

GUESSING QUANTUM STATES FROM IMAGES OF THEIR ZEROS IN THE COMPLEX PLANE

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Abstract The problem of determining the wave function of a physical system based on the graphical representation of its zeros is considered. It can be dealt with by invoking the Bargmann representation in which the wave functions are represented by analytic functions with an appropriate definition of the scalar product. The Weierstrass factorization theorem can then be applied. Examples of states that can be guessed from the pictorial representation of zeros by both the human eye and, possibly, by machine learning systems are given. The quality of recognition by the latter has been tested using Convolutional Neural Networks.

Keywords: scientific visualization, zeros of wave functions, Bargmann representation, Weierstrass factorization theorem, Convolutional Neural Networks

1. Introduction

It is, indeed, difficult to imagine physical sciences and their development without such or that pictorial representations of reality including representations of *states* of a physical system. Even solving problems in elementary or high-school physics almost always demands creating some figures to grasp the intuitive essence of the exercise. The situation in quantum mechanics is not different. As a matter of fact, graphical representations of physical states are even more needed because of several counter-intuitive features of that theory.

A basic way to represent states of quantum systems is by providing their wave functions. In many cases it is inconvenient, or even meaningless, to use the most standard representation of the wave functions as square-integrable functions defined on the suitable Cartesian product of the sets of real numbers. One of many possibilities is to consider the Bargmann representation in which the wave function belongs to the set of entire functions in the complex plane (or Cartesian product of many such planes).

Taking into account a special – “stiff” – behavior of entire functions in the complex planes, and the presence of several powerful theorems which, in principle, allows to reconstruct of the whole function from its values at specific points, one can reasonably ask whether it is possible to guess the “nature” of the quantum states just from a picture showing their zeros in the plane. The answer is, in principle, negative for the reasons specified later, but the number of specific interesting cases in which at least a qualitative description of the state can be done is sufficient to warrant further consideration.

The main body of the work is organized as follows. In Section 2 major facts about the

quantum states in the Bargmann representation are provided. Section 3 offers several examples of graphical representations of zeros of analytic wave functions that allow a trained human eye to easily guess what the quantum state is with a minimum of additional knowledge. Section 4 contains the description of the artificial neural network used in the paper and the results of its application. Some concluding remarks are contained in Section 5.

2. Quantum states in the Bargmann representation

After one of the major scientific revolutions which took places in years 1925-1935, quantum mechanics has been established as the most fundamental conceptual framework of the whole physics. Among its basic concepts is that of the wave function. A wave function is a complex function that represents the quantum state of a physical system. With the help of the wave function, we can calculate the probabilistic properties of the system, especially expectation values of observable physical quantities.

In the simplest case the wave function (also called state function or state vector) is a square-integrable complex function of four real variables including the time that serves as a parameter. The same wave function can, however, be represented in many different ways. A remarkable representation that is invoked in this work in which wave functions are holomorphic functions of complex variables is called *Bargmann* or *Bargmann-Segal* representation [2, 3, 7]. The state vectors are entire (i.e. holomorphic in the whole complex plane) functions of the complex variable z that are of the order one, that is, they cannot grow faster than

$$\exp(A|z|)$$

as the modulus $|z|$ goes to infinity with A being a constant.

One can define an important quantity called the scalar product of two functions $\psi(z)$ and $\phi(z)$ as follows:

$$\langle \phi(z) | \psi(z) \rangle = \frac{1}{\pi} \int \bar{\phi}(z) \psi(z) \exp(-|z|^2),$$

where we have restricted ourselves to functions of one complex variable z , and $\bar{\phi}(z)$ denotes the function that is complex-conjugated to $\phi(z)$. The integration is to be performed over the entire complex plane.

The quantity

$$Q(z) = \frac{1}{\pi} |\psi(z)|^2 \exp(-|z|^2)$$

is called (Husimi) Q -function [8]. It is sometimes used for visual representations of the quantum states as well as computation of expectation values of the so-called anti-normal products of operators.

The Bargmann representation is particularly well suited to describe the quantum aspects of electromagnetic fields in resonators or cavities. In such systems, it is very convenient to represent the quantized fields as system modes of oscillations (called just modes). If for some reason, we can restrict ourselves to precisely one such mode, the wave function in the Bargmann representation can be reduced to that of just one complex argument. If that single distinguished mode of electromagnetic oscillations is populated with just n quanta (photons in this case), the wave function is of the form:

$$\psi(z) = \psi_n(z) = \frac{1}{N} z^n,$$

where N is a normalization factor to ensure that the scalar product of $\psi_n(z)$ with itself is equal to 1. In the above simple case, we have $N = \sqrt{\pi n!}$.

The above state functions are called *Fock states*. These states are the most elementary ones. Remarkably, it is rather difficult (though possible) to obtain them in real-life experiments.

However, in many cases, the state functions are sums of the above elementary states. For instance,

$$\phi(z) = \frac{1}{N} (1 + z^2 + (1/2)z^3)$$

is a valid quantum state, being a *coherent superposition* of three Fock states. The first term, 1, corresponds to the state with zero photons (vacuum), the second – to the state with two photons, and the third – to the state with three photons. The coefficients (complex in the generic case) are weights with which elementary states contribute to the whole wave function.

Another important class of states consists of exponential functions of the form:

$$\psi_\alpha(z) = \exp(\alpha z),$$

where α is a complex number. They are called *coherent states*. The electromagnetic field produced by a laser is close to being in a coherent state. The light of a laser has excellent coherence properties; this justifies the name.

Let me now invoke the Weierstrass factorization theorem that allows one to build a holomorphic function from the location of its zeros.

To begin with, we follow Weierstrass as quoted by Rudin, and introduce the following *elementary factors* [6]:

$$E_p(z) = (1 - z) \exp\left(z + \frac{z^2}{2} + \dots + \frac{z^p}{p}\right).$$

Their only zero is at $z = 1$. They are all close to 1 if $|z| < 1$ and p is large.

Then the following holds.

Theorem (Weierstrass). *Let f be an entire function, suppose that $f(0) \neq 0$, and let $z_1, z_2, z_3, \dots$ be the zeros of f , listed according to their multiplicities. Then there exists an entire function g and a sequence $\{p_n\}$ of nonnegative integers, such that*

$$f(z) = e^{g(z)} \prod E_{p_n} \left(\frac{z}{z_n} \right).$$

Now, if f has a zero of the order k at $z = 0$, the above theorem applies to $f(z)/z^k$ so that the *non-zero* value at $z = 0$ is not an essential assumption. Unfortunately, the above factorization is *not* unique.

In the case of entire functions of the order q , the Weierstrass results has been strengthened by Hadamard:

Theorem (Hadamard). *If f is an entire function of finite order ρ and m is the order of the zero of f at $z = 0$, f admits a factorization:*

$$f(z) = z^m e^{g(z)} \prod_{n=1}^{\infty} E_{p_n} \left(\frac{z}{z_n} \right).$$

3. Examples of quantum states and pictorial representations of their zeros

Let me describe here what one can expect from the pictorial representations of the zeros of the (Bargmann-space) state functions. We can look for those zeros not in the whole plane but only inside a contour C . In what follows below we consider C to be a circle with the radius R .

In the case of a pure Fock state with an arbitrary photon number n , one can see only a single mark at $z = 0$ for any n . Unfortunately, using just one picture we cannot distinguish between various ns .

In the case of a coherent superposition of Fock states, i.e., a polynomial of the n th order in z , we can have up to n different zeros and n different marked points in the picture.

In the case of coherent states, the picture is *empty* because the simple exponential function has no zeros in the complex plane.

However, a superposition of the Fock and coherent states has, in the generic case, infinitely many zeros. Thus, with growing R we will see more and more points (and marks) to appear within the contour. What is more, the number of photons populating the most populated Fock state in the superposition can be easily guessed from the picture.

In this Section several examples of pictorial representations of the zeros of wave functions in the Bargmann representation are provided in Figs. 1-8.

Let us first observe that it would be quite difficult and sometimes impossible to find out the zeros of the wave function from the corresponding density given by the Q -function. Thus, the left-hand side of each of the figures has an independent value.

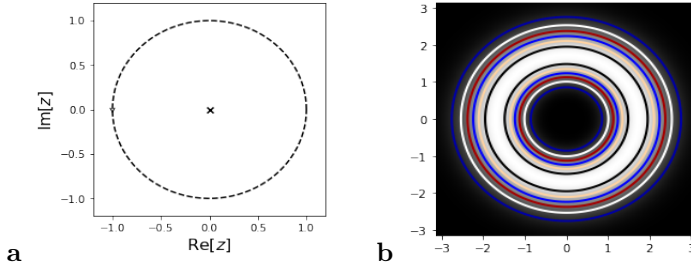


Fig. 1. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = z^3$. (a) Zeros of the wave function; (b) Q -function.

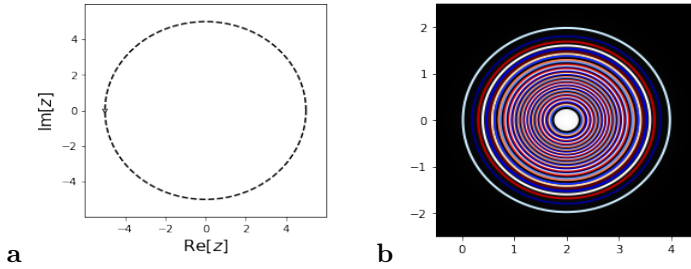


Fig. 2. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = \exp(2z)$. (a) Zeros of the wave function; (b) Q -function.

And let us now consider the principal problem stated in the previous section. Can we get at least some quantitative knowledge about the quantum state by just having a look at the left-hand sides of the figures contained in this section? Let us say that we know in advance that they show zeros of some state functions. In Fig. 1a we can

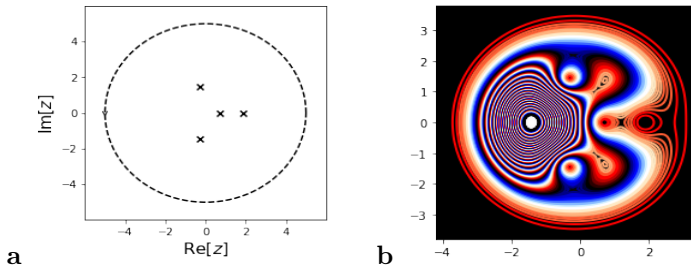


Fig. 3. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = z^4 - 2z^3 + 2z^2 - 5z + 3$. (a) Zeros of the wave function; (b) Q -function.

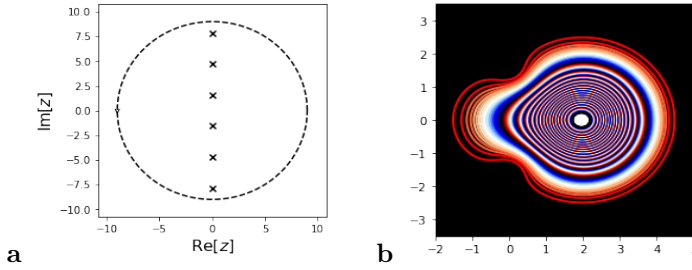


Fig. 4. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = 1 + \exp(2z)$. (a) Zeros of the wave function; (b) Q -function.

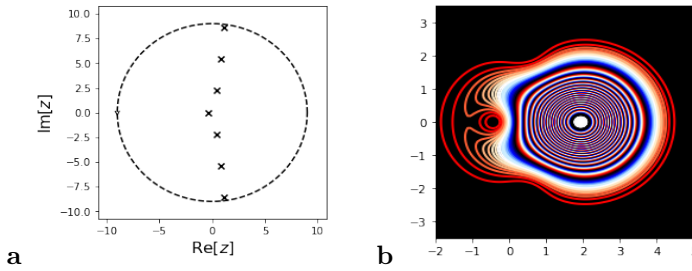


Fig. 5. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = z + \exp(2z)$. (a) Zeros of the wave function; (b) Q -function.

immediately infer that very likely, the state has just a single zero at $z = 0$. This means that it must be a Fock state with n photons though we cannot know what the number n is equal to. In Fig. 2a we see that a state has no zeros at all. Though there are, in principle, uncountably many such functions, an exponential one is clearly distinguished

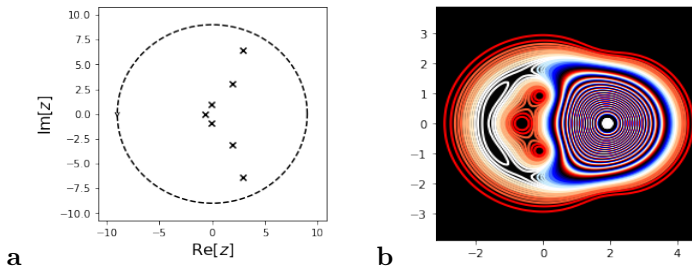


Fig. 6. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = z^3 + \exp(2z)$. (a) Zeros of the wave function; (b) Q -function.

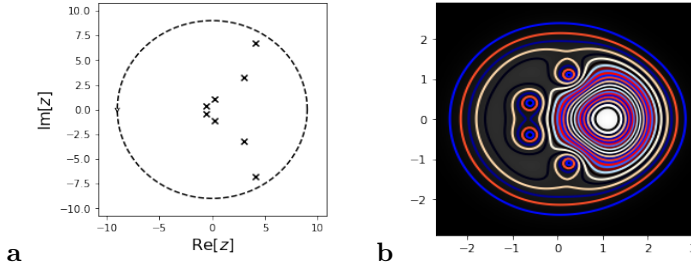


Fig. 7. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = z^4 + \exp(2z)$. (a) Zeros of the wave function; (b) Q -function.

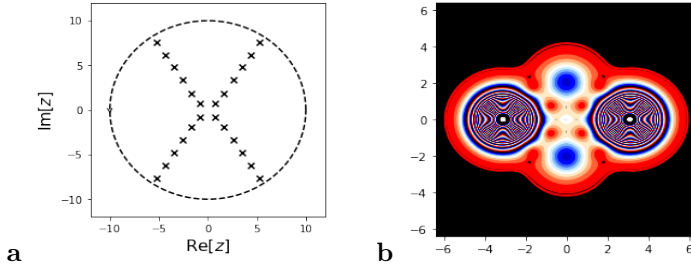


Fig. 8. Zeros and density in the complex plane associated with the (unnormalized) wave function $\psi(z) = 1 + z^2 + \cos(2z) + (1/4)\cos(3.15iz)$. (a) Zeros of the wave function; (b) Q -function.

by the physical context. Thus, we may reasonably suspect that we have to do with a coherent state (though we cannot say too much about the factor multiplying z in the exponent). Fig. 3a shows four zeros. If we can change the radius of the contour and there is no change in the number of zeros contained within it, we can claim with a reasonable margin of error that the state is a superposition of Fock states and the state which contributes the largest amount of quanta has precisely four of them. Looking at Figs. 4a-7 we can suspect that, on this occasion, the number of zeros is infinite (again, we would have to change the radius of the contour to confirm this). The difference in the number of photons carried by the Fock-state component is very nicely mirrored in the figures, though, in this case, the right-hand sides of the figures would be very helpful to establish the probable nature of the superposition. Finally, the X -like nature of the distribution of zeros in Fig. 8a suggests that a special combination of coherent states containing sines and/or cosines are involved.

4. Classification of states using convolutional neural networks

To check whether automatization of the recognition of quantum states based on the pictures of their zeros, we have decided to employ a convolutions neural network to solve the following classification problem.

We have generated pictures showing zeros of two families of functions.

The first family (denoted by (A)) has been of the form:

$$W_i(z) = \sum_{j=0}^K a_{i,j} z^j,$$

with $i = 0, 2, \dots, N - 1$. Several values of N has been tried from $N = 100$ to $N = 10000$. The degree of the polynomials K has been set equal to 5. All the coefficients $a_{i,j}$ have been real random numbers uniformly sampled from the interval $(0, 1)$. Physically, all $W_i(x)$ s correspond to a superposition of Fock states.

The second (B) family of functions and corresponding pictures of their zeros has been given by:

$$P_i(z) = \sum_{j=0}^K b_{i,j} z^j + c_i \exp(2z),$$

where again i runs from 0 to $N - 1$. The coefficients $b_{i,j}$ and c_i have again been real random numbers uniformly sampled from the interval $(0, 1)$. Physically, this function corresponds to a superposition of Fock states and a coherent state.

For both families of coefficients, $3N$ plots have been created with circular marks of zeros for three radii of circles within which the zeros have been determined. Those radii have been chosen equal to 3, 6, and 9. All together we generated $2 \cdot (3N)$ pictures.

Thus, our neural network has been trained to solve binary, balanced classification problems to distinguish between two families of triples of pictures corresponding to (A) and (B).

The training set has consisted of 80% of pictures, that is, $0.8 \cdot 2 \cdot 3N = 4.8 \cdot N$, the test set has had $1.2 \cdot N$ pictures.

The number of epochs in training the network has been 20. The architecture of the network has been illustrated in Fig. (9).

Despite this, the results are quite encouraging as can be seen from Figures (10, 11) as well as from the report contained in Figure (12).

The standard metrics took satisfactory values even for N as small as 300. The network has had no difficulties in classifying the plots.

In addition, we have also generated a family (denoted by (C)) similar to $P_i(z)$, but this time containing the sine function:

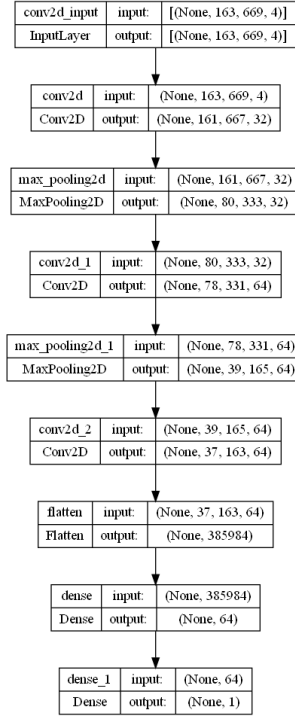


Fig. 9. Architecture of the convolutional neural network used in this work.

$$R_i(z) = \sum_{j=0}^K b_{i,j} z^j + c_i \sin(2z).$$

From the quantum-optical point of view such a (wave) function pertains to a superposition of several Fock states and two coherent states.

We have trained the convolutional neural network to solve the classification problem for triples of pictures belonging to (A) or (C).

The results for the $R_i(z)$ have been less impressive but they seem still to be quite satisfactory as can be seen from Figs. (13, 14, 15)

as well as from the report contained in Figure (12)

There is no need to stress that the above results have a rather preliminary character serving as a kind of “proof of concept”. Much more complex classification problems dealing with multiple classes and using more advanced classifiers will have to be considered.

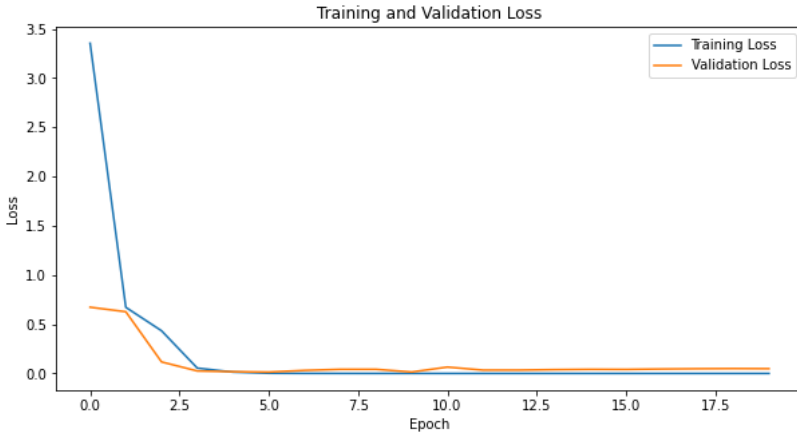


Fig. 10. Dependence of the loss function on the training epoch for the classification of images generated by zeros of the functions $W_i(z)$ and $P_i(z)$.

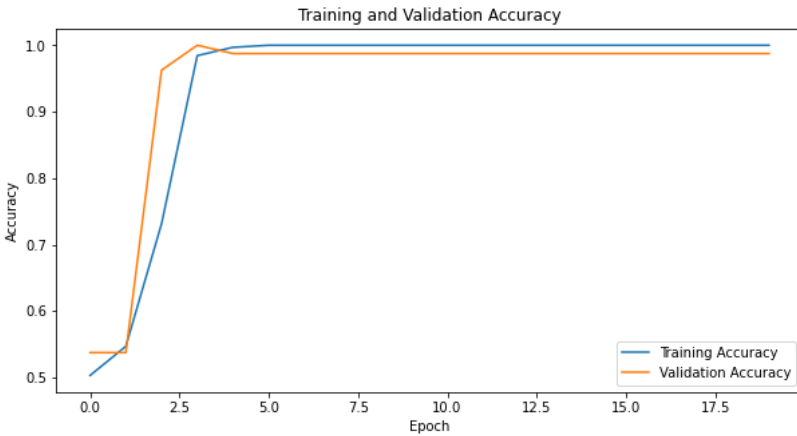


Fig. 11. Dependence of the classification accuracy on the training epoch for the images generated by zeros of the functions $W_i(z)$ and $P_i(z)$.

What is more, semi-supervised and/or self-supervised learning methods will likely be of advantage in the context of graphical recognition of quantum states in the context of quantum tomography [1, 9].

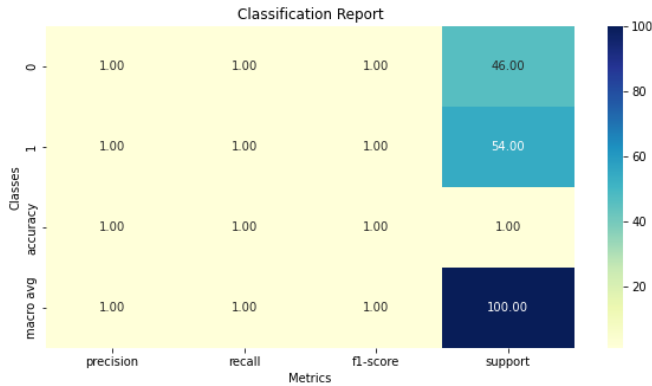


Fig. 12. Classification report for the images generated by zeros of the functions $W_i(z)$ and $P_i(z)$.

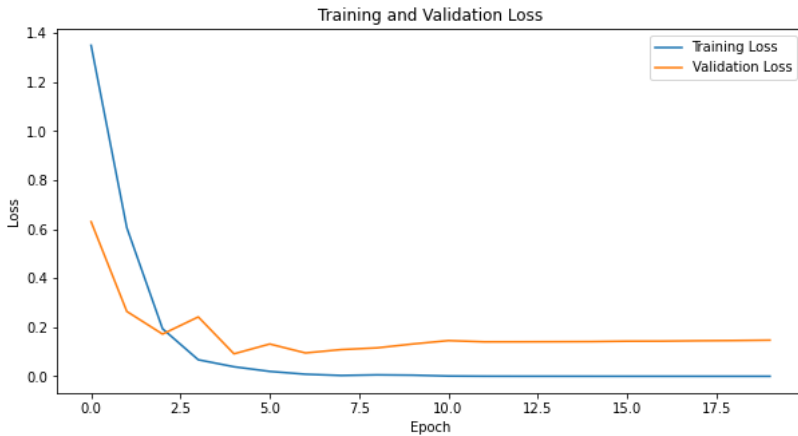


Fig. 13. Dependence of the loss function on the training epoch for the classification of images generated by zeros of the functions $W_i(z)$ and $R_i(z)$.

5. Concluding remarks

An obvious question is whether we can find a similar representation of multi-mode states. Let us first consider, another quantity (more general than the wave function) that characterizes a quantum system. This is the density matrix. For a single mode, the density matrix depends on two complex variables: $\rho = \rho(w^*, z)$. Of particular interest is often the *diagonal part* of the density matrix, $\rho(z^*, z)$. This means that, of course, ρ is not a holomorphic function and we have no reconstruction theorems like that of Weierstrass

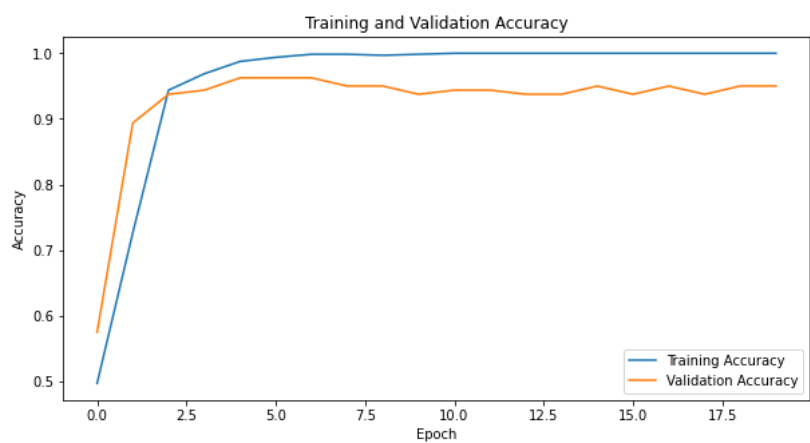


Fig. 14. Dependence of the classification accuracy on the training epoch for the images generated by zeros of the functions $W_i(z)$ and $R_i(z)$.

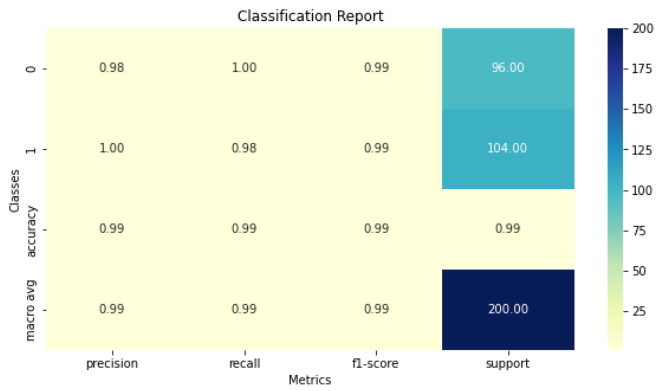


Fig. 15. Classification report for the images generated by zeros of the functions $W_i(z)$ and $R_i(z)$.

or Hadamard in our disposal. Still, zeros of such diagonal elements (being the zero of Q -functions) can be obtained and plotted to serve as a pictorial representation of the state.

Now, if we have a multi-mode wave function, then at least two routes are possible depending on the number of modes. If this number is equal to 2, we can obtain an interesting parallel with the knot theory [5]. Indeed, suppose (unnormalized) $\psi(z_1, z_2)$ is equal to, say, $z_1^2 + z_2^3$. In that case, the zeros satisfy the equations $z_1^2 = -z_2^3$ so that they say, $z_1^2 + z_2^3$, then In that case, the zeros satisfy the equations $z_1^2 = -z_2^3$ so that they

are located on a complex curve (there are no isolated zeros of holomorphic functions of many variables). The common part of this curve with a sphere S^3 forms a simple knot. Thus, in a certain sense, the knots can also serve as a two-dimensional generalization of the pictures in Figs. 1a-8a. Finally, let us mention here that there is a pretty obvious analogy of the zeros of multi-mode quantum states and the Calabi-Yau surfaces. They are known for their very complicated behavior and any visualization methods applied to them would be helpful or even desirable. One line of tackling this problem has been outlined in [4].

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