Towards Commoditised Near Infrared Spectroscopy

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ABSTRACT
Near Infrared Spectroscopy (NIRS) is a sensing technique in which near infrared light is transmitted into a sample, followed by light absorbance measurements at various wavelengths. This technique enables the inference of the inner chemical composition of the scanned sample, and therefore can be used to identify or classify objects. In this paper, we describe how to facilitate the use of NIRS by non-expert users in everyday settings. Our work highlights the key challenges of placing NIRS devices in the hands of non-experts. We develop a system to mitigate these challenges, and evaluate it in a user study. We show how NIRS technology can be successfully utilised by untrained users in an unsupervised manner through a special enclosure and an accompanying smartphone app. Finally, we discuss potential future developments of commoditised NIRS.

Author Keywords
Near Infrared Spectroscopy; sample identification; sensor accessibility; user-induced errors; pharmaceuticals; user study; gluten detection.

ACM Classification Keywords
H.5.m. Information interfaces and presentation (*e.g.*, HCI): Miscellaneous.

INTRODUCTION

As can been seen in consumer electronics, sophisticated hardware is becoming cheaper and more accessible to the modern customer (*e.g.*, smartphones), this includes Near Infrared Spectroscopy (NIRS) scanners. NIRS has the ability to penetrate the surface and traverse the physical structure of an object. It allows for the retrieval of information about the inner composition of a sample in the form of a spectrum, which acts as a proverbial fingerprint [48] of the sample. Thus, it enables accurate and detailed object identification.

While NIRS scanners have been used in research laboratories for decades [38], only recently has the technology matured enough to allow for end-user hardware which is both small and robust enough to be carried around, while still capable of producing reliable results. The NIRS device used in our study (DLP NIRscan Nano [15]) costs under 1000 US dollars at the time of writing and weighs just 80 grams – a fraction of the price and weight of high-end NIRS hardware. These numbers can be expected to continue to decline, which in turn encourages researchers to start considering everyday scenarios for this technology. For the first time, we argue, it can plausibly be placed in the hands of consumers. The main objective of our work is to explore the improvement of the accessibility of these devices for non-experts.

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Coupling NIRS hardware with commodity devices (*e.g.*, tablets, smartphones) opens a range of exciting research avenues to explore. An *in situ* scanner placed at supermarkets could enable classification of products while they are being weighted, and report to the users the current state of the product (*e.g.*, the level of ripeness of a fruit [45]). In a home scenario, augmented shelves can detect the food being stored, and even determine if it has gone bad [3]. In a domiciliary health scenario, a user can scan a pill or medicine to confirm that this pill is the correct one to take at that moment [9]. There are a vast number of potential use cases for an everyday device that can identify objects based on their physical composition and ingredients.

The contribution of our work is three-fold. First, we explore the challenges in obtaining reliable scanning results, namely the impact of user-induced errors on scan accuracy. This is an unexplored territory in the context of miniaturised NIRS scanning. Second, we map the complexity and required knowledge to carry out a full sample analysis [27]. Third, we design and evaluate a set of mechanisms to address these issues and make NIRS more accessible and usable to non-experts. Our design consists of a custom enclosure to physically guide the user in the scanning process, and a mobile application to assist the user, inform of scanning errors during usage, and encapsulate the sample analysis process. We evaluate our design in a user study to collect feedback and ideas for future improvements. Our findings show that non-experts can successfully use this technology when both *physical* and *procedural* guides are in place.

RELATED WORK

Making Sensors Accessible

Sensors play an increasingly larger role in consumer electronics. Today, consumers' personal devices are embedded with a plethora of different hardware sensors, such as accelerometer, gravity, gyroscope, light, and magnetic [47]. Beyond providing benefits to the users themselves, these sensors have proven to be valuable tools when conducting research in fields such as traffic management [5], HCI [41], localisation [10], and healthcare [32]. While these electronic components are now commoditised and embedded as an integral part in a variety of products, they were originally much larger standalone devices. For example, the first accelerometer weighted almost 0.5 kg and measured 1.90 x 4.76 x 21.59 cm in size [53]. The size, weight, and cost of the accelerometer was eventually reduced, while the use cases expanded [53]. Initially, the accelerometer was used mostly in industry, but now benefits end-users with service enhancement in numerous applications. Further, smart devices do not only serve as a host for embedded sensors, but frequently act as control points for smaller and mobile sensors. This, combined with the widespread nature of smartphones [42], allows for innovative services. For instance, smartphones can be connected to portable medical devices (*e.g.*, blood pressure, glucose, and pulse oximeter) to process, analyse, and present biohealth data [22,31]. It is increasingly feasible for end-users to self-monitor their health, without the need for trained healthcare personnel. In essence, the development of these sensors and their increased accessibility help bridge the gap between end-users and advanced medical equipment.

In another example, Samsung's Galaxy Note 7 includes an infrared iris sensor, which allows biometric authentication on consumers' devices for security and access control [43]. Similarly, while until recently only a few devices came with fingerprint sensors [19], this technology has become increasingly more accessible for end-users. Goel *et al.* [20] showcase how a hyperspectral sensor, previously used for research, can assist in a wider set of use cases. Using *functional* Near-Infrared Spectroscopy (fNIRS) for Brain–Computer Interfaces (BCI) has begun to proliferate in the HCI community [30,33,40,51]. Strait *et al.* [52] investigate the reliability of fNIRS in BCI through a user study, and highlight some of the obstacles. Yuksel *et al.* [54] develop a system that automatically adjusts musical learning tasks based on the user's cognitive workload measured by fNIRS. In our work, we take initial usability steps towards facilitating the use of NIRS scanners by non-experts and by using smartphones as a control point.

Near Infrared Spectroscopy

NIRS sends near infrared light into a sample and measures the absorbance at various wavelengths, thus allowing for object identification [7]. Because of the characteristics of the NIR band (780 nm to 2500 nm), it can penetrate objects up to several millimetres. This enables quick and accurate analysis of the inner composition of samples (*e.g.*, analysing if a food product contains gluten), something that cannot be attained using computer vision. NIRS has been shown to be a useful technique in research across many different fields [16,17,49]. One of the more popular use cases of NIRS is to verify the quality of food. Sinelli *et al. [49]* used NIRS to analyse the freshness of minced beef. By comparing scans taken at different times, they were able to accurately determine the expiry date of the product. Others have explored NIRS as a way of developing a non-destructive solution for analysing fruit quality [28]. NIRS methods can reveal information about the inside of the fruit, something impossible to achieve solely through visual inspection. The reflected spectra contain the information used to infer the fruit's maturity, pH factor, solid content, and flesh elasticity. Another distinct feature of NIRS is the possibility to scan an item with no manipulation or pre-treatment applied to the object itself [6]. For this reason, NIRS has also gained popularity in the pharmaceutical industry [4]. This industry is heavily regulated, with a need for fast and safe quality control. NIRS can also help to address the challenge of counterfeit drugs. It is estimated that around 7% of the pharmaceuticals sold in the world are fake [13]. These counterfeit drugs are typically defined as drugs that have active substances which have been modified [13]. Similarly, in textile industries there is a need to verify the fibres of clothes at different stages in the production and recycling. However, many of the current methods for textile classification are both time consuming and involve dangerous chemicals. Cleve *et al.* [12] report how they accurately identified fabrics using NIRS. Durand *et al.* [16] argue that NIRS can replace existing methods and report an identification accuracy of over 96% for textiles. The aforementioned use cases (*i.e.*, food, pharmaceutical, textile) provide realistic real-world usage scenarios and are suitable for testing in a miniaturised NIRS context.

Miniaturised Near Infrared Spectroscopy

Most of the previous examples rely on heavy desktop NIRS equipment or larger portable devices. Given their success, miniaturised versions for field use have recently been developed. For instance, a mobile NIRS device has been used to detect tomato's pathogen [1]. By scanning the fruit just before it is harvested, it is possible to avoid large losses of fruit being rejected in quality control. Instead of sending the sample to a lab and waiting for a report, results can be obtained *in situ* in a matter of seconds. Unlike many of the current *in situ* chemical approaches, NIRS is also a non-destructive method. However, farmers reported that they considered the equipment to be both too expensive and too difficult to use [13].

Recently, cheaper and smaller devices have entered the market. However, there is a lack of research that investigates the effects of user-noise and usability when the device is placed in the hands of non-expert. Specifically, the effect of device motion [26], sample distance [46], sample angle [35], sample surface [36], sample interference [56], and ambience [50] have not been tested in the context of end-user miniaturised NIRS usage. Therefore, in this paper we investigate the effect of these parameters and consider ways to overcome the challenges they may impose. Furthermore, we propose a non-expert assistance for end users.

CHALLENGES OF NIRS SCANNING

There are two main challenges that users face when utilising NIRS technologies: 1) the impact of user-induced errors on the reliability of the results, and 2) the complexity of the sample analysis process. The effect of the former is exacerbated when NIRS devices are placed in the hands of non-experts. The latter is a challenge pertaining to commoditising this technology, since we expect that everyday users lack the skills to extract, analyse, and interpret the output generated by the device. Next, we describe in detail the impact of both these challenges on the reliability of the results.

Challenge 1 – User-Induced Errors

We experimentally investigate the limitations of NIRS technology in terms of user-induced errors in a scanning scenario with everyday materials. When a user interacts with the device (*e.g.*, place an object, hold the device), the user may introduce some noise to the system that can degrade scan accuracy. This could for example be caused by improper sample placement or an (unintended) shaking motion. To support non-expert NIRS usage, we have to identify the magnitude of the various types of user-induced errors. Moreover, based on the data from these test, we can inform the design of our non-expert assistance.

To showcase the impact of each type of user-induced error, we chose three different sample types (fruit, pharmaceutical, textile) with varying characteristics, as shown in Table 1. In some cases, we used different items from the same sample type for a more appropriate evaluation of each parameter. For example, when testing sample surface, it would not make sense to test a round object with no edges or varying texture. A NIRS scan was deemed inadequate when it produced values that are significantly different from the values obtained under ideal conditions (significance tested through Wilcoxon signed-rank tests).

Sample	Properties	Test(s)
100% Cotton	Area (Square): 196 cm Height: 2,5 cm	1 - 6
Omega 3	Brand: Möller Weight: 1200 mg	2, 5, 6
Multivitamin Plus M	Brand: Orion Pharma Weight: 250 mg	1, 3, 4
Banana	Uncut Diameter: 20 cm Weight: 120 g	1 - 5
Apple	Uncut Diameter: 6 cm Weight: 80 g	5, 6
Grape	Uncut Diameter: 2 cm Weight: 5 g	5

Table 1. Selected samples, properties, and respective tests.

Scan setup and configuration

Our scan setup consists of a NIRS scanner (DLP NIRscan Nano [15]) and a camera tripod. We use a custom-built aluminium plate and the tripod's spirit level to align the scanner with the scanned object. We use a separate spirit level to ensure both an overall alignment and the incident beam hitting the sample orthogonally. Figure 1 depicts the scan setup. Our scan setup was installed in a room with controlled light conditions, and a lux meter was used to detect the amount of light visible in the room. The lux meter detects wavelengths within the visible light range (400-700nm). Fluorescent lamps, such as the ones in our testing room, mainly radiate within the same spectra [18]. Therefore, the level of stray light interference can be measured by the lux meter.

The DLP NIRscan Nano software allows the user to configure and calibrate the device before starting a scan. A reference scan was set using a labsphere Spectralon Diffuse Reflectance Standard. This calibration tool reflects up to 99% of incoming light, allowing the machine to adjust to changing hardware performance. The configuration during all experiments used the whole available NIRS wavelength range (900-1700nm). The resolution of the hardware describes the smallest spectral features that it is able to detect. In our case the hardware has an optical resolution of 10nm. The digital resolution can be increased at the cost of decreasing the Signal-to-Noise Ratio (SNR). The lowest setting with the manufacturer's software is 7.02nm without receiving warnings about degrading performance. Therefore this setting was chosen as literature suggests that a higher resolution helps to detect all spectral features [12,21,37]. The manufacturer ships the device with four typical scan configurations [15]. For a digital resolution of 7.02nm, it is suggested that the spectra should be sampled approximately 228 times, meaning that it will be oversampled by 2 to satisfy the Nyquist-Shannon Sampling Theorem [8].

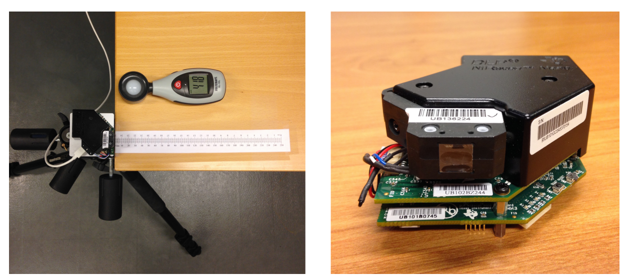

Figure 1. Left: Scanning platform with the DLP NIRscan Nano mounted and the lux meter. Right: DLP NIRscan Nano.

Specifically, the spectral bandwidth being sampled is 800nm (*i.e.*, 1700nm-900nm). With a digital resolution of 7.02nm, we need 114 (*i.e.*, 800nm / 7.02nm) patterns to sample the whole spectra. A common way to increase the SNR while sampling is by signal averaging [23]. We scan each object six times, as advised by the manufacturer. Each sample is recorded in the same manner, and all are averaged to increase the SNR. Each data point in Figure 2 – 7 represents the average mean absorbance of six individual scans.

There are two available scan methods for the device, which determine how the wavelengths are scanned: Hadamard scan and Column scan. Hadamard multiplexes several wavelengths together and decodes individual wavelengths. Noise in the incident signal is distributed evenly over the spectrum to minimize the effect. This method also collects more light and provides a greater SNR than the Column scan [15], and was therefore chosen for our study.

Test 1: Device Motion

The device could be used either as a handheld point and scan device (*e.g.*, baggage scanner) or as a stationary device (*i.e.*, mobile, but placed on a table when scanning). We investigated the effect of device motion on scan quality. If even small movements from events such as hand tremor cause inadequate scans, then the latter positioning technique would be the best solution when using these devices.

Movement of the NIRS while scanning can cause the lens window to lose contact with the sample. This may lead to unwanted reflections, distortion of the signal, and exposure to ambient light [26]. To explore the effect of device motion on scan accuracy, we scan each sample while the device is under three different levels of motion. First, we scan the sample with the device placed on the table. Second, we scan the sample while holding the device (*i.e.*, light movement). Lastly, we conduct scans with moderate motion to reflect careless usage.

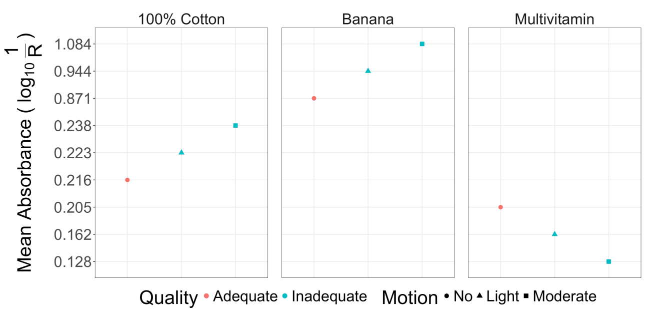

Figure 2. Mean absorbance of objects with different levels of device motion.

Figure 2 shows how the quality of the scans degrades when motion is applied to the NIRS when scanning. The absorbance also increases for both the 100% cotton and the banana sample, meaning less light is reflected. The multivitamin experiences a decrease in absorbance, likely caused by an increase in the lens exposure to ambient light.

Test 2: Sample Distance

Device positioning depends on the sample distance range for which it can deliver adequate results. Typically, lower ranges yield more accurate results, and in such cases the scanner should ideally be positioned upwards to enforce that the samples are directly on top of the lens window. However, a larger range would facilitate a more flexible design. The two lens-end broadband tungsten filament lamps in the NIRS hardware emit light through the device's sapphire window. Both the light source paths and the vision cone of the receiving lens intersect directly in front of the window. The further away the sample is positioned, the less light the system is able to collect because of path loss [44]. In addition, the reflected signal contains less information and is more prone to noise. NIRS scanners assume that all light which is not reflected has been absorbed, even though it may have radiated through or around the object. While different objects absorb at varying rate, lower absorbance (*i.e.*, a higher reflectance) often indicates that the object is closer and more ideally positioned. In addition, a sample positioned at close range will ensure less stray light entering the spectrometer, thereby increasing accuracy [46].

To test the accuracy of our scans over different distances, we attached a ruler to the table. Each sample was then measured from 0cm to 3cm with increments of 1mm. The effect of the distance on the absorbance is shown in Figure 3. All of the curves display a similar characteristic, with the main difference seen in the level of object absorbance (dependent on the chemical composition of the sample). We can see that pure cotton reflects back more light back than the omega-3 sample. This is because the omega-3 is transparent, with the majority of incoming light being scattered in multiple directions.

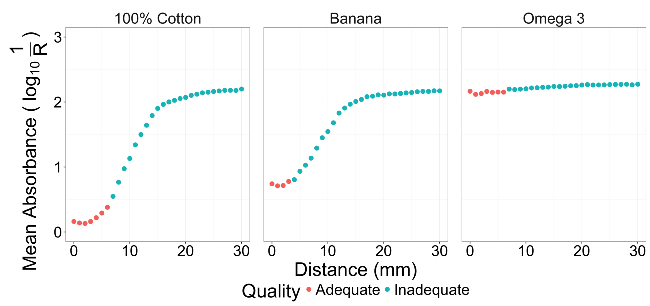

Figure 3. Mean absorbance of objects over different distances to the scanner

Test 3: Sample Angle

To design an appropriate sample holder for the hardware, we identify the sample angle range in which the device delivers adequate result. The holder needs to hold the sample flat down if the range is limited. With adequate results in a larger range, the design could be more universal with less focus on holding the sample in a certain angle.

For scans to be of high quality, the scanner needs to collect as much of the reflected light as possible. Ideally, the incident wave should hit a flat surface with an angle of 0°, following the law of reflection [35]. To measure the effects of scanning an item at various angles, we scan samples from 0° to 90° with increments of 15°. Figure 4 shows the effect of object angle on absorbance levels. For every increment of 15°, the quality deteriorates rapidly. While 0° is the optimal angle to retain all the spectral properties, small items (*e.g.*, multivitamins) reflect an adequate amount of light up to 15° (as shown in Figure 4) because of the illumination angle of the device.

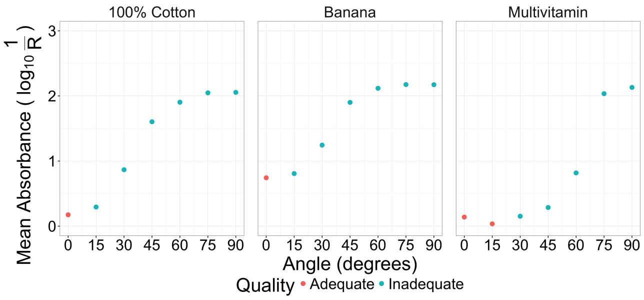

Figure 4. Mean absorbance of objects over different scanning angles.

Test 4: Sample Surface
The sample may have a surface with varying texture. It is crucial to know if the different textures will affect the scan accuracy. If the texture degrades scan accuracy significantly, the non-expert user should be instructed on how to correctly place the item to scan the most appropriate surface. A flat surface can reflect the signal in one direction, whereas a rough surface may cause signal scattering [36]. To investigate the consequences of scanning at various areas, we scanned the same samples from 3 reference points and 3 uneven surfaces. The reference scans are taken at 0mm distance and at a 0° angle at a flat surface covering most of the lens. The uneven surfaces consist of parts of the object that have edges or are rugged.

In Figure 5, we can observe that all the reference scans are of adequate quality and have little variance between them. In contrast, just one out of the nine uneven samples is of adequate quality. The uneven cotton samples also have a large variance compared to the rest. Since the cotton samples were placed unfolded in front of the lens, they had a varying thickness when we were scanning the three uneven samples.

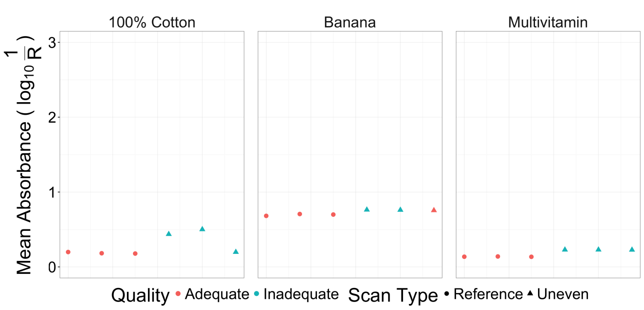

Figure 5. Mean absorbance of objects with different surface evenness

Test 5: Sample Interference
When scanning a sample, nearby objects may be a source of interference. If the magnitude of this noise causes inadequate scans, then the user should be instructed on correct scan behaviour (*i.e.*, only scan one sample at a time). Furthermore, this may also further encourage a stationary design, where the object is placed on a sample holder. The ratio of the NIRS waves that is reflected, absorbed, or passed through the scanned object depends on the object characteristics. Fruits [29], textiles [56], and pharmaceuticals [11] all have different penetration properties. Furthermore, a secondary object placed directly behind the sample might also reflect some light and affect the resulting spectra. To inspect the effects of this potential source of interference, we placed one object to be scanned in an ideal position while a secondary object was positioned directly behind the scanned object, moving up to 5cm away from the primary object at increments of 2mm.

Figure 6 shows how the distance of a secondary object to the scanned object can affect the quality of the signal. For the first and second graph, there was only one instance of interference when the secondary object (*i.e.*, apple, banana) was placed directly behind the sample (*i.e.*, cotton, grape). Finally, the level of interference from cotton on the omega-3 decreased in magnitude from 0mm to 37mm. This is because the omega-3 is transparent and therefore light is transmitted through the object and hits the cotton. It is then reflected back to the lens, causing the resulting spectra to be distorted.

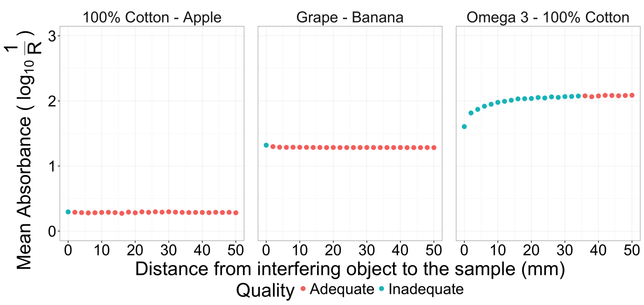

Figure 6. Mean absorbance of objects over different distances of interfering objects to the main object

Test 6: Ambience
The user may add noise to the spectrum by conducting scans with the NIRS in a context with unsuitable levels of ambient light, humidity, or temperature. We focus on light, as humidity and temperature's effect on the NIR spectra is limited in non-extreme climates [55]. The user should be instructed through the interface if the ambient light can cause the scan quality to drop significantly.

Radiation from nearby light sources can affect the accuracy of the NIRS [50]. The level of interference depends on the magnitude of the illuminance and the distance between scanner and sample. We use a 120W halogen lamp as an interference source and a lux meter to measure its illuminance. As the halogen lamp transmits on wavelengths beyond the lux meter's range, not all the light was detected. However, we still obtained a good indication of the illuminance level. We measured the effect of five different lux levels: 500 (bright office), 800, 1200 (daylight), 1600, and 2000 lux (shop window) [14]. The measurements were taken at four distances: 0, 10, 20, and 30mm. The effect of increased illuminance on SNR can be observed in Figure 7. The graphs are divided into bins. Samples in the same bin were taken at equal distance. Cotton and apple were unaffected by higher amounts of lux at 0mm range, while cotton showed varying results at 10, 20, and 30mm. For the apple, the scan contained substantial noise when increasing the lux beyond 0mm range. Omega-3 was affected more by stray light than the other two samples. Readings became noisy when the measured lux was above 500. This was expected as omega-3 is transparent and the interfering light can easily penetrate and cause noise.

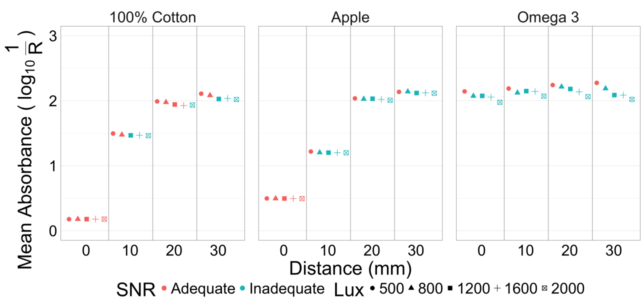

Figure 7. Mean absorbance of objects over different lux levels

Challenge 2 - Complexity of the Sampling Process

In addition to the challenges associated with user-induced errors when using NIRS, interaction with the scanning device is another important aspect. To facilitate novice end-user interaction with NIRS, a graphical user interface is required [27]. Figure 8 shows a procedural overview of the steps a user has to complete when using a NIRS device. The first two columns contain the steps and their respective descriptions. The third column indicates whether a user has to conduct that step when using a default NIRS device.

STEP	DESCRIPTION	ORDINARY NIRS USER INVOLVEMENT
Phone	UI Interaction	No
NIRS	SW / HW Interaction	Yes
Spectrum	Extract Raw Data	Yes
Analysis	Filtering Machine Learning	Yes
Results	Interpretation	Yes
Phone	Presentation	No

Figure 8. Necessary steps a user needs to complete with a typical NIRS device. Adapted from [26].

First, users have to operate the instrument through typically complex software (and sometimes hardware) operations. Current NIRS systems require users to configure the device, set scan parameters, and navigate complex menus. Following these steps, the user also has to handle information produced by the device. A major challenge for non-experts is that data is usually returned in a raw format, not revealing much information to the end user. To extract the data and turn it into understandable knowledge, analysis methods (*i.e.*, chemometrics) have to be applied to the dataset. This involves pre-processing the data when needed, and using multivariate analysis to classify the information [34]. Furthermore, a reference library is required to serve as training data for the classification model. The whole process hinders non-experts without strong analytical capabilities to interpret the information produced by the instrument. Consequently, training and education is a prerequisite for personnel wanting to utilise this technology in its present state. Our work is a step towards a future where users are not required to perform complex steps that require specific skills.

NON-EXPERT ASSISTANCE

To overcome the challenges related to scanning and identifying samples, we adopt a combined hardware-software approach. We address potential user-induced errors and the procedural complexities through a 3D printed enclosure and by guiding the user through a smartphone application capable of automating the required analysis.

Physical Assistance: Enclosure

We designed a 3D printed enclosure to both protect the scanner, reduce the effect of user-induced errors, and facilitate the scanning process. The design of our enclosure is informed by the findings of our tests. The design consists of a modular approach (protective casing and two different sample holders), which can be replaced by the user. The sample holders are distinctive in both shape and size to allow for different types of objects to be scanned. Figure 9 shows the final iteration of the enclosure and sample holders.

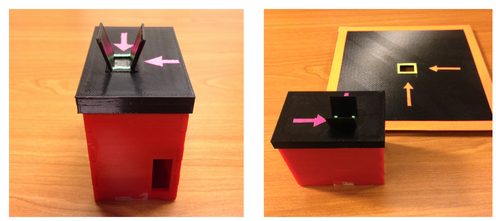

Figure 9. Enclosure and sample holders. The smaller sample holder contains two walls for small samples to be held in place.

The enclosure is formed to be positioned on the table, which removes the chance for device motion noise during operation. It is also pointing upwards, guaranteeing that object placement is within close proximity of the lens. This increases the accuracy as discovered in the sample distance test. Furthermore, it also the reduces the interference from ambient light, as the object is now covering the lens. The holder ensures that items are by default positioned at an even sample angle. In addition, our design prevents users from accidentally placing another object behind the scanned object, affecting the scan results (sample interference). Two arrows were placed on each platform to guide the user as to where the sample should be positioned.

The larger sample holder has a dimension of 20 x 20 cm. The considerable surface area enables comfortable placement of samples, without concern for the sample falling off. The smaller sample holder consists of two small walls placed at an incline, allowing for small samples to be held securely in place. This addition can be seen more in detail in Figure 12. The walls are covered using insulating tape with IR absorbing characteristics, to reduce light scattering and to shield from interference caused by any nearby objects. The base of the walls are positioned at the edge of the lens, so that any item positioned between the walls is covering the lens. The final setup as described above is the result of three iterations of design, 3D printing, and testing.

Procedural Assistance: Software

We developed a smartphone application to allow end-users to interact with the NIRS device. The application provides a single interaction point. Furthermore, it provides the user with instructions and warnings regarding scan quality issues in order to reduce the effect of user-induced errors. The software also automates and encapsulates all the complex analysis stages, thus reducing the burden for the user. Figure 10 displays the various screens of the application.

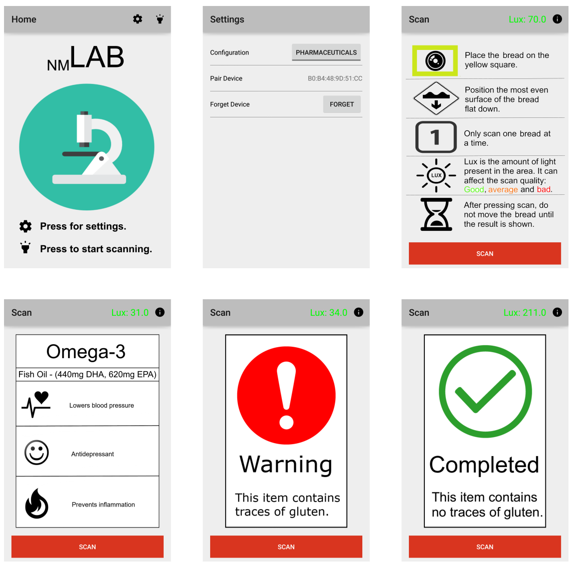

Figure 10. Top row from left: Initial screen, settings, example of scanning instructions. Bottom row from left: Example of sample identification result, example of scan result warning about the presence of a component, example of scan result regarding the absence of a component.

The home screen allows users to adjust the settings or start a new scan. In the settings screen, the user selects the type of sample that will be scanned. Instead of having to adjust a long list of parameters for the scan, the user can choose a pre-determined category. Based on this configuration, the scan screens will adjust to show the relevant instructions, guiding the user in correctly scanning the sample. For example, the text instructs the user to position an even surface down and only scan one sample at a time. These guidelines were based on our tests investigating user-induced errors. After a scan is completed, the application displays the results. We utilise the built-in lux sensor of the phone to infer the level of illuminance in the area. Lux is measured in luminous flux per square metre, so while the phone and sensor are not in the exact same position, it can still be used as a baseline for how much light is reaching the NIRS. The lux measurement (top right corner of scan screen) changes from green, to yellow, to red, depending on the level of illuminance based on our ambient light tests.

When the user presses the scan button, the button becomes disabled and a progress bar appears together with a text field describing the stage (*i.e.*, scanning, analysis, or processing). The whole process takes around 20 seconds (approximately 10 seconds for scan, 5 seconds for analysis, and 5 seconds for processing) to complete. Upon completion, the application will display the results and also vocalise the results using text-to-speech. The current version of the application has the ability to identify pharmaceuticals and detect whether a bread contains gluten. While the application could be implemented for a vast number of scenarios, we focus on the two aforementioned scenarios in our user study.

Communication (*e.g.*, starting a scan, receiving scan results) between the smartphone and the NIRS device occurs over Bluetooth Low Energy. When the application receives the scan results, they are sent to a server for processing (*e.g.*, filtering, classification, regression). After the sample is analysed, the results are sent back to the smartphone and presented to the user. In addition, there are four scenarios in which the application will display a warning message to the user. While the warnings are active (10s), the scan button is greyed out and disabled. This is to ensure that the user reads it and does not accidently press the scan button again. After ten seconds, the button becomes active again. Warnings are intended to correct scan behaviour and limit the effect of user-induced errors, and are displayed in Figure 11. The thresholds for triggering these warnings were informed by the user-induced errors tests.

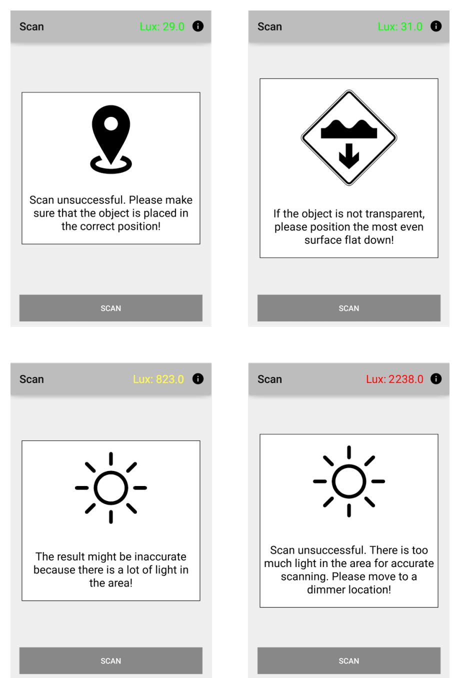

Figure 11. Warnings 1 - 4 from top left to bottom right.

Warning 1. If insufficient light is reflected back to the receiver, this is interpreted by the software as the object being misplaced.

Warning 2. If substantial noise is detected in the resulting spectra, this can be caused either by object transparency or uneven surfaces.

Warning 3. When the illuminance is larger than 800 lux, the text turns yellow and the user will be informed that the accuracy of the scans might be inaccurate.

Warning 4. When the illuminance is larger than 1200 lux, the text turns red and scanning is temporarily disabled until the user can find a darker location.

Evaluation

To evaluate our proposed software and physical guides, we conducted a user study with participants who had no prior experience with NIRS technology. The main goal was to investigate whether non-experts are able to successfully conduct the scanning procedure without training. We investigated how people interact with the technology through a scanning experiment, and conducted a semi-structured interview to capture their opinions and feedback. Thus, our objective here is to explore the practical usability and perceived usefulness of the developed solution.

Participants and Procedure

We recruited 15 people using mailing lists of our university (9 males, 6 females; ages: 20-34 years old, M=26.6). Participants had a diverse range of educational backgrounds (*e.g.*, Finance, Biology, Anthropology, and Computer Science). We carried out the experiments with each participant individually. The experiment duration was approximately 30 minutes per participant. Participants were rewarded for their participation with a movie voucher. After a short introduction to the experiment, participants were asked to scan a set of objects placed on the table before them using the NIRS scanner within the enclosure and a provided mobile phone running our application. The study was divided in two parts: 1) sample identification using 10 different pharmaceuticals, and 2) gluten detection using 10 pieces of bread. Both parts had items with varying characteristics (*e.g.*, shape, size, texture, and transparency) to thoroughly test our non-expert assistance. We counterbalanced the scanning order.

Participants did not receive any instructions on how to use the devices, as we wanted to assess the usability of our proposed solution in a realistic setting (*e.g.*, the user would encounter this device in a supermarket without additional guidance from the staff). The participants were asked to report the scan results to the observing researcher. During the experiment, we recorded the participants' answers and how they interacted with the non-expert assistance, as well as any comments from the participants while they scanned the objects. In addition, we also recorded any warning messages that were displayed by the application, for which object this warning message was displayed, and the user's reaction. After all scans were completed, we conducted a semi-structured interview in which we asked participants to comment on the application (*e.g.*, usage, instructions, warnings, results), the enclosure, and the technology in general. The interview was structured as follows.

Age, gender, occupation, background.

Statements ranked on a 5-point Likert scale.

- The scan time was acceptable.
- The instructions/warnings/results (asked individually) were easy to understand.
- The instructions/warnings (asked individually) had enough details.
- It was easy to understand where to place the object.
- It was easy to place the object in the correct position.
- I felt comfortable when I used the device.
- I would trust this type of technology.
- I can see myself using this technology daily.

Open-ended questions.

- What is your overall experience using our solution?
- Did you have any issues understanding how to use the application?
- Did you make any adjustments when you received the warnings?
- What steps would you take upon receiving a warning?
- What is your impression of the accuracy of the device?
- What type of information would you like to receive with the result?
- What features did you like on the enclosure?
- What features did you not like on the enclosure?
- What features would you change on the enclosure?
- What would you scan with a device like this?

Since not all the warnings were shown during the scans, we printed them on paper and showed them individually during the interview in order to collect feedback. We asked participants to envision receiving the warnings and describing their subsequent actions. In addition, we asked the participants what additional information they would like to receive in scenarios besides the two we presented. The main focus of the study was to investigate whether novice end-users would be able to successfully utilise a NIRS device using our design. We were also interested in collecting opinions on our design and the technology in general.

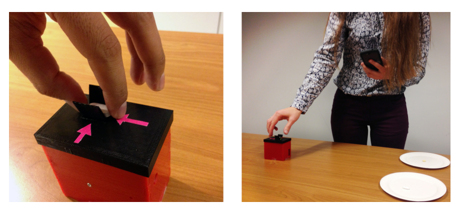

Figure 12. Left: Object placement on small sample holder. Right: Participant during the user study.

Results

Perceptions

The majority of participants (N=14) immediately understood the instructions and started using the application with no notable problems. One participant (P07) tried scanning the object by holding the phone towards it instead of placing the object on the platform. The participant quickly corrected his behaviour and explained that the confusion was due to having used several applications that rely on the camera. Participants strongly agreed that the instructions were easy to understand (M = 4.53, SD = 1.06), and also agreed that the instructions they were provided with by the smartphone were of sufficient detail (M = 4.40, SD = 0.91). Some participants commented that the instructions could be presented in a stepwise fashion, allowing for a more legible presentation: "I *would like stepwise instructions, where you swipe to show the next instructions. It would allow for bigger pictures and text.*" (P09). None of the participants reported having any issues with using the application and generally agreed that the scan time was acceptable (M = 3.80, SD = 0.68). Context was also deemed an important factor: "*A user in the supermarket would not be able to wait that long*" (P01).

Warnings

A few warnings were caused by participants pressing the scan button before positioning the sample, triggering Warning 1. In these cases, the users quickly recovered. There were also events in which transparent samples (omega-3) generated Warning 2. We showed each individual warning to the participants, and they generally agreed that they were understandable (M = 4.34, SD = 0.80) and contained enough details (M = 4.41, SD = 0.85). P04, P09, P11, and P12 commented that the icon for Warning 2 did not correlate with the text in the warning. "*The icon in Warning 2 does not indicate transparency*" (P04). P05 recommended more visual instructions, instead of text. P06 requested more information about the lux range and more distinct difference for the icons in warning 3 and 4. Regarding the actions they would take upon receiving a warning, the answers were in line with the steps we envisioned a user would take (*e.g.*, reposition object, place flat surface down, shade the machine from interfering light, or move to a darker area).

Scan Presentation

Participants strongly agreed that the results were easy to understand (M = 4.87, SD = 0.35). When questioned about what additional information participants would like to have included with the results, most answers were related to more nutritional information (*e.g.*, protein, carbohydrates, fats, sugar) but also other allergens (lactose). We received positive comments for the pharmaceutical results, such as "*I really like the vitamin feedback. It is cool that it tells you what it contains. Reminds me of a video game, where you can inspect items and see their stats*" (P05).

Physical Enclosure

Multiple participants positively commented on the enclosure, with comments such as, "*It's small, light, and portable*" (P04), and "*The large surface area makes it easy to position the bread*" (P01). Participants strongly agreed that it was easy to understand where to place the sample (M = 4.67, SD = 0.72). "*I liked the arrows and colour indications on the box*" (P05). They also agreed that it was easy to place the item in the correct position (M = 4.20, SD = 0.86). When asked about potential improvements to the enclosure, a few remarks about aesthetics were noted. "*Would change the package a bit, make it less bulky and more flat.*" (P08). Another participant believed the scanning process of smaller items could be improved with a redesign of the enclosure, "*Make the box so that you put the item inside and scan it, and change the platform to be a bowl, so the item falls to the middle.*" (P10).

Future Use

The participants reported being comfortable when using the device (M = 4.47, SD = 0.64), and the general consensus was that they would use the technology on a daily basis (M = 4.47, SD = 0.74). In addition, participants stated they would trust this type of technology (M = 4.53, SD = 0.64), "*I think it was accurate and made correct identifications. I trust this machine more than my own judgement or some labels*" (P12). However, a couple of participants expressed the importance of getting the scans right in certain situations, "*False classifications could potentially be dangerous for the user. In those cases, accuracy is really important.*" (P04).

When probed about potential scenarios where they would use this technology, several participants mentioned food, pharmaceuticals, textiles, and various chemicals. Three participants proposed creative ways of using the technology: "*It would be interesting to scan makeup to look for micro plastic. I don't use makeup that can potentially damage the nature.*" (P05). "*I would like to scan food products for gelatine. We Muslims don't eat products that contain it.*" (P12). *"It would be nice to have a survival scanner that could detect if food found in the nature (e.g., berries and mushrooms) are poisonous or safe to eat.*" (P13).

Typical information to look for could be nutritional content, Active Pharmaceutical Ingredient (API) percentages, allergens, and item quality. Multiple users would like to have the machine in a supermarket, to scan products and retrieve information about their quality (*e.g.*, fruit ripeness). "*Putting it in the supermarket would be really helpful, I can see a lot of people using it.*" (P12). "*It would be useful for dementia patients. Pharmaceuticals can look the same, but have strongly different effects.*" (P04). Several participants envisioned that in the future, NIRS could be a helpful sensor embedded in their smartphones. Multiple participants also expressed their desire to have such a device in their home for a number of different reasons. Throughout the study, people were enthusiastic about the technology, and commented positively on its potential.

DISCUSSION

Towards End-User Near Infrared Spectroscopy

Previous work on portable NIRS has mainly been concerned with testing performance under ideal conditions with domain experts [2,28,39]. However, there is a scarcity of research that highlights the potential use cases, design challenges, and solutions to enable non-experts to use NIRS. The effect of user-induced errors on NIRS can pose significant challenges, particularly for untrained users. Users currently have to operate the instrument through complex software and require knowledge about advanced analytical methods to understand the result. We argue that in order to make the technology more accessible and still produce reliable results, the scanner and its software/hardware controls must be designed to guide the user and avoid problematic scanning conditions. In this paper, we report and evaluate a hardware-software design that proved successful in guiding and facilitating the scanning process for non-expert end users.

Our application provided simplified instructions for users with no previous contact with the technology. The warnings were designed to help users overcome probable scanning errors, and were shown to help them overcome sample misplacement. Our design effectively provides an interactive way to train users of the equipment, and our user study shows that participants were able to quickly start using the technology reliably without any verbal instructions.

Furthermore, the 3D printed enclosure and sample holder enabled, for the most part, correct scanning behaviour by facilitating optimal object placement. Participants felt that the enclosure effectively guided them in correctly placing the samples, while at the same time protecting the device. One element of the scanning process that was rated slightly lower than others was the scanning time (M = 3.80, SD = 0.68). One potential reason for this is that the technology is quite new - it is possible that users have not yet formed an opinion on how long a scan should take. The scan time depends on the scan configuration (*e.g.*, resolution, width, and SNR). By increasing the precision or reliability of the scan, it takes a longer time to complete. Some configurations are more appropriate, depending on the nature of the analysis and the scanning environment. Ultimately, what constitutes a feasible and acceptable scan time will depend on the scenario (*e.g.*, supermarket, home) and the analysis requirements (*e.g.*, allergens, API, nutrition, ripeness, poisonous).

Moreover, one important challenge for end-user NIRS is the collection of reference scans. With our system, users have to indicate the type of objects that they are scanning so that the application can optimise the scanning configuration. This then loads the appropriate model depending on the user's choice. We envision that in the future, devices will come pre-loaded with models for commonly scanned objects. In addition, crowdsensing communities [24] can emerge to establish a shared repository of sample fingerprints to facilitate object identification. Furthermore, methods that enable use of existing knowledge-bases built by benchtop instruments can be used with acceptable performance [21].

Implications for Practice and Research

We tested a relatively cheap and miniaturised NIRS device on a wide set of everyday objects. We have shown how the device performs when scanning various objects with different physical characteristics. By better understanding these parameters, it is possible to design enclosures and applications that facilitate the correct usage of the technology. This would allow for a smartphone to be turned into an advanced scientific instrument by simply installing an application and coupling it to a NIRS device. As a result, even novice users would be able to conduct experiments, earlier limited only to trained lab personnel. For instance, farmers can be better informed on the best time to harvest their crops without relying on expensive or time-consuming methods. About 125,000 people die every year due to medication mismanagement and the estimated cost is around $300 billion [25]. Miniaturised NIRS could be implemented to help nurses or the users themselves (*e.g.*, old adults) administer medicine. Furthermore, a number of interesting use cases that we did not envision were identified by our participants, highlighting the potential of the technology for a wide variety of everyday scenarios. For researchers, our study opens multiple avenues to explore. Due to the small form factor, our solution can be carried around by the user for *in situ* sample analysis. Furthermore, a multitude of everyday objects, from cups and dishes to shelves and refrigerators can begin to be instrumented with NIRS hardware to identify objects. Ubiquitous scanning stations where the NIRS is bundled with tablets could be installed in public locations and serve a broad group of users. As NIRS devices decrease in size and price, it may become possible to bind them to smartphones in the future. This could create a range of opportunities for scanning "in-the-wild" without having to carry around an additional device.

Limitations

The work presented in this paper has several limitations. First, we conducted the user-induced errors experiments using visual alignment. While both careful precision and measuring tools were used to align the samples, there may still exist some human error. Second, we did not compare participant usage of the technology with and without our solution. It would be unreasonable to give the hardware with its default elements and expect a participant to be able to conduct any given step of the scan and analysis process. Also, discussion about classification models is considered to be out of scope for this paper. Finally, we only utilise one NIRS scanner in this paper. While our findings can be used as guidelines for a larger array of hardware, it would be interesting to test multiple devices from different vendors for a more thorough investigation.

CONCLUSION

Our work has systematically investigated the effect of user-induced errors and the complexity of the sampling process in the context of an affordable and miniaturised NIRS. We subsequently investigated the magnitude of these parameters to derive their potential impact on scanning quality and usability. Previous work has taken for granted that the instrument is used under ideal conditions by trained personnel. We show that NIRS can be successfully used by novice end-users, if the challenges explored in this paper are taken into consideration. This is validated through a user study where non-expert users test a NIRS equipped with a 3D printed enclosure and smartphone application. The results indicate that the accuracy and user experience when using NIRS for object detection and analysis is adequate when use is facilitated with our proposed non-expert assistance. In our ongoing work, we intend to deploy an *in situ* scanner in a variety of different scenarios.

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