



Homework 2
Due 5pm, Wednesday, September 14, 2022

Problem 1: *Logistic regression via SGD.* Use SGD to solve the logistic regression optimization problem

$$\underset{\theta \in \mathbb{R}^p}{\text{minimize}} \quad \frac{1}{N} \sum_{i=1}^N \log(1 + \exp(-Y_i X_i^\top \theta)),$$

where $X_1, \dots, X_N \in \mathbb{R}^p$ and $Y_1, \dots, Y_N \in \{-1, 1\}$. Use the data

```
N, p = 30, 20
np.random.seed(0)
X = np.random.randn(N, p)
Y = 2*np.random.randint(2, size = N) - 1
```

where $X_1^\top, \dots, X_N^\top$ are the rows of X .

Problem 2: *SVM via SGD.* Use SGD to solve the non-differentiable SVM optimization problem

$$\underset{\theta \in \mathbb{R}^p}{\text{minimize}} \quad \frac{1}{N} \sum_{i=1}^N \max\{0, 1 - Y_i X_i^\top \theta\} + \lambda \|\theta\|^2,$$

where $X_1, \dots, X_N \in \mathbb{R}^p$, $Y_1, \dots, Y_N \in \{-1, 1\}$, and $\lambda = 0.1$. Use the data of Problem 1. Empirically, does the SGD ever encounter a point of non-differentiability?

Problem 3: Consider the data generated by the Python code

```
N=30
np.random.seed(0)
X = np.random.randn(2, N)
y = np.sign(X[0, :]**2 + X[1, :]**2 - 0.7)
theta = 0.5
c, s = np.cos(theta), np.sin(theta)
X = np.array([[c, -s], [s, c]]) @ X
X = X + np.array([[1], [1]])
```

Observe (by plotting) that the data is not linearly separable. Consider the transformation

$$\phi\left(\begin{bmatrix} u \\ v \end{bmatrix}\right) = \begin{bmatrix} 1 \\ u \\ u^2 \\ v \\ v^2 \end{bmatrix}.$$

Using the logistic regression or SVM, show that the data $\phi(X_1), \dots, \phi(X_N) \in \mathbb{R}^5$ with labels $Y_1, \dots, Y_N \in \{-1, +1\}$ is linearly separable. Visualize in \mathbb{R}^2 the data and the decision boundary.

Hint. Visualize the decision boundary given by

```
0 == w[0]+w[1]*x+w[2]*(x**2)+w[3]*y+w[4]*(y**2)
```

with the code

```
xx = np.linspace(-4, 4, 1024)
yy = np.linspace(-4, 4, 1024)
xx, yy = np.meshgrid(xx, yy)
Z = w[0] + (w[1] * xx + w[2] * xx**2) + (w[3] * yy + w[4] * yy**2)
plt.contour(xx, yy, Z, 0)
```

Remark. This is the basis of kernel methods.

Problem 4: *Nonnegativity of KL-divergence.* A set $C \subseteq \mathbb{R}^m$ is said to be convex if

$$x_1, x_2 \in C \Rightarrow \eta x_1 + (1 - \eta)x_2 \in C, \quad \forall \eta \in (0, 1).$$

A function $\varphi: C \rightarrow \mathbb{R}$ is said to be convex if $C \subseteq \mathbb{R}^m$ is convex and

$$\varphi(\eta x_1 + (1 - \eta)x_2) \leq \eta \varphi(x_1) + (1 - \eta)\varphi(x_2), \quad \forall x_1, x_2 \in C, \eta \in (0, 1).$$

Jensen's inequality [1] states that if $X \in C$ is a random variable and φ is convex, then

$$\varphi(\mathbb{E}[X]) \leq \mathbb{E}[\varphi(X)].$$

Use this to show that

$$D_{\text{KL}}(p||q) \geq 0$$

for any probability mass functions $p, q \in \mathbb{R}^n$.

Hint. First show that $-\log(x)$ is a convex function.

Problem 5: *Positivity of KL-divergence.* A function $\varphi: C \rightarrow \mathbb{R}$ is said to be *strictly* convex if $C \subseteq \mathbb{R}^m$ is convex and

$$\varphi(\eta x_1 + (1 - \eta)x_2) < \eta \varphi(x_1) + (1 - \eta)\varphi(x_2), \quad \forall x_1, x_2 \in C, x_1 \neq x_2, \eta \in (0, 1).$$

Strict Jensen's inequality states that if $X \in C$ is a non-constant random variable and φ is strictly convex, then

$$\varphi(\mathbb{E}[X]) < \mathbb{E}[\varphi(X)].$$

Use this to show that

$$D_{\text{KL}}(p||q) > 0$$

for any probability mass functions $p, q \in \mathbb{R}^n$ such that $p \neq q$.

Problem 6: Differentiating 2-layer neural networks. Consider the 2-layer neural network

$$f_{\theta}(x) = u^{\top} \sigma(ax + b) = \sum_{j=1}^p u_j \sigma(a_j x + b_j),$$

where $a, b, u \in \mathbb{R}^p$ and $\theta = (a_1, \dots, a_p, b_1, \dots, b_p, u_1, \dots, u_p) \in \mathbb{R}^{3p}$. Assume the univariate function $\sigma: \mathbb{R} \rightarrow \mathbb{R}$ is differentiable. The notation $\sigma(ax + b)$ means σ is applied elementwise to the vector in \mathbb{R}^p . Show that

$$\begin{aligned}\nabla_u f_{\theta}(x) &= \sigma(ax + b) \\ \nabla_b f_{\theta}(x) &= \sigma'(ax + b) \odot u = \text{diag}(\sigma'(ax + b))u \\ \nabla_a f_{\theta}(x) &= (\sigma'(ax + b) \odot u)x = \text{diag}(\sigma'(ax + b))ux,\end{aligned}$$

where $\sigma'(ax + b)$ means the univariate function σ' is applied elementwise to the vector $ax + b$, \odot denotes the element-wise product, and $\text{diag}(\cdot)$ denotes the diagonal matrix with the diagonal elements equal to the elements of the input vector.

Problem 7: SGD with 2-layer neural networks. Consider the univariate function

$$f_{\star}(x) = (x - 2) \cos(4x).$$

Let

$$f_{\theta}(x) = \sum_{j=1}^p u_j \sigma(a_j x + b_j),$$

be the same 2-layer neural network as in the previous problem. For this problem, use the sigmoid activation function, i.e., $\sigma(x) = (1 + e^{-x})^{-1}$. Given data X_i generated as IID unit Gaussians and corresponding labels $Y_i = f_{\star}(X_i)$ for $i = 1, \dots, N$, define loss functions

$$\mathcal{L}(\theta) = \frac{1}{N} \sum_{i=1}^N \ell_{\theta}(X_i, Y_i)$$

and

$$\ell_{\theta}(X, Y) = \frac{1}{2} (f_{\theta}(X) - Y)^2.$$

Consider the minimization problem

$$\underset{\theta \in \mathbb{R}^{3p}}{\text{minimize}} \quad \mathcal{L}(\theta).$$

Without using PyTorch (so using NumPy), implement

$$\begin{aligned}i(k) &\sim \text{Uniform}\{1, \dots, N\} \\ \theta^{k+1} &= \theta^k - \alpha \nabla_{\theta} \ell_{\theta}(X_{i(k)}, Y_{i(k)}).\end{aligned}$$

Use the parameters $K = 10000$, $\alpha = 0.007$, $N = 30$, and $p = 50$ and use independent initializations with distributions $a_j^0 \sim \mathcal{N}(0, 4^2)$, $b_j^0 \sim \mathcal{N}(0, 4^2)$, and $u_j^0 \sim \mathcal{N}(0, 0.05^2)$ for $j = 1, \dots, p$. (These parameters and initializations are implemented in the starter code `twolayerSGD.py`.) Plot the final trained function with $f_{\theta^K}(x)$ as a function of x . How does it compare with $f_{\star}(x)$?

Remark. In order to fit the nonlinear function f_{\star} , it is essential that we use the nonlinear activation function σ ; without it,

$$f_{\theta}(x) = \sum_{j=1}^p u_j (a_j x + b_j),$$

will be linear in x , and a linear function cannot approximate the nonlinear function $f_{\star}(x)$ well.

References

- [1] J. L. W. V. Jensen, Sur les fonctions convexes et les inégalités entre les valeurs moyennes, *Acta Mathematica*, 1906.