

## **Regression Flow-B**

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### **Notes:**

1. This Jython script works in Sarchitect Designer version 2.3
2. Learn about Sarchitect Designer – <http://www.strandls.com/sarchitect/index.html>
3. Get Sarchitect – <http://www.strandls.com/sarchitect/freetrial.php>

***The actual script follows this discussion. It is also accessible directly from the webpage in .py format.***

### **Discussion:**

The script provided here automates regression modeling. It is an implementation of the modeling workflow depicted in Figure 2. The following steps get executed:

- 1) Top 400 descriptors are selected based on correlation with endpoint – a “Feature Ranking” report of all the descriptors is displayed as well as a “Ranked Subset” with top 400 descriptors gets created. (User can change the cutoff values in line #67 of the script.)
- 2) An auto-correlation filter is applied with a cutoff of 0.9 on this “Ranked Subset” – a report and a scatter-plot is shown on the “Non Redundant Features” as well as a “Non Redundant Descriptors” subset containing non-correlated descriptors gets created. (User can change the cutoff values in line #102 of the script.)
- 3) “Partial Least Squares Regression” modeling algorithm is called on the “Non Redundant Descriptors” – a “PLS Results” node is created displaying “PLS Scores” and “PLS Loadings” in a table format. Also, prediction results are displayed in a node title “Prediction” that contains the “Prediction Results” in a table, a scatter-plot of “Actual vs. Predicted” and the “Model Formula” that displays the independent variables and their coefficients. (As of now, user is prompted through a dialog-box to provide for PLS Regression parameters, mainly, the ‘number of components’.)

User can now save the PLS model.



Flow B  
The first shot quick regression flow with Partial Least Squares Regression

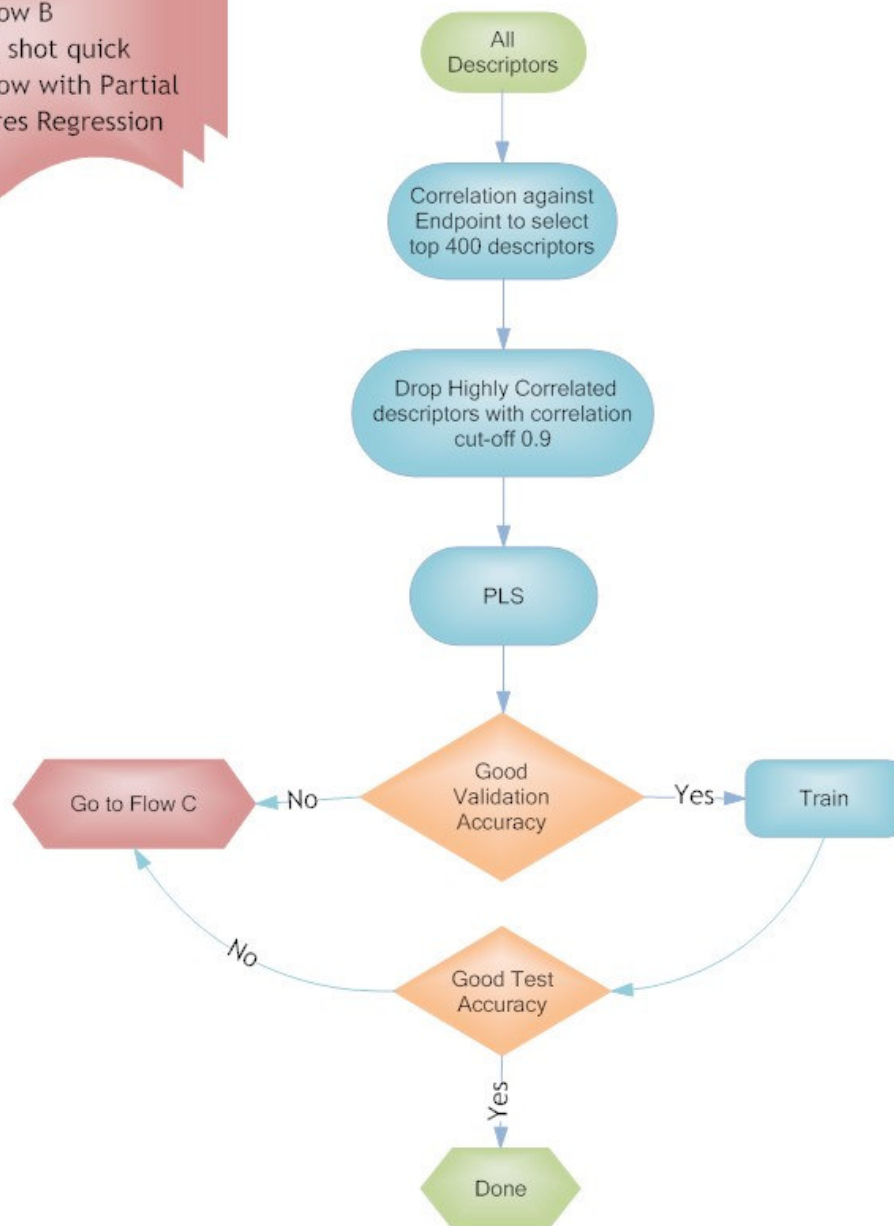


Figure 2

**Cite this as:**

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##-----
##
##
## Sarchitect Designer 2.3 script
## implementing "Regression Flow-B"
##
##
##
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##
##-----

import script
from script.dataset import *
from script.algorithm import *
from script.project import *
from script.view import *
from script.omega import createComponent, showDialog
from javax.swing import *
from com.strandgenomics.cube.dataset import *
import jarray

##-----
## GET LIST OF CONTINUOUS, UNMARKED COLUMNS
def getColumnList(dataset):
    ## Get columns, assumption: continuous and unmarked columns
    indices_continuous =
DatasetUtil.getContinuousColumnIndices(dataset)
    indices_nm_continuous =
script.project.removeMarkedColumns(dataset,indices_continuous)
    columnList = indices_nm_continuous
    #print columnList
    return columnList

##-----
##
def getIndexedIntArray(rowHeaderLabels,dataset):
    from com.strandgenomics.cube.framework.data import ArrayUtil,
DefaultIntArray
    size = rowHeaderLabels.getSize()
    array = DefaultIntArray(size)
    for i in range(size):
        colName = rowHeaderLabels.get(i)
        c = dataset.getColumn(colName)
        array.add(dataset.indexOf(c))
    return ArrayUtil.createIndexedIntArray(array)

##-----
##
def getStringArray(rowHeaderLabels):

```

```

    array = []
    from com.strandgenomics.cube.framework.data import DefaultIntArray
    size = rowHeaderLabels.getSize()
    for i in range(size):
        array.append(rowHeaderLabels.get(i))
    return array

##-----

dataset = script.project.getActiveDataset()

## Correlation against endpoint to select top N descriptors
result =
script.algorithm.FeatureSelection(test="correlation",select="Based on
rank", rank=400).execute()

inputs = result.getInputs()
dataset = inputs["dataset"]
rankDataset = result["results"]
rowHeaderLabels = result["rowHeaderLabels"]

nameColumn = ColumnFactory.createStringColumn("Descriptor",
getStringArray(rowHeaderLabels))
columnList = []
columnList.append(nameColumn)
for i in range(rankDataset.getColumnCount()):
    columnList.append(rankDataset.getColumn(i))

columns = jarray.array(columnList, IColumn)
newDataset =
DatasetFactory.createDataset(rankDataset.getName(), columns)

node = script.project.getActiveDatasetNode()

from com.strandgenomics.cube.framework.selection import
MappedSelectionModel, DummySelectionModel
from com.strandgenomics.cube.framework.filter import DummyFilterModel
selModel =
MappedSelectionModel(node.getContext().getColumnSelectionModel(),
getIndexIntArray(rowHeaderLabels, dataset))

newnode = script.project.addFolderNode("Feature Ranking", node)
script.view.RankFeaturesView(node=newnode, dataset=newDataset,
title=newDataset.getName(), rowSelectionModel=selModel,
columnSelectionModel = DummySelectionModel.INSTANCE, filterModel =
DummyFilterModel(newDataset.getRowCount())).show()

pvalue = inputs['pvalue']
rank = inputs['rank']
select = inputs['select']
script.algorithm.SelectFeatures(node = node, featureselection =
newDataset, dataset = dataset, pvalue = pvalue, rank = rank, select =
select).execute(displayResult=1)

```

```
## Drop auto-correlated descriptors with correlation more than cutoff
result =
script.algorithm.RemoveRedundant(options="Correlation").execute(interac
tive=0, displayResult=1, newThread=0)
non_corr = result['SelectedIndicesList'][89] ##count starts from zero,
89 is 90, => auto-correlation cut off of 0.90

colIndices = ArrayUtil.createIndexedIntArray(to_java(non_corr))
script.project.getActiveDatasetNode().addChildDatasetNode("Non
Redundant Descriptors", columnIndices=colIndices, setActive=1,
addMarkedColumns=1)
script.view.Table(rowHeight=80).show()

node = script.project.getActiveDatasetNode()
dataset=script.project.getActiveDataset()

collist = getColumnlist(dataset)
endpoint = DatasetUtil.getMarkedColumnIndices(dataset, "classlabel")
endpoint = ArrayUtil.createIndexedIntArray(endpoint)
endpoint = endpoint.get(0)

import thread
thread.start_new_thread(script.chem.models.pls_nipals.pls, ())

##
## END
##
```

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End of Document