



Article

The Sentinel 2 MSI Spectral Mixing Space

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Abstract: A composite spectral feature space is used to characterize the spectral mixing properties of Sentinel 2 Multispectral Instrument (MSI) spectra over a wide diversity of landscapes. Characterizing the linearity of spectral mixing and identifying bounding spectral endmembers allows the Substrate Vegetation Dark (SVD) spectral mixture model previously developed for the Landsat and MODIS sensors to be extended to the Sentinel 2 MSI sensors. The utility of the SVD model is its ability to represent a wide variety of landscapes in terms of the areal abundance of their most spectrally and physically distinct components. Combining the benefits of location-specific spectral mixture models with standardized spectral indices, the physically based SVD model offers simplicity, consistency, inclusivity and applicability for a wide variety of land cover mapping applications. In this study, a set of 110 image tiles compiled from spectral diversity hotspots worldwide provide a basis for this characterization, and for identification of spectral endmembers that span the feature space. The resulting spectral mixing space of these 13,000,000,000 spectra is effectively 3D, with 99% of variance in 3 low order principal component dimensions. Four physically distinct spectral mixing continua are identified: Snow:Firn:Ice, Reef:Water, Evaporite:Water and Substrate:Vegetation:Dark (water or shadow). The first 3 continua exhibit complex nonlinearities, but the geographically dominant Substrate:Vegetation:Dark (SVD) continuum is conspicuous in the linearity of its spectral mixing. Bounding endmember spectra are identified for the SVD continuum. In a subset of 80 landscapes, excluding the 3 nonlinear mixing continua (reefs, evaporites, cryosphere), a 3 endmember (SVD) linear mixture model produces endmember fraction estimates that represent 99% of modeled spectra with <6% RMS misfit. Two sets of SVD endmembers are identified for the Sentinel 2 MSI sensors, allowing Sentinel 2 spectra to be unmixed globally and compared across time and space. In light of the apparent disparity between the 11D spectral feature space and the statistically 3D spectral mixing space, the relative contribution of 11 Sentinel 2 MSI spectral bands to the information content of this space is quantified using both parametric (Pearson Correlation) and nonparametric (Mutual Information) metrics. Comparison of linear (principal component) and nonlinear (Uniform Manifold Approximation and Projection) projections of the SVD mixing space reveal both physically interpretable spectral mixing continua and geographically distinct spectral properties not resolved in the linear projection.



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1. Introduction

The Sentinel 2 constellation [1] extends the 50 year Landsat legacy of multispectral Earth imaging [2] with higher spatial, spectral and temporal resolution. The combined spatial and spectral resolution of a sensor is manifest in the spectral dimensionality and topology of the spectral feature space defined by dimensions corresponding to the imaging sensor's different spectral band measurements [3,4]. In the case of decameter-resolution broadband sensors we refer to this feature space as a spectral mixing space to explicitly acknowledge the optical processes which occur when upwelling radiance from more than one spectrally distinct material is aggregated within the Instantaneous Field of View (IFOV) of a single pixel.

Previous analyses of spectrally diverse mixing spaces of both multispectral and hyperspectral sensors with decameter spatial resolution reveal a consistent topology with 97% to 99% of spectral variance embedded within a 3D linear mixing subspace bounded by distinct spectral endmembers [5–9]. These studies indicate that the vast majority of ice-free landscapes on Earth can be modeled accurately as linear mixtures of rock, alluvia and soil substrates (S), photosynthetic vegetation (V) and optically transmissive/absorptive materials like deep clear water, wet soils and low albedo substrates (e.g., ferromagnesian rocks). In addition, both micro and macro-scale shadow is often indistinguishable from absorptive/transmissive materials. Together, these components of the landscape are referred to as Dark targets (D) and comprise the third spectral endmember of the SVD linear spectral mixture model.

Within spectrally diverse mixing spaces, these materials are associated with endmember (EM) reflectance spectra that reside at the apexes of a triangular point cloud bounded by binary mixing lines between the Dark EM and each of the Substrate and Vegetation EMs. While both of these binary mixing lines are conspicuous in their linearity, the mixing trend between the Substrate and Vegetation EMs is generally concave inward as a result of the ubiquitous presence of multiple scales of shadow on most landscapes. In some landscapes the diversity of substrates is sufficient to extend the planar triangular mixing space into a 3D tetrahedral mixing space also bounded by a plane of substrates of varying reflectance, sometimes referred to as the “soil line” [10,11]—although this third dimension rarely accounts for $> \sim 3\%$ of total spectral variance. The apparent linearity of spectral mixing within this Substrate, Vegetation, and Dark bounded mixing space renders it generally amenable to representation with linear spectral mixture models. The minimal linear model used to represent this mixing space is referred to here (and elsewhere) as the SVD model [5–9,12]. The utility of the SVD model is its ability to represent a wide variety of landscapes in terms of the areal abundance of their most spectrally and physically distinct components. Combining the benefits of location-specific spectral mixture models with standardized spectral indices, the SVD model offers simplicity, consistency, inclusivity and applicability. In contrast to spectral indices which map specific materials using only 2 or 3 spectral bands, spectral mixture models use all available spectral bands to map the areal abundance all spectrally distinct materials present within a pixel’s Instantaneous Field of View simultaneously.

The objective of this study is to quantify the information content, spectral dimensionality and topology of the spectral mixing space of a spectrally diverse compilation of Sentinel 2 MSI imagery collected over a wide range of terrestrial biomes. In anticipation of similar topology and linearity to the mixing spaces of other multispectral and hyperspectral sensors, we identify spectral endmembers and evaluate the validity and stability of the SVD model for the Sentinel 2 MSI sensors. In addition to the 3D spectral mixing space rendered by the (linear) principal components of the Sentinel 2 compilation, we also employ manifold learning to render nonlinear 2D embeddings of the mixing space to identify additional, more subtle spectral distinctions (clusters and mixing continua) among land cover subcategories that are not apparent in the principal component projections of the mixing space. This comparison of linear and nonlinear embeddings is extended to land cover-specific compilations of Sentinel 2 imagery in the companion analysis to that presented here [13].

2. Materials and Methods

2.1. Data

We construct a composite mixing space from a set of 110 Sentinel 2 MSI tiles collected from spectral diversity hotspots worldwide. The geographic locations and biome designations of these hotspots are shown in Figure 1. Unlike previous studies, we include numerous examples of cryospheric landscapes, evaporite basins and shallow marine environments, in addition to a range of anthropogenically modified landscapes (e.g., urban & agriculture). From this collection of (110 tiles \times 10,980² pixels =) 13.3×10^9 Sentinel 2

spectra we identify a second set of (12 categories \times 10 examples =) 120 subtiles from specific land cover subcategories. Diverse sets of either 5 or 10 subtiles, each 10×10 km in area, are chosen from agricultural (10), evaporite (10), cryospheric (10), volcanic (5), urban (5), shallow marine (10), sand dune (10), closed (10) and open (10) canopy forest, scrub/shrub (5), tundra (5), wetland (10), and igneous/sedimentary/metamorphic rock + alluvium (10 + 10) landscapes for a total 120,000,000 subcategory-specific spectra. False color composites of both of these aggregate mosaics are shown in Figure 2. Tile IDs and subcategory subtile locations are given in Appendix B. All data were downloaded free-of-charge as Level 1C exoatmospheric reflectance from the USGS EarthExplorer data portal (<https://earthexplorer.usgs.gov/>, accessed on 1 October 2022).

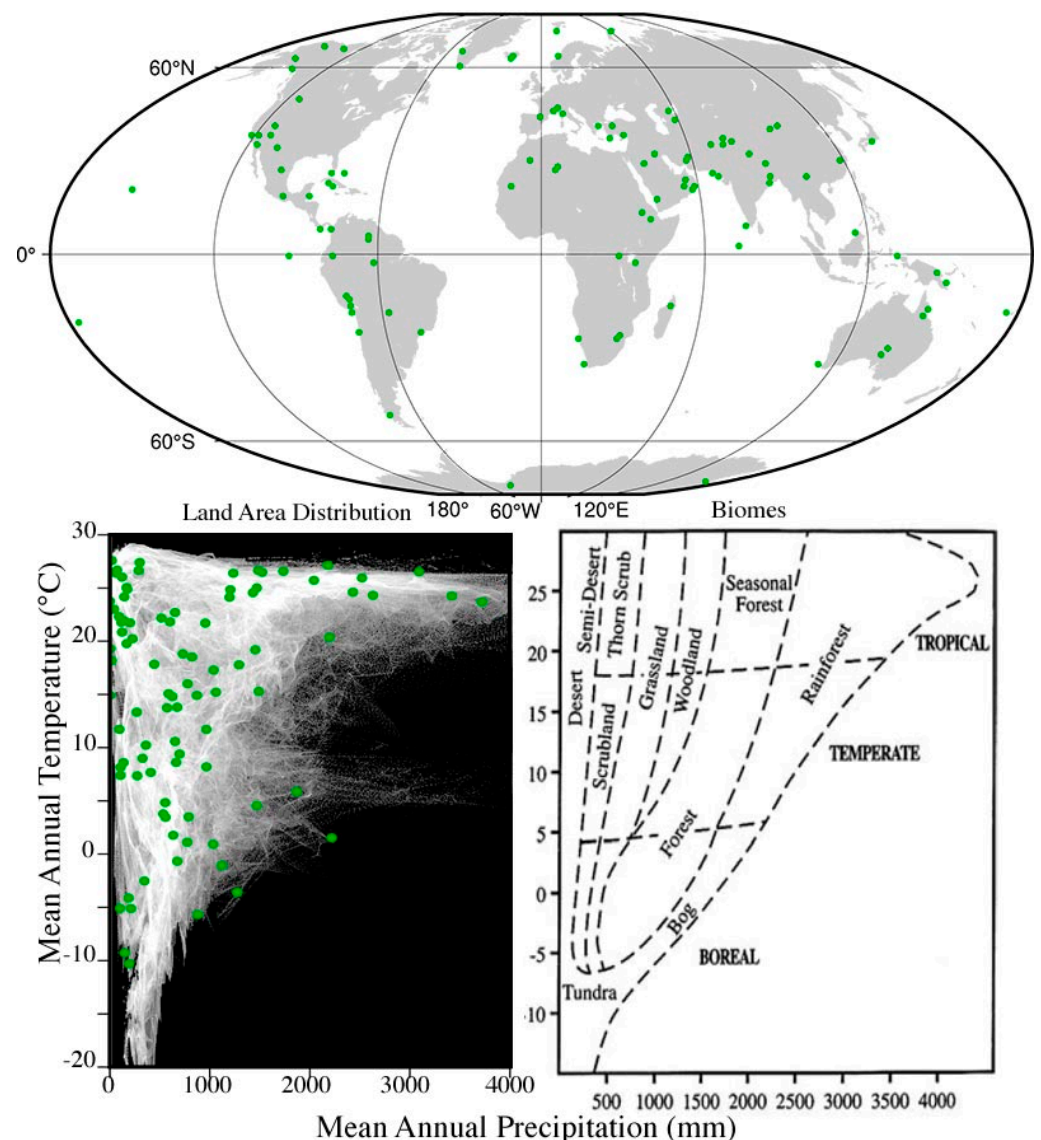


Figure 1. Geographic and climatic distributions of 110 Sentinel 2 tiles from spectral diversity hotspots. Geographic distribution of sample sites is guided by climatic and geologic diversity as well as overall species biodiversity. Individual tile selection criteria favor spectral diversity arising from land cover diversity within and across biomes. Tile geographic coverage corresponds well to global land area distribution within the climatic parameter space (lower left) from [14]. All biomes are well represented. Biome classification (lower right) adapted from [15].

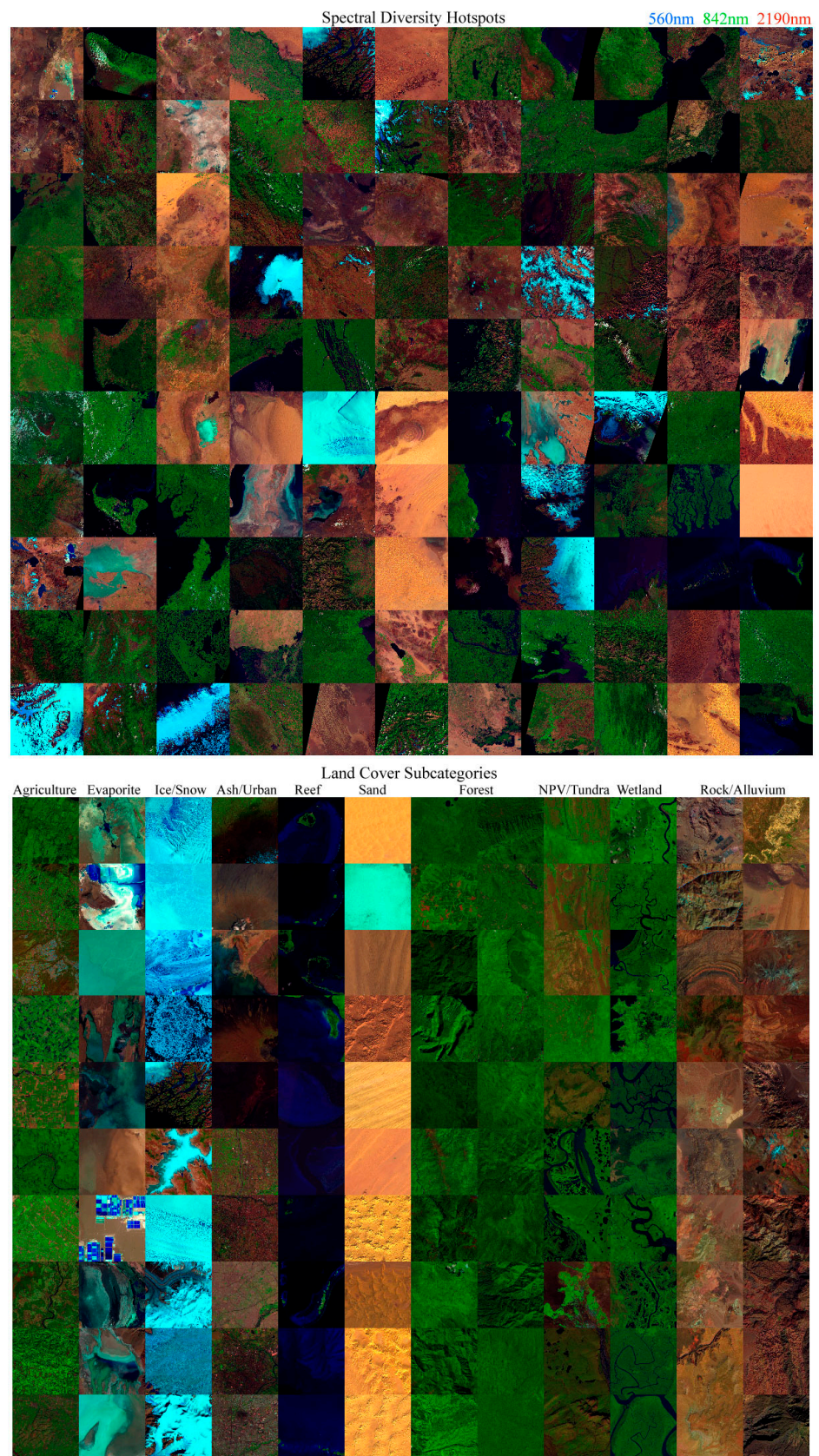


Figure 2. Sentinel 2 composites for 110 spectral diversity hotspot tiles (110 × 110 km) and specific land cover subcategories (10 × 10 km) selected from individual hotspot tiles. Identical 1% linear stretch applied to both mosaics.

The spectral diversity hotspots were chosen on the basis of climatic gradients, biome diversity, soil diversity, plant diversity and geologic diversity—both within and among individual tiles. Sources used include geologic (<https://mrdata.usgs.gov/geology/world/map-us.html>, accessed on 11 September 2021) and climatic (<https://storymaps.arcgis.com/stories/61a5d4e9494f46c2b520a984b2398f3b>, accessed on 11 September 2021) basemaps in conjunction with maps of soils (https://atlas-for-the-end-of-the-world.com/world_maps/world_maps_soils.html, accessed on 11 September 2021), biomes (<https://www.worldwildlife.org/publications/terrestrial-ecoregions-of-the-world>, accessed on 11 September 2021), plant biodiversity (<https://databasin.org/datasets/43478f840ac84173979b22631c2ed672/>, accessed on 11 September 2021) and crop wild relatives (<https://colostate.pressbooks.pub/cropwildrelatives/chapter/introduction-to-crop-wild-relatives/>, accessed on 11 September 2021).

2.2. Methods

All analyses described in this study use Sentinel 2 MSI bands 1, 2, 3, 4, 5, 6, 7, 8, 8a, 11, and 12. The 20 m and 60 m bands (1) are coregistered with and upsampled to the 10 m bands (2, 3, 4, 8) by bilinear interpolation.

The compilation of 13.3×10^9 Sentinel 2 spectra from 110 spectral diversity hotspots provides a basis for statistical assessment of the information content of the MSI spectral bands. The parametric Pearson correlation coefficient and the non-parametric Mutual Information metric were computed for all band pairs. The Pearson correlation coefficient, r_{xy} , is given as:

$$r_{xy} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (1)$$

where x and y are band-specific reflectances for each spectrum in the mosaic. Correlations are computed for all 55 band pairs.

The mutual information metric, as originally conceived by [16] and further formalized [17], is defined for two random variables X and Y as the Kullback–Leibler divergence from the product of the joint distribution from the product of the marginal distributions. That is,

$$MI = D_{KL}(p_{X,Y} \parallel p_X p_Y), \quad (2)$$

where MI is mutual information, D_{KL} is the Kullback–Leibler divergence, $p_{X,Y}$ is the joint distribution of X and Y , and p_X and p_Y are the marginal distributions of X and Y . The MI of a variable with itself is defined as its self-information. Both mutual and self-information are bounded by $[0, +\infty]$, and $MI \leq SI$. Conceptually, both self-information and MI can be understood as measures of “surprise”—the less probable are more surprising than probable events, and events with 100% probability are totally “unsurprising” (information = 0). Computation of MI was performed in Python using scikit-learn (package `sklearn.featureselection.mutual_info_regression`, with the implementation of [18,19]). As with the correlations, MI is computed for all 55 band pairs.

Spectral dimensionality is estimated from the variance partition of the eigenvalues of the spectra in the compilation mosaics described above. Variance partition by principal component dimension, given by the sum-normalized eigenvalues of the Singular Value Decomposition of the mosaics, and land cover subcategories, are shown in Figure 3. Because the tiles in the 120 tile spectral diversity hotspot mosaic are arranged in alphabetical order of the tile IDs (effectively random geographically), and most tiles are internally spectrally diverse, the mosaic can be subdivided into 5 subsets to assess the scaling of the spectral dimensionality of the compilation with number of spectra. Spectral dimensionality is estimated from variance partition for both the 110 tile Spectral Diversity Hotspot mosaic and the 120 subset land cover subcategory mosaic.

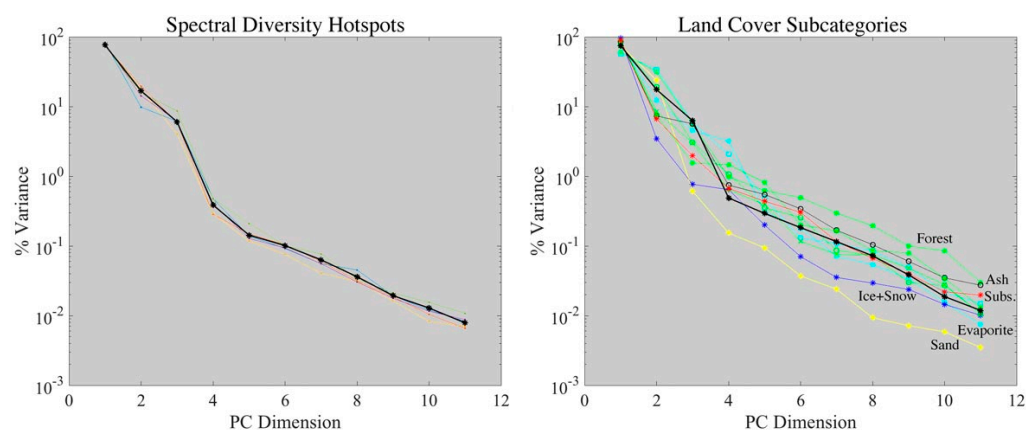


Figure 3. Spectral dimensionality from variance partition. Five 20 tile subsets (**left**) each have very similar variance partition to the full 110 tile aggregate (**black**) with 99% variance in the first 3 dimensions. The aggregate of 120 land cover subcategory subsets (**right-black**) also has very similar variance partition with 98% in the first 3 dimensions. The individual land cover subcategories vary somewhat, with sand and ice + snow having lower dimensionality than more heterogeneous categories. All have <1% variance in all dimensions >4. Both mosaics can be considered 3D in the sense that the 3 low order dimensions represent >98% of total variance.

The topology of the Sentinel 2 MSI spectral mixing space is characterized with the low order principal components identified by the variance partition. As described by [20], apexes of the mixing space indicate spectral endmembers and straight edges between apexes indicate binary mixing lines between the corresponding endmembers. Three pairwise combinations of the three low order PCs provide orthogonal planar projections of the 3D mixing space. Because the PC transform maximizes variance partition into the smallest number of uncorrelated dimensions, it reveals the “global” structure of the mixing space corresponding to differences in the shape of the spectral continuum of different endmembers. Therefore, different categories of land cover with physical properties form distinct limbs on the mixing space.

An alternative approach can be provided by manifold learning. Here, “local” structure is revealed by a nonlinear mapping of high-dimensional spectra into lower-dimensional embedding space. This mapping is constructed in such a way to optimally preserve local (statistical “nearest neighbor”) distance and/or connectivity structures. In this analysis we use the Uniform Manifold Approximation and Projection (UMAP) algorithm [21] to provide a complementary projection for comparison to the PC-derived mixing space. The UMAP algorithm assumes that the Sentinel-2 spectra are uniformly distributed on a locally connected Riemannian manifold with an (approximately) locally constant Riemannian metric. UMAP models this manifold using a fuzzy topological structure, then seeks a low-dimensional (2- or 3-D) embedding with an optimally similar fuzzy topological structure. In general, the resulting embedding is nonlinear and not invertible. For excellent background information on UMAP, see: <https://umap-learn.readthedocs.io/en/latest/> (accessed on 1 October 2022).

All UMAP computations were performed using the open source `umap-learn` Python package on a commercially available laptop computer with 32 GB RAM, 2GHz Quad-Core Intel Core i5 CPU, and a 1536 MB Intel Iris Plus Graphics GPU. Hyperparameter sensitivity was investigated by sweeps which looped through various choices of `n_components`, `n_neighbors`, and `min_dist`. Results were found to be relatively insensitive to all three hyperparameters, within at least 2 orders of magnitude of variability. All UMAP shown in this analysis used `n_components = 2`, `n_neighbors = 5` or `500`, and `min_dist = 0.1`.

Spectral EMs derived from the composite spectral mixing space provide the basis for the standardized SVD model, which is inverted to provide endmember fraction estimates for all spectra in the mosaic. The 3 EM linear spectral mixture model is given explicitly as a

set of 11 band-specific mixing equations. Because the number of mixing equations exceeds the number of unknown fractions, the system is overdetermined, allowing for inversion by minimization of model misfit.

$$\begin{matrix}
 F_S E_1 + F_V E_1 + F_D E_1 & O_1 \\
 \vdots & \vdots \\
 F_S E_{11} + F_V E_{11} + F_D E_{11} & O_{11}
 \end{matrix} = \begin{matrix} \vdots \\ \vdots \\ \vdots \end{matrix} \quad \text{In matrix notation: } O = FE + \varepsilon \quad (3)$$

where E is the 3 column matrix of 11-band endmember vectors, O is the observed spectral vector to be modeled, $F_{S|V|D}$ is the vector of endmember fractions to be estimated, and ε is the model misfit to be minimized by the inversion. In addition, a unit sum constraint equation is included. The least squares solution, $F = (E^T E)^{-1} E^T O$ [22] for the S,V,D endmember fraction estimates gives fractions well-bounded [0, 1]. Model validity is assessed by the Root Mean Square (RMS) of the difference between observed and modeled spectra using the S, V, D estimates and endmember spectra in the forward model (L_2 norm).

3. Results

Information content of the Sentinel 2 MSI bands is quantified using both Pearson’s r parametric correlation and the mutual information (MI) metric for all 55 band pairs for the 8×10 land cover subcategory mosaic. Tables 1 and 2 give the r and MI matrices for each band pair for the 80 tile subset. In both matrices, values ≥ 0.8 are shown in bold italic. As in previous studies, the highest correlations occur between adjacent bands within the visible, near infrared (NIR) and shortwave infrared (SWIR) wavebands. However, unlike the study of [12] which focused only on soils and agriculture, this analysis also finds high correlations between visible and SWIR bands as a result of the high albedo sands included in the mosaic. The mutual information matrix shows a similar pattern of higher MI between adjacent band pairs within wavebands, but more pronounced than for r . In comparing correlations and MI estimates for all 55 band pairs, the two metrics show a decidedly nonlinear relationship, with a correlation of 0.88 and MI of 1.195 (r on MI) and 1.16 (MI on r) (Appendix A).

Table 1. Sentinel 2 MSI Band Pearson Correlation (r).

1	2	3	4	5	6	7	8	8a	11	12
1	0.62	0.57	0.5	0.47	0.31	0.21	0.21	0.18	0.39	0.42
0.62	1	0.96	0.85	0.8	0.53	0.35	0.37	0.3	0.67	0.71
0.57	0.96	1	0.95	0.93	0.7	0.52	0.55	0.48	0.82	0.85
0.5	0.85	0.95	1	0.99	0.76	0.57	0.6	0.53	0.92	0.95
0.47	0.8	0.93	0.99	1	0.84	0.65	0.69	0.63	0.95	0.96
0.31	0.53	0.7	0.76	0.84	1	0.9	0.96	0.94	0.87	0.8
0.21	0.35	0.52	0.57	0.65	0.9	1	0.91	0.92	0.71	0.62
0.21	0.37	0.55	0.6	0.69	0.96	0.91	1	0.98	0.76	0.66
0.18	0.3	0.48	0.53	0.63	0.94	0.92	0.98	1	0.71	0.6
0.39	0.67	0.82	0.92	0.95	0.87	0.71	0.76	0.71	1	0.98
0.42	0.71	0.85	0.95	0.96	0.8	0.62	0.66	0.6	0.98	1

The spectral dimensionality of both the 110 tile spectral diversity hotspot mosaic and the 120 subset land cover subcategory mosaic are nearly identical (Figure 3), suggesting that the subcategories chosen encompass the salient structure of the larger spectral diversity hotspot mosaic. The variance partition in Figure 3 indicates that both mosaics are effectively 3D, containing 99% and 98% of spectral variance in the three low order dimensions and $\ll 1\%$ variance in all higher order dimensions. Figure 3 also shows the variance partition of 5 subsets of 20 tiles each, compared to the variance partition of the full 110 tile spectral diversity hotspot mosaic. The fact that all 5 subsets have nearly identical variance partition to the full mosaic suggests that each is sufficiently spectrally diverse to encompass the

diversity of the full spectral mixing space. The implication of this convergence is that the full 110 tile mosaic is more than sufficient to encompass full global spectral diversity. Figure 3 also shows the variance partition of each of the 12 land cover subcategories compared to the variance partition of the full mosaic. As expected, there is significant variation among the subcategories with more homogeneous land cover like snow and sand showing lower relative dimensionality and others like evaporites showing higher relative dimensionality.

Table 2. Sentinel 2 MSI Band Mutual Information (MI, 3 nearest neighbors).

1	2	3	4	5	6	7	8	8a	11	12
1.06	0.86	0.56	0.42	0.41	0.19	0.17	0.15	0.15	0.29	0.33
0.68	1.39	0.85	0.61	0.58	0.25	0.22	0.21	0.2	0.39	0.44
0.49	0.96	1.28	0.83	0.8	0.38	0.31	0.32	0.28	0.54	0.57
0.39	0.83	0.9	1.17	1.03	0.59	0.52	0.53	0.49	0.68	0.76
0.34	0.66	0.83	0.99	1.29	0.69	0.57	0.54	0.52	0.81	0.79
0.14	0.21	0.36	0.5	0.59	1.37	1.03	0.96	0.93	0.55	0.43
0.1	0.16	0.28	0.44	0.5	1.04	1.34	1.11	1.19	0.46	0.39
0.09	0.16	0.28	0.44	0.46	0.95	1.08	1.4	1.08	0.45	0.37
0.08	0.14	0.24	0.39	0.44	0.9	1.15	1.08	1.42	0.44	0.37
0.24	0.41	0.53	0.67	0.81	0.64	0.58	0.57	0.58	1.28	0.88
0.27	0.51	0.6	0.78	0.88	0.55	0.51	0.5	0.5	1.01	1.1

The topology of the spectral mixing spaces of both mosaics are very similar and consistent with their spectral dimensionality. Figure 4 shows the 3D mixing spaces of the 110 tile Spectral Diversity Hotspot mosaic and the 120 subset land cover subcategory mosaic as orthogonal projections of bivariate PC distributions, along with the most conspicuous spectral endmembers from each. Both mixing spaces show complete mixing continua spanning the Substrate, Vegetation and Dark endmembers (PC 3 vs. 2 projections)—although the greatest spectral variance is associated with the PC 1 vs. 2 projection, driven by the strong contrast of the two highest albedo endmembers, sand and snow. Snow/ice and reefs each form distinct mixing continua with the Dark endmember, while evaporites form more distinct clusters without a single dominant mixing continuum. This suggests a more complex spectral continuum that may not be as linear as the others. It is noteworthy that neither reefs nor evaporites generally represent linear spectral mixing among distinct land cover types. Whereas aggregate albedo of most landscapes is modulated by a combination of reflectance, illumination flux density and shadow, the albedo of reefs is also strongly influenced by water depth while the albedo of evaporite basins is most strongly modulated by moisture content and the presence of standing water. Purely cryospheric environments are distinguished from other environments by their more homogeneous gradients spanning the snow-firn-ice continuum. Partial snow cover in non-cryospheric environments (e.g., boreal forests) may exhibit linear or nonlinear spectral mixing, but is sufficiently complex to warrant a more focused investigation separately.

Because reefs, evaporite basins and cryospheric environments are geographically and spectrally distinct from the SVD continuum that encompasses the majority of Earth's biomes, the focus of the rest of the analysis is on the 8×10 column subset of the land cover subcategories spanning the SVD continuum. This mixing space is effectively 2D with $(81\% + 14\% =) 95\%$ of variance in the two low order PC dimensions. This triangular mixing space is dominated by the Substrate-Dark and Vegetation-Dark mixing continua as seen in Figure 5. Unlike previous studies, the Sentinel 2 MSI SVD space shows a clear distinction (kink & discontinuity) between high albedo sands and the lower albedo substrates that bound one side of the SVD continuum. Most non-forest biomes fall within this continuum, with varying amounts of nonphotosynthetic vegetation (NPV) and exposed substrate interspersed with herbaceous and woody photosynthetic vegetation.

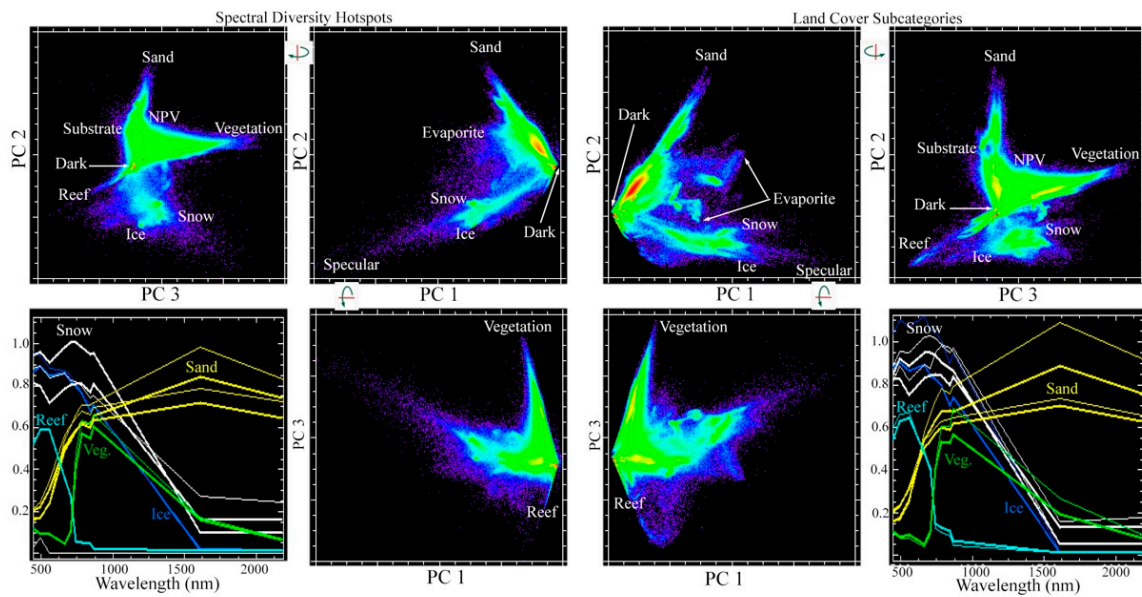


Figure 4. Spectral mixing spaces for Sentinel 2 mosaics. Orthogonal projections show the 3D topology of the PC spaces as continuous with clearly defined apexes corresponding to physically distinct spectral endmembers. Vegetation and Sand + Substrate endmembers show strongly linear mixing with the Dark (shadow or water) endmember. Both mosaics have very similar topology and endmembers in the 3D PC space, indicating that the 120 land cover subcategories capture the salient features of the 110 spectral diversity hotspots.

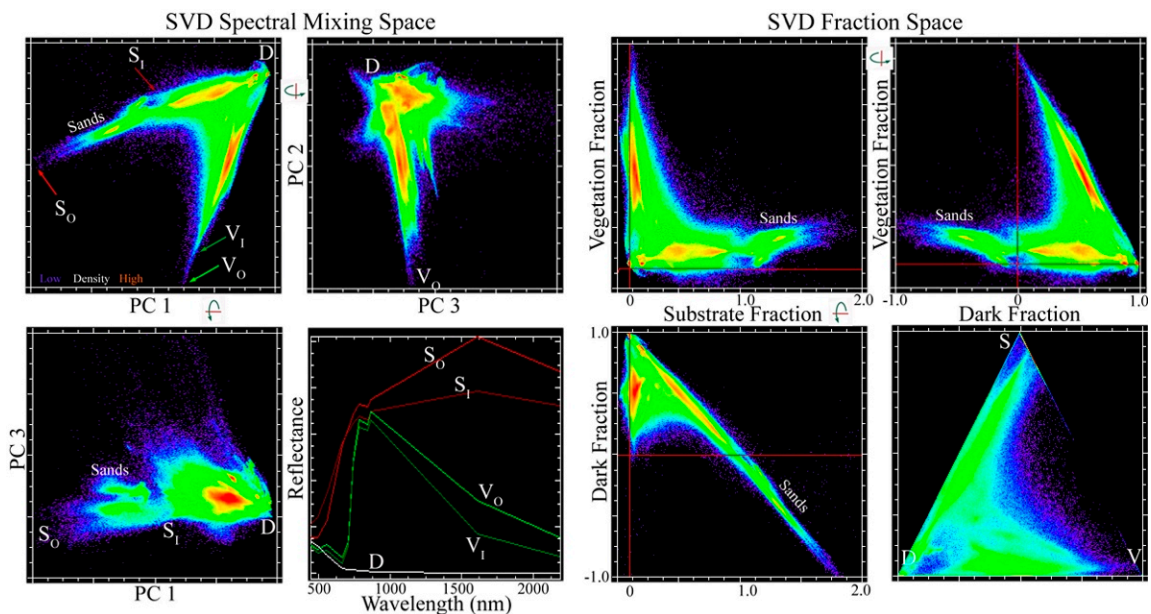


Figure 5. Sentinel 2 SVD spectral mixing space, spectral endmembers, and the corresponding SVD fraction space. An eight column (80,000,000 spectra) subset of the Land Cover Subcategory mosaic encompassing the SVD-bounded plane of the full mixing space is effectively 2D with PC dimensions 1 (81%) and 2 (14%) accounting for 95% of total variance, compared to PC 3 (2%). Maximum amplitude (Outer) and lower amplitude mean (Inner) endmember spectra for Substrate and Vegetation define bases for maximal and minimal SVD models (left). Inversion of the minimal model provides liberal estimates of SVD fractions (right), but excludes pure sand landscapes. Because sands lie outside the minimal SVD model, their Substrate fractions exceed 1.0 with Dark fractions < 0. The resulting planar SVD fraction distribution can be projected onto a 2D ternary diagram (lower right) with no loss of information.

The Substrate limb discontinuity, combined with the diffuse apex of the Vegetation limb suggest two different, but related, SVD models. Because pure sands (e.g., dunefields) rarely support vegetation communities, an SVD model using an inner Substrate endmember (S_i) is more physically plausible than an SVD model using an outer Substrate endmember (S_o) composed of pure sand. However, the outer Substrate endmember could be used for modeling landscapes where bright sands are prominent. Similarly, an outer Vegetation endmember (V_o) composed of a single pixel spectrum is less representative than an inner Vegetation endmember (V_i) composed of an average of several individual spectra at the more densely occupied inner Vegetation apex of the mixing space. Comparisons of inner and outer S and V endmembers are shown in Figure 5. All 5 endmember spectra are given in Table 3.

Table 3. Sentinel 2 MSI Spectral Endmembers (Exoatmospheric reflectance $\times 10,000$).

λ (nm)	S_i	V_i	D	S_o	V_o
443	1754	1084	1198	1536	1194
490	1799	827	946	1556	909
560	2154	892	739	2291	969
665	3028	410	280	5485	447
705	3303	1070	208	6236	1126
740	3472	4206	180	6889	4762
783	3656	5646	167	7323	6323
842	3566	5495	135	7176	6193
865	3686	6236	129	7530	6629
1610	5097	2101	26	10,252	1731
2190	4736	775	14	8745	712

Inversion of the SVD linear mixture model using the inner S_i and V_i endmembers yields the SVD fraction space shown in Figure 5. As expected, S fractions for the high albedo sands outside the triangular model exceed 1.0 with Dark fractions <0 , but all other fraction estimates are well-bounded $[0, 1]$. Relatively small percentages of the binary S-D and V-D mixtures have V and S (respectively) fractions are slightly negative, but almost all are within 5% of 0. As shown in Figure 6, the spectra with these slightly negative near-zero fractions are limited to a few spatially contiguous geographies (e.g., mangroves, dunes or volcanic ash deposits). The distribution of RMS misfit between the observed and modeled spectra for the 80 subcategory composite has $<6\%$ misfit for $>99\%$ of 80,000,000 Sentinel 2 spectra, with the upper tail of higher misfits also limited to a few specific land covers not represented in the SVD model (e.g., turbid water, evaporites and light snow).

The SVD fraction composite for the 8×10 land cover subcategories (Figure 7) is skewed toward RGB primaries, consistent with the S-D and V-D binary mixing continua seen in the SVD mixing space. The larger, more spatially heterogeneous collection of 110 spectral diversity hotspot tiles shows a wider range of intermediate spectral mixtures, as would be expected.

The spectral mixing space rendered by the 2D UMAP embedding preserves the binary S-D and V-D mixing trends that dominate the PC and fraction spaces. Figure 8 shows a broader mixing continuum for the V-D limb extending to NPV-dominant biomes near the distinct S-D continuum. However, both UMAP embeddings also show a number of distinct clusters located outside the S-D and V-D continua. Most obvious are the several distinct sand clusters associated with different dunefields with distinct sand mineralogies. Additionally, noteworthy are the single distinct clusters associated with two tundra sites in the Canadian and Alaskan arctic and the single cluster associated with two mangrove sites in the Bangladesh Sundarban. It is noteworthy that all of the distinct clusters are associated with

specific, spatially contiguous, areas within individual (sometimes multiple) subsets that are evident when labeled clusters in the UMAP space are back-projected to geographic space.

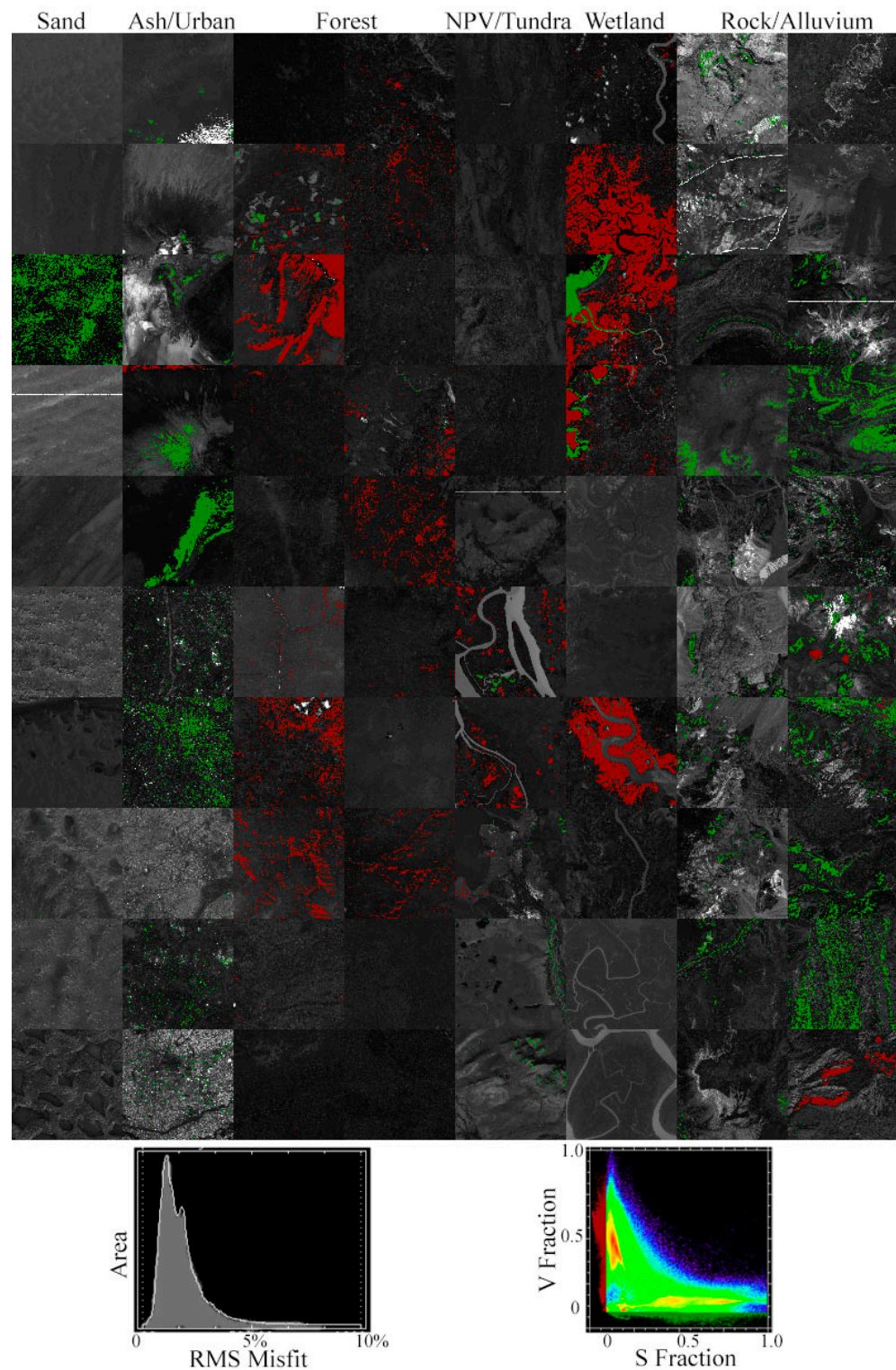


Figure 6. SVD model misfit and negative fraction distributions. RMS misfit map (linear stretch [0, 10%]) shows largest misfits associated with snow, evaporites and turbid water. RMS distribution shows 99% of spectra with <5% misfit (92% < 3%). Negative S (red) and V (green) fractions are well within 0.1 of zero.

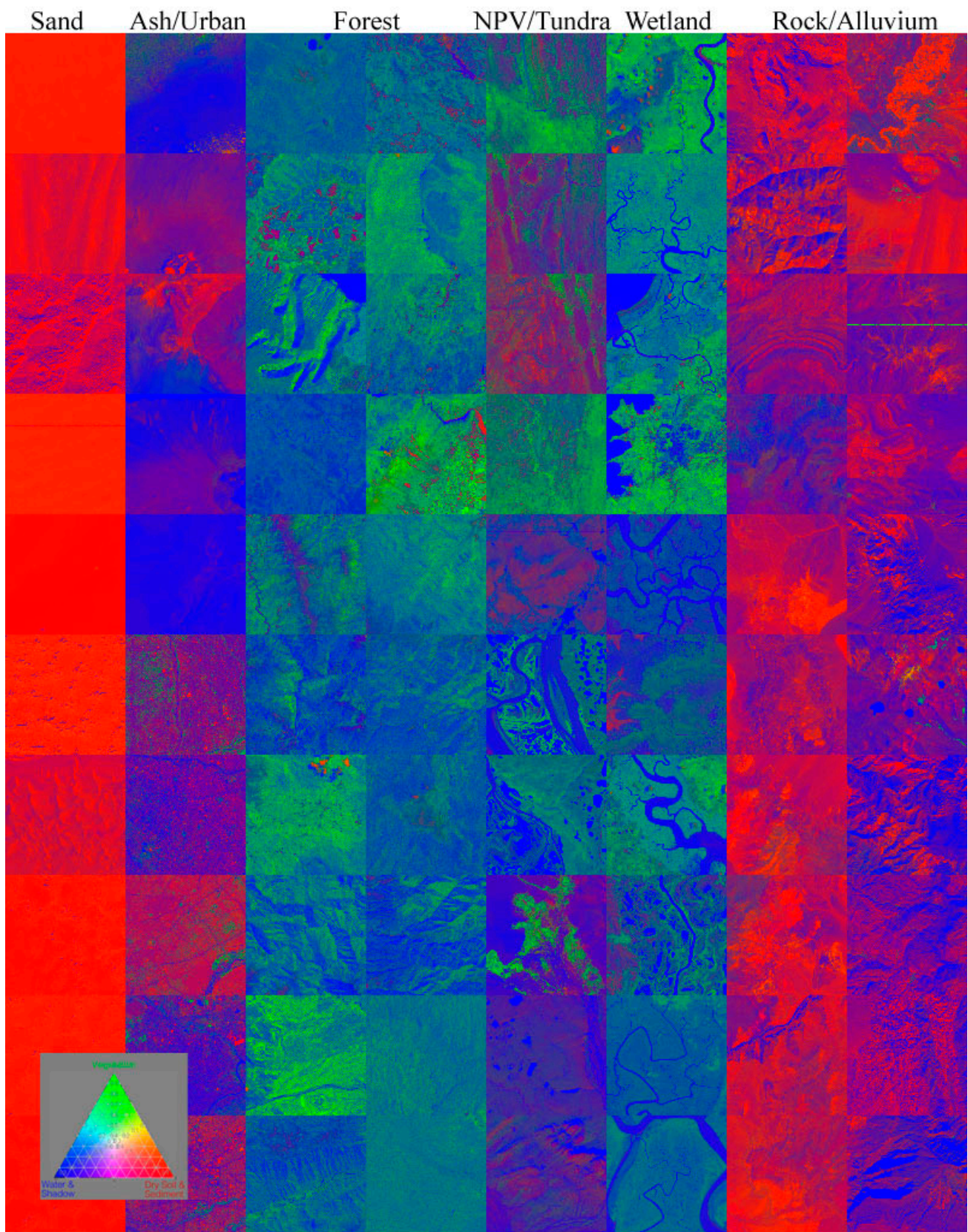


Figure 7. Minimal model SVD fraction mosaic for the primary land cover subset. Linear stretch [0, 1] for all fractions. Sands are saturated red because they are outside the minimal model with S_j fractions > 1 .

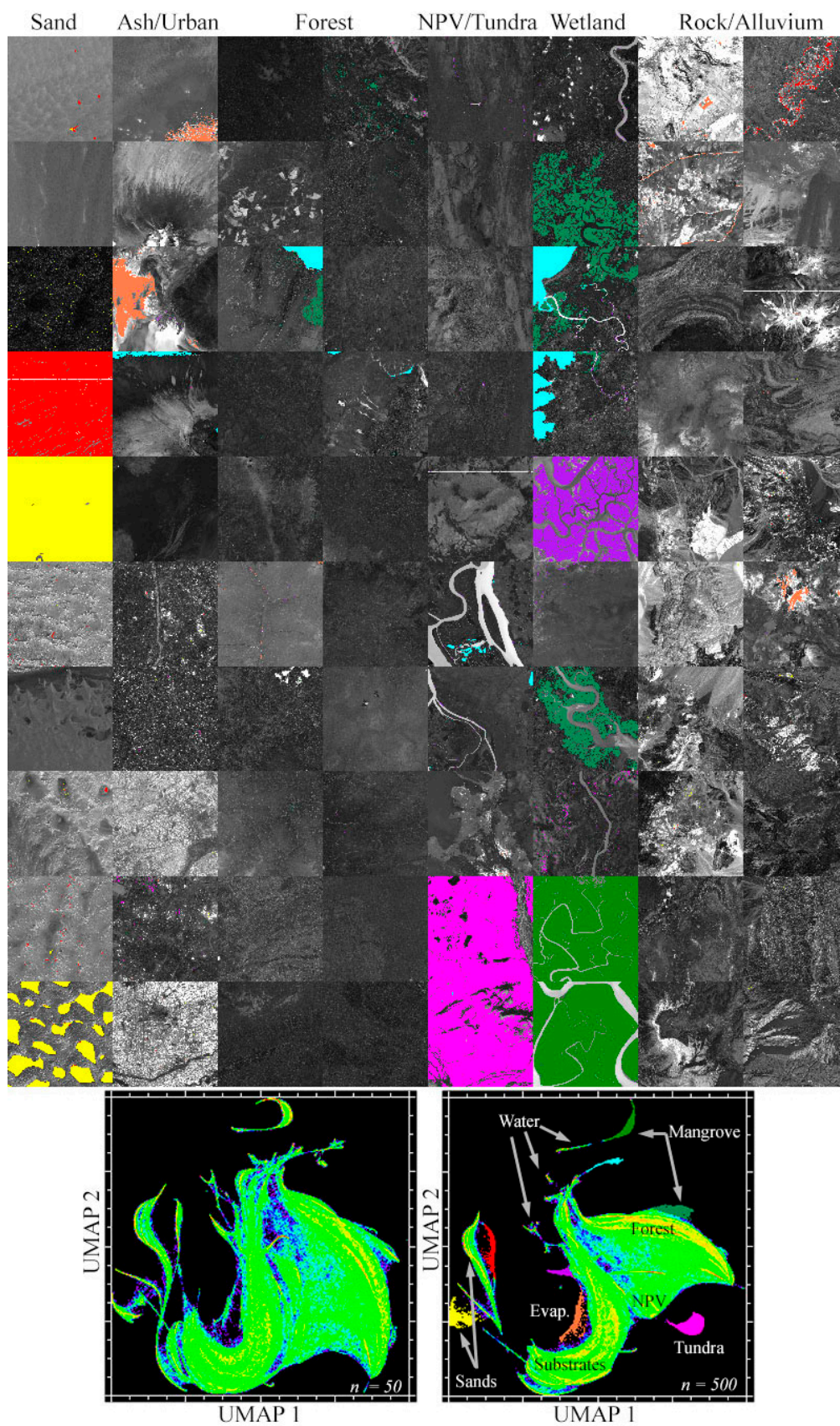


Figure 8. UMAP manifolds with distinct clusters labeled in mixing space then back-projected into geographic space (on RMS misfit map). Distinct clusters of spectra in the mixing space correspond to geographically distinct and spatially contiguous land cover.

4. Discussion

4.1. Spectral Information Content

The increased NIR spectral resolution of the Sentinel 2 MSI sensors contributes substantially to the spectral information content. While the correlations of adjacent spectral bands within the visible, NIR and SWIR are >0.8 , scatterplots of band pairs reveal conspicuous departures from linearity in all but the highest correlations ($>\sim 0.95$) which are reflected in correspondingly lower MI scores. A comparison of all bands with MSI band 8 in Appendix A illustrates a variety of such features, suggesting a diversity of spectra with significantly different reflectance (e.g., absorptions) between adjacent spectral bands. As in previous studies using Landsat multispectral and AVIRIS hyperspectral, the primary correlation structure clearly distinguishes visible, NIR and SWIR wavebands [12], but both r and MI suggest only moderate redundancy between adjacent spectral bands within each waveband. This may be partially responsible for the two clearly diverging lower limbs of the V-D continuum ($F_v < \sim 0.5$) trending toward the Dark endmember and toward the ternary mixing NPV + soil + shadow region near the S-D mixing continuum. Empirically, these mixing trends appear to correspond to closed and open canopy forest. Figure 5 also shows two distinct subparallel clusters on a single mixing trend on the V-D mixing continuum in the PC 3 vs. 2 space. These features are not seen in either the Landsat or MODIS mixing spaces [7,8].

Among the new VNIR bands provided by Sentinel 2 MSI, the greatest redundancy appears to be among bands 7, 8 and 8a, as indicated by some of the highest MI values. Whereas bands 4 and 5 have a correlation of 0.99, their MI is a comparatively lower 1.03, suggesting that the MI metric can resolve nonredundancies that correlation does not. The curvature of the log-linear relationship between the upper tails of the r and MI relationship (Appendix A) suggests that the two metrics are sensitive to different disparities between band reflectance distributions. Given the wide diversity of reflectances included in these mixing spaces, the similarities and differences in spectral continuum shape may overshadow meaningful differences in VNIR band information content. The fact that the UMAP embeddings identify a number of distinct clusters and apexes not apparent in the PC-derived feature space suggests that subtle differences in continuum curvature captured by the narrow NIR bands may indeed provide potentially useful resolving power to discriminate between otherwise similar reflectances within land cover subcategories.

4.2. Spectral Dimensionality and Mixing Space Topology

While the full mixing spaces shown in Figure 4 are both 3D, neither is amenable to a single mixture model containing 6+ endmembers (SVD + evaporite, reef, snow/ice). Such a mixture model would be both physically and mathematically implausible. Physically, as discussed above, reefs, evaporite basins and cryospheric landscapes are generally distinct from the continuum of biomes (Figure 1) in which a substrate continuum is interspersed with multiple scales of photosynthetic and nonphotosynthetic vegetation and structural shadow. Mathematically, the similarity of spectral shape of many evaporites with ice and snow spectra, and the inverse similarity of both to vegetation spectra will destabilize any inversion containing either two or all three of these endmembers because they are far from orthogonal, and often nearly colinear. The result is significant percentages of strongly negative (< -0.5) fractions in one or more of the fraction distributions. These are the primary reasons we focus on the 8×10 subset mosaic and the SVD model for the latter part of this analysis.

4.3. The SVD Model

The new, lower amplitude, Substrate endmember identified from the break in the S-D continuum supports a more physically plausible mixture model than earlier SVD models which used sand spectra for the Substrate EM. Using high albedo sand as an endmember has the undesirable consequence of likely underestimating the true substrate fraction in most situations where sand is not actually present. While we have advocated the use

of local Substrate endmembers in previous studies, we find the use of a more realistic standardized Substrate reflectance as a reasonable substitute in situations where a single local Substrate endmember cannot be identified. In many landscapes, a more distinct plane of substrates may be more apparent than in the mixing spaces of these unusually diverse collections of spectra. If so, local soil and NPV endmembers might be distinguishable, as we have found in similar analyses of compilations of hyperspectral data in agricultural environments [13]. Because we did not identify a distinct apex associated with NPV in either of the composite mixing spaces, and observe that NPV occupies an intermediate region on the Substrate-Dark mixing continuum, we find no reason to extend the SVD model to include a NPV endmember.

The use of a lower amplitude inner Substrate endmember also provides more dynamic range to the Substrate fraction distribution by eliminating the much brighter sands which compress the dynamic range of the Substrate fraction. Allowing greater dynamic range may also facilitate distinction between different dry soil reflectances and different moisture content within a single soil type. At present, variations in dry reflectance and variations in moisture content are accommodated by varying fractions of Dark endmember—representing a fundamental ambiguity in the SVD model specifically and broadband reflectance generally. While this distinction may be impossible in single date imagery, spatiotemporal variations in soil moisture (and hence the S-D fraction continuum) of a single location may facilitate distinguishing these two effects on soil reflectance.

4.4. Manifold Topology and Spectral Resolution

The use of nonlinear, nonparametric dimensionality reduction provides a new and potentially very useful approach to spectral feature/mixing space characterization [23]. The presence of numerous distinct clusters in the UMAP projections contrasts strongly to the much more continuous PC-derived feature spaces. While the latter are essential to identifying spectral endmembers and verifying linearity of spectral mixing, the variance maximization on which the PC transform is based is much more sensitive to the shape of the spectral continuum than the presence of more subtle (lower variance) absorption features. In contrast, manifold learning algorithms that preserve local structure in the form of nearest neighbor proximity (e.g., UMAP, t-SNE) make it possible to identify more subtle differences in spectral curvature and absorption features (often aliased in multispectral imagery) that convey real physical meaning and may considerably extend the usable information content of narrowband multispectral sensors like Sentinel 2 MSI. The companion study to this [24] carries this duality a step further by combining the physically interpretable structure of the SVD mixing space with the more subtle features of local scale manifolds in the form of a joint characterization of the spectral mixing space.

In summary, the construction of a diverse collection of Sentinel 2 MSI tiles from 110 spectral diversity hotspots worldwide provides a basis for a globally representative spectral feature space. Because spectral mixing is pervasive in most biomes, even at 10 m resolution, we refer to this aliased feature space as a spectral mixing space. Identification of more spectrally homogeneous examples of a variety of specific land cover subcategories makes it possible to separate landscapes dominated by nonlinear spectral mixing (reefs, evaporite basins and cryospheric landscapes) from the more linear SVD continuum that spans most terrestrial biomes. Global standardized SVD endmembers chosen from the inner apexes of the SVD mixing space provide the basis for a general model of fractional subpixel land cover that is applicable to most biomes. While the PC-based mixing space allows for unambiguous identification of spectral endmembers, and determination of linearity of mixing (and inversion of linear mixture models), the use of nonlinear manifold learning to project proximity-preserving embeddings of the higher dimensional mixing space allows for identification of both mixing continua and isolated clusters of spectrally distinct land covers that are not generally apparent in the PC-based mixing space.

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Data Availability Statement: The data supporting this manuscript can be downloaded free of charge from the web portals listed in the main text.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Correlation and Mutual Information

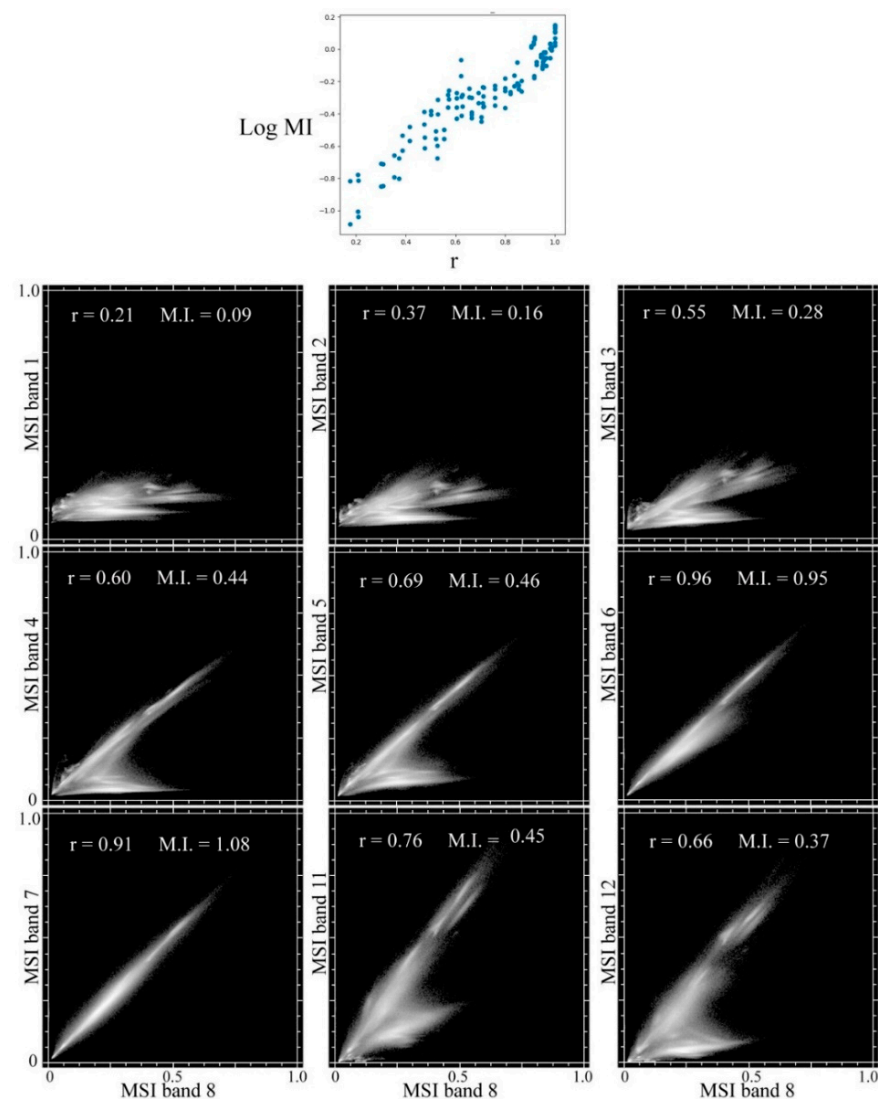


Figure A1. Correlation vs. Mutual Information estimates and band to band bivariate distributions for the 80 land cover specific subset mosaic. For all band to band pairs (top) correlation and Mutual Information estimates show a correlation of 0.88 and MI of 1.195 (r on MI) and 1.16 (MI on r), with some degree of Log-linear scaling on the lower tail of the distribution and clear nonlinearity on the upper tail. The range of both metrics suggests that almost all non-adjacent, and some adjacent, band combinations provide some discriminative utility for at least some land cover subcategories. Bivariate distributions of MSI band 8 with all other bands show considerable deviations from linearity for all but band 7.

Appendix B

Table A1. Sentinel 2 tileIDs.

c1	c2
S2A_MSIL1C_20160723T143750_T19KEQ	S2A_MSIL1C_20170205T210921_N0204_R057_T04QHH
S2A_MSIL1C_20160723T143750_T19KER	S2B_MSIL1C_20180311T185149_N0206_R113_T10SFJ
S2A_MSIL1C_20170118T081241_N0204_R078_T35MRV	S2A_MSIL1C_20170315T101021_N0204_R022_T32TPP
S2A_MSIL1C_20170119T074231_N0204_R092_T36JTT	S2A_MSIL1C_20170412T074611_N0204_R135_T37PDQ
S2A_MSIL1C_20170119T074231_N0204_R092_T36JUT	S2A_MSIL1C_20170427T021921_N0205_R060_T50HLH
S2A_MSIL1C_20170119T143731_N0204_R096_T20NNM	S2A_MSIL1C_20170427T153621_N0205_R068_T18NTP
S2A_MSIL1C_20170124T051101_N0204_R019_T43PGL	S2A_MSIL1C_20170428T215921_N0205_R086_T01KFS
S2A_MSIL1C_20170124T051101_N0204_R019_T44RQV	S2A_MSIL1C_20170506T054641_N0205_R048_T42QXM
S2A_MSIL1C_20170124T165551_N0204_R026_T14QQE	S2A_MSIL1C_20170508T012701_N0205_R074_T54STE
S2A_MSIL1C_20170125T202521_N0204_R042_T58CDU	S2A_MSIL1C_20170604T043701_N0205_R033_T45RYL
c3	c4
S2A_MSIL1C_20170613T182921_N0205_R027_T11SMB	S2A_MSIL1C_20170723T064631_N0205_R020_T41TKG
S2A_MSIL1C_20170620T181921_N0205_R127_T12TTK	S2A_MSIL1C_20170723T182921_N0205_R027_T11UQQ
S2A_MSIL1C_20170621T074941_N0205_R135_T37RGL	S2A_MSIL1C_20170724T145731_N0205_R039_T18LZL
S2A_MSIL1C_20170627T180911_N0205_R084_T12SUF	S2A_MSIL1C_20170830T125301_N0205_R138_T27WXM
S2A_MSIL1C_20170627T180911_N0205_R084_T12SUG	S2A_MSIL1C_20170830T131241_N0205_R138_T23KLP
S2A_MSIL1C_20170628T173901_N0205_R098_T13SCS	S2A_MSIL1C_20170908T063621_N0205_R120_T40QFK
S2A_MSIL1C_20170704T013711_N0205_R031_T52MHD	S2A_MSIL1C_20170914T065621_N0205_R063_T40TFQ
S2A_MSIL1C_20170705T022551_N0205_R046_T50NMN	S2A_MSIL1C_20170915T213531_N0205_R086_T06WVS
S2A_MSIL1C_20170718T210021_N0205_R100_T08WNB	S2A_MSIL1C_20170916T055631_N0205_R091_T42RUN
S2A_MSIL1C_20170719T084601_N0205_R107_T41XNE	S2A_MSIL1C_20170917T190351_N0205_R113_T10SFG
c5	c6
S2A_MSIL1C_20170919T142931_N0205_R139_T23VMH	S2A_MSIL1C_20171117T064141_N0206_R120_T40RFU
S2B_MSIL1C_20180328T183949_N0206_R070_T11SKA	S2A_MSIL1C_20171129T142031_N0206_R010_T18FXJ
S2A_MSIL1C_20170923T074231_N0205_R049_T37PHN	S2A_MSIL1C_20171201T150711_N0206_R039_T18LZH
S2A_MSIL1C_20171002T150621_N0205_R039_T19LBE	S2A_MSIL1C_20171203T034121_N0206_R061_T48QUM
S2A_MSIL1C_20171003T143321_N0205_R053_T20MQC	S2A_MSIL1C_20171207T082321_N0206_R121_T34HCH
S2A_MSIL1C_20171013T080931_N0205_R049_T25CEM	S2A_MSIL1C_20171208T111441_N0206_R137_T29QKD
S2A_MSIL1C_20171016T073911_N0205_R092_T36MZC	S2A_MSIL1C_20171209T072301_N0206_R006_T38QND
S2A_MSIL1C_20171017T103021_N0205_R108_T32TLQ	S2A_MSIL1C_20171210T065251_N0206_R020_T40QCJ
S2A_MSIL1C_20171107T070231_N0206_R120_T39LUC	S2A_MSIL1C_20160615T183312_N0204_R127_T11SPS
S2A_MSIL1C_20171117T064141_N0206_R120_T40RFU	S2A_OPER_PRD_MSIL1C_PDMC_20150813T101657
c7	c8
S2A_MSIL1C_20150813T101026_N0204_R022_T32UPU	S2A_OPER_MSI_L1C_TL_EPA_20161012T193400_A006777_T55KCB
S2A_MSIL1C_20151022T184002_N0204_R027_T115MA	S2B_MSIL1C_20170713T023549_N0205_R089_T51RTN
S2A_OPER_PRD_MSIL1C_PDMC_20151206T145051	S2B_MSIL1C_20170723T124309_N0205_R095_T28WDT
S2A_OPER_PRD_MSIL1C_PDMC_20160318T145513_01	S2B_MSIL1C_20170727T053639_N0205_R005_T43SFV
S2A_OPER_MSI_L1C_TL_SGS_20161011T162433_A006812_T32WPT	S2B_MSIL1C_20170730T040549_N0205_R047_T47SND
S2A_OPER_MSI_L1C_TL_SGS_20161013T032322_A006834_T56LKR	S2B_MSIL1C_20170816T005709_N0205_R002_T53JQJ
S2A_OPER_MSI_L1C_TL_EPA_20161012T193400_A006777_T55LCC	S2B_MSIL1C_20170817T114639_N0205_R023_T33XWF
S2A_OPER_MSI_L1C_TL_MTI_20161014T211238_A006858_T15MXV	S2B_MSIL1C_20170824T145909_N0205_R125_T22WEV
S2A_OPER_MSI_L1C_TL_SGS_20161017T100159_A006894_T45QYG	S2B_MSIL1C_20170826T155519_N0205_R011_T17NMJ
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S2B_MSIL1C_20170912T084549_N0205_R107_T36TUL	S2B_MSIL1C_20171019T083959_N0205_R064_T36STF
S2B_MSIL1C_20170912T170949_N0205_R112_T14RPL	S2B_MSIL1C_20171101T004649_N0206_R102_T54JTL
S2B_MSIL1C_20170916T215519_N0205_R029_T06WVB	S2B_MSIL1C_20171103T061009_N0206_R134_T42SWC
S2B_MSIL1C_20170918T054629_N0205_R048_T43SDT	S2B_MSIL1C_20171103T061009_N0206_R134_T42SWD
S2B_MSIL1C_20170918T205119_N0205_R057_T07VEG	S2B_MSIL1C_20171116T132219_N0206_R038_T23KPK
S2B_MSIL1C_20170919T140039_N0205_R067_T21KVA	S2B_MSIL1C_20171123T043059_N0206_R133_T45QYE
S2B_MSIL1C_20170929T222959_N0205_R072_T60KWF	S2B_MSIL1C_20171130T160619_N0206_R097_T17RMH
S2B_MSIL1C_20171008T105009_N0205_R051_T30TYN	S2B_MSIL1C_20171202T064229_N0206_R120_T40RGU
S2B_MSIL1C_20171009T003649_N0205_R059_T55MDP	S2B_MSIL1C_20171207T105419_N0206_R051_T30RVT
c11	
S2B_MSIL1C_20171208T052209_N0206_R062_T44SMD	
S2B_MSIL1C_20180729T141049_N0206_R110_T21LTC	
S2B_MSIL1C_20171208T084329_N0206_R064_T33JWN	
S2B_MSIL1C_20171212T064249_N0206_R120_T40QEL	
S2B_MSIL1C_20171212T064249_N0206_R120_T40QFH	
S2B_MSIL1C_20171212T100359_N0206_R122_T32RLQ	
S2B_MSIL1C_20180622T085559_N0206_R007_T34RGS	
S2B_MSIL1C_20171214T155519_N0206_R011_T18RUN	
S2B_MSIL1C_20171215T152629_N0206_R025_T18NUF	
S2B_MSIL1C_20171227T160459_N0206_R054_T17QME	

Table A2. TileIDs and NW corner coordinates of land cover subcategory subsets.

Agriculture			
<i>TileID</i>	<i>UTM Zone</i>	<i>Easting</i>	<i>Northing</i>
S2A_MSIL1C_20170205T210921_N0204_R057_T04QHH	4N	868610	2223190
S2A_MSIL1C_20170315T101021_N0204_R022_T32TPP	32N	623950	4864330
S2A_MSIL1C_20170508T012701_N0205_R074_T54STE	54N	269220	3988590
S2A_MSIL1C_20170723T064631_N0205_R020_T41TKG	41N	266210	4645260
S2A_MSIL1C_20170917T190351_N0205_R113_T10SFG	10N	688930	4167330
S2A_OPER_PRD_MSIL1C_PDMC_20161017T044357	45N	723470	2625060
S2B_MSIL1C_20170730T040549_N0205_R047_T47SND	47N	554190	4363690
S2B_MSIL1C_20170918T054629_N0205_R048_T43SDT	43N	459570	3800040
S2B_MSIL1C_20171008T105009_N0205_R051_T30TYN	30N	702100	4787760
S2B_MSIL1C_20171013T081959_N0205_R121_T36SYF	36N	778000	4095680
Sand			
<i>TileID</i>	<i>UTM Zone</i>	<i>Easting</i>	<i>Northing</i>
S2A_MSIL1C_20170628T173901_N0205_R098_T13SCS	13N	372290	3654900
S2A_MSIL1C_20170908T063621_N0205_R120_T40QFK	40N	653400	2447190
S2A_MSIL1C_20171119T040041_N0206_R004_T48TUK	48N	305540	4438710
S2A_MSIL1C_20171208T111441_N0206_R137_T29QKD	29N	291550	2399280
S2A_MSIL1C_20171209T072301_N0206_R006_T38QND	38N	527910	1890720
S2B_MSIL1C_20171207T105419_N0206_R051_T30RVT	30N	481880	3290910
S2B_MSIL1C_20171208T084329_N0206_R064_T33JWN	33S	541880	7265640
S2B_MSIL1C_20171212T100359_N0206_R122_T32RLQ	32N	339750	2966720
S2B_MSIL1C_20171212T100359_N0206_R122_T32RLR	32N	331950	3100020
Lava & Ash			
<i>TileID</i>	<i>UTM Zone</i>	<i>Easting</i>	<i>Northing</i>
S2A_MSIL1C_20170205T210921_N0204_R057_T04QHH	4N	861160	2206290
S2A_MSIL1C_20171016T073911_N0205_R092_T36MZC	36S	819250	9703580
S2A_MSIL1C_20171016T073911_N0205_R092_T36MZC	36S	834220	9768640
S2A_OPER_PRD_MSIL1C_PDMC_20161014T163303	15S	652170	9967520
S2B_MSIL1C_20170723T124309_N0205_R095_T28WDT	28N	399960	7200220
Urban			
<i>TileID</i>	<i>UTM Zone</i>	<i>Easting</i>	<i>Northing</i>
S2A_MSIL1C_20170508T012701_N0205_R074_T54STE	54N	269890	3950620
S2A_MSIL1C_20170830T131241_N0205_R138_T23KLP	23S	328970	7398470
S2A_MSIL1C_20170916T055631_N0205_R091_T42RUN	42N	300000	2758120
S2A_MSIL1C_20171017T103021_N0205_R108_T32TLQ	32N	390060	4999690
S2B_MSIL1C_20170912T170949_N0205_R112_T14RLP	14N	364980	2848280
Forest—1			
<i>TileID</i>	<i>UTM Zone</i>	<i>Easting</i>	<i>Northing</i>
S2A_MSIL1C_20170118T081241_N0204_R078_T35MRV	35S	831290	9963030
S2A_MSIL1C_20170119T074231_N0204_R092_T36JTT	36S	284150	7247210
S2A_MSIL1C_20170205T210921_N0204_R057_T04QHH	4N	847400	2230620
S2A_MSIL1C_20170427T021921_N0205_R060_T50HLH	50S	355240	6230970
S2A_MSIL1C_20170508T012701_N0205_R074_T54STE	54N	257880	3907290
S2A_MSIL1C_20170604T043701_N0205_R033_T45RYL	45N	794940	3088140
S2A_MSIL1C_20170705T022551_N0205_R046_T50NMMN	50N	450950	704020
S2A_MSIL1C_20170724T145731_N0205_R039_T18LZL	18S	875170	8546360
S2A_MSIL1C_20170724T145731_N0205_R039_T19LBF	19S	215640	8582190
S2A_MSIL1C_20170830T131241_N0205_R138_T23KLP	23S	321220	7348390
Forest—2			
<i>TileID</i>	<i>UTM Zone</i>	<i>Easting</i>	<i>Northing</i>
S2A_MSIL1C_20170917T190351_N0205_R113_T10SFG	10N	607440	4106660
S2A_OPER_PRD_MSIL1C_PDMC_20151206T145051	20N	469370	431170
S2B_MSIL1C_20170713T023549_N0205_R089_T51RTN	51N	231700	3257530
S2B_MSIL1C_20170718T101029_N0205_R022_T32TQS	32N	773730	5121020
S2B_MSIL1C_20170906T002659_N0205_R016_T55KCA	55S	353630	8006280
S2B_MSIL1C_20170912T084549_N0205_R107_T36TUL	36N	335150	4512660
S2B_MSIL1C_20171009T003649_N0205_R059_T55MDP	55S	469610	9317570
S2B_MSIL1C_20171013T081959_N0205_R121_T36SYF	36N	791100	4092030
S2B_MSIL1C_20171116T132219_N0206_R038_T23KKP	23S	215910	7344400
S2B_MSIL1C_20171215T152629_N0206_R025_T18NUF	18N	381240	26200
Senescent Vegetation			
<i>TileID</i>	<i>UTM Zone</i>	<i>Easting</i>	<i>Northing</i>
S2A_MSIL1C_20170119T074231_N0204_R092_T36JUT	36S	387540	7237130
S2A_MSIL1C_20170119T074231_N0204_R092_T36JUT	36S	381920	7259800
S2A_MSIL1C_20170119T074231_N0204_R092_T36JUT	36S	375110	7261040
S2A_MSIL1C_20170119T074231_N0204_R092_T36JUT	36S	379990	7209420
S2A_MSIL1C_20170516T154911_N0205_R054_T18TWQ	18N	563770	4938390

Table A2. Cont.

Tundra & Wetlands			
TileID	UTM Zone	Easting	Northing
S2A_MSIL1C_20170718T210021_N0205_R100_T08WNB	8N	508380	7654750
S2A_MSIL1C_20170718T210021_N0205_R100_T08WNB	8N	540940	7608620
S2A_OPER_PRD_MSIL1C_PDMC_20160318T145513	19S	495986	7997974
S2B_MSIL1C_20170916T215519_N0205_R029_T06WVB	6N	442210	7700040
S2B_MSIL1C_20170916T215519_N0205_R029_T06WVB	6N	458950	7676830
Mangroves			
TileID	UTM Zone	Easting	Northing
S2A_MSIL1C_20170427T153621_N0205_R068_T18NTP	18N	258620	824760
S2A_MSIL1C_20170704T013711_N0205_R031_T52MHD	52S	814620	9839210
S2A_MSIL1C_20170705T022551_N0205_R046_T50NMN	50N	498390	752360
S2A_MSIL1C_20170705T022551_N0205_R046_T50NMN	50N	423780	704730
S2A_MSIL1C_20170916T055631_N0205_R091_T42RUN	42N	319520	2736030
S2A_OPER_PRD_MSIL1C_PDMC_20161018T073751	38N	655730	3419140
S2B_MSIL1C_20170826T155519_N0205_R011_T17NMJ	17N	472220	875270
S2B_MSIL1C_20170919T140039_N0205_R067_T21KVA	21S	445610	8017250
S2B_MSIL1C_20171123T043059_N0206_R133_T45QYE	45N	756960	2481220
S2B_MSIL1C_20171123T043059_N0206_R133_T45QYE	45N	763390	2429410
Rock & Alluvium—1			
TileID	UTM Zone	Easting	Northing
S2A_MSIL1C_20160723T143750_T19KER	19S	506000	7534310
S2A_MSIL1C_20170124T051101_N0204_R019_T44RQV	44N	781870	3417600
S2A_MSIL1C_20170412T074611_N0204_R135_T37PDQ	37N	467190	1496550
S2A_MSIL1C_20170412T074611_N0204_R135_T37PDQ	37N	415880	1480390
S2A_MSIL1C_20170613T182921_N0205_R027_T11SMB	11N	478340	4162580
S2A_MSIL1C_20170613T182921_N0205_R027_T11SMB	11N	441920	4110190
S2A_MSIL1C_20170613T182921_N0205_R027_T11SMB	11N	424630	4194020
S2A_MSIL1C_20170613T182921_N0205_R027_T11SMB	11N	429810	4180830
S2A_MSIL1C_20170627T180911_N0205_R084_T12SUF	12N	310360	4011400
S2A_MSIL1C_20170627T180911_N0205_R084_T12SUF	12N	304930	4096250
Rock & Alluvium—2			
TileID	UTM Zone	Easting	Northing
S2A_MSIL1C_20170627T180911_N0205_R084_T12SUG	12N	393280	4169500
S2A_MSIL1C_20170908T063621_N0205_R120_T40QFK	40N	664760	2494790
S2A_MSIL1C_20171201T150711_N0206_R039_T18LZH	18S	866060	8213050
S2A_MSIL1C_20171207T082321_N0206_R121_T34HCH	34S	395100	6286480
S2A_OPER_PRD_MSIL1C_PDMC_20151022T184002	11N	516790	4027140
S2A_OPER_PRD_MSIL1C_PDMC_20160318T145513	19S	486817	8008443
S2B_MSIL1C_20171103T061009_N0206_R134_T42SWC	42N	576560	3774420
S2B_MSIL1C_20171103T061009_N0206_R134_T42SWD	42N	544220	3856340
S2B_MSIL1C_20171202T064229_N0206_R120_T40RGU	40N	768340	3304040
S2B_MSIL1C_20171212T064249_N0206_R120_T40QEL	40N	520620	2570980

References

1. Drusch, M.; Del Bello, U.; Carlier, S.; Colin, O.; Fernandez, V.; Gascon, F.; Hoersch, B.; Isola, C.; Laberinti, P.; Martimort, P. Sentinel-2: ESA's Optical High-Resolution Mission for GMES Operational Services. *Remote Sens. Environ.* **2012**, *120*, 25–36. [[CrossRef](#)]
2. Wulder, M.A.; Roy, D.P.; Radeloff, V.C.; Loveland, T.R.; Anderson, M.C.; Johnson, D.M.; Healey, S.; Zhu, Z.; Scambos, T.A.; Pahlevan, N. Fifty Years of Landsat Science and Impacts. *Remote Sens. Environ.* **2022**, *280*, 113195. [[CrossRef](#)]
3. Boardman, J.W.; Green, R.O. Exploring the Spectral Variability of the Earth as Measured by AVIRIS in 1999. In *Proceedings of the Summaries of the 8th Annual JPL Airborne Geoscience Workshop*; NASA: Pasadena, CA, USA, 2000; Volume 1, pp. 1–12.
4. Cawse-Nicholson, K.; Hook, S.J.; Miller, C.E.; Thompson, D.R. Intrinsic Dimensionality in Combined Visible to Thermal Infrared Imagery. *IEEE J. Sel. Top. Appl. Earth Obs. Remote Sens.* **2019**, *12*, 4977–4984. [[CrossRef](#)]
5. Small, C. The Landsat ETM+ Spectral Mixing Space. *Remote Sens. Environ.* **2004**, *93*, 1–17. [[CrossRef](#)]
6. Small, C.; Milesi, C. Multi-Scale Standardized Spectral Mixture Models. *Remote Sens. Environ.* **2013**, *136*, 442–454. [[CrossRef](#)]
7. Sousa, D.; Small, C. Global Cross-Calibration of Landsat Spectral Mixture Models. *Remote Sens. Environ.* **2017**, *192*, 139–149. [[CrossRef](#)]
8. Sousa, D.; Small, C. Globally Standardized MODIS Spectral Mixture Models. *Remote Sens. Lett.* **2019**, *10*, 1018–1027. [[CrossRef](#)]
9. Sousa, D.; Brodrick, P.G.; Cawse-Nicholson, K.; Fisher, J.B.; Pavlick, R.; Small, C.; Thompson, D.R. The Spectral Mixture Residual: A Source of Low-Variance Information to Enhance the Explainability and Accuracy of Surface Biology and Geology Retrievals. *J. Geophys. Res. Biogeosci.* **2022**, *127*, e2021JG006672. [[CrossRef](#)]
10. Kauth, R.J.; Thomas, G.S. The Tasseled Cap—A Graphic Description of the Spectral-Temporal Development of Agricultural Crops as Seen by Landsat. In *LARS Symposia*; Purdue University: West Lafayette, IN, USA, 1976; p. 159.

11. Crist, E.P.; Cicone, R.C. A Physically-Based Transformation of Thematic Mapper Data—The TM Tasseled Cap. *IEEE Trans. Geosci. Remote Sens.* **1984**, *GE-22*, 256–263. [[CrossRef](#)]
12. Sousa, D.; Small, C. Multisensor Analysis of Spectral Dimensionality and Soil Diversity in the Great Central Valley of California. *Sensors* **2018**, *18*, 583. [[CrossRef](#)] [[PubMed](#)]
13. Sousa, D.; Small, C. Linking Common Multispectral Vegetation Indices to Hyperspectral Mixture Models: Results from 5 Nm, 3 m Airborne Imaging Spectroscopy in a Diverse Agricultural Landscape. *arXiv* **2022**, arXiv:2208.06480.
14. Small, C. Global Population Distribution and Urban Land Use in Geophysical Parameter Space. *Earth Interact.* **2004**, *8*, 1–18. [[CrossRef](#)]
15. Houghton, J.T.; Meira Filho, L.G.; Callander, B.A.; Harris, N.; Kattenberg, A.; Maskell, K. *Climate Change 1995: The Science of Climate Change*; Cambridge University Press: Cambridge, UK, 1996; 572p.
16. Shannon, C.E. A Mathematical Theory of Communication. *Bell Syst. Tech. J.* **1948**, *27*, 379–423. [[CrossRef](#)]
17. Kozachenko, L.F.; Leonenko, N.N. Sample Estimate of the Entropy of a Random Vector. *Probl. Peredachi Inf.* **1987**, *23*, 9–16.
18. Kraskov, A.; Stögbauer, H.; Grassberger, P. Estimating Mutual Information. *Phys. Rev. E* **2004**, *69*, 066138. [[CrossRef](#)] [[PubMed](#)]
19. Ross, B.C. Mutual Information between Discrete and Continuous Data Sets. *PLoS ONE* **2014**, *9*, e87357. [[CrossRef](#)] [[PubMed](#)]
20. Boardman, J.W. Automating Spectral Unmixing of AVIRIS Data Using Convex Geometry Concepts. *AVIRIS Workshop* **1993**, *1*, 11–14.
21. McInnes, L.; Healy, J.; Melville, J. Umap: Uniform Manifold Approximation and Projection for Dimension Reduction. *arXiv* **2018**, arXiv:1802.03426.
22. Settle, J.J.; Drake, N.A. Linear Mixing and the Estimation of Ground Cover Proportions. *Int. J. Remote Sens.* **1993**, *14*, 1159–1177. [[CrossRef](#)]
23. Sousa, D.; Small, C. Joint Characterization of Multiscale Information in High Dimensional Data. *Adv. Artif. Intell. Mach. Learn.* **2021**, *1*, 196–212. [[CrossRef](#)]
24. Sousa, D.; Small, C. Joint Characterization of Sentinel-2 Reflectance: Insights from Manifold Learning. *Remote Sens.* **2022**, *14*, 5688. [[CrossRef](#)]