Semester: 2

Group: 2

Section: FB\_Monday\_10\_15

# Computer Programming Laboratory

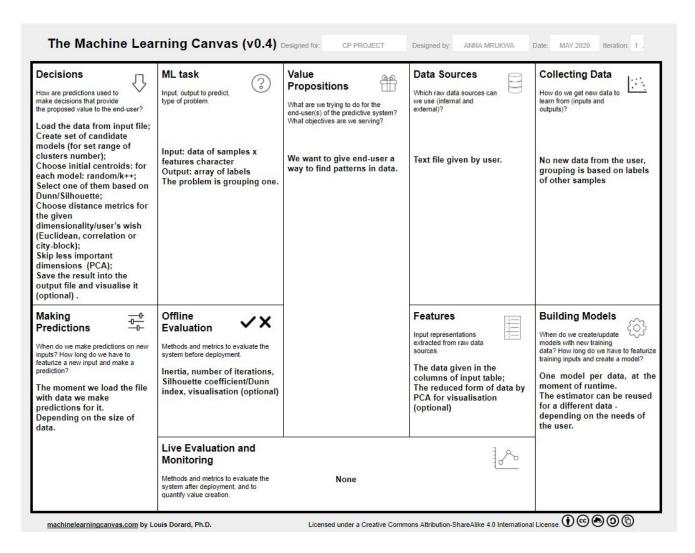
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## 1. Task topic

During the process of preparing my project I created ML Canvas dedicated to this programme. It helped me to get a clearer look at the architecture and applications of the whole composition. Because of that I place it below as an important part of the whole procedure.



## 2. Project analysis

As mentioned above, the problem to solve here is finding patterns in the data and grouping them accordingly into clusters, whose number does not have to be specified by the user. To do so, I am using the k-means algorithm. It is simple grouping algorithm that is based on the following steps:

- Initialize algorithm by choosing initial centroids I decided to implement both Mac Queen's random initialization, consisting of randomly chosen points from a given dataset and k++ initialization, explained below.
- To complete initialization, we label all the points belonging to the given set we assign them to the clusters based on their distance (measured in the

- Euclidean, correlation or cityblock metrics) to the closest one. Each such group consisting of data points is a cluster with a common label.
- After completing initialization recalculating the centroids begins. As the name
  of the method suggests, we choose new centroid coordinates based on the
  mean of coordinates in each dimension of all the points belonging to the
  cluster.
- By doing it, we possibly moved the centroids and previously assigned labels are no longer corresponding to the actual smallest distance between a point and a member of the centroid group. To fix this, we label all the points again.

The two last steps are repeated for the determined number of iterations. This improves the result of clustering. We provide the labels of each point to the user.

Most of the basic problems are already solved in <u>my implementation of this algorithm in C</u> and their solutions can be applied similarly. To describe new issues more precisely I skip discussing these problems and carry on with the rest of this implementation.

The part that proved to be more challenging was creating adequate assignment operators and appropriate constructors. As I created my own structure containing the dynamically allocated array and two parameters describing its dimensions, I could not simply copy a pointer from one object to another.

I also added another initialization method to k-means - it speeds up the algorithm, choosing not random, but more different initial centroids. K++ iniltialization chooses the first centroid at random. For the next ones, however, we compute the distance from each point to the closest centroid. Then we choose the next centroid using weighted probability proportional to this distance squared.

Moreover, to enhance the whole process and enable future visualisation, I implemented one more unsupervised learning algorithm - this one for feature extraction. Principal Component Analysis lets us rotate the coordinate system in which we position the data in such a way that each dimension is independent; more intuitional explanation would be a comparison to finding the best way to take a photo of a group of people: we want to see them as clearly as possible without unnecessary obscuring of the photo. To do so, we rotate the camera until we get the best version of the image. The line we project the people onto and the line orthogonal to it are what we are looking for. The implementation consists of calculating the covariance matrix for the input data and then calculating eigenvectors of this matrix. As we want to reduce the number of dimensions of our input and preserve as much of the initial information as possible, we sort the eigenvectors by their eigenvalues in the descending order. We preserve only the first N eigenvectors, where N is the number of dimensions we want the data to be reduced to. Then we multiply the initial data by the remaining eigenvectors.

I did not want to use any external libraries computing the eigenvectors and eigenvalues of the matrix, so I wrote QR decomposition combined with the power method. To ensure the orthonormalization every iteration, I also applied modified Gram-Schmidt algorithm to prevent numerical errors.

As I wanted the program to choose the best number of clusters by itself, not by the specification of the user, I also implemented Dunn Index and Silhouette score. Dunn Index calculates the smallest distance between two clusters in the current grouping and then divides it by the greatest defined distance within the cluster. The linkages can be chosen by the user. This shows us how much the points with the same labels are different and how much different clusters are mixed together. The bigger the index, the better the clustering. Silhouette score

informs us about the same. I calculate it for the whole set as the average score for every point belonging to this set. Silhouette score for one point is defined as:  $s = \frac{b-a}{max(a,b)}$ , where a mean intra cluster distance (from this point to all the other in the same cluster), b - mean distance to the closest cluster the sample does not belong to. Scores close to 1 mean great assignment, 0 - overlapping clusters, negative values - samples are in the wrong clusters.

## 3. External specification

The easiest way to download the program is by clicking <u>here</u>. I strongly recommend reading README and taking a look at the specially created <u>exemplary file</u>.

The input file is not checked in this implementation - the program will not inform you about the typos and will not work correctly. This is because I wanted to speed up the whole process, as loading the data takes up a lot of time.

Besides that, most of the basic functions (such as vector division) check for the incorrect behaviour, terminating with a message. This should help you diagnose the problem in case of possible different usage of the header parts.

K-means and PCA implementations imitate the parts of scikit-learn pipelines: you can use fit, predict for k-means, as well as fit\_predict, grouping your data and returning the labels, whereas for PCA you get fit, transform and fit\_transform, performing the decomposition and transforming your data.

While using GapSearch or SilhouetteSearch, remember that after fitting the estimator you used remained unchanged - the desired one with the best score is still inside the searching object and you have to extract the labels from it.

## 4. Internal specification

Here I present classes, methods and functions used in the project:

1. In the file <u>Vectors.h</u>:

```
enum class dist { Euclidean, correlation, cityblock };
```

this enum class holds all the possible distance metrics the user can choose from; it prevents unnecessary typos that could occur with the string names.

class vectors - class for storing matrices and possible operations on them.

public members:

```
int n_samples = 0; number of rows of the matrix, automatically set to 0
int n_features = 0; number of columns of the matrix, automatically set to 0
double* coords; pointer to array of doubles, dynamically allocated later on
```

vectors() = default; default constructor, creates NULL pointer, usage unadvised

vectors (int samples, int features, double\* data) - constructor creating the matrix of given dimensions: samples - number of rows, features - number of columns, data - a deep copy of a given array is created. The memory used by this parameter should be freed later on, this constructor doesn't free it.

vectors (int samples, int features) - constructor allocating the memory of the given size (samples\*features) and setting the dimensions.

vectors(int square\_dim) - convenience constructor for square matrices

vectors (const vectors v1) - copy constructor. Creates a deep copy of a given object - doesn't only copy pointer coords but creates a new one and copies the values in the array.

vectors(std::ifstream& datafile) - constructor loading the matrix from the stream datafile. Number of rows is the same as the number of lines in the file, the number of columns is the same as the number of entrances in each line. It does not check if the file is correct - errors may occur.

~vectors() - object destructor, frees the memory.

vectors& operator=(const vectors& v) - assigns the number of rows and columns to these numbers in v. Reallocates the coords, creates a deep copy of v.coords.

void shape show() - prints the matrix dimensions to the console: (n samples, n features).

double sum() - returns the sum of all elements of the array.

double sum\_of\_column(int column) - returns the sum of elements in the column of the given index (int column).

double sum\_of\_row(int row) const - returns the sum of elements in the row of the given
index (int row)

double mean\_of\_row(int row) const - returns the mean of elements in the row of the given index (int row)

double mean\_of\_column(int column) - returns the mean of elements in the column of the
given index (int column)

void change\_size(int samples, int features) - changes n\_samples to samples, n\_features to features and reallocates memory.

void substract (double value) - substracts value from all the elements of the array.

void substract (double value, int column) - substracts value from all the elements of the column given by the index (int column).

void substract (double\* v, int col) - substracts given vector from the column specified by given index (int col).

double\* substract(double value, int row) const - returns vector specified by the row index decreased by the given value.

void divide (double value, int column) - divides all the elements of the column specified by index (int column) by value.

void divide (double value) - divides all the elements of the matrix by value.

vectors transpose () - returns the transpose of the matrix.

void leave n cols(int col) - method preserving col columns out of matrix.

#### private:

void get\_dimensions(std::ifstream& datafile) - counts number of lines and columns in a given file and sets the dimensions of the object accordingly.

void load\_data(std::ifstream& datafile) - loads the data from the given file into the object. The dimensions of the vectors should be specified before the usage.

this header contains also functions operating on the vectors class:

vectors indices(int 1) - creates the matrix of 1 n\_features and and 1 n\_samples, returning it filled with the appropriate indices.

double length\_of\_column(const vectors& v1, int column) - returns the length of column under the index (int column) of object v1.

double length\_of\_row(const vectors& v1, int row) - returns the length of row under the index (int row) of object v1.

double length\_of\_row(double\* v, int dimension) - this function calculates length of given array on specified number of dimensions. Dimension shouldn't be bigger than the number of allocated doubles

void normalise (vectors\* v, int col) - normalises the column under given index (col) to the unit vector

```
void normalise (vectors* v) - normalises the whole matrix.
vectors center(const vectors@ v1) - returns centered matrix.
vectors standardise(const vectors& v1) - returns standardised matrix.
vectors std base (int dimension) - returns matrix being standard basis for dimension-space.
bool operator == (const vectors& v1, const vectors& v2) - compares n dimensions,
n features and variables in v1 and v2.
void operator<<(std::ostream& out, const vectors& some vector) - writes into out all the</pre>
elements in the array, preserving its specified dimensions.
double* operator* (const vectors & A, double* x) - returns the result of multiplication A*x.
x should not be shorter than A.n features. If longer, additional dimensions are skipped.
vectors operator*(const vectors& A, const vectors& B) - returns result of matrix
multiplication A*B. A.n features should be equal to B.n samples.
double row_product(double* d1, double* d2, int dimension) - returns result of dot
product of d1 and d2. Their lengths should be equal to dimension.
double col product (vectors x, int col1, int col2) - returns result of dot product of
columns under indexes col1 and col2.
double correlation distance(const vectors& v1, const vectors& v2, int row1, int
row2) - returns correlation distance between rows of two matrices: row1 in v1 and row2 in
v2.
double Euclidean distance(const vectors& v1, const vectors& v2, int row1, int row2)
- returns Euclidean distance between rows of two matrices: row1 in v1 and row2 in v2.
double cityblock distance(const vectors& v1, const vectors& v2, int row1, int row2)
- returns cityblock distance between rows of two matrices: row1 in v1 and row2 in v2.
double distance(const vectors& v1, const vectors& v2, int row1, int row2, dist
metric = dist :: Euclidean) - returns distance in dist metric between rows of two
matrices: row1 in v1 and row2 in v2. The default is Euclidean distance.
double min_distance(const vectors& v1, const vectors& v2, int row1, dist_ metric =
dist :: Euclidean) - returns distance in dist metric between row of two matrices: row1 in
```

v1 and closest row to row1 of v2.

double min\_distance(const vectors& v1, const vectors& v2, int row1, int index, dist\_ metric = dist\_::Euclidean) - returns distance in dist\_ metric between row of two matrices: row1 in v1 and closest row to v1 from rows in v2 up to index, exclusively.

int argmin\_distance(const vectors& v1, const vectors& v2, int row1, dist\_ metric =
dist\_::Euclidean) - returns index of row in v2 closest to row1 in v1 in dist\_ metric.

double abs (double a, double b) - returns absolute difference between a and b.

bool are\_same(const vectors& v1, const vectors& v2, double tol = 1e-4) - checks if the matrices are the same with some tolerance tol.

void orthogonalise (vectors\* x, int col1, int col2) - orthogonalises column col1 of x with respect to column col2 of x.

vectors  $Gram\_Schmidt(vectors x)$  - returns orthomalized x, assuming consecutive vectors are in columns, not rows.

#### 2. In the file initialization.h:

enum class init\_ {random, kpp}; - this enum class holds all the possible initialization methods the user can choose from; it prevents unnecessary typos that could occur with the string names.

void swap (double\* a, double\* b) - swaps a and b.

void fisher\_yates(int desired\_dimensions, vectors\* ind) - randomly swaps values in ind.coords up to desired\_dimensions index (exclusively) with all others values in ind.coords.

void random\_init(vectors\* centres, vectors x) - chooses centres->n\_samples samples
from x at random and fills centres->coords with them.

void first\_centroid(vectors\* centres, vectors x) - chooses 1 sample at random from x as the first centroid for k++ initialization and fills the first row of centres with the values.

int weighted\_random(vectors weights) - returns index of one of the points by probability based on the given weights.coords.

void next\_centroid(vectors\* centres, vectors x, vectors\* weights, int c\_index,
dist\_ metric) - chooses next centroid for k++ initialization from x based on metric and
appends it in c index row of centres.

void kpp\_init(vectors\* centres, vectors x, dist\_ metric) - chooses
centres->n samples samples from x by k++ method and fills centres->coords with them.

void initialize(vectors\* centres, vectors x, init\_ init, dist\_ metric) - chooses
centres->n samples samples from x by init and fills centres->coords with them.

#### 3. In the file kmeans.h:

void label\_points(vectors\* labels, vectors x, vectors centroids, dist\_ metric) fills labels->coords with indices of rows of centroids being closest to the consecutive samples
in x measured with metric.

void calculate\_centroids(vectors labels, vectors x, vectors\* centroids) - calculates centroids->coords as average on each axis of samples in x with the same labels.coords under the appropriate indices.

double calculate\_inertia(vectors labels, vectors x, vectors centroids, dist\_
metric) - returns inertia for given parameters.

void kmeans\_algorithm(vectors\* centroids, vectors\* labels, dist\_ metric, int
n\_clusters, init\_ initialization, double\* inertia, int max\_iter, int\* n\_iter,
vectors x) - performs k-means clustering on x for n\_clusters. Fills centroids and labels
matrices and counts n iter for this run. Calculates inertia of the model.

 ${\tt class}$  kmeans - k - means estimator.

#### public members:

vectors centroids - Coordinates of cluster centers and their dimensions.

dist metric - one of dist : Euclidean, correlation or cityblock.

int n\_clusters - the number of clusters to form as well as the number of centroids to generate, should be int greater than 1.

 $init\_initialization$  - one of  $init\_: random\ or\ kpp.$ 

double inertia - sum of squared distances of samples to their closest cluster center.

int max iter - maximum number of iterations of the k-means algorithm for a single run.

int n\_iter - number of iterations run.

vectors labels - labels of each point.

int n\_init - Number of times the k-means algorithm will be run. The final results will be the best output of n init consecutive runs in terms of inertia.

kmeans(int clusters\_n, dist\_ metrics = dist\_::correlation, init\_ init = init\_::kpp,
int iter = 1000, int init\_n = 10) - constructor setting all the parameters for the future
clustering.

kmeans() = default - default constructor, standalone usage not recommended.

~kmeans() - destructor.

kmeans (const kmeans & estim) - copy constructor; creates deep copy of all parameters, labels and centroids too.

kmeans (const kmeans estim, int clusters\_n) - copy constructor; creates copy of all parameters except estim.labels, estim.centroids and estim.n\_clusters. n\_clusters is set to clusters\_n. New estimator should be fitted independently later on.

kmeans& operator=(const kmeans& estim) - deep assignment operator.

void fit(vectors data) - compute k-means clustering for data.

vectors predict (vectors data) - predict the closest cluster each sample in data belongs to.

vectors fit\_predict(vectors data) - convenience method equivalent to calling fit and then predict on data.

#### 4. In the file sorting.h:

bool descending sort (int i, int j) - checks if i is bigger than j.

class sort\_indices - convenience class for sorting functions.

#### public members:

vectors b - vectors which coords is sorted

sort indices(vectors to sort) - constructor

bool operator()(int i, int j) const - checks if b.coords[i] is bigger than b.coords[j].

void sort\_by\_idx(vectors\* x, vectors idx) - sorts \*x by the order specified in idx.

void sort\_two(vectors\* basic, vectors\* dependent) - sorts \*basic in descending order and
the columns in \*dependent accordingly.

#### 5. In the file <u>pca.h</u>:

vectors covariance\_matrix(vectors data) - returns approximate covariance matrix of data. void  $QR_algorithm(vectors x, vectors* eigenvec, vectors* eigenvals, double tol, int iter) - finds eigenvectors and eigenvalues of x approximating to tol, iterating at most iter times. Uses QR algorithm combined with orthogonal power method.$ 

class PCA - performs Principal Component Analysis. Using standardised vectors is recommended for performance reasons.

#### public members:

```
int reduced_dims - number of features data should have left after the transformation

std::string reduce - if not "YES", keeps all features

vectors eigenvectors - reduced eigenvectors of the covariance matrix of data used to fit

vectors eigenvalues - reduced eigenvalues of the covariance matrix of data used to fit

double tol - tolerance for singular values of coords of eigenvectors

int n_iter - number of iterations for the QR method

PCA(std::string red = "YES", int dims = 2, double tolerance = 1e-6) - constructor

-PCA() - destructor

PCA(const PCAs t) - deep copy constructor

void fit(vectors data) - fit model with data

vectors transform(vectors data) - apply dimensionality reduction to data

vectors fit_transform(vectors data) - convenience method, equivalent to fitting model with data and applying dimensionality reduction on it.
```

#### 6. In the file dunn.h:

enum class inter\_ {centroid, closest, furthest, avg} - this enum class holds all the possible distances between clusters the user can choose from; it prevents unnecessary typos that could occur with the string names.

```
inter ::centroid - distance between centroids of the clusters
inter ::closest - distance between closest samples of two distinct clusters
inter ::furthest - distance between furthest samples of two distinct clusters
inter::avg - average distance between all of the samples of two distinct clusters
enum class inter {centroid, closest, furthest, avg} - this enum class holds all the
possible distances within the cluster the user can choose from; it prevents unnecessary typos
that could occur with the string names.
intra ::centroid - average distance from all the samples in the cluster to its centroid
intra ::furthest - distance between furthest samples of the cluster
intra ::avg - average distance between all of the samples within cluster
double single linkage(vectors labels, vectors data, int c1, int c2, dist metric) -
returns closest distance in metric distance between two samples of data belonging to clusters
c1 and c2 respectively.
double complete_linkage(vectors labels, vectors data, int c1, int c2, dist_ metric)
- returns the distance in metric distance between the most remote samples of data belonging to
clusters c1 and c2 respectively.
double avg_linkage(vectors labels, vectors data, int c1, int c2, dist_ metric) -
returns the average distance in metric distance between all of the samples of data belonging to
clusters c1 and c2 respectively.
double inter linkage (vectors labels, vectors data, int c1, int c2, dist metric,
inter link) - returns the distance between clusters c1 and c2 in metric, defined as link.
double inter_dist(kmeans* est, vectors data, inter_ metric) - returns smallest distance
between two clusters of *est, defined as one of: inter ::closest, inter:: furthest, inter ::avg.
double inter_centroid(vectors centroids, dist_ metric) - returns smallest distance
between centroids.
          inter distance(kmeans
                                     *estim,
                                                vectors
                                                            data,
                                                                     inter
inter ::centroid) - returns the smallest distance between two clusters of all clusters, defined
as metric.
```

double intra\_centroid(kmeans\* est, vectors data, int c) - returns the average distance of samples in data belonging to cluster c from centroid c.

double intra\_linkage(kmeans\* estim, vectors data, int c, intra\_ metric) - returns
distance within cluster c defined as metric.

double intra\_distance(kmeans\* est, vectors data, intra\_ metric= intra\_::avg) returns the biggest distance within a cluster of all clusters, defined as metric.

double dunn\_index(kmeans \*estim, vectors data, inter\_ metric1 = inter\_::centroid,
intra\_ metric2 = intra\_::avg) - returns Dunn Index for estim and the data in specified
linkage metrics.

class DunnSearch - chooses the best estimator and its number of clusters by computing Dunn Index for specified range.

#### public members:

kmeans estimator - after fitting, estimator of the greatest Dunn Index from min\_clusters to max clusters interval, before: template estimator given by user.

intra\_ intra - measurement method of distance within clusters.

inter\_ inter - measurement method of distance between clusters.

int max\_clusters - biggest number of clusters for estimator.

int min\_clusters - smallest number of clusters for estimator.

double index - Dunn Index value for estimator after fitting.

DunnSearch(kmeans est, inter\_ inter\_d = inter\_::centroid, intra\_ intra\_d =
intra\_::avg, int min = 2, int max = 20) - constructor; creates a deep copy of est.

~DunnSearch() - destructor.

DunnSearch (const DunnSearch& estim) - deep copy constructor.

double single\_idx(kmeans\* est, vectors data, int clusters\_n) - returns a single Dunn Index for \*est, automatically fits \*est and changes its number of clusters.

void fit (vectors data) - performs k-means clustering for kmeans estimators with n\_cluster between max\_clusters and min\_clusters, chooses the estimator with the highest Dunn Index.

#### 7. In the file <u>silhouette.h</u>:

double avg\_to\_cluster(vectors labels, vectors data, int sample, int c, dist\_
metric) - calculates the average distance of the sample in data to samples in cluster c in
metric.

double min\_avg(vectors labels, vectors data, int sample, int n\_clusters, dist\_metric) - calculates the distance of the sample in data to the closest cluster it doesn't belong to, in metric distance.

double \_for\_sample(kmeans\* est, vectors data, int sample) - returns Silhouette Score for sample in data, \*est should be fitted.

double silhouette (kmeans\* est, vectors data) - returns average Silhouette Score for data after clustering.

class SilhouetteSearch - chooses the best estimator and its number of clusters by computing Silhouette Score for specified range.

#### public members:

kmeans estimator - after fitting, estimator of the greatest Silhouette Score from min\_clusters. to max\_clusters interval, before: template estimator given by user.

int max clusters - biggest number of clusters for estimator.

int min clusters - smallest number of clusters for estimator.

double coefficient - Silhouette Score value for estimator

SilhouetteSearch(kmeans est, int min = 2, int max = 20) - constructor; creates a deep copy of est.

~SilhouetteSearch() - destructor.

SilhouetteSearch(const SilhouetteSearch& estim) - deep copy constructor.

double single\_coefficient(kmeans\* est, vectors data, int clusters\_n) - calculates a single Silhouette Score for \*est, automatically fits \*est and changes its number of clusters.

void fit (vectors data) - performs k-means clustering for kmeans estimators with n\_cluster between max\_clusters and min\_clusters, chooses the estimator with the highest Silhouette Score.

#### 5. Source code

I decided against putting the source code in this file for it would definitely lower its quality. All of the files are available in the already linked repository. It is organized in 8 source files, excluding tests:

- Vectors.h provides class and functions for operations on matrices.
- initialization.h entails functions choosing some part of given vectors (random or k++ initialization).
- kmeans.h runs k-means algorithm.
- dunn.h runs k-means algorithm with sweep by Dunn index
- silhouette.h runs k-means algorithm with sweep by Silhouette Score.
- sorting.h sorts two vectors in descending order of one of them.
- pca.h performs dimension reduction by Principal Component Analysis.
- Example.cpp contains main() function and shows exemplary flow of the program.

### 6. Testing

I decided to implement unit tests for this project so that debugging and manual tests will not be necessary so often. I used Native Unit Tests provided by Visual Studio. All of them can be seen <a href="here">here</a>. I will not put them here as it would obscur the whole report. I also performed a separate test on PCA, as I wanted to check its correctness on more complex data than small matrices. I checked whether the transformation of the iris dataset in this implementation and solution provided in the scikit-learn package gives the same result. My program proved to be successful. The same applies to DunnSearch (I checked this one with my own implementation in Python as well as some verified codes available on GitHub, as there is none in scikit-learn), and SilhouetteSearch - the values of the calculated numbers of clusters were the same.

#### 7. Additional remarks

To improve the stability and performance of the k-means algorithm, each training of the model is repeated 10 times - after that, I choose the version with the smallest inertia. This also made the choice of number of clusters in Search classes more stable - this value stopped jumping through the whole desired interval, settling for one characteristic value for the dataset.