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THREE FACTORS OF "PLANTNESS" — TRAIT SUMMARY SCORES GENERATED FROM A BIFACTOR MODEL WITH COMPLEX STRUCTURE

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ABSTRACT

This paper explores whether a data reduction technique used almost exclusively in psychometrics — i.e., bifactor latent trait modeling — provides any added value beyond unsupervised machine learning techniques already common in plant science. Using data from the TRY database and other public repositories, for 52,104 species I compiled 42 wide-ranging plant traits (e.g., growth form, plant height, leaf size, leaf dry mass, leaf phosphorus, vessel and fiber length, seed size, medicinal use, geographic distribution, protected species status, etc.) and conducted Exploratory Factor Analysis **(**EFA) with iterated target rotation to explore how the traits "cluster." Three factors were identified in the EFA, later modeled in a Quasi-Confirmatory Factor Analysis (CFA) using a bifactor configuration specifying three specific factors. The three factors could reasonably be called Leaf Size (defined most strongly by leaf dry and fresh mass), Vessel/Fiber Length, and SLA/Water Content (defined most strongly by specific leaf area, leaf water content, and the inverse of leaf dry matter content). The statistical model used to describe these three factors —i.e., the "bifactor" model— is named as such because each trait belongs to not only its specific factor (e.g., the trait "leaf fresh mass" belongs to the Leaf Size factor) but also to an overall "General" factor to which all traits belong. That is, in addition to the three factors from the article's title, there is a "fourth factor" (the General Factor of Plantness, or simply General Plantness) comprising all traits. The meaning of General Plantness (indicated most strongly by water content, plant height, and possibly tree/shrub form) is unclear without genetic research, and it is not one of the three factors of plantness. Rather, General Plantness would better be conceptualized as a "meta-factor" transcending the three factors of plantness from the title. I speculate that the General Factor of Plantness is a latent measure of genome age, or how long ago a species evolved to its current form.

The three factors of plantness (Leaf Size, Vessel/Fiber Length, and SLA/Water Content), along with the General Factor of Plantness, are plotted with examples and discussed. Examples included common (e.g. willow tree, fleabane), cultivated (e.g. corn, watermelon), unusual (e.g. venus fly trap, ginkgo), and scientifically well-known (e.g. thale cress, *Amborella*) species. Importantly, the examples were chosen independently of the traits or trait scores (to avoid choosing an example **because** it had a specific score). Of the examples, *Ephedra distachya* had the highest score on Vessel/Fiber Length, *Ginkgo biloba* had the highest score on SLA/Water Content, and *Zea mays* (corn) had the highest score on Leaf Size. The species *Amborella trichopoda*, *Cycas revoluta*, and *Ginkgo biloba* had the highest scores on General Plantness. The lowest scores on General Plantness were found in *Arabidopsis thaliana*, *Dionaea muscipula*, and *Papaver rhoeas*. Genome age is a common factor among the three species highest on plantness, suggesting that the General Factor of Plantness deserves further investigation. Critically, scores are provided (link below) for N = 52,104 species, many of which have scores more extreme than the few examples reported above. Further research using genetic data is strongly encouraged.

When measuring plant traits (e.g. leaf length, root depth, etc.), whether with a ruler or mass spectrometer or simple scale, it is common to take many related measurements. Especially in large-scale studies (Fiorani & Schurr 2013; Pieruschka & Schurr 2019; Zhang et al. 2019), many measurements of many traits are recorded. The result is often a data matrix where each row is a species and each column is a measurement (trait), such as leaf length or root depth. While this data matrix may be sufficient to answer the researcher's question, it contains much more information that is often discarded: meaningful patterns in the bivariate (1-on-1) relationships among the measurements. A whole branch of statistical methodology, unsupervised machine learning, is dedicated to uncovering such patterns, including in data characterizing plants and plant species.

Here, I explore whether a data reduction technique used almost exclusively in psychometrics — i.e., bifactor latent trait modeling — provides any added value to techniques already common in plant science (Chitwood & Topp 2015; Elavarasan et al. 2018; Feldmann et al. 2020; Furbank et al. 2019; Mendes et al. 2019; Saryan et al. 2020; Zhao et al. 2018; also see Butler et al. 2017). The idea behind data reduction techniques (elaborated below) is to start with a set of trait measurements (e.g., physical and chemical features) and determine which measurements are of traits that correlate with each other relative strongly, with the purpose of grouping them (not the species) into categories. For example, four traits might be root length, root thickness, phosphorus per mass of stem, and phosphorus per mass of leaf. Using the 4x4 matrix of bivariate relationships (often a correlation matrix with 1s on the diagonal and strengths of relationships ranging from -1 to 1 off the diagonal), most data reduction algorithms will "detect" that the first two traits (having to do with root size) are measurements of things that tend to correlate with each other more than with the things measured in the other two variables. Likewise for the latter two traits (having to do with phosphorus concentration) — the algorithm will detect that they are measurements of things that tend to correlate with each other more than with the two root-related variables. The result will be that the four variables have been "reduced" to two variables, one related to root size and another related to phosphorus concentration. Going from four to two variables is not very interesting or useful, but going from dozens or hundreds of variables to a much smaller number might provide interesting insights or at least serve a practical purpose for future researchers (see below). The technique used here is called "factor analysis."

Factor analysis is a type of data reduction technique ("unsupervised machine learning technique" is equivalent) that groups variables (plant traits in this case) into clusters according to some goal[1]. It is usually motivated by one of two goals.

1) Data reduction. Reducing the number of total variables used in analysis by creating (called "deriving") a smaller number of variables that combine information from the many variables. For example, if trying to use house characteristics to predict future selling price, one might have the following nine variables: square footage, number of bedrooms, number of bathrooms, cost of refrigerator, cost of oven, cost of microwave, neighborhood mean rents (1BR), school district quality score, and mean credit rating of neighborhood residents. Before running any analyses, in this very simple case, one could intuitively group the above variables into three categories—house size, appliance quality, and location desirability. This reduction in the number of variables is advantageous for reasons beyond the present scope, but also for the simple reason that it is more parsimonious. Importantly, in the above case, it is easy to intuit how the variables should group, but in many applied cases involving dozens or hundreds of variables, it is not possible for a human to reasonably group the variables into clusters. This is the purpose of factor analysis: using the data alone, the algorithm groups variables optimally without any input from the researcher except how many factors to extract (in the above example, three).
2) Theory testing. Testing or developing a theory based on some a priori expectations. For example, in psychometrics, one might have a hypothesis about how mental abilities tend to correlate — e.g., that tests of reading comprehension will tend to correlate more strongly with other verbal tasks than with quantitative tasks. This could be tested using factor analysis, because, if the theory generating the hypothesis is true, then a group of tests factor analyzed should cluster according to verbal-versus-quantitative rather than some other classification scheme (e.g. self-paced versus not, multiple-choice

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[1] In factor analysis specifically, the algorithm usually seeks a solution that has "simple structure", which is a set of rules defined by Thurstone (1947) listing out the characteristics of a matrix of numbers that is most likely to be interpretable by humans. That is, the "optimum criterion" is a solution that is most interpretable to humans, where interpretable is defined by a set of logical rules that can be interpreted by a computer (e.g., must be a specific number of zeros in each row). This ability to tell a computer what is interpretable (called "factor rotation") was one of the most important developments in psychometrics.

versus free response, etc.). An example, again from psychometrics, is the idea that psychiatric disorders and symptoms can be explained by a specific theory (Lahey et al. 2017) that can draw evidence (Lahey et al. 2012) from factor analysis.

Study Purpose

The current study is motivated mostly by #1 above, data reduction, insofar as I wish to generate a small set of phenotype scores for plant researchers, but #2 (theory generation or testing) is also relevant insofar as a secondary question of the study is whether the General Factor of Plantness has any meaning. The term "General Plantness" is admittedly opaque—after all, how could one species of plant have more "plantness" than another species of plant? Until further studies are done to investigate the phenomenon, I simply have no better name. Whatever it is, General Plantness is a dimension that runs through all plants, a latent meta-trait influencing all traits in all three factors mentioned in the title of this article. To be more concrete, I speculate that the General Factor of Plantness is a combination of genes that evolved early in plant evolution and therefore tend to have more relative influence in "old" plants—i.e. plants that evolved to their present form early. I present for testing the idea that there is a group of genes that collectively determine (including gene-gene interactions) the traits that are strongly associated with the General Factor of Plantness, and these genes will be evolutionarily old. This claim could easily be tested in a genome-wide association study (GWAS) using the General Plantness score, though I would like to emphasize the importance of gene-gene interactions in this case. I therefore recommend that geneticists identify *a priori* the genes known to be "old" and include interactions among them in the GWAS; this, as opposed to approaching it from the other way, starting with the plants that we already know are old in form. Regardless, this is a theoretical question that will be answered only by genetic data, and once further research into the General Factor of Plantness is completed, perhaps it will be renamed to better reflect what it is actually capturing. However speculative, a strength of the above claim is the falsifiability: the only feasible explanation for a General Factor of Plantness to exist is that the various sizes of loadings on the general factor are caused by a specific constellation of genes and their interactions; otherwise, General Plantness does not exist. For this reason, in addition to the bifactor scores I provide, I also provide the analogous scores using the exact same method minus the bifactor component (no general factor). Even if it does turn out that the bifactor scores are suboptimal, the correlated-traits scores will still be usable. Scores are available at <https://www.mooremetrics.com/3fp/>.

METHODS

Data and sources

Data were obtained from the TRY database (32 traits from the main database; Kattge et al. 2011, 2020), growth form data from the GIFT database (Weigelt, König, & Kreft 2020), protected status data from the IUCN "Red List" (Species Survival Commission 2001-2020), "climber" status data from the Jena experiment (Roscher et al. 2018), and medicinal use data collected firsthand from multiple public sources (European Medicines Agency 2020; Wikipedia.org 2020; World Health Organization 2007). The data set used here includes a total of 52,104 species and 42 traits (listed in Table 1). Factor scores available at <https://mooremetrics.com/3fp/>.

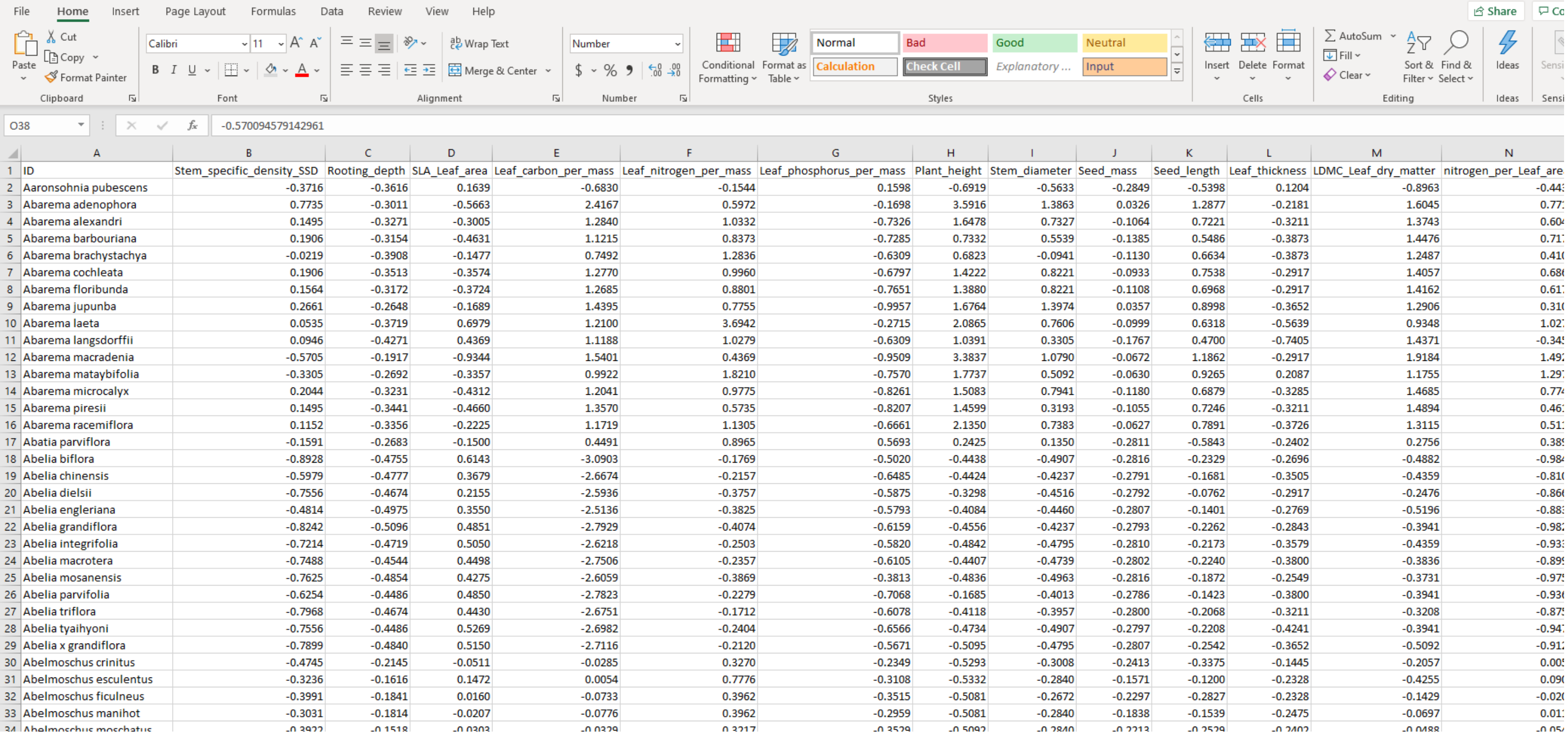
TRY database. The relevant trait data in the TRY database can be represented by a two-dimensional matrix: the species × trait matrix, with species in rows and traits in columns. It is large but sparse: high numbers of species and traits in TRY make the two matrices large, but many cells in the matrices are empty. For this reason, I used "gap-filled" data provided by TRY (Kattge, personal communication, 22 July 2020), which was estimated by Bayesian hierarchical probabilistic matrix factorization (BHPMF) (Fazayeli et al. 2014; Schrodt 2015; Shan et al. 2012). In the TRY database, traits are grouped into eight main clusters: biodiversity, climate change, plant traits, functional diversity, carbon cycle, community, vegetation, and environmental filtering. Note that this cluster specification is unique to the TRY database and is not used here.

GIFT database (growth form data). GIFT integrates plant distributions, functional traits, phylogenetic information, and region-level geographic, environmental, and socio-economic data. It currently holds species lists for 2,893 regions across the globe, including about 315,000 taxonomically standardized species names and about 3 million species-by-region occurrences. In addition, GIFT contains information about the floristic status (native, endemic, alien, and naturalized) and takes advantage of the wealth of trait information in the regional Floras, complemented by data from global trait databases. Based on a hierarchical and taxonomical derivation scheme, GIFT holds information for 83 functional traits and more than 2.3 million trait-by-species combinations, and it achieves unprecedented coverage in categorical traits such as woodiness (~233,000 spp.) and growth form (~213,000 spp.).

IUCN "Red List" (protected status data). This classifies species at high risk of global extinction, each species categorized as follows: Not Evaluated, Data Deficient, Least Concern, Near Threatened, Vulnerable, Endangered, Critically Endangered, Extinct in the Wild, and Extinct. More than 120,000 species have been assessed (as of August 2020).

Jena experiment ("climber" status data). The Jena data was obtained through the TRY database with permission from the authors (Roscher et al. 2018). Many of the Jena traits overlapped with those from other databases, but one that did not (or at least with only a very few) was whether the plant was a “climber.” Briefly, the “Jena experiment” was designed on a trait-based a priori definition of functional groups (grasses, legumes, small herbs, tall herbs), based on means, extent of variation (coefficient of variation across communities), and other metrics for nine functional traits (only one of which is used here, climber vs. non-climber).

Medicinal use data from public sources. This sample underestimates the number of plants with medicinal use, and this underestimation could be substantial. For example, even if it is likely that multiple species within a genus were used medicinally, the only species marked medicinal will be those that happen to be documented. Nonetheless, I opted to include this variable here, and specific sources are listed above. For example, Wikipedia.org (2020) lists *Achillea millefolium* (common yarrow) as a diaphoretic and stimulant (https://en.wikipedia.org/wiki/List_of_plants_used_in_herbalism); the European Medicines Agency (2020) lists *Echinacea angustifolia* (narrow-leaved coneflower) as an herb used to alleviate cough/cold symptoms (https://www.ema.europa.eu/sites/default/files/Medicines_output_herbal_medicines. xlsx), etc. If a plant was not listed on any “list” like the ones above, it was classified as “non-medicinal,” which causes the unavoidable underestimation mentioned above.



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	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	ID	Stem_specific_density_SSD	Rooting_depth	SLA_Leaf_area	Leaf_carbon_per_mass	Leaf_nitrogen_per_mass	Leaf_phosphorus_per_mass	Plant_height	Stem_diameter	Seed_mass	Seed_length	Leaf_thickness	LDMC_Leaf_dry_matter	nitrogen_per_Leaf_are
2	Aaronsohnia pubescens	-0.3716	-0.3616	0.1639	-0.6830	-0.1544	0.1598	-0.6919	-0.5633	-0.2849	-0.5398	0.1204	-0.8963	-0.44
3	Abarema adenophora	0.7735	-0.3011	-0.5663	2.4167	0.5972	-0.1698	3.5916	1.3863	0.0326	1.2877	-0.2181	1.6045	0.77
4	Abarema alexandri	0.1495	-0.3271	-0.3005	1.2840	1.0332	-0.7326	1.6478	0.7327	-0.1064	0.7221	-0.3211	1.3743	0.60
5	Abarema barbouriana	0.1906	-0.3154	-0.4631	1.1215	0.8373	-0.7285	0.7332	0.5539	-0.1385	0.5486	-0.3873	1.4476	0.71
6	Abarema brachystachya	-0.0219	-0.3908	-0.1477	0.7492	1.2836	-0.6309	0.6823	-0.0941	-0.1130	0.6634	-0.3873	1.2487	0.41
7	Abarema cochleata	0.1906	-0.3513	-0.3574	1.2770	0.9960	-0.6797	1.4222	0.8221	-0.0933	0.7538	-0.2917	1.4057	0.68
8	Abarema floribunda	0.1564	-0.3172	-0.3724	1.2685	0.8801	-0.7651	1.3880	0.8221	-0.1108	0.6968	-0.2917	1.4162	0.61
9	Abarema jupunba	0.2661	-0.2648	-0.1689	1.4395	0.7755	-0.9957	1.6764	1.3974	0.0357	0.8998	-0.3652	1.2906	0.31
10	Abarema laeta	0.0535	-0.3719	0.6979	1.2100	3.6942	-0.2715	2.0865	0.7606	-0.0999	0.6318	-0.5639	0.9348	1.02
11	Abarema langsdorffii	0.0946	-0.4271	0.4369	1.1188	1.0279	-0.6309	1.0391	0.3305	-0.1767	0.4700	-0.7405	1.4371	-0.34
12	Abarema macradenia	-0.5705	-0.1917	-0.9344	1.5401	0.4369	-0.9509	3.3837	1.0790	-0.0672	1.1862	-0.2917	1.9184	1.49
13	Abarema mataybifolia	-0.3305	-0.2692	-0.3357	0.9922	1.8210	-0.7570	1.7737	0.5092	-0.0630	0.9265	0.2087	1.1755	1.29
14	Abarema microcalyx	0.2044	-0.3231	-0.4312	1.2041	0.9775	-0.8261	1.5083	0.7941	-0.1180	0.6879	-0.3285	1.4685	0.77
15	Abarema piresii	0.1495	-0.3441	-0.4660	1.3570	0.5735	-0.8207	1.4599	0.3193	-0.1055	0.7246	-0.3211	1.4894	0.46
16	Abarema racemiflora	0.1152	-0.3356	-0.2225	1.1719	1.1305	-0.6661	2.1350	0.7383	-0.0627	0.7891	-0.3726	1.3115	0.51
17	Abatia parviflora	-0.1591	-0.2683	-0.1500	0.4491	0.8965	0.5693	0.2425	0.1350	-0.2811	-0.5843	-0.2402	0.2756	0.38
18	Abelia biflora	-0.8928	-0.4755	0.6143	-3.0903	-0.1769	-0.5020	-0.4438	-0.4907	-0.2816	-0.2329	-0.2696	-0.4882	-0.98
19	Abelia chinensis	-0.5979	-0.4777	0.3679	-2.6674	-0.2157	-0.6485	-0.4424	-0.4237	-0.2791	-0.1681	-0.3505	-0.4359	-0.81
20	Abelia dielsii	-0.7556	-0.4674	0.2155	-2.5936	-0.3757	-0.5875	-0.3298	-0.4516	-0.2792	-0.0762	-0.2917	-0.2476	-0.86
21	Abelia engleriana	-0.4814	-0.4975	0.3550	-2.5136	-0.3825	-0.5793	-0.4084	-0.4460	-0.2807	-0.1401	-0.2769	-0.5196	-0.88
22	Abelia grandiflora	-0.8242	-0.5096	0.4851	-2.7929	-0.4074	-0.6159	-0.4556	-0.4237	-0.2793	-0.2262	-0.2843	-0.3941	-0.98
23	Abelia integrifolia	-0.7214	-0.4719	0.5050	-2.6218	-0.2503	-0.5820	-0.4842	-0.4795	-0.2810	-0.2173	-0.3579	-0.4359	-0.93
24	Abelia macrotera	-0.7488	-0.4544	0.4498	-2.7506	-0.2357	-0.6105	-0.4407	-0.4739	-0.2802	-0.2240	-0.3800	-0.3836	-0.89
25	Abelia mosanensis	-0.7625	-0.4854	0.4275	-2.6059	-0.3869	-0.3813	-0.4836	-0.4963	-0.2816	-0.1872	-0.2549	-0.3731	-0.97
26	Abelia parvifolia	-0.6254	-0.4486	0.4850	-2.7823	-0.2279	-0.7068	-0.1685	-0.4013	-0.2786	-0.1423	-0.3800	-0.3941	-0.93
27	Abelia triflora	-0.7968	-0.4674	0.4430	-2.6751	-0.1712	-0.6078	-0.4118	-0.3957	-0.2800	-0.2068	-0.3211	-0.3208	-0.87
28	Abelia tyaihyoni	-0.7556	-0.4486	0.5269	-2.6982	-0.2404	-0.6566	-0.4734	-0.4907	-0.2797	-0.2208	-0.4241	-0.3941	-0.94
29	Abelia x grandiflora	-0.7899	-0.4840	0.5150	-2.7116	-0.2120	-0.5671	-0.5095	-0.4795	-0.2807	-0.2542	-0.3652	-0.5092	-0.91
30	Abelmoschus crinitus	-0.4745	-0.2145	-0.0511	-0.0285	0.3270	-0.2349	-0.5293	-0.3008	-0.2413	-0.3375	-0.1445	-0.2057	0.00
31	Abelmoschus esculentus	-0.3236	-0.1616	0.1472	0.0054	0.7776	-0.3108	-0.5332	-0.2840	-0.1571	-0.1200	-0.2328	-0.4255	0.09
32	Abelmoschus ficulneus	-0.3991	-0.1841	0.0160	-0.0733	0.3962	-0.3515	-0.5081	-0.2672	-0.2297	-0.2827	-0.2328	-0.1429	-0.02
33	Abelmoschus manihot	-0.3031	-0.1814	-0.0207	-0.0776	0.3962	-0.2959	-0.5081	-0.2840	-0.1838	-0.1539	-0.2475	-0.0697	0.01
34	Abelmoschus moschatus	-0.3922	-0.1518	-0.0303	-0.0329	0.3217	-0.3529	-0.5092	-0.2840	-0.2213	-0.2529	-0.2402	-0.0488	-0.05

Figure 1. Example of data used in this analysis, in Microsoft Excel (screenshot). Measures have been z-transformed, so units are standard deviations (not native units, such as millimeters).

Statistical Analysis

General Approach. All the data sets listed above have a column in common — i.e., species name ("Genus species") — which allowed the data sets to be linked into a single matrix. Figure 1 shows a screenshot of a portion of the data open in Microsoft Excel, where each row is a species and each column is a trait (e.g. seed length). Many unsupervised machine learning algorithms (not used here) attempt to group the rows — e.g., since each row is a species, perhaps the algorithm will try to group species into genera. By contrast, the goal in the present paper was to group the columns (traits). The purpose of grouping columns is discussed below, but the idea is that the columns relate to each other (e.g. seed mass correlates with plant height). Another benefit of clustering columns is that each species then receives a score for each cluster; for example, if traits 1, 2, and 3 cluster to form Variable Cluster 1, each plant will receive a score for Variable Cluster 1 that is on the same scale as all other species' scores (and therefore comparable to them). These scores can then be used in subsequent analyses, whether genetic or otherwise (e.g., using trait scores to predict crop viability).

Missing data imputation. When the data matrices described above were merged by species, this introduced gaps into the data, because some species will have data for only some of the data types. For example, *Aaronsohnia pubescens* has complete data from the main TRY database but is missing data on growth form. To fill these gaps, I first excluded any species missing from the main TRY database ("TRY database" above), which left N=52,104 species. Of these, most (87%) had at least one missing value from the remaining data sets (growth form from the GIFT database, etc.). Missing data were imputed using the random forest algorithm (Svetnik et al. 2003) in the *missForest* package (Stekhoven 2013).

Bivariate (1-on-1) relationships. I first estimated the correlations among traits, and because the traits are a mix of continuous and categorical (yes/no) variables, the result is a mixed correlation matrix. That is, correlations between continuous variables are standard Pearson correlations, correlations between categorical variables are tetrachoric, and correlations between continuous and categorical variables are biserial[2]. All three correlation types (Pearson, tetrachoric, and biserial) are on the same scale and span the full theoretical range from -1 to 1 (unlike point-biserial correlations, for example).

Exploratory Factor Analysis (EFA). The above correlation matrix was used as input for exploratory factor analysis (Gorsuch 1983; Kim & Mueller 1978a, 1978b), where the term "factor" is equivalent to the term "Variable Cluster" used above in the "General Approach" subsection. The number of factors was determined by subjective examination of the scree plot, which clearly suggested three factors. For thoroughness I also estimated the appropriate number of factors using many conventional methods: Cattell-Nelson-Gorsuch (Gorsuch & Nelson 1981), multiple regression (Zoski & Jurs 1993), optimal coordinate (Raiche et al. 2013), acceleration factor (Raiche et al. 2013), Bartlett index (Bartlett 1950), Bentler-Yuan index (Bentler & Yuan 1998), and the minimum Bayesian Information Criterion (Schwarz 1978). These methods suggest 3, 4, 7, 7, >20, >20, and >20 factors, respectively. Nonetheless, the scree plot is clear in suggesting three factors, so in the interest of parsimony, I opted for that as the final number.

With the number of factors decided, it's necessary to choose a rotation. Because I did not necessarily expect simple structure (Thurstone 1947) — i.e., I did not believe *a priori* that each phenotype would load on one and only one factor — iterated target rotation (ITR) was employed (Moore 2013; Moore et al. 2015), which is more likely to detect complex structure (cross-loadings) than are traditional simple structure rotations such as oblimin or promax. Specifics of ITR are beyond the present scope, but the idea is to start with a conventional simple structure rotation (here, promax)

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[2] Note that these are biserial, not point-biserial. See Kemery, Dunlap, & Griffeth (1988) for details.

and use that rotated solution (pattern matrix) to construct a partially-specified[3] target matrix for use in a subsequent target rotation. This subsequent target-rotated solution is then used in the same way as the analytic rotation was first used, to build another target matrix. This third target-rotated solution is used to build another target, and so on, until a constructed target matches one that was previously used in the sequence, indicating algorithm convergence. Note that target matrices created in the above sequence are not limited to one estimated element per row — a configuration that would correspond with simple structure — but rather are specified to allow whatever level of complexity is suggested by the previous solution in the target-iteration sequence. Indeed, if a solution includes a row with salient (> 0.20) loadings on all factors, the resulting target would be completely unspecified for that row (allowing free estimation of all elements in that row). The opposite — all row elements specified as zero — is also possible.

Quasi-Confirmatory[4] Factor Analysis (CFA). The final ITR solution was used to construct and estimate a Bayesian CFA. The first step of the CFA was to decide how to model the multidimensionality. In any multidimensional factor model, the multiple factors will undoubtedly correlate with each other, and there are three ways to model this phenomenon (see Reise, Moore, & Haviland 2010, Figure 1).

1) Simply allow the factors to correlate. This is called a “correlated traits” model, and there is no “overall” factor in common among all traits. If I had several measurements of airplanes and factor analyzed them, I might find that there was a factor clearly related to wing size (wing length, wing width, wing deadweight, etc.) and another factor related to capacity (number of seats, number of cargo holds, fuselage diameter, etc.), among others. In this scenario, a correlated-traits model makes sense because airplane capacity and wing size are correlated out of physical necessity. More load requires more aerodynamic surface area and possibly more engines, which are usually held by the wings. So, they correlate; end of story.
2) Suppose the inter-factor correlation is caused by a higher-level phenomenon influencing both factors; this is called a “higher-order” (or “second-order”) model. If I factor analyzed several measurements of adult athletes, I might find a factor related to basketball ability (total points per game, number of rebounds, etc.) and another related to food (weekly sugar intake, weekly niacin intake, etc.), among others. Here, there is a clear reason these two factors would correlate: total body mass. An athlete’s size influences both his/her ability at basketball and his/her nutritional intake, making “size” the higher-order factor in this case.
3) Suppose the inter-factor correlation is caused by a higher-level phenomenon directly influencing all traits, which are themselves also influenced by factors unique to them. This is called a “bifactor” model (Reise 2012; Holzinger & Swineford 1937) because all variables are influenced by two phenomena simultaneously: a “general” factor causing all inter-variable correlations, and a “specific” factor causing inter-variable correlations only among variables that cluster together. If I had question responses (correct/incorrect) to a test of human cognitive abilities, I might find a factor related to memory (episodic memory, list memorization, etc.) and one related to complex reasoning (progressive matrices, verbal analogies, etc.), among others. All of these tests would correlate because of the well-documented “g” factor of human intelligence, affecting all test responses of any kind. Thus, it makes sense to have a general factor directly influencing all tests (episodic memory, progressive matrices, etc.) rather than having a higher-order factor that influences the latent phenomena of memory and complex reasoning. In addition to the general factor, however, there will undoubtedly be some unique influence of the specific abilities of

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[3] Partially-specified targets include only two types of elements: either “0”, indicating that the rotation should “try” to get that element as close to 0 as possible, or “?” (unspecified), indicating that the rotation should freely estimate that element.

[4] “Quasi-” because there is no real, cross-validated confirmation here.

memory and complex reasoning causing the tests to correlate slightly more strongly with tests in the same cluster (memory or complex) than with all tests in general. Specific factors are therefore needed to account for said unique influence. Importantly, when the general factor is modeled as in the bifactor, there is no need to allow the specific factors to correlate. The bifactor model is therefore orthogonal.

Here, I model plant traits as a bifactor model (#3 above) for two main reasons. First, if there is a “general” factor influencing all plant phenotypes, I want to know the extent to which that general factor influences some specific traits more than others. In a higher-order model (#2 above), there would be no direct relationships between the general factor and the traits. All relationships have to be “routed” through the lower-level factors, meaning that if two traits belong to the same sub-factor (e.g., leaf size) there is no way to determine whether one traits (e.g. leaf dry mass) relates more strongly to the general factor than does another (e.g. leaf width) except to multiply their loadings by each other, in which case there is a built-in constraint whereby both traits’ loadings must be multiplied by the same higher-order loading. The bifactor model does not have this constraint, called a “proportionality constraint.” The second reason I use a bifactor model is that I wish to produce phenotype factor scores for public use, and one of the most convenient features of bifactor scores is that they are orthogonal (independent), allowing them to be used simultaneously as predictors in a statistical model without having to worry about collinearity. Note that a bifactor model is the only way[5] to sensibly model correlated phenomena as though they were independent. The above bifactor model was used to generate orthogonal phenotype scores for public use.

RESULTS

Table 1 shows the unidimensional, 2- and 3-factor exploratory solutions, plus the Bayesian-estimated quasi-CFA. The unidimensional model is determined most strongly by terrestrial status, plant height, and leaf dry mass. The forb and herb growth form variables also have moderate negative loadings on the unidimensional model, suggesting this model essentially captures “tree-ness” or a contrast factor between “treeness” and “herbness.” The two-factor model in Table 1 shows us what happens when the traits are allowed to dissociate into two groups: they separate into one factor dominated by leaf size, and a second factor dominated by leaf dry matter content, probability of being in the Australasian realm, and (inversely) specific leaf area. The three-factor model comprises two factors virtually identical to the two factors above, with a third factor dominated by wood fiber and vessel lengths. Finally, the three rightmost columns in Table 1 (highlighted yellow) show the Bayesian model from which scores were generated. The results are similar enough to the three-factor exploratory model to not warrant further description, but note again that the correlated-traits scores corresponding to the “Bayes 3-Factor” model in Table 1 are included in the score release and can be assumed just as valid as the bifactor scores.

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[5] It is easy to overlook the difficulty of this problem — i.e. trying to produce orthogonal scores from phenomena that are correlated. Using an orthogonal rotation (e.g. varimax) does not accomplish the task, because orthogonal rotations force orthogonality where there is none. For example, there simply is no such thing as psychosis independent of anxiety, genetic risk independent of ancestry, verbal ability independent of quantitative ability, etc., so if a model has produced these things orthogonal to one another, then whatever those things are, they are not the phenomena one set out to measure. The bifactor model solves the problem by including an additional factor (the “general”) to account for the inter-factor correlations. Orthogonality is therefore not forced on the solution, but rather follows from the specific factors’ competing with the general factor for variance explained in each individual phenotype.

Figure 2. Path diagram showing the bifactor measurement model. Note. Exact loadings can be found in Table 2; items with very low communalities have been removed from the diagram for ease of visualization but were not removed before score-creation; green indicates positive loading (association); red indicates negative loading; thickest lines represent loadings with absolute value > 0.70; second-thickest lines represent loadings with absolute value 0.50-0.70; thinnest lines represent all other loadings (even those < 0.01); dotted lines indicate cross-loadings (complex structure); direction of arrows (from factors to traits) is consistent with the latent trait theory (factor analysis) whereby the latent factors cause the traits, itself consistent with the idea that genes cause traits.

Table 2 shows the results of the bifactor model using the same item-factor configuration suggested by the exploratory models above but with the addition of a General Factor of Plantness. **Factor 1** is Leaf Size, determined most strongly by dry and fresh leaf mass. **Factor 2** is SLA/Water Content (specific leaf area and water content), indicated most strongly by leaf water content and the inverse of leaf dry matter content. **Factor 3** is Vessel/Fiber Length. Finally, the factor of **General Plantness** (leftmost column in Table 2 and right side of Figure 2) is most strongly indicated by greater seed length, greater seed mass, greater dispersal vehicle length, greater plant height, greater leaf dry matter content, lower water content per leaf mass, greater probability of being a tree or shrub, and greater probability of a strictly terrestrial habit. As with the unidimensional model described in the paragraph above, the General Factor of Plantness is definitely aligned with “treeness,” but note the difference in emphasis on terrestrial status and plant height (for the unidimensional[6]) versus dry matter content and seed size (for bifactor General Plantness). Figure 2 shows the bifactor model in the traditional way, via a path diagram, but with strengths of associations represented graphically (by color and line thickness) rather than by numerical coefficients (available in Table 2).

Figures 3-6 show the frequencies (histograms) of the four factor scores generated from the bifactor model in Table 2. All, including examples, make intuitive sense although interpretation of the General Plantness factor is risky at this stage.

Figure 7 shows the bivariate relationships among factor scores from both the correlated-traits model and the bifactor model. The specific bifactor factors for leaf size and Fiber/Vessel Length are highly correlated with the equivalent scores from the correlated-traits model (correlations 0.90+). Also of note, the general bifactor factor correlated 0.81 with the water content factor from the correlated-traits model. This provides a hint that the General Plantness factor is some combination of water content (or lack thereof), plant height, and possibly tree form, among others.

Figures 8-13 show scatterplots of a few selected species (mix of famous, common, and scientifically important) plotted with respect to two dimensions at a time (e.g. Leaf Size and General Plantness). The diagonal dotted line is the identity line (y = x), and while the scatters appear to show some positive or negative correlations, all data viewed together does not show such patterns (see Figure 7, where the only clear correlations are between equivalent corr-traits//bifactors scores, never between bifactor//bifactor scores). Indeed, if all species were plotted together in Figures 6-11, there would be no clear relationship at all—simply a cloud of points—which is one of the strengths of the bifactor model. When developing scores for use in secondary analyses, it is best if those scores are uncorrelated.

Table 1. Unidimensional, 2-factor, and 3-factor exploratory solutions for the TRY+ Database, with 3-factor quasi-confirmatory solution.

		Exploratory 2-Factor		Exploratory 3-Factor			Bayes 3-Factor		
Variable (trait)	Uni	F1	F2	F1	F2	F3	F1	F2	F3
Leaf_area	0.68	0.87		0.88			0.92		
Leaf_fresh_mass	0.67	0.86		0.84			0.97		
Leaf_dry_mass	0.78	0.83		0.82			0.96		
Leaflet_area	0.60	0.81		0.82			0.83		
other_leaf_area	0.62	0.80		0.78			0.80		
Leaf_width	0.59	0.76		0.76			0.74		
Seed_length	0.77	0.47	0.52	0.53	0.45		0.39	0.44	
Leaf_length	0.41	0.58		0.52			0.54		
Plant_height	0.80	0.48	0.57	0.52	0.50		0.42	0.46	
Disp_vehicle_length	0.69	0.42	0.48	0.48	0.40		0.35	0.41	
Neotropical_realm	0.53	0.43		0.48			0.42		
Seed_mass	0.56	0.35	0.37	0.40	0.31		0.31	0.27	

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[6] It is tempting to view the unidimensional model as "General Plantness" just like we're viewing the bifactor general factor. However, unidimensional models estimated in multidimensional data (as here) yield biased loadings (Reise, Moore, & Maydeu-Olivares, 2011; Reise, Cook, & Moore, 2015). Correct loadings on the general factor can be identified only by estimating the multidimensional group factors along with it (in a full bifactor model, as here).

N_isotope_signature_Leaf	0.25	0.27		0.31			0.21		
climber	0.05	0.14		0.18			0.06		
LDMC_Leaf_dry_matter	0.57		0.84		0.84			0.93	
SLA_Leaf_area	-0.35		-0.71		-0.78			-0.66	
Australasian_realm	0.19	-0.44	0.72	-0.44	0.76		-0.25	0.65	
water_content_per_leaf_mass	-0.48		-0.71		-0.71			-0.84	
strictly_terrestrial	0.87	0.47	0.68	0.50	0.61		0.40	0.45	
Leaf_phosphorus_per_mass	-0.35		-0.57		-0.60			-0.52	
form_Forb	-0.56		-0.60		-0.59			-0.55	
Stem_specific_density_SSD	0.38		0.60		0.59			0.53	
form_Herb	-0.66		-0.59	-0.34	-0.53		-0.25	-0.53	
Leaf_carbon_per_mass	0.39		0.47		0.49			0.47	
Leaf_nitrogen_per_mass	-0.13		-0.40	0.31	-0.49		0.10	-0.41	
nitrogen_per_Leaf_area	0.27		0.45		0.48			0.41	
Stem_diameter	0.48		0.44		0.45			0.37	
Rooting_depth	0.41		0.39		0.36			0.34	
form_Shrub_or_SubShrub	-0.03	-0.35	0.31	-0.34	0.34		-0.32	0.26	
Specific_root_length_SRL	-0.29		-0.36		-0.34			-0.34	
endangered_or_worse	0.25		0.28		0.29			0.27	
Nearctic_realm	-0.28		-0.23		-0.20			-0.13	
documented_medicinal	0.00		-0.13		-0.15			-0.11	
Wood_vessel_length	0.17	0.33				0.85			0.98
Wood_fiber_lengths	0.38	0.41				0.63			0.75
Seed_number_per_unit	0.07	0.15				0.48			0.48
chromosome_number	-0.08		-0.24			0.46			0.45
Stem_conduit_density	-0.27		-0.22			0.37			0.25
cpDNA_content	-0.10		-0.15			0.36			0.33
Leaf_thickness	-0.04	-0.16				0.33			0.16
Stem_conduit_diameter	0.23	0.34				0.32			0.39
Seed_germination_rate	-0.13	-0.12				-0.24			-0.17

Table 2. Quasi-confirmatory bifactor solution for the TRY+ Database, with three specific factors and one general (overall) factor.

Variable	**Gen**	**F1**	**F2**	**F3**
Leaf_area	0.33	0.85		
Leaf_fresh_mass	0.29	0.94		
Leaf_dry_mass	0.42	0.87		
Leaflet_area	0.25	0.79		
other_leaf_area	0.25	0.76		
Leaf_width	0.28	0.67		

Seed_length	**0.92**	0.06	-0.40	
Leaf_length	0.21	0.49		
Plant_height	**0.68**	0.25	-0.01	
Disp_vehicle_length	**0.83**	0.05	-0.35	
Neotropical_realm	0.35	0.30		
Seed_mass	**0.64**	0.06	-0.35	
N_isotope_signature_Leaf	0.20	0.13		
climber	0.02	0.05		
LDMC_Leaf_dry_matter	**0.73**		0.60	
SLA_Leaf_area	-0.45		-0.50	
Australasian_realm	0.40	-0.14	0.51	
water_content_per_leaf_mass	**-0.63**		-0.61	
strictly_terrestrial	**0.68**	0.25	0.02	
Leaf_phosphorus_per_mass	-0.38		-0.37	
form_Forb	-0.57		-0.17	
Stem_specific_density_SSD	0.42		0.30	
form_Herb	**-0.70**	-0.13	-0.06	
Leaf_carbon_per_mass	0.43		0.19	
Leaf_nitrogen_per_mass	-0.21	0.04	-0.36	
nitrogen_per_Leaf_area	0.27		0.31	
Stem_diameter	0.35		0.12	
Rooting_depth	0.35		0.08	
form_Shrub_or_SubShrub	-0.03	-0.19	0.34	
Specific_root_length_SRL	-0.33		-0.12	
endangered_or_worse	0.25		0.06	
Nearctic_realm	-0.14		-0.03	
documented_medicinal	-0.03		-0.14	
Wood_vessel_length	0.05			0.96
Wood_fiber_lengths	0.32			0.74
Seed_number_per_unit	0.00			0.49
chromosome_number	-0.20			0.48
Stem_conduit_density	-0.27			0.26
cDNA_content	-0.08			0.34
Leaf_thickness	-0.10			0.17
Stem_conduit_diameter	0.12			0.39
Seed_germination_rate	-0.08			-0.19

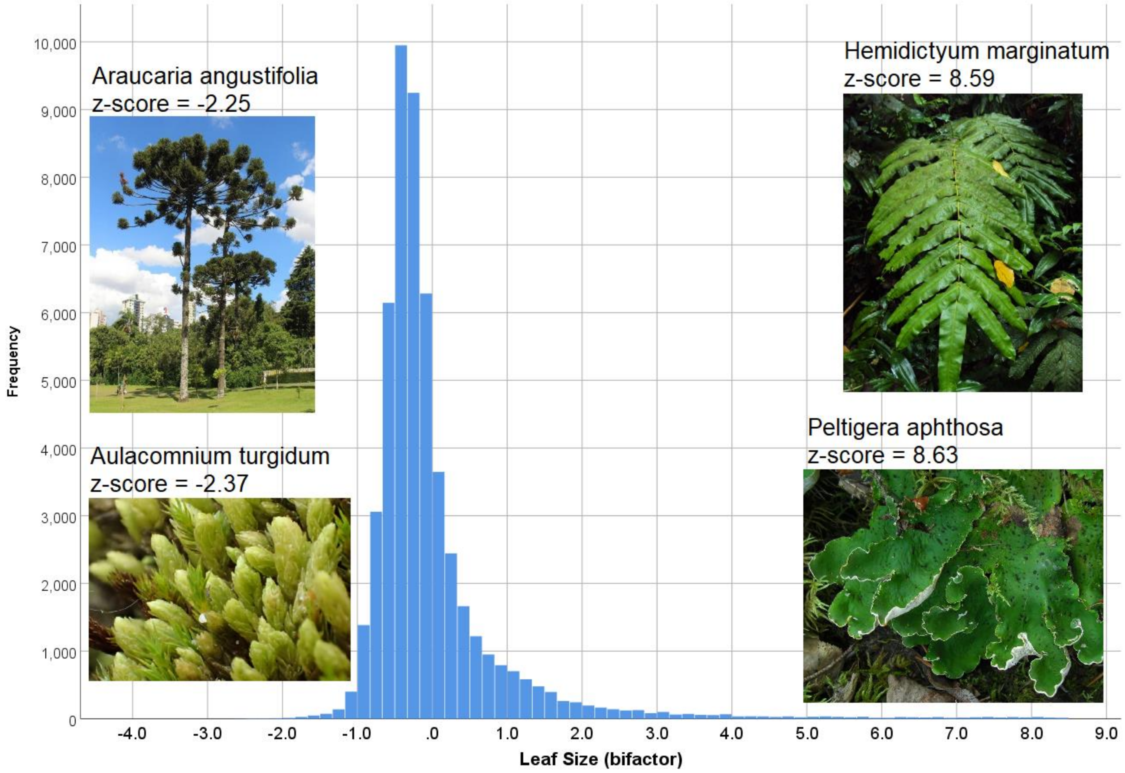

Figure 3. Histogram of Leaf Size factor score from the bifactor model, with extreme examples.

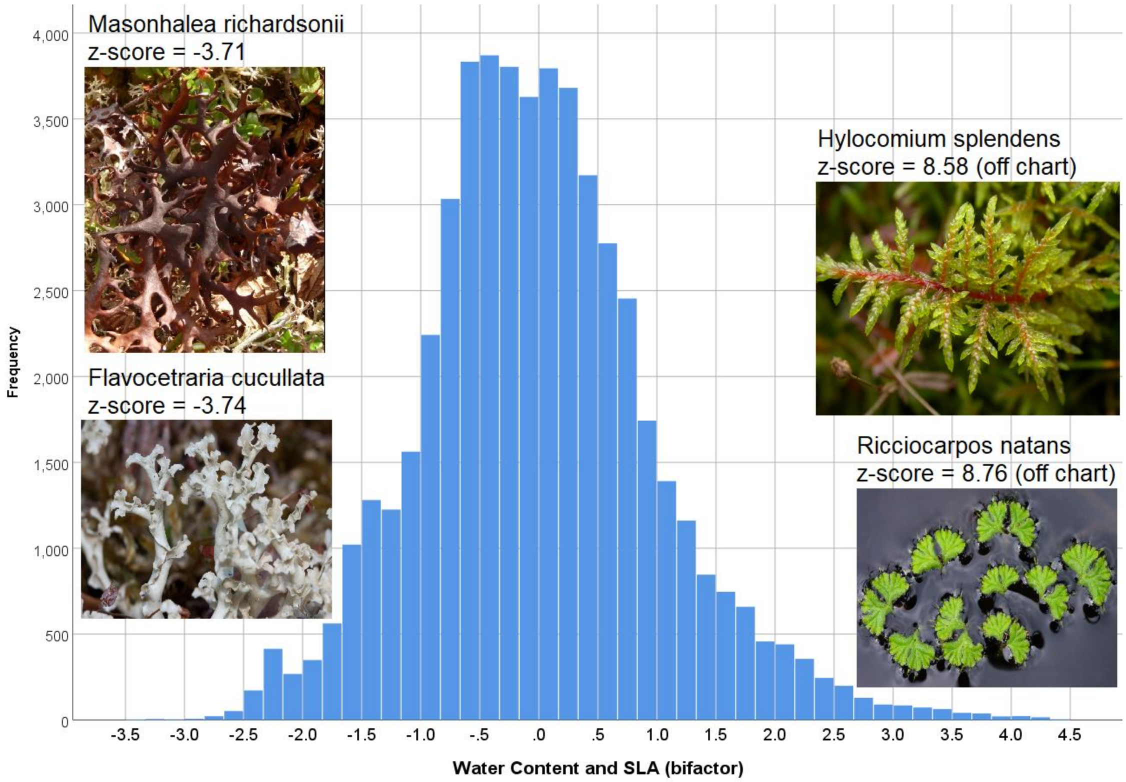

Figure 4. Histogram of Water Content and SLA (specific leaf area) factor score from the bifactor model, with extreme examples.

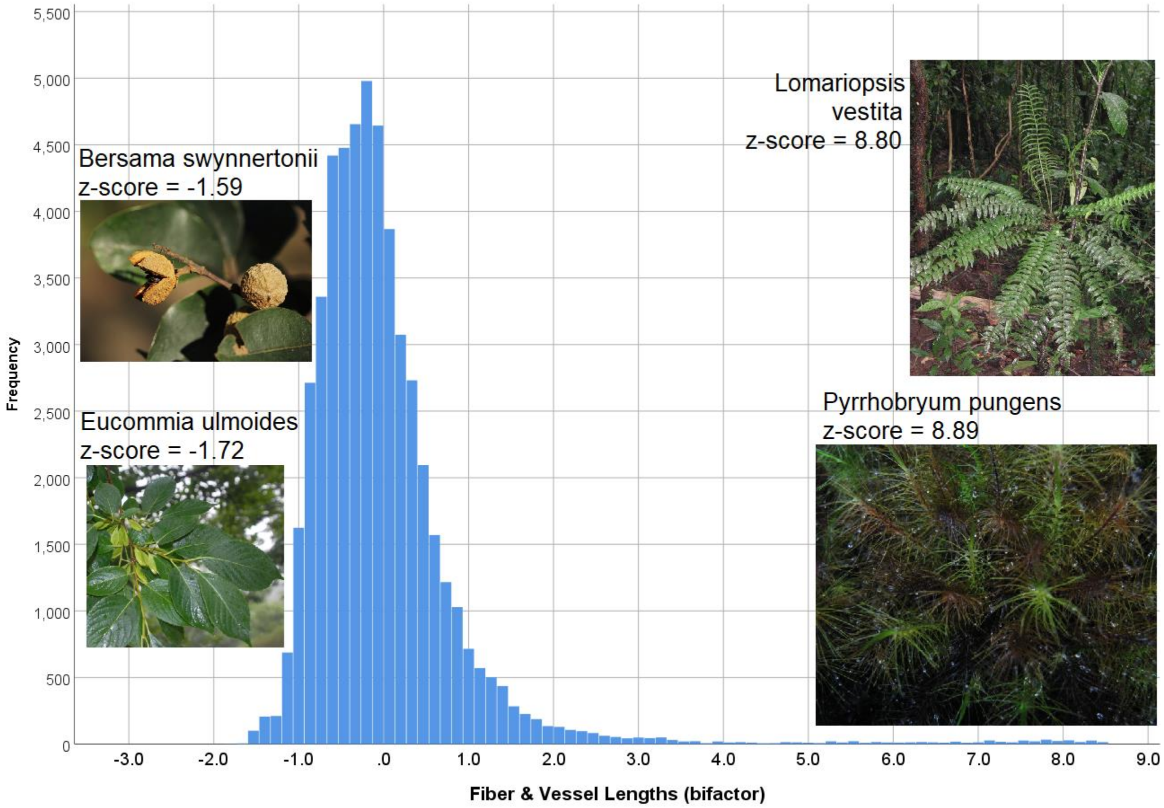

Figure 5. Histogram of Vessel/Fiber Lengths score from the bifactor model, with extreme examples.

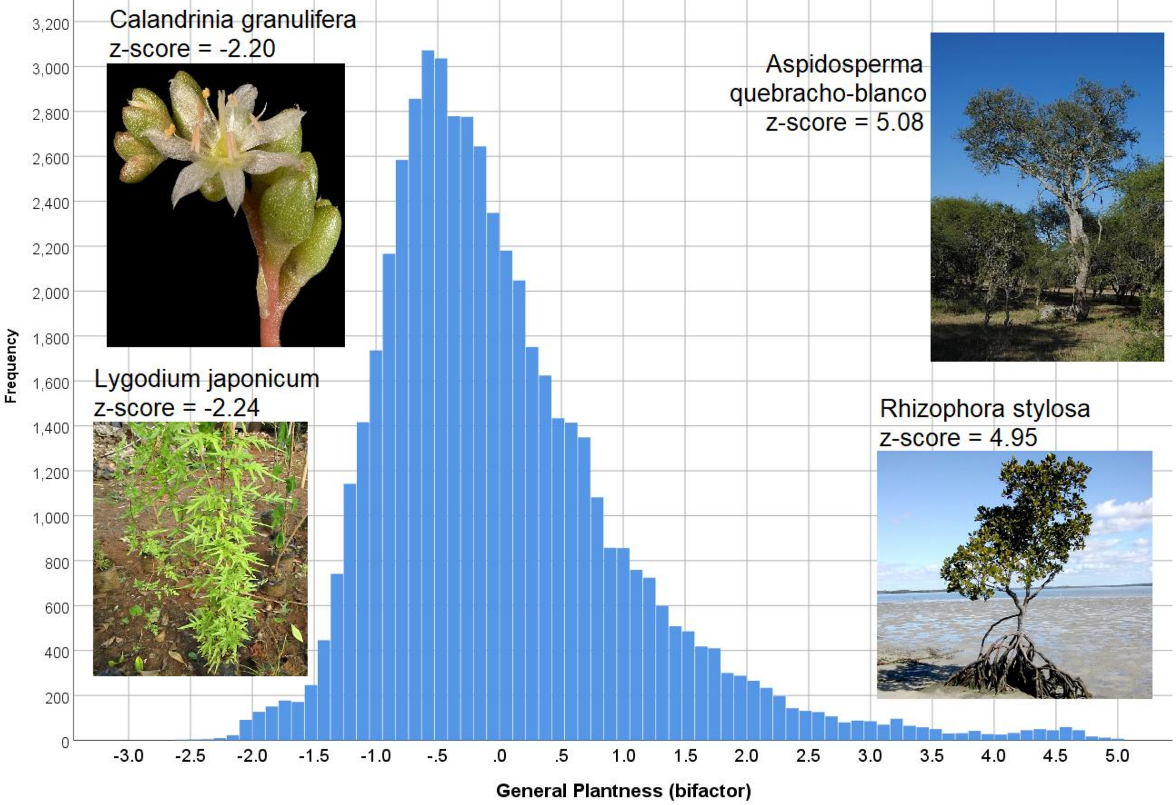

Figure 6. Histogram of General Plantness score from the bifactor model, with extreme examples.

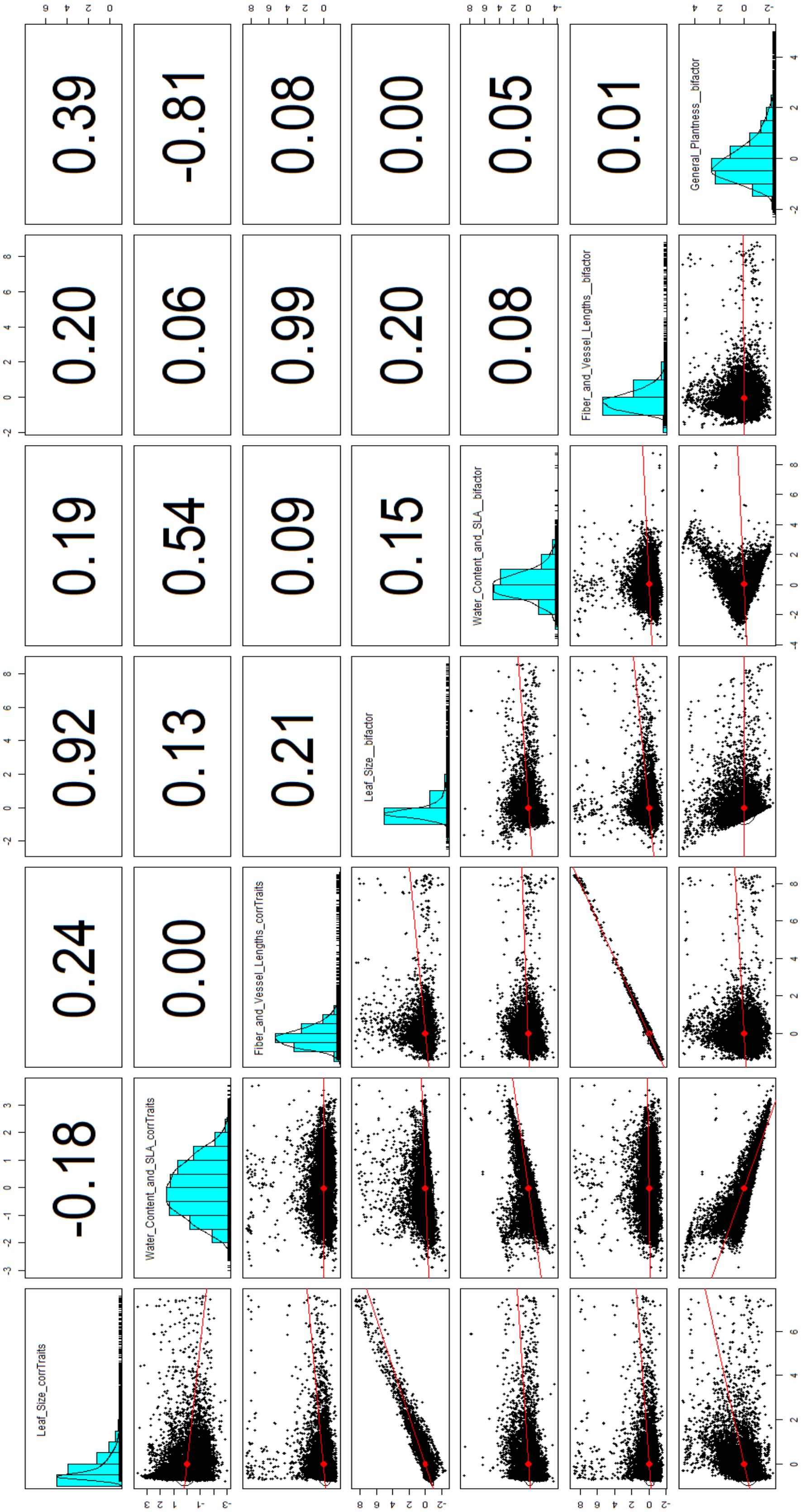

Figure 7. Correlations among plant factor scores from the correlated-traits and bifactor models.

DISCUSSION

The current study adds to the methodological and plant trait literature in two ways. First, I present the bifactor model as a possible solution to the problem of inter-factor collinearity, a problem not solved by any existing orthogonalization method. Second, I allow complex structure (cross-loadings) at the exploratory phase, allowing a model that more closely represents the sample (albeit at a cost to parsimony). The latter contribution, use of iterated target rotation, is quite novel and may grow to replace existing simple structure rotations if detection of complex structure (as here) proves useful. The fact that ITR will detect simple structure as well as complex structure—i.e., if ITR is overkill, it will return a simple structure solution—is all the more reason to expect the shift away from rotations that force simple structure. The bifactor model, likewise, introduces the idea of a single factor/dimension underlying all plant traits, which, if supported through genetic studies, will provide another dimensional trait score for use in prediction studies (e.g. predicting crop yields or any other plant-related outcome). From the botany perspective, the most important output from this project is the set of factor scores for use in subsequent studies. These scores likely differ from existing plant trait scores in that (1) they are orthogonal, and (2) they include a General Factor of Plantness.

The current study has some notable limitations. First, analyses were entirely exploratory, leaving for later studies investigation of the veracity of the measurement model arrived at through exploration. A more common pipeline for development of measurement models is to conduct exploratory analyses in one random portion of the sample and then *test* the model(s) in the other (non-overlapping) portion of the sample. I made the judgment call here that the exploratory models alone are enough for the present report, and I intend to investigate the reproducibility of the models in the same sample (analogous to the pipeline above) using bootstrapping. Nonetheless, even after this second study, it will have been done only in this sample. A true test of the measurement model presented here will be in a new sample — i.e., because there is natural variation within species, it would be optimal to collect more specimens of the same species used here and re-run these analyses. More realistically, these analyses should be redone after the TRY database has been expanded (as it constantly will be). This would add not only more specimens of the same species, but more species overall. A second limitation of the present study is that the imputation of missing data for growth form, region, endangeredness, medicinal use, and climber status was done without consideration of the multilevel (clustered) nature of the data — i.e., species within genera within families, etc. Clustering and other multilevel structure affects standard errors more than point estimates (Peugh 2005; see Equation 5), so the hope is that ignoring the nesting will increase only error, not bias. However, this “hope” could be tested by future researchers by comparing random forest imputation to an imputation method that considered the nested data structure (e.g. BHPMF mentioned above; also see Moreno-Martinez et al. 2018). Third, given the novelty of the present problem (does General Plantness “exist”?), it is possible that use of iterated target rotation complicates the problem unnecessarily at this early stage. I suggest that the approach used here — i.e., if there is any reason to doubt simple structure, use ITR — is best practice, but future researchers should examine simple structure rotations of these solutions, nonetheless. Indeed, the small-to-moderate cross loadings in Table 2 (only one reaching absolute value = 0.40) hint that ITR might not be necessary. Finally, I had to make many “executive decisions” while collecting, merging, and analyzing these data, and the decisions could not all feasibly be documented. Examples include decisions about whether to delete (versus manually correct) ambiguously misspelled species names, whether to distinguish among variations and subspecies in the analyses (decision was no on both counts), how to aggregate across multiple samples of the same species (decision was to take the mean), and dozens more. Documentation was foregone in some cases simply for the sake of speed, and any study performed by an individual in this way should be viewed with caution and replicated by a team, if possible.

This paper addresses an important methodological issue related to the bifactor model, which is the question of whether it makes sense to estimate one even when the correlated-traits model provides no evidence for a general factor. Shilton et al. (under review) provide some evidence for the potential utility of bifactor models even when preliminary analyses might suggest that a hierarchical approach like the bifactor is unnecessary. They take a correlated-traits model presented in Moore et al. (2020) and apply a bifactor model (in a different data set) even though the inter-factor correlations from the models in Moore et al. were quite weak. Unsurprisingly, the general factor in Shilton's bifactor model is determined by a mixture of items across group factors, with item loadings on the general factor varying substantially across and *within* group factor. This in itself provides no evidence for or against a bifactor model necessarily, but it does suggest that if there is a general factor underlying item responses to some extent, it would not be noticeable in the correlated-traits (or higher-order) models. Most importantly, Shilton et al. found that the general factor score from the bifactor model had better criterion validity than any other score in the model. This provides one piece of evidence in favor of "trying" bifactor models even when inter-factor correlations suggest there is no general factor (obviating a bifactor model). If it turns out that no items have strong loadings on the general factor, then the researcher will know that the original hint (weak inter-factor correlations) was correct. On the other hand, if some specific items within the group factors have strong loadings on the general factor, the above study suggests that the general factor score might be a valid metric. In the present study, the question remains, is the General Factor of Plantness a valid measure of something interesting or useful (as turned out in the Shilton et al. study)? Further research is needed, but I speculate that the answer is yes, "General Plantness" is interesting and useful and the corroborating evidence for its existence will come (or already is available) from genetics.

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ELECTRONIC MATERIAL

Factor scores are available for download at <https://www.mooremetrics.com/wp-content/uploads/2020/08/Plant_Factor_Scores.csv>. Note that scores ending in "__bifactor" are the bifactor scores used here. Scores ending in "__corrTraits" are generated from a model that does not include a general factor (i.e. a correlated-traits model). The .r file for conducting iterated target rotation, along with the Mplus files for conducting the Bayesian CFAs are available at <http://www.mooremetrics.com/wp-content/uploads/2020/08/Iterated_Target_Rotation_and_Mplus_scripts.zip>. All files and figures are available at <https://mooremetrics.com/3fp/>.

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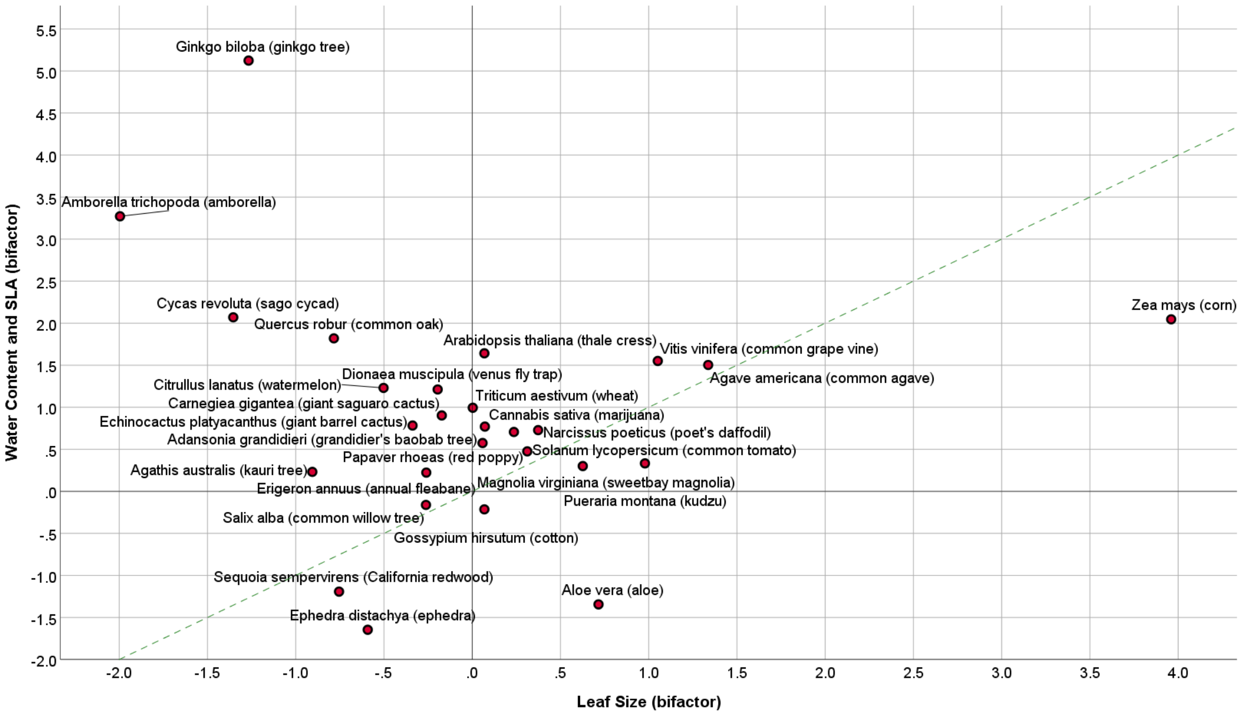

Figure 8. Selected species examples showing relative standing on Leaf Size and SLA/Water Content scores produced from a bifactor model. Scores are independent (uncorrelated); any visual hint of a relationship between scores is due only to this specific set of examples; the purpose of the plot is only to show where some common plants score relative to one another, not to show a bivariate relationship; dotted line is identity line (x = y)**, not line of best fit**.

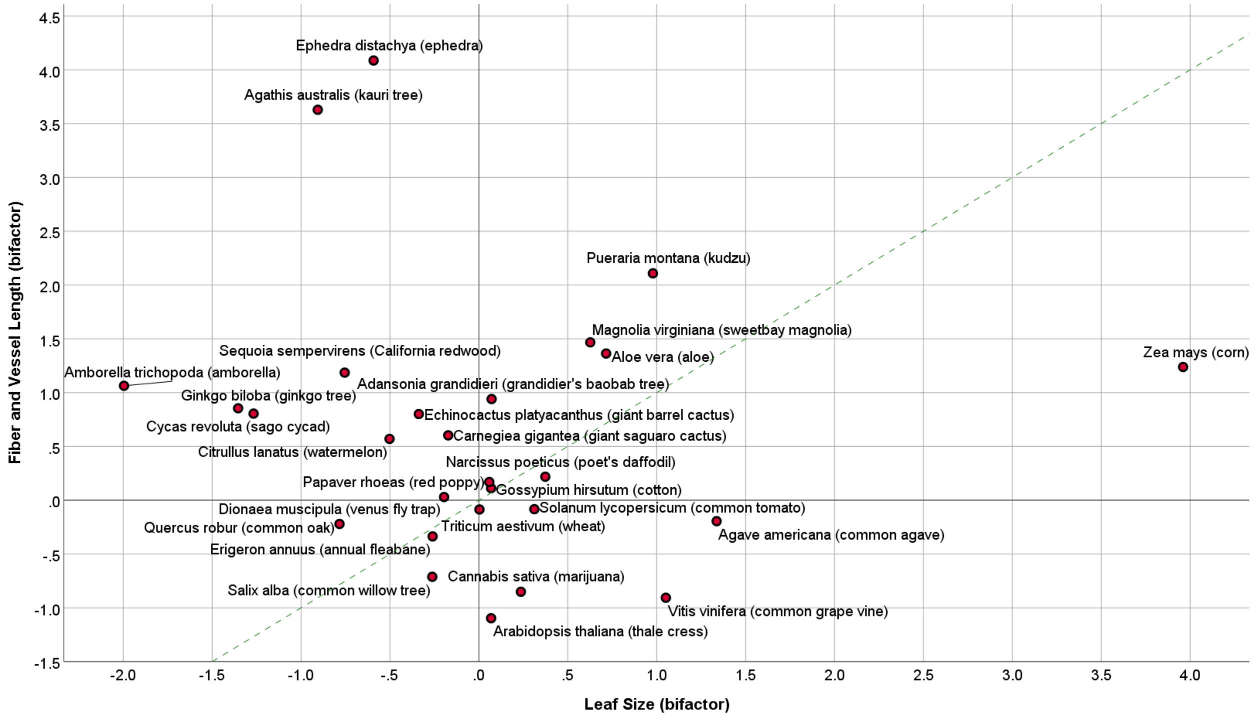

Figure 9. Selected species examples showing relative standing on Leaf Size and Fiber/Vessel Length scores produced from a bifactor model. Scores are independent (uncorrelated); any visual hint of a relationship between scores is due only to this specific set of examples; the purpose of the plot is only to show where some common plants score relative to one another, not to show a bivariate relationship; dotted line is identity line (x = y)**, not line of best fit**.

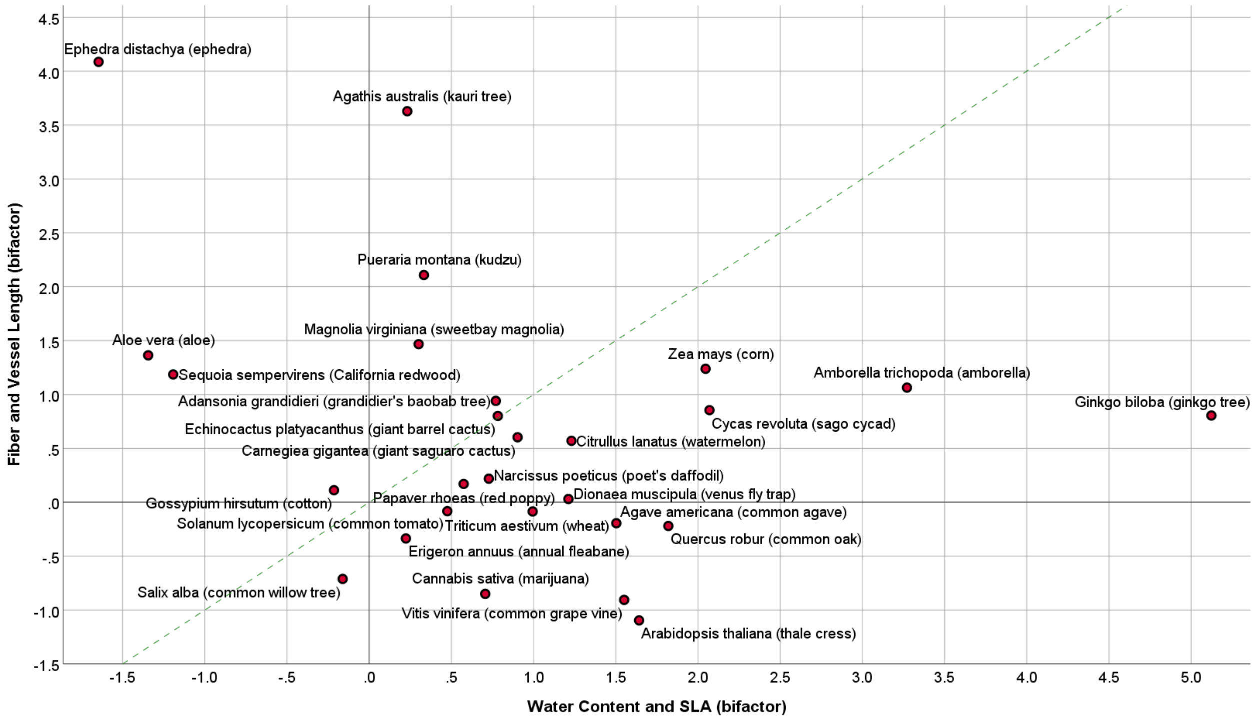

Figure 10. Selected species examples showing relative standing on SLA/Water Content and Vessel/Fiber Length scores produced from a bifactor model. Note: scores are independent (uncorrelated); any visual hint of a relationship between scores is due only to this specific set of examples; the purpose of the plot is only to show where some common plants score relative to one another, not to show a bivariate relationship; dotted line is identity line (x = y)**, not line of best fit**.

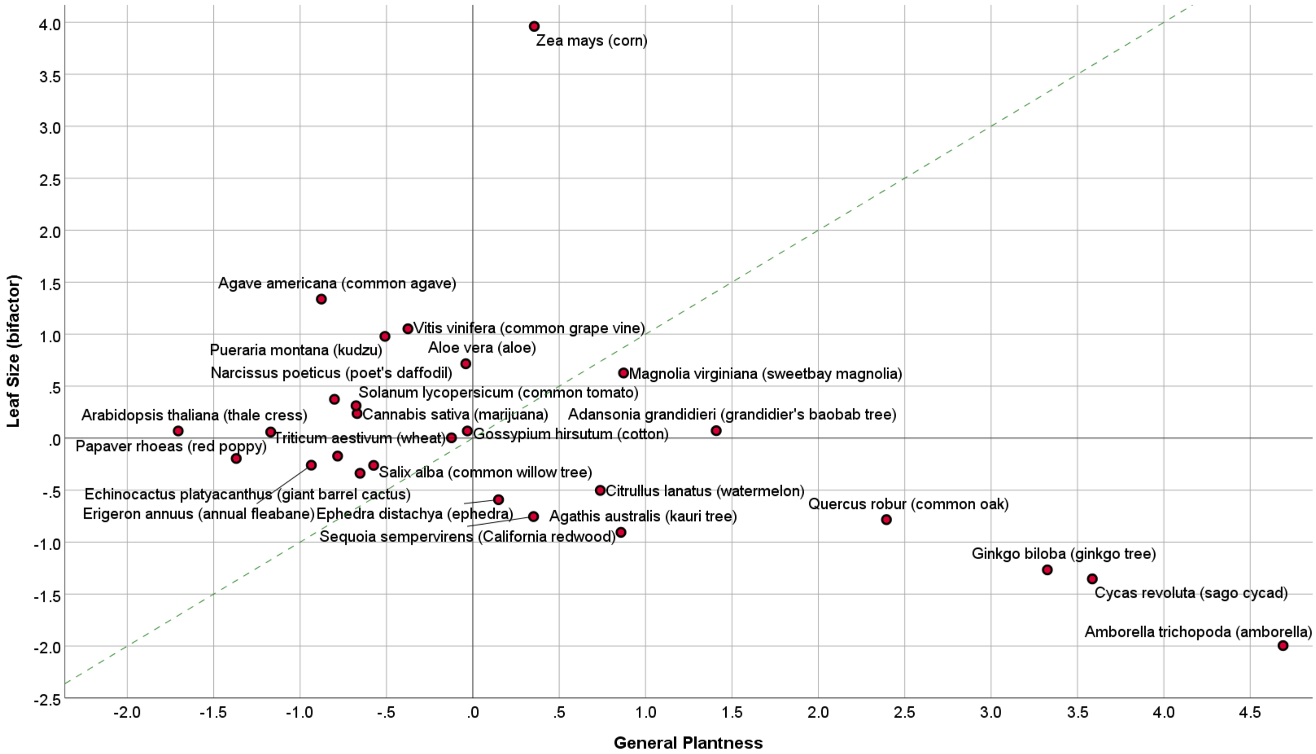

Figure 11. Selected plant examples showing relative standing on General Plantness and Leaf Size scores produced from a bifactor model. Note: scores are independent (uncorrelated); any visual hint of a relationship between scores is due only to this specific set of examples; the purpose of the plot is only to show where some common plants score relative to one another, not to show a bivariate relationship; dotted line is identity line (x = y)**, not line of best fit**.

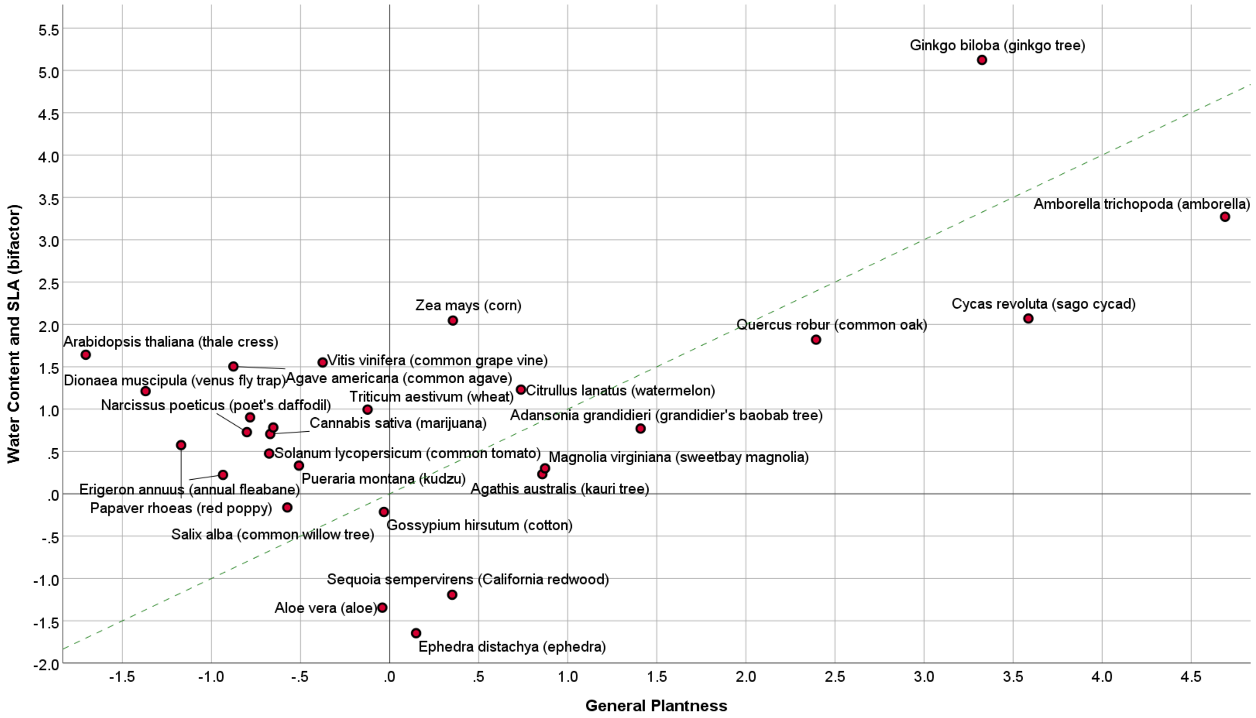

Figure 12. Selected plant examples showing relative standing on General Plantness and SLA Water Content scores produced from a bifactor model. Note: scores are independent (uncorrelated); any visual hint of a relationship between scores is due only to this specific set of examples; the purpose of the plot is only to show where some common plants score relative to one another, not to show a bivariate relationship; dotted line is identity line (x = y)**, not line of best fit**.

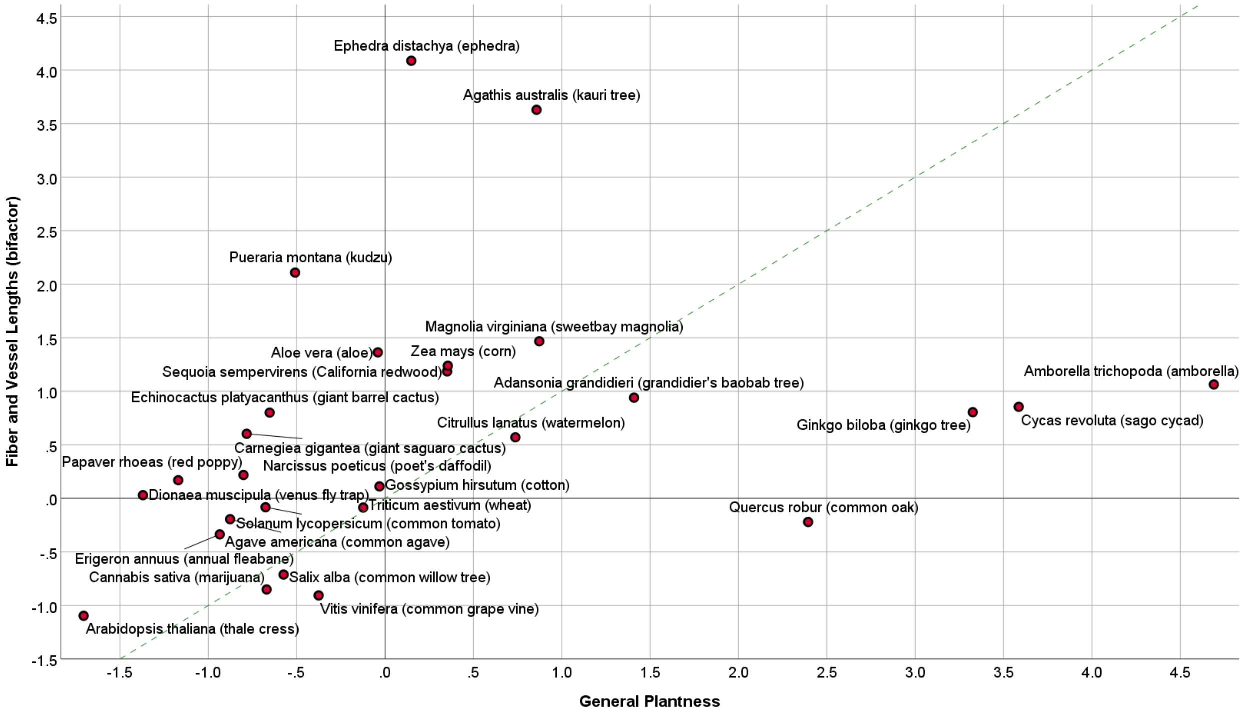

Figure 13. Selected plant examples showing relative standing on General Plantness and Fiber/Vessel Length scores produced from a bifactor model. Note: scores are independent (uncorrelated); any visual hint of a relationship between scores is due only to this specific set of examples; the purpose of the plot is only to show where some common plants score relative to one another, not to show a bivariate relationship; dotted line is identity line (x = y)**, not line of best fit**.