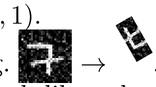
The objective of this lab is for you to program in Matlab gradient descent (GD) and stochastic gradient descent (SGD) for two linear models (for regression and for classification), apply them to some datasets and observe their behavior. The TA will first demonstrate the results of the algorithms on several datasets, and then you will program them, replicate those results, and further explore the datasets with the algorithms. You can use the textbook, lecture notes and your own notes.

Important: develop your code so it works with inputs $\mathbf{x} \in \mathbb{R}^D$ for any dimension D (and, for regression, with outputs $\mathbf{y} \in \mathbb{R}^{D'}$ for any dimension D'). It is as easy as for dimension 1 if you use vectorized code in Matlab, and it should look very similar to the actual equations. Start with the easiest case, which is linear regression, on a toy dataset where $x_n, y_n \in \mathbb{R}$. Test your GD and SGD code there, make sure they work as expected and understand their behavior as a function of their parameters (learning rate and minibatch size). Then move on to logistic regression, which is a bit more complicated, and to higher-dimensional datasets.

I Datasets

Firstly, construct your own toy datasets to visualize the result easily and be able to get the algorithm right. Take the input instances $\{\mathbf{x}_n\}_{n=1}^N$ in $\mathbb{R}$ or $\mathbb{R}^2$ and the labels $\{y_n\}_{n=1}^N$ in $\mathbb{R}$ (regression) or $\{0, 1\}$ (classification).

Then, try the MNIST dataset of handwritten digits, with instances $\mathbf{x} \in \mathbb{R}^D$ (where $D = 784$). For classification with logistic regression, use the labels $y_n \in \{0, \dots, 9\}$ (for binary classification, pick instances from only two digit classes and use labels $y_n \in \{0, 1\}$). For linear regression, create a ground-truth mapping $\mathbf{y} = \mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$ as follows:

- A random mapping with output dimension D', e.g. take $\mathbf{A}_{D' \times D}$ and $\mathbf{b}_{D' \times 1}$ with elements in $\mathcal{N}(0, 1)$.
- A mapping that rotates, scales, shifts and possibly clips the input image $\mathbf{x}$ and adds noise to it, e.g. . This makes it easy to visualize the result, since the desired output $\mathbf{f}(\mathbf{x})$ for an image $\mathbf{x}$ should look like $\mathbf{x}$ but transformed accordingly.

II (Stochastic) gradient descent for linear regression

Review Consider first the case of a single output dimension, $y \in \mathbb{R}$. Given a sample $\{(\mathbf{x}_n, y_n)\}_{n=1}^N$ with $\mathbf{x}_n \in \mathbb{R}^D$ and $y_n \in \mathbb{R}$, we solve a linear least-squares regression problem by minimizing:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} (y_n - \mathbf{w}^T \mathbf{x}_n)^2 = \sum_{n=1}^{N} e(\mathbf{w}; \mathbf{x}_n, y_n) \qquad \text{with} \qquad e(\mathbf{w}; \mathbf{x}_n, y_n) = \frac{1}{2} (y_n - \mathbf{w}^T \mathbf{x}_n)^2$$

where we assume the last element of each $\mathbf{x}_n$ vector is equal to 1, so that w_D is the bias parameter (this simplifies the notation). $E(\mathbf{w})$ is a quadratic objective function over $\mathbf{w}$ with a unique minimizer that can be found in closed form by solving the normal equations (obtained by computing the gradient of E wrt $\mathbf{w}$, setting it to zero and solving for $\mathbf{w}$):

$$\mathbf{X}\mathbf{X}^T \mathbf{w}^* = \mathbf{X}\mathbf{y} \Leftrightarrow \mathbf{w}^* = (\mathbf{X}\mathbf{X}^T)^{-1} \mathbf{X}\mathbf{y}, \text{ where } \mathbf{X}_{D \times N} = (\mathbf{x}_1, \dots, \mathbf{x}_N), \ \mathbf{w}^*_{D \times 1} = (w_1, \dots, w_D)^T, \ \mathbf{y}_{N \times 1} = (y_1, \dots, y_N)^T.$$

This can be done with a routine for solving linear systems, e.g. in Matlab, use `linsolve` or the "\" operator. You can also use `inv` but this is numerically more costly and less stable.

The minimizer $\mathbf{w}^*$ of E can also be found iteratively by gradient descent (GD) and stochastic gradient descent (SGD), starting from an initial $\mathbf{w}$. These use the following updates (obtained by computing the gradient $\nabla E(\mathbf{w})$ of E wrt $\mathbf{w}$):

$$\text{GD: } \Delta\mathbf{w} = \eta \sum_{n=1}^{N} (y_n - \mathbf{w}^T \mathbf{x}_n)\, \mathbf{x}_n \qquad \qquad \text{SGD: } \Delta\mathbf{w} = \eta \sum_{n \in \mathcal{B}} (y_n - \mathbf{w}^T \mathbf{x}_n)\, \mathbf{x}_n$$

where η is the learning rate (step size) and $\mathcal{B}$ is a minibatch (i.e., a subset of $1 < |\mathcal{B}| < N$ points). For GD, at each iteration we set $\mathbf{w} \leftarrow \mathbf{w} + \mathbf{\Delta w}$ with $\mathbf{\Delta w} = -\eta \nabla E(\mathbf{w})$. For SGD, after each minibatch we set $\mathbf{w} \leftarrow \mathbf{w} + \mathbf{\Delta w}$ with $\mathbf{\Delta w} = -\eta \sum_{n \in \mathcal{B}} \nabla e(\mathbf{w}; \mathbf{x}_n)$, and repeat over all minibatches to complete one iteration (one epoch), which passes over the whole data once. If the minibatches contain a single data point ($|\mathcal{B}| = 1$), then there are N minibatches and we do pure online learning. If there is a single minibatch containing all points ($|\mathcal{B}| = N$), we do pure batch learning (identical to GD). The fastest training occurs for an intermediate (usually small) minibatch size. It also helps to reorder at random (shuffle) the data points at the beginning of each epoch (so the minibatches vary, and are scanned in a different order), rather than using the same, original order at every epoch (helpful Matlab function: `randperm`).

Consider now the general case of several output dimensions and a sample $\{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$ with $\mathbf{x}_n \in \mathbb{R}^D$, $\mathbf{y}_n \in \mathbb{R}^{D'}$. This is equivalent to D' independent single-output regressions. The corresponding equations are as follows, where $\mathbf{X}_{D\times N} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$, $\mathbf{Y}_{D'\times N} = (\mathbf{y}_1, \dots, \mathbf{y}_N)$, $\mathbf{W}_{D'\times D}$ and $\mathbf{w}_d^T$ is the dth row of $\mathbf{W}$:

$$\text{Objective function: } E(\mathbf{W}) = \frac{1}{2}\sum_{n=1}^N \|\mathbf{y}_n - \mathbf{W}\mathbf{x}_n\|^2 = \sum_{n=1}^N e(\mathbf{W}; \mathbf{x}_n, \mathbf{y}_n) \quad \text{with} \quad e(\mathbf{W}; \mathbf{x}_n, \mathbf{y}_n) = \frac{1}{2}\sum_{d=1}^{D'} (y_{nd} - \mathbf{w}_d^T\mathbf{x}_n)^2$$

$$\text{Gradient: } \frac{\partial E}{\partial \mathbf{W}} = -\sum_{n=1}^N (\mathbf{y}_n - \mathbf{W}\mathbf{x}_n)\,\mathbf{x}_n^T \qquad \text{GD: } \Delta\mathbf{W} = \eta\sum_{n=1}^N (\mathbf{y}_n - \mathbf{W}\mathbf{x}_n)\,\mathbf{x}_n^T \qquad \text{SGD: } \Delta\mathbf{W} = \eta\sum_{n\in\mathcal{B}} (\mathbf{y}_n - \mathbf{W}\mathbf{x}_n)\,\mathbf{x}_n^T$$

$$\text{Normal equations: } (\mathbf{X}\mathbf{X}^T)\mathbf{W} = \mathbf{X}\mathbf{Y}^T \Leftrightarrow \mathbf{W} = (\mathbf{X}\mathbf{X}^T)^{-1}\mathbf{X}\mathbf{Y}^T.$$

Implementation and exploration: toy problem Firstly, verify that the GD/SGD updates above are correct, by obtaining the gradient of $E(\mathbf{w})$ with pen and paper. Then, implement GD and SGD by programming the updates with a "for" loop. Run them for, say, 100 iterations $\mathbf{w}^{(0)}, \mathbf{w}^{(1)}, \dots, \mathbf{w}^{(100)}$ from an initial $\mathbf{w} = \mathbf{w}^{(0)}$ (equal to small random numbers, e.g. uniform in $[-0.01, 0.01]$). To visualize the results, create the following plots for each algorithm (GD and SGD):

- Plot the dataset (y_n vs $\mathbf{x}_n$) and the regression line $f(\mathbf{x}) = \mathbf{w}^T\mathbf{x}$.
- Plot the error $E(\mathbf{w})$ over iterations, evaluated on the training set, and also on a validation set.
- Do a contour plot of the error $E(\mathbf{w})$ and the iterates $\mathbf{w}^0, \mathbf{w}^{(1)}, \dots$

Consider the following questions:

- Does the error $E(\mathbf{w})$ approach the optimal error $E(\mathbf{w}^*)$ (where $\mathbf{w}^*$ is the solution to the normal equations)? How fast does it approach it? Does $E(\mathbf{w})$ decrease monotonically? Or does it oscillate or even diverge?
- Vary the learning rate $\eta > 0$. What happens if it is very small or if it is very big? Try to determine the value of η that gives the fastest convergence for your toy dataset by trial and error. Note: practical values of η are usually (quite) smaller than 1.
- For SGD with fixed η, vary the minibatch size $|\mathcal{B}|$ between 1 and N. How does this affect the speed of convergence?
- For both GD and SGD we keep the learning rate η constant. How does this affect the behavior of SGD as we keep training? What should we do to improve that?
- Repeat all of the above in the following situations:
  - Use a dataset having 10 times as many points.
  - Use a dataset having 3 times larger noise.
  - Use a different initial $\mathbf{w}^{(0)}$.

  Are the best values of η the same as before for GD? How about SGD? What other changes do you observe?

See the end of file `lab06_linregr.m` for suggestions of things to explore.

Implementation and exploration: MNIST Select a small enough subset of MNIST as training inputs (using the whole dataset will be slow). Apply the ground-truth linear transformation to the data to generate the output labels $\mathbf{y} = \mathbf{f}(\mathbf{x}) = \mathbf{A}\mathbf{x} + \mathbf{b}$. Then proceed as with the toy dataset to compute the optimal solution exactly by solving the normal equations, and approximately by running GD and SGD. Then, consider the same questions as with the toy dataset. Note that the appropriate values for η, etc. may now be significantly different. To visualize the results, create the following plots for each algorithm (GD and SGD):

- Plot the training and validation error $E(\mathbf{w})$ over iterations, as with the toy dataset.
- For each of the 4 results (true mapping, optimal mapping from the normal equations, and the mappings learned by GD and SGD), plot:
  - The parameters of the linear mapping using `imagesc(A)` and `imagesc(b)`. These are signed values, so use `colormap(parula(256))`.
  - If using as linear mapping the rotation/shift/scale/clip transformation, which produces as output a (possibly smaller) image $\mathbf{y}_n$, plot the following for a few sample images: the input image $\mathbf{x}_n$, and the outputs $\mathbf{y}_n$ under the 4 mappings.

III (Stochastic) gradient descent for logistic regression (= classification)

Review We consider the two-class case, given a sample $\{(\mathbf{x}_n, y_n)\}_{n=1}^N$ with $\mathbf{x}_n \in \mathbb{R}^D$ and $y_n \in \{0,1\}$. Again we assume the last element of each $\mathbf{x}_n$ vector is equal to 1, so that w_D is the bias parameter in the sigmoid $\sigma(\mathbf{w}^T\mathbf{x}_n) = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x}_n)}$. The objective functions $E(\mathbf{w})$ below do not admit a closed-form solution, so we need iterative algorithms. We apply GD and SGD, whose updates are obtained by computing the gradient $\nabla E(\mathbf{w})$ of E wrt $\mathbf{w}$. We can learn $\mathbf{w}$ by maximum likelihood, or by regression.

- By *maximum likelihood*: we minimize the cross-entropy

$$E(\mathbf{w}) = \sum_{n=1}^N e(\mathbf{w}; \mathbf{x}_n, y_n) \qquad \text{where} \qquad \begin{cases} e(\mathbf{w}; \mathbf{x}_n, y_n) = -y_n \log \theta_n - (1-y_n)\log(1-\theta_n) \\ \theta_n = \sigma(\mathbf{w}^T\mathbf{x}_n) = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x}_n)}. \end{cases}$$

  With GD and SGD we have the following updates:

$$\text{GD: } \mathbf{\Delta w} = \eta \sum_{n=1}^N (y_n - \theta_n)\mathbf{x}_n \qquad\qquad \text{SGD: } \mathbf{\Delta w} = \eta \sum_{n\in\mathcal{B}} (y_n - \theta_n)\mathbf{x}_n.$$

- By *regression*: we minimize the least-squares error

$$E(\mathbf{w}) = \sum_{n=1}^N e(\mathbf{w}; \mathbf{x}_n, y_n) \qquad \text{where} \qquad \begin{cases} e(\mathbf{w}; \mathbf{x}_n, y_n) = \frac{1}{2}(y_n - \theta_n)^2 \\ \theta_n = \sigma(\mathbf{w}^T\mathbf{x}_n) = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x}_n)}. \end{cases}$$

  With GD and SGD we have the following updates:

$$\text{GD: } \mathbf{\Delta w} = \eta \sum_{n=1}^N (y_n - \theta_n)\theta_n(1-\theta_n)\mathbf{x}_n \qquad\qquad \text{SGD: } \mathbf{\Delta w} = \eta \sum_{n\in\mathcal{B}} (y_n - \theta_n)\theta_n(1-\theta_n)\mathbf{x}_n.$$

Implementation and exploration: toy problem Proceed as in the linear regression case. The differences now are: 1) the problem is classification rather than regression; 2) the objective function $E(\mathbf{w})$ and hence its gradient and GD/SGD updates are different; and 3) the model is $\sigma(\mathbf{w}^T\mathbf{x})$ rather than $\mathbf{w}^T\mathbf{x}$. Some additional questions to consider:

- How do the contours of the objective function (cross-entropy or least-squares error) look like compared with each other, and compared with the contours of the least-squares error for the linear regression case?
- Try datasets where the two classes are linearly separable, and where they are not linearly separable. Do the contours of the objective function look the same in both cases? Why? How does this affect the optimal parameters? More specifically: in the linearly separable case, what happens to $\|\mathbf{w}\|$ as the number of iterations increases? Will the algorithm ever converge?
- Try using as initial weights $\mathbf{w} \in \mathbb{R}^D$ random numbers uniformly distributed in $[-u, u]$. Try a small value of u (say, 0.01) and a large one (say, 100). What happens, and why? Which initialization is better?

See the end of file `lab06_logregr.m` for suggestions of things to explore.

Once this works, you can implement logistic regression for the $K > 2$ classes case, if you feel adventurous.

Implementation and exploration: MNIST As in the linear regression case.

IV What you have to submit

We provide you with 4 scripts `lab06_linregr.m`, `lab06_linregr_MNIST.m`, `lab06_logregr.m`, `lab06_logregr_MNIST.m` which set up the problem (toy dataset or MNIST) and plot the figures mentioned earlier. You have to code the normal equations and the (stochastic) gradient descent algorithms, and explore their behavior.

Follow these instructions strictly. Email the TA the following packed into a **single** file (`lab06.tar.gz` or `lab06.zip`) and with email subject `[CSE176] lab06`:

- Matlab code for the functions:
  - `linfexact.m`, `linfgd.m` and `linfsgd.m`. They train a linear regressor (from D dimensions to D' dimensions) by solving the normal equations, by gradient descent, or by stochastic gradient descent, respectively.
  - `slinfgd.m` and `slinfsgd.m`. They train a logistic regressor for binary classification (from D dimensions to one output in $[0, 1]$) by gradient descent or by stochastic gradient descent, respectively.

  Use the templates provided. Read them carefully to understand what the functions should do, and the functions `linf.m`, `slinf.m` and `sigmoid.m` (which we provide). The functions should work when called from the scripts `lab06*.m` listed above.
  Note: you are not allowed to use any functions from the Matlab Toolboxes (in particular, the Statistics and Machine Learning Toolbox, or the Neural Network Toolbox). You can only use basic Matlab functions.

- A brief report (2 pages) in PDF format describing your experience with the algorithms. The more extensive and insighful your exploration, the higher the grade. Be concise. Don't include code or figures, we can recreate them by running your functions. Indicate the part that each member of the group did.