EE-559 – Deep learning

5.2. Stochastic gradient descent

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So far, to minimize a loss of the form

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

we have considered the gradient-descent algorithm, of the form

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

A straight-forward implementation would be

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

    model.zero_grad()
    loss.backward()
    with torch.no_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”:

```
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])
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- It takes time to compute (more exactly **all our time!**).
- It is an empirical estimation of an hidden quantity, and any partial sum is also an unbiased estimate, although of greater variance.
- It is computed incrementally

$$\nabla \mathscr{L}(w_t) = \sum_{n=1}^{N} \nabla \ell_n(w_t),$$

and when we compute ℓ_n, we have already computed $\ell_1, \dots, \ell_{n-1}$, and we could have a better estimate of w^* than w_t.

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&= \sum_{k=1}^{K} \sum_{m=1}^{M} \ell(f(x_m; w), y_m) \\
&= K \sum_{m=1}^{M} \ell(f(x_m; w), y_m).
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So instead of summing over all the samples and moving by η, 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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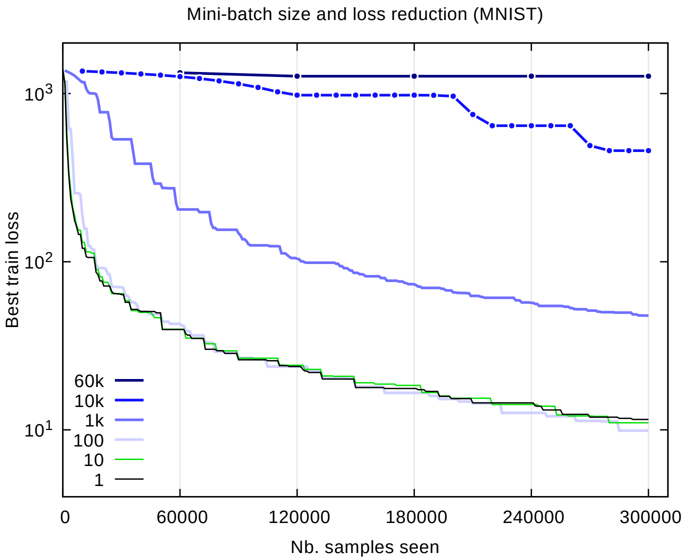

Mini-batch size and loss reduction (MNIST)
Best train loss
10^3
10^2
10^1
60k
10k
1k
100
10
1
0
60000
120000
180000
240000
300000
Nb. samples seen

Limitation of the gradient descent

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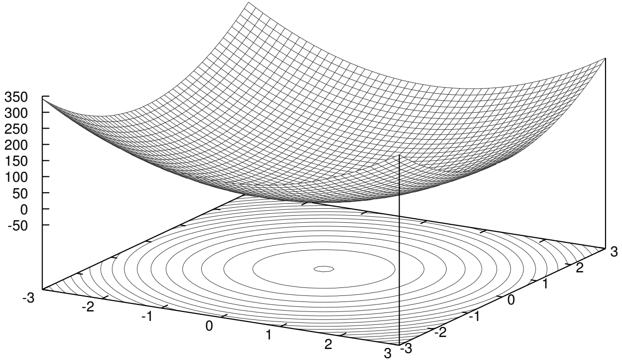

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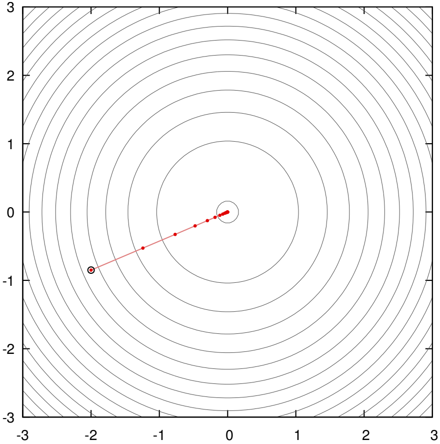
$\eta = 1.0e - 2$



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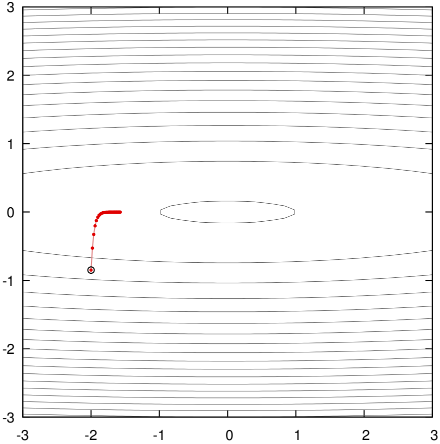

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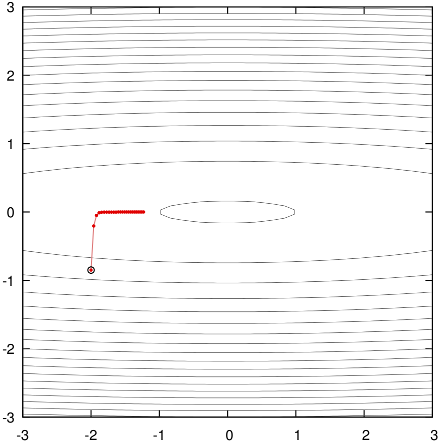

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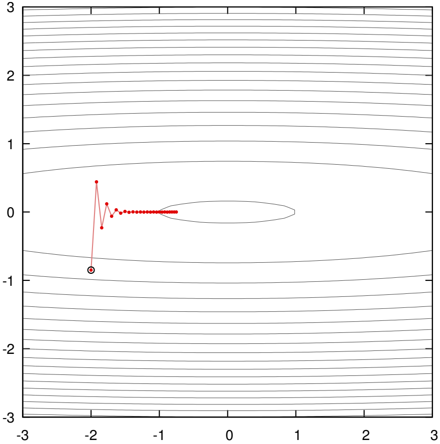

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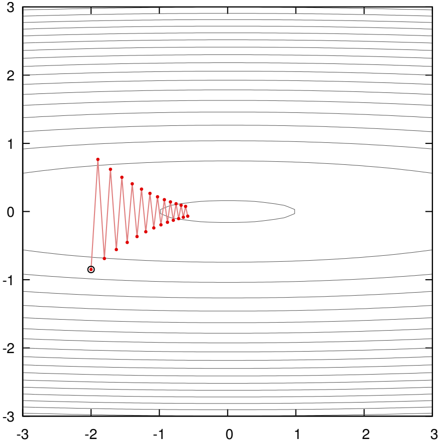

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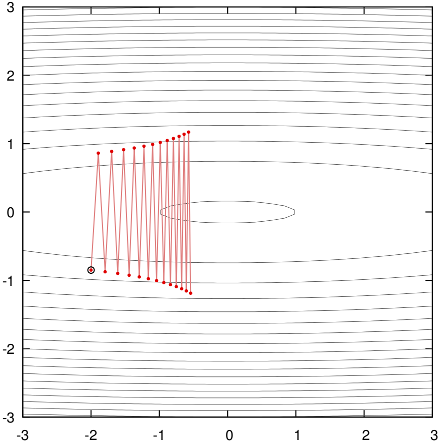

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Deep-learning generally relies on a smarter use of the gradient, using statistics over its past values to make a “smarter step” with the current one.

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

$$
\begin{aligned}
u_t &= \gamma u_{t-1} + \eta g_t \\
w_{t+1} &= w_t - u_t .
\end{aligned}
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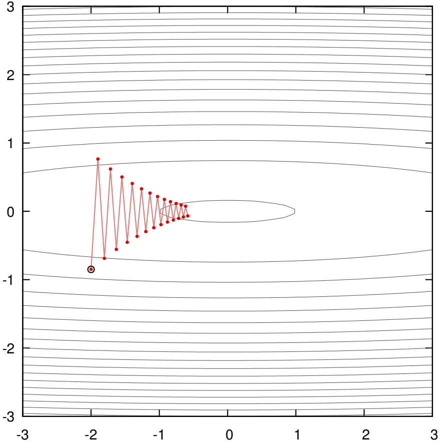
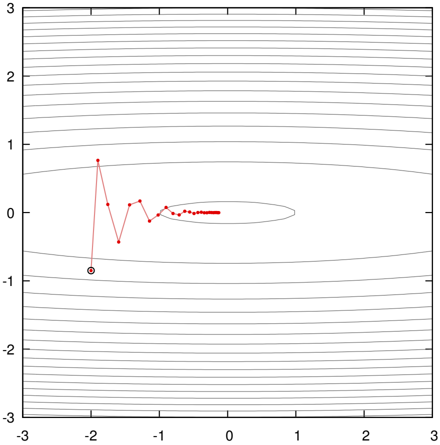
$$

- it dampens oscillations in narrow valleys.

$$\eta = 5.0e - 2, \gamma = 0$$



$$\eta = 5.0e - 2, \gamma = 0.5$$



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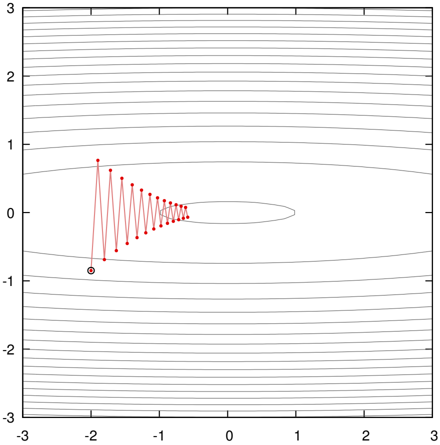
The update rule is, **on each coordinate separately**

$$
\begin{aligned}
m_t &= \beta_1 m_{t-1} + (1-\beta_1) g_t \\
\hat{m}_t &= \frac{m_t}{1-\beta_1} \\
v_t &= \beta_2 v_{t-1} + (1-\beta_2) g_t^2 \\
\hat{v}_t &= \frac{v_t}{1-\beta_2} \\
w_{t+1} &= w_t - \frac{\eta}{\sqrt{\hat{v}_t} + \epsilon} \hat{m}_t
\end{aligned}
$$

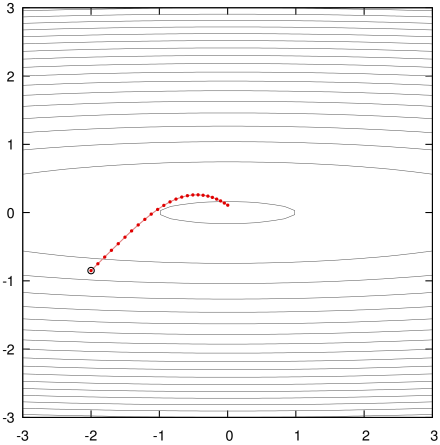
(Kingma and Ba, 2014)

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

$\eta = 5.0e - 2$



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 ...

The end

References

D. Kingma and J. Ba. Adam: A method for stochastic optimization. *CoRR*, abs/1412.6980, 2014.

D. E. Rumelhart, G. E. Hinton, and R. J. Williams. Learning representations by back-propagating errors. *Nature*, 323(9):533–536, 1986.