Near Infra-Red Spectroscopy Predicts Crude Protein in Hemp Grain

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Abstract

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Plain Language Summary

- Earthquake data for the island of La Palma from the September 2021 eruption is
- found ...

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incomplete: may contain errors, run-ons, half-thoughts, etc.

0.1 INTRODUCTION

- Hemp (Cannabis sativa L.) is an annual crop with potential uses as a source of
- $_{20}$ food or feed from grain, and bast fiber or hurd from the stalk. Hemp cultivars are
- commonly grown for one or both purposes and a cultivar may be referred to as a
- grain, fiber, or dual-purpose type. Because of protein's nutritional importance, the
- protein content of a grain crop is an prime consideration for researchers, producers,
- 24 and consumers. Whole hemp grain typically contains approximately 25-30% protein
- ²⁵ (Bárta et al., 2024; Ely & Fike, 2022). Crude protein (CP) is often used as a proxy
- for the direct measurement of protein concentration and consists of the multiplica-
- tion of nitrogen concentration by a conversion factor because measuring nitrogen
- concentration is relatively easy and cheap via laboratory assay (Hayes, 2020).
- Near-infrared spectroscopy (NIRS) technology is rapid, non-destructive, and cheap,
- $_{\rm 30}$ $\,$ and consists of the measurement of NIR radiation reflected from a sample (Roberts
- et al., 2004). NIR spectra from many samples are related to laboratory values
- for components such as moisture, protein, fat, or fiber [Roberts et al. (2004)].
- NIRS technology has been used since the 1970's to assess forage CP (Reeves, 2012;
- Williams, 1975). A NIRS calibration set often consists of samples from one species
- grown in many environments encompassing the range of expected values from the
- analyte or analytes (Chadalavada et al., 2022). Partial least squares regression
- (PLSR) is a typical method used in the agricultural and food sciences to relate spec-
- tra to analyte (Roberts et al., 2004).
- A NIRS-scanned sample of undamaged grain may subsequently be grown, an im-
- portant consideration for a plant breeder. In wheat and corn, grain protein content
- has been shown to be heritable [Giancaspro et al. (2019); Geyer et al. (2022)]. This
- suggests (at least potentially) that NIRS technology could serve as resource to more
- rapidly identify high CP hemp germplasm, senabling the delivery of higher CP hemp
- grain cultivars faster.
- For this study, a benchtop NIR spectrometer was used to develop a model to predict
- 46 CP content based on a data set representing multiple years, locations, and cultivars
- using PLSR.

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0.2 MATERIALS AND METHODS

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0.2.1 Hemp Grain Sample Background

- Spectral data were obtained from whole (unground) hemp grain samples, harvested
- at maturity, collected from 2017 2021 from 18 cultivar trials in New York (NY)
- 53 (149 samples). Grain samples were obtained by hand sampling or mechanical har-
- vest and were cleaned of chaff and dried at 30 C for six days in a forced-air dryer.

- In total, 38 cultivars were represented in the data set. Cultivars were grain or dualpurpose types and included both commercially available and experimental material.
- All cultivar trials were planted in randomized complete block design with each culti-
- $_{58}$ $\,$ var replicated four times. The 2017 data were comprised of samples from the same
- thirteen cultivars sampled from six NY locations. For those trials, grain was har-
- vested from each plot individually and aggregated by cultivar within each trial. Four
- subsamples were drawn from each aggregated sample and scanned separately. These
- spectra were averaged at each 2 nm increment. All remaining samples from 2018-
- 2021 were collected on a per-plot basis. All possible cultivars and possible locations
- were represented in 2017, but only a selected subset of cultivars and locations were
- represented in 2018-2021.

66 0.2.2 Spectral Data Collection and Preprocessing

- A benchtop NIR spectrometer (FOSS/ NIR FOSS/ NIR Systems model 5000) was
- used to obtain the spectra (FOSS North America, Eden Prairie, MN, USA). Spec-
- tra were collected every 2 nm from 1100-2498 nm and the logarithm of reciprocal
- reflectance was recorded.
- VINISI software version 1.02A (Infrasoft International, Port Matilda, PA, USA) was
- used to average the spectra in 2017, as well as to select samples for laboratory assay.
- Samples were selected according to their spectral distance from their nearest neigh-
- bor within the calibration data set with a cutoff of a distance of 0.6 H, where H is
- $_{75}$ $\,$ approximately equal to the squared Mahalanobis distance divided by the number
- of principal components used in the calculation (Garrido-Varo et al., 2019). Prior
 - to selection selection, spectra were preprocessed using SNV-detrend with settings
- 1,4,4,1 for the derivative, gap, smooth, and smooth 2 settings respectively.

0.2.3 Additional software used:

- We used R version 4.3.3 (R Core Team, 2024) and the following R packages: data.table
- v. 1.15.2 (Barrett et al., 2024), randomForest v. 4.7.1.1 (Liaw & Wiener, 2002),
- rmarkdown v. 2.26 (Allaire et al., 2024; Xie et al., 2018, 2020), tidyverse v. 2.0.0
- ⁸³ (Wickham et al., 2019).
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0.2.4 Preprocessing

- Multiplicative scatter correction (MSC)
- standard normal variate (SNV) transformation
- The calibration set consisted of
- The validation set consisted of

90 0.2.5 Laboratory Validation

- Laboratory assays were performed by Dairy One Forage Laboratory (Ithaca, NY).
- For those assays, 1mm ground samples were analyzed by combustion using a CN628
- or CN928 Carbon/Nitrogen Determinator. Samples from 2017 were aggregated as
- described above, but
- Prior to In 2017, an in
- 0.3 RESULTS AND DISCUSSION
- o.4 ACKNOWLEDGMENTS
- 98 0.5 SUPPLEMENTAL MATERIAL
- 99 0.6 OPTIONAL SECTIONS
- 0.7 REFERENCES
- 101 0.8 FIGURES AND TABLES
- 102 Source: Article Notebook

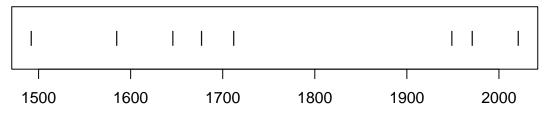


Figure 1: Timeline of recent earthquakes on La Palma

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Based on data up to and including 1971, eruptions on La Palma happen every 79.8 years on average.

Studies of the magma systems feeding the volcano, such as (marrero2019?), have proposed that there are two main magma reservoirs feeding the Cumbre Vieja volcano; one in the mantle (30-40km depth) which charges and in turn feeds a shallower crustal reservoir (10-20km depth).

Eight eruptions have been recorded since the late 1400s (Figure 1).

Data and methods are discussed in Section 0.9.

Let x denote the number of eruptions in a year. Then, x can be modeled by a Poisson distribution

$$p(x) = \frac{e^{-\lambda}\lambda^x}{x!} \tag{1}$$

where λ is the rate of eruptions per year. Using Equation 1, the probability of an eruption in the next t years can be calculated.

Table 1: Recent historic eruptions on La Palma

| | ar |
|------------------------|----|
| C | |
| Current 20 | 21 |
| Teneguía 19 | 71 |
| Nambroque 19 | 49 |
| El Charco 17 | 12 |
| Volcán San Antonio 16 | 77 |
| Volcán San Martin 16 | 46 |
| Tajuya near El Paso 15 | 85 |
| Montaña Quemada 14 | 92 |

Table 1 summarises the eruptions recorded since the colonization of the islands by Europeans in the late 1400s.

La Palma is one of the west most islands in the Volcanic Archipelago of the Canary Islands (Figure 2).



Figure 2: Map of La Palma

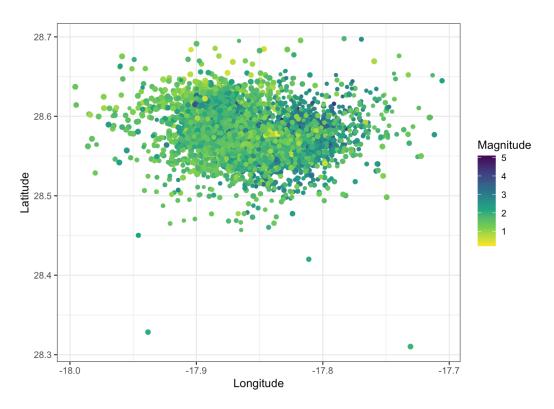


Figure 3: Locations of earthquakes on La Palma since 2017

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Figure 3 shows the location of recent Earthquakes on La Palma.

Source: Explore Earthquakes

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0.9 Data & Methods
0.10 Conclusion
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