# SITS: Data Analysis and Machine Learning for Data Cubes using Satellite Image Time Series

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Using time series derived from big Earth Observation data sets is one of the leading research trends in Land Use Science and Remote Sensing. One of the more promising uses of satellite time series is its application for classification of land use and land cover, since our growing demand for natural resources has caused major environmental impacts. Here, we present an open source *R* package for satellite image time series analysis called sits. Package sits provides support on how to use statistical learning techniques with image time series obtained from data cubes. These methods include linear and quadratic discrimination analysis, support vector machines, random forests, boosting, deep learning and convolution neural networks.

#### Introduction

Earth observation satellites provide a regular and consistent set of information about the land and oceans of the planet. Recently, most space agencies have adopted open data policies, making unprecedented amounts of satellite data available for research and operational use. This data deluge has brought about a major challenge: *How to design and build technologies that allow the Earth observation community to analyse big data sets?* 

The approach taken in the current work is to develop data analysis methods that work with satellite image time series, obtained by taking calibrated and comparable measures of the same location in Earth at different times. These measures can be obtained by a single sensor (e.g., MODIS) or by combining different sensors (e.g., Landsat 8 and Sentinel-2). If obtained by frequent revisits, the temporal resolution of these data sets can capture important land use changes.

Time series of remote sensing data show that land cover can occur not only in a progressive and gradual way, but they may also show discontinuities with abrupt changes [Lambin et al., 2003]. Analyses of multiyear time series of land surface attributes, their fine-scale spatial pattern, and their seasonal evolution leads to a broader view of land-cover change. Satellite image time series have already been used in applications such

as mapping for detecting forest disturbance [Kennedy et al., 2010], ecology dynamics [Pasquarella et al., 2016], agricultural intensification [Galford et al., 2008], and its impacts on deforestation [Arvor et al., 2012]. Algorithms for processing image time series include BFAST for detecting breaks [Verbesselt et al., 2010], TIMESAT for modelling and measuring phenological attributes [Jönsson and Eklundh, 2004] and methods based on Dynamic Time Warping (DTW) for land use and land cover classification [Petitjean et al., 2012][Maus et al., 2016].

In this work, we present SITS, an open source R package for satellite image time series analysis. It provides support on how to use machine learning techniques with image time series. These methods include linear and quadratic discrimination analysis, support vector machines, random forests, and neural networks. One important contribution of the SITS package is to support the complete cycle of data analysis for time series classification, including data acquisition, visualisation, filtering, clustering, classification, validation and post-classification adjustments.

Most studies using satellite image time series for land cover classification use a *space-first, time-later* approach. For multiyear studies, researchers first derive best-fit yearly composites and then classify each composite image. For a review of these methods for land use and land cover classification using time series, see [Gomez et al., 2016]. As an alternative to *Space-first, time-later* methods, the SITS package provides support for classification of time series, preserving the full temporal resolution of the input data, using a *time-first, space-later* approach. SITS uses all data in the image time series to create larger dimensional spaces for machine learning. The idea is to have as many temporal attributes as possible, increasing the dimension of the classification space. Each temporal instance of a time series is taken as an independent dimension in the feature space of the classifier. To the authors' best knowledge, the classification techniques for image time series included in the package are not previoulsy available in other R or python packages. Furthermore, the package includes methods for filtering, clustering and post-processing that also have not been published in the literature.

#### Image data cubes as the basis for big Earth observation data analysis

In broad terms, the cloud computing model is one where large satellite-generated data sets are archived on cloud services, which also provide computing facilities to process them. By using cloud services, users can share big Earth observation databases and minimize the amount of data download. Investment in infrastructure is minimised and sharing of data and software increases. However, data available in the cloud is best organised for analysis by creating data cubes.

Generalising Appel and Pebesma [2019], we consider that a data cube is a four-dimensional structure with dimensions x (longitude or easting), y (latitude or northing), time, and bands. Its spatial dimensions refer to a single spatial reference system (SRS). Cells of a data cube have a constant spatial size (with regard to the cube's SRS). The temporal dimension is specified by a set of intervals. For every combination of dimensions, a cell has a single value. Data cubes are particularly amenable for machine learning techniques; their data cane be transformed into arrays in memory, which can be fed to

training and classification algorithms. Given the widespread availability of large data sets of Earth observation data, there is a growing interest in organising large sets of data into "data cubes".

As explained below, a data cube is the data type used in sits to handle dense raster data. Many of the operations involve creating, transforming and analysing data cubes.

# Using Web Data Services to Access Image Data Cubes

One of the distinguishing features of SITS is that it has been designed to work with big satellite image data sets which reside on the cloud and with data cubes. Many *R* packages that work with remote sensing images require data to be accessible in a local computer. However, with the coming of age of big Earth observation data, it is not always practical to transfer large data sets. Users have to rely on web services to provide access to these data sets. In this context, SITS is based on access to data cubes using web services.

A web service is software system designed to support remote access to image collections through APIs. These are machine-to-machine protocols that allow access to image collections and to generate *data cubes*. Currently, sits uses the WTSS ("Web Time Series Serice"). WTSS is a light-weight service for retrieval of time series data for selected locations and periods [Vinhas et al., 2016]. The WTSS R client is available in the CRAN archive using the wtss package.

These services are set on the SITS configuration file, which is described later in this document. For each services, the above function lists the names of the data cubes available and additional information.

# Defining a data cube using the WTSS service

To define a data cube for the WTSS, in principle the following parameters should be provided: (a) the type of the service ("WTSS"); (b) the URL; (c) the satellite and sensor associated to the cube, and (d) name of the data cube in the remote service. The package will retrieve the information about the cube from the WTSS service.

MODIS

## 1 WTSS http://www.esensing.dpi.inpe.br/wtss TERRA

```
# spatial dimensions of the data cube
wtss_cube %>% dplyr::select(xmin, xmax, ymin, ymax)
## # A tibble: 1 x 4
##
      xmin xmax ymin ymax
     <dbl> <dbl> <dbl> <dbl> <
## 1 -81.2 -30.0 -40.0 10.0
# temporal dimension of the data cube
timeline <- sits_timeline(wtss_cube)</pre>
# first date of the data cube
timeline[1]
## [1] "2000-02-18"
# last date of the data cube
timeline[length(timeline)]
## [1] "2019-09-30"
# number of steps in the data cube
length(timeline)
## [1] 452
# bands of the data cube
sits_bands(wtss_cube)
## [1] "mir" "blue" "nir"
```

## Defining a data cube using files organised as raster bricks

The SITS package enables uses to create data cube based on files. In this case, these files should be organized as raster bricks. A RasterBrick is a multi-layer raster object used by the *R* raster package. Each brick is a multi-layer file, containing different time instances of one spectral band. To allow users to create data cubes based on files, SITS needs to know what is the timeline of the data sets and what are the names of the files that contain the RasterBricks. The example below shows one bricks containing 392 time instances of the "ndvi" band for the years 2000 to 2016. The timeline is available as part of the SITS package. In this example, as in most cases using raster bricks, images are stored as GeoTiff files.

Since GeoTiff files do not contain information about satellites and sensors, it is best practice to provide information on satellite and sensor.

```
# get information on the data cube
raster_cube %>% dplyr::select(type, URL, satellite, sensor)
## # A tibble: 1 x 4
##
     type URL
                            satellite sensor
                            <chr>
                                      <chr>
##
    <chr> <chr>
## 1 BRICK http://127.0.0.1 TERRA
                                      MODIS
# get information on the coverage
raster_cube %>% dplyr::select(xmin, xmax, ymin, ymax)
## # A tibble: 1 x 4
##
          xmin
                              ymin
                    xmax
                                        ymax
##
         <dbl>
                   <dbl>
                             <dbl>
                                       <dbl>
## 1 -6054361. -6051117. -1282895. -1280347.
```

To create the raster cube, we a set of consistent raster bricks (one for each satellite band) and a timeline that matches the input images of the raster brick. Once created, the coverage can be used either to retrieve time series data from the raster bricks using sits\_get\_data() or to do the raster classification by calling the function sits\_classify.

#### Data structures for satellite image time series

The sits package requires a set of time series data, describing properties in spatiotemporal locations of interest. For land use classification, this set consists of samples provided by experts that take *in-situ* field observations or recognize land classes using high resolution images. The package can also be used for any type of classification, provided that the timeline and bands of the time series (used for training) match that of the data cubes.

For handling time series, the package uses a sits tibble to organize time series data with associated spatial information. A tibble is a generalization of a data. frame, the usual way in *R* to organise data in tables. Tibbles are part of the tidyverse, a collection of R packages designed to work together in data manipulation [Wickham and Grolemund, 2017]. As a example of how the sits tibble works, the following code shows the first three lines of a tibble containing 2,115 labelled samples of land cover in Mato Grosso state of Brazil. It is the most important agricultural frontier of Brazil and it is the largest producer of soybeans, corn, and cotton. The samples contain time series extracted from the MODIS MOD13Q1 product from 2000 to 2016, provided every 16 days at 250-meter spatial resolution in the Sinusoidal projection. Based on ground surveys and high resolution imagery, it includes 425 samples of nine classes: "Forest", "Cerrado", "Pasture", "Soybean-fallow", "Fallow-Cotton", "Soybean-Cotton", "Soybean-Corn", "Soybean-Millet", and "Soybean-Sunflower".

```
# data set of samples
data(samples_mt_4bands)
samples_mt_4bands[1:3,]
```

```
## # A tibble: 3 x 9
    id_sample cluster_label longitude latitude start_date end_date label cube
##
       <int> <chr>
                             <dbl>
                                     <dbl> <date>
                                                     <date>
                                                                <chr> <chr>
## 1
          1 Pasture
                            -55.2 -10.8 2013-09-14 2014-08-29 Past~ MOD1~
                                   -9.76 2006-09-14 2007-08-29 Past~ MOD1~
## 2
          2 Pasture
                            -57.8
                           -51.9 -13.4 2014-09-14 2015-08-29 Past~ MOD1~
## 3
          3 Pasture
    ... with 1 more variable: time_series <list>
```

A sits tibble contains data and metadata. The first six columns contain the metadata: spatial and temporal information, label assigned to the sample, and the data cube from where the data has been extracted. The spatial location is given in longitude and latitude coordinates for the "WGS84" ellipsoid. For example, the first sample has been labelled "Cerrado, at location (-58.5631, -13.8844), and is considered valid for the period (2007-09-14, 2008-08-28). Informing the dates where the label is valid is crucial for correct classification. In this case, the researchers involved in labeling the samples chose to use the agricultural calendar in Brazil, where the spring crop is planted in the months of September and October, and the autumn crop is planted in the months of February and March. For other applications and other countries, the relevant dates will most likely be different from those used in the example. The time\_series column contains the time series data for each spatiotemporal location. This data is also organized as a tibble, with a column with the dates and the other columns with the values for each spectral band.

```
# print the first time series records of the first sample
sits_time_series(samples_mt_4bands[1,])[1:3,]
```

The sits package provides functions for data manipulation and displaying information for sits tibbles. For example, sits\_labels() shows the labels of the sample set and their frequencies.

## sits\_labels(samples\_mt\_4bands)

```
## # A tibble: 9 x 3
##
     label
                   count
                            prop
     <chr>
##
                   <int>
                           <dbl>
## 1 Cerrado
                     379 0.200
                      29 0.0153
## 2 Fallow_Cotton
## 3 Forest
                     131 0.0692
## 4 Pasture
                     344 0.182
## 5 Soy_Corn
                     364 0.192
## 6 Soy_Cotton
                     352 0.186
## 7 Soy_Fallow
                      87 0.0460
## 8 Soy_Millet
                     180 0.0951
## 9 Soy_Sunflower
                      26 0.0137
```

In many cases, it is useful to relabel the data set. For example, there may be situations when one wants to use a smaller set of labels, since samples in one label on the original set may not be distinguishable from samples with other labels. We then could use sits\_relabel(), which requires a conversion list (for details, see ?sits\_relabel).

Given that we have used the tibble data format for the metadata and and the embedded time series, one can use the functions from dplyr, tidyr and purrr packages of the tidyverse [Wickham and Grolemund, 2017] to process the data. For example, the following code uses sits\_select\_bands() to get a subset of the sample data set with two bands (NDVI and EVI) and then uses the dplyr::filter() to select the samples labelled either as "Cerrado" or "Pasture". We can then use the plot.sits() function (or use plot() directly) to display the time series. Given a small number of samples to display, plot.sits() tries to group as many spatial locations together. In the following example, the first 15 samples of "Cerrado" class refer to the same spatial location in consecutive time periods. For this reason, these samples are plotted together.

```
# select NDVI band
samples_ndvi.tb <- sits_select_bands(samples_mt_4bands, ndvi)
# select only samples with Cerrado label
samples_cerrado.tb <-
    dplyr::filter(samples_ndvi.tb, label == "Cerrado")
# plot the first sample
plot(samples_cerrado.tb[1,])</pre>
```

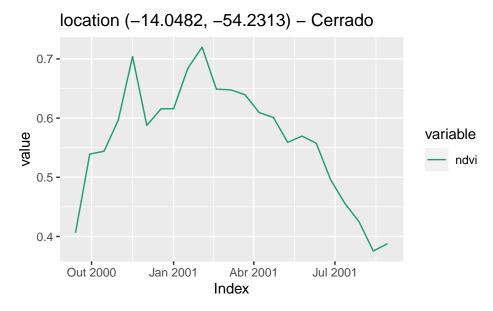


Figure 1: Plot of the first 'Cerrado' sample from data set

For a large number of samples, where the amount of individual plots would be substantial, the default visualization combines all samples together in a single temporal interval (even if they belong to different years). All samples with the same band and label are aligned to a common time interval. This plot is useful to show the spread of values for the time series of each band. The strong red line in the plot shows the median of the values, while the two orange lines are the first and third interquartile ranges. The documentation of plot.sits() has more details about the different ways it can display data.

```
# plot all cerrado samples together
plot(samples_cerrado.tb)
```

## Obtaining time series data

To get a time series in SITS, one has to create a data cube first, as described above. Alternatively, the time series can also be converted from data stored in the ZOO format [Zeileis and Grothendieck, 2005]. Users can request one or more time series points from a data cube by using sits\_get\_data(). This function provides a general means of



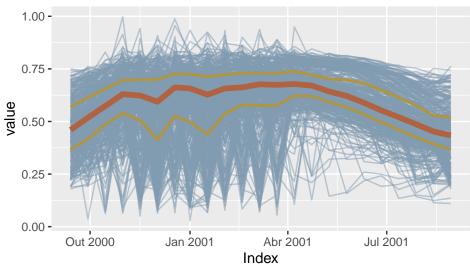


Figure 2: Plot of all Cerrado samples from data set

access to image time series. Given data cue, the user provides the latitude and longitude of the desired location, the bands, and the start date and end date of the time series. If the start and end dates are not provided, it retrieves all the available period. The result is a tibble that can be visualized using plot().

A useful case is when a set of labelled samples are available to be used as a training data set. In this case, one usually has trusted observations which are labelled and commonly stored in plain text CSV files. Function sits\_get\_data() can get a CSV file path as an argument. The CSV file must provide, for each time series, its latitude and longitude, the start and end dates, and a label associated to a ground sample. An example of a CSV file used is shown below:

```
# print the first line of a CSV file used to retrieve data
csv_sinop <- system.file("extdata/samples/samples_matogrosso.csv", package = "sits")
head(read.csv(csv_sinop))

## # A tibble: 6 x 6
## id longitude latitude start_date end_date label
## <int> <dbl> <dbl> <chr> <chr> <chr>
```

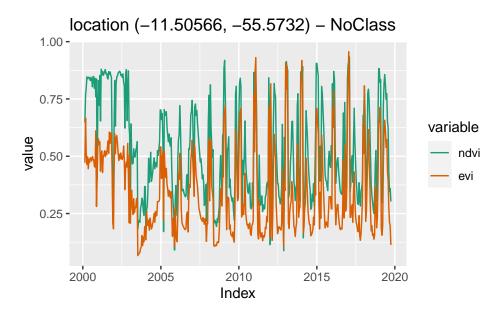


Figure 3: NDVI and EVI time series fetched from WTSS service.

```
## 1
               -55.0
                         -15.2 2015-09-14 2016-08-28 Pasture
         2
               -55.0
                         -15.2 2015-09-14 2016-08-28 Pasture
##
## 3
         3
               -55.0
                         -15.2 2015-09-14 2016-08-28 Pasture
## 4
         4
               -46.6
                         -10.4 2004-09-13 2005-08-29 Cerrado
## 5
         5
               -46.4
                         -10.9 2007-09-13 2008-08-29 Cerrado
## 6
               -46.4
                         -10.9 2006-09-13 2007-08-29 Cerrado
# read the first three samples from the CSV file
csv_data <- sits_get_data(cube = wtss_cube, file = csv_sinop, .n_max_csv = 3)</pre>
```

## All points have been retrieved from WTSS service

csv\_data

```
## # A tibble: 3 x 7
##
     longitude latitude start_date end_date
                                                label
                                                         cube
                                                                 time_series
##
                   <dbl> <date>
                                     <date>
                                                <chr>
                                                         <chr>
                                                                 st>
       -55.0
## 1
               -15.2 2015-09-14 2016-08-28 Pasture MOD13Q1 <tibble [23 x 7]>
## 2
       -55.0
               -15.2 2015-09-14 2016-08-28 Pasture MOD13Q1 <tibble [23 x 7]>
## 3
       -55.0
               -15.2 2015-09-14 2016-08-28 Pasture MOD13Q1 <tibble [23 x 7]>
```

A common situation is when users have samples available as shapefiles in point format. Since shapefiles contain only geometries, we need to provide information about the start and end times for which each label is valid. in this case, one should use the function sits\_get\_data() to retrieve data from a data cube based on the contents of the shapefile. The parameter shp\_attr (optional) indicates the name of the column on

the shapefile which contains the label to be associated to each time series; the parameter .n\_shp\_pol (defaults to 20) determines the number of samples to be extracted from each polygon.

```
# define the input shapefile (consisting of POLYGONS)
shp_file <- system.file("extdata/shapefiles/parcel_agriculture.shp",</pre>
                         package = "sits")
# set the start and end dates
start_date <- lubridate::ymd("2012-08-29")</pre>
end_date <- lubridate::ymd("2013-08-13")</pre>
# define the name of attribute of the shapefile that contains the label
shp_attr <- "ext_na"</pre>
# define the number of samples to extract from each polygon
.n_shp_pol <- 10
# read the points in the shapefile and produce a CSV file
data <- sits_get_data(cube = wtss_cube,</pre>
                       file = shp_file,
                       start_date = start_date,
                       end_date = end_date,
                       shp_attr = shp_attr,
                       .n_{shp_pol} = .n_{shp_pol}
```

 $\hbox{\it \#\# although coordinates are longitude/latitude, st\_relate\_pattern assumes that they are planar}$ 

```
## Linking to GEOS 3.7.2, GDAL 2.4.2, PROJ 5.2.0
```

## although coordinates are longitude/latitude, st\_intersects assumes that they are planar
## although coordinates are longitude/latitude, st\_intersects assumes that they are planar

## although coordinates are longitude/latitude, st\_relate\_pattern assumes that they are planar

## although coordinates are longitude/latitude, st\_intersects assumes that they are planar
## although coordinates are longitude/latitude, st\_intersects assumes that they are planar

## although coordinates are longitude/latitude, st\_relate\_pattern assumes that they are planar

## although coordinates are longitude/latitude, st\_intersects assumes that they are planar
## although coordinates are longitude/latitude, st\_intersects assumes that they are planar

```
data
```

```
## # A tibble: 10 x 7
## longitude latitude start_date end_date label cube time_series
## <dbl> <dbl> <date> <chr> <chr> chr> <list>
```

```
-15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
## 1
       -55.2
##
   2
        -55.2
                -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
               -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
##
   3
       -55.2
       -55.2
               -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
##
   5
        -55.2
               -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
##
##
   6
        -55.2
               -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
##
   7
        -55.2
               -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
        -55.2
## 8
               -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
## 9
        -55.2
                -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
## 10
        -55.2
               -15.4 2012-08-29 2013-08-13 Soja_Algodao MOD13~ <tibble [22 x 7~
```

## Filtering techniques

The literature on satellite image time series have several applications of filtering to correct or smooth vegetation index data. The following filters are available in SITS and are described in more detail in the vignette "Satellite Image Time Series Filtering with SITS":

- Savitzky–Golay filter (sits\_sgolay)
- Whittaker filter (sits\_whittaker)
- Envelope filter (sits\_envelope)
- ARIMA filter for cloud removal in NDVI band (sits\_ndvi\_arima)
- Cloud filter (sits\_cloud\_removal)
- Kalman filter (sits\_kalman)

The SITS package uses a common interface to all filter functions with the sits\_filter. The function has two parameters: data for the dataset to be filtered and filter for the filter to be applied. To aid on data visualisation, all bands which are filtered have a suffix which is appended, as shown in the examples below. Here we show an example using the Whittaker smoother, which has been proposed in literature [Atzberger and Eilers, 2011] as arguably the most appropriate one to use for satellite image time series. The Whittaker smoother attempts to fit a curve that represents the raw data, but is penalized if subsequent points vary too much [Atzberger and Eilers, 2011]. As such, it balances between the residual to the original data and the "smoothness" of the fitted curve. It uses the parameter lambda to control the degree of smoothing. I

```
# Take a NDVI time series, apply Whittaker filter and plot the series
point_whit <- sits_filter(point_ndvi, filter = sits_whittaker(lambda = 5.0))
# merge with original data and plot the original and the filtered data
point_whit %>%
    sits_merge(point_ndvi) %>%
    plot()
```

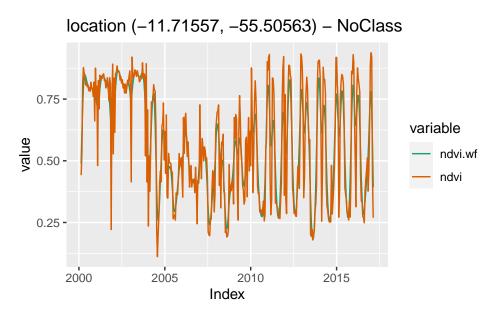


Figure 4: Whittaker smoother filter applied on one-year NDVI time series. The example uses default  $\lambda = 3$  parameter.

## Clustering for sample quality control using self-organizing maps

One of the key challenges of machine learning classification models is assessing the quality of the training data sets. It is useful to apply pre-processing methods to improve the quality of the samples and to remove those that might have been wrongly labeled or that have low discriminatory power. Good samples lead to good classification maps. sits provides support for two clustering methods to test sample quality: (a) Agglomerative Hierarchical Clustering (AHC); (b) Self-organizing Maps (SOM). In what follows, we briefly describe the use of SOM for clustering, which is applicable for large data sets such as those used in machine learing. Full details of the cluster methods used in SITS are available in the vignette 'Clustering of Satellite Image Time Series with SITS'.

Self-organizing maps (SOM) is a dimensionality reduction technique [Kohonen et al., 2001], where high-dimensional data is mapped into two dimensions, keeping the topological relations between data patterns. The input data is a set of training samples which are typically of a high-dimension. For example, a time series of 25 instances of 4 spectral bands is a 100-dimensional data set. The output layer is a 2D grid of neurons, each associated to a weight vector of the same dimension as the input space. The general idea of SOM-based clustering is that, by projecting the high-dimensional data set of training samples into a 2D map, good quality samples of each class should be close together in the resulting map. SITS provides the convenience function sits\_cluster\_som to perform clustering using SOM, This function uses self-organized maps to find clusters in satellite image time series for quality control of the samples.

```
# clustering time series using SOM
# return a tibble with all samples and which cluster it belongs
som_cluster.tb <-</pre>
```

```
sits::sits_cluster_som(prodes_226_064,
    grid_xdim = 10,
    grid_ydim = 10,
    alpha = 1.0,
    distance = "euclidean",
    iterations = 20,
    conditonal_threshold = 0.8,
    posterior_threshold = 0.6)
```

```
## [1] " -- There is no sample to be analyzed! == "
```

## Classification using machine learning

There has been much recent interest in using classifiers such as support vector machines [Mountrakis et al., 2011] and random forests [Belgiu and Dragut, 2016] for remote sensing images. Most often, researchers use a *space-first, time-later* approach, in which the dimension of the decision space is limited to the number of spectral bands or their transformations. Sometimes, the decision space is extended with temporal attributes. To do this, researchers filter the raw data to get smoother time series [Brown et al., 2013, Kastens et al., 2017]. Then, using software such as TIMESAT [Jönsson and Eklundh, 2004], they derive a small set of phenological parameters from vegetation indexes, like the beginning, peak, and length of the growing season [Estel et al., 2015, Pelletier et al., 2016].

In a recent review of machine learning methods to classify remote sensing data [Maxwell et al., 2018], the authors note that many factors influence the performance of these classifiers, including the size and quality of the training dataset, the dimension of the feature space, and the choice of the parameters. We support both *space-first, time-later* and *time-first, space-later* approaches. Therefore, the sits package provides functionality to explore the full depth of satellite image time series data.

When used in *time-first, space-later* approache, sits treats time series as a feature vector. To be consistent, the procedure aligns all time series from different years by its time proximity considering an given cropping schedule. Once aligned, the feature vector is formed by all pixel "bands". The idea is to have as many temporal attributes as possible, increasing the dimension of the classification space. In this scenario, statistical learning models are the natural candidates to deal with high-dimensional data: learning to distinguish all land cover and land use classes from trusted samples exemplars (the training data) to infer classes of a larger data set.

The SITS package provides a common interface to all machine learning models, using the sits\_train function. this function takes two parameters: the input data samples and the ML method (ml\_method), as shown below. After the model is estimated, it can be used to classify individual time series or full data cubes using the sits\_classify function. In the examples that follow, we show how to apply each method for the classification of a single time series. Then, we disscuss how to classify full data cubes.

When a dataset of time series organised as a SITS tibble is taken as input to the classifier, the result is the same tibble with one additional column ("predicted"), which contains the information on what labels are have been assigned for each interval. The following example illustrate how to train a dataset and classify an individual time series. First we use the sits\_train function with two parameters: the training dataset (described above) and the chosen machine learning model (in this case, a random forest classifier). The trained model is then used to classify a time series from Mato Grosso Brazilian state, using sits\_classify. The results can be shown in text format using the function sits\_show\_prediction or graphically using plot.

#select the data for classification

```
# get a point to be classified
point_4bands <- sits_select_bands(point_mt_6bands, ndvi, evi, nir, mir)</pre>
# Train a machine learning model using Random Forest
model <- sits_train(data = samples_mt_4bands, ml_method = sits_rfor())</pre>
# Classify using random forest model and plot the result
class.tb <- sits_classify(point_4bands, model)</pre>
# show the results of the prediction
sits_show_prediction(class.tb)
## # A tibble: 17 x 3
##
      from
                 to
                             class
                            <chr>
##
      <date>
                 <date>
   1 2000-09-13 2001-08-29 Forest
##
   2 2001-09-14 2002-08-29 Forest
##
##
   3 2002-09-14 2003-08-29 Forest
##
   4 2003-09-14 2004-08-28 Pasture
##
   5 2004-09-13 2005-08-29 Pasture
##
   6 2005-09-14 2006-08-29 Pasture
##
   7 2006-09-14 2007-08-29 Pasture
##
  8 2007-09-14 2008-08-28 Pasture
##
   9 2008-09-13 2009-08-29 Pasture
## 10 2009-09-14 2010-08-29 Sov_Corn
## 11 2010-09-14 2011-08-29 Soy_Corn
## 12 2011-09-14 2012-08-28 Soy_Corn
## 13 2012-09-13 2013-08-29 Soy_Corn
## 14 2013-09-14 2014-08-29 Soy_Corn
## 15 2014-09-14 2015-08-29 Soy_Corn
## 16 2015-09-14 2016-08-28 Soy_Corn
## 17 2016-09-13 2017-08-29 Soy_Corn
# plot the results of the prediction
plot(class.tb)
```

The following methods are available in SITS for training machine learning models:

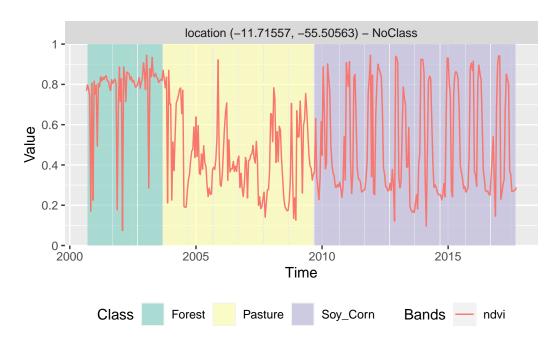


Figure 5: Random forest classification of a 16 years time series. The location (latitude, longitude) shown at the top of the graph is in geographic coordinate system (WGS84 *datum*).

- Linear discriminant analysis (sits\_lda)
- Quadratic discriminant analysis (sits\_qda)
- Multinomial logit and its variants 'lasso' and 'ridge' (sits\_mlr)
- Support vector machines (sits\_svm)
- Random forests (sits\_rfor)
- Extreme gradient boosting (sits\_xgboost)
- Deep learning (DL) using multi-layer perceptrons (sits\_deeplearning)
- DL with 1D convolutional neural networks (sits\_CNN),
- DL combining 1D CNN and multi-layer perceptron networks (sits\_tempCNN)
- DL using 1D version of ResNet (sits\_ResNet).
- DL using a combination of long-short term memory (LSTM) and 1D CNN (sits\_-LSTM\_FCN)

For more details on each method, please see the vignette "Machine Learning for Data Cubes using the SITS package".

# Validation techniques

Validation is a process undertaken on models to estimate some error associated with them, and hence has been used widely in different scientific disciplines. Here, we are interested in estimating the prediction error associated to some model. For this purpose, we concentrate on the *cross-validation* approach, probably the most used validation technique [Hastie et al., 2009].

To be sure, cross-validation estimates the expected prediction error. It uses part of the available samples to fit the classification model, and a different part to test it. The so-called k-fold validation, we split the data into k partitions with approximately the same size and proceed by fitting the model and testing it k times. At each step, we take one distinct partition for test and the remaining k-1 for training the model, and calculate its prediction error for classifying the test partition. A simple average gives us an estimation of the expected prediction error.

A natural question that arises is: *how good is this estimation?* According to Hastie et al. [2009], there is a bias-variance trade-off in choice of k. If k is set to the number of samples, we obtain the so-called *leave-one-out* validation, the estimator gives a low bias for the true expected error, but produces a high variance expectation. This can be computational expensive as it requires the same number of fitting process as the number of samples. On the other hand, if we choose k = 2, we get a high biased expected prediction error estimation that overestimates the true prediction error, but has a low variance. The recommended choices of k are 5 or 10 [Hastie et al., 2009], which somewhat overestimates the true prediction error.

sits\_kfold\_validate() gives support the k-fold validation in sits. The following code gives an example on how to proceed a k-fold cross-validation in the package. It perform a five-fold validation using SVM classification model as a default classifier. We can see in the output text the corresponding confusion matrix and the accuracy statistics (overall and by class).

```
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction Cerrado Pasture
##
      Cerrado
                   395
                             15
##
      Pasture
                     5
                            331
##
##
             Accuracy : 0.9732
```

```
## 95% CI : (0.9589, 0.9835)
##

## Kappa : 0.946

##

## Prod Acc Cerrado : 0.9875

## Prod Acc Pasture : 0.9566

## User Acc Cerrado : 0.9634

## User Acc Pasture : 0.9851

##
```

#### **Cube classification**

The continuous observation of the Earth surface provided by orbital sensors is unprecedented in history. Just for the sake of illustration, a unique tile from MOD13Q1 product, a square of 4800 pixels provided every 16 days since February 2000 takes around 18GB of uncompressed data to store only one band or vegetation index. This data deluge puts the field into a big data era and imposes challenges to design and build technologies that allow the Earth observation community to analyse those data sets [Câmara et al., 2017].

To classify a data cube, use the function sits\_classify() as described below. This function works with cubes built from raster bricks. The classification algorithms allows users to choose how many process will run the task in parallel, and also the size of each data chunk to be consumed at each iteration. This strategy enables sits to work on average desktop computers without depleting all computational resources. The code bellow illustrates how to classify a small raster brick image that accompany the package.

# Steps for cube classification

Once a data cube which has associated files is defined, the steps for classification are:

- 1. Select a set of training samples.
- 2. Train a machine learning model
- 3. Classify the data cubes using the model, producing a data cube with class probabilities.
- 4. Label the cube with probabilities, including data smoothing if desired.

## Adjustments for improved performance

To reduce processing time, it is necessary to adjust sits\_classify() according to the capabilities of the server. The package tries to keep memory use to a minimum, performing garbage collection to free memory as often as possible. Nevertheless, there is

an inevitable trade-off between computing time, memory use, and I/O operations. The best trade-off has to be determined by the user, considering issues such disk read speed, number of cores in the server, and CPU performance.

The first parameter is memsize. It controls the size of the main memory (in GBytes) to be used for classification. The user must specify how much free memory will be available. The second factor controlling performance of raster classification is multicores. Once a block of data is read from disk into main memory, it is split into different cores, as specified by the user. In general, the more cores are assigned to classification, the faster the result will be. However, there are overheads in switching time, especially when the server has other processes running.

Based on current experience, the classification of a MODIS tile (4800 x 4800) with four bands and 400 time instances, covering 15 years of data, using SVM with a training data set of about 10,000 samples, takes about 24 hours using 20 cores and a memory size of 60 GB, in a server with 2.4GHz Xeon CPU and 96 GB of memory to produce the yearly classification maps.

## Smoothing of raster data after classification

Post-processing is a desirable step in any classification process. Most statistical classifiers use training samples derived from "pure" pixels, that have been selected by users as representative of the desired output classes. However, images contain many mixed pixels irrespective of the resolution. Also, there is a considerable degree of data variability in each class. These effects lead to outliers whose chance of misclassification is significant. To offset these problems, most post-processing methods use the "smoothness assumption" [Schindler, 2012]: nearby pixels tend to have the same label. To put this assumption in practice, smoothing methods use the neighbourhood information to remove outliers and enhance consistency in the resulting product.

Smoothing methods are an important complement to machine learning algorithms for image classification. Since these methods are mostly pixel-based, it is useful to complement them with post-processing smoothing to include spatial information in the result. For each pixel, machine learning and other statistical algorithms provide the probabilities of that pixel belonging to each of the classes. As a first step in obtaining a result, each pixel is assigned to the class whose probability is higher. After this step, smoothing methods use class probabilities to detect and correct outliers or misclassified pixels. SITS uses a Bayesian smoothing method, which provides the means to incorporate prior knowledge in data analysis. For more details on the smoothing procedure, please see the vignette "Post classification smoothing using Bayesian techniques in SITS".

Doing post-processing using Bayesian smoothing in SITS is straightforward. The result of the sits\_classify function applied to a data cube is set of more probability images, one per requested clasification interval. The next step is to apply the sits\_label\_classification function. By default, this function selects the most likely class for each pixel considering only the probabilities of each class for each pixel. To allow for Bayesian smooting, it suffices to include the smoothing = bayesian parameter. If desired, the variance parameter (associated to the hyperparameter  $\sigma_k^2$  described above) can control the degree of smoothness. The following example takes the previously produced classification output and applies a Bayesian smoothing.

#### Final remarks

Current approaches to image time series analysis still use limited number of attributes. A common approach is deriving a small set of phenological parameters from vegetation indices, like beginning, peak, and length of growing season [Brown et al., 2013], [Kastens et al., 2017], [Estel et al., 2015], [Pelletier et al., 2016]. These phenological parameters are then fed in specialized classifiers such as TIMESAT [Jönsson and Eklundh, 2004]. These approaches do not use the power of advanced statistical learning techniques to work on high-dimensional spaces with big training data sets [James et al., 2013].

Package sits can use the full depth of satellite image time series to create larger dimensional spaces. We tested different methods of extracting attributes from time series data, including those reported by Pelletier et al. [2016] and Kastens et al. [2017]. Our conclusion is that part of the information in raw time series is lost after filtering. Thus, the method we developed uses all the data available in the time series samples. The idea is to have as many temporal attributes as possible, increasing the dimension of

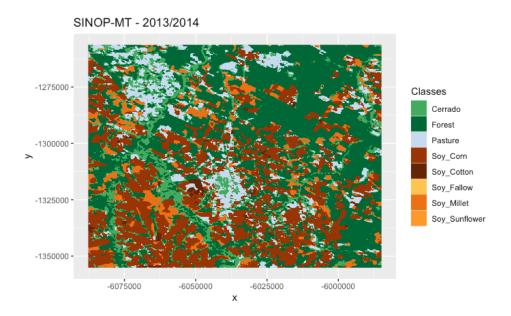


Figure 6: Classified image post-processed with Bayesian smoothing. The image coordinates (*meters*) shown at vertical and horizontal axis are in MODIS sinusoidal projection.

the classification space. Our experiments found out that modern statistical models such as support vector machines, and random forests perform better in high-dimensional spaces than in lower dimensional ones.

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