Inf2B Coursework 2

(Ver. 1.2)

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1 Outline

The coursework consists of two tasks, Task 1 – PCA and clustering, Task 2 – classification with K-NN and Bayes classification with Gaussian distributions, in which we use a data set of handwritten characters (digits).

You are required to submit (i) two reports, one for each Task, (ii) code, and (iii) results of experiments if specified, using the electronic submission command. Details are given in the corresponding task sections below. Some of the code and results of experiments submitted will be checked with an automated marking system in the DICE computing environment, so that it is essential that you follow the syntax of function and file format specified. No marks will be given if it does not meet the specifications. Efficiency of code and programming style (e.g. comments, indentation, and variable names) count. Those pieces of code that do not run or that do not finish in approximately five minutes (excluding Task 1.5 when k=20) on a standard DICE machine will not be marked. This coursework is out of 100 marks and forms 12.5% of your final Inf2b grade.

This coursework is individual coursework - group work is forbidden. You should work alone to complete the coursework. You are not allowed to show any written materials, the data provided to you, results of your experiments, or code to anyone else. This includes posting your coursework to the internet and making it accessible to other people not only during the coursework period, but also after that. Never copy-and-paste material of other people (including those available on the internet) into your coursework and edit it. You can, however, use the code provided in the lecture notes, slides, and labs of this course, excluding some functions described later. High-level discussion that is not directly related to this coursework is fine.

Please note that assessed work is subject to University regulations on academic misconduct:

http://web.inf.ed.ac.uk/infweb/admin/policies/academic-misconduct

For late coursework and extension requests, see the page: http://web.inf.ed.ac.uk/infweb/student-services/ito/admin/coursework-projects/late-coursework-extension-requests

Note that any extension request must be made to the ITO, and not to the lecturer.

Programming: Write code in Matlab(R2018a)/Octave or Python(version 2.7)+Numpy+Scipy+Matplolib. Your code should run on standard DICE machines without the need of any additional software. There are some functions that you should write the code by yourself rather than using those of standard libraries available. See section 4 for details.

This document assumes programming in Matlab. For Python, put all the specified functions into a single file for each Task, so that task1.py for Task 1, and task2.py for Task 2. Output data should be stored in Matlab's MAT binary format.

2 Data

The coursework employs the MNIST handwritten digits data set http://yann.lecun.com/exdb/mnist. Each character image is represented as 28-by-28 pixels in gray scale, being stored as a row vector of 784 elements $(28 \times 28 = 784)$. A subset of the original MNIST data set is considered in this coursework.

You data set is stored in your coursework-data directory (denoted as Your Data Dir hereafter):

/afs/inf.ed.ac.uk/group/teaching/inf2b/cwk2/d/UUN/

where \underline{UUN} denotes your UUN (DICE login name). In the directory, you will find the following four files:

File name	Matlab variable (Class)	Description
'tron-images-idx3-ubyte'	Xtrn[Ntrn,784] (uint8)	training samples
'trn-labels-idx1-ubyte'	Ytrn[Ntrn,1] (uint8)	class labels of training samples
'tst-images-idx3-ubyte'	Xtst[Ntst,784] (uint8)	test samples
'tst-labels-idx1-ubyte'	Ytst[Ntst,1] (uint8)	class labels of test samples

where Ntrn and Ntst denote the total number of training samples and test samples, respectively, which are smaller than the original ones. The file formats are the same as the original ones.

A sample code to load the data files will be provided in the following directory.

/afs/inf.ed.ac.uk/group/teaching/inf2b/cwk2/matlab_codes/

There are ten classes, C_1, \ldots, C_{10} , (C_1 corresponds to digit '0', C_{10} to '9'), and each class has about 4200 training samples and 300 test samples on the average, respectively, but exact number of samples may be different among different classes.

Each pixel value is represented as an unsigned byte integer (uint8) with the range in [0, 255]. Note that, after you load the data in your program, you should at first convert the image data to floating point (double) numbers. Additionally, you should divide the numbers by 255.0 so that the maximum value is less than or equal to 1.0.

A class label is represented as an 8-bit unsigned integer (uint8) number between 0 and 9, where 0 denotes '0' and 9 '9', respectively. For Matlab programming, you should change the original labels so that class number starts at 1 rather than 0.

3 Task specifications

Task1 – PCA and Clustering [50 marks]

Task 1.1 [5 marks]

(a) Write a Matlab function that displays the images of the first ten samples for each class using montage() function, so that each figure shows the ten samples for class C_k , where k = 1, ..., 10. Save your code as 'task1_1.m'. Note that file names and function names are case sensitive. The syntax of the function should be as follows.

function task1_1(X, Y)

where

- X M-by-D data matrix (of floating-point numbers in double-precision format, which is the default in Matlab), where M is the number of samples, and D is the number of elements in a sample. Note that each sample is represented as a row vector rather than a column vector.
- Y M-by-1 label vector (of uint8) for X. Y(i) is the class number of X(i,:).
- (b) Run the following:

```
task1_1(Xtrn, Ytrn);
```

and save the image (hardcopy) for each class as 'task1_1_imgs_class \underline{K} .pdf', where K = 1, ..., 10. (e.g. task1_1_imgs_class3.pdf is a hardcopy for C_3 in PDF format.) In your report, show the ten figures.

Task 1.2 [5 marks]

(a) Write a Matlab function that calculates a mean vector of data for each class (k = 1, ..., K, where K = 10) and for all, and displays the images of K + 1 mean vectors in a single graph using montage() function. Save your function as 'task1_2.m'. The syntax of the function should be as follows.

```
function M = task1_2(X, Y)
```

where X and Y are the same formats as in Task 1.1.

- M (K+1)-by-D mean vector matrix (double), where K is the number of classes, and D is the same as in Task 1.1. M(K+1,:) is the mean vector of the whole data.
- (b) Run the following:

```
M = task1_2(Xtrn, Ytrn);
```

and save M as 'task1_2_M.mat', save the figure as 'task1_2_imgs.pdf'. In your report, show the figure.

Task 1.3 [7 marks]

(a) Write a Matlab function that computes the principal components of a data set, and save it as 'comp_pca.m'. The syntax of the function is as follows:

```
function [EVecs, EVals] = comp_pca(X)
```

X is the same format as in Task 1.1. EVecs are the eigenvectors (stored in a D-by-D matrix EVecs), and EVals are the corresponding eigen values $\{\lambda_i\}_{i=1}^D$ (stored in a D-by-1 vector). The eigenvalues should be sorted in descending order, so that λ_1 is the largest and λ_D is the smallest, and i'th column of EVecs should hold the eigenvector that corresponds to λ_i . Eigenvectors are not unique by definition in terms of scale (length) and sign, but we make them unique in this coursework by putting the following additional constraints, which your comp-pca() should satisfy.

- The first element of each eigenvector is non-negative. If it is not the case, i.e. if the first element is negative, multiply -1 to the eigenvector (i.e. $\mathbf{v} \leftarrow -\mathbf{v}$) so that it gets the opposite direction.
- Each eigenvector is a unit vector, i.e. $\|\mathbf{v}\| = 1$, where \mathbf{v} denotes an eigenvector. As far as you use Matlab's eig() or Python's numpy.linalg.eig(), you do not need to care about this, since either function ensures unit vectors.
- (b) Write a Matlab function task1_3() that
 - carries out PCA (i.e. calls comp_pca),
 - computes cumulative variances, and plots them,
 - finds the minimum number of PCA dimensions to cover 70%, 80%, 90%, 95% of the total variance,

and save it as 'task1_3.m'. The syntax of the function should be as follows.

```
function [EVecs, EVals, CumVar, MinDims] = task1_3(X)
```

Where Evecs Evals the same as in part (a),

Cumvar D-by-1 vector (double) of cumulative variance.

MinDims 4-by-1 vector (int32) showing the minimum number of PCA dimensions shown above.

(c) Run the following:

```
[EVecs, EVals, CumVar, MinDims] = task1_3(Xtrn);
```

and save the graph as 'task1_3_graph.pdf', and save EVecs, Evals, CumVar, MinDims as 'task1_3_evecs.mat', 'task1_3_evals.mat', 'task1_3_cumvar.mat', and 'task1_3_mindims.mat' respectively.

In your report, show the figure of commutative covariance, and show the values of MinDims.

Task 1.4 [5 marks]

(a) Write a Matlab function that displays the images of the first ten principal axes of PCA using montage() so that all the images are shown in a single graph. Save your code as 'task1_4.m'. The syntax of the function should be as follows.

```
function task1_4(EVecs)
```

where EVecs is the same format as in Task 1.3.

(b) Run task1_4(EVecs) and save the figure as 'task1_4_imgs.pdf', where EVecs is the eigenvector matrix obtained in Task 1.3.

In your report, show the images.

Task 1.5 [6 marks]

(a) Write a Matlab function that carries out the k-means clustering, and save it as my_kMeansClustering.m. The syntax of the function should be as follows.

function [C, idx, SSE] = $my_kMeansClustering(X, k, initialCentres, maxIter)$ where X is the same format as in Task 1.1.

k The target number of clusters (int32) initial Centres Initial cluster centres in the k-by-D matrix (double), where each row represents a cluster centre.

 $\begin{array}{ll} \text{maxIter} & \text{Maximum number of iterations (optional)} \\ \text{C} & \text{Cluster centres in the k-by-$D matrix (double)}. \end{array}$

idx Cluster indices in the N-by-1 vector (int32), where idx[i] indicates the cluster number (starting from 1) of i-th data

point.

SSE The sum squared error (the one shown in slide 21 for

Lecture 3) for each iteration in the (L+1)-by-1 vector (double), where the first element is the SSE for the initial cluster centres, and L is the number of iterations done.

(b) Write a Matlab function that calls the k-mean clustering function for each k in a vector Ks, using the first k samples in the data set X as the initial cluster centres, and saves the returned C, idx, and SSE as 'task1_5_c_ \underline{k} .mat', 'task1_5_idx_ \underline{k} .mat', and 'task1_5_sse_ \underline{k} .mat', respectively. Save your code as 'task1_5.m'. The syntax of the the function should be as follows.

function task1_5(X, Ks)

where X is the same as in Task 1.1, Ks is a 1-by-L vector (int32) of the numbers of nearest neighbours.

(c) Run the following:

```
Ks = [1,2,3,4,5,7,10,15,20];

task1_5(Xtrn, Ks);
```

In your report, show a graph of SSE vs k, and show the time taken for each k.

Task 1.6 [5 marks]

(a) Write a Matlab function that displays the image of each cluster centre, where you should use montage() function to put all the images into a single figure. Save your code as 'task1_6.m'. The syntax of the function should be as follows.

```
function task1_6(MAT_ClusterCentres)
```

where MAT_ClusterCentres is a MAT binary file that contains C, the cluster centre matrix shown in Task 1.5.

(b) Run task1_6('task1_5_c_ \underline{k} .mat') for k in Ks defined in Task 1.5, and save each figure as 'task1_6_imgs_ \underline{k} .pdf'.

In your report, show the figures.

Task 1.7 [7 marks]

(a) Write a Matlab function that visualises cluster regions on the 2D-PCA plane, where the position of the plane is specified by a point vector. The plotting range should be $m \pm 5\sigma$, where m is the mean and σ is the standard deviation of the data on the corresponding PCA axis. Save your code as 'task1_7.m'. The syntax of the function should be as follows.

```
function Dmap = task1_7(MAT_ClusterCentres, MAT_M, MAT_evecs, MAT_evals,
posVec, nbins)
```

where the first three arguments are MAT files of cluster centres, eigenvectors, and eigenvalues. posVec is a 1-by-D vector (double) to specify the position of the 2D-PCA plane. We assume that nbins by nbins square grid points are used to plot the cluster regions. The output, Dmap is a nbin-by-nbin matrix (uint8), each element represents the cluster number that the point belongs to.

(b) Run the following for k = 1, 2, 3, 5, 10,

```
\label{eq:def:Dmap} $$\operatorname{task1_7('task1_5_c_{\underline{k}.mat', 'task1_2_M.mat', 'task1_3_evecs.mat', 'task1_3_evals.mat', mean(Xtrn), 200);}
```

and save Dmap as 'task1_7_dmap_ \underline{k} .mat', and save the figure of cluster regions as 'task1_7_imgs_ \underline{k} .pdf'.

(c) In your report, show the images, and describe the method implemented for visualising the regions.

Task 1.8 [10 marks]

This is a mini research project, in which you are asked to investigate the k-means clustering in terms of initial cluster centres, i.e. how different initial cluster centres result in different cluster centres, for which employ SSE to measure the clustering performance. Report your experiments and findings in your report, and save your code as 'task1_8.m'.

Task 2 - Classification [50 marks]

In the following classification experiments, assume a uniform prior distribution over class, and use the maximum likelihood estimation (MLE) to estimate model parameters. In programming, you can assume that the number of classes is equal to the maximum value of labels for training data, given that label values start at 1 rather than 0.

Task 2.1 [7 marks]

(a) Write a Matlab function for the classification with k-NN, save it as 'run_knn_classifier.m'. The syntax of the function should be as follows.

```
function [Ypreds] = run_knn_classifier(Xtrain, Ytrain, Xtest, Ks)
where
```

Ks 1-by-L vector of the numbers of nearest neighbours.

Ypreds N-by-L matrix (uint8) of predicted class labels for Xtest.

Ypreds(i,j) is the predicted class for Xtest(i,:) with the number of nearest neighbours being Ks(j).

(b) Write a Matlab function that creates a confusion matrix, and save the code as 'comp_confmat.m'. The syntax of the function should be as follows.

```
function [CM, acc] = comp_confmat(Ytrues, Ypreds, K)
where
```

Ytrues N-by-1 vector (uint8) of ground truth (target) class labels

Ypreds N-by-1 vector (uint8) of predicted class labels

K The number of classes (which is 10 for our data set)

CM K-by-K confusion matrix (int32), where CM(i,j) is the number of samples classified as j'th class among those whose true class label is i

acc A scalar variable (double) representing the accuracy (i.e. correct classification rate) with the range in [0, 1].

(c) Write the following Matlab function, and save it as 'task2_1.m'. The syntax of the function is as follows

```
function task2_1(Xtrain, Ytrain, Xtest, Ytest, Ks)
```

The specifications of the script are as follows.

• Runs a classification experiment on the data set using run_knn_classifier.

- Measures the user time taken for the classification experiment, and display the time (in seconds) to the standard output (i.e. display).
- Saves the confusion matrix for each k to a matrix variable cm, and save it with the file name 'task2_1_cm\(\bar{k}\).mat', where \(\bar{k}\) denotes the number of nearest neighbours (i.e. k) specified in Ks.
- Displays the following information (to the standard output).

k The number of nearest neighbours

N The number of test samples

Nerrs The number of wrongly classified test samples

acc Accuracy (i.e. correct classification rate)

(d) Run the following:

```
Ks = [1,3,5,10,20];
task2_1(Xtrn, Ytrn, Xtst, Ytst, Ks);
```

In your report, report the information shown on the display.

Task 2.2 [6 marks]

(a) Write a Matlab function that visualises decision regions of k-NN on a 2D PCA plane, where the position of the plane is specified by a point vector. Use the same specifications for plotting as in Task 1.7. The syntax of the function is as follows.

```
function Dmap = task2_2(Xtrain, Ytrain, k, MAT_evecs, MAT_evals, posVec,
nbins)
```

where k is the number of nearest neighbours in k-NN.

(b) Run the following for k=1,3.

```
N = 2000;
Xtrn2 = Xtrn(1:N,:); Ytrn2 = Ytrn(1:N,:);
Dmap = task2_2(Xtrn2, Ytrn2, k, 'task1_3_evecs.mat', 'task1_3_evals.mat',
mean(Xtrn), 200);
```

and save each Dmap as 'task2_2_dmap_ \underline{k} .map', and save the figure of decision regions as 'task2_2_imgs_k.pdf'.

In your report, show the figures.

Task 2.3 [7 marks]

(a) Write a Matlab function that transforms data to the ones in 2D PCA space and plots a contour of Gaussian distribution for each class. Save your code as 'task2_3.m'. The syntax of the function should be as follows.

```
function task2_3(Xtrain, Ytrain)
```

The specifications of the function are as follows.

- Transform X to the data in the 2D space spanned by the first two principal components.
- Estimate the parameters (mean vector and covariance matrix) of Gaussian distribution for each class in the 2D space.
- On a single graph, plot a contour of the distribution for each class using plot() function. Do not use functions for plotting contours such as contour(). The lengths of longest / shortest axis of an ellipse should be proportional to the standard deviation for the axis. (Please note that that contours of different distributions plotted by this method do not necessary give the set of points of the same pdf value.)
- (b) Run task2_3(Xtrn, Ytrn) and save the figure in 'task2_3_img.pdf'. In your report, show the figure.

Task 2.4 [5 marks]

(a) Write a Matlab function that calculates correlation r_{12} on 2D-PCA for each class and for all the classes (i.e. whole data). Note that the whole data (Xtrain shown below) should be used for PCA. Save your code as 'task2-4.m'. The syntax of the function is as follows.

```
function [Corrs] = task2_4(Xtrain, Ytrain)
```

where Corrs is a 11-by-1 vector (double) - Corrs(k) holds the correlation for class k (k = 1, ..., 10), and Output(11) holds the correlation for the whole data.

(b) Run task2_4(Xtrn, Ytrn) and save Corrs as 'task2_4_corrs.mat'. In your report, show the correlations.

Task 2.5 [6 marks]

(a) Write a Matlab function for the classification with a single Gaussian distribution per class, and save the code as 'run_gaussian_classifiers.m'. The syntax of the function should be as follows.

[Ypreds, Ms, Covs] = run_gaussian_classifiers(Xtrain, Ytran, Xtest, epsilon) where Xtrn, Ytrn, Xtst, and Ypreds are the same as those in Task1. epsilon is a scalar (double) for the regularisation of covariance matrix described in Lecture 8, in which we add a small positive number (ϵ) to the diagonal elements of covariance matrix, i.e. $\Sigma \leftarrow \Sigma + \epsilon I$, where I is the identity matrix.

Ms K-by-D matrix of mean vectors, where Ms(k,:) is the sample mean vector for class k.

Covs K-by-D-by-D 3D array of covariance matrices, where Cov(k,:,:) is the covariance matrix (after the regularisation) for class k.

Note that, as opposed to Tasks 2.3 and 2.4 that use PCA, we do not apply PCA to the data in this task.

(b) Write a Matlab function for a classification experiment, and save the code as 'task2_5.m'. The syntax of the function is as follows.

```
function task2_5(Xtrain, Ytrain, Xtest, Ytest, epsilon)
```

The specifications of the function are as follows.

- Calls the classification function with epsilon=0.01.
- Measures the user time taken for the classification experiment, and display the time (in seconds) to the standard output.
- Obtains the confusion matrix, stores it to a matrix variable cm, and saves it with the file name 'task2_5_cm.mat'.
- Copy the mean vector and covariance matrix for Class 10, i.e., Ms(10,:) and Covs(10,:,:), to new variables, M10 and Cov10, respectively, in the following manner:

```
M10 = Ms(10,:); Cov10 = Covs(10,:,:);
```

and save them as 'task2_5_m10.mat' and 'task2_5_cov10.mat', respectively.

• Displays the following information (to the standard output).

N The number of test samples

Nerrs The number of wrongly classified test samples

acc Accuracy (i.e. correct classification rate)

(c) Run task2_5(Xtrn, Ytrn, Xtst, Ytst, 0.01). In your report, report the information you obtained.

Task 2.6 [6 marks]

(a) Write a Matlab function that visualises decision regions of the Gaussian classifiers on a 2D-PCA plane. Save your code as 'task2_6.m'. The syntax of the function is as follows.

function Dmap = task2_6(X, Y, epsilon, MAT_evecs, MAT_evals, posVec, nbins) where MAT_evecs, MAT_evals, posVec, and nbins are the same as in Task 1.7.

(b) Run the following.

```
Dmap = task2_6(Xtrn, Ytrn, 0.01, 'task1_3_evecs.mat', 'task1_3_evals.mat',
mean(Xtrn), 200);
```

and save Dmap as 'task2_6_dmap.mat', and save the figure of decision regions as 'task2_6_img.pdf'.

In your report, show the figure.

Task 2.7 [5 marks]

This task aims to investigate the effect of amount of training data on classification performance for Gaussian classifiers.

(a) Write a Matlab function that run an experiment using a subset of training data, and save your code as 'task2_7.m'. The syntax of the function is as follows.

function [CM, acc] = task2_7(Xtrain, Ytrain, Xtest, Ytest, epsilon, ratio) where ratio specifies the ratio of training data to use. If it is 0.9, use the first 90% of samples in Xtrain.

(b) Run the following for ratio = 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3.

```
task2_7(Xtrn, Ytrn, Xtst, Ytst, 0.01, ratio);
```

and save each CM as 'task2_7_cm_ \underline{R} .mat', where \underline{R} = ratio * 100, so that 'task2_7_cm_90.mat' for ratio=0.9.

In report, report the result.

Task 2.8 [8 marks]

In this task, you

(a) Write a Matlab function that applies k-means clustering to each class to obtain multiple Gaussian classifiers per class, and carries out classification. Save the function as 'run_mgcs.m'

The syntax of the function is as follows.

function [Ypreds, MMs, MCovs] = run_mgcs(Xtrain, Ytrain, Xtest, epsilon,
L)

where L denotes the number of clusters per class.

MMs L*K-by-D matrix (double) of mean vectors.

MCovs (L*K)-by-D-by-D 3D array (double) of covariance matrices.

(b) Write a Matlab function that runs an experiment, and save the code as 'task2_8.m'. The syntax of the function is as follows.

function task2_8(Xtrain, Ytrain, Xtest, Ytest, epsilon, L)

The specifications of the function are as follows.

- Calls the classification function.
- Measures the user time taken for the classification experiment, and display the time (in seconds) to the standard output.
- Obtains the confusion matrix, stores it to a matrix variable cm, and saves it with the file name 'task2_8_cm_L.mat'.
- Copy the mean vectors and covariance matrices for Class 1, i.e., MMs(1:L,:) and MCovs(1:L,:,:), to new variables, Ms1 and Covs1, respectively, in the following manner:

```
Ms1 = MMs(1:L,:); Covs1 = MCovs(1:L,:,:);
```

Save Ms1 and Covs1 as 'task2_8_gL_m1.mat' and 'task2_8_gL_cov1.mat', respectively.

• Displays the following information (to the standard output).

N The number of test samples

Nerrs The number of wrongly classified test samples

acc Accuracy (i.e. correct classification rate)

(c) Run run_mgcs(Xtrn, Ytrn, Xtst, Ytst, 0.01, L); for L=2,5,10. In your report, report the information you obtained.

4 Functions that are not allowed to use

Since one of the objectives of this coursework is to understand and implement basic algorithms for machine learning, you are not allowed to use those functions in standard libraries listed below. You should write the code by yourself using the basic operations of arithmetic for scalars, vectors, and matrices. If it is the case, use a different function name from the original one in standard libraries (e.g. MyCov() for cov() as shown in the table below). You may, however, use them for comparison purposes, i.e. to check your code.

Description of function	Typical names	Suggested name to implement
Pairwise (squared) Euclidean distance	pdist2()	MySqDist()
Compute the mean	mean()	MyMean()
Compute the covariance matrix	cov()	MyCov()
Compute Gaussian probability densities	mvnpdf()	
K-NN classification	fitcknn()	$run_knn_classifier()$
K-means clustering	kmeans()	$my_kMeansClustering()$
Compute confusion matrix	confusion()	$comp_confmat()$
Other utilities for classification		

You may use those functions or operations:

Description	Typical names	
Sum function	sum()	
Cumulative sum	cumsum()	
Square root function	$\operatorname{sqrt}()$	
Exponential function	e, exp()	
Logarithmic function	$\log(), \ln()$	
Matrix transpose	transpose(), '	
Matrix inverse	inv()	
Determinant	$\det()$	
Log determinant	logdet() · · · available in Inf2b cwk2 directory	
Eigen values/vectors	$\operatorname{eig}()$	
Sort	$\operatorname{sort}()$	
Sample mode	mode()	
Vectorisation helpers	bsxfun(), arrayfun()	
(NB: the list is not exhaustive)		

5 Submission

You should submit your work electronically via the DICE submit command by the deadline. No submission of printed document is required.

Since marking for each task will be done separately, you should prepare separate reports for the two tasks, and save your report files in PDF format and name them 'report_task1.pdf' and 'report_task2.pdf'. Remember to place your student number and the task name prominently at the top of each report. Do not indicate your name anywhere. Your report should be concise and brief for each task.

Create a directory named LearnCW, copy all of the requested files to the the directory, but do NOT put the data set files in it.

A checklist will be available from the coursework web page. Submit your coursework from a DICE machine using:

submit inf2b cw2 LearnCW