Deep learning

5.2. Stochastic gradient descent

François Fleuret

https://fleuret.org/dlc/
To minimize a loss of the form

\[ \mathcal{L}(w) = \sum_{n=1}^{N} \ell_n(f(x_n; w), y_n) \]

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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While it makes sense in principle to compute the gradient exactly, in practice:

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\nabla \mathcal{L}(w_t) = \sum_{n=1}^{N} \nabla l_n(w_t),
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and when we compute \(\nabla l_n\), we have already computed \(\nabla l_1, \ldots, \nabla l_{n-1}\), and we could have a better estimate of \(w^*\) than \(w_t\).
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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

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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.
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**The stochastic behavior of this procedure helps evade local minima.**
So our exact gradient descent with mini-batches

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can be modified into the mini-batch stochastic gradient descent as follows:

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Limitation of the gradient descent
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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 can “go through” local barriers,
- it accelerates if the gradient does not change much:

\[ (u = \gamma u + \eta g) \Rightarrow \left( u = \frac{\eta}{1 - \gamma} g \right), \]
- it dampens oscillations in narrow valleys.
\[ \eta = 5.0e^{-2}, \gamma = 0 \]
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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.

\[
\hat{m}_t = \beta_1 m_{t-1} + (1 - \beta_1) g_t \\
\hat{v}_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t^2 \\
w_{t+1} = w_t - \eta \sqrt{\hat{v}_t} + \epsilon \hat{m}_t
\]

(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

\[
\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
\end{align*}
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This can be seen as a combination of momentum, with \(\hat{m}_t\), and a per-coordinate re-scaling with \(\hat{v}_t\).
$\eta = 5.0e - 2$
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 ...

There is unfortunately no best general optimizer. Although a default choice such as Adam with default parameter values usually gives good results, it can be beneficial to test alternatives and optimize meta-parameters.
The end
References
