Multiple Nonlinear Regression-Based Adaptive Colour Model for Smartphone Colorimeter

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Abstract: A self-contained smartphone-based colorimetric sensing platform adaptable for multiple analytes is demonstrated. Concurrent variation of multiple optical sensing parameters is addressed using multiple nonlinear regression analysis. © 2020 The Author(s)

1. Introduction

The majority of reported smartphone-based optical sensing instruments use simple colorimetric based detection or methods that are based on digitizing colour information of an emitter onto the smartphone complementary metal-oxide-semiconductor (CMOS) camera detector. Because of its simplicity, the technique has been used as an effective and reliable approach to serving across a range of biological and chemical sensing. The use of a smartphone's embedded features have driven the development of the lab-in-a-phone technology further, creating a platform for next-generation portable smart sensor networks for Internet-of-Things (IoT) applications.

Smartphone-based colorimetric detection often involves challenges associated with the fluctuation of light under ambient illuminations and, more seriously, unwanted colour correction by the camera itself. The corrections are often manufacturer sensitive posing a significant practical problem for high-end performance. These wider issues have been addressed partially by, for example, introducing a 3D-printed enclosure for controlling the environment and illumination or adding references into the measurements, posing other physical challenges [1, 2]. Appropriate colour models that reduce sensitivity to camera auto-corrections are also reported [3-5]. Both wavelength (λ) and intensity (I) information of emission change in many applications [6]. They may contain a differential change of colour parameter with the sample. The combination of these methods helps to address significantly some of the practical aspects of the instruments. Nevertheless, the combined solution ideally requires a generalized and adaptive correction algorithm considering the weight of all variables and advance statistical tools to optimize the algorithm. In this work, a robust and adaptive colour correction algorithm is developed by combining the orders of intensity and wavelength variations through multiple nonlinear regression. The technique is applied to detect and quantify colour information of two different solutions: pH-probe and KI-starch solution on a 3D-printed simple smartphone colorimeter.

2. Smartphone Colorimeter: Materials and Method

1.1. Optical Design and Fabrication

The optical layout of the simple smartphone colorimeter is shown in Fig. 1(a) which mainly contains a smartphone and an optical enclosure with sample cuvette. The enclosure is designed to fit with the rear-facing camera unit of the smartphone and hold a 10 mm sample cuvette at a fixed distance (d = 35 mm) in front of the camera. A pinhole (ϕ = 4 mm) allows illumination from the smartphone LED (λ = 400 ~ 700 nm) and a round slot allows the collection of reflected light onto the smartphone camera. The entire optical enclosure was fabricated using an FDM desktop 3D printer with white PLA (Polylactic Acid) material that suitably isolates the measuring platform from ambient illumination by blocking unwanted optical signals from the environment. The rough surface diffuses all reflection in all directions, improving the uniformity of sample illumination.

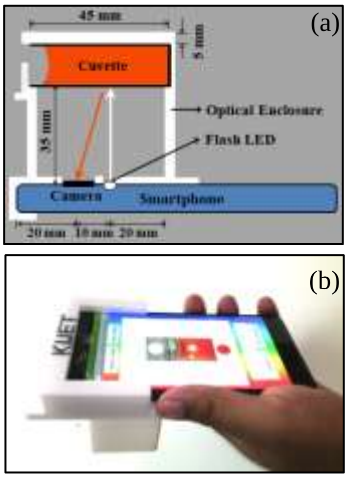

Fig. 1. Smartphone colorimeter: (a) the optical layout, and (b) the 3D printed final device installed on an Android smartphone.

1.2. Multiple Nonlinear Regression in Colorimetric Detection

Most smartphone-based colorimetric detections reported to date have been designed around a single explanatory variable utilizing simple linear or nonlinear regression analysis. But in actual measurements, every colorimetric change is associated with nonlinear concurrent variation of λ and I. So, multiple variables such as hue (H), saturation (S) and value (V) need to be addressed using nonlinear regression to extract the actual colour information. An adaptable generalized equation (Eq. 1) is formulated to relate the study variable (Y) with multiple independent explanatory variables (H, S, and V) through regression coefficients matrices and using a third-order polynomial fit. An ordinary least squares (OLS) method is implemented to estimate the regression coefficients of this model.

$$[Y] = [a_0 \quad a_1 \quad a_2 \quad a_3]\begin{bmatrix} 1 \\ H \\ S \\ V \end{bmatrix} + [H \quad S \quad V]\begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{bmatrix}\begin{bmatrix} H \\ S \\ V \end{bmatrix} + [H \quad S \quad V]\begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}\begin{bmatrix} H^2 \\ S^2 \\ V^2 \end{bmatrix} + d\,[HSV] \qquad (1)$$

1.3. Samples and Device Calibration

To calibrate the colorimeter as a pH meter, 11 buffer solutions ranging from pH 4.0 to 9.0 are prepared by shifting the pH value of standard acetate and phosphate buffer using 0.1 M NaOH at an average temperature of *T* ~ 25 °C. The pH value of each is confirmed by using a standard pH meter. 0.2 ml of universal indicator is added to 10 ml of each buffer solution as the chemosensor dye for the colorimetric detection of pH. To use the colorimeter for measuring chlorine (Cl) concentration, the instrument is calibrated against 24 chlorine solutions of different concentrations ([Cl] ~ 0.1 to 8.0 PPM) prepared by dissolving calcium hypochlorite [$Ca(ClO)_2$] in deionised water. The working sample for colorimetric Cl measurement is obtained by adding 150 µl of KI-starch solution to 10 ml of each chlorine sample. A customised Android app records the images of different samples and find the concurrent and nonlinear variation of *H*, *S*, and *V* as shown in Fig. 2(a) and (b). These parameters are considered as the independent variables of multiple nonlinear regression analysis for both cases. Regression coefficients matrices of Eq. 1 are estimated to adequately calibrate this instrument as a pH meter and [Cl] quantifier and thus two multi order polynomials are formulated with determination coefficient R^2 = 0.9999 and R^2 = 0.9998 respectively. Although this reflects a high degree of accuracy, it is noted that any nonlinear statistical analysis centered around three independent variables has to be done with a degree of caution. Finally, these calibration equations are incorporated into the detection algorithm of the customised app to quantify pH and [Cl] of unknown samples using the smartphone-based colorimeter.

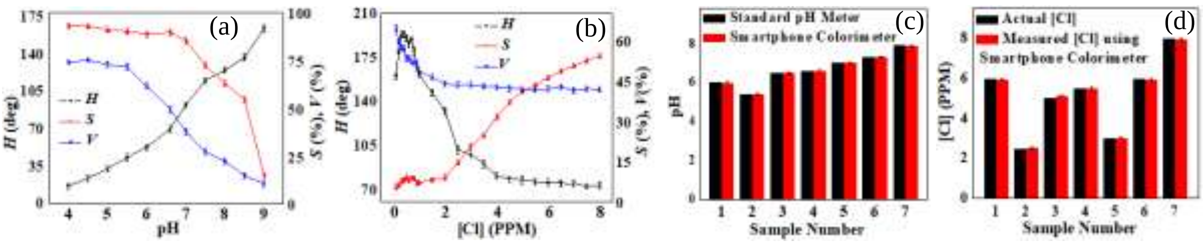

Fig. 2. Calibration of smartphone colorimeter as (a) pH meter and (b) [Cl] quantifier; results of (c) pH and (d) [Cl] measurement.

3. pH and Chlorine Detection in Water

Seven different water samples were collected from different sources in KUET campus to evaluate the performance of pH measurement as shown in Fig. 2(c). Average error of detection in pH measurement is about 0.20% with respect to a standard pH meter. Similarly, the performance of the chlorine concentration quantifier was justified by measuring [Cl] of seven water samples collected from different types of fish ponds in Khulna, Bangladesh and compared with the actual [Cl] of the samples as shown in Fig. 2(d) (average error ~1.01%). The error bars represent a negligible standard deviation over three consecutive measurements of each sample that highlights the exact repeatability of the sensing instrument to determine pH and [Cl].

4. Conclusion

An adaptive colour detection algorithm based on multiple nonlinear regression of colour parameters is developed for smartphone colorimetric applications with superior accuracy. The concept was successfully demonstrated for pH and [Cl] detection of waters from different agricultural sources. This can be applied in other forms of smart colorimetric detection with high-end applications.

5. References

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