3.5. Gradient descent

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

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

leads to the loss

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

which cannot be minimized analytically.
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The general minimization method used in such a case is the **gradient descent**.
Given a functional

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

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

its gradient is the mapping

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

\[ x \mapsto \left( \frac{\partial f}{\partial x_1}(x), \ldots, \frac{\partial f}{\partial x_D}(x) \right). \]
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.
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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 \( \mathcal{L} \).
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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.
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Diagram showing the loss functions \( \mathcal{L} \) and \( \tilde{\mathcal{L}} \) with a point at \( w_1 \).
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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

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

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

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

and the gradient descent as

```
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
```
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```
With 100 training points and $\eta = 10^{-1}$.
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$n = 10^3$
With 100 training points and $\eta = 10^{-1}$.
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The end