

NIPALS_PCA

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NIPALS_PCA

A Julia package for calculating PCA and PLS using the NIPALS implementation. Both models handles missing values

The package contains data structures for models and datasets

Installation

In Julia add https://gitlab.moffitt.usf.edu:8000/Bios2Projects/NIPALS_PCA as [unregistered package](#)

```
using Pkg
Pkg.add("https://gitlab.moffitt.usf.edu:8000/Bios2Projects/NIPALS_PCA")
```

Running Julia REPL

Julia can be started using

1. The base installation
2. From Singularity container (in progress, details pending)
3. Utilizing the downloaded folder as a local environment.

To activate NIPALS_PCA as local environment

```
cd path/to/cloned/NIPALS_PCA
julia --project=.
```

Loading package

```
using NIPALS_PCA
```

Example

```
(base) ~/tmp > git clone https://gitlab.moffitt.usf.edu:8000/Bios2Projects/NIPALS_PCA
Cloning into 'NIPALS_PCA'...
Username for 'https://gitlab.moffitt.usf.edu:8000': patterhf
Password for 'https://patterhf@gitlab.moffitt.usf.edu:8000':
warning: redirecting to https://gitlab.moffitt.usf.edu:8000/Bios2Projects/NIPALS_PCA.git/
remote: Enumerating objects: 164, done.
remote: Counting objects: 100% (164/164), done.
remote: Compressing objects: 100% (162/162), done.
remote: Total 164 (delta 80), reused 105 (delta 54), pack-reused 0
Receiving objects: 100% (164/164), 97.56 KiB | 1.99 MiB/s, done.
Resolving deltas: 100% (86/86), done.
(base) ~/tmp > cd NIPALS_PCA
(base) ~/tmp/NIPALS_PCA > ? develop julia --project=.

Documentation: https://docs.julialang.org
Type "?" for help, "]" for Pkg help.
Version 1.5.3 (2020-11-09)
Official https://julialang.org/ release

julia> using NIPALS_PCA
[ Info: Precompiling NIPALS_PCA [6d34e894-ae79-4b37-8bb1-32484f02c67]

julia> loadIrisData()
100x9 DataFrame
 Row Column1 Column2 Column3 Column4 Column5 Column6 Column7 Column8 Column9
  Float64 Float64 Float64 Float64 Float64 Float64 Float64 Float64 String
1      5.1  0.222222      3.5  0.625      1.4  0.0077960      0.2  0.0410657  setosa
```

On cluster using Singularity

A prebundled singularity container for Julia can be accessed at

/share/data2/applications/singularity_images/bbsrTools.sif

-C, Is required to utilize packages installed in the container. If this flag is not used, Julia will load packages from the users home directory

-B, binds folders to be accessible to the container

```
module load singularity/3.10
sudo singularity run -C -B ../data/ data bbsrTools.sif
```

Tutorial

PCA modelling

From Julia REPL

1)Load package

```
using NIPALS_PCA
```

2)Load dataset from .csv file to DataFrame

```
x_df = loadIrisData()
```

3>Create dataset and apply normalize to mean center data

```
xdataset = parseDataFrame(x_df) |> normalize
```

4)Calculate PCA model

```
pca = calcPCA(xdataset, 3)
```

5)Calculate variances for model

```
calcVariances(xdataset,pca)
```

PLS normalization

The PLS normalization workflow can either be run from a script or from an interactive Julia session. The default script can be find in src/scripts/plsnorm.jl

Run from script

```
julia src/scripts/plsnorm.jl \
--xfile /path/to/xmatrix.txt \
--yfile /path/to/ymatrix.txt \
--ycategorical "colname" \
--ycontinuous "colname1,colname2" \
--mode calibrate \
--modelfile model.jld2 \
--outfile output_file.csv
```

Run from interactive session

```
using NIPALS_PCA

parsed_args=Dict{String,Any}{"xfile" => "/path/to/xmatrix.txt","ycategorical" => "colname","yfi
#to calibrate
calibrate_model(parsed_args)

#to correct
correct(parsed_args)
```

Run on cluster using Singularity image

The folder(s) used for reading and writing needs a Bind. In the example below
 -B ../data/::data
 data will be accessible from the root level within the container. Multiple folders can be bound.

```
module load singularity/3.10

sudo singularity run --app plsnorm -C -B ../data/::data bbsrTools.sif \
--xfile /data/xmatrix.txt \
--yfile /data/ymatrix.txt \
--ycategorical "colname" \
--ycontinuous "colname1,colname2" \
--mode calibrate \
--modelfile model.jld2 \
--outfile output_file.csv
```

Get help

```
julia plsnorm.jl --help
```

Structures

NIPALS_PCA.Dataset — Type

```
struct Dataset
```

- `X::Array{Union{Missing, Float64},2}`
- `means::Array{Float64,1}`
- `stdeys::Array{Float64,1}`
- `value_columns::Array{String,1}`
- `xmask::BitArray{2}`
- `mv::Bool`

NIPALS_PCA_PCA — Type

```
struct PCA <: NIPALS_PCA.MultivariateModel
```

- `T::DataFrames.DataFrame`
- `P::DataFrames.DataFrame`

NIPALS_PCA_PLS — Type

```
struct PLS <: NIPALS_PCA.MultivariateModel
```

- `T::DataFrames.DataFrame`
- `P::DataFrames.DataFrame`
- `C::DataFrames.DataFrame`
- `W::DataFrames.DataFrame`
- `U::DataFrames.DataFrame`

Functions

General functionality

NIPALS_PCA.calcPCA — Function

calcPCA(dataset::Dataset, comps::Int64)

Calculates a PCA model

Examples

```
julia> calcPCA(dataset,3)
```

NIPALS_PCA.calcPLS — Function

calcPLS(xdataset::Dataset,dataset::Dataset,comps::Int64,incsamples::Array{Int64,1}=collect(1:size(xdataset.X)[1]))

Calculates a PLS model

NIPALS_PCA.calcVariances — Function

calcVariances(dataset::Dataset, model::PCA)::NamedTuple

Calculates r2x, r2x_cum and eigenvalues for all components in PCA model

Examples

```
julia> r2x,r2x_cum,eigenvalues = calcPCA(datset,model)
```

NIPALS_PCA.loadmodel — Function

loadmodel(path::String)::Tuple{MultivariateModel,Array{Float64,1},Array{Float64,1}}

Load PCA or PLS model from JLD2 file into a tuple containing the model, variable standard d

NIPALS_PCA.savemodel — Function

savemodel(model::T, dataset::Dataset, name::String) where T <: MultivariateModel

Save PCA or PLS model as JLD2 file

PLS normalization

NIPALS_PCA.calibrate_model — Function

calibrate_model(x::DataFrame::DataFrame,A::Int64,modelfile::String)

Calibrates PLS model based on datatypes in DataFrame for y

Columns of type CategoricalArray is handled by one-hot procedure

The calibrated model is saved to specified locations

NIPALS_PCA.correct — Function

correct(model::T, dataset::Dataset, name::String) where T <: MultivariateModel

Save PCA or PLS model as JLD2 file

NIPALS_PCA.predict_xres — Function

predict_xres(modelfile::String,xfile::String,outfile::String)

Loads model from jld2 file, predicts using xfile and exports residual matrix into .csv file