

# USING SMARTPHONES AS A COLORIMETRIC SENSORS: CASE STUDY FOR WINE ANALYZES

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## ABSTRACT

Over the years mobile phones, specifically smartphones, have undergone in major changes, making them tools capable of collecting and processing data that was only possible a few years ago using several devices together: camera, computer, etc.

The purpose of this dissertation is to demonstrate how the use of a smartphone, for conducting spectral and colorimetric analyzes, allows us to evaluate the color of a wine sample.

In order to treat and study the results obtained with the smartphone, it was studied, developed and improved a method of spectral inversion that through the characteristic values of a color, XYZ, can present a spectral representation coincident with the one obtained in the laboratory.

Several solutions were tested as the inversion through normalized and non-normalized values and the division into asymmetric and symmetric sets. For each of these solutions, several samples were tested before the final experiment with a wine sample, such as: LED of an iPhone and dyes with different colors. The Root Mean Square Error (RMSE) value was calculated to serve as an additional term of evaluation for the spectral inversion method.

In the final experiment, wine sample, the best result for the RMSE value was reached using the spectral division with asymmetric sets (25 and 45 samples), the error was 0.1466, while the best spectral representation is obtained through the use of normalized values.

**Keywords:** Smartphone, Wine, XYZ

## 1. INTRODUCTION

### 1.1. Motivation

The smartphone, probably the technological invention most used by the world's population, is still considered a new technology nowadays, despite the high market penetration observed since 2015 (147%) [1].

In Portugal, around 70% of the population used a smartphone in 2017, a value that increased by 40% compared to the year 2012, as can be seen in Figure 1 [2].

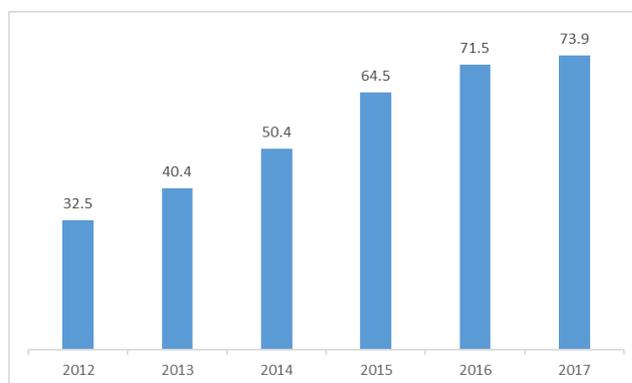


Figure 1: Time evolution of smartphone usage in Portugal (% of population) (extracted from [3])

One of the components in mobile phones that has evolved the most in recent years is the camera, being initially characterized by its low resolution (0.11 Megapixels [4]). In addition to the positive evolution verified in the cameras, the sensors that are inside a smartphone have undergone an improvement, being nowadays equipped with sensors of movement, position, image, among others. The evolution of sensors in mobile phones, in addition to enabling smartphones for various technical applications, has also made them more appealing to end consumers, giving them the possibility to store all kinds of functions and tools in a single device.

It is possible to perceive the usefulness of a smartphone for the case study of this thesis, because it prevents that there are charges in the acquisition of software and hardware to collect and treat all type of information necessary and due to its size and accessibility, it facilitates the whole process involved.

## 1.2. Goals

The objective of this dissertation is the demonstration of the possibility of using a smartphone to perform several spectral and colorimetric analyzes applied to a specific scenario, the wine monitoring, with a view to future application.

To achieve this goal, it will be necessary to develop tools that will allow the evaluation of the wine's quality. In this way, the first tool consists in the representation of the white light spectrum, which will serve as a basis for comparison throughout the project. The white light source, together with the use of a camera of a mobile phone, will allow us to obtain an image to collect the values of the corresponding components of each color. Subsequently, these values should be spectrally represented, making them comparable with the spectrum of the light source. Finally, using these comparisons, it will be possible to obtain and identify the color absorption spectra of each wine sample, which will serve as the basis for a qualitative analysis of the results.

## 2. STATE OF ART

### 2.1. Evolution of sensors in smartphones

About 24 years ago, in 1994, the first smartphone, the IBM Simon, was launched. In addition to the basic features of other conventional mobile phones, IBM Simon featured touchscreen technology, the ability to run some software applications, and the ability to connect to a fax machine [5]. Over the years, several devices that aimed to combine the functionality of a computer and a mobile phone were developed. With increasing popularity, suppliers have been investing more and more in the design and functionality of the equipment, in line with the new needs of consumers, being one of the biggest innovations the ability to connect to the internet [6].

As time goes by and with the evolution observed in the hardware and software of the equipment, there was a development of many sensors for this type of mobile phone, improving its performance in several aspects, and nowadays it is possible to find several sensors, as the example [7]:

- Accelerometer;
- Gyroscope;
- Magnetometer;
- GPS (Global Positioning System);
- Barometer;
- Proximity sensor;
- Ambient light sensor;
- Illumination sensor.

In addition to the sensors, the camera of the mobile phones has also suffered several updates with the goal of approaching it even more to a digital camera, and may even serve as its substitute.

### 2.2. Application areas of smartphones sensors

All sensors available on a smartphone, as well as its camera, can be used for different purposes and in different areas of human life such as:

- Health care - in the last decades the aged population (over 65 years) represents about 20% of the world population, and this age group needs regular or continuous monitoring. The combination of body sensors with mobile phones allows to control various indicators of the health of an individual [8];
- Augmented reality - possibility to place digital objects in real world locations and interact with them with precise movements, making it easier to choose furniture to have in a house, for example [9];
- Traffic control - traffic can affect both the environment and human productivity, so it is important to detect the fastest and least congested paths in a trip [7];
- Environmental control – measuring the pollution levels and monitoring individual actions that affect both exposure and contribution to problems such as carbon emissions [7];
- Behavioral monitoring – abnormal activity detection applications draw a lot of attention among scientists. It is possible to feel the environment and perceive various human behaviors [10];
- Food control – detection of nutrients and chemicals present in food consumed by humans that benefit or harm their health [11].

### 2.3. Wine monitoring

Viticulture has been present in the daily life of the human being since the fourth millennium B.C. With the expansion of the Greeks and Romans, it spread throughout Europe and eventually throughout the world, being the old continent the one with the greatest extension, expansion and tradition of this culture [12]. With the passage of time and new demands of consumers, it has become imperative to control and regulate the quality of the vine and wine. The wine's color represents a unique characteristic in the definition of quality, since it is the first characteristic in which consumers focus and can influence the perception of the wine's taste, through the expectations created by the human being, by the association of colors with flavors [13].

Currently, the new standards created in Portugal require the use of spectroscopic techniques to determine the wine's color. All experiments are performed in the range of 360 nm to 830 nm using an illuminant, usually D65, and using a spectral step of 1 nm [14].

### 3. THEORETICAL FOUNDATION

#### 3.1. Human Visual System

Color is a fundamental attribute of human visual perception, and the human eye is only sensitive to a small band of the electromagnetic spectrum between 380 nm and 780 nm [15]. The human visual system consists of two parts, the eye and the brain. While the eye functions as a kind of camera, the brain plays the role of image processing. The human eye, Figure 2, has a spherical shape of about 24 mm in diameter. The incident light hits the cornea and the iris, that regulates the amount of light that is allowed to pass into the retina, retains part of it. The retina, in turn, contains two types of light sensitive cells, named according to their shape: the cones and rods. Rods (about 100 million) allow the perception of different brightness levels, and are mainly responsible for the night vision (Scotopic). The cones (about 4-6 million) allow to recognize different colors, especially in relatively bright environments [15].

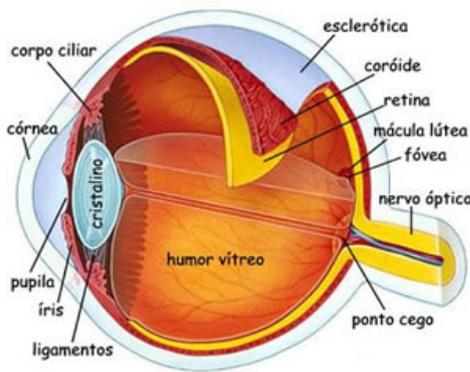


Figure 2: Human eye (extracted from [15])

Based on the visual system, we can make a first evaluation of a sample of wine, since if it presents a different color from the usual we can soon conclude that probably that wine is damaged or has some abnormal mixture and it is not necessary to resort to a detailed spectral analysis to arrive at that conclusion.

#### 3.2. Optical Receivers

Charge-Coupled Devices (CCDs) are silicon matrices based on MOS (Metal-Oxide-Silicon) diodes that have the ability to store and transfer information across multiple load packets [16]. Although they were originally invented as a memory device, the CCDs are intended to be used as an image sensor, enjoying its sensitivity to light. They receive as an input the light from an object or an electric charge, captured through small light detectors, the pixels, which work as a bucket of electrons that during the exposure time

fill up in proportion to the amount of light captured [17] and then convert it into an electronic signal. The output signal is then processed by other equipment and/or software to produce an image or to provide information [18].

The sensitivity of these devices varies depending on the light source, since the gain of conversion depends on the wavelength of the optical signal. From a certain point, the output voltage reaches a limit value, even if the intensity of the incident light continues to increase (saturation), causing the sensitivity to become zero and to lose information, causing the need for limiting the output voltage to its saturation value [19].

CDD cameras are very useful from the scientific point of view, as they are widely used in laboratory to capture small details that an ordinary camera would not be able, since they are very sensitive to light [17].

#### 3.3. Radiometry, Photometry and Trichromatic Vision

Radiometry is the science that studies the amount of light in the visible region of the electromagnetic spectrum.

Photometry, in turn, is the art of measuring visible light taking into account the characteristics of the human visual system. It is a quantitative science based on a statistical model of visual response to light on carefully controlled conditions [20]. In photometry, we do not measure power or radiated energy, but rather the subjective impression produced by stimulation of the visual system with radiated energy. This task becomes quite complicated since the human eye does not have a linear response to light, since it depends on several variables, among which: wavelength, amount of radiated flux, intermittent light, complexity of the observed scene, the adaptation of the retina and the iris, among others [21].

For the development of this dissertation, we are only interested in the photometric measurements, since the whole process of analysis is based on the colors and values representative of these colors of different samples. In 1931, the CIE (*Commission Internationale de l'Éclairage*) created two color spaces, RGB and XYZ. The CMF (Color Matching Functions) of each of these spaces are represented in Figure 4, and if the values are all the same, white color is produced. In the case of XYZ, the CMF of Y matches the luminous efficiency function of the human eye.

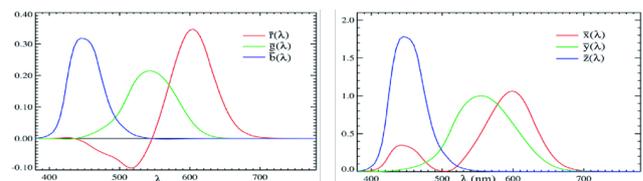


Figure 3: a) CIE RGB CMF; b) CIE XYZ CMF (extracted from [15])

It is possible to obtain the XYZ values from the spectral data as follows:

$$X = \frac{K}{N} \int S(\lambda) I(\lambda) \bar{x}(\lambda) d\lambda \quad (1)$$

$$Y = \frac{K}{N} \int S(\lambda) I(\lambda) \bar{y}(\lambda) d\lambda \quad (2)$$

$$Z = \frac{K}{N} \int S(\lambda) I(\lambda) \bar{z}(\lambda) d\lambda \quad (3)$$

Where  $S(\lambda)$  is the spectral reflectance,  $I(\lambda)$  is the power distribution,  $N = \int I(\lambda) \bar{y}(\lambda) d\lambda$ ,  $K$  is a scaling factor (usually 1 or 100) and  $\lambda$  is the wavelength. From these results, it is possible to normalize XYZ in the chromaticity coordinates ( $x$ ,  $y$ ) and represent them in the  $xy$  plane, since  $x + y + z = 1$ :

$$x = \frac{X}{X+Y+Z} \quad (4)$$

$$y = \frac{Y}{X+Y+Z} \quad (5)$$

$$z = \frac{Z}{X+Y+Z} \quad (6)$$

### 3.4. Inversion of XYZ values to Spectrum

The first step to do this inversion is the definition of the proportionality constant. To do this, it is necessary to multiply the second column of matrix A (matrix CMF CIE 1931 corresponding to the values of XYZ with the spectral step of 5 nm in the region between 380 nm and 720 nm) by the light spectrum of a light source, followed by the sum of all values of the generated vector. To the constant resulting from this sum we give the name of scaling factor, which is later used to calculate a new vector (B) with three coordinates [22], obtained by multiplying the scaling factor by each of the XYZ components.

Then, it is necessary to obtain an E matrix, where each column represents each of the three components (XYZ), used as the basis for the calculation and representation of the spectrum [23]. For the calculation of this matrix, in a first phase, it is necessary to calculate the multiplication of matrix A by its transpose, to later calculate, the inverse of this multiplication. The value obtained, is then multiplied by the transpose of matrix A and finally transposed, resulting in a new matrix, as can be seen in equation 7 [22]:

$$E = ((A^T \times A)^{-1} \times A^T)^T \quad (7)$$

Finally, by combining the values of the matrix E with the vector B, as we can see in equation 8, it is possible to obtain the final values used to represent the spectrum [23].

$$f = B \times E \quad (8)$$

Based on the method described above, using the XYZ values corresponding to each sample, we will proceed to its inversion to try to arrive at the representative initial sample of the study sample.

## 4. RESULTS

### 4.1. Testing the spectral inversion procedure of an LED lighting from an iPhone 4

In order to demonstrate the feasibility of using a smartphone to quantify the colorimetric characteristics of a sample an algorithm was implemented. It aims to use light from a white light source in a given sample and analyze the image obtained from the sample. With these values, and following the method described in section 3.4, it will be possible to obtain the absorption spectrum of the sample under study which, when compared to the white light power spectrum, allows us to reach the color absorption spectrum of the specimen under investigation. It is from this absorption spectrum that we will carry out the qualitative analysis of this wine and see if it meets the minimum quality requirements imposed by law [14]. The description of this method is shown in Figure 5.

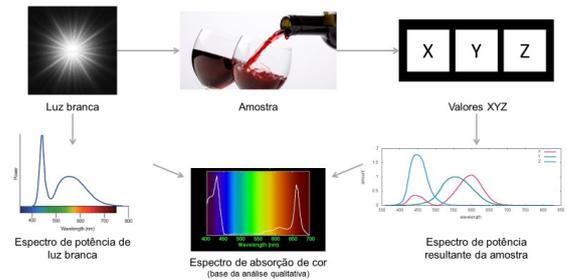


Figure 4: Method for analyzing a sample of wine

The preliminary task to implement this method, is the realization of a method for the spectral inversion of the color coordinate values.

Thus, the Oceanview S09500 spectrometer, with a resolution of 1024 pixels and an integration time of 1 second, is used to obtain the emission spectrum of the illumination LED of an iPhone 4. The experimental data is interpolated to the spectral region between 380 and 720 nm with a spectral step of 5 nm according to the requirements of the CIE to be able to represent the spectrum shown in Figure 6.

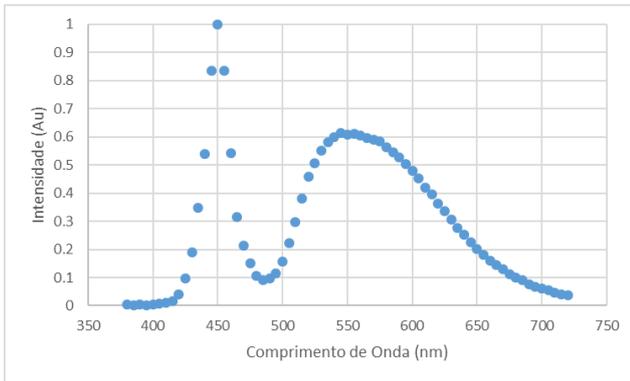


Figure 5: White LED spectrum

The next step is trying to reach the spectrum of the studied LED by inverting the values of XYZ. For this, and taking into account the whole process enumerated in the previous section, a script was implemented, which solves all the calculations and presents as a result the graph of Figure 7.

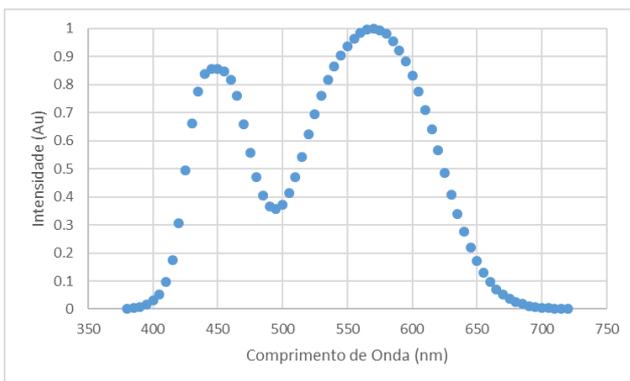


Figure 6: White LED spectrum obtained by inversion of XYZ values (RMSE = 0.2485)

The expectation was that both graphs would be identical, since the inversion of the XYZ values is being done for a white light source. However, as it is possible to observe, it does not happen and if we calculate the root mean square error [24] between the values of both spectra, we can confirm this same difference, since we obtain the value of 0.2485. It is possible to verify that this value differs from the ideal (0) which represents an equality of the obtained data. These differences are mainly due to the loss of information in obtaining the XYZ values and their consequent inversion, mainly due to the need to reduce the initial number of 1024 samples to those necessary to use the CIE 1931 XYZ matrix with a spectral spacing of 5 nm.

#### 4.2. Improving the spectral inversion method

After the inconclusive and mismatched results obtained in the previous section, it became imperative to try to change the outcome of the spectral inversion method. The first step was to reduce the spectral spacing from 5 nm to 1 nm to try to figure out whether if increasing the number of samples, and consequently losing less information, would be possible to achieve better results. To perform this test, it was necessary to re-interpolate the values obtained in the laboratory so that they were eligible to be apply to the inversion method of the XYZ values.

As can be seen from Figure 8, little or no results differ from those achieved previously, and it is therefore possible to infer that the use of a more or less narrow spectral step does not contribute to the loss of information and to an unadjusted representation of the initial spectrum.

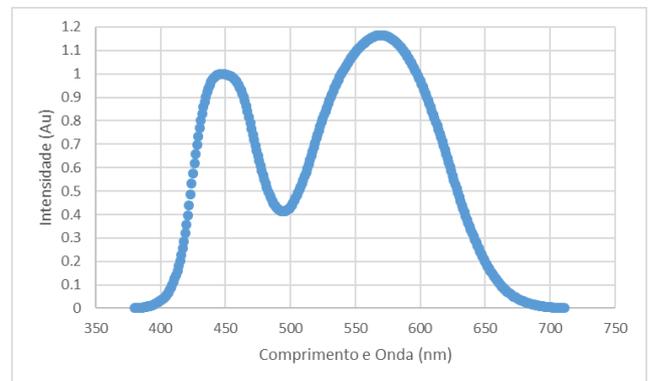


Figure 7: White LED spectrum obtained by inversion of XYZ values (RMSE = 0.4177)

The next step, in the attempt to discover the origin of the spectral differences, was the creation of a routine that could minimize the value of the root mean square error using only, as parameters to change, the values of the three coordinates that represent the color of the studied LED, XYZ. Using the Solver tool of Excel [23] it was verify that the value of RMSE decreases from 0.2485 to 0.2108, which causes some differences in the inverted spectrum graph, as we can see in Figure 9.

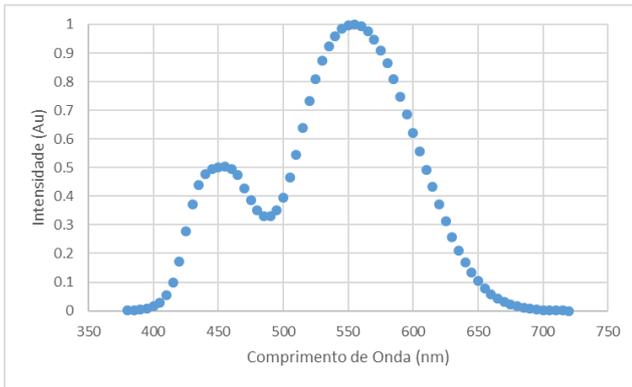


Figure 8: White LED spectrum after minimization (RMSE = 0.2108)

As can be seen from comparing both graphs, the spectral representation has improved somewhat, but not enough. The intensity values at the two maximum are almost the same as the original chart, but they are shifted in terms of wavelengths. Since no major improvements were achieved in relation to the spectral inversion method, we decided to apply this method to different samples in the expectation that using different color samples, the results produced would be different. The three specimens of the CIE emission, which represent the RGB colors, were put to test and the results showed some improvements compared to the white light, which can be verified by Figures 10, 11 and 12.

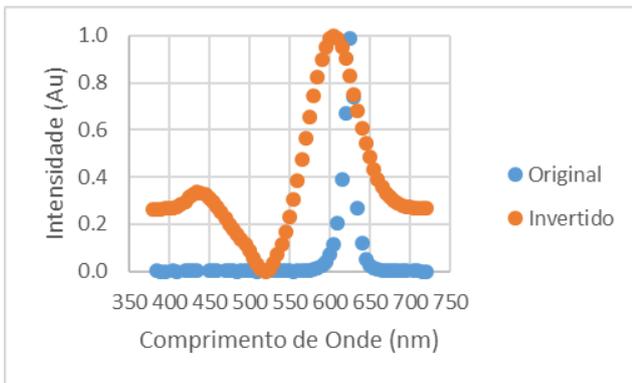


Figure 9: Original and inverted spectrum for Red color (RMSE = 0.3256)

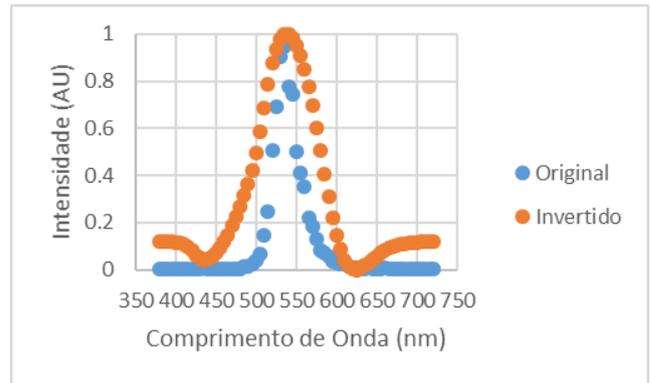


Figure 10: Original and inverted spectrum for Green color (RMSE = 0.2964)

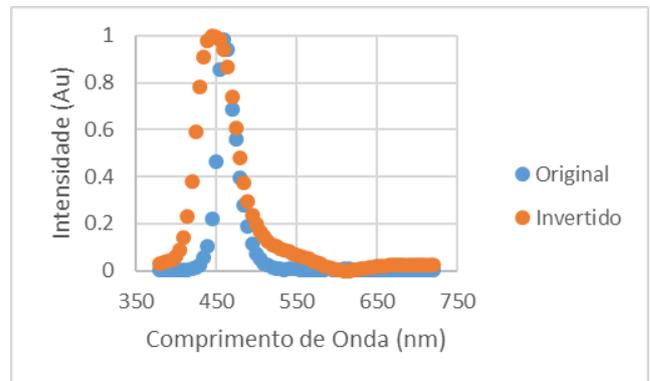


Figure 11: Original and inverted spectrum for Blue color (RMSE = 0.3452)

We can conclude that, as the wavelength that characterizes a color decreases, the quality of the inverted spectrum increases, being the blue color spectrum the closest to the original. After all these experiments we came to the conclusion that one of the possible reasons for the inaccuracy of the root mean square error minimization is that Solver only performs five iterations, thus limiting the progress of the minimization routine.

#### 4.3. Improving the spectral inversion method using MatLab (fminsearch)

Finding the results achieved to this point somewhat imprecise, we felt the need to implement this RMSE minimization routine in MatLab, in the expectation that increasing the number of iterations the results produced would be more satisfactory. To implement this routine we developed two scripts, one that calculates the root mean square error and another that minimizes it through the `fminsearch` function [24].

The next step, in an attempt to improve the final value of RMSE, was the recombination of the parameters to be

altered. We then tested seven hypotheses for the same LED of the iPhone:

1. Change the values of XYZ;
2. Change the values of XY;
3. Change the values of XZ;
4. Change the values of YZ;
5. Change the values of X;
6. Change the values of Y;
7. Change the values of Z.

For the purposes of information summary and reduction of images, only the solutions with the lowest root mean square error and highest graphic similarity values are presented, Figure 13 and 14.

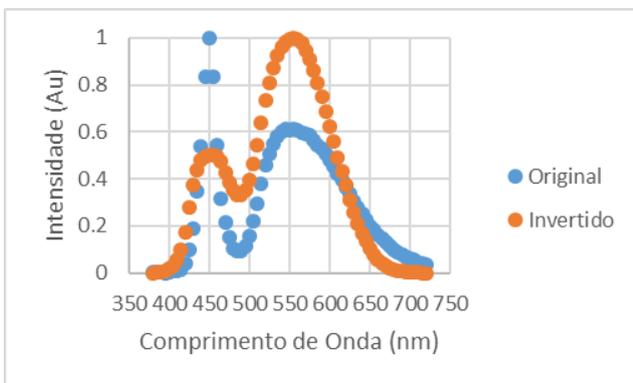


Figure 12: Original and inverted spectrum (Minimization with XYZ, RMSE = 0.2108)

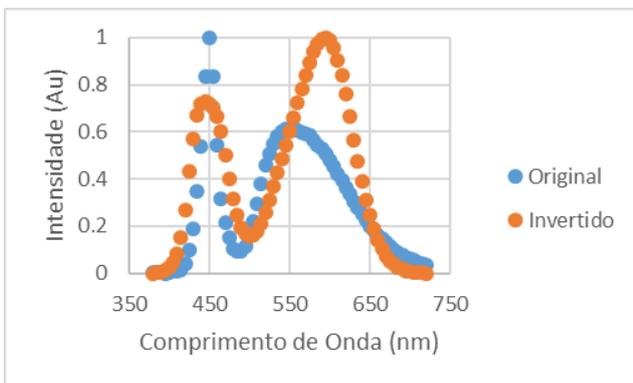


Figure 3: Original and inverted spectrum (Minimization with X, RMSE = 0.2246)

If only the different RMSE values are taken into account, with each of the seven combinations and based on the initial value of 0.2485, one can conclude that using the assumptions 1, 2 and 4, the lowest possible error value is achieved (0.2108). If the graphical comparison between the two spectrums is used, the result is different from the previous one. For this evaluation method, tests 1, 2, and 4 are equal to each other and identical to the solution using the Excel Solver tool, which was expected since all have the

same root mean square error value. In the third case, the first maximum of the chart improves substantially, while the second one worsens. The combinations where the inverted spectrum most closely resembles the initial spectrum are five and six, where in the first of these cases, the first maximum is the one that improves the most and the second one worsens very little. In the second case, 6, both maximums improve when compared to the first hypothesis. These results appear to be discrepant with the expected, since it should be assumed that as the RMSE value decreases the similarities between the spectra increased, which did not occur. The main reason for such occurrences is that white light has a spectrum too wide, 380 nm to 720 nm, thus comprising too much information for the correct application of the spectral inversion method. After these conclusions were drawn, the sample was changed in order to understand if the routine would achieve better results using a color with a narrower spectrum and with less information. The first color chosen was blue and for it, the value of the RMSE, changing the three coordinates, was 0.2259. This is the lowest value that the error reaches, and this situation was verified in hypotheses 1, 2, 3 and 4. When the graphical comparison is used as the weighting term, changing only the values of X or Z, experiences 5 and 7, we can notice a slight worsening, which is more pronounced in case 7. Changing only the value of Y we reach the best situation, again being strange confronted with the value of the root mean square error. For the case of yellow color, the results were identical, where hypotheses 1, 2, 3 and 4 were the ones with the best root mean square error values, 0.0751.

Although spectral representation continues to exhibit some imperfections when using a color other than white, it is possible to notice that there is a significant improvement in its representation for the reason described above. Figures 15 and 16 confirm this, where the graphs of the original and inverted spectrum are represented, when there is a change of the three parameters (XYZ).

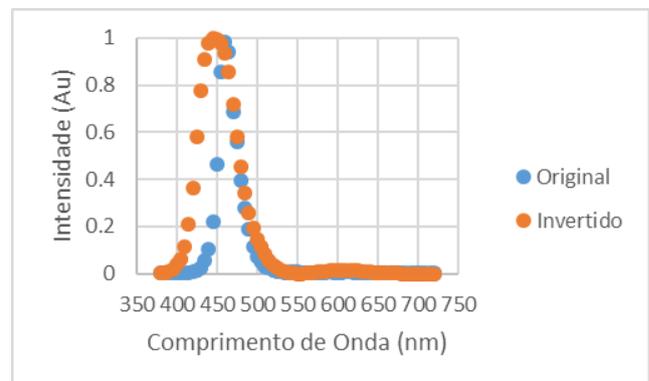


Figure 4: Original and inverted spectrum for Blue color (RMSE = 0.2259)

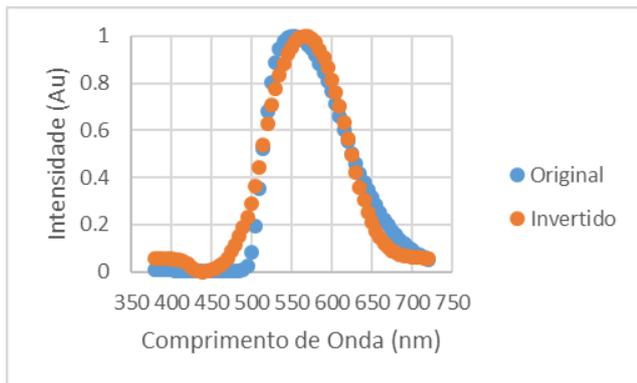


Figure 5: Original and inverted spectrum for Yellow color (RMSE = 0.0751)

After these conclusions were drawn, and re-using the iPhone LED, the two scripts were changed to not normalize the results of the spectral inversion method and it was found that the root mean square error value decreased from 0.2485 to 0.1148. As for the graphical representation of the spectrum, and as we can see from Figure 17, it improved significantly in the second maximum.

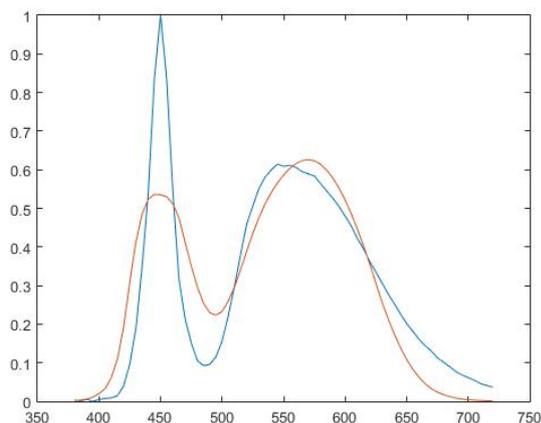


Figure 6: Original and inverted spectrum with non-normalized data (White LED)

After this experience, it can be concluded that one was going in the right direction in perfecting the method of spectral inversion. In order to try to improve the method, we decided to make two more new experiences involving the division of the total spectrum:

1. Division with 25 sample, between 380 nm and 500 nm, and 45 samples, between 500 nm and 720 nm;
2. Division with 35 samples, between 380 nm and 550 nm, and 35 samples, between 550 nm and 720 nm.

Obviously, in order to calculate the root mean square error value, the RMSE of each block of samples was added, and each one of them must be multiplied by a value, alpha and

beta. The sum of alpha and beta must be equal to one, and initially the value of 0.7 and 0.3 was assigned to alpha and beta, respectively. In the first case, the value of the error was 0.2329, while in the second one it was 0.1373. Figures 18 and 19 show the original and inverted spectrum of these two tests.

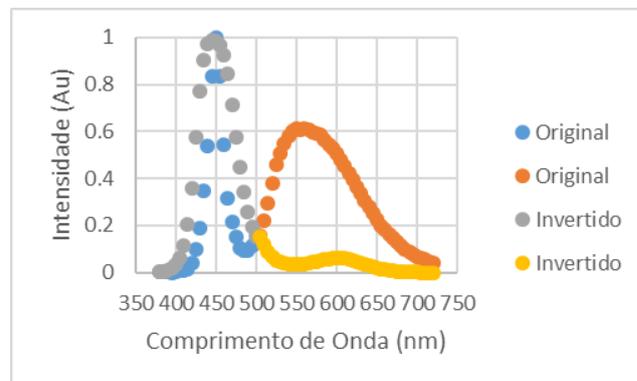


Figure 7: Original and inverted spectrum for asymmetric assemblies (RMSE = 0.2329)

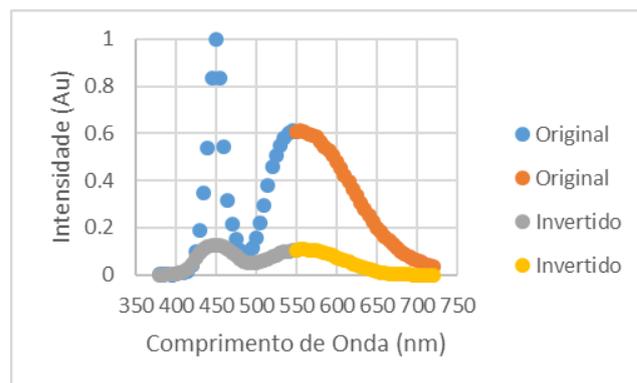


Figure 8: Original and inverted spectrum for symmetric assemblies (RMSE = 0.1371)

Once more, and as we can see from the two figures, the RMSE values do not match what was graphically expected. In the case of the first division, we can notice that there is a significant improvement in the first maximum, but also a regression in the second one. For the second case, where one would expect a slight improvement, once again there is a total worsening of the inverted spectrum.

#### 4.4. Application for the characterization of a wine sample

After several attempts and tests, it was impossible to put alpha as a parameter to change and then we chose to leave the program as it was and test the actual sample. The wine chosen for this sample was a red, *Grand 'Arte Alicante Bouschet*, from the region of Lisbon of 2014.

The first step was to calculate the XYZ coordinates from this sample by using the equations 9 to 12, and to do so we collected the RGB values to apply to them.

$$\begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} 0.488718 & 0.31068 & 0.200602 \\ 0.176204 & 0.812985 & 0.010811 \\ 0 & 0.010205 & 0.989795 \end{bmatrix} \times \begin{bmatrix} R \\ G \\ B \end{bmatrix} \quad (9)$$

$$x = \frac{X}{X+Y+Z} \quad (10)$$

$$y = \frac{Y}{X+Y+Z} \quad (11)$$

$$z = 1 - x - y \quad (12)$$

For this wine, the RGB values were [224;27;3] and when applied to the four equation we achieved the following results, X=0.647, Y=0.336 and Z=0.017.

After testing all the solutions presented throughout the chapter we conclude that the lowest value of the root mean square error is reached when using the spectral division with 25 and 45 samples, asymmetric sets, obtaining a value of 0.1466. If we take into account, the representation of the inverted spectrum the best solution is reached when using normalized values of the spectrum and only changing the Z value, Figure 20, although the value of RMSE in this case is 0.3838.

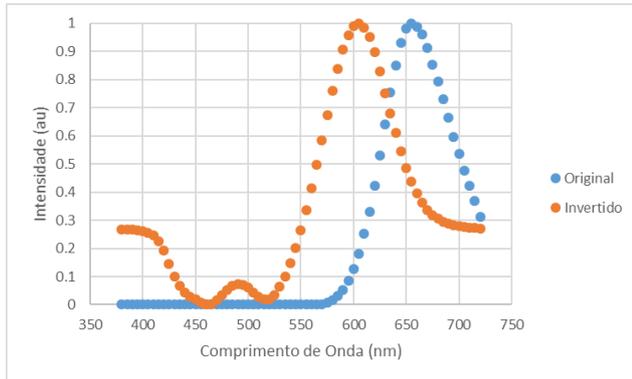


Figure 9: Original and inverted spectrum (Minimization with Z, RMSE = 0.3838)

Once again, and as it has been verified several times throughout all the experiments and tests carried out, the lowest value of the root mean square error did not correspond to the best graphical representation, although it is possible to observe from the image that the absorption peak is similar, but it is at a different wavelength.

## 5. CONCLUSIONS

After two semesters dedicated to this project, some conclusions can be drawn about the work developed.

First, we can concluded that the spectral inversion method used is a relatively simple process. This uses the

manipulation of the matrix CMF CIE 1931 and doing some simple calculations comes to the final solution.

As all the calculations regarding the method were consolidated, the method was implemented to study the lighting LED of an iPhone. The results obtained were not as expected, presenting some unwanted flaws. In order to study the discrepancies of the results, the root mean square error was calculated and throughout the project, the value of RMSE for the different experiments always served as an evaluation and comparison term.

Since the results did not meet the desired ones, we decided that the spectral inversion method needed to be improved, by trying to minimize the root mean square error value using only the values representing a color, XYZ, as parameters to be altered. The first step in optimizing this process was made using the Excel Solver tool, because it is a simple and easy program to use. We realized that this tool did few iterations and little or nothing improved in the spectral representation, even though it improved slightly when the samples used were altered. It was then necessary to use MatLab, more specifically the fminsearch function, to try to mitigate the error value and thus improve the representation of the inverted spectrum in relation to the original one. Using this tool the results improved somewhat, since the number of iterations went from five to one hundred and thirteen, in the case of LED.

After the three experiments were made, use of normalized values, use of non-normalized values and division of the spectrum into two, we concluded that the method continued to fail. In the case of the illumination LED the differences are the greater, since the white light is the one that has more information and it uses the total bandwidth of the electromagnetic spectrum, whereas when they use specific colors the spectrum only have a peak of absorption and contain much less information. These failures are due to errors in the acquisition of the original color spectrum in the laboratory (container containing poorly sealed sample, off-center fiber optics, excessive sunlight in the room, etc.), most of them due to human error. They are also due to the loss of information during the entire calculation process of the spectral inversion method and error mitigation.

The final experience of a wine sample corroborated all the results concluded until then and confirmed what was expected, the red wine had the same behavior as the red color. The lowest RMSE value obtained with this sample was 0.1466 and it was obtained by using the three parameters to minimize the error, in the experiment where the spectrum was divided into two asymmetric sets, one with 25 samples and the other with 45 samples. As for the graphical representation, and although it was expected that for this solution also the best result of the spectral inversion method was presented, this was not confirmed. The greatest similarity between the original and the inverted spectrum was achieved using only the parameter Z to mitigate the root mean square error, which was carried out when using the

normalized values resulting from the spectral inversion method.

It is possible to conclude that by not using normalized values, experiences suffer a huge setback. This is because, even reaching the lowest values for the root mean square error, the non-normalization of the results causes large changes that lead to the unfeasibility of its use as an evaluation tool. The best spectral representations can be achieved by using the normalized values, without using spectral divisions. It is therefore possible to conclude that, in none of the experiments performed, the best spectral representation corresponded to the lowest RMSE value.

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