EE-559 – Deep learning

3.5. Gradient descent

François Fleuret
https://fleuret.org/ee559/
May 16, 2020
We saw that training consists of finding the model parameters minimizing an empirical risk or loss, for instance the mean-squared error (MSE)

\[ \mathcal{L}(w, b) = \frac{1}{N} \sum_n (f(x_n; w, b) - y_n)^2. \]

Other losses are more fitting for classification, certain regression problems, or density estimation. We will come back to this.
We saw that training consists of finding the model parameters minimizing an empirical risk or loss, for instance the mean-squared error (MSE)

$$\mathcal{L}(w, b) = \frac{1}{N} \sum_n (f(x_n; w, b) - y_n)^2.$$ 

Other losses are more fitting for classification, certain regression problems, or density estimation. We will come back to this.

So far we minimized the loss either with an analytic solution for the MSE, or with *ad hoc* recipes for the empirical error rate (*k*-NN and perceptron).
There is generally no \textit{ad hoc} method. The logistic regression for instance

\[ P_w(Y = 1 \mid X = x) = \sigma(w \cdot x + b), \quad \text{with} \quad \sigma(x) = \frac{1}{1 + e^{-x}} \]

leads to the loss

\[ \mathcal{L}(w, b) = -\sum_n \log \sigma(y_n(w \cdot x_n + b)) \]

which cannot be minimized analytically.
There is generally no *ad hoc* method. The logistic regression for instance

\[ P_w(Y = 1 \mid X = x) = \sigma(w \cdot x + b), \quad \text{with} \quad \sigma(x) = \frac{1}{1 + e^{-x}} \]

leads to the loss

\[ \mathcal{L}(w, b) = -\sum_n \log \sigma(y_n(w \cdot x_n + b)) \]

which cannot be minimized analytically.

The general minimization method used in such a case is the **gradient descent**.
Given a functional

\[ f : \mathbb{R}^D \to \mathbb{R} \]

\[ x \mapsto f(x_1, \ldots, x_D), \]

its gradient is the mapping

\[ \nabla f : \mathbb{R}^D \to \mathbb{R}^D \]

\[ x \mapsto \left( \frac{\partial f}{\partial x_1}(x), \ldots, \frac{\partial f}{\partial x_D}(x) \right). \]
To minimize a functional

\[ \mathcal{L} : \mathbb{R}^D \rightarrow \mathbb{R} \]

the gradient descent uses local linear information to iteratively move toward a (local) minimum.
To minimize a functional

\[ \mathcal{L} : \mathbb{R}^D \to \mathbb{R} \]

the gradient descent uses local linear information to iteratively move toward a (local) minimum.

For \( w_0 \in \mathbb{R}^D \), consider an approximation of \( \mathcal{L} \) around \( w_0 \)

\[ \tilde{\mathcal{L}}_{w_0}(w) = \mathcal{L}(w_0) + \nabla \mathcal{L}(w_0)^\top (w - w_0) + \frac{1}{2\eta} \|w - w_0\|^2. \]

Note that the chosen quadratic term does not depend on \( \mathcal{L} \).
To minimize a functional 

\[ \mathcal{L} : \mathbb{R}^D \rightarrow \mathbb{R} \]

the gradient descent uses local linear information to iteratively move toward a (local) minimum.

For \( w_0 \in \mathbb{R}^D \), consider an approximation of \( \mathcal{L} \) around \( w_0 \)

\[
\tilde{\mathcal{L}}_{w_0}(w) = \mathcal{L}(w_0) + \nabla \mathcal{L}(w_0)^\top (w - w_0) + \frac{1}{2\eta} \|w - w_0\|^2.
\]

Note that the chosen quadratic term does not depend on \( \mathcal{L} \).

We have

\[
\nabla \tilde{\mathcal{L}}_{w_0}(w) = \nabla \mathcal{L}(w_0) + \frac{1}{\eta} (w - w_0),
\]

which leads to

\[
\arg\min_w \tilde{\mathcal{L}}_{w_0}(w) = w_0 - \eta \nabla \mathcal{L}(w_0).
\]
The resulting iterative rule, which goes to the minimum of the approximation at the current location, takes the form:

\[ w_{t+1} = w_t - \eta \nabla \mathcal{L}(w_t), \]

which corresponds intuitively to “following the steepest descent”.

This [most of the time] eventually ends up in a local minimum, and the choices of \( w_0 \) and \( \eta \) are important.
\[ \eta = 0.125 \]
$\eta = 0.125$
\( \eta = 0.125 \)
\( \eta = 0.125 \)
\[ \eta = 0.125 \]
$\eta = 0.125$
$\eta = 0.125$
$\eta = 0.125$
\[ \eta = 0.125 \]
\[ \eta = 0.125 \]
$\eta = 0.125$

$\tilde{\mathcal{L}}$
$\eta = 0.125$
$\eta = 0.125$
\( \eta = 0.125 \)
$\eta = 0.125$
\( \eta = 0.125 \)
\[ \eta = 0.125 \]
$\eta = 0.125$
\[ \eta = 0.125 \]
\[ \eta = 0.125 \]
\[ \eta = 0.125 \]
\eta = 0.125
\[ \eta = 0.125 \]
\[ \eta = 0.125 \]
\( \eta = 0.5 \)

\( \mathcal{L} \)

\( \mathcal{L}^\sim \)

\( w_0 \)
\[ \eta = 0.5 \]
$\eta = 0.5$

Diagram showing two loss functions $\mathcal{L}$ and $\tilde{\mathcal{L}}$ with a point $w_2$.
$\eta = 0.5$
\[ \eta = 0.5 \]
\[ \eta = 0.5 \]
\[ \eta = 0.5 \]
$\eta = 0.5$
\( \eta = 0.5 \)
\( \eta = 0.5 \)
\( \eta = 0.5 \)
\[ \eta = 0.5 \]
We saw that the minimum of the logistic regression loss

\[ \mathcal{L}(w, b) = -\sum_n \log \sigma(y_n (w \cdot x_n + b)) \]

does not have an analytic form.
We can derive

\[
\frac{\partial \mathcal{L}}{\partial b} = - \sum_n y_n \sigma(-y_n(v \cdot x + b)),
\]

\forall d, \quad \frac{\partial \mathcal{L}}{\partial w_d} = - \sum_n x_{n,d} y_n \sigma(-y_n(v \cdot x + b)),
\]
We can derive

\[
\frac{\partial \mathcal{L}}{\partial b} = - \sum_n y_n \sigma(-y_n(w \cdot x_n + b)),
\]

\[
\forall d, \frac{\partial \mathcal{L}}{\partial w_d} = - \sum_n x_{n,d} y_n \sigma(-y_n(w \cdot x_n + b)),
\]

which can be implemented as

```python
def gradient(x, y, w, b):
    u = y * (-y * (x.mv(w) + b)).sigmoid()
    v = x * u.view(-1, 1)  # Broadcasting
    return - v.sum(0), - u.sum()
```
We can derive

\[
\frac{\partial L}{\partial b} = - \sum_n y_n \sigma\left(-y_n(w \cdot x_n + b)\right),
\]

\[
\forall d, \frac{\partial L}{\partial w_d} = - \sum_n x_{n,d} y_n \sigma\left(-y_n(w \cdot x_n + b)\right),
\]

which can be implemented as

```python
def gradient(x, y, w, b):
    u = y * (-y * (x.mv(w) + b)).sigmoid()
    v = x * u.view(-1, 1)  # Broadcasting
    return - v.sum(0), - u.sum()
```

and the gradient descent as

```python
w, b = torch.empty(x.size(1)).normal_(), 0
eta = 1e-1
for k in range(nb_iterations):
    print(k, loss(x, y, w, b))
    dw, db = gradient(x, y, w, b)
    w -= eta * dw
    b -= eta * db
```
With 100 training points and $\eta = 10^{-1}$.
With 100 training points and $\eta = 10^{-1}$.
With 100 training points and $\eta = 10^{-1}$.
With \textbf{100} training points and $\eta = 10^{-1}$. 

\[ n = 10^3 \]
With 100 training points and $\eta = 10^{-1}$. 

$n = 10^4$
With 100 training points and $\eta = 10^{-1}$. LDA.
The end