Deep learning hands-on

Lecture 2 Optimising feed-forward neural networks

Ole Winther

Dept for Applied Mathematics and Computer Science
Technical University of Denmark (DTU)

August 17, 2018

Objectives of lecture

- Feed-forward neural network (FFNN) training with
- error back-propagation
- We only need to understand the principles
- Autograd - automated differentiation handles the derivation for us!

Training criterion

Find parameters

$$\theta = \{\mathbf{W}^{(l)}, \mathbf{b}^{(l)}\}_{l=1}^{L}$$

that minimize expected negative log-likelihood:

$$C = -\sum_{i=1}^{n} \log P(\mathbf{y}_i|\mathbf{x}_i, \theta) \ .$$

Learning becomes optimization.

Say we have a true distribution $P(\mathbf{y} \mid \mathbf{x})$ and we would like to find a model $Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta})$ that matches P. Let us study how maximizing expected negative log-likelihood $C = \mathbb{E}_P[-\log Q]$ works as a learning criterion.

$$\boldsymbol{\theta}^* = \operatorname*{argmin}_{\theta} C(\theta) = \operatorname*{argmin}_{\theta} \mathbb{E}_{P(\mathbf{y}|\mathbf{x})}[-\log Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta})] \ .$$

Let us assume that there is a $\boldsymbol{\theta}^*$ for which $Q(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta}^*) = P(\mathbf{y}|\mathbf{x})$. We can note that the gradient at $\boldsymbol{\theta}^*$

$$\begin{aligned}
&\frac{\partial}{\partial \boldsymbol{\theta}} \mathbb{E}_{P(\mathbf{y}|\mathbf{x})}[\log Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}^*)] \\
&= \mathbb{E}_{P(\mathbf{y}|\mathbf{x})}\left[\frac{\partial}{\partial \boldsymbol{\theta}} \log Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}^*)\right] \\
&= \int P(\mathbf{y} \mid \mathbf{x}) \frac{\frac{\partial}{\partial \boldsymbol{\theta}} Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}^*)}{Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}^*)} \mathrm{d}\mathbf{y} \\
&= \int \frac{\partial}{\partial \boldsymbol{\theta}} Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}^*) \mathrm{d}\mathbf{y} \\
&= \frac{\partial}{\partial \boldsymbol{\theta}} \int Q(\mathbf{y} \mid \mathbf{x}, \boldsymbol{\theta}^*) \mathrm{d}\mathbf{y} = \frac{\partial}{\partial \theta} 1 = 0
\end{aligned}$$

becomes zero, that is, the learning converges when $Q = P$. Therefore the expected log-likelihood is a reasonable training criterion.

Classification - one hot encoding and cross-entropy

- MNIST, output labels: $0, 1, \ldots, 9$.
- Convenient to use a sparse one hot encoding:

$$0 \to \mathbf{y} = (1,0,0,0,0,0,0,0,0,0)^T$$
$$1 \to \mathbf{y} = (0,1,0,0,0,0,0,0,0,0)^T$$
$$2 \to \mathbf{y} = (0,0,1,0,0,0,0,0,0,0)^T$$
$$\ldots.$$
$$9 \to \mathbf{y} = (0,0,0,0,0,0,0,0,0,1)^T$$

- Output

$$P(\mathbf{y}|\mathbf{x},\theta) = \mathbf{h}^{(3)} = \text{softmax}(\mathbf{W}^{(3)}\mathbf{h}^{(2)} + \mathbf{b}^{(3)})$$

  interpreted as class(-conditional) probability.
- Cross-entropy cost - sum over data and label

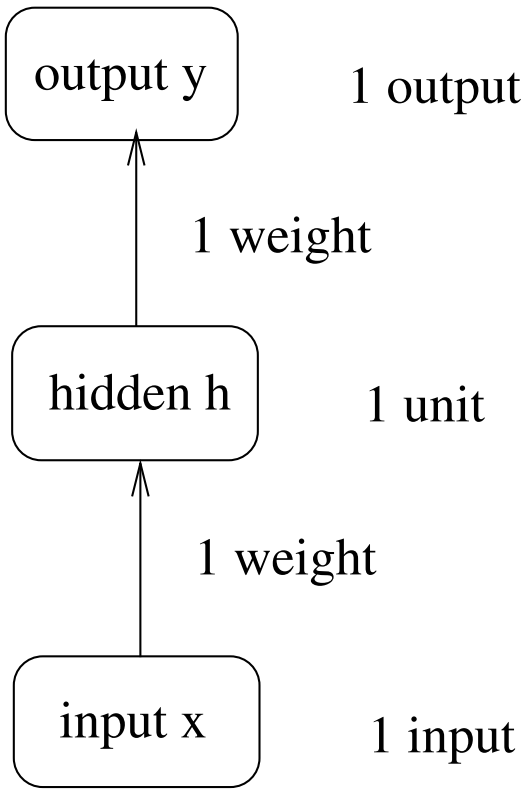
$$C = -\sum_{n=1}^{N}\sum_{k=1}^{K} y_{nk} \log h_{nk}^{(3)}$$

Gradient descent

- Simple algorithm for minimizing the training criterion C.
- Gradient $\mathbf{g} = \nabla_{\boldsymbol{\theta}} C(\theta) = \begin{pmatrix} \frac{\partial C}{\partial \theta_1} \\ \vdots \\ \frac{\partial C}{\partial \theta_n} \end{pmatrix}$
- Iterate $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta_k \mathbf{g}_k$
- Notation: iteration k, stepsize (or learning rate) η_k

Backpropagation (Linnainmaa, 1970)

Computing gradients in a network.



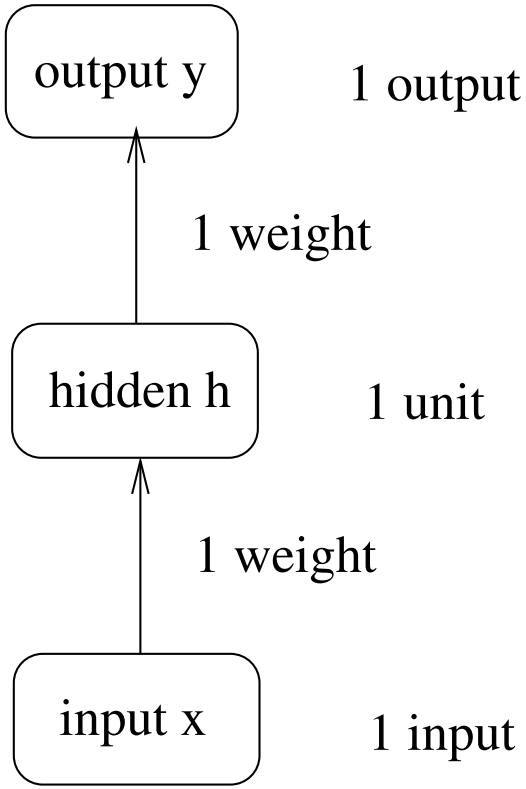
- First with scalars. Use chain rule:

$$\frac{\partial C}{\partial w_2} = \frac{\partial C}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial w_2}$$

$$\frac{\partial C}{\partial w_1} = \frac{\partial C}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial w_1}$$

- Chain rule: $\frac{\partial h^{(2)}}{\partial x} = \frac{\partial h^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial x}$

Tiny example I



- Chain rule:

$$\frac{\partial C}{\partial w_2} = \frac{\partial C}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial w_2}$$

$$\frac{\partial C}{\partial w_1} = \frac{\partial C}{\partial h^{(2)}} \frac{\partial h^{(2)}}{\partial h^{(1)}} \frac{\partial h^{(1)}}{\partial w_1}$$

- Example: $C = \left(y - h^{(2)}\right)^2$

$$h^{(2)} = w_2 h^{(1)}$$

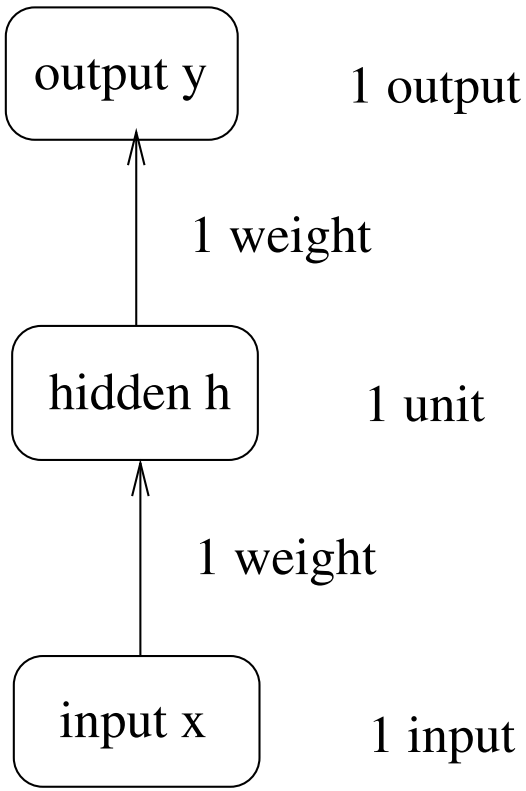
$$h^{(1)} = \text{relu}(w_1 x) = \max(0, w_1 x)$$

- Derivatives:

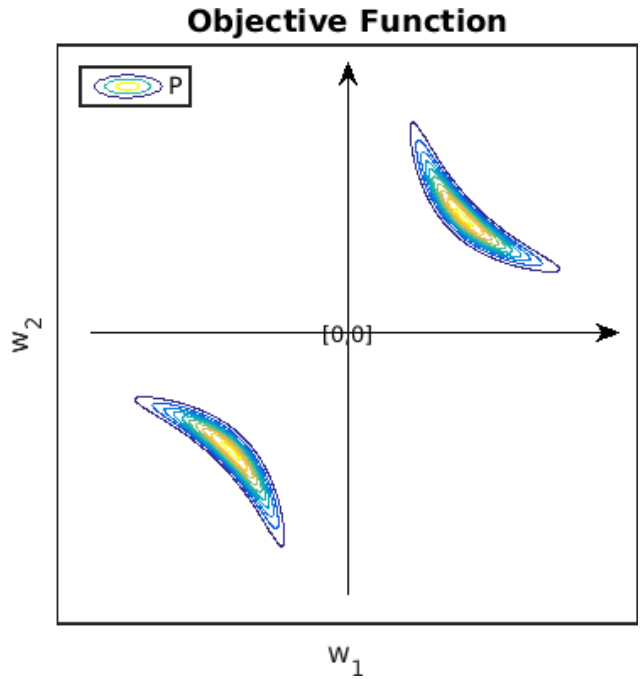
$$\frac{\partial C}{\partial w_2} = -(y - h^{(2)})\, h^{(1)}$$

$$\frac{\partial C}{\partial w_1} = -(y - h^{(2)})\, w_2\, 1(w_1 h^{(1)} > 0) x$$

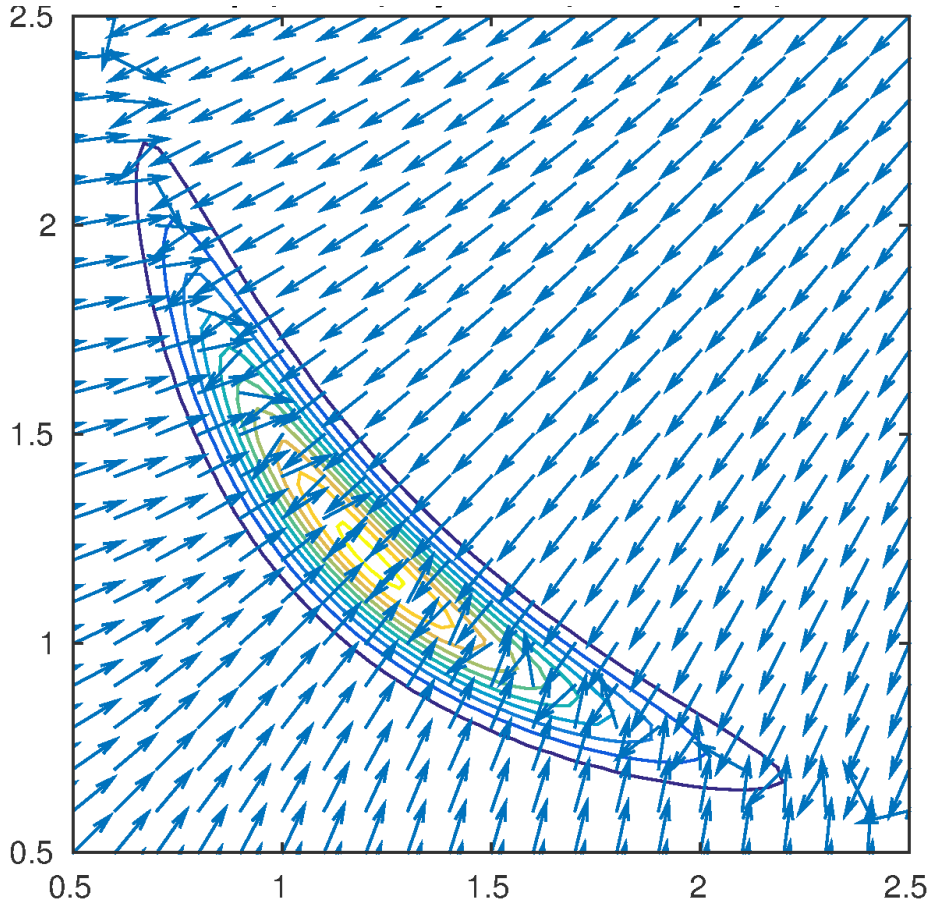
Tiny Example II



- $y \sim \mathcal{N}(w_2 h, 1)$
- $h = w_1 x$
- "Data set": $\{x = 1, y = 1.5\}$
- Some weight decay.
- $C = (w_1 w_2 - 1.5)^2 + 0.04(w_1^2 + w_2^2)$

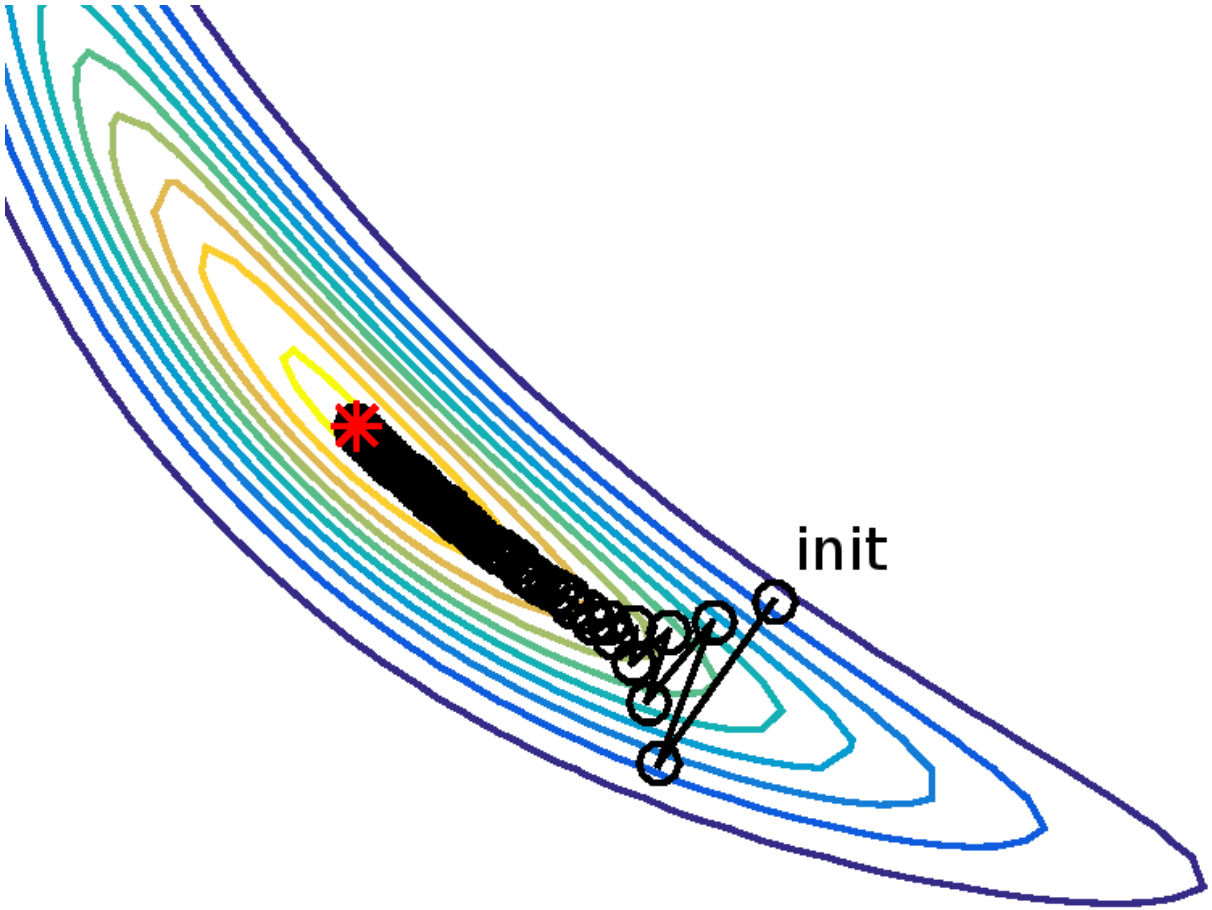


Gradient $\mathbf{g} = \nabla_\theta C(\theta) = \begin{pmatrix} \frac{\partial C}{\partial \theta_1} \\ \vdots \\ \frac{\partial C}{\partial \theta_n} \end{pmatrix}$



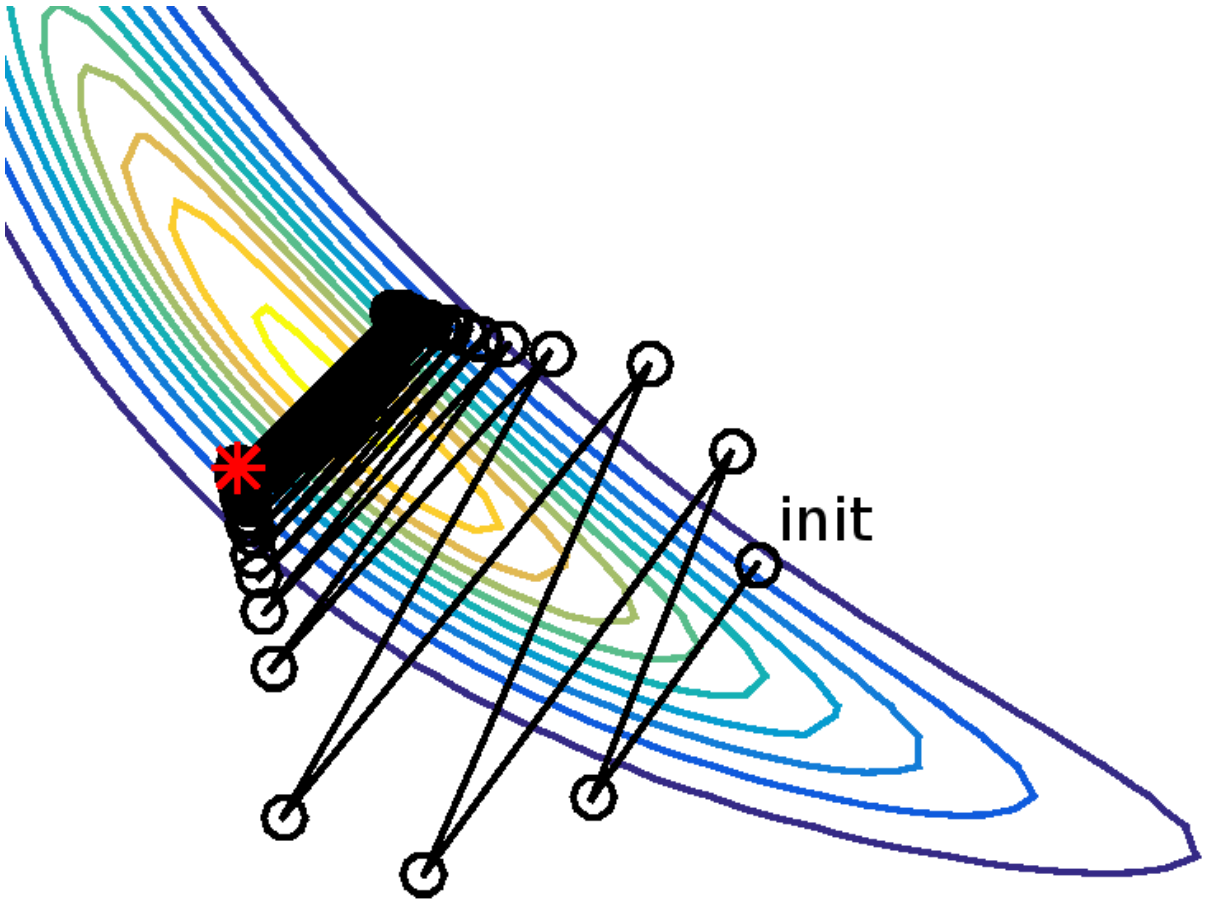
Gradient descent, $\eta_k = 0.25$ ($\rightarrow$ too slow)

$\theta_{k+1} = \theta_k - \eta_k \mathbf{g}_k$, iteration k, stepsize (or learning rate) η_k



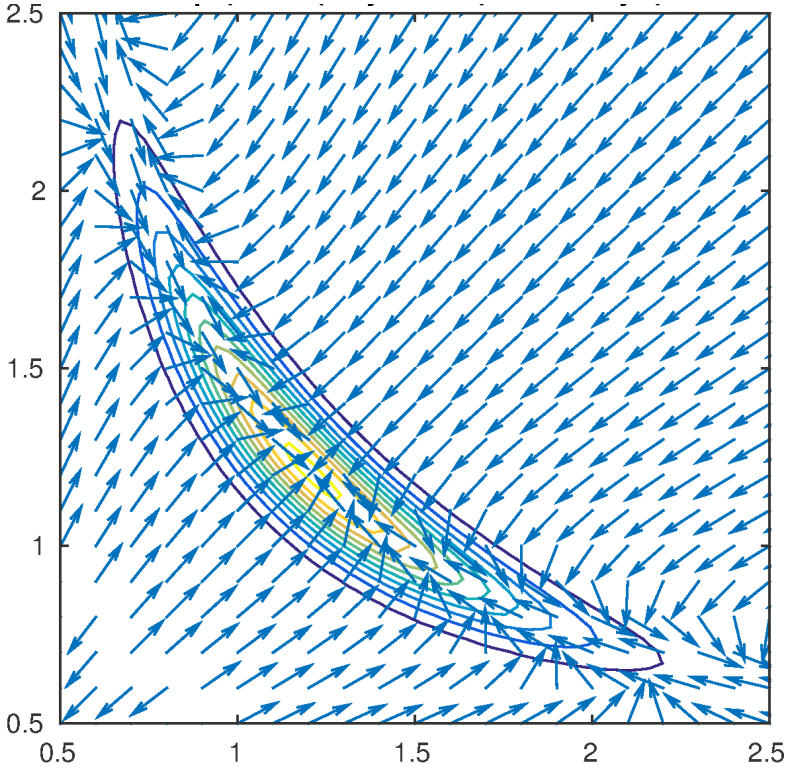
Gradient descent, $\eta_k = 0.35$ ($\rightarrow$ oscillates)

$$\theta_{k+1} = \theta_k - \eta_k \mathbf{g}_k$$



Newton's method, too complex

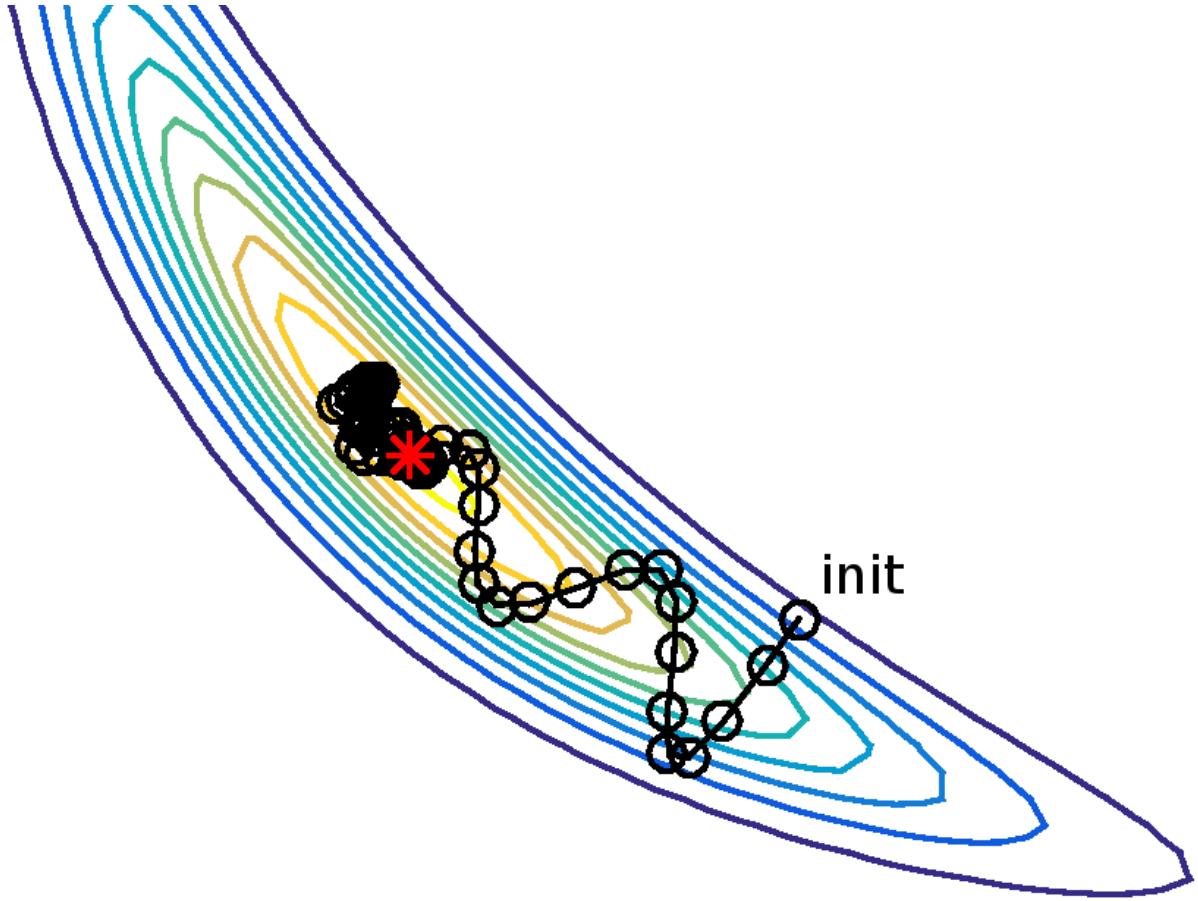
$$\theta_{k+1} = \theta_k - \mathbf{H}_k^{-1}\mathbf{g}_k, \quad \mathbf{H} = \begin{pmatrix} \frac{\partial^2 C}{\partial\theta_1\partial\theta_1} & \cdots & \frac{\partial^2 C}{\partial\theta_1\partial\theta_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 C}{\partial\theta_n\partial\theta_1} & \cdots & \frac{\partial^2 C}{\partial\theta_n\partial\theta_n} \end{pmatrix}$$



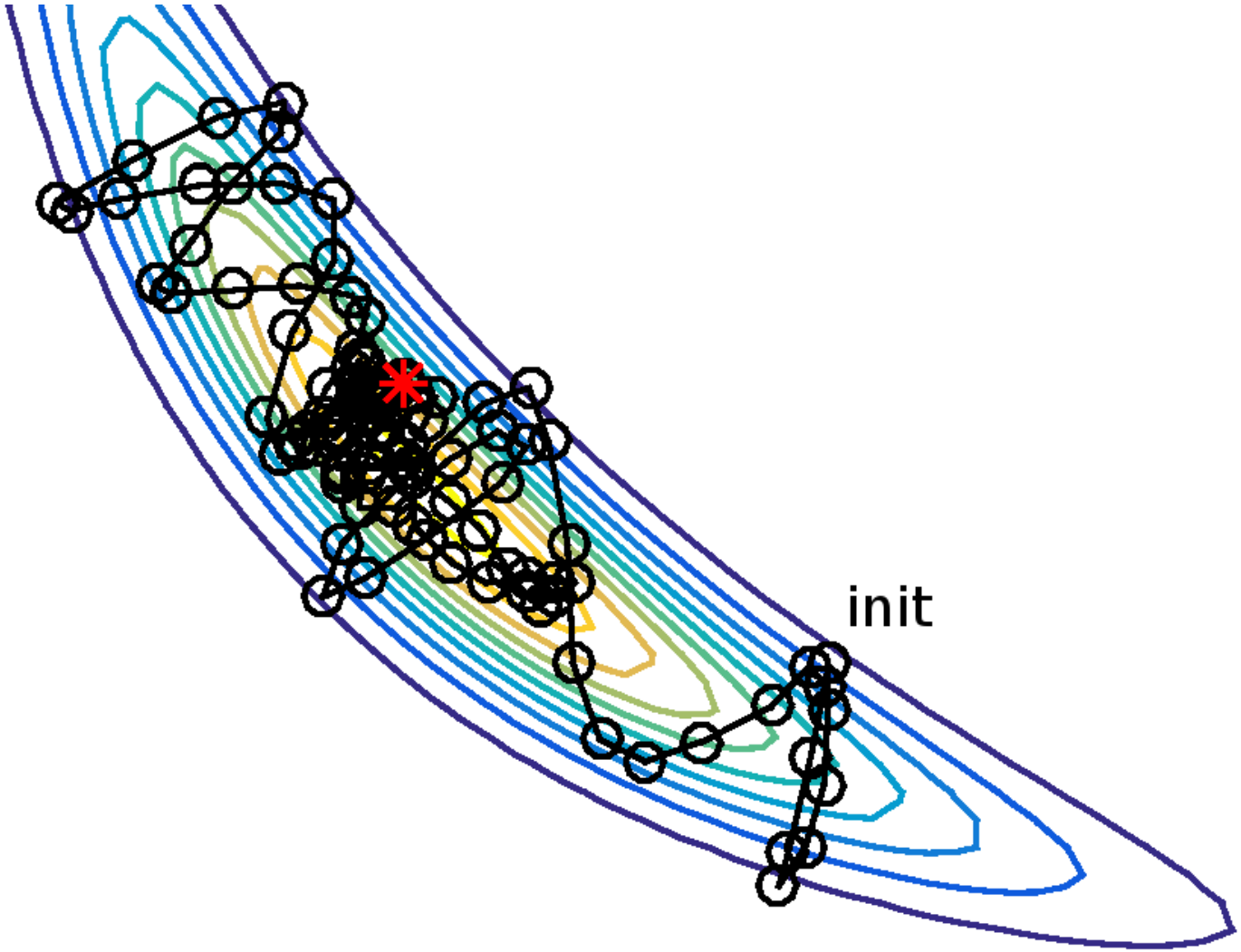
- Less oscillations.
- Points to the wrong direction in places (solvable).
- Computational complexity: #params^3 (prohibitive).
- There are approximations, but not very popular.

Momentum method (Polyak, 1964)

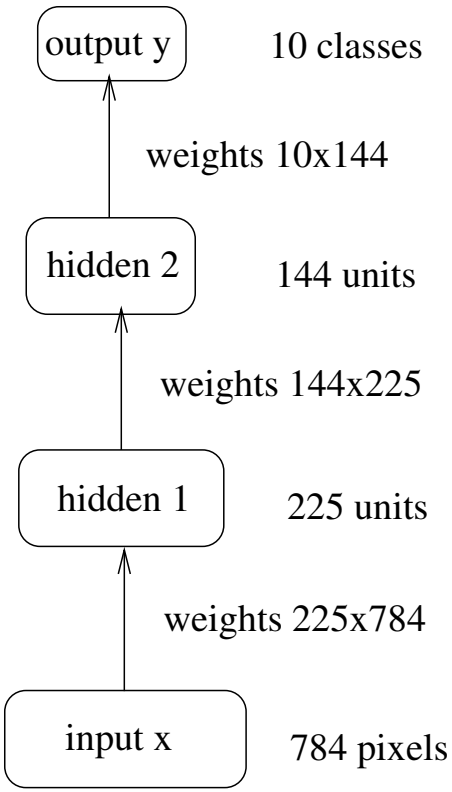
$$\mathbf{m}_{k+1} = \alpha \mathbf{m}_k - \eta_k \mathbf{g}_k$$
$$\theta_{k+1} = \theta_k + \mathbf{m}_{k+1}$$



Momentum method with noisy gradient



Backpropagation



- Multi-dimensional:

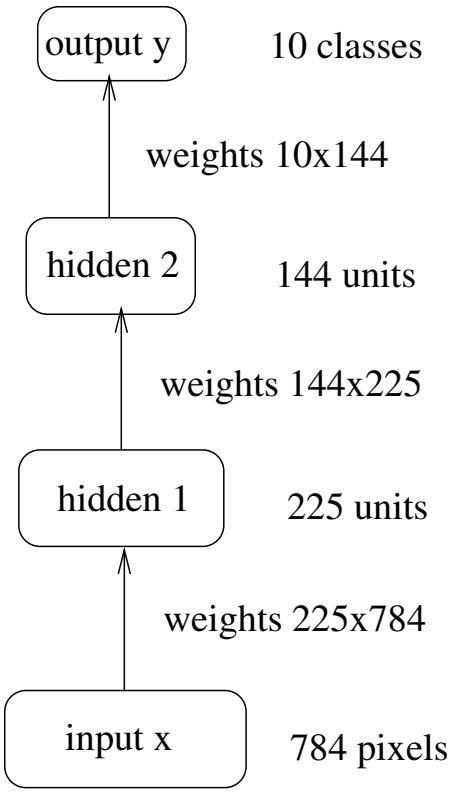
$$\frac{\partial C}{\partial W_{ij}^{(3)}} = \frac{\partial C}{\partial h_i^{(3)}} \frac{\partial h_i^{(3)}}{\partial W_{ij}^{(3)}}$$

$$\frac{\partial C}{\partial W_{jk}^{(2)}} = \sum_i \frac{\partial C}{\partial h_i^{(3)}} \frac{\partial h_i^{(3)}}{\partial h_j^{(2)}} \frac{\partial h_j^{(2)}}{\partial W_{jk}^{(2)}}$$

$$\frac{\partial C}{\partial W_{kl}^{(1)}} = \sum_j \sum_i \frac{\partial C}{\partial h_i^{(3)}} \frac{\partial h_i^{(3)}}{\partial h_j^{(2)}} \frac{\partial h_j^{(2)}}{\partial h_k^{(1)}} \frac{\partial h_k^{(1)}}{\partial W_{kl}^{(1)}}$$

- *How many paths - for two hidden layers*
- *as a function of depth?*
- Modern software (autograd) handles this derivation!

Backpropagation



- Multi-dimensional:

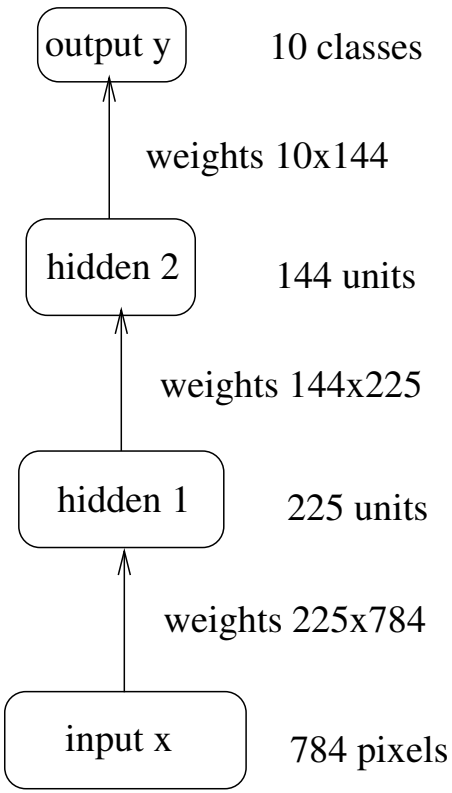
$$\frac{\partial C}{\partial W_{ij}^{(3)}} = \frac{\partial C}{\partial h_i^{(3)}} \frac{\partial h_i^{(3)}}{\partial W_{ij}^{(3)}}$$

$$\frac{\partial C}{\partial W_{jk}^{(2)}} = \sum_i \frac{\partial C}{\partial h_i^{(3)}} \frac{\partial h_i^{(3)}}{\partial h_j^{(2)}} \frac{\partial h_j^{(2)}}{\partial W_{jk}^{(2)}}$$

$$\frac{\partial C}{\partial W_{kl}^{(1)}} = \sum_j \sum_i \frac{\partial C}{\partial h_i^{(3)}} \frac{\partial h_i^{(3)}}{\partial h_j^{(2)}} \frac{\partial h_j^{(2)}}{\partial h_k^{(1)}} \frac{\partial h_k^{(1)}}{\partial W_{kl}^{(1)}}$$

- *How many paths - for two hidden layers*
- *as a function of depth?*
- Modern software (autograd) handles this derivation!

Backpropagation - dynamic programming



- Store intermediate results

$$\frac{\partial C}{\partial h_j^{(2)}} = \sum_i \frac{\partial C}{\partial h_i^{(3)}} \frac{\partial h_i^{(3)}}{\partial h_j^{(2)}}$$

$$\frac{\partial C}{\partial h_k^{(1)}} = \sum_j \frac{\partial C}{\partial h_j^{(2)}} \frac{\partial h_j^{(2)}}{\partial h_k^{(1)}}$$

- In general

$$\frac{\partial C}{\partial h_j^{(l)}} = \sum_i \frac{\partial C}{\partial h_i^{(l+1)}} \frac{\partial h_i^{(l+1)}}{\partial h_j^{(l)}}$$

- and gradient:

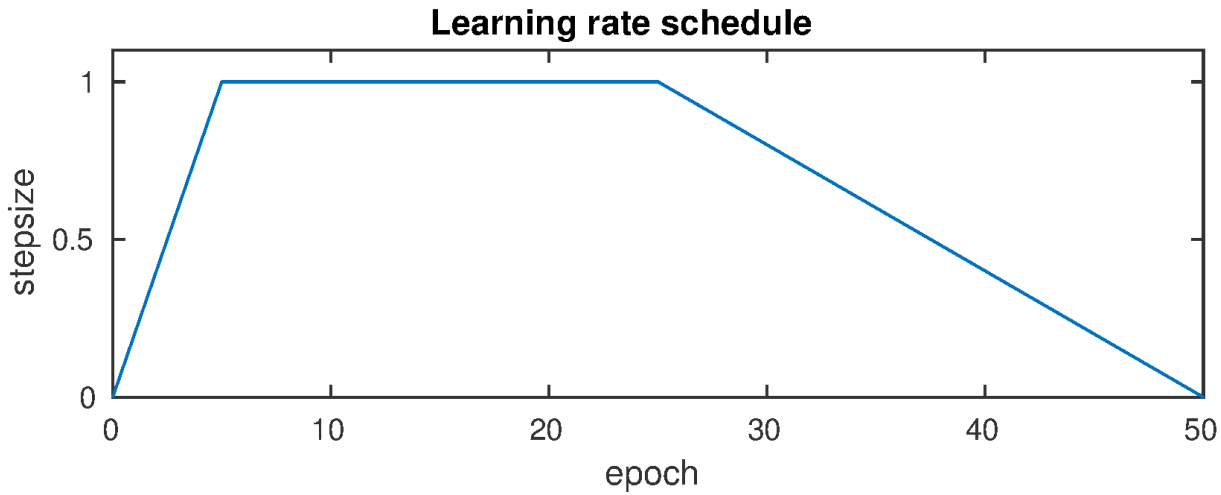
$$\frac{\partial C}{\partial W_{ij}^{(l)}} = \frac{\partial C}{\partial h_i^{(l)}} \frac{\partial h_i^{(l)}}{\partial W_{ij}^{(l)}}$$

Mini-batch training

- No need to have an accurate estimate of $\mathbf{g}$.
- Use only a small batch of training data at once.
- Leads into many updates per epoch (=seeing data once).
- E.g. 600 updates with 100 samples per epoch in MNIST.

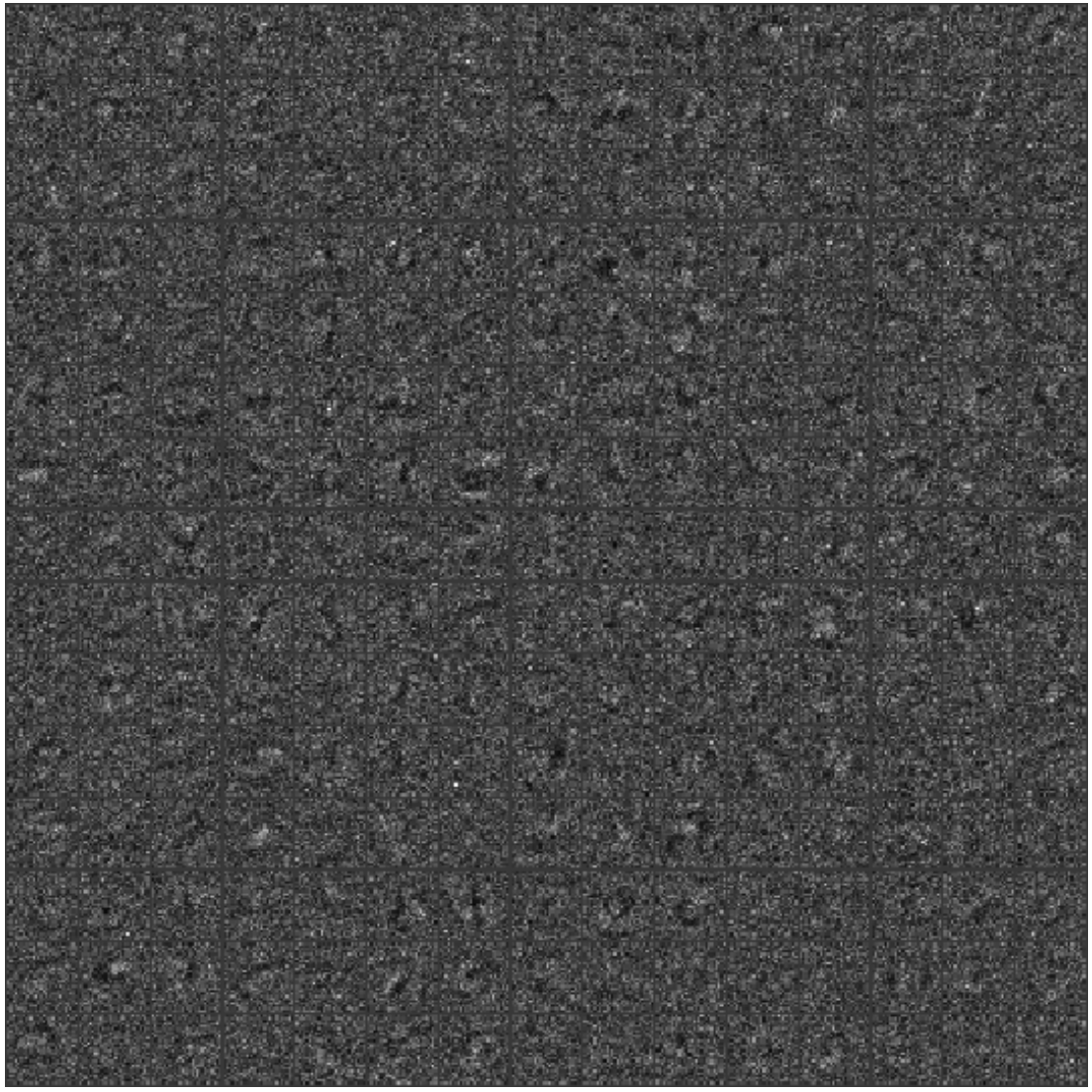
Mini-batch training

- No need to have an accurate estimate of **g**.
- Use only a small batch of training data at once.
- Leads into many updates per epoch (=seeing data once).
- E.g. 600 updates with 100 samples per epoch in MNIST.
- Important to anneal stepsize η_k towards the end, e.g.

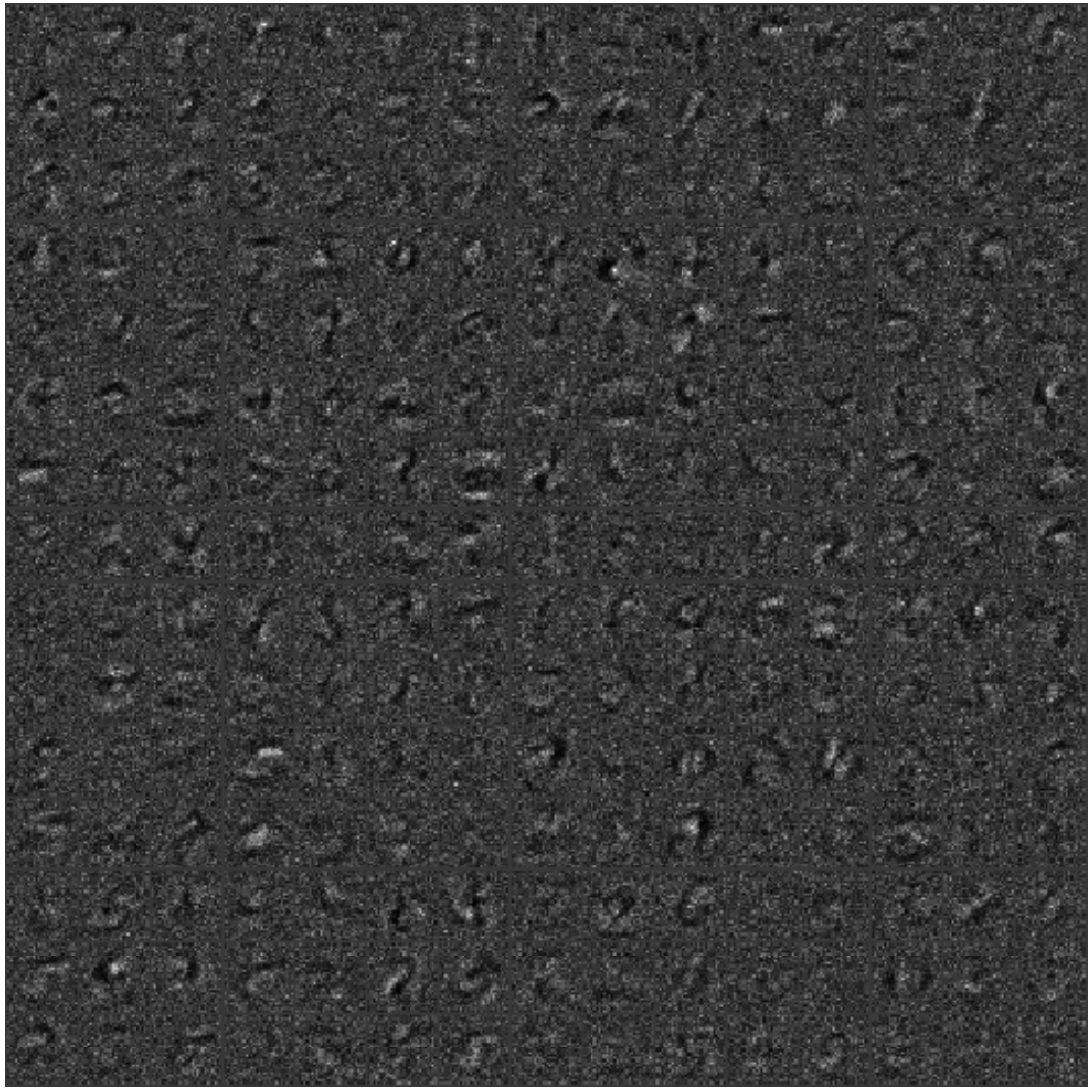


- Adaptation of η_k possible (Adam, Adagrad, Adadelta).

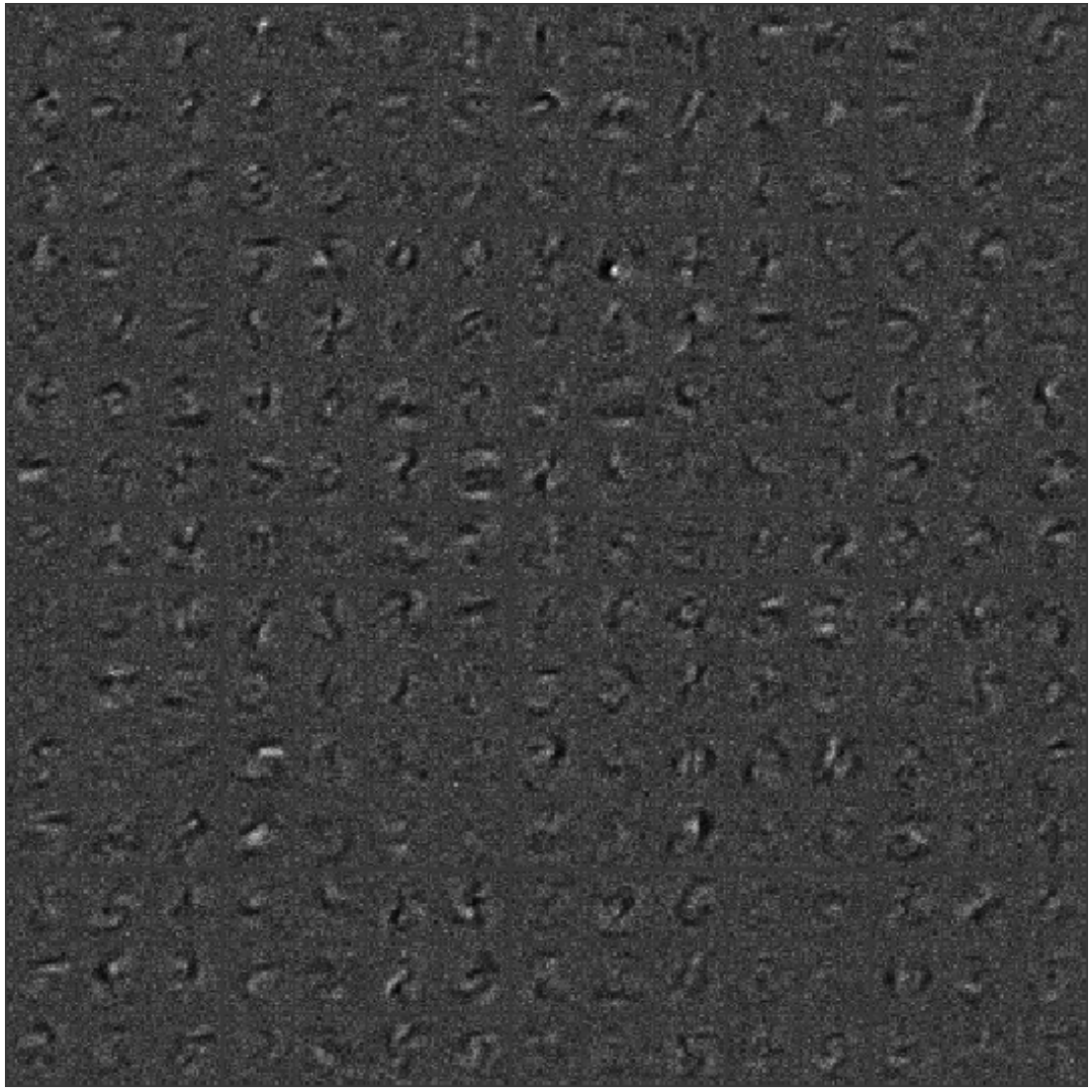
$\mathbf{W}^{(1)}$ after epoch 1



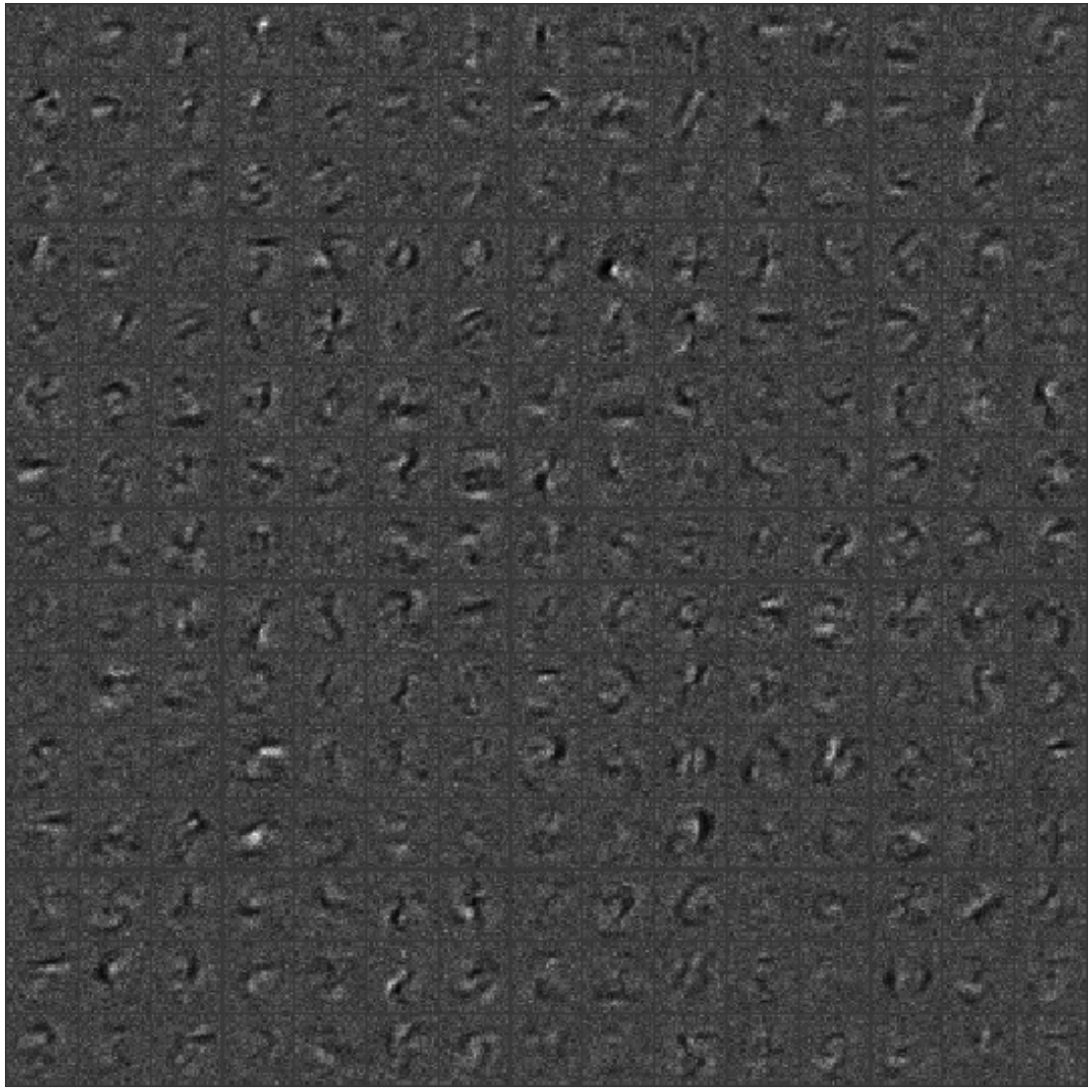
$\mathbf{W}^{(1)}$ after epoch 2



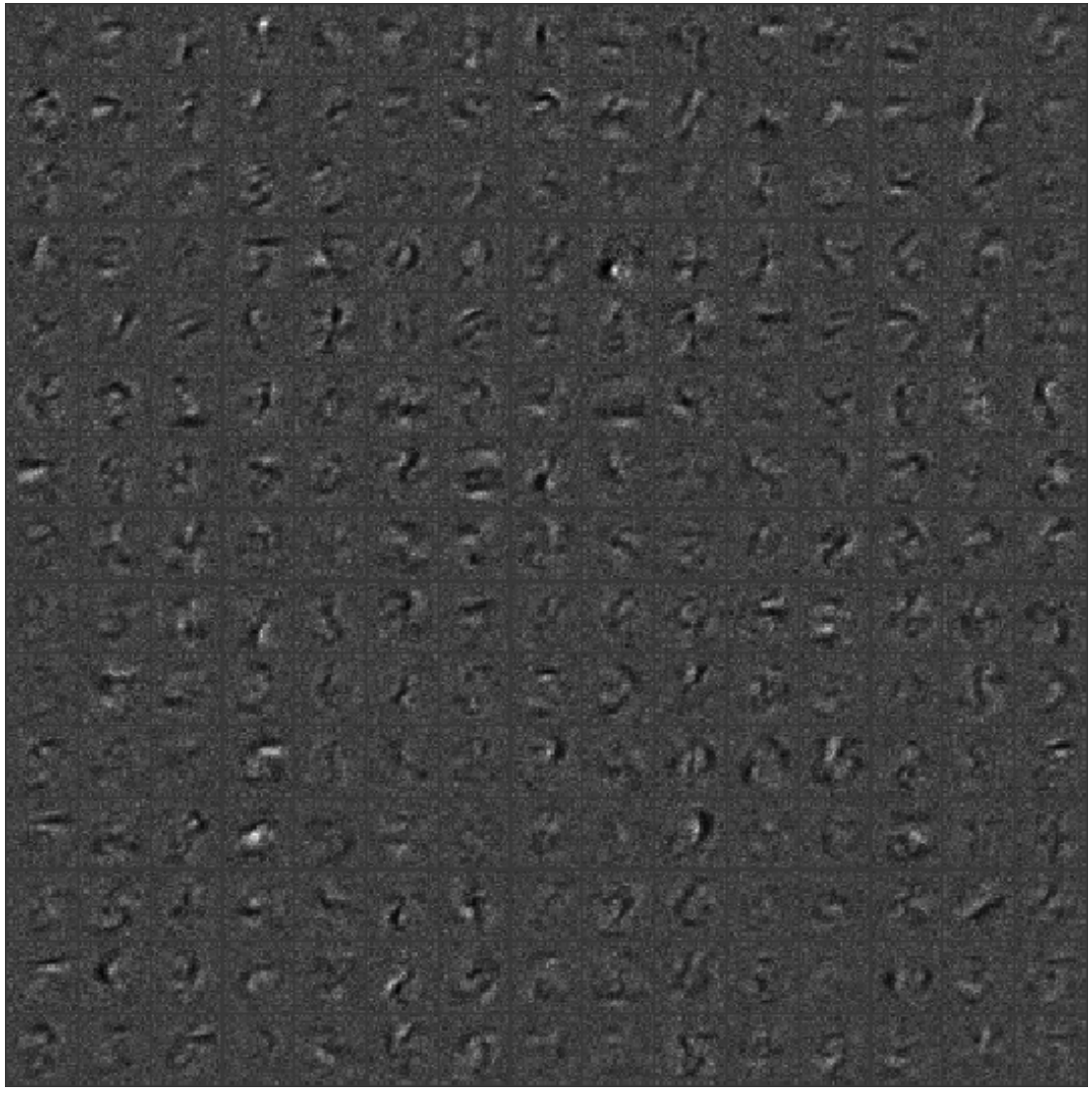
$\mathbf{W}^{(1)}$ after epoch 3



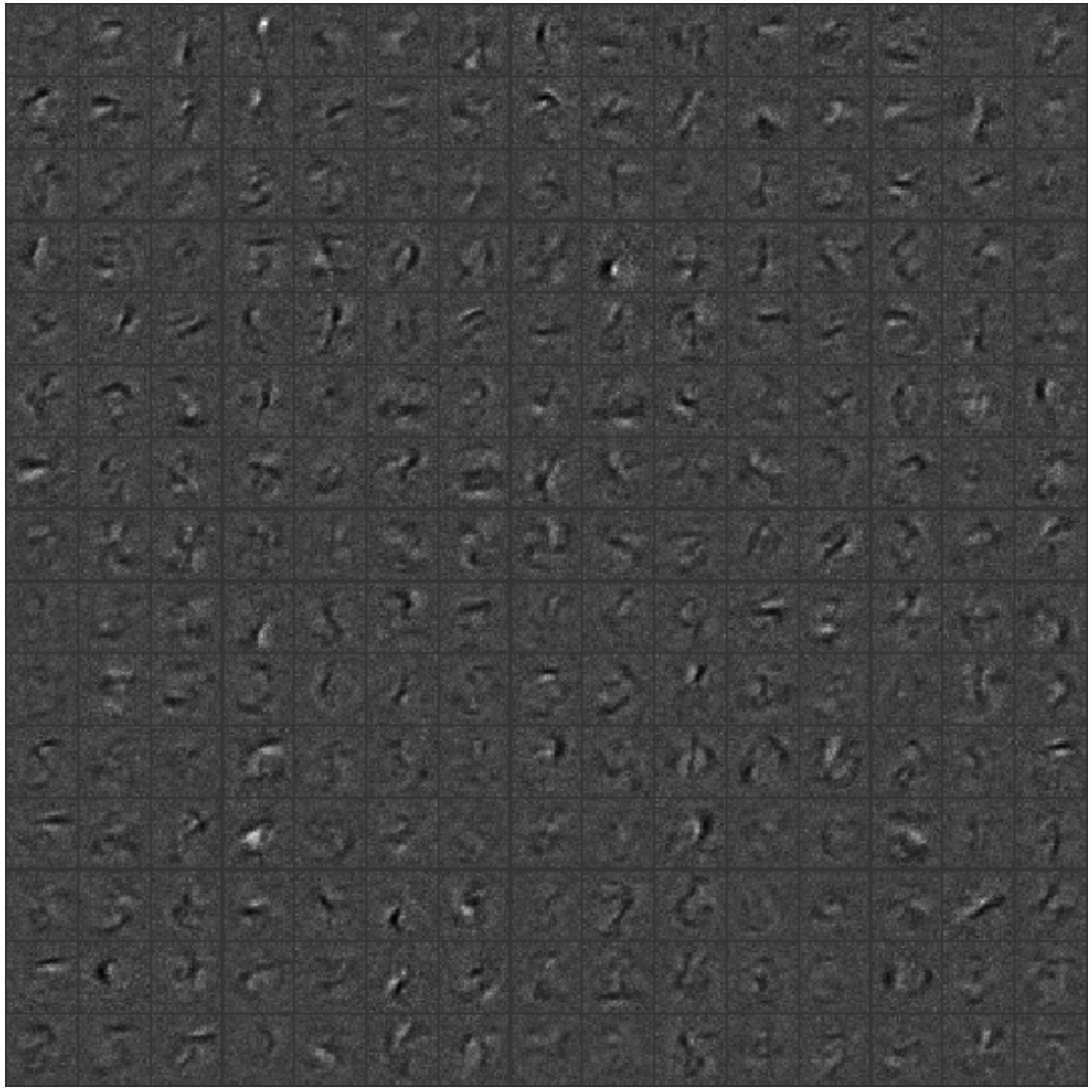
$\mathbf{W}^{(1)}$ after epoch 4



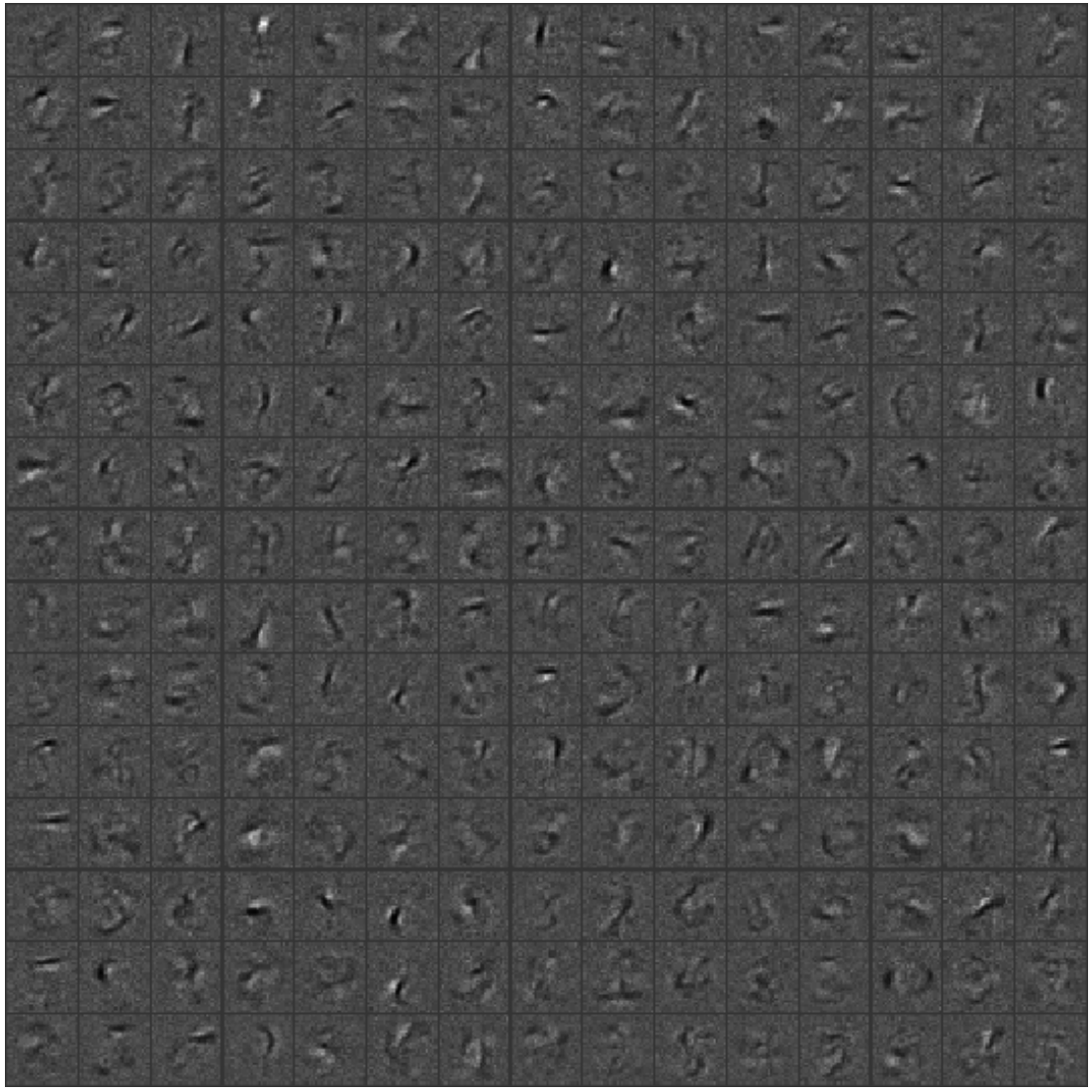
$\mathbf{W}^{(1)}$ after epoch 5



$\mathbf{W}^{(1)}$ after epoch 10

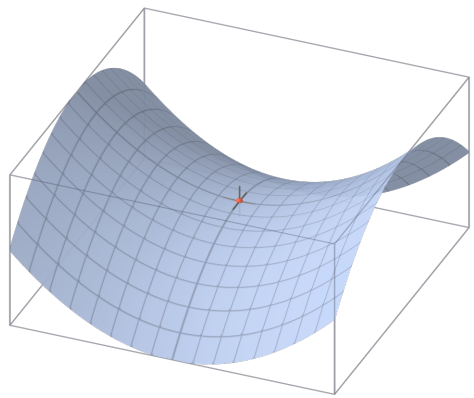


$\mathbf{W}^{(1)}$ after epoch 50 (final)



Definitions

- Learning stops at a critical point (gradient $\mathbf{g} = 0$)
- If all eigenvalues of Hessian **H** are positive it is a local minimum
- If all eigenvalues of Hessian **H** are negative it is a local maximum



- If Hessian has both positive and negative eigenvalues it is a **saddle point**

Theory: Local minima not an issue

(Dauphin et al., 2014, Choromanska et al., 2015)

- Local minima dominate in low-dimensional optimization, but saddle points dominate in high dimensions
- Most local minima are close to the global minimum

- Noisy gradient $\mathbf{g}$ helps in escaping saddle points

Backpropagation, tiny example

$$
\begin{aligned}
y &= w_2 h + \text{noise} \\
h &= w_1 x \\
C &= (y - 1.5)^2 \\
\frac{\partial C}{\partial w_2} &= 2(w_2 w_1 x - 1.5) w_1 x \\
\frac{\partial C}{\partial w_1} &= 2(w_2 w_1 x - 1.5) w_2 x
\end{aligned}
$$

Note a scaling issue: If w_1 is doubled and w_2 is halved,
- output y stays the same.
- system is twice as sensitive to changes in w_2.
- gradient of w_2 is doubled!

Exponential growth/decay forward

- Recall the model

$$\begin{aligned}\mathbf{y} &= \text{softmax}(\mathbf{W}^{(3)}\mathbf{h}^{(2)} + \mathbf{b}^{(3)}) \\ \mathbf{h}^{(2)} &= \text{relu}(\mathbf{W}^{(2)}\mathbf{h}^{(1)} + \mathbf{b}^{(2)}) \\ \mathbf{h}^{(1)} &= \text{relu}(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)})\end{aligned}$$

- Ignoring softmax and biases, we can write

$$y_i = \sum_{j,k,l} \mathbf{1}\left(h_j^{(2)} > 0\right) \mathbf{1}\left(h_k^{(1)} > 0\right) W_{ij}^{(3)} W_{jk}^{(2)} W_{kl}^{(1)} x_l$$

- Exponential growth/decay of forward signals!

Exponential growth/decay backward

- Given indicators $\mathbf{1}(\cdot)$, model is linear

$$y_i = \sum_{j,k,l} \mathbf{1}\left(h_j^{(2)} > 0\right) \mathbf{1}\left(h_k^{(1)} > 0\right) W_{ij}^{(3)} W_{jk}^{(2)} W_{kl}^{(1)} x_l$$

$$\frac{\partial y_i}{\partial x_l} = \sum_{j,k} \mathbf{1}\left(h_j^{(2)} > 0\right) \mathbf{1}\left(h_k^{(1)} > 0\right) W_{ij}^{(3)} W_{jk}^{(2)} W_{kl}^{(1)}$$

- Exponential growth/decay of gradient, too!
- $\Rightarrow$ Scale of initialization important.

References

- S. Linnainmaa. The representation of the cumulative rounding error of an algorithm as a Taylor expansion of the local rounding errors. Master's Thesis (in Finnish), Univ. Helsinki, 1970.
- Polyak, B.T. Some methods of speeding up the convergence of iteration methods. USSR Computational Mathematics and Mathematical Physics, 4(5):1–17, 1964.
- Kingma, D. and Ba, J. (2015). ADAM: A method for stochastic optimization. In the International Conference on Learning Representations (ICLR), San Diego. arXiv:1412.6980.
- Dauphin, Pascanu, Gulcehre, Cho, Ganguli, and Bengio. Identifying and attacking the saddle point problem in high dimensional non-convex optimization. In NIPS 2014.
- Choromanska, Henaff, Mathieu, Ben Arous, and LeCun. The Loss Surface of Multilayer Nets. In AISTATS 2015.
- Glorot, Xavier, and Yoshua Bengio. "Understanding the difficulty of training deep feedforward neural networks." International conference on artificial intelligence and statistics. 2010.
- Martens, J. Deep learning via Hessian-free optimization. In ICML, 2010.

Thanks!
Ole Winther