Deep learning

5.2. Stochastic gradient descent

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To minimize a loss of the form

$$\mathcal{L}(w) = \sum_{n=1}^{N} \ell(f(x_n; w), y_n)$$

the standard gradient-descent algorithm update has the form

$$w_{t+1} = w_t - \eta \nabla \mathcal{L}(w_t).$$
A straight-forward implementation would be

```python
for e in range(nb_epochs):
    output = model(train_input)
    loss = criterion(output, train_target)

    model.zero_grad()
    loss.backward()
    with torch.no_grad():
        for p in model.parameters(): p -= eta * p.grad
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However, the memory footprint is proportional to the full set size. This can be mitigated by summing the gradient through “mini-batches”:

```python
for e in range(nb_epochs):
    model.zero_grad()

    for b in range(0, train_input.size(0), batch_size):
        output = model(train_input[b:b+batch_size])
        loss = criterion(output, train_target[b:b+batch_size])
        loss.backward()

    with torch.no_grad():
        for p in model.parameters(): p -= eta * p.grad
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- It takes time to compute (more exactly all our time!).
- It is an empirical estimation of a hidden quantity, and any partial sum is also an unbiased estimate, although of greater variance.
- It is computed incrementally

\[ \nabla \mathcal{L}(w_t) = \sum_{n=1}^{N} \nabla \ell_n(w_t), \]

and when we compute \( \nabla \ell_n \), we have already computed \( \nabla \ell_1, \ldots, \nabla \ell_{n-1} \), and we could have a better estimate of \( w^* \) than \( w_t \).
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So instead of summing over all the samples and moving by $\eta$, we can visit only $M = N/K$ samples and move by $K\eta$, which would cut the computation by $K$.

Although this is an ideal case, there is redundancy in practice that results in similar behaviors.
The **stochastic gradient descent** consists of updating the parameters $w_t$ after every sample

$$w_{t+1} = w_t - \eta \nabla \ell_{n(t)}(w_t).$$

However this does not benefit from the speed-up of batch-processing.

The mini-batch stochastic gradient descent is the standard procedure for deep learning. It consists of visiting the samples in "mini-batches", each of a few tens of samples, and updating the parameters each time.
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The stochastic behavior of this procedure helps evade local minima.
So our exact gradient descent with mini-batches

for $e$ in range(nb_epochs):
    model.zero_grad()

    for $b$ in range(0, train_input.size(0), batch_size):
        output = model(train_input[b:b+batch_size])
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    with torch.no_grad():
        for $p$ in model.parameters():
            $p -= \eta \times p.grad$
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can be modified into the mini-batch stochastic gradient descent as follows:

```python
for e in range(nb_epochs):
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```
Mini-batch size and loss reduction (MNIST)

Best train loss vs. number of samples seen for different mini-batch sizes:
- 60k
- 10k
- 1k
- 100
- 10
- 1

The graph shows the best train loss over the number of samples seen for each mini-batch size.
Limitation of the gradient descent
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Some optimization methods leverage higher-order moments, in particular second order to use a more accurate local model of the functional to optimize.
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Deep-learning generally relies on a smarter use of the gradient, using statistics over its past values to make a “smarter step” with the current one.
Momentum and moment estimation
The “vanilla” mini-batch stochastic gradient descent (SGD) consists of

\[ w_{t+1} = w_t - \eta g_t, \]

where

\[ g_t = \sum_{b=1}^{B} \nabla \ell_{n(t,b)}(w_t) \]

is the gradient summed over a mini-batch.
The first improvement is the use of a “momentum” to add inertia in the choice of the step direction

\[ u_t = \gamma u_{t-1} + \eta g_t \]
\[ w_{t+1} = w_t - u_t. \]

(Rumelhart et al., 1986)

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- it accelerates if the gradient does not change much:

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(u = \gamma u + \eta g) \Rightarrow \left( u = \frac{\eta}{1 - \gamma} g \right),
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  \[ (u = \gamma u + \eta g) \Rightarrow \left( u = \frac{\eta}{1 - \gamma} g \right), \]
- it dampens oscillations in narrow valleys.
$\eta = 5.0 \times 10^{-2}, \gamma = 0$
\[ \eta = 5.0 \times 10^{-2}, \gamma = 0.5 \]
Another class of methods exploits the statistics over the previous steps to compensate for the anisotropy of the mapping.

The Adam algorithm uses moving averages of each coordinate and its square to rescale each coordinate separately.

\[
\begin{align*}
    m_t &= \beta_1 m_{t-1} + (1 - \beta_1) g_t \\
    \hat{m}_t &= m_t^1 - \beta_1 t \\
    v_t &= \beta_2 v_{t-1} + (1 - \beta_2) g_t^2 \\
    \hat{v}_t &= v_t^1 - \beta_2 \\
    w_{t+1} &= w_t - \eta \sqrt{\hat{v}_t} + \epsilon \hat{m}_t
\end{align*}
\] (Kingma and Ba, 2014)

This can be seen as a combination of momentum, with $\hat{m}_t$, and a per-coordinate re-scaling with $\hat{v}_t$. 

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The update rule is, **on each coordinate separately**

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\begin{align*}
    m_t &= \beta_1 m_{t-1} + (1 - \beta_1) g_t \\
    \hat{m}_t &= \frac{m_t}{1 - \beta_1^t} \\
    v_t &= \beta_2 v_{t-1} + (1 - \beta_2) g_t^2 \\
    \hat{v}_t &= \frac{v_t}{1 - \beta_2^t} \\
    w_{t+1} &= w_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t
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(Kingma and Ba, 2014)

This can be seen as a combination of momentum, with \( \hat{m}_t \), and a per-coordinate re-scaling with \( \hat{v}_t \).
$\eta = 5.0 \times 10^{-2}$
Adam, $\beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 1e^{-8}, \eta = 1.0e^{-1}$
These two core strategies have been used in multiple incarnations:

- Nesterov’s accelerated gradient,
- Adagrad,
- Adadelta,
- RMSprop,
- AdaMax,
- Nadam ...
The end
References
