brainSimulator Documentation

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CONTENTS

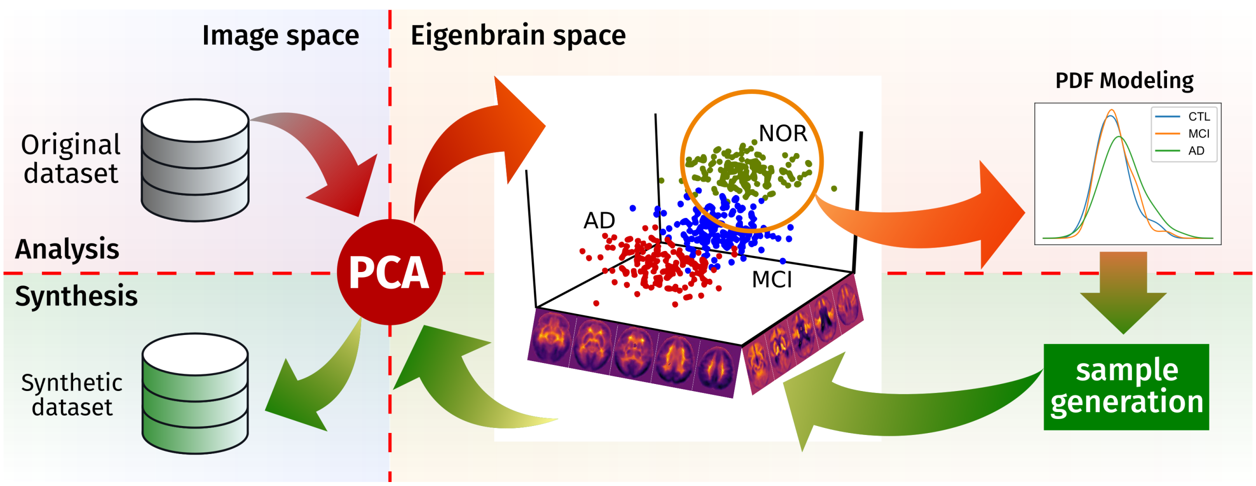
Functional brain image synthesis using the KDE or MVN distribution. Currently in beta. Python code.

brainSimulator is a brain image synthesis procedure intended to generate a new image set that share characteristics with an original one. The system focuses on nuclear imaging modalities such as PET or SPECT brain images. It analyses the dataset by applying PCA to the original dataset, and then model the distribution of samples in the projected eigenbrain space using a Probability Density Function (PDF) estimator. Once the model has been built, anyone can generate new coordinates on the eigenbrain space belonging to the same class, which can be then projected back to the image space.

CHAPTER ONE

BRAINSIMULATOR'S OVERVIEW

brainSimulator is a brain image synthesis procedure intended to generate a new image set that share characteristics with an original one. The system focuses on nuclear imaging modalities such as PET or SPECT brain images. It analyses the dataset by applying PCA to the original dataset, and then model the distribution of samples in the projected eigenbrain space using a Probability Density Function (PDF) estimator. Once the model has been built, anyone can generate new coordinates on the eigenbrain space belonging to the same class, which can be then projected back to the image space.



1.1 Quickstart

1.1.1 The "stack"

The first key concept here is a **stack**. A *stack* is a bidimensional *numpy.ndarray* of size *N*'x'*K*, where *N* is the number of brain images available and *K* is the number of voxels in each image. It is **important** to remark that all images must have been registered to the same brain space (*recommendation: use MNI space*). Use a similar code to this to generate a stack:

```
import os
import nibabel as nib
import numpy as np

def create_stack(list_images):
        i=0
        labels = np.array(len(list_images))
```

```
        for im in list_images:
                image = nib.load(im)
                labels[i] = get_label(im) # get the image label
                if i==0:
                        stack = np.zeros((datos.shape[0],image.shape[0], image.
↪shape[1], image.shape[2]))
                stack[i, :,:,:] = image.get_data()
        return stack, labels
```

1.1.2 Creating the brainSimulator object

With the new version, the whole interface has been switched to an object. This allows to train the model once and then perform as many sample drawings as required. To do so, we simply navigate to the folder where the simulator.py is located (if that folder is added to the path, that is not necessary), and import the module:

```
#navigate to the folder where simulator.py is located
import brainSimulator as sim

simulator = sim.BrainSimulator(algorithm='PCA', method='mvnormal')
```

There are different PDF modelling methods: *mvnormal*, *gaussian* and *kde*. Other methods based on alpha-stable distribution are planned for the future. The most accurate method is the *mvnormal*, but it requires some further tuning of the parameters. A high number of components may lead to overfitting, producing, when n_comp tends to infinity, always the average image of each class. For its part, the *kde* method is less accurate, but it works essentialy *out of the box*. Use them at your discrection.

1.1.3 Fitting the model

Once the object has been created, we use the *stack* and its labels to fit the model:

```
simulator.fit(stack, labels)
```

This procedure may take some time, depending on the PDF estimation method.

1.1.4 Generating a new dataset

Once the fitting procedure has finalised, you can generate a new dataset using the trained object:

```
new_stack, new_labels = simulator.generateDataset(N=200, classes=[0, 1, 2])
```

This will generate 200 new samples for each class in 0, 1 and 2, ready to use in our favourite machine learning algorithm.

CHAPTER TWO

BRAINSIMULATOR'S API

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@author: Francisco J. Martinez-Murcia <fjesusmartinez@ugr.es>

2.1 class brainSimulator

class brainSimulator.**BrainSimulator**(*method='kde'*, *algorithm='PCA'*, *N=100*, *n_comp=-1*, *regularize=False*, *verbose=False*)

createNewBrains(*N*, *kernel*, *components=None*)

Generates new samples in the eigenbrain space and projects back to the image space for a given kernel and a specified number of components.

Parameters

- **N** (*integer*) – Number of samples to draw from that class
- **kernel** (*KDEestimator*, *MVNormalEstimator* or *GaussianEstimator*) – kernel or list of kernels to generate new samples
- **components** (*int*) – Number of components to be used in the reconstruction of the images.

Returns **simStack** - a *stack* or numpy.ndarray containing *N* vectorized images in rows.

decompose(*stack*, *labels*)

Applies PCA or ICA decomposition of the dataset.

Parameters

- **stack** (*numpy.ndarray*) – stack of vectorized images comprising the whole database to be decomposed
- **labels** (*list or numpy.ndarray*) – labels of each subject in *stack*

Returns

- **SCORE** - A matrix of component scores
- **COEFF** - The matrix of component loadings.
- **MEAN** - If standardized, the mean vector of all samples.
- **VAR** - If standardized, the variance of all samples.

`estimateDensity`(*X*)

Returns an estimator of the PDF of the current data.

Parameters **`X`** (*`numpy.ndarray`*) – the data from which the different kernels are fitted.

Returns the trained kernel estimated for *X*

`fit`(*stack*, *labels*)

Performs the fitting of the model, in order to draw samples afterwards. It applies the functions *self.decompose* and *self.model*

Parameters

- **`stack`** (*`numpy.ndarray`*) – stack of vectorized images comprising the whole database to be decomposed
- **`labels`** (*`list or numpy.ndarray`*) – labels of each subject in *stack*

`generateDataset`(*stack=None*, *labels=None*, *N=100*, *classes=None*, *components=None*)

Fits the model and generates a new set of N elements for each class specified in "classes".

Parameters

- **`stack`** (*`numpy.ndarray`*) – the stack from which the model will be created
- **`labels`** (*`numpy.ndarray`*) – a vector containing the labels of the stacked dataset
- **`N`** (either int (the same N will be generated per class) or a list of the same length as *classes* containing the number of subjects to be generated for each class respectively.) – the number of elements (per class) to be generated
- **`classes`** (a list of the classes to be generated, e.g.: *[0, 2]* or *['AD', 'CTL'].*) – the classes that we aim to generate
- **`components`** (*`integer`*) – the number of components used in the synthesis. This parameter is only valid if *components* here is smaller than the *n_comp* specified when creating and fitting the *BrainSimulator* object.

Returns

- **labels** - numpy.ndarray vector with labels for *stack*
- **stack** - a *stack* or numpy.ndarray containing all synthetic images (N per clas *clas*) in rows.

`model`(*labels*)

Models the per-class distribution of scores and sets the kernels. Uses the internally stored *SCORE* matrix, once the decomposition is applied

Parameters **`labels`** (*list* or numpy.ndarray) – labels of each subject in *stack*

Returns

- **kernels** - a multivariate *kernel* or list of kernels, depending on the model.
- **uniqLabels** - unique labels used to create a standard object.

sample(*N*, *clas=0*, *n_comp=None*)
Standard method that draws samples from the model.

Parameters

- **N** (*integer*) – number of samples to be generated for each class.
- **clas** (*integer*) – class (according to *self.uniqLabels*) of the images to be generated.
- **n_comp** (*int*) – Number of components to be used in the reconstruction of the images.

Returns

- **labels** - numpy.ndarray vector with *N* labels of *clas*
- **stack** - a *stack* or numpy.ndarray containing *N* vectorized images of clas *clas* in rows.

2.2 auxiliary classes

These auxiliary classes define the PDF models that will be applied in the analysis and synthesis of brain images. All feature a set of methods *.fit* and *.sample* that in the case of MVN and Gaussian are a simple interface for their *scipy* counterparts, while for the KDE, it uses automatic estimation of bandwidth and defines more auxiliary functions. See a further discussion of these in the original paper.

class brainSimulator.**MVNormalEstimator**(*mean=0.0*, *cov=1.0*)
This class creates an interface for generating random numbers according to a given multivariate normal parametrization, estimated from the data Works only with python 3.4+ (due to numpy matrix multiplication)

class brainSimulator.**GaussianEstimator**(*mean=0.0*, *var=1.0*)
This class generates an interface for generating random numbers according to a per-component gaussian parametrization, estimated from the data

class brainSimulator.**KDEestimator**(*bandwidth=1.0*)
An interface for generating random numbers according to a given Kernel Density Estimation (KDE) parametrization based on the data.

botev_bandwidth(*data*)
Implementation of the KDE bandwidth selection method outline in:

26. (a) Botev, J. F. Grotowski, and D. P. Kroese. *Kernel density estimation via diffusion.* The Annals of Statistics, 38(5):2916-2957, 2010.

Based on the implementation of Daniel B. Smith, PhD. The object is a callable returning the bandwidth for a 1D kernel.

Forked from the package PyQT_fit.

Parameters **data** (*numpy.ndarray*) – 1D array containing the data to model with a 1D KDE.

Returns Optimal bandwidth according to the data.

2.3 auxiliary functions

brainSimulator.**applyPCA**(*X*, *regularize=True*, *n_comp=-1*)
This function applies PCA decomposition to a matrix containing all subjects to be modeled.

Parameters

- **X** (*numpy.ndarray*) – The bidimensional array containing one image per row (conveniently vectorized)
- **regularize** (*bool*) – Whether or not to regularize (standardize) X. default=True.
- **n_comp** (*int*) – Number of components to extract. If not specified, it will compute all available components except one.

Returns

- **Spca** (numpy.ndarray): Array with the PCA decomposition of X.
- **Components** (numpy.ndarray): Array with the eigenvalues of the PCA decomposition of X.
- **Mean** (numpy.ndarray): Vector with per-column average value.
- **Variance** (numpy.ndarray): Vector with per-column variance value.

brainSimulator.**applyICA**(*X*, *regularize=True*, *n_comp=-1*)

This function applies ICA decomposition to a matrix containing all subjects to be modeled.

Parameters

- **X** (*numpy.ndarray*) – The bidimensional array containing one image per row (conveniently vectorized)
- **regularize** (*bool*) – Whether or not to regularize (standardize) X. default=True.
- **n_comp** (*int*) – Number of components to extract. If not specified, it will compute all available components except one.

Returns

- **Spca** (numpy.ndarray): Array with the ICA decomposition of X.
- **Components** (numpy.ndarray): Array with the eigenvalues of the ICA decomposition of X.
- **Mean** (numpy.ndarray): Vector with per-column average value.
- **Variance** (numpy.ndarray): Vector with per-column variance value.

CHAPTER

THREE

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CHAPTER

FOUR

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F.J. Martinez-Murcia et al (2017). “Functional Brain Imaging Synthesis Based on Image Decomposition and Kernel Modelling: Application to Neurodegenerative Diseases.” Frontiers in neuroinformatics (online). DOI: 10.3389/fninf.2017.00065

CHAPTER

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