Unconstrained optimization

GECD / MIRI - BarcelonaTech

Lab Assignment Pattern recognition with Single Layer Neural Network (SLNN) v4.0-02/21

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Pattern recognition with SLNN

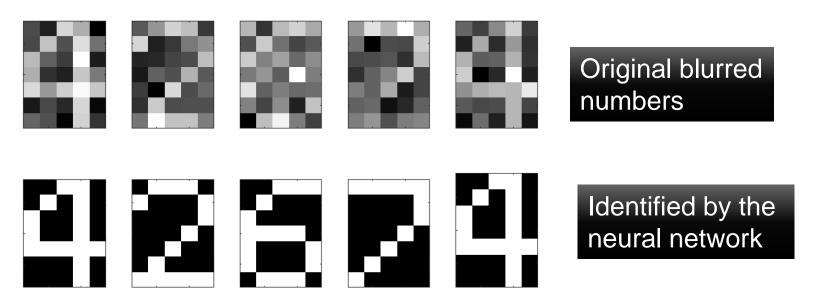
- 1. Presentation.
- 2. Single Layer Neural Network (SLNN).
 - Architecture and loss function.
 - Training and testing.
 - Gradient of the loss function.
 - Backtracking line search.
- 3. Pattern recognition with SLNN.
 - Problem statement and modelling.
 - Generation of training and test data sets.
 - Coding the loss function and gradient.
- 4. Assignment.
 - Part 1: pattern recognition with GM, CGM and QNM.
 - Part 2: pattern recognition with stochastic gradient.
 - Part 3: computational study of the performance.
 - Report.
- 5. Summary of supporting codes.





Presentation

 The aim of this project is to develop an application, based on the unconstrained optimization algorithms studied in this course, that allow to recognize the numbers in a sequence of blurred digits:



Sequence=42674; Identified=42674

The procedure to achieve that goal will be to formulate a Single Layer
 Neural Network that is going to be trained to recognize the different
 numbers with First Derivative Optimization methods.





Summary of supporting material

Documents

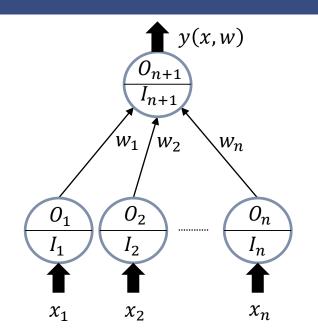
uo_nn_v40.pdf: this document.

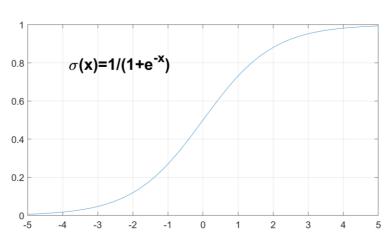
Function/script	Page
uo_nn_main.m: run a single recognition.	<u>link</u>
uo_nn_batch: run a batch of recognitions.	<u>link</u>
<pre>function [X,y] = uo_nn_dataset(seed, ncol, target, freq): generates the dataset x,y.</pre>	<u>link</u>
function uo_nn_Xyplot(X,y,w): plots the dataset X,y. If w is not [], the plot tells right from wrong predictions of the SLNN.	<u>link</u>
<pre>function [alpha,iout] = uo_BLSNW32(f,g,x,d,almax,c1,c2,kBLSmax,epsal): Algorithm 3.2 of Nocedal & Wright (backtracking line search with SWC and curve fitting).</pre>	<u>link</u>





Single layer Neural Network (SLNN): architecture





Input signal:

$$I_i = x_i, i = 1, 2, ..., n$$
; $I_{n+1} = \sum_{i=1}^n w_i \cdot O_i$

Activation function (sigmoid function) :

$$O_i = \sigma(I_i)$$
, $\sigma(x) = 1/(1 + e^{-x})$

· Output signal: assumed to be binary

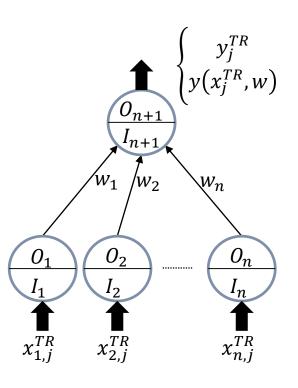
$$y(x,w) = \sigma(I_{n+1}) = \sigma\left(\sum_{i=1}^{n} w_{i} O_{i}\right) = \sigma\left(\sum_{i=1}^{n} w_{i} \cdot \sigma(x_{i})\right)$$
$$= \left(1 + e^{-\left(\sum_{i=1}^{n} w_{i} \cdot \sigma(x_{i})\right)\right)^{-1}}$$
$$= \left(1 + e^{-\left(\sum_{i=1}^{n} w_{i} \cdot (1 + e^{-x_{i}})^{-1}\right)\right)^{-1}}$$





SLNN: training

Training data set, size p:



$$\underbrace{ \begin{cases} y_j^{TR} & \text{data} \\ y(x_j^{TR}, w) & \text{model} \end{cases} }_{X^{TR}} = \begin{bmatrix} x_1^{TR}, x_2^{TR}, \dots, x_p^{TR} \end{bmatrix} = \begin{bmatrix} x_{1,1}^{TR} & x_{1,2}^{TR} & \cdots & x_{1,p}^{TR} \\ x_{2,1}^{TR} & x_{2,2}^{TR} & \cdots & x_{2,p}^{TR} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1}^{TR} & x_{n,2}^{TR} & \cdots & x_{n,p}^{TR} \end{bmatrix}$$

$$y^{TR} = \begin{bmatrix} y_1^{TR} & y_2^{TR} & \cdots & y_p^{TR} \end{bmatrix}^T$$

Mean loss function: for a given (X^{TR}, Y^{TR})

$$L(X^{TR}, y^{TR}) = \min_{w \in \mathbb{R}^n} L(w; X^{TR}, y^{TR}) = \frac{1}{p} \sum_{i=1}^{p} (y(x_j^{TR}, w) - y_j^{TR})^2$$

 L^2 regularization or weight decay⁽¹⁾:

$$\tilde{L}(X^{TR}, y^{TR}, \lambda) = \min_{w \in \mathbb{R}^n} \tilde{L}(w; X^{TR}, y^{TR}, \lambda) = L(w; X^{TR}, y^{TR}) + \lambda \cdot \frac{\|w\|^2}{2}$$

(1): AKA ridge regression or Tikhonov regularization.

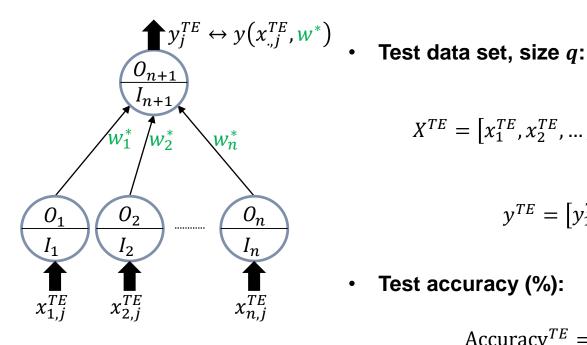
Training accuracy (%): $Accuracy^{TR} = \frac{100}{p} \cdot \sum_{j=1}^{p} \delta_{\left[y\left(x_{j}^{TR}, w^{*}\right)\right], y_{j}^{TR}}$

where
$$\delta_{x,y} = \begin{cases} 1 & \text{if } x = y \\ 0 & \text{if } x \neq y \end{cases}$$
 (Kronecker delta). $w^* = \operatorname{argmin}_{w \in \mathbb{R}^n} \tilde{L}(w; X^{TR}, y^{TR}, \lambda)$





SLNN: testing



$$X^{TE} = \begin{bmatrix} x_1^{TE}, x_2^{TE}, \dots, x_q^{TE} \end{bmatrix} = \begin{bmatrix} x_{1,1}^{TE} & x_{1,2}^{TE} & \cdots & x_{1,q}^{TE} \\ x_{2,1}^{TE} & x_{2,2}^{TE} & \cdots & x_{2,q}^{TE} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n,1}^{TE} & x_{n,2}^{TE} & \cdots & x_{n,q}^{TE} \end{bmatrix}^{T}$$

$$y^{TE} = \begin{bmatrix} y_1^{TE} & y_2^{TE} & \cdots & y_q^{TE} \end{bmatrix}^{T}$$

Test accuracy (%):

$$Accuracy^{TE} = \frac{100}{p} \cdot \sum_{j=1}^{p} \delta_{\left[y\left(x_{j}^{TE}, w^{*}\right)\right], y_{j}^{TE}}$$

Overfitting: if Accuracy $^{TR} \gg \text{Accuracy}^{TE}$

SLNN: gradient (1/2)

Mean loss function with regularization (objective function):

$$\tilde{L}(w; X^{TR}, y^{TR}, \lambda) = \frac{1}{p} \sum_{i=1}^{p} (y(x_j^{TR}, w) - y_j^{TR})^2 + \frac{\lambda}{2} \cdot \sum_{i=1}^{n} w_i^2$$

Gradient:

$$\frac{\partial \tilde{L}(w; X^{TR}, y^{TR}, \lambda)}{\partial w_i} = \frac{1}{p} \sum_{j=1}^{p} 2 \cdot \left(y(x_j^{TR}, w) - y_j^{TR} \right) \cdot \frac{\partial y(x_j^{TR}, w)}{\partial w_i} + \lambda \cdot w_i \quad (1)$$

with

$$y(x_i^{TR}, w) = \left(1 + e^{-\left(\sum_{i=1}^n w_i \cdot \left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}\right)\right)^{-1}}$$
(2)





SLNN: gradient (2/2)

• Let us find $\partial y(x_i^{TR}, w)/\partial w_i$:

$$\frac{\partial y(x_{j}^{TR}, w)}{\partial w_{i}} = \frac{\partial}{\partial w_{i}} \left(1 + e^{-\left(\sum_{i=1}^{n} w_{i} \cdot \left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}\right)} \right)^{-1} = \frac{-y(x_{j}^{TR}, w)^{2}}{\left(1 + e^{-\left(\sum_{i=1}^{n} w_{i} \cdot \left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}\right)}\right)^{-2}} \cdot \frac{\left(y(x_{j}^{TR}, w)^{-1} - 1\right)}{\left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}} \cdot \left(-\left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}\right) \cdot \left(-\left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}\right) \cdot \left(1 + e^{-x_{i,j}^{TR}}\right)^{-1} = y(x_{j}^{TR}, w) \cdot \left(1 - y(x_{j}^{TR}, w)\right) \cdot \left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}$$

$$= y(x_{j}^{TR}, w) \cdot \left(1 - y(x_{j}^{TR}, w)\right) \cdot \left(1 + e^{-x_{i,j}^{TR}}\right)^{-1}$$

Therefore:

$$\frac{\partial \tilde{L}\left(w; X^{TR}, y^{TR}, \lambda\right)}{\partial w_{i}} = \frac{1}{p} \sum_{j=1}^{p} 2 \cdot \left(y\left(x_{j}^{TR}, w\right) - y_{j}^{TR}\right) \cdot y\left(x_{j}^{TR}, w\right) \cdot \left(1 - y\left(x_{j}^{TR}, w\right)\right) \cdot \left(1 + e^{-x_{i,j}^{TR}}\right)^{-1} + \lambda \cdot w_{i}$$





SLNN: backtracking line search

- The backtracking line search algorithm Alg.BLS cannot handle conveniently the SLNN problem. We need to introduce two modifications in the computation of the line search:
 - 1. The maximum step length cannot be a constant for every iteration. Instead, it must be updated dynamically using information of the local behaviour of f near the iterated point at each iteration, using some of the formulas (N&W page 58):

$$\alpha_1^{max} = \alpha^{k-1} \frac{\nabla f^{k-1}^T d^{k-1}}{\nabla f^{k}^T d^k}; \quad \alpha_2^{max} = \frac{2(f^k - f^{k-1})}{\nabla f^{k}^T d^k}.$$

2. A BLS based on interpolations must be used (see N&W 3.4), as the one proposed in Alg 3.2 and 3.3 of N&W, implemented in function uo_BLSNW32:

```
function [alpha,iout] =
```

where f,g,d,x,almax,c1,c2 are as usual, iout=0 if the procedure succeeds and:

- * kBLSmax is the maximum number of iterations of the BLS algorithm: if exceeded, the algorithm stops with iout=1.
- * epsal is the minimum variation between two consecutive reductions of α^k , meaning that the algorithm will stop with iout=2 whenever $|\alpha^{k+1} \alpha^k| < epsal$.





Pattern recognition with SLNN (1/2)

-10

-10

10

-10

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-10

10 10

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-10

10

-10

-10

-10

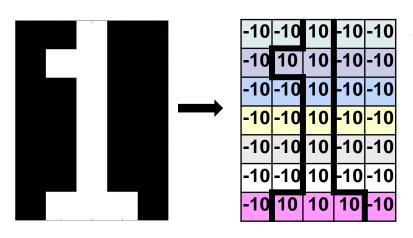
-10

10

 We are going to use the SLNN to solve a problem of pattern recognition over a small 7x5 pixels matrix picturing the 10 digits:

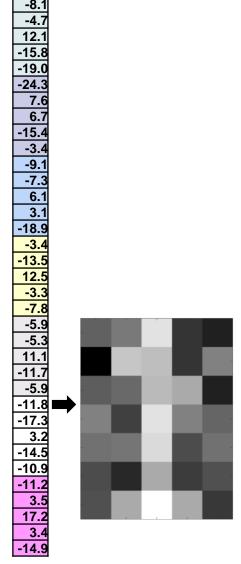


To obtain the input data of the SLNN x, each white pixel is assigned with a value of 10 and each black pixel with a value of -10 then vectorized and blurred with a Gaussian noise with $\mu = 0$ and $\sigma = \sigma_{rel} \cdot 10$.



Vectorization x =

-10 -10 -10 Gaussian blur -10 10 $x \leftarrow x + \epsilon =$ -10 -10 -10 -10 10 $\epsilon \sim N(0,5)$ -10 $\sigma_{rel} = 0.5$ -10 -10 10



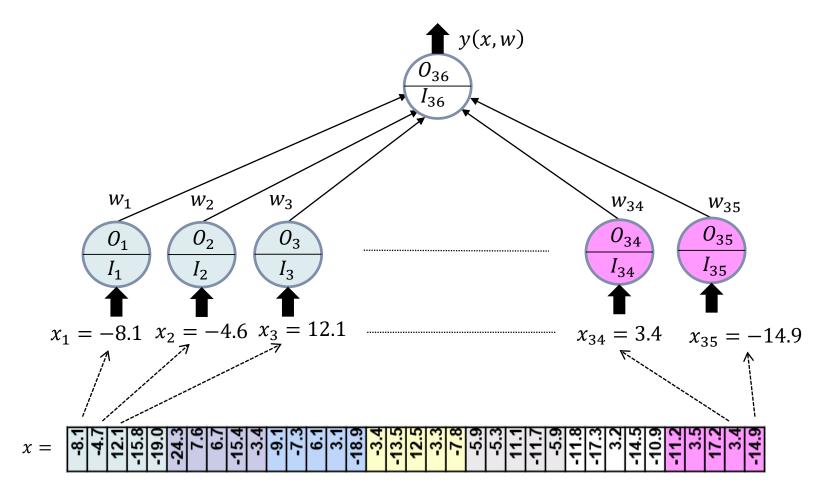




10 10

Pattern recognition with SLNN (2/2)

• The resulting vectorised and blurred digit *x* are going to be taken as the inputs of a SLNN:







Training and test data set (1/2)

- The objective of the SLNN is to recognize a set of target numbers, num target, for instance num target = [1 3 5 7 9] will recognize the odd numbers between 0 and 9.
- To this end, the training and test data sets:

$$X^{TR} = \left[x_1^{TR}, x_2^{TR}, \dots, x_p^{TR}\right] \equiv \text{Xtr}(1:35,1:\text{tr_p}) \text{ and } y^{TR} \equiv \text{ytr}(1:\text{tr_p})$$

$$X^{TE} = \left[x_1^{TE}, x_2^{TE}, \dots, x_p^{TE}\right] \equiv \text{ Xte} (1:35, 1:te_q) \text{ and } y^{TE} \equiv \text{ yte} (1:te_q)$$

must be generated with the help of function

This function will generate a dataset, where:

- x,y are the generated data sets (xtr, ytr or xte, yte).
- seed is the seed for the Matlab random numbers generator. The numbers in the dataset are randomly choosed, guaranteeing a frequency of the digits in target close to freq. The value σ_{rel} for each digit is also randomly selected within the range [0.25, 1].
- number number of columns/elements of array x/y.
- target is the set of digits to be identified.
- freq is the frequency of the digits target in the data ser. For instance, if target=[1 2] and freq=0.5, the digits 1 and 2 will be, approximately, half of the total digits in the data set x. If freq≤0.0, every digit is (approx.) equally represented in the dataset: this is the value to be used when generating the test dataset X^{TE} , y^{TE} .





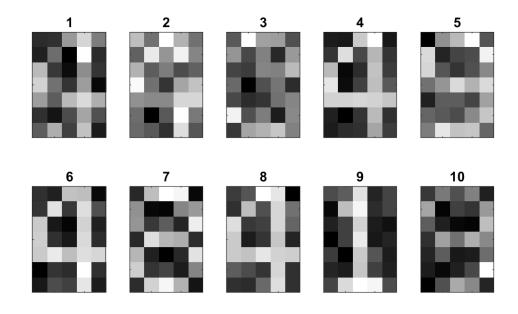
Training and test data set (2/2)

• Exemple: let seed=1234, number=10, target=[4], freq=0.5 then:

```
>> [X,y]=uo nn dataset(1234,10,[4],0.5)
x =
  -11.5323
                       -8.2363
                                 -11.4127
                                           -31.3497
                                                      -9.9915
                                                                -10.0134
                                                                           -9.8603
              8.5784
                                                                                     -5.8843
                                                                                                -5.6767
  -11.0925
             -6.6966
                       46.1249 -11.9861
                                             2.8732 -12.0420
                                                                  8.8078
                                                                           -6.9858
                                                                                     -4.5738
                                                                                                 6.4063
    3.5013
             21.9754
                       15.0901
                                   9.6655
                                            11.6102
                                                       7.1156
                                                                17.6479
                                                                           14.5913
                                                                                      9.2044
                                                                                                -1.3036
 -13.9129 -12.5358
                       5.2724
                                 -7.4084
                                           -7.6072 -12.5149 -12.5704 -11.6329
                                                                                    -6.2185
                                                                                               -9.5339
y =
                                                             0
     1
```

and the graphical representation:

- function uo_nn_Xyplot(X,y,w)
 plots a set of vectorised digits, and the recognition brought by a vector w:
 - x an array of vectorised digits.
 - y associated output of the SLNN.
 - w vector of weights w (optional).







Loss function and its gradient (1/2)

- Let xtr, ytr be the training data set:
 - [Xtr,ytr] = uo_nn_dataset(tr_seed, tr_p, num_target, tr_freq);
- Defining the row vector of predictions $y(X^{TR}, w)$ and the sigmoid matrix of inputs $\sigma(X^{TR})$ as

$$y(X^{TR}, w) \stackrel{\text{def}}{=} \left[y(x_1^{TR}, w), \dots, y(x_p^{TR}, w) \right]; \quad \sigma(X^{TR}) = \begin{bmatrix} \sigma(x_{11}^{TR}) & \cdots & \sigma(x_{1p}^{TR}) \\ \vdots & \ddots & \vdots \\ \sigma(x_{n1}^{TR}) & \cdots & \sigma(x_{np}^{TR}) \end{bmatrix}$$

the value of the loss function \tilde{L} and its gradient $\nabla \tilde{L}$ can be expressed as

$$\tilde{L}(w; X^{TR}, y^{TR}, \lambda) = \frac{1}{p} ||y(X^{TR}, w) - y^{TR}||^2 + \lambda \frac{||w||^2}{2}$$

$$\nabla \tilde{L}(w; X^{TR}, y^{TR}, \lambda) = \frac{1}{p} 2\sigma(X^{TR}) \left((y(X^{TR}, w) - y^{TR}) \circ y(X^{TR}, w) \circ \left(1 - y(X^{TR}, w) \right) \right)^T + \lambda w$$

where \circ stands for the **element-wise** (or **Hadamard**) **product** $\binom{u}{v} \circ \binom{x}{y} = \binom{ux}{vy}$). These expressions can be easily coded in Matlab with the **element-wise operators** ". / " and ". * ":

_	•	
	σ	sig = @(Xds) 1./(1+exp(-Xds));
	у	y = 0 (Xds, w) sig(w'*sig(Xds));
	$ ilde{L}$	$L = @(w,Xds,yds) (norm(y(Xds,w)-yds)^2)/size(yds,2) + (la*norm(w)^2)/2;$
	$ abla ilde{L}$	gL = @(w,Xds,yds) (2*sig(Xds)*((y(Xds,w)-yds).*y(Xds,w).* (1-y(Xds,w)))')/size(yds,2)+la*w;

Assignment.

There are three different parts in this assignment:

- Part 1: to develop a code uo_nn_solve for the recognition of some specific target with GM and QNM).
- Part 2: to extend code uo_nn_solve with the stochastic gradient method (SGM).
- Part 3: to conduct a comparation of the performance of the abovementioned methods.



Part 1: pattern recognition

Matlab script to solve the recognition of a given num_target

```
uo nn main.m : recognition of num target digits.
clear:
% Parameters for dataset generation
num target =[1];
tr freq
          = .5;
          = 250;
tr p
te q
          = 250;
tr seed = 123456;
te seed = 789101;
% Parameters for optimization
la = 0.0;
                                                              % L2 regularization.
epsG = 10^-6; kmax = 10000;
                                                              % Stopping criterium.
ils=3; ialmax = 2; kmaxBLS=30; epsal=10^-3; c1=0.01; c2=0.45; % Linesearch.
isd = 1; icq = 2; irc = 2; nu = 1.0;
                                                              % Search direction.
sq seed = 565544; sq al0 = 2; sq be = 0.3; sq qa = 0.01;
                                                              % SGM iteration.
sg emax = kmax; sg ebest = floor(0.01*sg emax);
                                                              % SGM stopping condition.
% Optimization
t1=clock;
[Xtr,ytr,wo,fo,tr acc,Xte,yte,te acc,niter,tex]=uo nn solve(num target,tr freq,tr seed,tr p,te seed,te q,la
,epsG,kmax,ils,ialmax,kmaxBLS,epsal,c1,c2,isd,sg al0,sg be,sg ga,sg emax,sg ebest,sg seed,icg,irc,nu);
t2=clock;
fprintf('wall time = %6.1d s.\n', etime(t2,t1));
```

Part 1: pattern recognition

- Function uo_nn_solve called inside uo_nn_main.m must solve the instance corresponding to a particular combination of parameters. The actions to be taken inside this function are:
 - i. To generate the training data set (X^{TR}, y^{TR}) and the test dataset (X^{TE}, y^{TE}) with function **uo_nn_dataset.m**.
 - ii. To find the value of w^* minimizing $\tilde{L}(w; X^{TR}, y^{TR}, \lambda)$ with your own optimization routines developed during the course.
 - iii. To calculate $Accuracy^{TR}$ and $Accuracy^{TE}$.



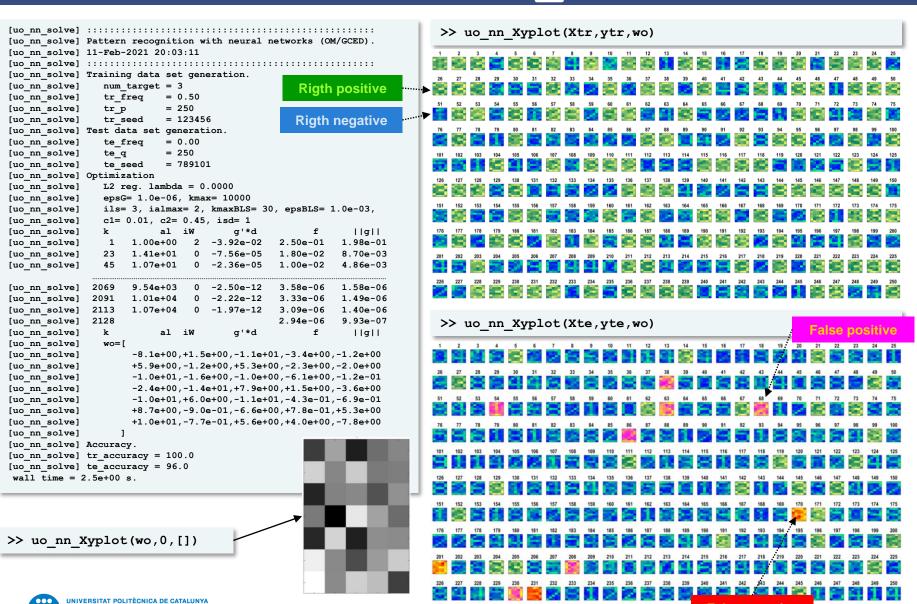


Part 1: example 1, num_target=[1]

```
>> uo nn Xyplot(Xtr,ytr,wo)
[uo nn solve]
             Pattern recognition with neural networks (OM/GCED).
[uo nn solve] 11-Feb-2021 19:34:47
[uo nn solve] Training data set generation.
[uo nn solve]
                num target = 1
                                                 Rigth positive
[uo nn solve]
                tr freq
                          = 0.50
[uo nn solve]
                tr p
                          = 250
                                                 Rigth negative
[uo nn solve]
                tr seed
                          = 123456
[uo nn solve] Test data set generation.
                          = 0.00
[uo nn solve]
                te freq
                          = 250
[uo nn solve]
                te q
                          = 789101
[uo nn solve]
                te seed
[uo nn solve] Optimization
                L2 \text{ reg. } lambda = 0.0000
[uo nn solve]
                epsG= 1.0e-06, kmax= 10000
[uo nn solve]
[uo nn solve]
                ils= 3, ialmax= 2, kmaxBLS= 30, epsBLS= 1.0e-03,
[uo nn solve]
                c1=0.01, c2=0.45, isd= 1
[uo nn solve]
                                      g'*d
                                                          HgH
                    1.00e+00
[uo nn solve]
                               2 -1.18e-01
                                             2.50e-01
                                                        3.44e-01
                                  -5.81e-02
                                             1.50e-01
                                                        2.41e-01
[uo nn solve]
                     3.44e+00
[uo nn solve]
                     5.22e+01
                                  -4.37e-03
                                             3.59e-02
                                                        6.61e-02
[uo nn solve]
                    3.09e+04
                                  -9.68e-12
                                             1.08e-06
                                                        3.11e-06
                    2.18e+05
                                  -1.47e-12
                                             9.17e-07
                                                        1.21e-06
[uo nn solve]
[uo nn solve]
                     6.95e+04
                                  -1.75e-12
                                             6.74e-07
                                                        1.32e-06
                45
                                             6.11e-07
                                                        9.80e-07
[uo nn solve]
                                                                         >> uo nn Xyplot(Xte,yte,wo)
                                      g'*d
[uo nn solve]
                         al iW
                                                          llgll
[uo nn solve]
                1=0w
[uo nn solve]
                     -1.1e+00,-1.6e+00,-2.3e-01,-2.4e+00,-1.4e+00
                     -1.3e+00,+1.5e+00,+2.7e+00,+1.3e-01,-1.4e+00
[uo nn solve]
                     -1.7e+00,-9.3e-02,+3.0e+00,-7.9e-01,-7.6e-01
[uo nn solve]
[uo nn solve]
                     -2.1e+00,-1.7e+00,+2.7e+00,-2.4e+00,-1.4e-01
[uo nn solve]
                     -1.8e+00,-4.8e-01,+2.0e+00,-1.4e+00,-2.0e+00
[uo nn solve]
                     -9.6e-01,-1.2e+00,+2.2e+00,-1.1e+00,-3.6e-01
                     -2.5e-01,-2.1e-02,+2.7e-01,+7.4e-01,-7.4e-01
[uo nn solve]
[uo nn solve]
[uo nn solve] Accuracy.
[uo nn solve] tr accuracy = 100.0
[uo nn solve] te accuracy = 100.0
wall time = 1.6e-01 s.
>> uo nn Xyplot(wo,0,[])
```

BY-NC-ND

Part 1: example 2, num_target=[3]



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False negative

PRSLNN - 20

SGM

BARCELONATECH

Departament d'Estadística i Investigació Operativa BY-NC-ND

Part 1: example 3, num target=[1 3 5 7 9]

```
[uo nn solve] Pattern recognition with neural networks (OM/GCED).
[uo nn solve] 11-Feb-2021 20:14:05
[uo nn solve] Training data set generation.
                num target = 1 3 5 7
[uo nn solve]
[uo nn solve]
                tr freq
                           = 0.50
[uo nn solve]
                tr p
                           = 250
[uo nn solve]
                tr seed
                           = 123456
[uo nn solve] Test data set generation.
                           = 0.00
[uo nn solve]
                te freq
                           = 250
[uo nn solve]
                te q
                           = 789101
[uo nn solve]
                te seed
[uo nn solve] Optimization
                L2 \text{ reg. } lambda = 0.0000
[uo nn solve]
                epsG= 1.0e-06, kmax= 10000
[uo nn solve]
[uo nn solve]
                ils= 3, ialmax= 2, kmaxBLS= 30, epsBLS= 1.0e-03,
[uo nn solve]
                c1=0.01, c2=0.45, isd= 1
[uo nn solve]
                          al iW
                                      g'*d
                                                          HgH
                    1.00e+00
[uo nn solve]
                               2 -3.41e-02
                                              2.50e-01
                                                        1.85e-01
                                 -1.56e-03
                                              4.89e-02
                                                        3.95e-02
[uo nn solve]
                     3.36e+00
              1821
                                 -2.31e-12
                                              4.02e-06
                                                        1.52e-06
                     1.56e+04
[uo nn solve]
[uo nn solve]
              1841
                     1.49e+04
                                  -1.90e-12
                                              3.70e-06
                                                        1.38e-06
                     1.53e+04
[uo nn solve]
              1861
                                 -1.71e-12
                                              3.43e-06
                                                        1.31e-06
[uo nn solve]
              1881
                     1.55e+04
                                 -1.57e-12
                                              3.17e-06
                                                        1.25e-06
                     1.55e+04
                                  -1.47e-12
                                              2.94e-06
                                                        1.21e-06
[uo nn solve]
              1901
                                              2.79e-06
[uo nn solve]
              1914
                                                        9.90e-07
                          al iW
                                      g'*d
[uo nn solve]
                k
                                                          llgll
[uo nn solve]
                1=ow
                     +6.1e+00,-7.3e-01,-2.3e+00,+4.1e+00,+9.4e-01
[uo nn solve]
                     -1.5e+00,-3.6e+00,+1.2e+01,-6.0e+00,-4.5e-01
[uo nn solve]
[uo nn solve]
                     -3.1e+00,+1.6e+00,+1.3e+01,+5.3e-01,+3.9e+00
[uo nn solve]
                     -8.5e+00,+8.0e-01,+1.4e+01,+1.8e+00,+6.4e+00
[uo nn solve]
                     -1.8e+01,-5.4e-01,+3.1e+00,-5.4e+00,+2.3e+00
                     +2.9e+00,-3.4e+00,+4.0e+00,+6.4e+00,+6.3e+00
[uo nn solve]
[uo nn solve]
                     +2.4e+00,-1.1e+01,-4.8e+00,-5.5e+00,+8.7e-02
[uo nn solve]
[uo nn solve] Accuracy.
[uo nn solve] tr accuracy = 100.0
[uo nn solve] te accuracy = 95.6
 wall time = 2.2e+00 s.
>> uo nn Xyplot(wo,0,[])
```

```
>> uo nn Xyplot(Xtr,ytr,wo)
>> uo nn Xyplot(Xte,yte,wo)
```





Part 2: Stochastic Gradient (1/6)

- Stochastic Gradient Method (SGM). (https://www.deeplearningbook.org/, chapter 8)
 - **Principle:** it is possible to obtain an unbiased estimate of the gradient by taking the average gradient on a minibatch of m examples drawn i.i.d. from the training dataset.
 - **Procedure:** given w^0 and $\alpha_0^{SG} > 0$, β^{SG} , $\gamma^{SG} \in [0,1]$ and $e_{max}^{SG} > 0$. $k \leftarrow 0$.
 - 1. Take a random permutation of the training data set: $P \leftarrow \{p_1, p_2, ..., p_p\}$
 - 2. Define the size of the minibatch: $\mathbf{m} \coloneqq |\mathbf{y}^{SG} \cdot p| (\ll p)$.
 - 3. Define a minibatch of observations associated to the first m indexs of P:
 - o Indexes of the minibatch: $S \leftarrow \{s_1, s_2, ..., s_m\} \equiv \{p_1, p_2, ..., p_m\}$.
 - Observations of the minibatch: $\begin{cases} X_{\mathbf{s}}^{TR} \leftarrow \left[x_{\mathbf{s_1}}^{TR}, x_{\mathbf{s_2}}^{TR}, \dots, x_{\mathbf{s_m}}^{TR} \right] \\ y_{\mathbf{s}}^{TR} \leftarrow \left[y_{\mathbf{s_1}}^{TR} \quad y_{\mathbf{s_2}}^{TR} \quad \cdots \quad y_{\mathbf{s_m}}^{TR} \right]^T \end{cases}$
 - 4. Estimate the gradient search direction : $d^k \leftarrow -\nabla \tilde{L}(w^k; X_s^{TR}, y_s^{TR}, \lambda)$
 - 5. Update the parametres: $w^k \leftarrow w^k + \alpha^k d^k$ with *learning rate* $\alpha^k \cdot k \leftarrow k + 1$
 - Repeat steps 3 to 5 k_e^{SG} : = $\lceil p/m \rceil$ iterations, taking at every iteration the next bunch of m indexes of P until every observation is used (epoch).
 - 7. Generate a new permutation P and repeat the steps 2 to 6 for a number of e_{max}^{SG} epochs (a total of k_{max}^{SG} : $= e_{max}^{SG} \cdot k_e^{SG}$ iterations).

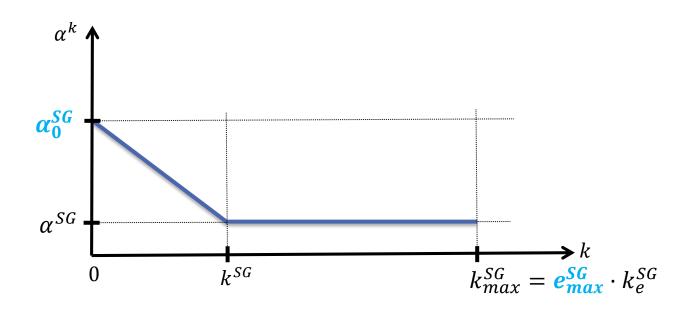




Part 2: Stochastic Gradient (2/6)

- Learning rate α^k : linear decay until iteration k^{SG} of a total of k_{max}^{SG} iterations, then constant α^{SG}

$$\alpha^{k} \leftarrow \begin{cases} \left(1 - \frac{k}{k^{SG}}\right) \alpha_{0}^{SG} + \frac{k}{k^{SG}} \alpha^{SG} & \text{if } k \leq k^{SG} \\ \alpha^{SG} & \text{if } k > k^{SG} \end{cases}, \qquad \begin{cases} \alpha^{SG} := 0.01 \cdot \alpha_{0}^{SG} \\ k^{SG} := \left\lfloor \beta^{SG} \cdot k_{max}^{SG} \right\rfloor \end{cases}$$







Part 2: Stochastic Gradient (3/6)

- **Stopping criterion:** the usual stopping condition $\|\nabla f(x^k)\| \approx 0$ is no longer suitable, as the SGM does not compute the true gradient $\nabla f(x)$. One of the most commonly regularization stopping condition is the *early stopping condition*. The rationale of this stopping criterion is:
 - 1. To check the value of the loss function for the **test data set** after each epoch *e*:

$$\tilde{L}^{TE} \leftarrow \tilde{L}\left(w^{e \cdot k_e^{SG}}, \boldsymbol{X^{TE}}, \boldsymbol{y^{TE}}, \lambda\right).$$

2. Every time the new value \tilde{L}^{TE} improves the best value so far (\tilde{L}_{best}^{TE}) , \tilde{L}^{TE} and the associated solution $w^{e \cdot k_e^{SG}}$ is saved :

$$\tilde{L}^{TE} < \tilde{L}_{best}^{TE} \stackrel{\text{def}}{=} \min_{j=1,\dots,e-1} \left\{ \tilde{L} \left(w^{j \cdot k_e^{SG}}, \boldsymbol{X^{TE}}, \boldsymbol{y^{TE}}, \lambda \right) \right\} \Rightarrow \begin{cases} \tilde{L}_{best}^{TE} \leftarrow \tilde{L}^{TE} \\ \boldsymbol{w^*} \leftarrow \boldsymbol{w^{e \cdot k_e^{SG}}} \end{cases}$$

3. If the value of \tilde{L}_{best}^{TE} has not been improved (updated) for the last e_{best}^{SG} epochs, the algorithm is terminated, and the solution of the last update w^* is declared optimal.





Part 2: Stochastic Gradient (4/6)

Algorithm SGM: Stochastic Gradient Method.

```
w^* \leftarrow \mathsf{SGM}(w^0, \lambda, \tilde{L}, \nabla \tilde{L}, X^{TR}, y^{TR}, X^{TE}, y^{TE}, \alpha_0^{SG}, \beta^{SG}, \gamma^{SG}, e_{max}^{SG}, e_{hest}^{SG})
                            p := \text{columns}(X^{TR});
                            \mathbf{m} \coloneqq |\mathbf{y}^{SG} \cdot p|; k_e^{SG} \coloneqq [p/m]; k_{max}^{SG} \coloneqq \mathbf{e}_{max}^{SG} \cdot k_e^{SG}; e \coloneqq 0; S \coloneqq 0; \tilde{L}_{hest}^{TE} \coloneqq +\infty; k \coloneqq 0;
                            While e \leq e_{max}^{SG} and s < e_{hest}^{SG} do
                                          P \leftarrow \{p_1, p_2, ..., p_n\};
                                        For i = 0, 1, ..., \lceil p/m - 1 \rceil do
                                                       S \leftarrow \{s_1, s_2, ..., s_m\} \equiv \{p_{i \cdot m+1}, p_{i \cdot m+2}, ..., p_{\min\{(i+1) \cdot m, p\}}\};
                                                      X_{s}^{TR} \leftarrow \begin{bmatrix} x_{s_1}^{TR}, x_{s_2}^{TR}, ..., x_{s_m}^{TR} \end{bmatrix}; \ y_{s}^{TR} \leftarrow \begin{bmatrix} y_{s_1}^{TR} & y_{s_2}^{TR} & \cdots & y_{s_m}^{TR} \end{bmatrix}^T;
                                                       d^k \leftarrow -\nabla \tilde{L}(w^k; X_s^{TR}, y_s^{TR}, \lambda);
                                                      \alpha^{k} \leftarrow \begin{cases} \left(1 - \frac{k}{k^{SG}}\right) \alpha_{0}^{SG} + \frac{k}{k^{SG}} \alpha^{SG} & \text{if } k \leq k^{SG} \\ \alpha^{SG} & \text{if } k > k^{SG} \end{cases}, \qquad \begin{cases} \alpha^{SG} \coloneqq 0.01 \cdot \alpha_{0}^{SG} \\ k^{SG} \coloneqq \left\lfloor \beta^{SG} \cdot k_{max}^{SG} \right\rfloor \end{cases}
                                                       w^k \leftarrow w^k + \alpha^k d^k: k \leftarrow k + 1:
                                         End For
                                          e \leftarrow e + 1; \tilde{L}^{TE} \leftarrow \tilde{L}(w^k, X^{TE}, y^{TE}, \lambda);
                                           If \tilde{L}^{TE} < \tilde{L}^{TE}_{hest} then (\tilde{L}^{TE}_{hest} \leftarrow \tilde{L}^{TE}, w^* \leftarrow w^k, s \leftarrow 0) else s \leftarrow s+1 End If
                           End While
            End SGM
```





Part 2: Stochastic Gradient (5/6)

Script uo nn solve.m with isd = 7 now applies the SGM:

```
uo nn main.m : recognition of num target digits.
clear;
% Parameters for dataset generation
num target =[1];
tr freq
           = .5;
tr p
          = 250;
te q
          = 250;
tr seed = 123456;
te seed = 789101;
% Parameters for optimization
la = 0.0;
                                                              % L2 regularization.
epsG = 10^-6; kmax = 10000;
                                                              % Stopping criterium.
ils=3; ialmax = 2; kmaxBLS=30; epsal=10^{-3}; cl=0.01; c2=0.45; % Linesearch.
isd = 7; icq = 2; irc = 2; nu = 1.0;
                                                              % Search direction.
sq seed = 565544; sq al0 = 2; sq be = 0.3; sq qa = 0.01;
                                                              % SGM iteration.
sg emax = kmax; sg ebest = floor(0.01*sg emax);
                                                              % SGM stopping condition.
% Optimization
t1=clock;
global iheader; iheader = 1;
[Xtr,ytr,wo,fo,tr acc,Xte,yte,te acc,niter,tex]=uo nn solve(num target,tr freq,tr seed,tr p,te seed,te q,la
,epsG,kmax,ils,ialmax,kmaxBLS,epsal,c1,c2,isd,sg al0,sg be,sg ga,sg emax,sg ebest,sg seed,icg,irc,nu);
t2=clock;
fprintf('wall time = %6.1d s.\n', etime(t2,t1));
```





Part 2: Stochastic Gradient (6/6)

```
>> uo nn Xyplot(Xtr,ytr,wo)
[uo nn solve] Pattern recognition with neural networks (OM/GCED).
[uo nn solve] 26-Apr-2021 16:45:24
[uo nn solve] Training data set generation.
[uo nn solve]
                num target = 3
                                                 Rigth positive
[uo nn solve]
                tr freq
                           = 0.50
[uo nn solve]
                           = 250
                tr p
[uo nn solve]
                tr seed
                           = 123456
                                                 Rigth negative
[uo nn solve] Test data set generation.
                           = 0.00
[uo nn solve]
                te freq
[uo nn solve]
                te q
                           = 789101
[uo nn solve]
                te seed
[uo nn solve] Optimization
[uo nn solve]
                L2 \text{ reg. } lambda = 0.0000
                epsG= 1.0e-06, kmax= 10000
[uo nn solve]
                ils= 3, ialmax= 2, kmaxBLS= 30, epsBLS= 1.0e-03,
[uo nn solve]
[uo nn solve]
                c1=0.01, c2=0.45, isd=7
[uo nn solve]
                sg al0= 2.00, sg be= 0.3, sg ge= 0.01
[uo nn solve]
                sg emax= 10000, sg ebest= 100
[uo nn solve]
                                                    f
                                                           llgll
[uo nn solve]
                     2.00e+00
                                  -8.34e-02
                                              2.50e-01
                                                        1.98e-01
                                 -1.25e-03
                                                         8.60e-02
[uo nn solve]
                     2.00e+00
                                              3.43e-02
[uo nn solve]
                     2.00e+00
                                  +1.07e-05
                                                         1.41e-02
[uo nn solve]
                     2.00e+00
                                  +1.91e-07
                                              7.41e-03
                                                         3.10e-03
                                  -4.22e-05
[uo nn solve]
                     2.00e+00
                                              7.31e-03
                                                         1.08e-02
                                                                         >> uo nn Xyplot(Xte,yte,wo)
[uo nn solve]
                     2.00e+00
                                  -1.34e-04
                                              1.07e-02
                                                         1.99e-02
[uo nn solve] 12673
                     1.93e+00
                                  -2.21e-08
                                              3.56e-04
                                                         1.78e-04
[uo nn solve] 12751
                                              4.40e-04
                                                        1.60e-03
[uo nn solve]
                          al iW
                                      a'*d
                                                           Hall
[uo nn solve]
[uo nn solve]
                     -5.6e-01,-1.7e-02,-1.3e+00,-2.8e-01,-1.2e+00
[uo nn solve]
                     +9.3e-01,-1.3e-01,-2.1e-01,-9.6e-03,+3.3e-01
[uo nn solve]
                     -2.8e+00,-6.4e-01,-6.1e-01,-8.9e-01,-1.8e-01
                     -6.2e-01,-3.1e+00,+1.6e+00,+5.7e-01,-1.8e+00
[uo nn solve]
[uo nn solve]
                     -2.1e+00,+4.4e-01,-2.1e+00,-2.5e-01,+2.6e-01
                     +2.4e+00,-9.4e-01,-4.9e-01,+2.4e-01,+7.6e-01
[uo nn solve]
[uo nn solve]
                     -5.0e-01,-3.6e-01,+2.1e-01,+2.8e-01,-6.9e-01
[uo nn solve]
[uo nn solve] Accuracy.
[uo nn solve] tr accuracy = 98.8
[uo nn solve] te accuracy = 98.8
 wall time = 2.8e-01 s.
>> uo nn Xyplot(wo,0,[])
                                                                                                     210 211 212 213 214 215 216 217 218 219 220 221
                                                                                  229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250
```



BY-NC-ND

GM

Part 3: computational study (1/3)

- In this third part we want to conduct a series of computational experiments to study:
 - i. How the regularization parameter λ affects the results.
 - ii. The relative performance of the different algorithms (GM, QNM,SGM)
- To this end, an instance of the SLNN problem must be solved:
 - For every one of the individual digits, 0 to 9.
 - For every value of the regularization parameter $\lambda \in \{0.0, 0.01, 0.1\}$.
 - For every optimization algorithm: **GM, QNM** and **SGM**.

That makes a total of $10 \times 3 \times 3 = 90$ instances to be solved.

We will use a small size dataset with

Max. number of iterations for GM and QNM will be kmax = 1000. To do a fair comparison with SGM, sg_emax = kmax, so that every method is allowed to spend a similar computational effort (number of gradient evaluations).





Part 3: computational study (2/3)

• To organize the computational experiments you can use function uo nn batch.m:

uo nn batch.m: run a batch of SLNN instances. clear: % Parameters. tr seed = 123456; te seed = 789101; tr p = 250; te q = 250; tr freq = 0.5;% Datasets generation $epsG = 10^-6; kmax = 1000;$ % Stopping condition. ils=3; ialmax = 1; kmaxBLS=10; epsal=10^-3; c1=0.01; c2=0.45; % Linesearch. icg = 2; irc = 2; nu = 1.0; % Search direction. sg seed = 565544; sg al0 = 2; sg be = 0.3; sg ga = 0.01; % SGM iteration. sg emax = kmax; sg ebest = floor(0.01*sg emax); % SGM stopping condition. % Optimization global iheader; iheader = 1; csvfile = strcat('uo nn batch ',num2str(tr seed),'-',num2str(te_seed),'.csv'); fileID = fopen(csvfile ,'w'); t1=clock; for num target = [1:10] for la = [0.0, 0.01, 0.1]for isd = [1,3,7][Xtr,ytr,wo,fo,tr acc,Xte,yte,te acc,niter,tex]=uo nn solve(num target,tr freq,tr seed,tr p,te seed,te q,la ,epsG,kmax,ils,ialmax,kmaxBLS,epsal,c1,c2,isd,sg al0,sg be,sg ga,sg_emax,sg_ebest,sg_seed,icg,irc,nu); if iheader == 1 fprintf(fileID, 'num target; la; isd; niter; tex; tr acc; te acc; L*;\n'); end %1i; %7.4f; %1i; %6i; %7.4f; %5.1f; %5.1f; %8.2e;\n', fprintf(fileID,' mod(num target,10), la, isd, niter, tex, tr acc, te acc, fo); iheader=0; end end t2=clock; fprintf(' wall time = 6.1d s. n', etime(t2,t1)); fclose(fileID);





Part 3: computational study (3/3)

• The outcome of uo_nn_batch.m is the log file
uo_nn_batch_tr_seed-te_seed.csv with the following content:

```
num target;
                 la; isd;
                           niter;
                                      tex; tr acc; te acc;
                                                                   L*;
             0.0000;
                       1;
                              75;
                                   0.1055;
                                            100.0;
                                                     100.0;
                                                             5.72e-07;
             0.0000;
                       3;
                               6;
                                   0.0099;
                                            100.0;
                                                     100.0;
                                                            2.91e-50;
         1;
             0.0000;
                       7; 125001;
                                  1.5164;
                                            100.0;
                                                     100.0;
                                                            1.41e-05;
                                           100.0;
         1;
             0.0100;
                       1;
                              58; 0.0955;
                                                     100.0; 2.76e-02;
                                           100.0;
         1;
             0.0100;
                       3;
                              45;
                                   0.1026;
                                                     100.0;
                                                             2.76e-02;
         1;
             0.0100;
                       7;
                            3751;
                                   0.0464; 96.4; 99.6;
                                                             6.74e-02;
             0.1000;
                              36;
                                   0.0645;
                                             99.6;
                                                      98.4;
                                                             1.45e-01;
         0;
                       1;
             0.1000;
                                   0.0520;
         0;
                       3;
                              20;
                                           99.6;
                                                      98.4;
                                                             1.45e-01;
         0;
             0.1000;
                       7;
                            2751;
                                   0.0336;
                                              53.6;
                                                      92.4;
                                                             6.37e-01;
```

The data included in this file will be the base for the analysis of the performance of the different optimization algorithms that you have to perform in this project.





Report (1/3)

- 1) Study of the convergence: first, we are going to study the global and local convergence of the three algorithms only in terms of the objective function \tilde{L} :
 - a) **Global convergence**: compare the value at the optimal solution of the loss function \tilde{L} for every combination λ -algorithm. According to the information in the log file Are the three algorithms able to identify a stationary solution of the loss function \tilde{L} ?
 - b) Local convergence:
 - Compare the speed of convergence of the three algorithms in terms of the execution time and number of iterations.
 - ii. Analyse how the speed of convergence of the three algorithms depend on the value of λ and try to find an explanation for the observed dependence, if any.
 - iii. Analyse the running time per iteration (tex/niter) and try to find an explanation for the different values among the three algorithms.
 - c) Finally, according to the previous study, discuss the general performance of the three algorithms in terms of local and global convergence and justify which is the most efficient for the minimization of \tilde{L} .





Report (2/3)

2) Study of the recognition accuracy: now, we are going to analyse the recognition accuracy of the SLNN, $Accuracy^{TE}$ (te_acc) for the different algorithmic options with a more realistic dataset with:

Run the training process for the ten digits with these parameters and every algorithm, GM, QNM, SGM, using, for each one of them, the value of λ showing the best $Accuracy^{TE}$ in the results of the previous section 1- a) with the smaller dataset (tr_p = 250).

- a) Analyse the results. Based on this analyse, tell if there is a method that clearly outperforms the others in terms of speed and recognition accuracy.
- b) Does the best combination λ -algorithm with respect to the maximization of $Accuracy^{TE}$ coincide with best combination with respect to the minimization of \tilde{L} observed in the previous study 1-c)? Discuss the reasons for the discrepancy, in case the combinations do not coincide.



Report (3/3)

- This assignment must be done in groups of two. Use a value of tr_seed and te_seed based on your student's ID number. You must upload to Atenea a file with the name surname-student-1 surname-student-2.zip containing:
 - A report (.pdf file) with your answers to the different sections of tasks 1)
 "Convergence" and 2) "Accuracy".
 - The report must have a cover with the name of the two students and the values of tr_seed, te_seed and sg_seed
 - The source of all the codes used to do the assignment. The codes must be self-contained and must allow the replication of all the results included in the report.

 Grading criteria
- The mark will take into account formal quality, understandability and reading easiness, as long as the evidences provided to support the results of the analysis performed in the project (numerical values, tables, plots, ...).

ı	1) Study of the convergence:	Points
	a) Global convergence.	1,5
	b) Local convergence.	2,5
	c) Discussion.	1,0
	2) Study of the accuracy for large porblems.	
	 a) Best method for large problems. 	2,0
	b) Discussion $Accuracy^{TE}$ - $ ilde{L}$	2,0



3) Overall quality of the report.

1,0