The goals of this homework are (*i*) to acquire practice with real data and (*ii*) to explore various optimization methods for solving classification problems and understand how their performance is affected by their settings.

What to submit. Please submit a report with figures and comments. Link your codes to the report pdf. These can be e.g. Dropbox links or GitHub links, etc. All optimizers should be coded from scratch.

Programming language. You can use Matlab or Python.

- If you are using Matlab, you use MNIST data saved in `mnist.mat` and my codes `mnist_2categories_quadrati` and `LevenbergMarquardt.m` to get started.
- If you are using Python, you use MNIST data saved in `mnist2.mat` and my codes `mnist_2categories_quadra` and `LevenbergMarquardt.py` to get started.

1 MNIST dataset

You will experiment with the MNIST dataset of handwritten digits 0, 1, . . . , 9 available at `http://yann.lecun.com/exdb/mnist/`. The training set has 60000 28 x 28 grayscale images of handwritten digits (10 classes) and a testing set has 10000 images. I removed the 4-pixel paddings with zero from these images, making them 20-by-20, with the aid of the code `readMNIST.m` written by Siddharth Hegde.

2 Classification problem

The task is to select all images with digits 1 and all images with digits 7 from the training set, find a dividing surface that separates them, and test this dividing surface on the 1's and 7's from the test set. A sample of 1's and 7's from the training set is shown in Fig. 1.

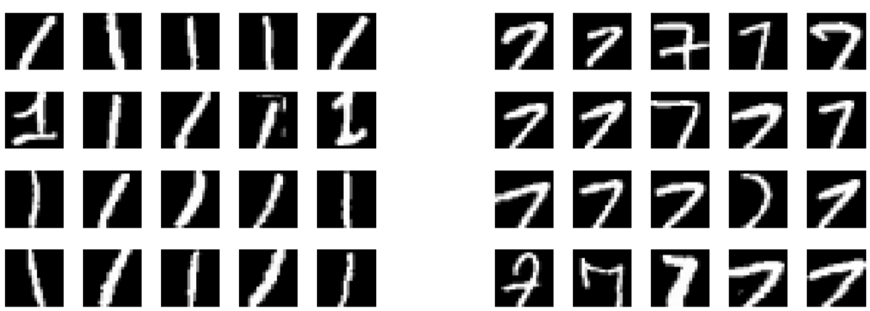


Figure 1: Samples of 20-by-20 images of 1's (left) and 7's (right) from MNIST.

Each image is a point in $\mathbb{R}^{400}$ (the images with stripped paddings are 20-by-20). It is convenient to reduce the dimensionality of data by using SVD and mapping the set to $\mathbb{R}^d$ where $d \ll 400$, e.g. $d = 3$, $d = 10$, $d = 20$, etc.

We pose three kinds of unconstrained optimization problems.

2.1 A smooth loss function for the optimal hyperplane with Tikhonov regularization

In the simplest setting, we aim at finding a dividing hyperplane $w^\top x+b=0$ with that $w^\top x_j+b>0$ for all (almost all) x_j corresponding to 1 (labelled with $y_j=1$) and $w^\top x_j+b<0$ for all (almost all) x_j corresponding to 7 (labelled with $y_j=-1$). Hence, x_j is classified correctly if

$$\mathsf{sign}(y_j(w^\top x_j+b))=1.$$

Instead of the discontinuous sign function, we use a smooth sigmoid-type function (we call it *residual*)

$$r_j \equiv r(x_j;\{w,b\}) \coloneqq \log\left(1+e^{-y_j(w^\top x_j+b)}\right) \tag{1}$$

that is close to zero if $y_j(w^\top x_j+b)>0$ and grows linearly in the negative range of the aggregate $y_j(w^\top x_j+b)$. For brevity, we will denote the $d+1$-dimensional vector of parameter $\{w,b\}$ by $\mathbf{w}$. We form the loss function by averaging up the residuals and adding a Tikhonov regularization term:

$$f(\mathbf{w})=\frac{1}{n}\sum_{j=1}^{n}\log\left(1+e^{-y_j(w^\top x_j+b)}\right)+\frac{\lambda}{2}\|\mathbf{w}\|^2. \tag{2}$$

Here n is the number of data points, and λ is a parameter for the Tikhonov regularization. λ should be a small number. Its purpose is to prevent the entries of w from being too large.

2.2 A smooth loss function for the optimal quadratic hypersurface with Tikhonov regularization

As you will see, a quadratic dividing hypersurface may lead to much fewer misclassified digits. We are seeking a quadratic hypersurface of the form:

$$x^\top Wx+v^\top x+b.$$

Hence, the quadratic test function is

$$q(x_j;\mathbf{w}) \coloneqq y_j(x^\top Wx+v^\top x+b). \tag{3}$$

The loss function is defined in a similar manner:

$$f(\mathbf{w})=\frac{1}{n}\sum_{j=1}^{n}\log\left(1+e^{-q(x_j;\mathbf{w})}\right)+\frac{\lambda}{2}\|\mathbf{w}\|^2. \tag{4}$$

Here $\mathbf{w}$ denotes the d^2+d+1-dimensional vector of coefficients of $\{W,v,b\}$.

2.3 A nonlinear least squares problem for the optimal quadratic hypersurface

Finally, we can design the loss function to fit the framework of the nonlinear least squares problem:

$$f(\mathbf{w})=\frac{1}{2}\sum_{j=1}^{n}[r_j(\mathbf{w})]^2, \quad r_j(\mathbf{w})=\log\left(1+e^{-q(x_j;\mathbf{w})}\right). \tag{5}$$

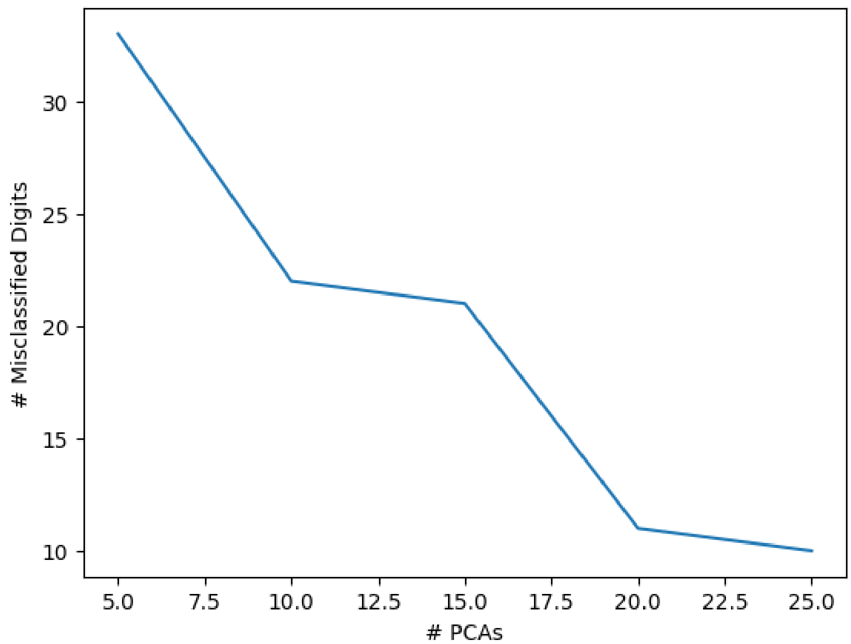
The provided codes solve this nonlinear least squares problem and find a dividing quadratic hypersurface using the Levenberg-Marquardt algorithm.

3 Tasks

3.1 Task 1

Experiment with **the number of PCAs** using the provided codes. Find out how the number of PCAs affects the number of misclassified digits. Plot a graph of the number of misclassified digits in the test set vs the number of PCAs.

Solution: We plot below the number of misclassified digits with each number of PCAs in $\{5, 10, 15, 20, 25\}$. As expected, we find that as the number of PCAs increases, the number of misclassified digits decreases.

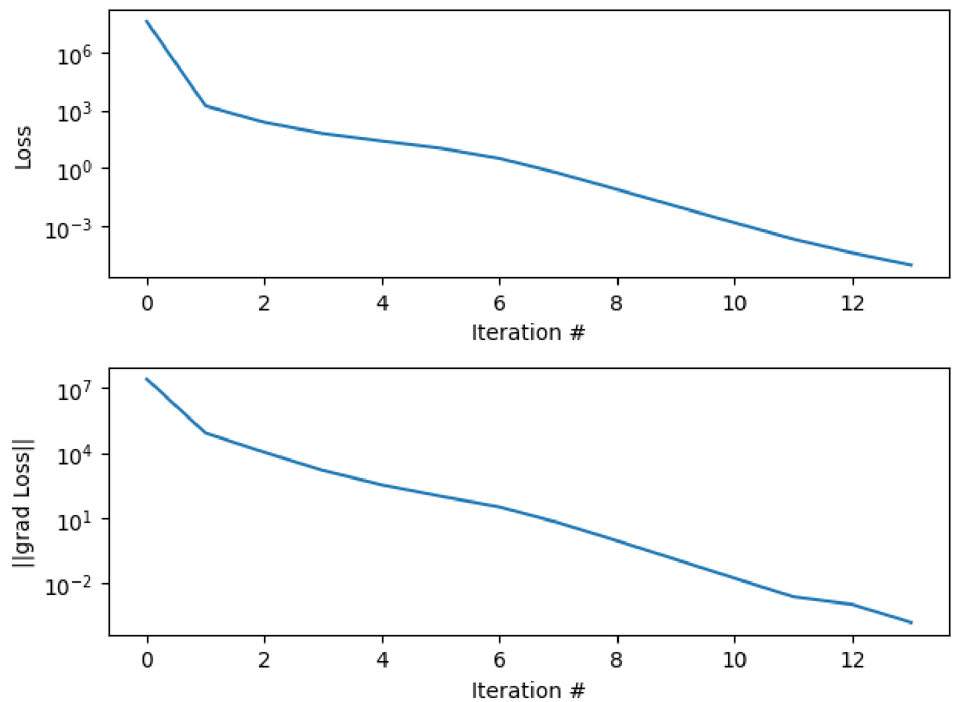


3.2 Task 2

Set the number of PCAs to 20. Program the **Gauss-Newton** algorithm and solve the nonlinear least squares problem in Section 2.3 using your routine. Plot the graphs of the loss and the norm of the gradient versus iteration number. To avoid problems with inverting the matrix $J^\top J$, you can regularize it by changing it to

$$J^\top J + I \cdot 10^{-6}.$$

Solution: We implement the Gauss-Newton algorithm here. With a tolerance of 10^{-3}, we find that the algorithm misclassifies 20 iterations digits in the test set. We plot the loss and the norm of the gradient of the loss below.

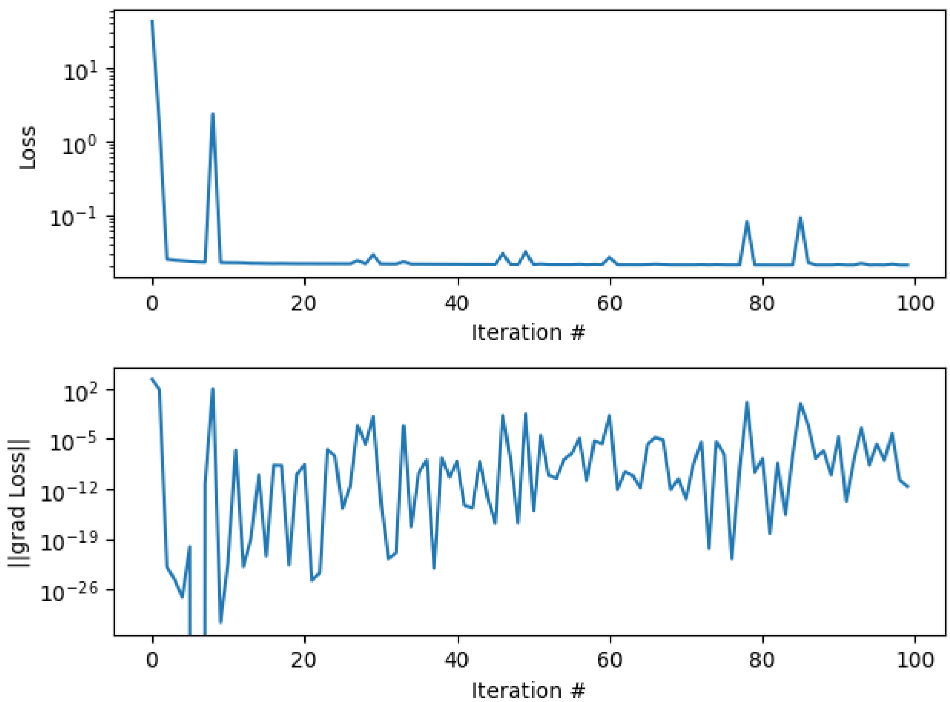


3.3 Task 3

Define the loss function as in (4). Implement **Stochastic Gradient Descent**. Experiment with various batch sizes and step sizes. Also, try a few stepsize decreasing strategies. Plot the graphs of the loss and the norm of the gradient versus iteration number. Write a summary of your observations. Conclude which batch sizes are reasonable, which stepsizes are reasonable, and how many epochs are enough. Is it beneficial for this problem to use a decreasing step size?

Solution: Trying several different values of batch size, step size, and λ in the Tikhonov regularization, we find that the best performance occurs with batch size 10, constant $\alpha = 10^{-3}$, and $\lambda = 10^{-4}$, after 100 epochs we misclassify only 11 digits.

Somewhat counterintuitively, we were unable to best this performance using a decreasing step size, although a decreasing step size should in theory yield better results. We plot the loss and the norm of the gradient of the loss below.



Loss
10^1
10^0
10^{-1}
0 20 40 60 80 100
Iteration #
||grad Loss||
10^2
10^{-5}
10^{-12}
10^{-19}
10^{-26}
0 20 40 60 80 100
Iteration #