Project in *First-order methods for large-scale machine learning*

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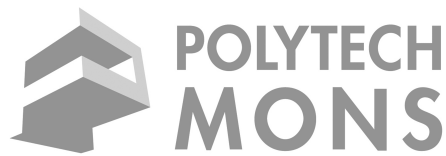

27 February 2024

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   - Ideally groups of 2, groups of > 3 are not accepted

Schedule

- Tuesday 27/02 08h30-12h30: presentation of the project, team building
- Tuesday 05/03 08h30-12h30: work by group, Q&A
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Deadline of the project is June 14th (the Kaggle deadline).

What's the project ?!

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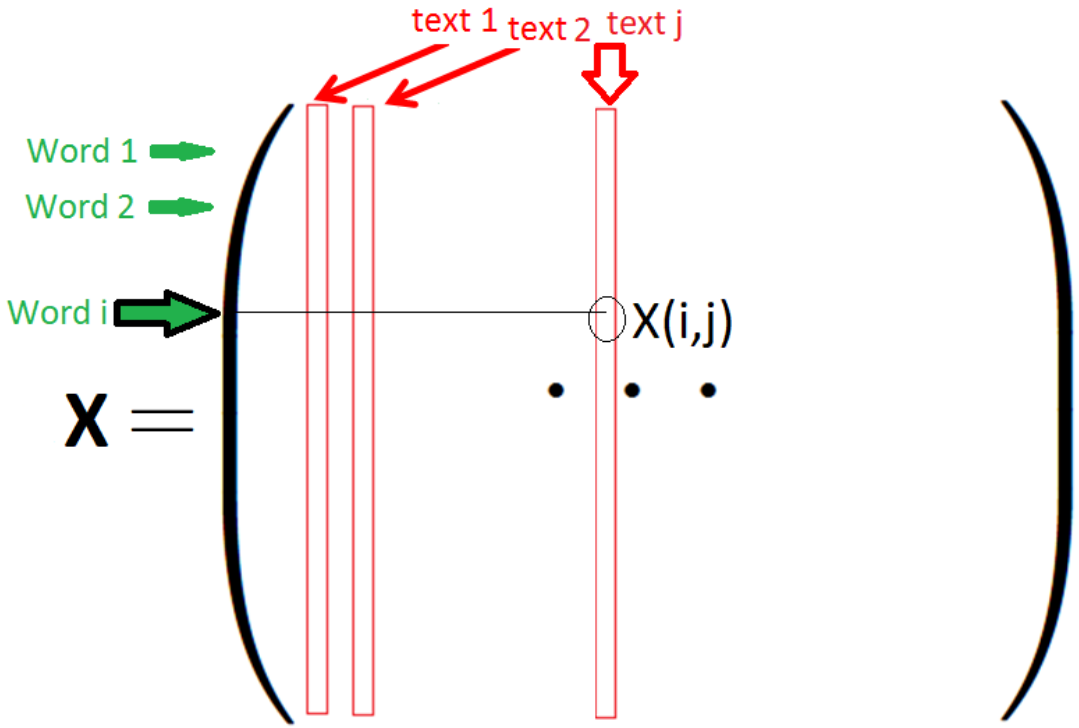
- Each document is represented by a "bag of words" i.e. the number of occurrences of each word in this document
- In summary, in the data matrix $X \in \mathbb{R}^{m \times n}$, each column corresponds to a document (text) and each row to a word. $X(i,j)$ $(i = 1, ..., m,$ $j = 1, ..., n)$ is the number of occurrences of word i in text j



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- Data are available on Kaggle website: see *https://www.kaggle.com/competitions/docum-classi/*.

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- It would be odd to consider it as the target for our model, since its numerical value has little interest in itself (e.g. class "3" is not better than class "1", other codings would be possible)
- "One hot encoding": for all j, transform each label y_j into a vector $Y(:, j)$ of length p (p is the number of classes) such that $Y(k, j) = 1$ iff $k = y_j$ and 0 otherwise. Consequently, $Y \in \mathbb{R}^{p \times n}$

Model

- "0-hidden-layer neural network": the output layer directly follows the input one $\rightarrow$ only one weight matrix $W_1 \in \mathbb{R}^{m \times p}$ and a bias vector $b_1 \in \mathbb{R}^p$

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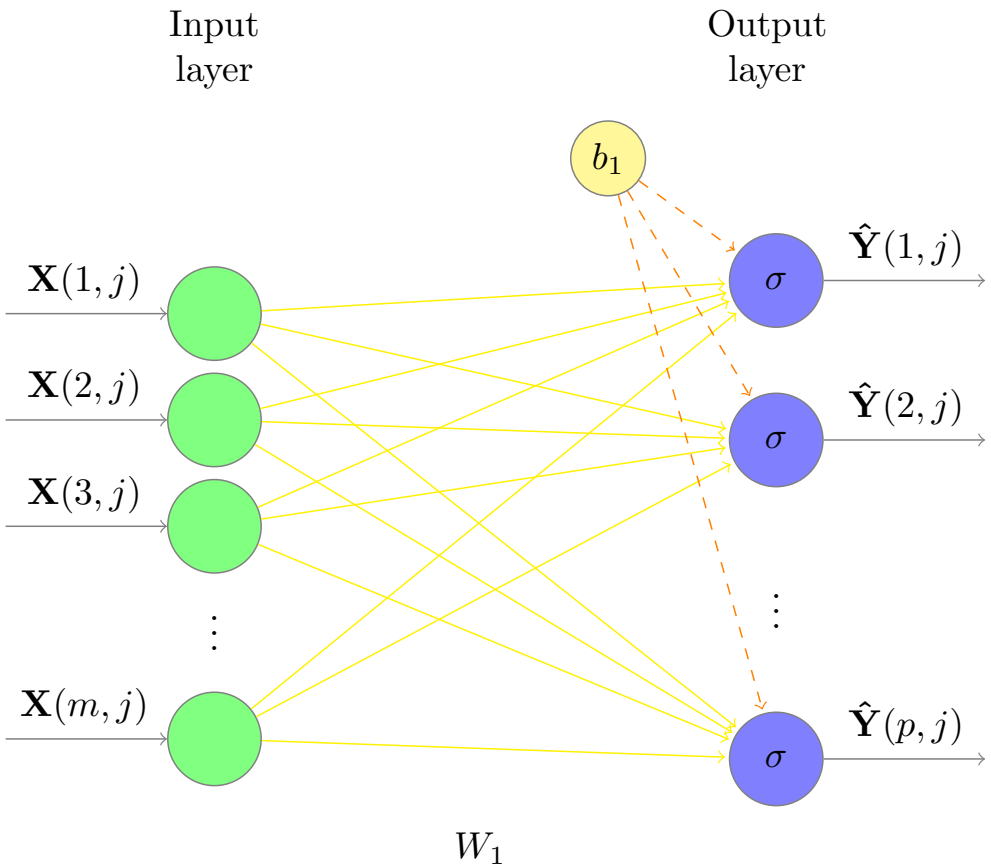
- Illustration of the workflow for the j-th data point:



The model in practice

- Predicted one-hot-encoded vector $\hat{Y}_j$ of document j given by $\hat{Y}(k,j) = \sigma(\sum_{i=1}^{m} W_1(i,k)X(i,j) + b_1(k))\ \forall k = 1, ..., p \Rightarrow \hat{Y}(:,j) = \sigma(W_1^T X(:,j) + b_1)$ where the activation σ is taken element-wise [1].

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- In matrix form, $\hat{Y} = \sigma(W_1^T X + B_1)$ where again, σ is element-wise and B_1 is a matrix whose each column is b_1 (see *repmat* function in Matlab)

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- Loss function: minimize the mean squared error between the prediction and the expected output: $\mathcal{L}(Y, \hat{Y}) = \frac{1}{n}\sum_{j=1}^{n} \| Y_j - \hat{Y}_j \|^2$ or, in matrix form, $\mathcal{L}(Y, \hat{Y}) = \frac{1}{n}\| Y - \hat{Y} \|_F^2$ (Rmq: a factor $\frac{1}{2}$ can be introduced (more convenient for derivation))

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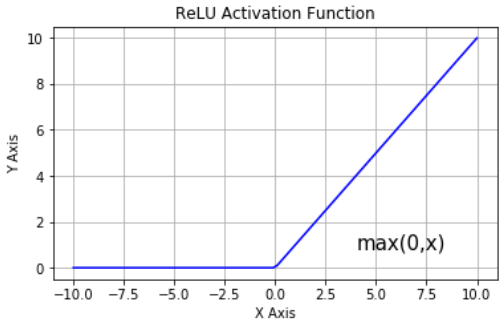

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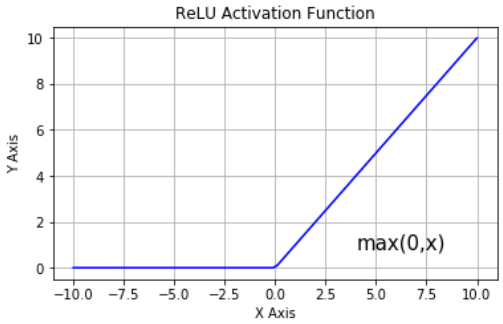

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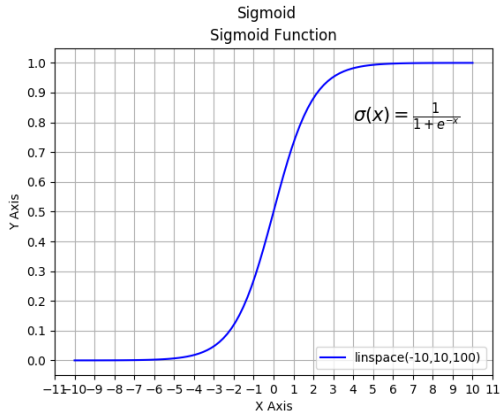

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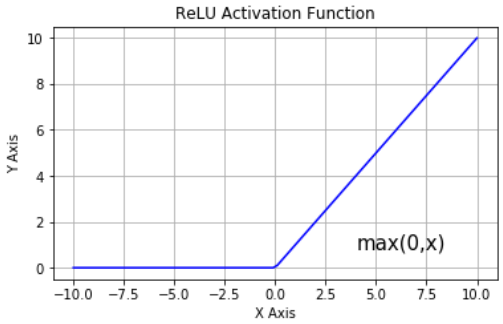

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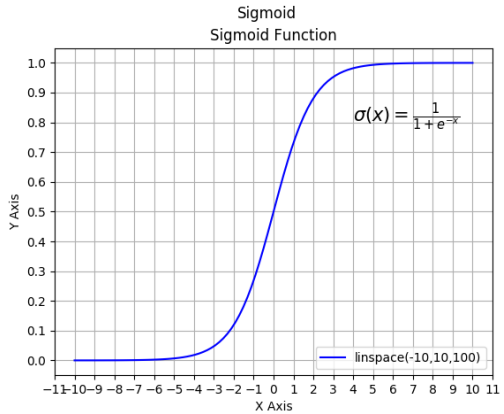

- Softmax, ELU (exponential linear unit), P-RELU (parametric RELU)

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Idea of the resolution schemes

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- Idea of resolution: alternatively optimize W_1 and b_1 until some stopping criterion is met (see last slide)

Algorithm Block coordinate descent

1: Initialize somehow W_1 and b_1
2: **for** $k = 0, \ldots$ **do**
3: Optimize W_1 while fixing b_1
4: Optimize b_1 while fixing W_1
5: **end for**

How to solve the optimization problem ?

- First-order (i.e. gradient-based) methods: second-order methods such as Newton's one are computationally too expensive (computing the Hessian is $\mathcal{O}(d^2)$ where d is the number of parameters to update) though they have a better convergence rate of the iterates (quadratic vs linear)

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Let's compute the gradient

- Recall of the loss function:
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- The same can be applied for the gradient w.r.t. B_1 (only the last factor changes)

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- $\frac{\partial \hat{Y}}{\partial Z} = \sigma'(Z)$ (simply apply the derivative of the sigmoid): should be applied element-wise

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Putting all together and taking care to the dimensions, we have

$\frac{\partial \mathcal{L}}{\partial W_1} = X\left\{\frac{1}{n}(\sigma(W_1^T X + B_1) - Y) \odot \sigma'(W_1^T X + B_1)\right\}^T$ where $\odot$ is an element-wise multiplication.

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- For B_1, remember that it comes from the bias vector b_1. So you will be updating b_1 and then using repmat to get B_1.

- Having said that, the derivative with respect to b_1 is $\frac{\partial \mathcal{L}}{\partial b_1} = \left(\frac{1}{n}(\sigma(W_1^T X + B_1) - Y) \odot \sigma'(W_1^T X + B_1) \right) \mathbf{1}$, where $\mathbf{1}$ is a vector of all ones.

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- Dummy backtracking line search (BLS):

Algorithm Basic Backtracking line search

Set initial step α_0 to a huge value (for example $\alpha_0 = 1$ or $\alpha_0 = 0.1\frac{||x_0||}{||\nabla f(x_0)||}$ to ensure that the decay term is the same order as x)
for $k = 0, \ldots$ **do**
  $\alpha_k = 1.5\alpha_k$ % Avoid vanishing learning rate
  $x_{k+1} = x_k - \alpha_k \nabla f(x_k)$
  while $f(x_{k+1}) > f(x_k)$ **do**
    $\alpha_k = \alpha_k/2$
    $x_{k+1} = x_k - \alpha_k \nabla f(x_k)$
  end while
  $\alpha_{k+1} = \alpha_k$
end for

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- Armijo backtracking line search is an alternative to that end.

Algorithm Armijo Backtracking line search

1: Let $a^{(0)} = a_{init}$ (e.g. $a_{init} = 1$), $k = 0$, $\beta \in (0, 1)$ and $\tau \in (0, 1)$
2: **while** $f(\mathbf{x}_k + a^{(k)} \nabla f(\mathbf{x}_k)) > f(\mathbf{x}_k) + a^{(k)} \beta \|\nabla f(\mathbf{x}_k)\|_2^2$ **do**
3: set $a^{(k+1)} = \tau a^{(k)}$
4: $k = k + 1$
5: **end while**

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- Gradient descent is simple but is still relatively costly: the computation involves all the data points
- Convergence is "slow"

$\Rightarrow$ We will see methods that solve these problems

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  - Stochastic gradient descent (SGD): compute the gradient with only one data point at the time
  - Mini-batch gradient descent (MBGD): compute the gradient with only some data points (=mini-batch) at the time (compromise between the expensiveness/"wholeness" of GD and the quickness/"stochasticness" of SGD)
- How to decrease the objective function faster ? Accelerated Gradient Descent (AGD): objective function decreases in $\mathcal{O}(\frac{1}{k^2})$ vs $\mathcal{O}(\frac{1}{k})$ for GD (in the convex case) ! (the best you can achieve with first-order methods)

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- Idea of the following methods: avoid computing the whole $\mathcal{L}$ and the whole gradient, just limit to a few data points (i.e. a few functions ℓ). In the following, $f_j = \ell(Y_j, \hat{Y}_j)$.

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- Some remarks:
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  - The step size can no longer be chosen through backtracking as the direction at each iteration may not lead to a decrease of the overall cost function (at most, you could do a BLS on a given f_{u_k} but it would be costly and without any guarantee) $\rightarrow$ fixed (small) step size or diminishing step size $\alpha_k = \frac{\beta}{\gamma + k}$ for some β, γ.

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2: Choose a MBGD size m_k and pick up randomly a subset B_k of size m_k in $\{1, \ldots, n\}$
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- Pay attention ! When you will compare the results of GD and SGD, *of course* one iteration of GD will decrease more the objective function than one iteration of SGD (though being $\sim n$ times more expensive). To be fair, you need to compare the results of one iteration of GD with the results of n iterations of SGD (and similarly for any mini-batch size)

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- Stochastic approximation with gradient aggregation (SAGA):
  - Rather than averaging the iterates, average the gradients: at iteration k, consider the mean of the stochastic gradients computed so far $g(k+1) = g(k) + \gamma(\nabla f_{u_k}(x_k) - g(k))$ with $g(0) = 0$ (set $\gamma = \frac{1}{k+1}$ if you want same weights for all the iterates, other if not)

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- Nesterov method: add momentum to the GD iterate **and in the gradient**

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- Replace gradient iteration by [3] $x_{k+1} = x_k - t_k \nabla f(x_k) + \beta_k (x_k - x_{k-1})$

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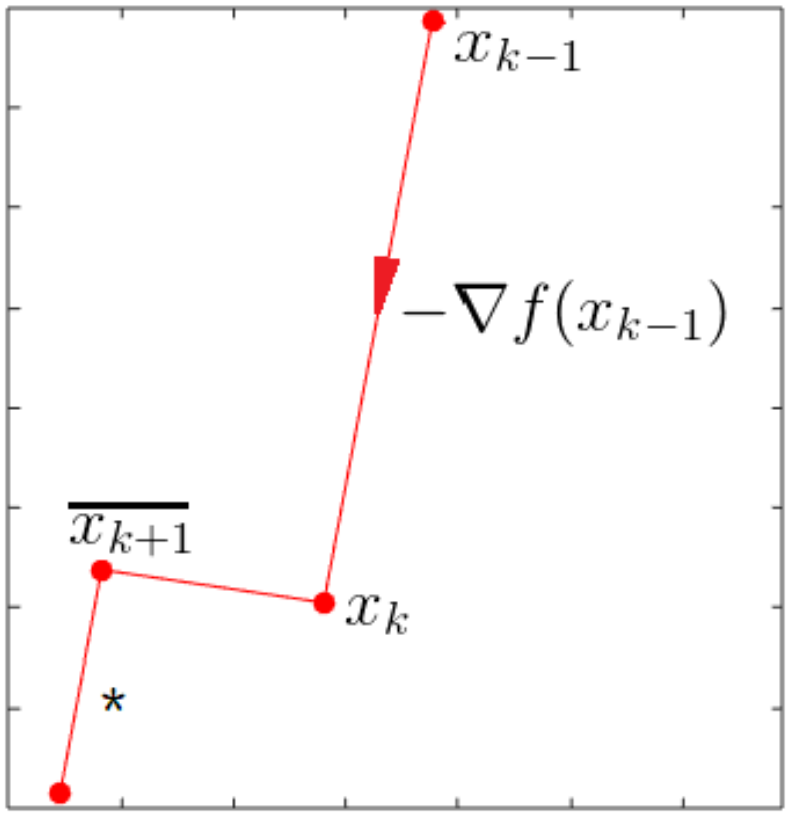

Figure taken from Andersen's notes `https://angms.science/notes.html`

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- Other way to see it: build a sequence y_k's such that
  $y_k = x_k + \beta_k(x_k - x_{k-1})$, we have $x_{k+1} = y_k - t_k \nabla f(y_k)$

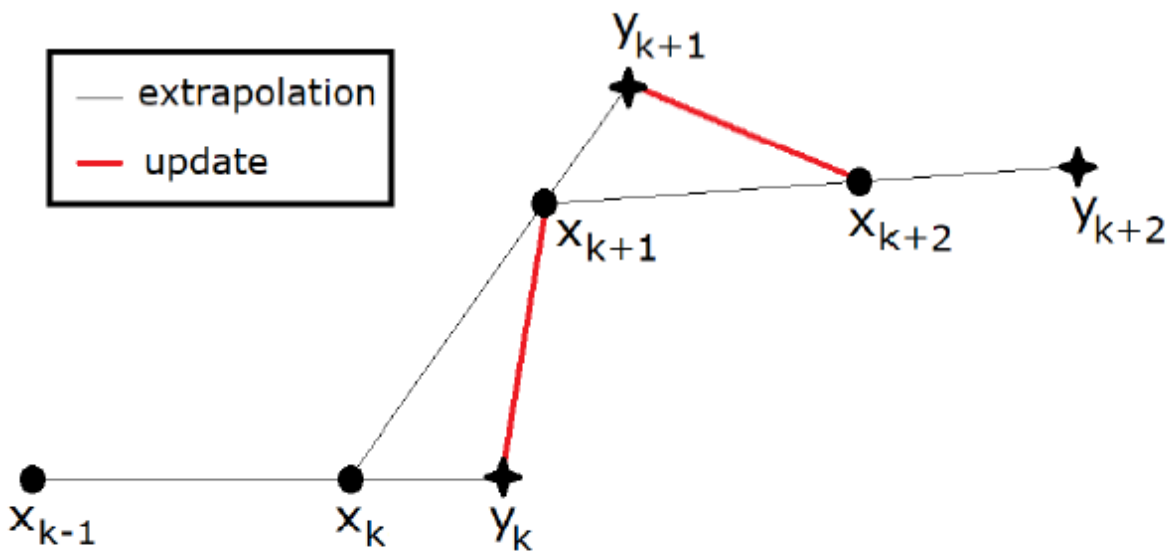

Figure taken from *ANG et GILLIS Accelerating nonnegative matrix factorization algorithms using extrapolation.*

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- Paul Tseng scheme: $\beta_k = \frac{k-1}{k+2}$

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- Restart procedure in the case of Nesterov's acceleration:

Algorithm Adaptive restart

Suppose you have the 2 first iterates x_0, x_1 (see above) and therefore y_1
for $k = 1, \ldots$ **do**
    Compute somehow β_{k+1}
    $x_{k+1} = y_k - t_k \nabla f(y_k)$
    $y_{k+1} = x_{k+1} + \beta_{k+1}(x_{k+1} - x_k)$
    if $f(x_{k+1}) > f(x_k)$ **then**
        $y_{k+1} = x_{k+1}$ % at the next iteration, we will have classical GD
    end if
end for

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- Typical accuracy measure: percentage of the well classified data

$$ACC = \frac{\sum_{j=1}^{n} \mathbb{1}(\hat{y\_test}_j, y\_test_j)}{n}$$

where $\mathbb{1}(a,b) = 1$ if $a = b$ and 0 otherwise (indicator function)

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