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Data Article

Dataset of chemical and near-infrared spectroscopy measurements of fresh and dried poultry and cattle manure

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ABSTRACT

Combined with multivariate calibration methods, near-infrared (NIR) spectroscopy is a non-destructive, rapid, precise and inexpensive analytical method to predict chemical contents of organic products. Nevertheless, one practical limitation of this approach is that performance of the calibration model may decrease when the data are acquired with different spectrometers. To overcome this limitation, standardization methods exist, such as the piecewise direct standardization (PDS) algorithm.

The dataset presented in this article consists of 332 manure samples from poultry and cattle, sampled from farms located in major regions of livestock production in mainland France and Reunion Island. The samples were analysed for seven chemical properties following conventional laboratory methods. NIR spectra were acquired with three spec-

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trometers from fresh homogenized and dried ground samples and then standardized using the PDS algorithm. This important dataset can be used to train and test chemometric models and is of particular interest to NIR spectroscopists and agronomists who assess the agronomic value of animal waste.

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Specifications Table

Subject	Chemistry, Near-Infrared (NIR) Spectroscopy
Specific subject area	Cattle and poultry manure composition
Type of data	.CSV and Excel files, figures, tables
How data were acquired	Absorbance spectra were acquired with 3 NIR spectrometers (2 XDS Foss, 1 NIRFlex Buchi). Conventional laboratory analyses (dry matter (DM), total ammonium nitrogen (NH_4), total nitrogen (N), phosphorus pentoxide (P2O5), calcium oxide (CaO), magnesium oxide (MgO) and potassium oxide (K2O))
Data format	Chemical analysis data, raw and standardized spectral data of standard cells, standardized spectral data of manure
Parameters for data collection	332 manure samples were analysed by NIR spectroscopy using 3 spectrometers. Both fresh homogenized and dried ground samples were scanned to acquire spectra.
Description of data collection	The 7 chemical contents were determined using conventional laboratory methods. NIR spectroscopy was combined with chemometric tools to standardize the spectral data, using the XDS Foss spectrometer of CIRAD as the reference instrument.
Data source location	Manure samples were collected from different farms in mainland France and Reunion Island (French overseas territory)
Data accessibility	Data presented in .CSV and Excel file formats are available in this article. Data are deposited in a public repository. Repository name: Data INRAE Data identification number: 10.15454/JIGO8R Direct URL to data: https://doi.org/10.15454/JIGO8R

Value of the Data

- This dataset provides results of analyses of NIR spectroscopy and chemical composition of a large sample of cattle and poultry manures (collected from different livestock production regions). This dataset thus integrates the high compositional variability of these materials, which can be valuable in studies interested in assessing the agronomic value of these types of manure.
- The data are of particular utility to NIR spectroscopists who test chemometric methods (e.g. regression, standardization) or agronomists who assess the agronomic value of animal waste.
- The data are also particularly useful for studying effects of manure sample preparation (moisture, particle size) on standardized NIR spectra.
- This article presents a case study of application of the piecewise direct standardization (PDS) algorithm, which can standardize data acquired with different spectrometers.

1. Data Description

The contents of dry matter (DM), total ammonium nitrogen (NH_4), total nitrogen (N), phosphorus pentoxide (P2O5), calcium oxide (CaO), magnesium oxide (MgO) and potassium oxide

Table 1
Statistics of contents of dry matter and chemical properties of manure samples (% of wet weight). SD: standard deviation

Property	n	Mean	SD	Min	Max	Range
DM	332	37.28	20.06	11.25	82.48	71.22
NH_4	332	0.262	0.276	0.001	1.086	1.085
N	332	1.36	1.09	0.25	4.15	3.90
CaO	158	0.57	0.56	0.09	3.11	3.01
K_2O	158	1.02	0.65	0.19	3.84	3.66
MgO	158	0.23	0.19	0.06	1.05	0.99
P_2O_5	158	0.48	0.58	0.09	3.02	2.93

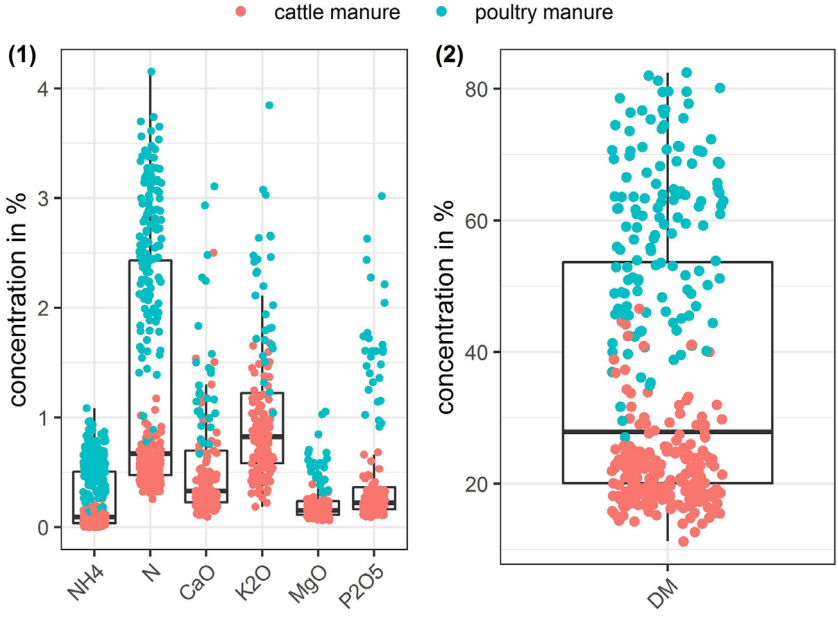


Fig. 1. Boxplots of contents (% of wet weight) of chemical properties of manure samples.

Table 2
Basic features of the near-infrared spectrometers.

Instrument	Foss XDS (CIRAD and ARVALIS)	Buchi NIRFlex (LDAR)
Technology	Dispersive	Fourier transform
Spectral range	400–2500 nm	4000–12,500 cm^{-1}
Spectral resolution	2 nm	8 cm^{-1}
Scans	32	32

(K_2O) of 332 poultry and cattle manure samples are available in this article (Table 1, Fig. 1). The samples were also analysed by NIR spectroscopy using three instruments (Table 2): two XDS Foss (belonging to CIRAD and ARVALIS, respectively) and one NIRFlex Buchi (belonging to LDAR), on fresh homogenized and dried ground samples. The XDS spectrometer of CIRAD was the reference instrument to which the other two were related. The absorbance spectra (1100–2498 nm) were standardized by the mean of three standard sealed cells (commercial compost, green waste compost and poultry litter) (Fig. 2) and the PDS algorithm in order to use them in calibration models for future processing (Fig. 3).

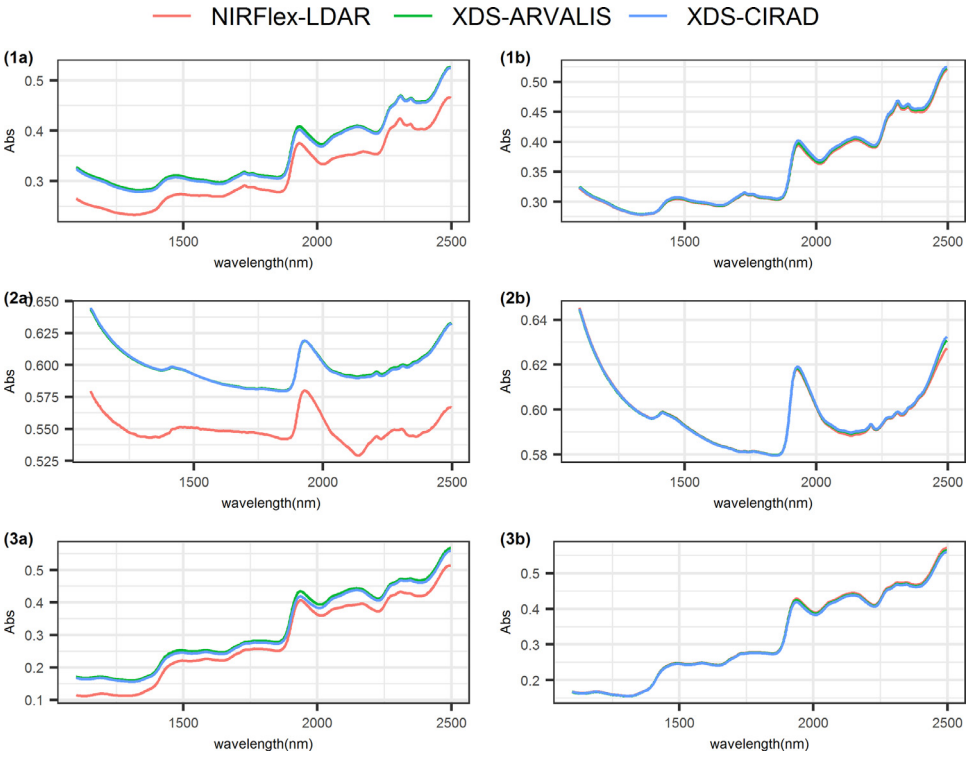


Fig. 2. Near-infrared spectra of the three standard sealed cells measured with the three spectrometers before (commercial compost (1a), green waste compost (2a) and poultry litter (3a)) and after piecewise direct standardization (commercial compost (1b), green waste compost (2b) and poultry litter (3b)).

Table 3
Contents of the dataset

File name	Contents
chemical_analysis.xlsx	Sample name (sample_name) Dry matter (% of wet weight).DM Total ammonium nitrogen (% of wet weight).NH4 Total nitrogen (% of wet weight).N Calcium oxide (% of wet weight).CaO Potassium oxide (% of wet weight).K2O Magnesium oxide (% of wet weight).MgO Phosphorus pentoxide (% of wet weight).P2O5 Type of manure (type_manure) Spectrometer Township Country
spectra_standard_cells.csv	The first column contains the sample identification code. The next two contain the spectrometer used for acquisition and whether the data are standardized or not, respectively. The other columns contain the absorbance data recorded by the spectrometers from 1100–2498 nm for the three standard sealed cells.
spectra_FH_Abs_STD_1100_2498 nm_STD.xlsx	The first column contains the sample identification code, and the others contain the standardized absorbance data recorded from 1100–2498 nm for the 332 fresh homogenized samples.
spectra_DG_Abs_STD_1100_2498 nm_STD.xlsx	The first column contains the sample identification code, and the others contain the standardized absorbance data recorded from 1100-2498 nm for the 332 dried ground samples.

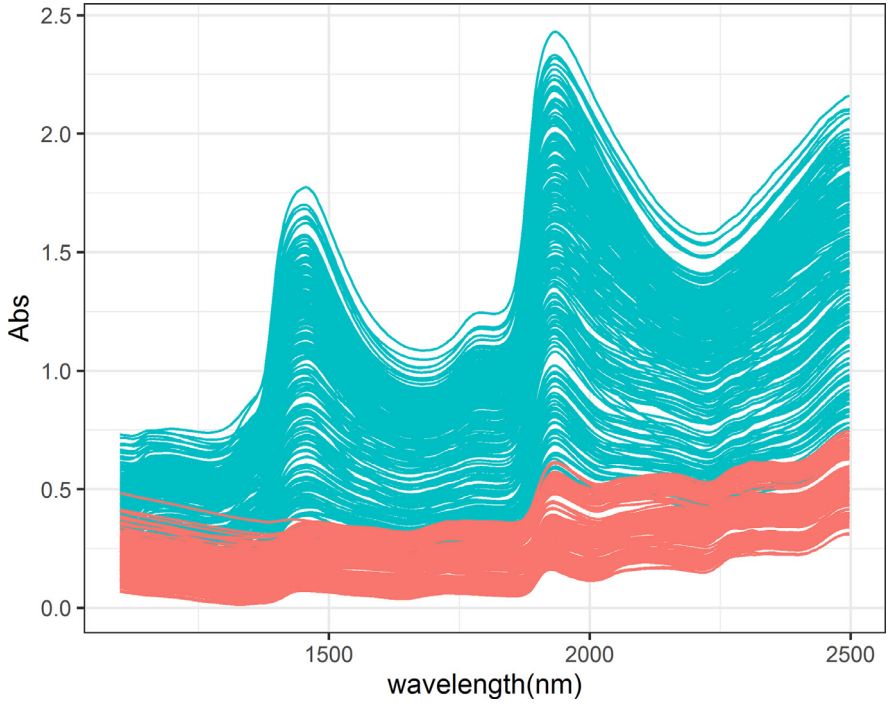


Fig. 3. Standardized near-infrared spectra for fresh homogenized samples (red) and dried ground samples (blue).

The dataset is composed of .CSV and 3 Excel files (Table 3). One .CSV file contains raw and standardized data of the three standard sealed cells acquired with the three spectrometers. Two Excel files contain standardized data of the 332 solid manures acquired from fresh homogenized and dried ground samples. One Excel file contains the chemical data. The dataset is available via the Data INRAE portal.

2. Experimental Design, Materials and Methods

2.1. Sample collection

A total of 196 cattle manure and 136 poultry manure samples were collected from major regions of livestock production in mainland France and Reunion Island. Broiler chicken were fed a mixture of cereals (wheat, maize, barley), oilseeds and their meals, vitamins and minerals in mainland France and on Reunion Island (the same feed). Dairy and feedlot cattle were fed hay or silage plus concentrated feed in mainland France and sugarcane residues plus concentrated feed on Reunion Island. Broiler chicken litter consisted of wheat straw in mainland France and Cryptomeria japonica woodchips on Reunion Island. The samples were sampled, collected along routes, prepared, preserved and analysed according to the following procedure adopted by the laboratories involved in this project. The samples were promptly frozen after collection to stop microbiological activity, which induces chemical transformations, and mineralization, which process that leads to causes NH4 losses during storage. In the laboratory, they were homogenized by crushing them in frozen form in a blender-cutter (Blixer Dito K45, Electrolux, Senlis, France). A subsample of each sample was dried in a forced-convection oven (at 40°C for 4 days) and then ground (to 1 mm) in a cyclone mill (Cyclotec 1093, Foss, Silver Spring, MD, USA).

2.2. Chemical analytical methods

The samples collected in mainland France were analysed by LDAR, AUREA and ARVALIS laboratories, while those collected on Reunion Island were analysed by CIRAD's laboratory. In each laboratory, manure samples were analysed according to international (ISO) or French (NF) standards [1] for seven chemical components: DM, NH_4, N, P_2O_5, CaO, MgO and K_2O (Table 1). DM was obtained by oven drying the partly dried (40°C) samples at 103 ± 2°C until they reached a constant weight. NH_4 and total N contents were measured by the Kjeldahl method (NF T90-015-AFNOR 1975). P_2O_5, CaO, MgO and K_2O contents of only 158 of the 332 samples were measured by Inductively Coupled Plasma (Element XR Thermo Scientific). To address agronomic and environmental issues, we analysed N, NH4 and DM contents in all samples. To decrease analysis costs, the mineral compounds were analysed only in a subset of 158 samples that covered the variety manure types, farm types and sample-collection areas. All analyses were performed in duplicate, and values of the duplicates were averaged.

2.3. Spectroscopic analysis

Samples were scanned in triplicate using one of three spectrometers, depending on the laboratory: 80 samples scanned by an XDS device of CIRAD (Foss, Silver Spring, MD, USA), 96 samples scanned by the other XDS device of ARVALIS and 156 samples scanned by a NIRFlex device of LDAR (Büchi, Flawil, Switzerland). Each replicated measurement was the mean of 32 scans and was recorded in absorbance (Abs) using the following equation: Abs = log(1/Reflectance). For each sample, the final spectrum used in data processing and analysis was the mean of the triplicate.

NIR spectra were recorded for 1) fresh homogenized samples in a rectangular quartz cell (250 ml) and 2) dried ground samples in a Petri dish (10 cm diameter) for those scanned by ARVALIS and a circular quartz cell (5 cm diameter) for those scanned by CIRAD.

2.4. Standardization procedure

The spectral response (e.g. amplitude, wavelength shift) of a given sample analysed by NIR spectroscopy can differ among the types of instrument used (e.g. different technologies) and even between two spectrometers of the same brand (e.g. different production batches). Standardization methods ([2–6]) allow spectra measured by one instrument to be transformed as if they had been measured by another instrument.

The NIRFlex, based on Fourier-transform technology, measures absorbance as a function of wavenumber (cm^{-1}), while the XDS Foss, based on dispersive technology, measures absorbance as a function of wavelength (nm). The wavenumber (4000–12,500 cm^{-1}) was converted to wavelength (800–2500 nm). As the resolution step of wavelength of the NIRFlex was not constant after this conversion, the absorbance was recalculated at the wavelength of the XDS Foss using a shape-preserving piecewise cubic interpolation that preserves the convexity of scattered convex data.

To standardize the spectra measured by the spectrometers, three standard sealed cells (commercial compost, green waste compost and poultry litter) were measured with the three instruments. The common spectral range from 1100–2498 nm was maintained. The PDS algorithm [7] was used to standardize the spectra from the three instruments. The algorithm transforms data measured by a "slave" instrument to data that appears to have been measured by a "master" instrument. The algorithm has two steps: (1) wavelengths of the "slave" instrument are matched to those of the "master" instrument to correct for a possible wavelength shift, and (2) a transformation matrix F is created from the three spectra of the standard sealed cells measured by both the "slave" and "master" instruments. The transformation matrix F is composed

of regression coefficients of multivariate linear (partial least squares) regression between the absorbance values at each λ_i of the "master" spectra and those at (λ_{i-k}, λ_{i+k}) of the "slave" spectra, for the three spectra of the standard sealed cells ($k = 3$ is the size of the wavelength window). Finally, the transformation is applied to the spectra of the samples measured by the "slave" instrument. In this study, the Foss XDS of CIRAD was the "master" instrument, while the two others were the "slave" instruments. Fig. 2 shows effects of the standardization based on the standard sealed cell spectra. Fig. 3 shows the standardized spectra for the fresh homogenized and dried ground samples.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that have, or could be perceived to have, influenced the work reported in this article.

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