the Probability of Improvement (PI) function was chosen. The PI function quantifies the probability that the objective function value at a candidate point will be an improvement over the current best-known value. Finally the last two hyperparameters are the number of optimization calls and the number of initial random points.

The objective function and optimisation procedure can be summarised in the following pseudo code.

Algorithm 2 Objective function

Input: a, b, c, d
Output: Inner product $\langle\Phi|\Psi\rangle$
$\alpha_1 \leftarrow \cos\left(\frac{\theta_1}{2}\right)$
$\alpha_2 \leftarrow \cos\left(\frac{\theta_2}{2}\right)$
$\beta_1 \leftarrow e^{i\phi_1} \cdot \sin\left(\frac{\theta_1}{2}\right)$
$\beta_2 \leftarrow e^{i\phi_2} \cdot \sin\left(\frac{\theta_2}{2}\right)$
$\langle\Phi|\Psi\rangle \leftarrow \alpha_1\alpha_2 a + \alpha_1\beta_2 b + \beta_1\alpha_2 c + \beta_1\beta_2 d$
return -$\langle\Phi|\Psi\rangle$
=0

Algorithm 3 Optimization Process

Input: Objective function f, Search space S, Hyperparameters
Output: $\theta_1, \theta_2, \phi_1, \phi_2$ ▷ Optimal solution
Procedure:
  Initialize random points in S
  Evaluate the objective function f for the initial points
  Set the current best solution as the initial points
for each optimization iteration **do**
    Select a candidate point in S based on the acquisition function
    Evaluate f for the candidate point
  if Objective value at candidate point is better **then**
      Update the current best solution
  end if
    Update the surrogate model based on the observed points
end for
Return: $\theta_1, \theta_2, \phi_1, \phi_2$

4 Results

By first taking into consideration the pure states derived from the family

$$|\Psi\rangle = \sqrt{p}|00\rangle + \sqrt{1-p}|11\rangle$$

presented in Section 2.6. We first began by discretizing the parameter p into 30 intervals. This discretization allowed us to generate a corresponding family of pure states

$$|\Psi\rangle = \begin{pmatrix} \sqrt{p} \\ 0 \\ 0 \\ \sqrt{1-p} \end{pmatrix}. \tag{18}$$

For each state within the family, we computationally determined the global maxima using our algorithm. Subsequently, we plotted the obtained results alongside analytical results. In Figure 3 the results are presented.

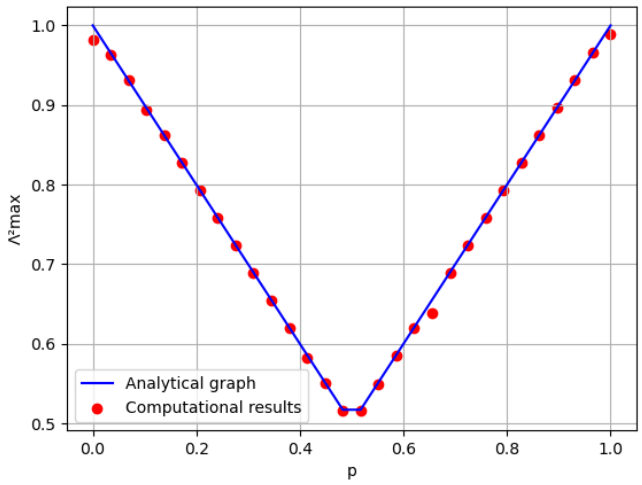

Figure 3: Comparison of Computational and Analytical Results

5 Discussion and Conclusions

The results closely align, as indicated by an error of approximately 0.003 percent in the worst cases compared to the expected theoretical results. Given that the computational outcomes closely mirror the expected analytical results, the utilization of this algorithm enables precise measurement of entanglement in a two-qubit pure system.

In this work, we have designed an algorithm for characterizing the entanglement measure of quantum states using Bayesian optimization and the geometric measure of entanglement. The algorithm has the ability to accurately describe the entanglement measure thus marking it as a good starting point, opening avenues for the potential extension of this approach to address the problems posed by systems involving multiple qubits. Notably, it addresses a significant challenge inherent in these systemsthat as the number of qubits increases, the complexity of the system grows exponentially. This phenomenon is a result of the intricate entanglements and interactions that occur between qubits, creating a computational problem that becomes exponentially expensive to compute. Furthermore another fundamental challenge in multiple qubit systems—the lack of analytical solutions. Unlike classical computing problems and the 2-qubit problem, where analytical solutions can often be derived, these systems pose a unique challenge due to their inherent probabilistic nature and the principles of superposition and entanglement. The absence of analytical solutions means that traditional methods for solving problems may not be directly applicable to quantum systems.

The algorithm aims to tackle both problems by efficiently characterise those systems using the geometric measure and efficiently using the Bayesian method.

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