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# The spectral treasure house of miniaturized instruments for food safety, quality and authenticity applications: A perspective

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ABSTRACT

*Background:* Optical technologies, relying on spectral analysis, are more and more implemented in portable devices for food analysis. Thereby, each food safety, quality or authenticity provision as well as each technology requires the generation of a dedicated spectral database with reference data. Currently, knowledge on how these databases might be connected or transferred across food commodities, targeted compounds or devices are very limited. Hence, repetitive work is conducted and technologies are not optimally used.

*Scope and approach:* This perspective focuses on the currently available technologies and approaches for data handling and database transfer across miniaturized devices and technologies for food safety, quality and authenticity assessments.

*Key findings and conclusions:* For almost every food commodity or target compound a miniaturized spectroscopic device can be applied with the respective database to compare findings. Recent developments in optical spectroscopy allow more possibilities for their use as well as facilitate the production of portable devices. A multifunctional device hyphenating several sensors and broadening the application range is still not marketed. Newly developed software architecture, accessing and extracting data, helps to overcome sample heterogenicity or spurious measured data. In addition, several data fusion approaches using machine learning and deep learning strategies are available to fuse spectroscopic data with itself or other non-spectroscopic data. Following the research results presented in this field, spectral data can possibly be re-used and shared across instruments and locations, highly increasing the applicability of data sets. Thereby, obstacles such as policy or confidentiality are taken into account.

## 1. Introduction

Currently, point-and-shoot optics hardware is being constantly miniaturized, the storage capacity of electronic devices is increasing, spectral multivariate statistics applications in spectral cloud databases and smartphones are being implemented and very short measurement and response time (seconds) is targeted. New devices should be easy to use and applied in a non-invasive manner. Hence, there should be no need to pre-process samples in an extensive preparation or the addition of reagents. Due to their real-time data acquisition and processing, novel devices may be applied on- or in-line in processing plants or *in situ*. Using small optical devices as an on-site decision support system for screening of samples fits into the lab-to-the-sample approach, where only suspect samples are transported to a laboratory facility for confirmation by a reference method. (Chapman, Gangadoo, Truong, & Cozzolino, 2019; Cozzolino, 2015; Ellis et al., 2012; Ellis, Muhamadali, Haughey, Elliott, & Goodacre, 2015; Esteki, Shahsavari, & Simal-Gandara, 2018; Hussain, Sun, & Pu, 2019; Lohumi, Lee, Lee, & Cho, 2015; Oliveira, Cruz-Tirado, & Barbin, 2019; Tahir et al., 2019; Wadood, Boli, Xiaowen, Hussain, & Yimin, 2020; Yeong, Jern, Yao, Hannan, & Hoon, 2019). Tremendous amounts of resources and time are being spent on the construction of spectral databases for ultraviolet–visible (UV-VIS), fluorescence,

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(Fourier transformation-) near-infrared (FT-NIR), mid-infrared (MIR) and Raman spectroscopic instruments. These optical spectroscopic approaches are widely used in the characterization of food products and screening of food quality, safety and authenticity. Either they are applied in the targeted approach by classification or quantification of specific commodity provisions or in the non-targeted approach for creating so-called fingerprints. In principle, for each food product, desired target compound and optical device a dedicated spectral database needs to be constructed. A typical spectral database should contain a sufficient number of certified samples covering the natural variability, i.e. season, geographical origin, processing steps and the concentration range of the analyte or classification range of interest. In addition, the appropriate application of multivariate statistics is crucial for the correct functioning of the application for which the spectral database is built. Although the advantages of a fast, non-destructive optics screening method are numerous, the spectral databases are specific for one food product, targeted compound, and type of optics hardware combination. If a new or updated optical device hardware version or new optical device type is implemented, a (partial) re-work of the spectral application is in most cases required including a so-called calibration transfer. Moreover, reference values from a validated laboratory-based analysis method, certified sampling sources or certified paper work are needed for (re-)calibration too. Despite all efforts in the scientific world to construct databases and setting the first steps towards interesting applications for food product assessments (McGrath et al., 2018), many of them are not in use or are not maintained any more due to hardware updates, lack of transferability to other devices or lack of interest or financial means. Thus, construction and re-construction of spectral databases which form the spectral 'treasure house' and the core of the applications are dear processes which are often dead ended. Consequently, they have become a significant bottleneck in the widespread application of fast portable optical screening devices for food applications.

It seems that we do not unleash the full power of our (largely scattered and fragmented) spectral treasure house to the full extent. In this perspective, we discuss the developments in spectroscopic and chemometric science regarding the re-use of previously recorded spectral data in spectral screening applications for food. We specifically focus on (1) hardware developments in portable devices using spectroscopic approaches, (2) developments in data handling via software architecture to access and extract information, (3) spectral data fusion, transfer and exchange approaches and (4) interchange of information and knowledge without sharing the actual database.

## 2. "The acquisition": outlook on hardware developments of portable devices to acquire spectral data

Among current miniaturized spectroscopic approaches integrable in portable devices, those using illumination wavelengths between UV and MIR range are the most widely and increasingly used in food analysis as reviewed recently by Crocombe (2018), Deidda et al. (2019), and Yeong et al. (2019). Optical spectroscopy may record spectra either in transmittance mode through clear or opaque samples such as beverages, hence deriving the optical absorbance by the investigated materials, or in the (diffuse) reflectance mode acquiring scattered radiation from solid or pastry food samples. The recorded physical effects span from electronic excitation of fluorophore molecules to elastic scattering. In the following, a synthesis of the functionality of available spectroscopic hardware is reported together with limitations, perspectives and data format and dimensions (see also Table 1).

A very well established approach is the use of *longwave ultraviolet* (UV 200–400 nm wavelength) and *visible* (VIS 400–750 nm wavelength) radiation, to explore the presence and quantity of molecules that bear the possibility to absorb light. Electronic transitions between molecular

**Table 1**
Overview of advantages, limitations and further research aspects of optical technologies currently used in food sensing.

| Sensor/Spectral range | Advantage | Limitations | Further research |
|---|---|---|---|
| UV-VIS | Available sensors in miniaturized sugar cube dimension;<br>Characteristic spectra for specific food components;<br>Available in combination with spectral imaging (SI);<br>Very short acquisition times (range of ms);<br>Spectral data in exportable text format;<br>File dimensions in the range of a few kBytes;<br>Low cost; | Only longwave UV possible;<br>Only fluorescent or colourful molecules may be detected;<br>Low chemical specifity;<br>No spatial information about the sample;<br>Interference of packaging; | Sensors covering more UV wavelengths;<br>More stable low cost light sources; |
| NIR and MIR | Available sensors in miniaturized sugar cube dimension;<br>Available in combination with SI;<br>Spectral data in exportable text format;<br>File dimensions in the range of a few kBytes; | Interference of water from samples and packaging;<br>Broad overlapping spectra;<br>Thermal noise which is possibly hampering measurements;<br>Cooling required when applying longer wavelengths;<br>Necessity of multivariate statistics.<br>Long acquisition times (range of seconds) and spectra averages needed; | MIR, FT-NIR and FIR sensors and illumination sources should be miniaturized; |
| Raman | Available portable (0.25–2 kg instruments);<br>Available in hyphenated devices;<br>Measurements possible through packaging;<br>No interference of water content;<br>Spectral data in exportable text format; File dimensions in the range of a few kBytes; | Laser needed;<br>Long acquisition times (range of minutes) due to the weakness of the physical process; | Further miniaturization of sensors;<br>Miniaturization of light sources; |
| Imaging (monochromatic-color, camera based) | Available in miniaturized versions (chip size);<br>Fast acquisition times (ms to s);<br>Coupling of spatial and chemical information; | Large data dimensions (order of MB or more);<br>Multivariate statistics necessary;<br>Low specificity; | Multivariate statistics and federate learning updates;<br>New interfaces to handle data transmission (i.e. USB, wireless connections); |
| Spectral imaging and microRaman | Available in miniaturized versions (chip size);<br>Really versatile, couples spatial and chemical information; | Very large datasets (up to GB);<br>Dedicated algorithms requested for data analysis;<br>Difficult miniaturization (high cost);<br>In some approaches, moving parts inside the sensor are necessary at the expenses of robustness; | Further miniaturization and combination with different technologies;<br>New interfaces to handle data transmission (i.e. USB, wireless connections); |

orbitals are triggered and give as response a fluorescence, a transmittance or a reflectance spectrum. It is worth mentioning that only longwave UV is possible to use in the previously described manner, as shortwave UV is too energetic and may cause instead of electronic excitation, molecular bond breaks and ionization of molecules. A possibility for development is, thus, exploring further wavelengths and broadening the range of wavelengths applied. An advantage of the UV-VIS approach is the large amount of literature present on its applications in food analysis for example: fruit products quality assessment (Cortés, Blasco, Aleixos, Cubero, & Talens, 2019), sugar and soluble solids content (Suhandy et al., 2010; Włodarska, Szulc, Khmelinskii, & Sikorska, 2019), characterization of pigments (Hempel, Müller-Maatsch, Carle, & Schweiggert, 2018), authenticity of varieties (Chang et al., 2016), as well as fat and protein content of milk (Bogomolov, Belikova, Galyanin, Melenteva, & Meyer, 2017). Beneficial is as well that UV-VIS wavelengths may be detected by one- and two-dimensional (1D, 2D) sensors, CCDs (charge-coupled devices), and CMOSs (complementary metal-oxide semiconductors) based on silicon. Detectors may be implemented in both MOEMS (micro-opto-electrical mechanical systems) or MEMS (micro-electrical mechanical systems). In combination with Light Emitting Diode (LED) for UV-VIS radiation, the manufacturing of micro and nano-scale spectrometers in miniaturized devices at low-cost is enabled. Nevertheless, further research is conducted developing novel, miniaturized sensors and light weight, miniaturized illumination sources (see also, Table 1). The currently available, low-cost devices constructed for UV-VIS may also be applied to measure *photoluminescence*. After excitation at a specific wavelength caused by longwave UV (200–400 nm wavelength) or VIS (400–500 nm wavelength) radiation, some molecules emit photons in the relaxing process at a wavelength usually longer than the excitation one. This causes a detectable signal, being fluorescence or phosphorescence according to the lifetime of the relaxing process. The detected excitation and emission can be used to identify molecules even in a complex material (Bertani et al., 2020) when the fluorescence emission of the specific molecule is known *a priori* and the non-specific fluorescence contribution from matrix molecules is taken into account. Furthermore, spectroscopic fingerprints may be applied to study food products' authenticity, discriminate between different quality grades and geographical origins, and detect adulterations for example olive oils with low-grade olive oils or other vegetable oils (Mishra, Lleó, Cuadrado, Ruiz-Altisent, & Hernández-Sánchez, 2018; Sikorska, Khmelinskii, & Sikorski, 2012, 2019). So, fluorescence spectroscopy has become an increasingly used approach for assessing food characteristics.

To overcome the limitations of UV-VIS spectroscopy with only specific molecules giving a response, *near-infrared* and *mid-infrared* technology may be applied. Molecular bonds vibrational level excitation is triggered by near-infrared (NIR 750–2500 nm wavelength) and mid infrared (MIR 2500–25000 nm wavelength) radiation, giving as a result a spectrum. NIR may be roughly divided in 2 regions from 750 (or 780) nm to 1900 nm and from 1900 to 2500 nm. In the first region, secondary vibrations or overtone energy levels due to non-harmonic contributions of molecular vibrations are excited. This is a less efficient effect than fundamental vibration excitation, which is excited by radiation from the second region and above (MIR). However, the detection below 1900 nm can be performed at ambient temperature since sensors based on silicon (2D, CCD or CMOS) or point detectors have a reasonable signal to noise ratio and cooling is not necessary. Second range NIR and MIR may further be detected using InGaAs (Indium gallium arsenide) and mercury cadmium telluride based arrays. NIR typical sources are halogen lamps but in miniaturized/portable NIR spectroscopy LEDs (monochromatic or white) are used in combination with phosphor converters. As NIR wavelengths penetrate fairly deep in solid samples (with low scattering) and most constituents in foods are sensitive to NIR, the resulting spectra are often broad, overlapping and complex, necessitating chemometric analysis (Petronijević, Velebit, & Baltić, 2017). In brief, beneficial of the NIR approach is that besides the identification of specific molecules or molecular groups, NIR reflectance spectrum may be used to predict complex characteristics in food analysis as listed by Chapman et al. (2019) and Wang, Sun, Pu, and Cheng (2017).

*Raman* spectroscopy has the advantage that water is not interfering and it may be applied through food packaging but only on small sample sizes. The technique is based on the scattering of a small number of photons from samples in response of a laser beam with defined wavelength and polarization (Qin et al., 2019; Yaseen, Sun, & Cheng, 2017). Predominately the scattered radiation is elastically scattered light in the same frequency as the incident light, while a small fraction is inelastically scattered light (Raman scattering). The energy or frequency of the Raman scattering is altered from that of the incident light by molecular bonds' vibrational energy being decreased or increased from the interaction of photon-molecule (Stokes shift) (Jones, Hooper, Zhang, Wolverson, & Valev, 2019). The obtained spectra carry the basic molecular information about the sample or provide a fingerprint of certain food commodities (Tahir et al., 2019). In this methodological approach miniaturized sensors (CCD, CMOS, linear or 2D array, in some cases also InGaAs arrays) and ultra-compact modules integrating the laser source (785 nm or 532 nm) are already commercially available. Recent applications of portable devices include the detection of food adulteration (Beganović et al., 2020; Du et al., 2020), assessment of foods' texture (Chen et al., 2020), nutritional content (Krimmer, Farber, & Kurouski, 2019), and authenticity and geographical origin (Liu, Chen, Shi, Yang, & Han, 2020; Yan, Xu, Siesler, Han, & Zhang, 2019).

### 2.1. Perspectives in hardware development

In the future tailored applications of optical technologies, hyphenations of multiple spectroscopy approaches or combinations with imaging approaches are necessary. To the best of our knowledge, a portable optical device that combines all previously mentioned miniaturized spectral techniques has not been marketed yet. One approach combining visible, NIR, fluorescence spectroscopy was outlined by Groβ et al. (2019) and applied at prototype-stage by Weesepoel, Alewijn, Wijtten, and Müller-Maatsch (2020), detecting adulterations of extra virgin olive oils. All previous mentioned spectroscopic techniques may be coupled with imaging systems such as spectral imaging. The advantage that most of them are available in miniaturized version at prototype-stage, allows the forecast that easy-to-use, field ready integrated devices will be available in the very next future. These coupled systems (could) simultaneously acquire and link the spectrally determined chemical information with spatial information of a sample. Thereby, the latter is obtained from the digital image and includes the shape and size, surface texture and color of a sample. Multiple applications have been explored and applied such as the chemical and physical analysis of food samples, monitoring food processes, and food safety evaluation (Dong et al., 2019) as well as the characterization of single cells (Ma, Sun, Pu, Cheng, & Wei, 2019). Prominently UV-VIS and IR spectroscopy is linked, but recently also Raman chemical imaging was explored (Yaseen et al., 2017). Besides these hyphenations or coupling attempts, novel technologies such as MIR and far infrared spectroscopy (Su & Sun, 2019) as well as terahertz (Gowen, O'Sullivan, & O'Donnell, 2012; Pawar, Sonawane, Erande, & Derle, 2013; Ren et al., 2019; Wang, Sun, & Pu, 2017) are under current development to be miniaturized and explored.

Developments on the sensors and technology approaches, devices carrying optical spectroscopic technologies are novated to enable measurements in remote locations and rough environments. Novel casings and mechanics are water- or splash and dust-proof and robust after shaking or falling down and during temperature changes. As measurements should be cost-efficient the availability of low-cost device components such as light sources, detectors, control electronics, analysis software is part of the research. Furthermore, in line with the attempt to offer the possibility for measurements for everyone i.e., laymen (do-it-yourself sensing), it is needed to link personal devices like smartphones to measurement tools and kits (Nelis et al., 2019), or directly use them as measurement tool (Rateni, Dario, & Cavallo, 2017). In order to perform actual implementation of spectroscopy in the coming years for control authorities and private entities, scientific developments target optical sensor hyphenation creating the universal optical sensor as well as data fusion, i.e., combining spectral data from different sensors, database transferability (i.e. calibration transfer) and open data and knowledge data exchange using for example a federated learning approach as depicted in Fig. 1 and outlined in the following sections.

## 3. "The data handling": current developments of software architecture to access and extract information from spectral data

Despite the availability of numerous spectroscopic approaches, food sensing has many burdens. One critical aspect in spectral data analysis of food is the foods' intrinsic heterogeneity. The conditions of a food commodity or raw material might differ due to differences in geographic origin, harvesting periods, processing or storage conditions and might even have differences within the same food sample. Such heterogeneity not only affects the results' reproducibility of measurements, but above all impacts the storage and transmission capability of the resulting spectral data. These capabilities are crucial when the acquired spectral data from a given sample is sent to a central machine intelligence station that processes all the data (Callao & Ruisánchez, 2018). Current developments of software architecture designed for automated food quality monitoring and spectral measurements are accounting for this aspect. Several examples, being open source tools or licensed ones are listed in Table 2. Beyond the heterogeneity of the foods' spectral data acquired, the data commonly presents in addition a discrete variation within nominally equal samples. For example contamination in food does appear different in every sample when ambient conditions as well as the commodity properties influence toxin distribution or bacteria proliferation. To maintain stable and high classification performances also in the presence of the described noisy features and fault occurrences, software data analysis architecture is part of research, embedding strategies for dynamic feature selection (DFS). A DFS algorithm selects in an unsupervised way for each new test sample the optimal feature set from an initial training set that will be used to train a classifier for the sample prediction. Optimal features should carry most of the information contained in a training sample-set and exclude variables that are not informative. This results in a simpler model with improved discrimination or prediction capacity. Dai, Cheng, Sun, and Zeng (2015) reviewed multiple approaches of feature selection that are currently applied in the food industry. Nevertheless, the development or selection of the most appropriate approach for each model depends on the samples, the size of the dataset, and the spectroscopic technology applied. In the heterogeneous scenario of food analysis, a unique approach is hardly the optimal one for any set of data features, thus, this is a matter of ongoing research. DFS has been successfully applied in some clinical scenarios (Mencattini et al., 2018; Mosciano et al., 2017) and also in food control (Lianou et al., 2019).

In addition, another critical aspect current research projects account for is the presence of spurious measured data, i.e., the presence of any artifact in static images or spectral data. Spurious data, often denoted as outliers, can impact the decision system performance and introduce an unpredictable drift of classification results. To construct a more reliable and robust recognition model, approaches for data reduction strategies are implemented in turns over the training data (Ifrim, Iuga, Pop, Wallace, & Poulopoulos, 2018). An example is the presence of pixels in the digital image that are saturated towards extreme value for example due

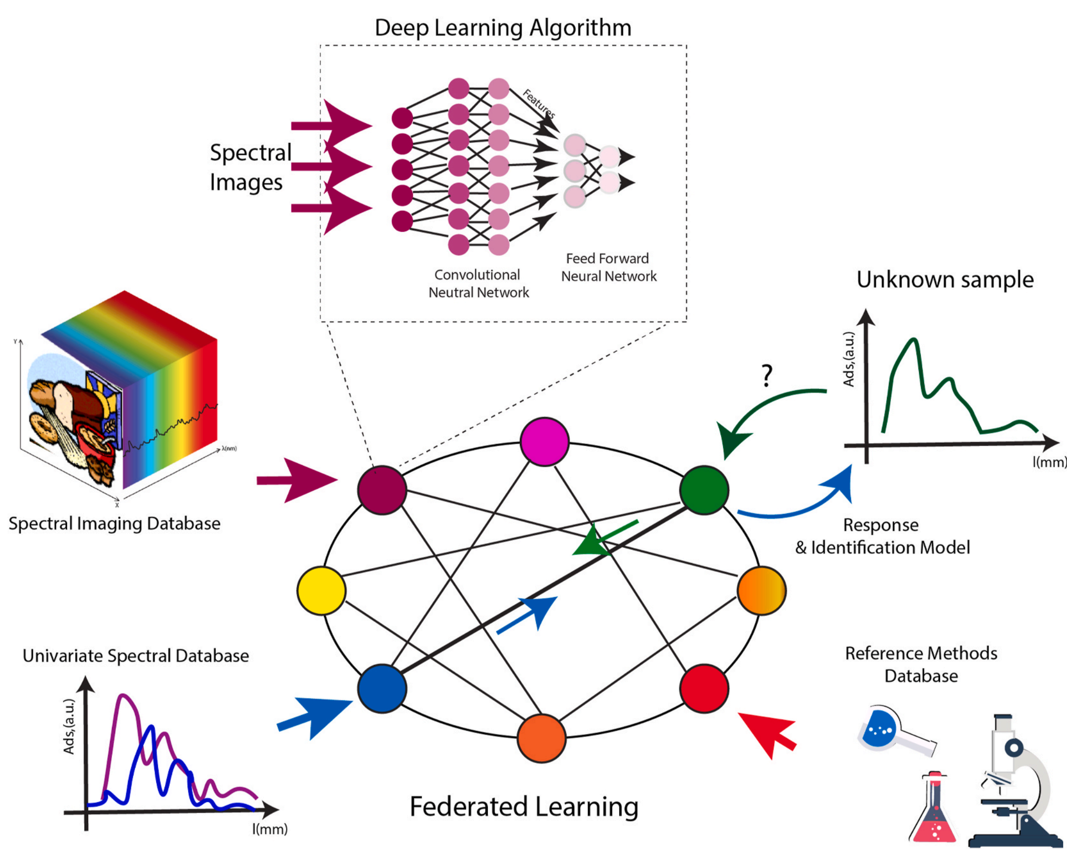


**Fig. 1.** Schematic figure of federated learning applied in food analysis. Data from an unknown sample coming from one or more instruments is send in the federated learning network. Here, sensors and their corresponding instrumental data in a specific database are represented by one or more network nodes. As an example, spectral images may be processed and by means of deep learning algorithms. After a machine learning decision strategy including reference method comparisons, the final response is generated to the initial node.

**Table 2**
Open source and licensed software tools for image analysis.

| Name | Developer | License | Usage | Functionalities | Requested Skills | Image analysis | |
|---|---|---|---|---|---|---|---|
| OPEN SOURCE TOOLS | | | | | | | |
| **ImageJ** | National Institutes of Health and Laboratory for Optical and Computational Instrumentation at the University of Wisconsin, USA | Open source Java-based | GUI | Image and video processing functionalities | Java Programming skills for extended research usage | Semi-automatic | Schneider, Rasband, and Eliceiri (2012) |
| Cell profiler | Broad Institute of Massachusetts Institute of Technology, USA, and Harvard, USA | Open Source Matlab based | GUI | Basic image processing functionalities and image measurements | No programming skills | Manual | Lamprecht, Sabatini, and Carpenter (2007) |
| Ilastik | The Ilastik developers | Open source | GUI | Basic segmentation and classification through Random Forest models | No programming skills | Semi-automatic | Sommer, Straehle, Köthe, and Hamprecht (2011); The Ilastik developers (2020) |
| **Orbit** | N/A | Open source | N/A | Built-in image analysis algorithms for tissue quantification using machine learning techniques, object/cell segmentation, and object classification | No programming skills | Semi-automatic | Stritt, Stadler & Vezzali (2020) |
| **Icy** | Institut Pasteur and France-BioImaging, France | Open source | GUI | Visualization, annotation and quantification of bioimaging data | No programming skills | Semi-automatic | de Chaumont et al. (2012) |
| **LICENSED TOOLS** | | | | | | | |
| **Matlab ®** | The Mathworks Inc., USA | Academy Licensed/ Commercial | Inline programming | Image/video analysis, visualization, segmentation, classification, measurement, and annotations | Matlab language | Automatic | Mathworks (2020) |
| **AMIRA** | Zuse Institute Berlin, Germany Thermo Fisher Scientific Inc., USA | Commercial | GUI | 3D and 4D data visualization, processing, and analysis | C++ skills for extended functionalities | Manual | Stalling, Westerhoff, and Hege (2012) |
| **IMARIS** | Oxford Instrument plc, UK (Bitplane, Switzerland) | Commercial | GUI | Visualization, segmentation and interpretation of 3D and 4D microscopy datasets Analysis includes cell counting, cell tracking, neuron tracing image segmentation, co-localization and 4D movie generation microscopy datasets | Skills different according to specific tools | Manual | Imaris (2020) |
| **HUYGENS** | Scientific Volume Imaging, the Netherlands | Commercial | GUI | Image processing and image analysis software for deconvolution, colocalization, object analysis and visualization. Supporting file formats from most major microscope manufactures | Skills different according to specific tools | Manual | ScientificVolumes Imaging (2020) |

to overexposure. Those pixels may alter the values of some global descriptors extracted from the digital image. Therefore, descriptor values that are in the tails of the distribution extracted over the training dataset (i.e., outside the interquartile range) are eliminated. Data reduction is having an important role not only for static data analysis, but also for time-varying observation of food quality, i.e. for food monitoring (He, Sun, & Wu, 2014). Current developments cover the fact that any change in food commodity or the kind of contamination and the related dynamics does require a sort of data adaptation process of the software platform. DFS is again a way to provide a robust tool for the analysis of food data along time.

Last but not least, novel devices are equipped with software to access spectral data and give results tailored to the end-user. As most handheld spectroscopic approaches are now targeting laymen, suitable designs have been outlined in detail by Gardner and Green (2014) including a self-repairing option (Magna, Di Natale, & Martinelli, 2019).

## 4. “The data transfer, fusion & exchange”: possibilities of combining, transferring and exchanging spectral information using machine learning approaches

The perfect transfer from one instrument to another, for example from benchtop to portable devices, should include the re-use of already established spectral databases including the calibration with reference samples in statistically retained accuracy and precision. Workman (2018) reviewed multiple approaches, being conventional and unconventional, and concluded that the differences between old and new instruments may cause significant variations in the predicted results after the transfer. These variations may be mitigated by statistically aligning the instrument spectral profiles which is part of current research. In particular, relating data from wet-chemical reference methods or other non-spectroscopic data to the one predicted by spectroscopy remains challenging. Transfer of calibration between instruments with similar principles has been shown by Eliaerts et al. (2020) and by Salguero-Chaparro, Palagos, Peña-Rodríguez, and Roger (2013) in the field of pharmaceuticals and food, respectively. In addition a calibration transfer between instruments with differing principles was evaluated by Pu et al. (2018) for NIR spectrometry and hyperspectral imaging and between two similar matrices in different aggregation state by Pereira, Carneiro, Botelho, and Sena (2016). Another option for data transfer, which is under ongoing development, is the fusion of multiple data streams, thereby the same sample is measured by different instruments and the data combined to complete its description (see also Fig. 1). Callao and Ruisánchez (2018) and Borràs et al. (2015) reviewed multiple ways to fuse data at low-, mid- or high-level. In low-level fusion, data from all instruments are concatenated sample-wise into a single matrix that has as many rows as samples analyzed and as many columns as variables supported by the respective instruments. Data fusion at mid-level performs a preprocessing of data by extracting principal or latent variables using for example Principal Component Analysis (PCA) or Partial Least Square-Discriminant Analysis techniques (Biancolillo, Bucci, Magrì, Magrì, & Marini, 2014). Finally, in high-level (or decision-level) fusion, classification or regression models are individually constructed from each data source, and the results from each individual model are combined in a framework that is usually referred to as *cooperative learning.* By data fusion from different technologies, a transfer of classification results might be possible from one instrument or technology to another. As a different data fusion approach is suitable for every food product, desired target compound and optical device, its tackling is of great research interest. An example for data fusion is the combination of spatial information from imaging and spectral information from UV-VIS or NIR technology. Whereas spectral food data are crucial for the investigation of food composition at molecular and cellular levels, imaging information completes the data representation and may support the control of samples' heterogeneity. Due to the huge amount of imaging data available, data reduction approaches such as PCA are developed to map the data into a domain with reduced dimensionality and maximum information (Del Fiore et al., 2010). However, this does not allow to extract and exploit the spatial correlation among the adjacent portion of the sample visualized. Therefore, Deep Learning (DL) architecture represents an important aid towards the analysis of image data, either static (single image acquisition) (Chen, Lin, Zhao, Wang, & Gu, 2014; Yu, Tang, Wu, & Lu, 2018) and variable over time. It offers the possibility to process large amounts of image data and to classify them according to a learning phase separately performed on data similar to those acquired. In a novel extended logic, the so-called *transfer learning*, DL allows using a pretrained network for example AlexNET (Alom et al., 2018) or ResNET (Wu, Shen, & van den Hengel, 2019) to code the available image into a vector of numerical descriptors without a retraining step. Hence, machine learning may lead to "universal" classification models that are not limited by the differences in hardware and sample sets. The strength of the cited approach is even more crucial when dealing with big data storage where re-training a network can be computationally prohibitive. Not less relevant, pre-trained networks have already learned to recognize more than 22, 000 distinct categories from 15 million labelled images and hence represent a robust tool for independent data representation. Recent examples in food application of such networks can be found in soft-shell shrimp quality (Liu, 2020) or general food quality studies (Yiğit & Ozyildirim, 2018). The strength of such networks is the capability to retrieve from a given image the information that optimally represent it in an unsupervised manner, thus providing a sort of signature of the image that can be used for further processing such as image classification (Alom et al., 2018). In addition, the use of image data allows for advanced data transferring procedures in case image acquisition is done at different spatial resolutions in particular novel imaging systems can use improved spatial resolution thus generating images with different sizes. Image re-sampling and re-sizing, as well as super-resolution approaches (Li, Hu, Zhao, Xie, & Li, 2017), permit to equalize data dimension in order to transfer old models to new data. The potential adaptation of a platform to diversified and changing scenarios is crucial also in context when large amount of (image or spectral) data have been already acquired and cannot be lost. However, the heterogeneity of large dataset acquired at different locations and times may represent a challenging aspect. More general, the huge amount of measured data already acquired represents knowhow to be saved and re-used. Data mining techniques (Garcia, 2013) may have a crucial role in the extraction of relevant information from the available dataset and the integration with newly acquired data. Such approaches may represent a valid alternative to re-formulate the *data transfer & exchange paradigm*. Instruments for food quality and monitoring change continuously from one locus to another within the same station, as technology progresses, leading to the exploiting of the novel more performing instruments.

## 5. "The information and knowledge exchange": possibilities to interchange knowledge and model information without sharing data (the actual database)

Privacy, as well as computer memory constraints, represents a serious bottleneck for data sharing and knowledge exchange, thus, research activities are targeting to overcome it. The newly developed machine learning architecture, named *federated learning* (FL) or *collaborative learning* represents a possible key solution to interchange knowledge and model information without sharing the actual database (Wang et al., 2019). In cooperation with blockchain technology, it allows validating the trustiness of the data along supply chains. FL trains a machine learning algorithm across multiple displaced centers where data are stored without exchanging data. The goal of current research is that the learned network is shared across the data acquisition loci and learned until it reaches acceptable results (Li, Sahu, Talwalkar, & Smith, 2019). An example application of a federated learning approach is in next generation mobile phone predictors. Thereby, a predictor is trained in a distributed fashion, preserving the privacy of the sent data and reducing the network traffic. Remote devices periodically connect to a central server to train a global model. At each connection, local training on some devices' non-identically-distributed user data is performed and updates are sent to the server. After incorporating these updates by the server, a new global model is distributed to other devices. This iterative training and updating process continues across the network. When convergence is reached or some stopping criterion is met it stops.

The developed FL approaches only work when an efficient exchange of spectral data sets, and the clear understandable metadata associated with those spectral datasets, is properly standardized and facilitated. Therefore, the FAIR-data principle (Findable, Accessible, Interoperable and Re-usable) was developed and introduced in 2016, advocating the re-use of digital assets with an emphasis on machine implementation. The findability (or 'FAIRification') of data implies that metadata and spectral data should be made available in a format that is understood by both humans and machines and that automated indexing of datasets is possible. Once the data is found, the accessibility on where the data is located and how this data can be accessed needs to be cleared to ensure the security of data. As (inter)operability of data is often a tedious task, terms such as controlled vocabulary organized in a hierarchical fashion (ontologies) play an important role in combining data sets without significant (meta)data loss. This leads to the main goal of FAIR: the (re) usability of data, focusing on the quality of the metadata description so that they can be combined under different scenarios. The proper implementation of FAIR data is vital for FL networks to function in the future and to re-use the generated spectral data from different devices and industry and academia (Mons et al., 2017; Wilkinson et al., 2016). Developments including the FL strategy in combination with the FAIR approach might firstly solve privacy problems and data access rights and in addition, solve the issue of foods' spectral data heterogeneity and the large amount of information displaced in different places.

## 6. Conclusions

The developments of the last years in sensor technologies and illumination sources and innovations in data handling, storage, accessing and transfer lead to miniaturized and portable versions that are commercially available at decreasing cost and increasing performances. With the increase of device availability, also the number of spectral databases increased. However, most versions are no longer in use, due to the constant need for updating, aligning with new devices or device versions and a lack of handling procedure of all this data. Novel approaches using machine learning, have been developed to tackle large amount of data and fuse multiple data streams, being spatial or spectroscopic. Current research conducted on data accessibility and data sharing focuses not only on the usage of spectral databases from a scientific point of view but includes privacy and confidentiality constraints of industrial and governmental players. The possibility to apply metadata analysis in combination or as an alternative to the universal machine learning approach is hence followed up. Last but not least, the previously mentioned developments and perspectives are not only restricted to agriculture and food production (Beganovic, Hawthorne, Bach, & Huck, 2019; Power, Truong, Chapman, & Cozzolino, 2019). Novel, portable and increasingly sensitive devices are in need to be adapted as fast techniques to pre-screen samples also in mining and metal industry, environmental science, healthcare and pharmaceuticals (Ciza et al., 2019) as well as in motor- (Sales et al., 2019) and space science (Nelis, Elliott, & Campbell, 2018).

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## Declaration of competing interest

The authors claim no conflict of interest.

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