Integrating GIScience and Crop Science datasets: a study involving genetic, geographic and environmental data

Roberto Santos[1,2], Adam Algar[1], Richard Field[1], and Sean Mayes[3]

[1]**School of Geography, University of Nottingham, UK**
[2]**Nottingham Geospatial Institute, University of Nottingham, UK**
[3]**Plant and Crop Sciences, University of Nottingham, UK**

ABSTRACT

Sharing and reusing data in research is a welcome and encouraged practice since it maximises the scientific outcomes given limited financial, material and human resources. Interdisciplinary research is considered to benefit from this practice, uniting researchers and data from two or more disciplines to advance fundamental understanding or tackle problems whose solution is beyond the limit of an individual body of knowledge. Here we discuss the challenges of combining data across disciplines, focusing in particular on associating geographic location data with genetic data in the context of a project involving Crop Science and Geospatial Information Science disciplines. This project aims to improve understanding of how geographical, environmental and anthropocentric factors affect the genetic variation in a neglected and underutilised crop called Bambara groundnut.

Keywords: Data integration, GIScience, Crop Science, Landscape Genetics, Bambara groundnut

INTRODUCTION

Research challenges in the 21st century require an interdisciplinary approach, to advance fundamental understanding or to tackle problems whose solutions are beyond the scope of a single discipline or body of knowledge (Academies, 2004). Interdisciplinarity is encouraged, with funding organisations recently increasing support for research that integrates multiple disciplines. Interdisciplinary science represents the current reality for increasing numbers of scientists, through the composition of research teams and the nature of the hypotheses being examined (Dyer, 2015). In this context, sharing and reusing datasets from different disciplines is common practice and aims to strength the research by adding new dimensions to the data available or verifying the results obtained from a different perspective. However, integration of discipline-associated datasets is not a smooth process and is subject to varying concepts of quality and abundance.

Geographic Information Science (GIScience) explores the location property of entities such as objects, events and processes, associating them with co-ordinates, such as longitude and latitude (Goodchild, 2010; Stevens and Pfeiffer, 2015). This process may seem straightforward, given the increasing presence of location-based sensors and mapping technologies in our daily lives. However, it is still a challenge because of the nature and contexts of the facts examined. In museums and herbaria, artefacts and specimens have usually been collected over decades or centuries and their finding location is often ambiguous or very imprecise (van Erp et al., 2015). In Health Science, investigation of historical records of disease occurrence in individuals relies on the names of locations and vague addresses. The lack of historical address databases undermines the potential use of those health data (Lash et al., 2012). In Crop Science, breeding programs rely on the collections of seeds available to germplasm banks. Knowledge about the origin of these seeds is necessary to characterise the environment around their collection location, and to go beyond basic measurements of diversity. However, again, location information about their origin may be vague or associated with markets where the seeds were obtained instead of where they grew or were originally sourced from (Richards, 2011).

A MODEL FOR INTEGRATION OF MULTIPLE DISCIPLINE DATA

In the cases just mentioned, integration of data from other disciplines with GIScience is not straightforward. In fact, the integration often involves transformation and filtering operations using arbitrary criteria. Given two datasets from

PeerJ Preprints | https://doi.org/10.7287/peerj.preprints.2248v3 | CC BY 4.0 Open Access | rec: 26 Sep 2016, publ: 26 Sep 2016

different disciplines, these operations typically discard or reduce records or items, often greatly, resulting in a relative subset of the original dataset that can be used in both disciplines. In Figure 1, a Venn diagram shows this concept using three distinct disciplines. Given the initial amount of data in a discipline (D1), only a subset (D1 ∩ D2 or D1 ∩ D3) fits the criteria of both disciplines (D1 and D2 or D1 and D3). As the number of disciplines involved increases, so there is further diminution of the available data.

These criteria involve requirements common and unique to the disciplines involved. Examples include the following cases: exclusion of records with missing data (i.e. records must have longitude and latitude or postcode); temporal scales (e.g. growing season must match respective weather data to investigate potential plant stress); spatial scales (e.g. association of soil and disease resistance among individuals in a small to medium farm demands detailed soil maps); sample units (e.g. if the location is available at the population level, the genetic information for individuals must be grouped by the same definition of the population).

Another issue with integrating data from distinct disciplines concerns variation of concepts such as abundance and diversity. A dataset may fit criteria of relatively high abundance and diversity in discipline D1, but be classed as scarce and uniform in discipline D2. Figure 2A shows one seedling being planted in the glasshouse. Cultivating seeds from different populations would provide a better representation of the geographic space. However, it would be necessary to investigate the characteristics of interest around this location in order to guarantee a reasonable representation of environmental variables. Experiment design and sampling strategy are important, and should be discussed taking into account the characteristics of the data of the disciplines involved.

THE BAMBARA GROUNDNUT STUDY CASE

Bambara groundnut is classed as a neglected and underutilised species of legume, mainly cultivated in Sub-Saharan Africa. It is believed that the process of its domestication and further cultivation started thousands of years ago. However, despite its long history, this crop is still cultivated from landraces (locally developed mixtures of genotypes) (Molosiwa et al., 2015). The development of proper varieties of Bambara groundnut demands a better understanding of its genetic structure and diversity. Despite being a human-associated species cultivated in human-managed landscapes, we expected that the genetic resources of Bambara groundnut still have an influence of geographic and environmental factors. Initially, we mapped the results clustering analysis on the genetic data to explore potential spatial patterns of genetic variation. In the next step, we investigated the correlation between genetic, geographic and environmental by performing the Mantel test using three measures of distance among the samples. The next section includes a description of these analyses.

The proposed pipeline

We developed a pipeline to assimilate and analyse the genetic, geographic and environmental data using a mix open source tools such as Python, R and their respectively libraries and packages running in a Linux environment (see Figure 3). By adopting open source software in our project, we pursued a set of best practices in computational research (Wilson et al., 2014; Joppa et al., 2013). One practice, in particular, was critical since the start, the ability to automate all steps of the analysis. As new data would frequently arrive, we would like to rerun the analysis with minimum human interference, avoiding unintentional mistakes such as forgetting to follow particular steps of the analysis and being flexible to explore the computational resources available.

Both environments, Python and R, have seen an increasing amount of tools to deal with the integration of genetic and geographic data, mixing complete open source software and open source and proprietary software (Jombart and Ahmed, 2011; Gruber and Adamack, 2015; van Etten, 2012; Etherington, 2011; Brown, 2014; Dick et al., 2014). See Figure 3 for an explanation of the data flow in the proposed pipeline.

So far, we have conducted exploratory analyses using the datasets and process presented here. We identified some imprecision in the location data that did not affect the initial analyses (mostly PCA and k-means cluster analysis of the genetic data and mapping of the first and second axes); however, future investigations of distance matrices to include anthropocentric factors may require the exclusion of the most compromised samples. Although the environmental and genetic datasets were large, putting the two together led to a small dataset that was only just big enough to analyse.

CONCLUSIONS

If, as a scientific community, we are serious about interdisciplinarity then we need a lot more work in co-ordinating data-collection activities, to guarantee the data acquired are useful for all disciplines involved. We propose that existing research on interoperability, an established concept in GIScience, be extended to other areas of science, and particularly the co-ordination of data collection. It holds potential for helping to address the challenges presented in the integration of multidisciplinary data.

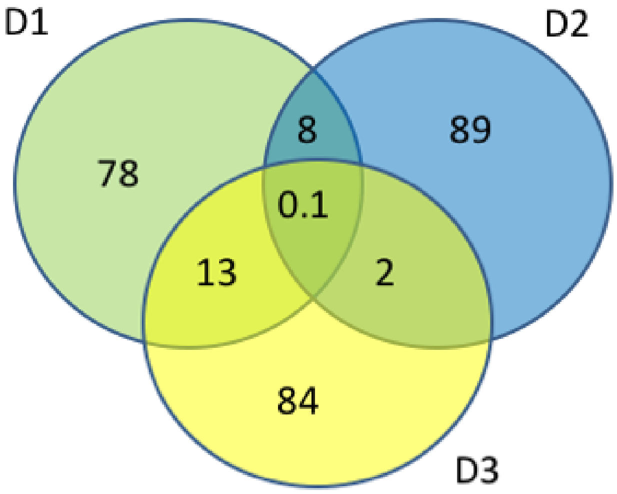


Figure 1. This figure shows a model for integration of data from distinct disciplines. Circles in the Venn diagram represent various disciplines (D1, D2 and D3) and their respective data criteria. Numbers represent a hypothetical amount (%) of the data that only fit the criteria of each discipline (D1 = 78, D2 = 89 and D3 = 84), or the combined criteria of two disciplines ($D1 \cap D2 = 8$, $D1 \cap D3 = 13$, $D2 \cap D3 = 2$), or the combined criteria of all disciplines ($D1 \cap D2 \cap 3 = 0.1$). Given two or more datasets from different disciplines, the combined criteria typically discard or reduce records or items, often greatly, resulting in a relatively small subset of the original datasets that can be used by the combined bodies of knowledge.

REFERENCES

Academies, N. (2004). *Facilitating Interdisciplinary Research*. National Academies Press, Washington, District of Columbia.

Brown, J. L. (2014). SDMtoolbox: a python-based GIS toolkit for landscape genetic, biogeographic and species distribution model analyses. *Methods in Ecology and Evolution*, 5(7):694–700.

Dick, D. M., Walbridge, S., Wright, D. J., Calambokidis, J., Falcone, E. A., Steel, D., Follett, T., Holmberg, J., and Baker, C. S. (2014). geneGIS : Geoanalytical Tools and Arc Marine Customization for Individual-Based Genetic Records. *Transactions in GIS*, 18(3):324–350.

Dyer, R. J. (2014). gstudio package.

Dyer, R. J. (2015). Is there such a thing as landscape genetics? *Molecular Ecology*, 24(14):3518–3528.

Etherington, T. R. (2011). Python based GIS tools for landscape genetics: visualising genetic relatedness and measuring landscape connectivity. *Methods in Ecology and Evolution*, 2(1):52–55.

Goodchild, M. F. (2010). Twenty years of progress: GIScience in 2010. *Journal of Spatial Information Science*, (1).

Gruber, B. and Adamack, A. T. (2015). landgenreport : a new r function to simplify landscape genetic analysis using resistance surface layers. *Molecular Ecology Resources*, 15(5):1172–1178.

Hijmans, R. J., Cameron, S. E., Parra, J. L., Jones, P. G., and Jarvis, A. (2005). Very high resolution interpolated climate surfaces for global land areas. *International Journal of Climatology*, 25(15):1965–1978.

Jombart, T. and Ahmed, I. (2011). adegenet 1.3-1: new tools for the analysis of genome-wide SNP data. *Bioinformatics*, 27(21):3070–3071.

Joppa, L. N., McInerny, G., Harper, R., Salido, L., Takeda, K., O'Hara, K., Gavaghan, D., and Emmott, S. (2013). Troubling Trends in Scientific Software Use. *Science*, 340(6134):814–815.

Lash, R., Carroll, D. S., Hughes, C. M., Nakazawa, Y., Karem, K., Damon, I. K., and Peterson, A. (2012). Effects of georeferencing effort on mapping monkeypox case distributions and transmission risk. *International Journal of Health Geographics*, 11(1):23.

Molosiwa, O., Aliyu, S., Stadler, F., Mayes, K., Massawe, F., Kilian, A., and Mayes, S. (2015). SSR marker development, genetic diversity and population structure analysis of Bambara groundnut [Vigna subterranea (L.) Verdc.] landraces. *Genetic Resources and Crop Evolution*, 62(8):1225–1243.

Nei, M. (1972). Genetic Distance between Populations. *The American Naturalist*, 106(949).

Richards, G. M. V. C. M. (2011). Integration of Georeferencing, Habitat, Sampling, and Genetic Data for Documentation of Wild Plant Genetic Resources. *HortScience*, 46(11):1446–1449.

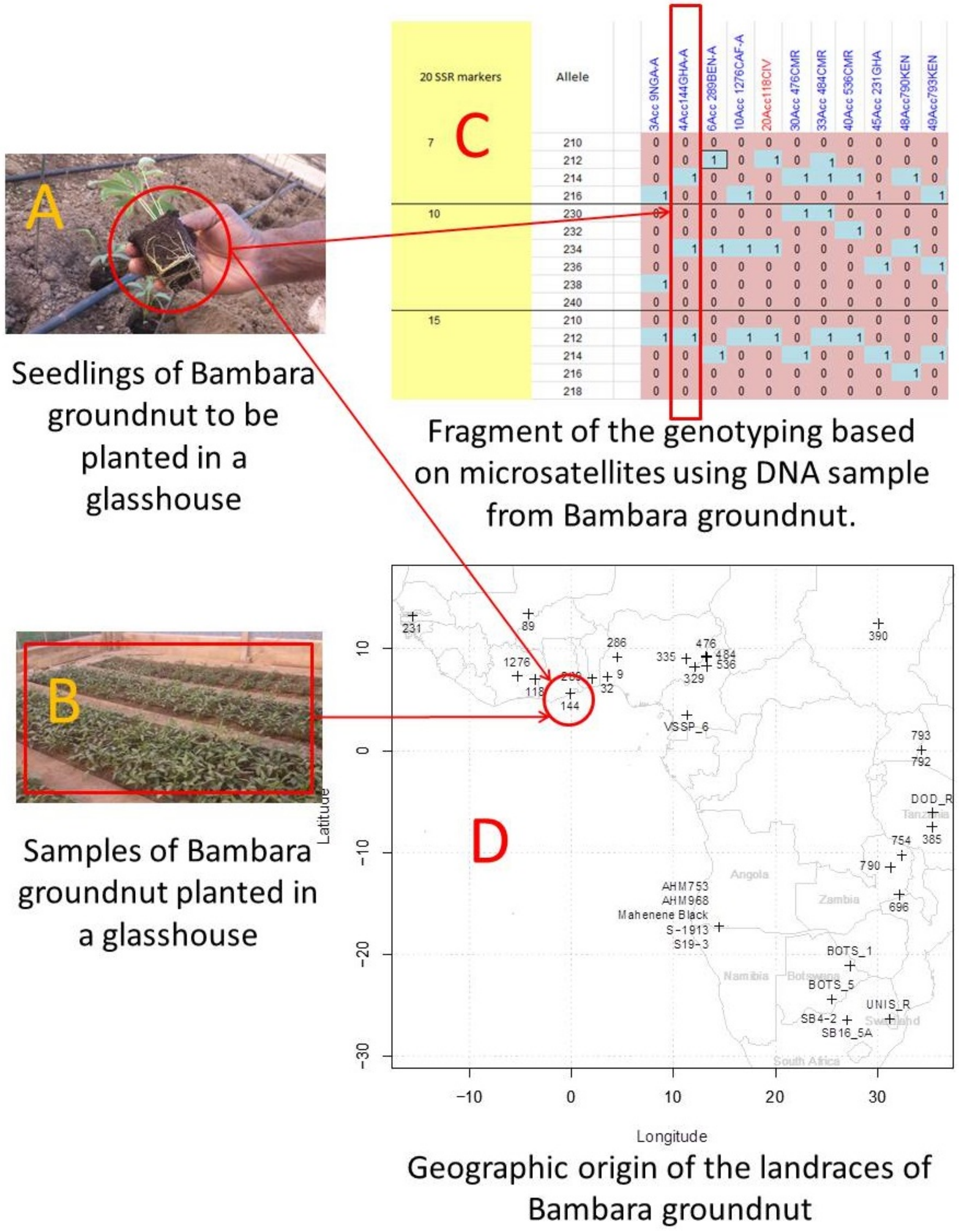
Stevens, K. B. and Pfeiffer, D. U. (2015). Sources of spatial animal and human health data: Casting the net wide to deal more effectively with increasingly complex disease problems. *Spatial and Spatio-temporal Epidemiology*, 13:15–29.

van Erp, M., Hensel, R., Ceolin, D., and van der Meij, M. (2015). Georeferencing Animal Specimen Datasets. *Transactions in GIS*, 19(4):563–581.

van Etten, J. (2012). gdiatnce: Distances and routes on geographical grids. R package version 1.1-4.

Wagner, J. O., Blanchet, F. G., Friendly, M., Kindt, R., Legendre, P., McGlinn, D., Minchin, P. R., O'Hara, R. B., Simpson, G. L., Solymos, P., Stevens, M. H. H., Szoecs, E., and Helene (2016). vegan: Community Ecology Package.

Wilson, G., Aruliah, D. A., Brown, C. T., Chue Hong, N. P., Davis, M., Guy, R. T., Haddock, S. H. D., Huff, K. D., Mitchell, I. M., Plumbley, M. D., Waugh, B., White, E. P., and Wilson, P. (2014). Best Practices for Scientific Computing. *PLoS Biology*, 12(1):e1001745.



Seedlings of Bambara groundnut to be planted in a glasshouse

20 SSR markers	Allele	3Acc 9NGA-A	4Acc144GHA-A	6Acc 289BEN-A	10Acc 1276CAF-A	20Acc118CIV	30Acc 476CMR	33Acc 484CMR	40Acc 536CMR	45Acc 231GHA	48Acc790KEN	49Acc793KEN
7	210	0	0	0	0	0	0	0	0	0	0	0
	212	0	0	1	0	1	0	1	0	0	0	0
	214	0	1	0	0	0	1	1	1	0	1	0
	216	1	0	0	1	0	0	0	0	1	0	1
10	230	0	0	0	0	0	1	1	0	0	0	0
	232	0	0	0	0	0	0	0	1	0	0	0
	234	0	1	1	1	1	0	0	0	0	1	0
	236	0	0	0	0	0	0	0	0	1	0	1
	238	1	0	0	0	0	0	0	0	0	0	0
	240	0	0	0	0	0	0	0	0	0	0	0
15	210	0	0	0	0	0	0	0	0	0	0	0
	212	1	1	0	1	1	0	1	1	0	0	0
	214	0	0	1	0	0	1	0	0	1	0	1
	216	0	0	0	0	0	0	0	0	0	1	0
	218	0	0	0	0	0	0	0	0	0	0	0

Fragment of the genotyping based on microsatellites using DNA sample from Bambara groundnut.

Samples of Bambara groundnut planted in a glasshouse

Geographic origin of the landraces of Bambara groundnut

Figure 2. Integration of geographic and genetic datasets of Bambara groundnut. (A) shows a seedling to be planted in the glasshouse. (B) shows a trial of Bambara groundnut planted in the glasshouse. (C) genotyping results with highlighted data of a specific sample. (D) geographic localisation of the landraces (populations) of Bambara groundnut used in this study. In the context of Crop Science, this individual has the potential to generate a significant amount of genetic data through genotyping or sequencing processes (see figure 2C), and the resulting dataset could be considered abundant. However, genetic information among individuals of the same species can be very similar and in order to get data that represents the differences it is important to choose highly polymorphic molecular markers in the genotyping process. In the context of GIScience, this individual seedling, whose origin information is available at the population level, has only one associated location, and would be considered scarce if the objective were to analyse the genetic data over a broad geographic area. Even if more seedlings from the same population were cultivated (see figure 2B), the number of population locations is still one, and all the genetic data generated from these samples are still associated with one point in space (see figure 2D).

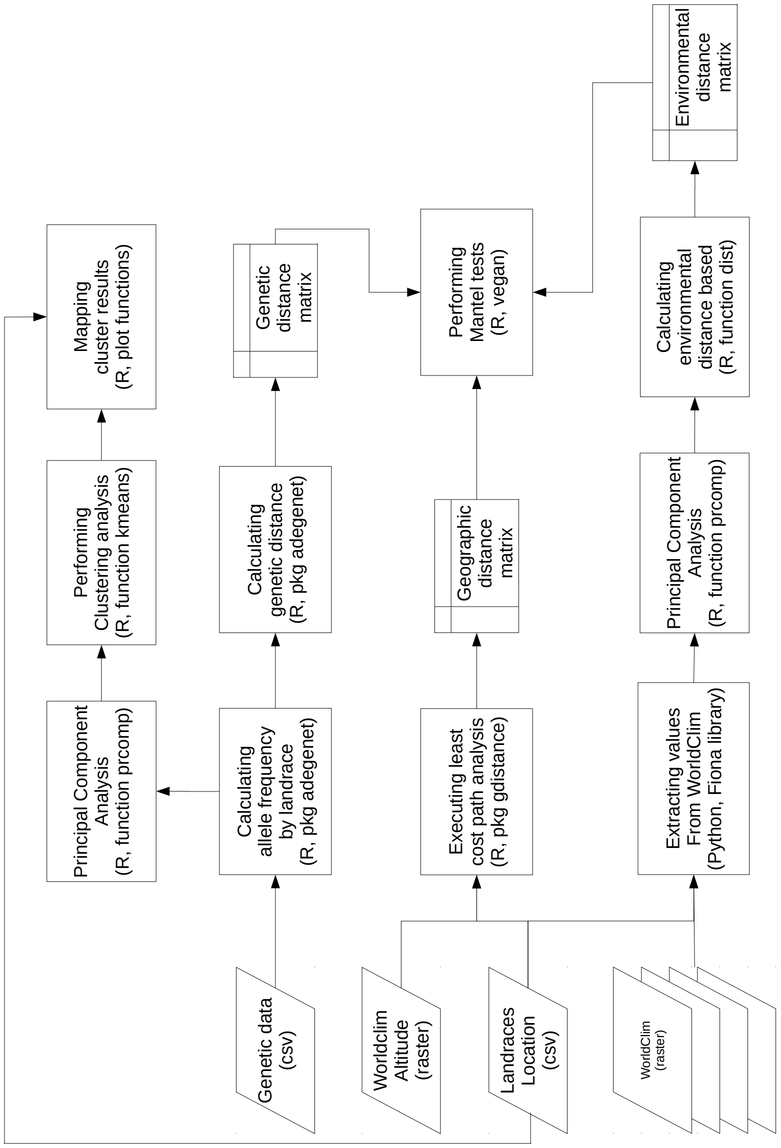


Figure 3. We used genetic and geographic datasets to explore spatial patterns of genetic variation. We included environmental datasets to examine distinct measures of distance (geographic, genetic and environmental) of Bambara groundnut landraces. The genetic dataset was composed of the genotyping information about the presence or absence of twenty Single Sequence Repeat (SSR) molecular markers of 33 distinct landraces of Bambara groundnut, with a total of 128 samples. Using the package adegenet (Jombart and Ahmed, 2011), we calculated the allele frequency for each group of landraces and based on the allele frequency we produced a matrix of genetic distance among each pair of landraces using Nei's genetic distance method (Nei, 1972). The geographic information about the origin of these seeds was provided by the International Institute of Tropical Agriculture (IITA) at landrace level. Using the package gdistance (van Etten, 2012), we performed a least cost path analysis based on the altitude data of WorldClim (Hijmans et al., 2005). Therefore, we produced a matrix of cost among each group of landraces. We also used the location of the landraces to characterise temperature, rainfall and altitude using the WorldClim layers BIO 5, 6, 13 and 14. The correlation among the matrices of distance (genetic, geographic and environmental) were assessed performing the Mantel test (Wagner et al., 2016). Although the environmental and genetic dataset were large, putting the two together led to a small dataset that was only just big enough to analyse.

PeerJ Preprints | https://doi.org/10.7287/peerj.preprints.2248v3 | CC BY 4.0 Open Access | rec: 26 Sep 2016, publ: 26 Sep 2016