

ITMAL

Hand-in: Journal 2

Af Gruppe 12

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Gradient descent

Qa:

Qa The Gradient Descent Method (GD)

Explain the gradient descent algorithm using the equations [HOML] p.114-115. and relate it to the code snippet

```
X_b, y = GenerateData()

eta = 0.1
n_iterations = 1000
m = 100
theta = np.random.randn(2,1)

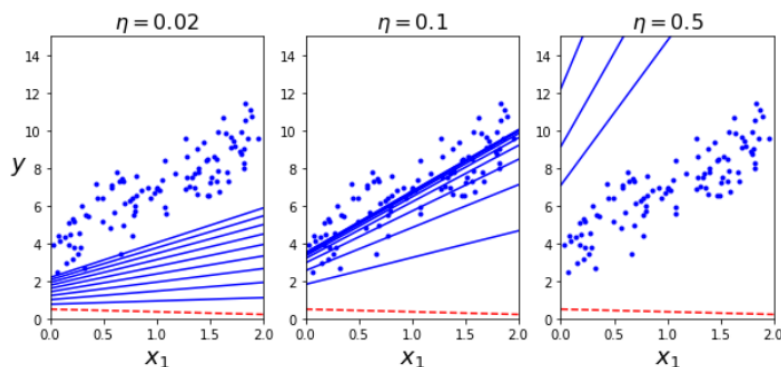
for iteration in range(n_iterations):
    gradients = 2/m * X_b.T.dot(X_b.dot(theta) - y)
    theta = theta - eta * gradients
```

in the python code below.

As usual, avoid going too much into details of the code that does the plotting.

What role does `eta` play, and what happens if you increase/decrease it (explain the three plots)?

stochastic gradient descent theta=[3.86865647 2.98760205]



OK

Forklaring:

On the left, the learning rate is too low: the algorithm will eventually reach the solution, but it will take a long time. In the middle, the learning rate looks pretty good: in just a few iterations, it has already converged to the solution. On the right, the learning rate is too high: the algorithm diverges, jumping all over the place and actually getting further and further away from the solution at every step.

Qb:

Qb The Stochastic Gradient Descent Method (SGD)

Now, introducing the *stochastic* variant of gradient descent, explain the stochastic nature of the SGD, and comment on the difference to the *normal* gradient descent method (GD) we just saw.

Also explain the role of the calls to `np.random.randint()` in the code,

HINT: In detail, the important differences are, that the main loop for SGC is

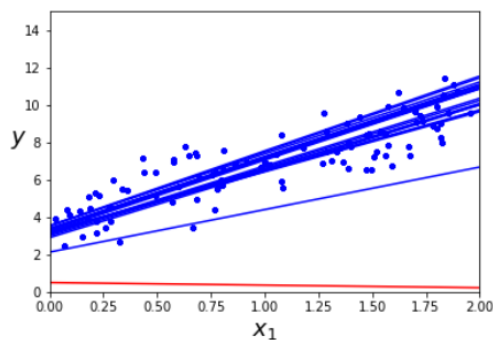
```
for epoch in range(n_epochs):
    for i in range(m):
        .
        .
        .
        gradients = 2 * xi.T.dot(xi.dot(theta) - yi)
        eta = ...
        theta = ...
```

where it for the GD method was just

```
for iteration in range(n_iterations):
    gradients = 2/m * X_b.T.dot(X_b.dot(theta) - y)
    theta = ..
```

NOTE: the call `np.random.seed(42)` resets the random generator so that it produces the same random-sequence when re-running the code.

stochastic gradient descent theta=[3.88230298 2.9898987]
Scikit-learn SGDRegressor "thetas": sgd_reg.intercept_[3.87342226], sgd_reg.coef_[3.00024641]



OK

`np.random.randint()` Bruges til at vælge en ny hældning, for at hurtigere kunne finde en korrekt hyperparameter. samtidig med at kunne have en større chance for at ramme det globale minimum på error function.

Qd:

Qd Mini-batch Gradient Descent Method ¶

Finally explain what a **mini-batch** SG method is, and how it differs from the two others.

Again, take a peek into the demo code below, to extract the algorithm details...and explain the **main differences**, compared with the GD and SGD.

Forklaring:

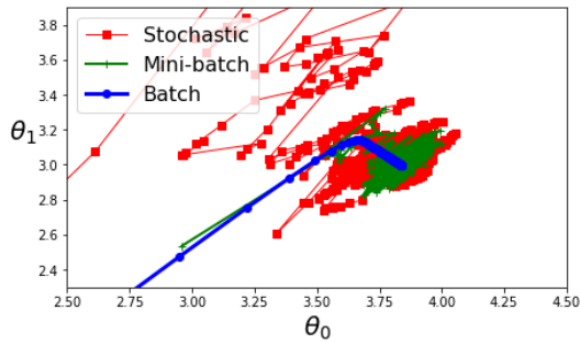
mini-batch theta=[3.86814831 3.02878845]
OK

Mini batch, som navnet lyder, shuffler dataen hver gang den når til outer loop igen, dette vil sige, den prøver m gange, hvorefter den som i SGD får chancen for at ramme det globale minimum hver gang inner loop er done!

Qe:

Qe Choosing a Gradient Descent Method

Explain the $\theta_0 - \theta_1$ plot below, and make a comment on when to use GD/SGD/mini-batch gradient descent (pros and cons for the different methods).



OK

Her ses det tydeligt at batch passer bedst til dette dataset, denne ville dog ikke kunne undslippe et lokal minimum. SGD passer bedre til flere minima i en error function da den kan undslippe de lokale minima, mens MGD får lov at arbejde længere tid på specifikke områder, derfor mere præcis, men dog måske langsommere.

Capacity under overfitting

Qa:

Qa Explain the polynomial fitting via code review

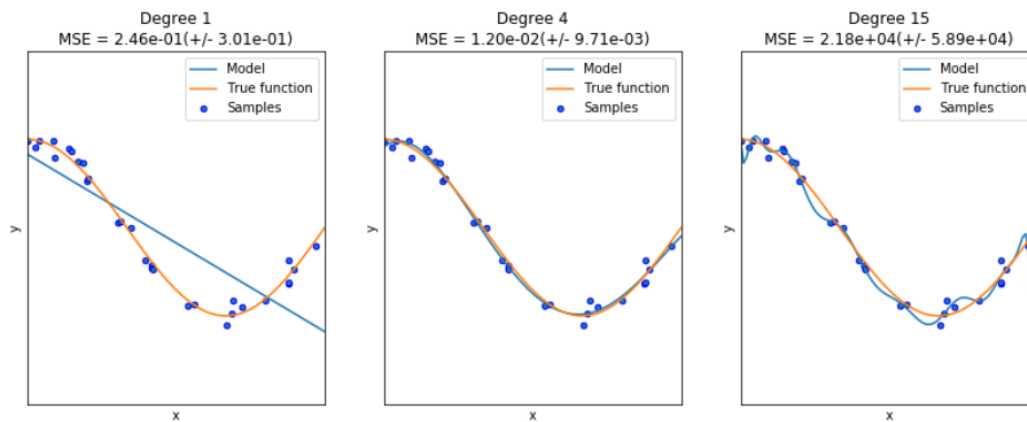
Review the code below, write a **short** code review summary, and explain how the polynomial fitting is implemented?

Do not dig into the plotting details, but explain the outcome of the plots.

```

Iterating...degrees= [1, 4, 15]
degree= 1, score_mean=0.25, PolynomialFeatures(degree=1, include_bias=False, interaction_only=False)
degree= 4, score_mean=0.01, PolynomialFeatures(degree=4, include_bias=False, interaction_only=False)
degree= 15, score_mean=21826.29, PolynomialFeatures(degree=15, include_bias=False, interaction_only=False)

```



OK

Der genereres data i form af sample punkterne X og y, ud fra en funktion, plus støj. Denne data bruges til fitting af de 2 modeller der er i pipelinen. Dette køres igennem 3 gange med forskellige degrees i polynomial features. (1 , 4 og 15)

Det ses at det første billede med 1 degree er meget underfittet, da resultatet stort set er en linær streg, hvor den skulle følge cosinus

Billede 3 er Overfittet, her ses det at modellen har "lært støjen" den tror den rammer rigtig, men i virkeligheden er den meget overfittet.

billede 2, passer meget bedre til hvad vi forventer at få ud, da den passer til funktionen, og ikke støjen.

Qb:

Qb Explain the capacity and under/overfitting concept

Write a textual description of the capacity and under/overfitting concept using the plots in the code above.

What happens when the polynomial degree is low/medium/high with respect to under/overfitting concepts? Explain in details.

Overfitting betyder at den har "lært af" støjen, dvs den passer perfect på støjen, og ikke funktionen, overfitting har en høj evne til at tilpasse sig (capacity). Underfitting, betyder af den nærmere rammer middel værdierne imellem punkterne, og minder mere om en linær line. Underfitting kan ikke generalisere godt, og derved ikke lære af dataen (capacity)

Generalization error

Qa:

Write a detailed description of figure 5.3 (above) for your journal.

All concepts in the figure must be explained

- training/generalization error,
- underfit/overfit zone,
- optimal capacity,
- generalization gap,
- and the two axes: x/capacity, y/error.

Forklaring

Generalisation error er hvor god algoritmen er til at predicte ud fra test data. Training error, er hvor god algoritmen er til at predicte ud fra trænings data.

Underfitting zone, er hvor generalisation error og training error er høj, fordi, da der ikke er fittet nok endnu.'

Optimal capacity, er hvor underfitting og overfitting er lige tilpas, så errors ikke er særlige høje på både test og trænings data

Overfitting zone, er hvor der er fittet for meget, og derfor passer "for godt" til træningsdataen, men passer rigtig dårlig på nyt data(test data)

Generalization gap, Jo mere overfittet, jo større gap, da det bliver alt for specifi

Qb:

Review the code for plotting the RMSE vs. the iteration number or epoch below (two cells, part I/II).

Write a short description of the code, and comment on the important points in the generation of the (R)MSE array.

The training phase output lots of lines like

```
epoch= 104, mse_train=1.50, mse_val=2.37
epoch= 105, mse_train=1.49, mse_val=2.35
```

What is an **epoch** and what is `mse_train` and `mse_val` ?

NOTE: the generalization plot in figure 5.3 and the plots below have different x-axis, and are not to be compared directly!

```
X_train.shape= (25, 1)
X_val .shape= (25, 1)
y_train.shape= (25,)
y_val .shape= (25,)
OK
```

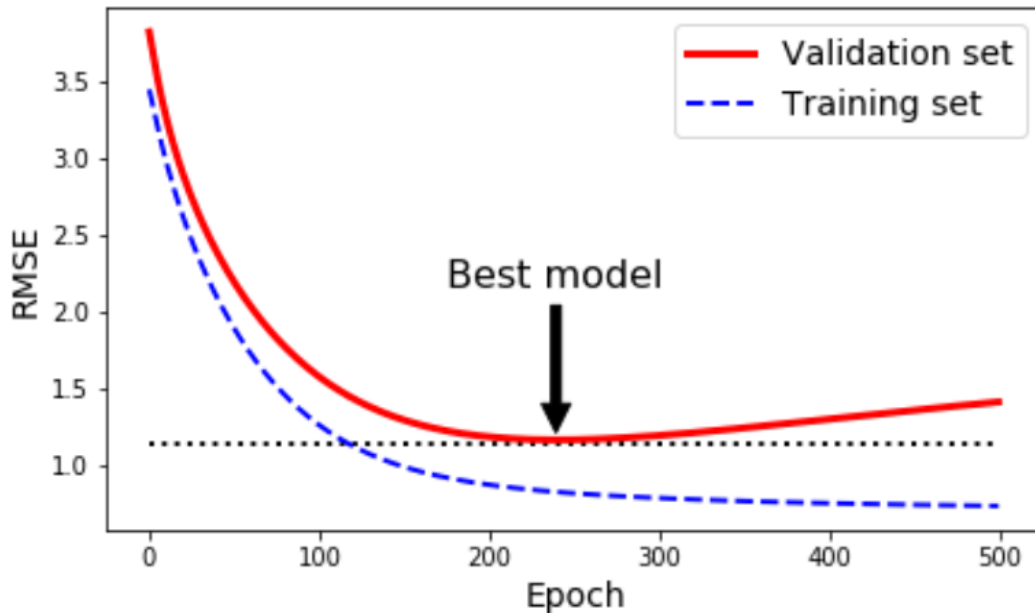
Epoch is the iteration it goes through in the descent MSE_Train is the Mean Square Error in the training set at the epoch MSE_val is the Mean Square Error in the test set at the epoch

`poly_scaler.fit_transform`, finder ud af hvad der skal til for at komme ned omkring nul, og transformere dataen ned til omkring nul.

Qb part II:

epoch= 498, mse_train=0.54, mse_val=1.98

epoch= 499, mse_train=0.54, mse_val=1.99



I koden overfor køres igennem fra vores data fra før, i et stokastisk gradient decent. Dette gøres (ud fra vores valg) 500 gange. for hver gang, springer random til et nyt sted, og tilnærmer sig det globale minimum, denne fremgangsmåde forhindre modellen i at ramme de lokale minima, og blive "stuck" der, her tilnærmer sig den det globale minimum, i starten, og "graver sig ned der". Hvir der er "for mange epoker" riskiere vi igen overfitting, som også kan ses på billedet ovenfor. Her ses det at trænings sættets RMSE bliver mindre og mindre, og tilsyneladende bedre og bedre, men langsomt, stiger RMSE for validations sættet.

Naïve Bayes

```
def MNIST_GetDataSet():
    return (mnist['data'], mnist['target'])

X, y = MNIST_GetDataSet()

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)

modelGaus = GaussianNB()
ModelMulti = MultinomialNB()

modelGaus.fit(X_train, y_train)
ModelMulti.fit(X_train, y_train)

y_predGaus = modelGaus.predict(X_test)
y_predMulti = ModelMulti.predict(X_test)
```

```
# accuracy
from sklearn.metrics import accuracy_score

ModelAccuracy = accuracy_score(y_predGaus, y_test)
print(ModelAccuracy)

ModelAccuracy = accuracy_score(y_predMulti, y_test)
print(ModelAccuracy)
```

```
0.5515714285714286
0.829
```

```
# f1 score
from sklearn.metrics import f1_score

Modelf1 = f1_score(y_test, y_predGaus, average='weighted')
print(Modelf1)

Modelf1 = f1_score(y_test, y_predMulti, average='weighted')
print(Modelf1)
```

```
0.5061920628495427
0.8296318905479115
```

```
ModelPresicion = precision_score(y_test, y_predGaus, average='weighted')
print(ModelPresicion)

ModelPresicion = precision_score(y_test, y_predMulti, average='weighted')
print(ModelPresicion)
```

```
0.6770364512150268
0.836251187274071
```

Regulizers

Qa:

Now, lets examine what $||\mathbf{w}||_2^2$ effectively mean? It is composed of our well-known \mathcal{L}_2^2 norm and can also be expressed as

$$||\mathbf{w}||_2^2 = \mathbf{w}^T \mathbf{w}$$

Construct a penalty function that implements $\mathbf{w}^T \mathbf{w}$, re-using any functions from `numpy` (implementation could be a tiny *one-liner*).

Take w_0 into account, this weight factor should NOT be included in the norm. Also checkup on `numpy s dot` implementation, if you have not done so and are using it: it is a typical pythonic *combo* function, doing both dot op's (inner product) and matrix multiplication (outer product) dependent on the shape of the input parameters.

Then run it on the three test vectors below, and explain when the penalty factor is low and when it is high.

```
def Omega(w):
    temp = w[1:]
    return (temp.T).dot(temp)

# weight vector format: [w_0 w_1 .. w_d], ie. elem. 0 is the 'bias'
w_a = np.array([1, 2, -3]) #
w_b = np.array([1E10, -3E10])
w_c = np.array([0.1, 0.2, -0.3, 0])

p_a = Omega(w_a)
p_b = Omega(w_b)
p_c = Omega(w_c)
```

$P(w_0)=13$
 $P(w_1)=9e+20$
 $P(w_2)=0.13$

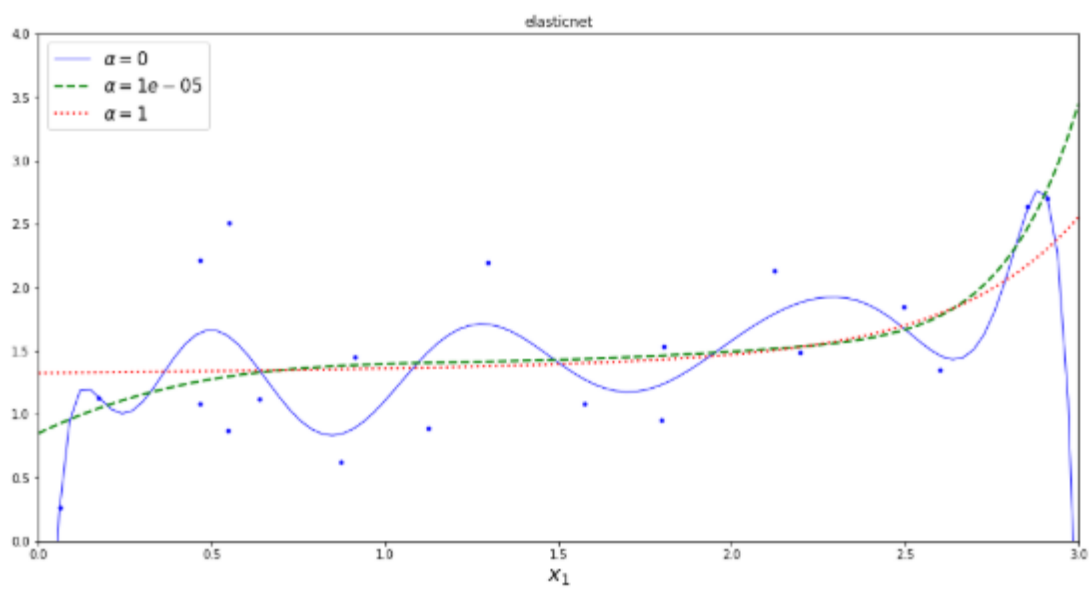
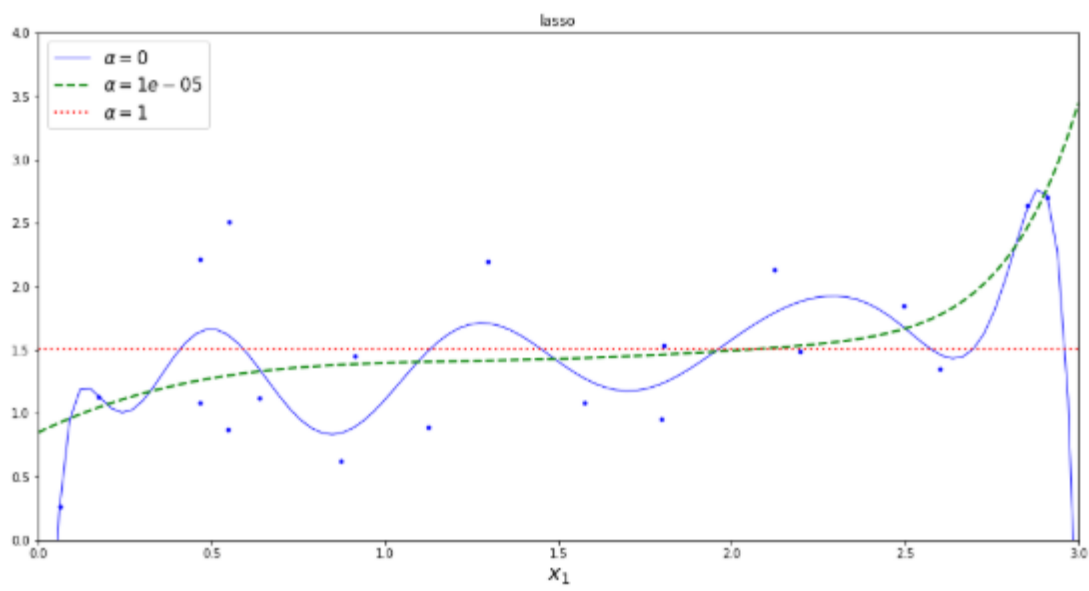
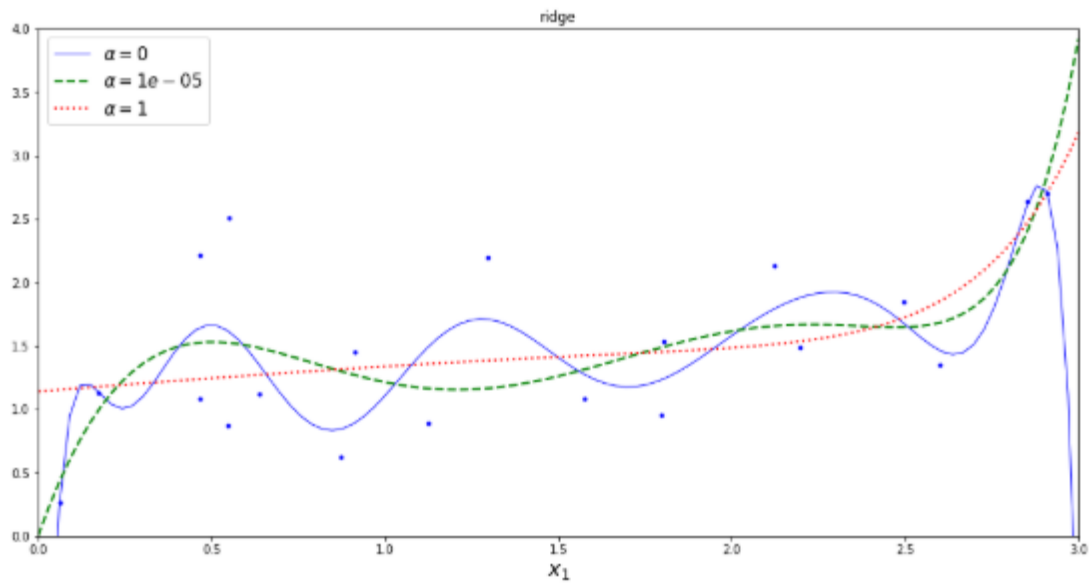
$P(w_0)$ er høj fordi tallene i arrayet er højere $p(w_1)$ er meget lav, da værdierne i arrayet også er meget lave.

Straffens vægt skal passe til talene!

Qb:

First take a peek into the plots (and code) below, that fits the Ridge, Lasso and ElasticNet to a polynomial model. The plots show three fits with different α values (0, 10^{-5} , and 1).

First, explain what the different α does to the actual fitting for the Ridge model in the plot.



Ridge bruges når penalty vægten skal være høj og straffen lille (da den er summen af de kvadratiske værdier) lasso bruges når vægten skal være lav, og straffen hård! (summen af de absolute værdier)

elastic net er kombinationen af ridge og lasso.

Alpha afgør straffen for træningen. Dette kan bruges til at sortere støj fra datasættet

Qc:

Then explain the different regularization methods used for the Ridge, Lasso and ElasticNet models, by looking at the math formulas for the methods in the Scikit-learn documentation and/or using [HOML].

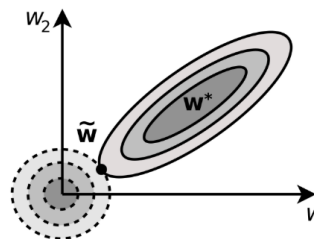
Lasso regression eliminere automatisk ubetydelige features, hvilket giver en renere model. hvor det flat liner ved vægten 1 Ridge regression, beholder vægterne så små som muligt og bevare features meres. hvis α er 0 fungerer ridge som en linear regression. hvis α er for stor, flat liner det.

Elastic net er en kombination af de 2 andre.

Qd:

Finally, comment on how regularization may be used to reduce a potential tendency to overfit the data

Describe the situation with the tug-of-war between the MSE and regularizer terms in \tilde{J} and the potential problem of \mathbf{w}^* being far, far away from the origin (with $\alpha = 1$ in regularizer term).



Would data preprocessing in the form of scaling, standardization or normalization be of any help to that particular situation? If so, describe.

Forklaring

Regularization kan bruges hvis f.eks. dataen er overfittet, til at sortere ubetydelige features / støj fra dataen!

ja, man kan preprocess for at fjerne en del af den støj der ligger i dataen, hvilket vil give bedre fitting og dermed MSE ..

Gridsearch

Qa

There are two code cells below: 1:) function setup, 2) the actual grid-search.

Review the code cells and write a **short** summary. Mainly focus on **cell 2**, but dig into cell 1 if you find it interesting (notice the use of local-function, a nifty feature in python).

In detail, examine the lines:

```
grid_tuned = GridSearchCV(model, tuning_parameters, ..
grid_tuned.fit(X_train, y_train)
..
FullReport(grid_tuned, X_test, y_test, time_gridsearch)
```

and write a short description of how the GridSearchCV works: explain how the search parameter set is created and the overall search mechanism (without going into too much detail)

What role does the parameter `scoring='f1_micro'` play in the GridSearchCV, and what does `n_jobs=-1` mean?

Cell 1

```

return X_train, X_test, y_train, y_test

print('OK')

```

OK

Cell 2

DATA: iris..

```

org. data: X.shape      =( 150;   4), y.shape      =( 150)
train data: X_train.shape=( 105;   4), y_train.shape=( 105)
test data: X_test.shape =(  45;   4), y_test.shape =(  45)

```

SEARCH TIME: 0.05 sec

Best model set found on train set:

```

best parameters={'C': 1, 'kernel': 'linear'}
best 'f1_micro' score=0.9714285714285714
best index=0

```

Best estimator CTOR:

```

SVC(C=1, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma='scale', kernel='linear',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)

```

Grid scores ('f1_micro') on development set:

```

[ 0]: 0.971 (+/-0.048) for {'C': 1, 'kernel': 'linear'}
[ 1]: 0.952 (+/-0.084) for {'C': 1, 'kernel': 'rbf'}
[ 2]: 0.952 (+/-0.084) for {'C': 10, 'kernel': 'linear'}
[ 3]: 0.971 (+/-0.048) for {'C': 10, 'kernel': 'rbf'}

```

Detailed classification report:

The model is trained on the full development set.
The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	1.00	1.00	1.00	16
1	1.00	0.94	0.97	18
2	0.92	1.00	0.96	11
micro avg	0.98	0.98	0.98	45
macro avg	0.97	0.98	0.98	45
weighted avg	0.98	0.98	0.98	45

```

CTOR for best model: SVC(C=1, cache_size=200, class_weight=None, coef0=0.0,
decision_function_shape='ovr', degree=3, gamma='scale', kernel='linear',
max_iter=-1, probability=False, random_state=None, shrinking=True,
tol=0.001, verbose=False)

```

```
best: dat=iris, score=0.97143, model=SVC(C=1, kernel='linear')
```

OK

Forklaring

grid search cv bruges til at pgle sig ind på de bedste parameter til en model, ved at prøve sig frem i mange forsøg, dog kan nogle parametre vælges i forvejen.

scoring f1_micro er den score der bruges til at regulere med. n_jobs=-1 kører parallelt.

Qb

Now, replace the `svm.SVC` model with an `SGDClassifier` and a suitable set of the hyperparameters for that model.

You need at least four or five different hyperparameters from the `SGD` in the search-space before it begins to take considerable compute time doing the full grid search.

```

18]: # TODO: Qb..
      model = SGDClassifier()

```

SEARCH TIME: 0.22 sec

Best model set found on train set:

```

      best parameters={'alpha': 10.0, 'average': False, 'n_iter_no_change': 1}
      best 'f1_micro' score=0.7619047619047619
      best index=39

```

Best estimator CTOR:

```

      SGDClassifier(alpha=10.0, average=False, class_weight=None,
early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None,
n_iter=None, n_iter_no_change=1, n_jobs=None, penalty='l2',
power_t=0.5, random_state=None, shuffle=True, tol=None,
validation_fraction=0.1, verbose=0, warm_start=False)

```

Grid scores ('f1_micro') on development set:

```

      [ 0]: 0.695 (+/-0.031) for {'alpha': 0.5, 'average': True, 'n_iter_no_change': 1}
      [ 1]: 0.743 (+/-0.137) for {'alpha': 0.5, 'average': False, 'n_iter_no_change': 1}
      [ 2]: 0.705 (+/-0.052) for {'alpha': 1.0, 'average': True, 'n_iter_no_change': 1}

```

Detailed classification report:

The model is trained on the full development set.
The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	0.67	1.00	0.80	16
1	0.00	0.00	0.00	18
2	0.52	1.00	0.69	11
micro avg	0.60	0.60	0.60	45
macro avg	0.40	0.67	0.50	45
weighted avg	0.37	0.60	0.45	45

```

CTOR for best model: SGDClassifier(alpha=10.0, average=False, class_weight=None,
    early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
    l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None,
    n_iter=None, n_iter_no_change=1, n_jobs=None, penalty='l2',
    power_t=0.5, random_state=None, shuffle=True, tol=None,
    validation_fraction=0.1, verbose=0, warm_start=False)

best: dat=iris, score=0.76190, model=SGDClassifier(alpha=10.0,average=False,n_iter_no_change=1)

OK

```

Qc

Now, add code to run a `RandomizedSearchCV` instead.



Conceptual graphical view of randomized search for two distinct hyperparameters.

Use the same parameters for the random search, but add and investigate the new `n_iter` parameter

```

random_tuned = RandomizedSearchCV(model, tuning_parameters, random_state=42, n_iter=20, cv=CV, scoring='f1_micro', verbose=VERBOSE, n_jobs=-1, iid=True)

```

Comparison of time (seconds) to complete `GridSearch` versus `RandomizedSearchCV`, does not necessarily give any sense, if your grid search completes in seconds (for the Iris tiny-data).

But you could compare the best-tuned parameter set and best scoring for the two methods. Is the random search best model close to the grid search?

```

random_tuned = RandomizedSearchCV(model, tuning_parameters, random_state=42, n_iter=1100,
    cv=CV, scoring='f1_micro', verbose=VERBOSE, n_jobs=-1, iid=True)

random_tuned.fit(X_train, y_train)
t = time()-start
# Report result
b0, m0= FullReport(random_tuned , X_test, y_test, t)

print(random_tuned)

```

SEARCH TIME: 5.22 sec

Best model set found on train set:

```

best parameters={'n_iter_no_change': 11, 'average': False, 'alpha': 0.5}
best 'f1_micro' score=0.7714285714285715
best index=26

```

Best estimator CTOR:

```

SGDClassifier(alpha=0.5, average=False, class_weight=None,
    early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
    l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None,
    n_iter=None, n_iter_no_change=11, n_jobs=None, penalty='l2',
    power_t=0.5, random_state=None, shuffle=True, tol=None,
    validation_fraction=0.1, verbose=0, warm_start=False)

```


Detailed classification report:

The model is trained on the full development set.

The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	1.00	1.00	1.00	16
1	0.00	0.00	0.00	18
2	0.38	1.00	0.55	11
micro avg	0.60	0.60	0.60	45
macro avg	0.46	0.67	0.52	45
weighted avg	0.45	0.60	0.49	45

CTOR for best model: SGDClassifier(alpha=0.5, average=False, class_weight=None, early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True, l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None, n_iter=None, n_iter_no_change=11, n_jobs=None, penalty='l2', power_t=0.5, random_state=None, shuffle=True, tol=None, validation_fraction=0.1, verbose=0, warm_start=False)

best: dat=iris, score=0.77143, model=SGDClassifier(alpha=0.5,average=False,n_iter_no_change=11)

```
RandomizedSearchCV(cv=5, error_score='raise-deprecating',
    estimator=SGDClassifier(alpha=0.0001, average=False, class_weight=None,
    early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
    l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None,
    n_iter=None, n_iter_no_change=5, n_jobs=None, penalty='l2',
    power_t=0.5, random_state=None, shuffle=True, tol=None,
    validation_fraction=0.1, verbose=0, warm_start=False),
    fit_params=None, iid=True, n_iter=1100, n_jobs=-1,
    param_distributions={'n_iter_no_change': array([ 1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16])},
    'alpha': array([ 0.5,  1. ,  1.5,  2. ,  2.5,  3. ,  3.5,  4. ,  4.5,  5. ,  5.5,
    6. ,  6.5,  7. ,  7.5,  8. ,  8.5,  9. ,  9.5, 10. , 10.5, 11. ,
    11.5, 12. , 12.5, 13. , 13.5, 14. , 14.5, 15. , 15.5, 16. , 16.5])}, 'average': (True, False)},
    pre_dispatch='2*n_jobs', random_state=42, refit=True,
    return_train_score='warn', scoring='f1_micro', verbose=0)
```

Qd

Finally, we create a small competition: who can find the best model+hyperparameters for MNIST dataset?

You change to the MNIST data by calling `LoadAndSetupData('mnist')`, and this is a completely other ball-game that the *tiny-data* iris: it's much larger (but still far from *big-data*)!

- You might opt for an exhaustive grid search, or a faster but-less optimal random search...your choice.
- You are free to pick any classifier in Scikit-learn, even algorithms we have not discussed yet, but keep the score function at `f1_micro`, otherwise, we will be comparing 'æbler og pærer'.
- And, you may also want to scale you input data for some models to perform better (neural networks in particular).
- DO NOT USE Keras or Tensorflow models...not yet, and there are too many examples on the net to cut-and-paste from!

Check your result by printing the first *return* value from `FullReport()`

```
b1, m1 = FullReport(random_tuned , X_test, y_test, time_randomsearch)
print(b1)
```

that will display a result like

```
best: dat=iris, score=0.97143, model=SVC(C=1, kernel='linear')
```

Now, check if your score (for MNIST) is better that the currently best score on Blackboard: "L07: Optimization and searching" | "Search Quest for MNIST"

https://blackboard.au.dk/webapps/blackboard/content/listContentEditable.jsp?content_id=2117394_1&course_id=124256_1&content_id=2179138_1

and paste your best model into the message box, like

```
best(Mr.Itmal): dat=mnist, score=0.47090, model=MLPClassifier(random_state=42, max_iter=10, activation='tanh')
```

Remember to provide a *custom* name manually, like 'best(joe)', 'best(john)' or 'best(it256)', so we can identify a winner!

For the journal, report your progress in scoring choosing different models, hyperparameters to search and how you might need to preprocess your data...

```
# TODO: Qd..
#from libitmal import utils as itmalutils
from libitmal import dataloaders_v2 as itmaldataloaders
X_train, X_test, y_train, y_test = LoadAndSetupData('mnist')
model = SGDClassifier()

random_tuned = RandomizedSearchCV(model, tuning_parameters, random_state=42, n_iter=5, cv=CV, scoring='f1_micro',
                                  verbose=VERBOSE, n_jobs=-1, iid=True)

random_tuned.fit(X_train, y_train)
t = time()-start
# Report result
b0, m0 = FullReport(random_tuned , X_test, y_test, t)

print(random_tuned)
```

```
DATA: mnist..
org. data: X.shape      =(70000; 784), y.shape      =(70000)
train data: X_train.shape=(49000; 784), y_train.shape=(49000)
test data: X_test.shape =(21000; 784), y_test.shape =(21000)
```

SEARCH TIME: 104.13 sec

Best model set found on train set:

```
best parameters={'n_iter_no_change': 1, 'average': True, 'alpha': 0.5}
best 'f1_micro' score=0.8949795918367347
best index=2
```

Best estimator CTOR:

```
SGDClassifier(alpha=0.5, average=True, class_weight=None,
early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None,
n_iter=None, n_iter_no_change=1, n_jobs=None, penalty='l2',
power_t=0.5, random_state=None, shuffle=True, tol=None,
validation_fraction=0.1, verbose=0, warm_start=False)
```

Grid scores ('f1_micro') on development set:

```
[ 0]: 0.870 (+/-0.040) for {'n_iter_no_change': 1, 'average': True, 'alpha': 14.0}
[ 1]: 0.881 (+/-0.028) for {'n_iter_no_change': 1, 'average': True, 'alpha': 16.0}
[ 2]: 0.895 (+/-0.005) for {'n_iter_no_change': 1, 'average': True, 'alpha': 0.5}
[ 3]: 0.885 (+/-0.017) for {'n_iter_no_change': 1, 'average': False, 'alpha': 11.5}
[ 4]: 0.861 (+/-0.035) for {'n_iter_no_change': 1, 'average': False, 'alpha': 1.5}
```

Detailed classification report:

The model is trained on the full development set.
The scores are computed on the full evaluation set.

Detailed classification report:

The model is trained on the full development set.
The scores are computed on the full evaluation set.

	precision	recall	f1-score	support
0	0.91	0.98	0.94	2077
1	0.94	0.97	0.96	2385
2	0.90	0.88	0.89	2115
3	0.90	0.86	0.88	2117
4	0.89	0.91	0.90	2004
5	0.89	0.76	0.82	1900
6	0.94	0.93	0.94	2045
7	0.92	0.91	0.92	2189
8	0.81	0.86	0.83	2042
9	0.84	0.88	0.86	2126
micro avg	0.90	0.90	0.90	21000
macro avg	0.90	0.89	0.89	21000
weighted avg	0.90	0.90	0.90	21000

CTOR for best model: SGDClassifier(alpha=0.5, average=True, class_weight=None, early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True, l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None, n_iter=None, n_iter_no_change=1, n_jobs=None, penalty='l2', power_t=0.5, random_state=None, shuffle=True, tol=None, validation_fraction=0.1, verbose=0, warm_start=False)

best: dat=mnist, score=0.89498, model=SGDClassifier(alpha=0.5, average=True, n_iter_no_change=1)

```
RandomizedSearchCV(cv=5, error_score='raise-deprecating',
estimator=SGDClassifier(alpha=0.0001, average=False, class_weight=None,
early_stopping=False, epsilon=0.1, eta0=0.0, fit_intercept=True,
l1_ratio=0.15, learning_rate='optimal', loss='hinge', max_iter=None,
n_iter=None, n_iter_no_change=5, n_jobs=None, penalty='l2',
power_t=0.5, random_state=None, shuffle=True, tol=None,
validation_fraction=0.1, verbose=0, warm_start=False),
fit_params=None, iid=True, n_iter=5, n_jobs=-1,
param_distributions={'n_iter_no_change': array([1]), 'alpha': array([ 0.5, 1. , 1.5, 2. , 2.5, 3. , 3.5, 4. ,
4.5, 5. , 5.5,
6. , 6.5, 7. , 7.5, 8. , 8.5, 9. , 9.5, 10. , 10.5, 11. ,
11.5, 12. , 12.5, 13. , 13.5, 14. , 14.5, 15. , 15.5, 16. , 16.5])}, 'average': (True, False)},
pre_dispatch='2*n_jobs', random_state=42, refit=True,
return_train_score='warn', scoring='f1_micro', verbose=0)
```

Speed up by compression

See how much you can speed up the above while retaining similar performance, by training on compressed data. (Don't forget to transform your test data too).

```
logisticRegr = LogisticRegression(solver = 'lbfgs',max_iter = 1000, multi_class = 'multinomial')
X_reduced_test = pca.fit_transform(X_test)

time_start = time.time()
logisticRegr.fit(X_reduced, y_train)
print('logisticRegr done! Time elapsed: {} seconds'.format(time.time()-time_start))

logisticRegr.score(X_reduced_test, y_test)

logisticRegr done! Time elapsed: 55.25297522544861 seconds
```

0.6372571428571429

forklaring

med komprimeret data ved at bibeholde samme PCA performance for vi en hurtigere træning men en væsentlig værre score

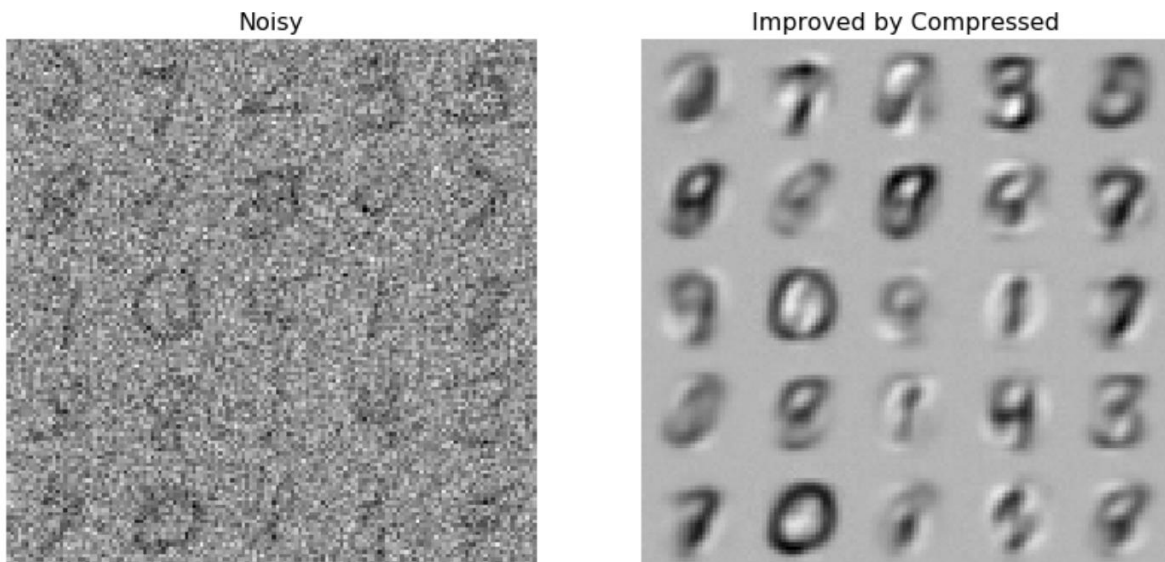
Noise reduction

Add some noise to MNIST (done below already), then compare a classifier trained and tested on:

Case 1: The noisy data.

Case 2: A PCA reduced version of the noisy data (remember to transform your test data too).

Can you find a reduced number of components that boosts performance? Different classifiers may handle noise more or less well by themselves. I tested with the SGDClassifier.



forklaring

Ved at sætte PCA n_components til at have 5% variance for vi et tydeligere billede af dataen.

```
clf = linear_model.SGDClassifier(max_iter=1000, tol=1e-3)
X_fit = clf.fit(X_train_noisy, y_train)
clf.score(X_test_noisy, y_test)
```

0.6383428571428571

forklaring

SGD kan bruges til at fitte dataen, men for en score på 0.63, som er væsentlig værre end vores PCA på ca 0.9.

PCA -> t-SNE features

From the above visualizations it seems reasonable that "PCA -> t-SNE" will perform much better than PCA alone as feature extraction by compression as input to a classifier (and be faster than t-SNE alone too).

Try if you can train and test with "PCA -> t-SNE" components (like we did earlier with PCA components). If not, explain why.

forklaring

man kan ikke træne og teste da t-SNE kun har funktionaliteten til fit_transform og ikke en transform til at bruge den fittede model og kan derfor ikke bruges til at transforme generelt data, men kun på dens egen fit_transformede data.

Neurons

Qa:

In broad terms, how does a neuron communicate?

Then explain, again with the wording of an engineer, not a biologist, how the neurons are structured in the brain.

Forklaring

Et neuron kommunikerer ved at "tilfældige" energi udladninger sender besked til neuronen om at videresende eller produceret et stof (en besked), som den sender videre til enten andre neuroner eller ud i kroppen, dette sker i synapsen. synapsen er mellemrummet mellem to neuroner. et neuron transmitter et stof over synapsen til en receptor i en anden neuron. dette er den besked, som der kommunikeres med mellem neuroner.

en meget kort forklaring om neuroner set fra en ingeniør, ville nok være at se neuroner som microchips, hvor synapser er de gates, som forbinder selv samme chips, så der kommer en energiladning med en besked fra en microchip som genereres "tilfældigt" og alt efter sammen faldet mellem energi udledning og hvilket gate, den rammer bestemmer beskeden. dette er mere struktureret end "tilfældigt", men dette kræver en bedre forståelse af biologi til at kunne beskrive i store detalje.

Qb:

Now, explaining cognition is still a pretty impossible philosophical question to answer. So you should answer this question: **what is your understanding of cognition?**

If we reproduce biological neurons, and just make enough of them, in your opinion, will a machine ever be able to have *cognition*?

Forklaring

kognition er evnen til at forstå, det er i sig selv et filosofisk beskrivelse. men for at gøre det så simpelt som muligt, så er forståelse mere end bare at kunne genkende, det er lige såvel at kunne associere det man ser og oplever med tilsvarende oplevelse at kunne skabe forbindelser imellem umiddelbare usammenhængende ting, igennem det man ville kunne intuition. Der er grader til den slags. dyr har en kognativ forståelse for visse opgaver og deres association. (godbider) dette er dog en slags intuition. hvor mennesker intuition er væsentlig anderledes. da der findes sociale og dyriske associationer samt intellektuel intuition (logisk). Disse intuitioner kan ikke genskabes ved at skabe flere neuroner, da desto store hjernen er, er ikke lig med ens kognitive evner. man kan sige at ML tillader maskiner at have dyriske associationer, i form af supervised/ semi-supervised learning / back-propagation. ved at bekræfte overfor maskinen at den laver den rigtige association. Som vil kunne skabe en form for intuition til at løse specifikke opgaver. men maskinen lærer ikke at associere på et højere plan. Som ikke løses ved mere hjernekapacitet. muligvis ved en anden forståelse af læring af maskinen eller hukommelse og evnen til at skabe "tilfældige" associationer.

Perceptron

Qa:

Load the moon data, split it into a train-and-test set, and train a `sklearn.linear_model.Perceptron` with default parameters (and with no cross-val this time).

What is the default score metric for the perceptron and what score do reach on the test data?

```
X, y = itmaldata loaders.MOON_GetDataSet(n_samples=1000)

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)

model = Perceptron();
model.fit(X_train, y_train);
model.score(X_test, y_test)
```

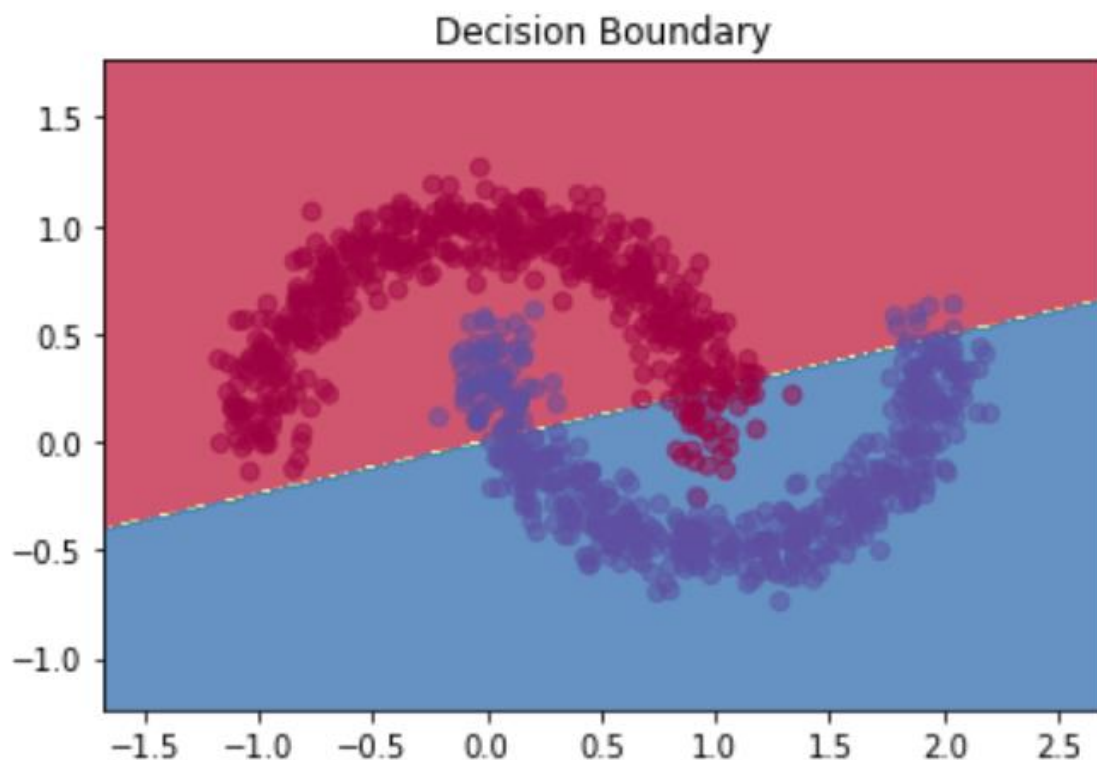
0.8533333333333334

Forklaring

Som det kan ses får vi en score på 0,85 med default settings som er `max_iter=1000` og `tol=None`.

Qb:

Use the helper code below to plot the decision boundary for the perceptron on the moon-data.



Qc:

How does the moon data relate to the well-known *XOR*-problem in machine learning?

Is it possible for a single neuron or perceptron to solve the moon/*XOR* problem satisfactorily?

Elaborate on the reason why not, and give a comment on how to overcome the *XOR*-problematic using more perceptrons.

Forklaring

En *XOR* tager to input og samlinger dem. Hvis de to input er forskellige giver det en false og hvis de er det samme giver den true.

En enkel Neuron/perceptron kan ikke løse dette problem. At den ikke kunne løse dette var også grunden til at man på et tidspunkt ikke mente at man kunne bruge neuroner til noget avanceret ML. Problemet er at neuronerne virker via en lineær model. Den lineære model kan ikke komme med to et enten eller output

Qd:

On the same train-test data train an SGD with perceptron compatible parameters. Give both models a `random_seed=42` and `tol=1e-3` parameters.

Are the SGD and Perceptron score metrics also compatible?

Does the SGD yield the same score as the Perceptron?

(100% similar scores, nearly similar or not at all similar?)

```
SGDModel = SGDClassifier(loss='perceptron', eta0=1, learning_rate='constant', penalty=None, random_state=42, tol=1e-3)
SGDModel.fit(X_train, y_train);
SGDScore = SGDModel.score(X_test, y_test)

PerceptronModel = Perceptron(random_state=42, tol=1e-3);
PerceptronModel.fit(X_train, y_train);
PerceptronScore = PerceptronModel.score(X_test, y_test)

print("SGDScore: ", SGDScore)
print("PerceptronScore: ", PerceptronScore)
```

```
SGDScore:  0.7933333333333333
PerceptronScore:  0.7933333333333333
```

Som vi kan se har begge model den samme score. Både SGD og Perceptron score bruger mean accuracy så det kan sagtens sammenlignes.

Multi-layers Perceptrons (MLP)

Qa:

Run the three cells below, and inspect the plots. I get an accuracy of 0.96 using the setup below.

Now, change the optimizer from `Adam` to our well-known `SGD` method, using

```
optimizer = SGD(lr=0.1)
```

instead of `ADAM(lr=0.1)`.

Does it still produce a good score, in form of the `categorical_accuracy`? My accuracy now drops to 0.88, and the new decision boundary looks like a straight line!

Find a way to make the `SGD` produce a result similar to the `ADAM` optimizer: Maybe you need to crank up the number of `EPOCHS` during training to get a better result using the `SGD` optimizer?

Cell 1

OK, training time=2.7

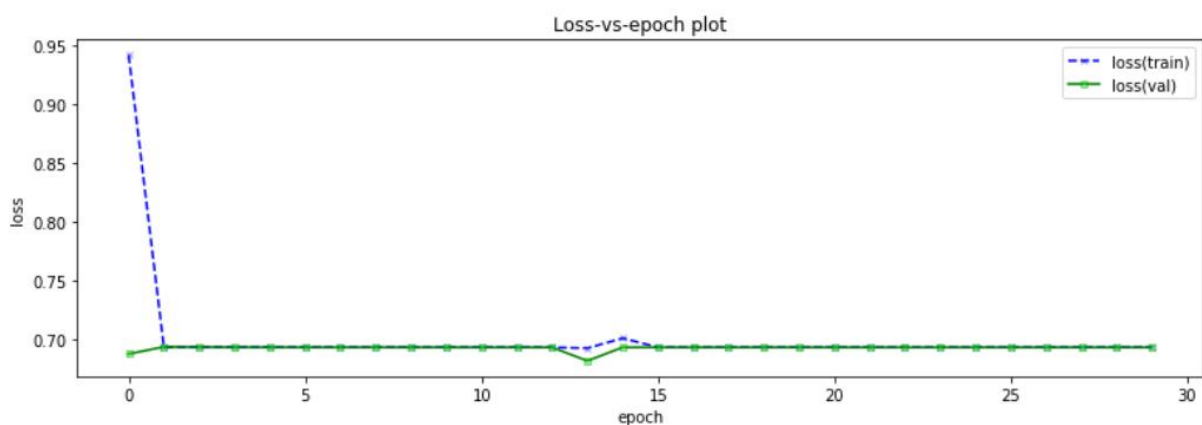
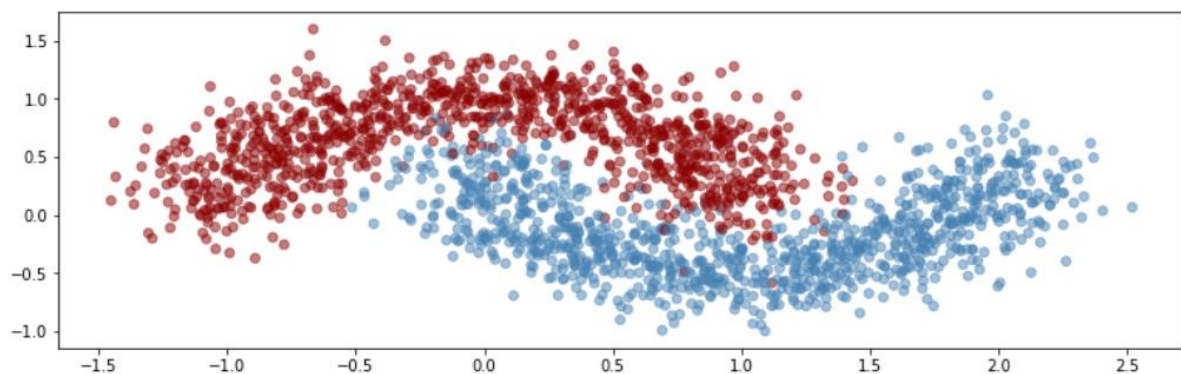
Cell 2

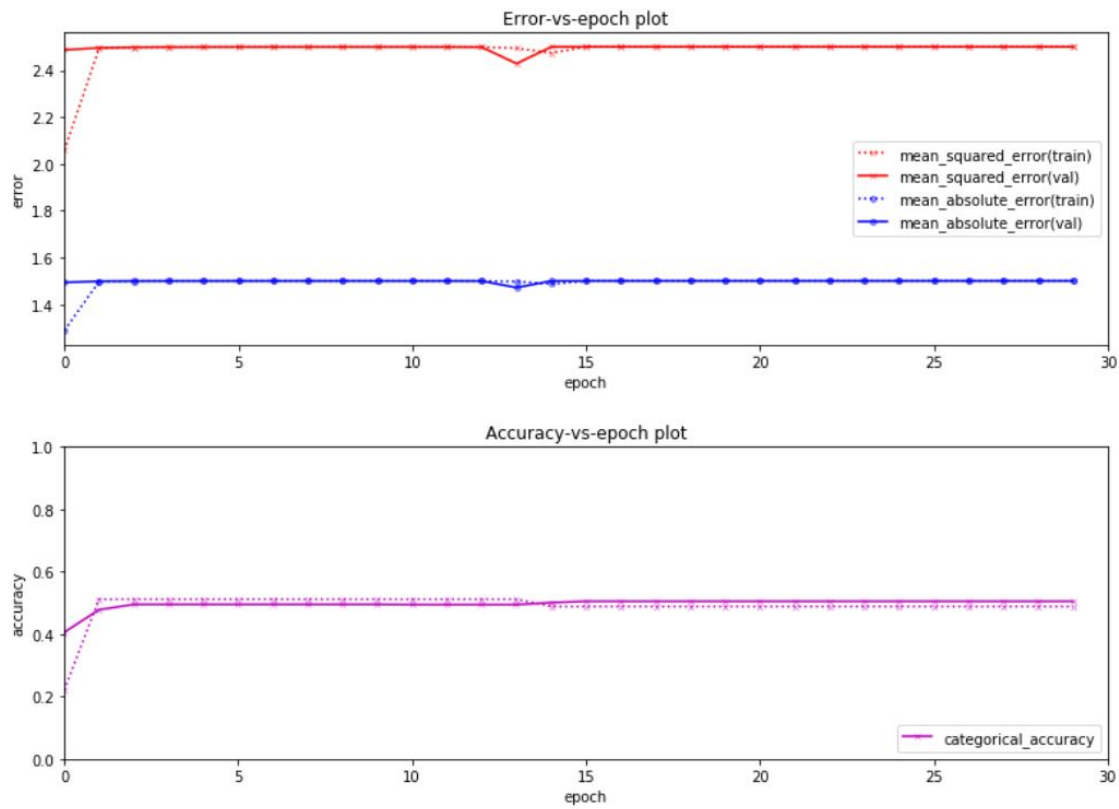
Training time: 2.7 sec

Test loss: 0.6931432207425435

Test accuracy: 0.48833333293596903

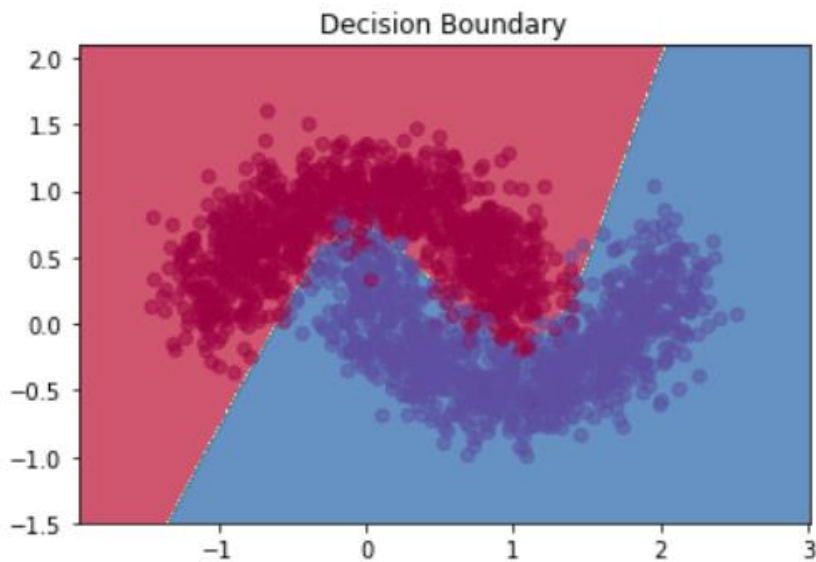
All scores in history: [0.6931432207425435, 0.48833333293596903, 2.499981838862101, 1.499992618560791]





Efter ca. 800 epoker ses det at sgd classifier matcher adam classifier igen. Hvor adam kun skulle bruge ca. 10 epoker for samme resultat.

Cell 3



Qb:

It is customary practice to convert both binary and multiclass classification labels to a one-hot encoding.

Explain one-hot encoding and the

```
y_train_binary = to_categorical(y_train)
y_test_binary = to_categorical(y_test)
```

and the used categorical metric (compare it to our well know accuracy function),

```
metrics=['categorical_accuracy',..
```

NOTE: Keras' `categorical_accuracy` is implemented as

```
def categorical_accuracy(y_true, y_pred):
    return K.cast(K.equal(K.argmax(y_true, axis=-1), K.argmax(y_pred, axis=-1)), K.floatx())
```

but also used internal TensorFlow tensors instead of `numpy.arrays` and these are right now difficult to work with directly.

Forklaring

In order to do a better job in predictions, one could use one-hot encoding, this works both for binary or multiclass classification!

the methods, converts the data sets catagorial binary data, and so the set will be reduced to a vector, that can match the output value into binary neurons.

Qc:

Now, try to optimize the model by

- increasing/decreasing the number of epochs,
- adding more neurons per layer,
- adding whole new layers,
- changing the activation functions in the layers,
- changing the output activation from `activation="softmax"` to something else,

Comment on your changes, and relate the resulting accuracy, accuracy-vs-epochs, loss-vs-epoch and decision boundary plots to your changes, ie. try to get a feeling of what happens when you modify the model hyperparameters.

NOTE: Many times the model seems to get stuck on an extreme flat loss plateau, and the decision boundary displays just a 'dum' straight line through the moons!

OPTIONAL: should the moon data be standardized or normalized to say range `[-1;1]` in both **x**-dimensions? Will it help, or is the data OK as-is?

```

np.random.seed(42)

# Build Keras model
model = Sequential()
model.add(Dense(input_dim=2, units=10, activation="tanh", kernel_initializer="normal"))
model.add(Dense(units=20, activation="tanh"))
model.add(Dense(units=2, activation="softmax"))

#optimizer = SGD(lr=0.1)
optimizer = Adam(lr=0.1)
model.compile(loss='categorical_crossentropy',
              optimizer=optimizer,
              metrics=['categorical_accuracy', 'mean_squared_error', 'mean_absolute_error'])

# Make data
X, y = datasets.make_moons(2000, noise=0.20, random_state=42)

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=42)

y_train_binary = to_categorical(y_train)
y_test_binary = to_categorical(y_test)

assert y.ndim==1
assert y_train_binary.ndim==2
assert y_test_binary.ndim ==2

# Train
VERBOSE = 0
EPOCHS = 5

start = time()
history = model.fit(X_train, y_train_binary, validation_data=(X_test, y_test_binary), epochs=EPOCHS, verbose=VERBOSE)
t = time()-start

print(f"OK, training time={t:0.1f}")

```

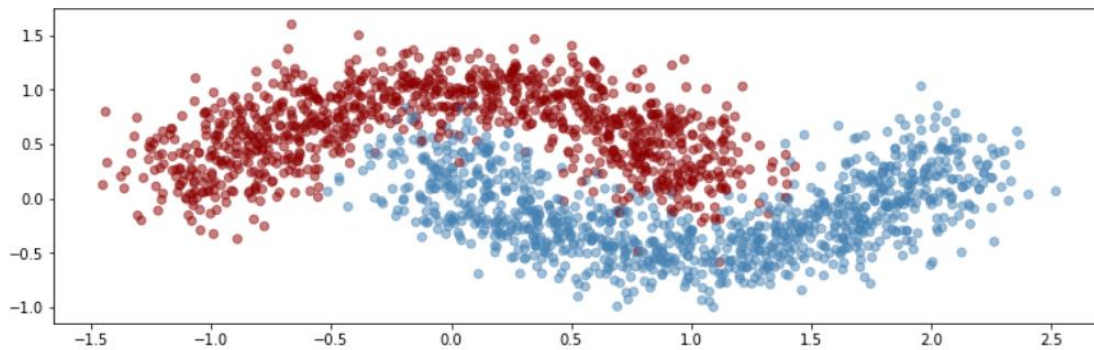
OK, training time=1.5

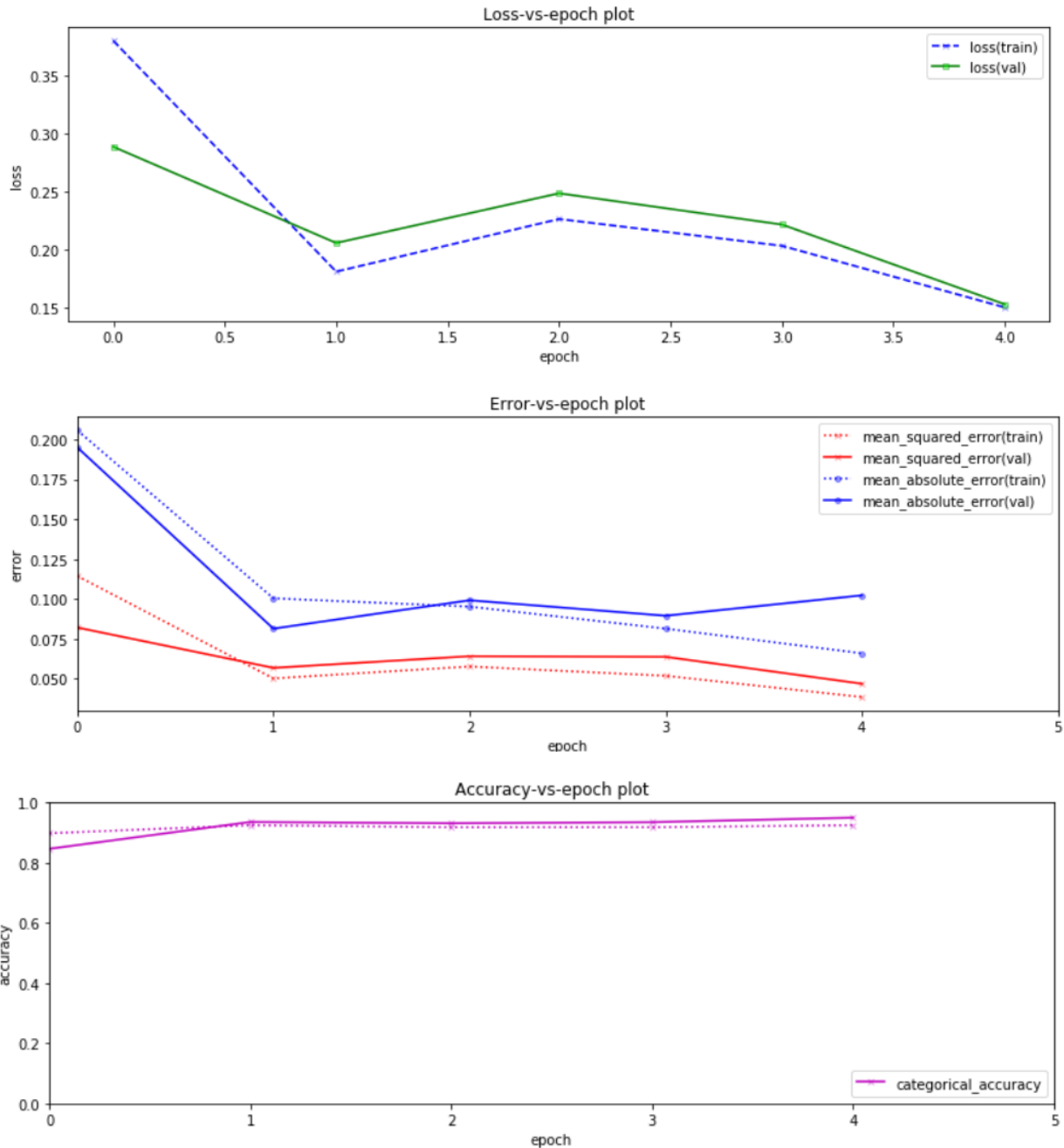
Training time: 1.5 sec

Test loss: 0.15305599172910053

Test accuracy: 0.9249999992052714

All scores in history: [0.15305599172910053, 0.9249999992052714, 0.04688500295082728, 0.10227124442656835]





Forklaring

Som det kan ses ud fra billeder på det nye data, har vi opnået en accuracy op ca. 0.9 allerede i første epoke. vi valgte at sætte 5 på for at vise, at det ikke var brug for flere epoker. Denne optimering er også opnået ved at indsætte et lag i midten af indgang og udgangen.

Keras Multi-Layer Perceptrons (MLP's) on MNIST-data

Qa:

Now, make a Keras `Sequential` model and fit it to the MNIST data, re-using as much of the code from the `mlp_moon.ipynb` as you can.

NOTE: you probably need to scale/normalize the MNIST data before a fit, and no 2D-decision boundaries can be drawn from the 784-dimension MNIST data.

```
np.random.seed(42)

# Build Keras model
model = Sequential()
model.add(Dense(input_dim=784, units=1200, activation="tanh", kernel_initializer="normal"))
model.add(Dense(units=1000, activation="tanh"))
model.add(Dense(units=10, activation="softmax"))

optimizer = SGD(lr=0.1)
#optimizer = Adam(lr=0.1)
model.compile(loss='categorical_crossentropy',
              optimizer=optimizer,
              metrics=['categorical_accuracy', 'mean_squared_error', 'mean_absolute_error'])

X_train, X_test, y_train, y_test = LoadAndSetupData('mnist') # or 'moon', or 'mnist'

scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

y_train_binary = to_categorical(y_train)
y_test_binary = to_categorical(y_test)

assert y.ndim==1
assert y_train_binary.ndim==2
assert y_test_binary.ndim ==2

# Train
VERBOSE = 1
EPOCHS = 5

start = time()
history = model.fit(X_train_scaled, y_train_binary, validation_data=(X_test_scaled, y_test_binary), epochs=EPOCHS,
                   verbose=VERBOSE)
t = time()-start

print(f"OK, training time={t:0.1f}")

DATA: mnist..
  org. data: X.shape      =(70000; 784), y.shape      =(70000)
  train data: X_train.shape=(49000; 784), y_train.shape=(49000)
  test data: X_test.shape =(21000; 784), y_test.shape =(21000)

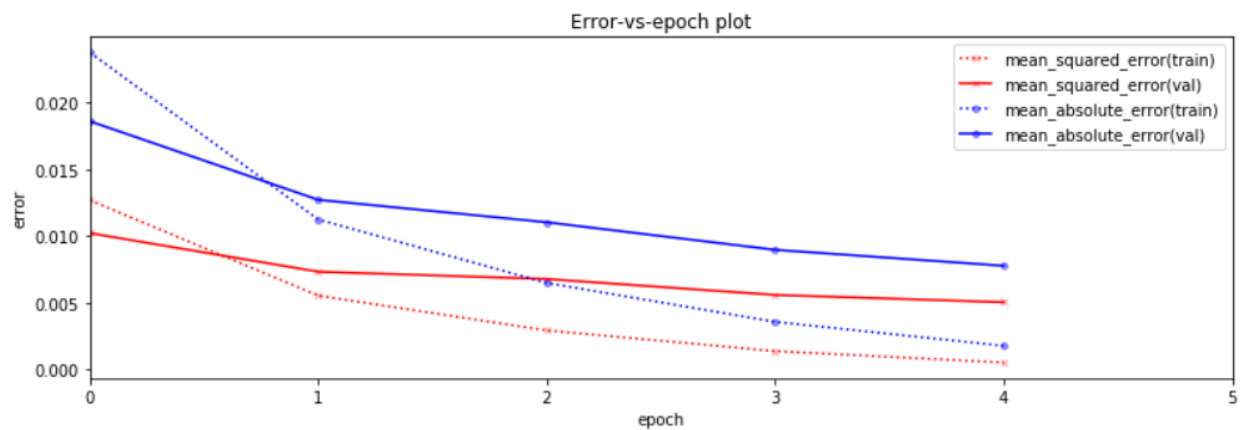
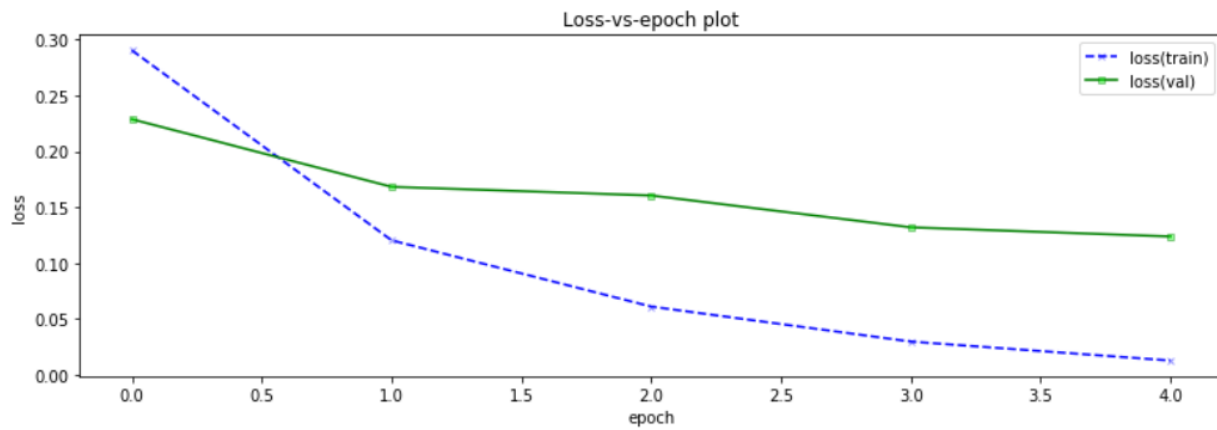
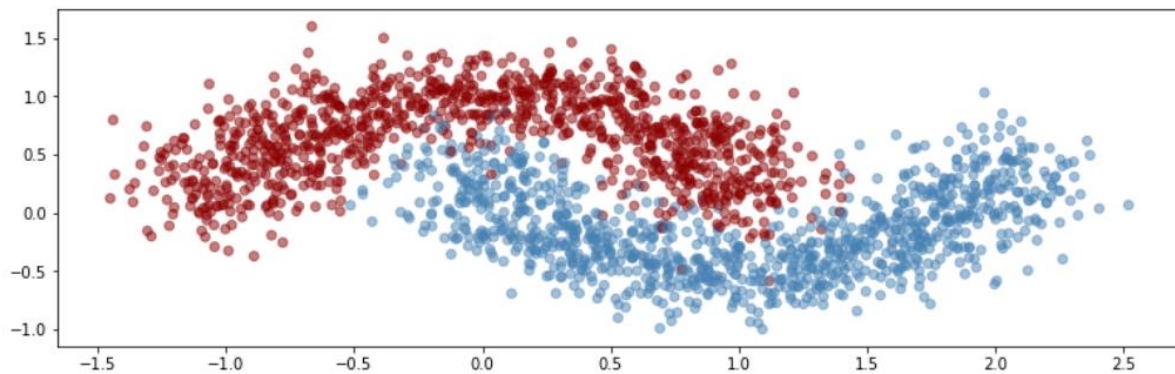
Train on 49000 samples, validate on 21000 samples
Epoch 1/5
49000/49000 [=====] - 9s 180us/step - loss: 0.2903 - categorical_accuracy: 0.9153 - mean_squared_error: 0.0127 - mean_absolute_error: 0.0238 - val_loss: 0.2287 - val_categorical_accuracy: 0.9323 - val_mean_squared_error: 0.0102 - val_mean_absolute_error: 0.0186
Epoch 2/5
49000/49000 [=====] - 7s 141us/step - loss: 0.1203 - categorical_accuracy: 0.9636 - mean_squared_error: 0.0055 - mean_absolute_error: 0.0112 - val_loss: 0.1682 - val_categorical_accuracy: 0.9521 - val_mean_squared_error: 0.0073 - val_mean_absolute_error: 0.0127
Epoch 3/5
49000/49000 [=====] - 6s 130us/step - loss: 0.0609 - categorical_accuracy: 0.9809 - mean_squared_error: 0.0029 - mean_absolute_error: 0.0065 - val_loss: 0.1604 - val_categorical_accuracy: 0.9559 - val_mean_squared_error: 0.0068 - val_mean_absolute_error: 0.0110
Epoch 4/5
49000/49000 [=====] - 7s 136us/step - loss: 0.0296 - categorical_accuracy: 0.9918 - mean_squared_error: 0.0014 - mean_absolute_error: 0.0036 - val_loss: 0.1319 - val_categorical_accuracy: 0.9637 - val_mean_squared_error: 0.0056 - val_mean_absolute_error: 0.0090
Epoch 5/5
49000/49000 [=====] - 7s 138us/step - loss: 0.0126 - categorical_accuracy: 0.9974 - mean_squared_error: 5.0283e-04 - mean_absolute_error: 0.0018 - val_loss: 0.1237 - val_categorical_accuracy: 0.9677 - val_mean_squared_error: 0.0050 - val_mean_absolute_error: 0.0078
OK, training time=35.8
```

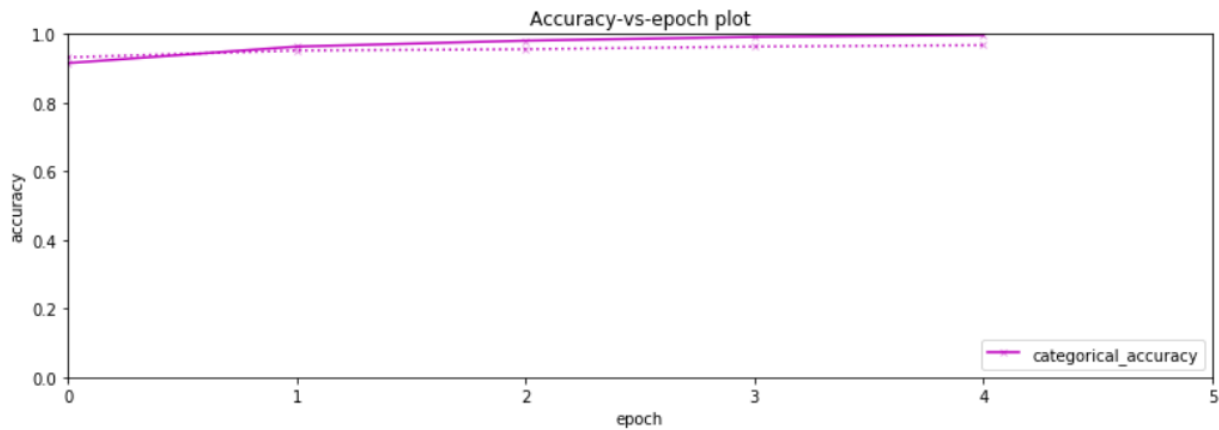
Training time: 35.8 sec

Test loss: 0.2893871153234726

Test accuracy: 0.9213809523809524

All scores in history: [0.2893871153234726, 0.9213809523809524, 0.012015223920333006, 0.01910299241786734]





Qb:

Now, try to crank up the accuracy for the model using the MNIST data, you could follow the NN layout found by ITMAL Grp10 using an MLP in the Scikit-learn framework.

Basically, they created a seven-layer `sklearn.neural_network.MLPClassifier`, with layer sizes 20-50-70-100-70-50-20. Their Scikit-learn `MLPClassifier` constructor looked like

```
CTOR for best model: MLPClassifier(activation='relu', alpha=0.05, batch_size='auto', beta_1=0.9,
    beta_2=0.999, early_stopping=False, epsilon=1e-08,
    hidden_layer_sizes=(20, 50, 70, 100, 70, 50, 20),
    learning_rate='adaptive', learning_rate_init=0.001, max_iter=500,
    momentum=0.9, n_iter_no_change=10, nesterovs_momentum=True,
    power_t=0.5, random_state=None, shuffle=True, solver='sgd',
    tol=0.0001, validation_fraction=0.1, verbose=False,
    warm_start=False)
```

See, if you can create a somewhat similar model in Keras, but feel free to replace any of the other hyperparameters (where some are not even present in Keras).

That best accuracy can you get from your model---for your validation or test set?

For the journal describe your investigation methods and results in your quest-quest for a higher accuracy score on MNIST.

```

from sklearn.neural_network import MLPClassifier

# TODO: Qb...
MLPClassifier(activation='relu', alpha=0.05, batch_size='auto', beta_1=0.9,
              beta_2=0.999, early_stopping=False, epsilon=1e-08,
              hidden_layer_sizes=(20, 50, 70, 100, 70, 50, 20),
              learning_rate='adaptive', learning_rate_init=0.001, max_iter=500,
              momentum=0.9, n_iter_no_change=10, nesterovs_momentum=True,
              power_t=0.5, random_state=None, shuffle=True, solver='sgd',
              tol=0.0001, validation_fraction=0.1, verbose=False,
              warm_start=False)

# Build Keras model
model1 = Sequential()
model1.add(Dense(input_dim=784, units=1200, activation="tanh", kernel_initializer="normal"))
model1.add(Dense(units=20, activation="tanh"))
model1.add(Dense(units=50, activation="tanh"))
model1.add(Dense(units=70, activation="tanh"))
model1.add(Dense(units=100, activation="tanh"))
model1.add(Dense(units=70, activation="tanh"))
model1.add(Dense(units=50, activation="tanh"))
model1.add(Dense(units=20, activation="tanh"))
model1.add(Dense(units=10, activation="softmax"))

optimizer = SGD(lr=0.1)
#optimizer = Adam(lr=0.1)
model1.compile(loss='categorical_crossentropy',
               optimizer=optimizer,
               metrics=['categorical_accuracy', 'mean_squared_error', 'mean_absolute_error'])

# Train
VERBOSE = 1
EPOCHS = 250

start1 = time()
history = model1.fit(X_train_scaled, y_train_binary, validation_data=(X_test_scaled, y_test_binary), epochs=EPOCHS, verbose=VERBOSE)
t1 = time() - start1

Epoch 247/250
49000/49000 [=====] - 4s 73us/step - loss: 0.0250 - categorical_accuracy: 0.9929 - mean_squared_error: 0.0011 - mean_absolute_error: 0.0020 - val_loss: 0.2464 - val_categorical_accuracy: 0.9567 - val_mean_squared_error: 0.0076 - val_mean_absolute_error: 0.0092
Epoch 248/250
49000/49000 [=====] - 4s 73us/step - loss: 0.0195 - categorical_accuracy: 0.9947 - mean_squared_error: 8.5324e-04 - mean_absolute_error: 0.0016 - val_loss: 0.2412 - val_categorical_accuracy: 0.9565 - val_mean_squared_error: 0.0076 - val_mean_absolute_error: 0.0092
Epoch 249/250
49000/49000 [=====] - 4s 73us/step - loss: 0.0180 - categorical_accuracy: 0.9950 - mean_squared_error: 8.1524e-04 - mean_absolute_error: 0.0016 - val_loss: 0.2309 - val_categorical_accuracy: 0.9584 - val_mean_squared_error: 0.0072 - val_mean_absolute_error: 0.0088
Epoch 250/250
49000/49000 [=====] - 4s 73us/step - loss: 0.0136 - categorical_accuracy: 0.9960 - mean_squared_error: 6.3707e-04 - mean_absolute_error: 0.0013 - val_loss: 0.2365 - val_categorical_accuracy: 0.9579 - val_mean_squared_error: 0.0073 - val_mean_absolute_error: 0.0089
OK, training time=928.5

```

Som der kan ses opnår vi en mean absolute error på 0.0013 som må siges at være ret godt. Og tæt på de 100 % som gruppe 10 havde lavet