Back-propagation Optimization

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Content of the lecture: Optimisation Approaches

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1. Vanishing Gradient activation functions and initialization

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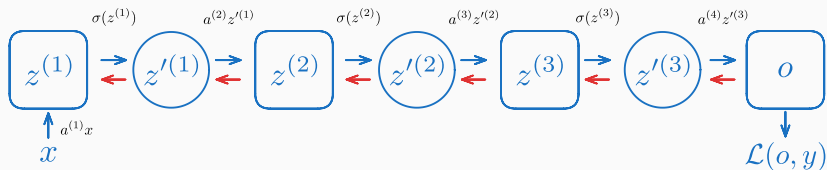
2. Regularization

Content of the lecture: Optimisation Approaches

1. Vanishing Gradient activation functions and initialization

2. Regularization

3. Gradient Descent variants

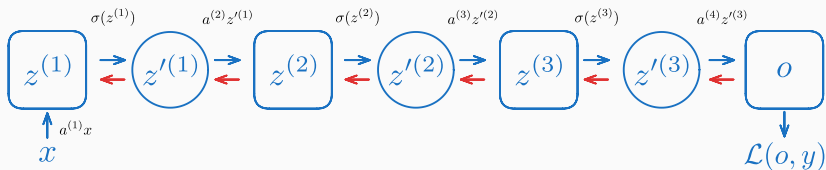# Vanishing Gradient actuvation function and initialization

Consider a MLP with only a single neuron in each layer (scalar network)

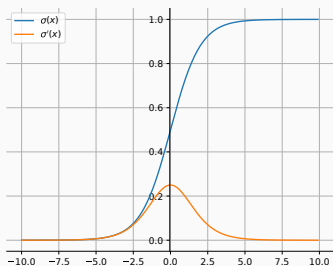**What is the gradient $\mathcal{L}(o, y)$ with respect to $a^{(1)}$?**

Consider a MLP with only a single neuron in each layer (scalar network)

What is the gradient $\mathcal{L}(o, y)$ with respect to $a^{(1)}$?

$$\frac{d\mathcal{L}(o, y)}{da^{(1)}} = \frac{d\mathcal{L}(o, y)}{do} \frac{do}{dz'^{(3)}} \times \frac{dz'^{(3)}}{dz^{(3)}} \times \frac{dz^{(3)}}{dz'^{(2)}} \times \frac{dz'^{(2)}}{dz^{(2)}} \times \frac{dz^{(2)}}{dz'^{(1)}} \times \frac{dz'^{(1)}}{dz^{(1)}} \times \frac{dz^{(1)}}{da^{(1)}}$$

$$= \frac{d\mathcal{L}(o, y)}{do} \times a^{(4)} \times \frac{d\sigma(z^{(3)})}{dz^{(3)}} \times a^{(3)} \times \frac{d\sigma(z^{(2)})}{dz^{(2)}} \times a^{(2)} \times \frac{d\sigma(z^{(1)})}{dz^{(1)}} \times a^{(1)}$$

Figure 1: The sigmoid function and its derivative ("logistic function")
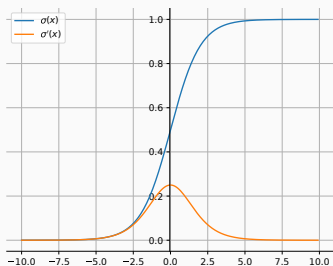
Sigmoid function (logistic function)

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$
$$\sigma'(x) = \sigma(x)(1 - \sigma(x))$$

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- In the best cases, we multiply successively by 0.25

Figure 2: The TanH (Hyperbolic tangent) function and its derivative

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- Better that sigmoid around 0
  - → Still vanishing gradient issues for strong values
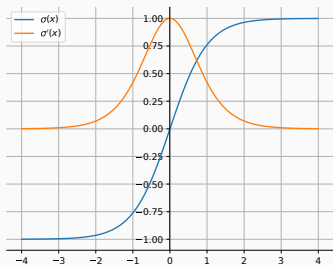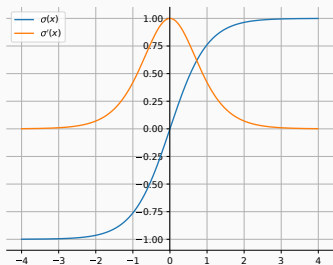
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- Popular in Natural Language Processing (e.g. in RNN architectures)

activation and Gradient: ReLU

Figure 3: The ReLU (Rectified Linear Unit) function and its derivative
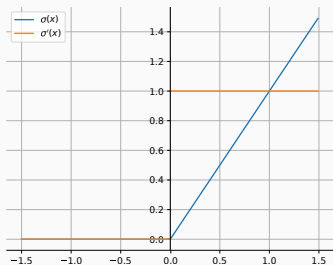
ReLU function (Rectified Linear Unit)

$$\sigma(x) = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

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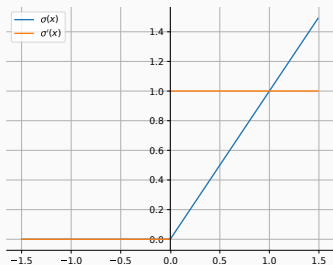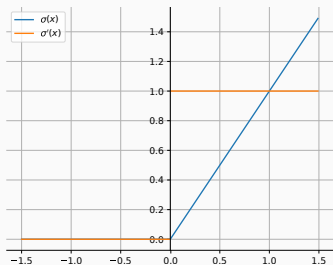- "Dead units" problems (when $x << 0$ for instance a very low bias)

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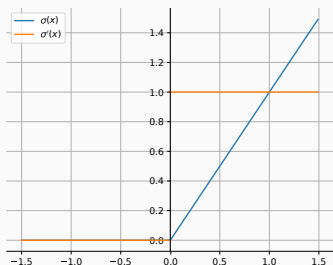$$\sigma'(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases}$$

Vanishing gradient

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- "Dead units" problems (when $x << 0$ for instance a very low bias)

- Used a lot in computer vision (CNN)

What do we want?

- Value close to zero often prevent vanishig gradient
  $\rightarrow$ Ensure input of activation close to zero at the begining of the training

- Having a similar gradient magnitude for all layers
  $\rightarrow$ Avoid one layer to do all the works while others are useless

Vanishing Gradient: How to prevent it?

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Hyperbolic Tangent
Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$:

- A sampled uniformly between
  $\left[-\frac{\sqrt{6}}{\sqrt{m+n}}, \frac{\sqrt{6}}{\sqrt{m+n}} \right]$

- b initialized to 0

Called Xavier or Glorot initialization
→ "Understanding the difficulty of training deep
feedforward neural networks", Glorot, X. and
Bengio, Y. (2010)

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Rectified Linear Unit
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- A sampled uniformly between $\left[-\frac{\sqrt{6}}{\sqrt{n}}, \frac{\sqrt{6}}{\sqrt{n}} \right]$

- b initialized to 0 (or $b = 0.01$)

Called Kaiming or He initialization
$\rightarrow$ "Delving deep into rectifiers: Surpassing human-level performance on imagenet classification.", He, K. et.al. (2015)

Regularization approaches

Principle of generalization

Overparameterized neural networks

Networks where the number of parameters exceed the training dataset size.

- Can learn by heart the dataset,
  i.e. **overfit the data** $\rightarrow$ does not generalize well to unseen data

- Are easier to optimize in practice

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Monitoring the training process

- Loss should go down $\quad\Rightarrow\quad$ otherwise your step-size is probably too big!

- Training accuracy should go up

- Dev accuracy should go up $\quad\Rightarrow\quad$ otherwise the network is overfitting!

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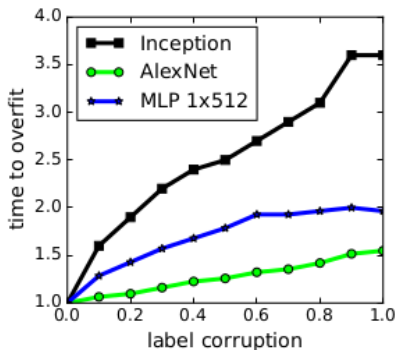
Regularization

Techniques to control parameters during learning and prevent overfitting

model	# params	random crop	weight decay	train accuracy	test accuracy
Inception	1,649,402	yes	yes	100.0	89.05
		yes	no	100.0	89.31
		no	yes	100.0	86.03
		no	no	100.0	85.75
(fitting random labels)		no	no	100.0	9.78
Inception w/o BatchNorm	1,649,402	no	yes	100.0	83.00
		no	no	100.0	82.00
(fitting random labels)		no	no	100.0	10.12
Alexnet	1,387,786	yes	yes	99.90	81.22
		yes	no	99.82	79.66
		no	yes	100.0	77.36
		no	no	100.0	76.07
(fitting random labels)		no	no	99.82	9.86
MLP 3x512	1,735,178	no	yes	100.0	53.35
		no	no	100.0	52.39
(fitting random labels)		no	no	100.0	10.48
MLP 1x512	1,209,866	no	yes	99.80	50.39
		no	no	100.0	50.51
(fitting random labels)		no	no	99.34	10.61
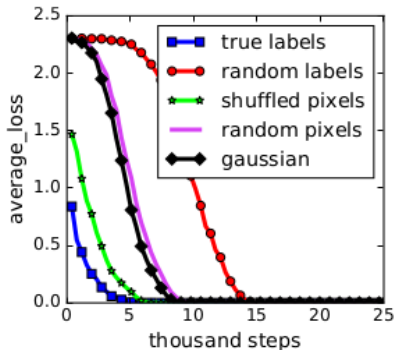
(a) learning curves

(b) convergence slowdown

Regularization L2, gaussian or with weight decay

Regularisation term:

$$\hat{\Theta} = \arg\min_{\Theta} \mathcal{L}(f(x; \Theta), y) + \frac{\lambda}{2} ||\Theta||^2$$
$$= \arg\min_{\Theta} \mathcal{L}(f(x; \Theta), y) + \mathcal{R}(\Theta; \lambda)$$

The right term is called the regularization term it can be equivalently interpreted as:

- A soft constraint on the magnitude of parameters (**L2 regularization**)

- A Gaussian prior on parameters $\mathcal{N}(0, \frac{1}{\lambda})$ (**Gaussian regularization**)

- A re-scaling of the parameters during gradient-descent (**weight-decay**)

Using "classical" gradient descent algorithm

Regularization L2, gaussian or with weight decay

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$$= \arg\min_{\Theta} \mathcal{L}(f(x;\Theta), y) + \mathcal{R}(\Theta; \lambda)$$

During the gradient update:

$$\Theta^{t+1} = \Theta^t - \epsilon\nabla_{\Theta^t}\mathcal{L} - \epsilon\nabla_{\Theta^t}\mathcal{R}(\Theta; \lambda)$$

$$= \Theta^t - \epsilon\left(\nabla_{\Theta^t}\mathcal{L} - \nabla_{\Theta^t}\mathcal{R}(\Theta; \lambda)\right)$$

What is the gradient of the regularization term

$$\frac{\partial\mathcal{R}(\Theta; \lambda)}{\partial\Theta} = \frac{\partial\frac{\lambda}{2}||\Theta||^2}{\partial\Theta} = \frac{2\lambda\Theta}{2} = \lambda\Theta$$

The update $\Theta^{t+1} = \Theta^t - \lambda\Theta^t$ is called weight decay
$\rightarrow$ ⚠ **It is coupled with the optimisation of a loss !!!**

Regularization L2, gaussian or with weight decay: Implementation

Implementation from Pytorch (with minor modifications)
:

```
class SGD(Optimizer):
  def step(self, closure=None):
    """Performs a single optimization step."""
    for group in self.param_groups: # iterate over parameters
      for p in group['params']:
        if p.grad is None:
          continue

      d_p = p.grad.data # get gradient
      weight_decay = group['weight_decay']
      if weight_decay != 0:
        d_p.add_(weight_decay, p.data) # add weight decay to
   gradient
      p.data.add_(-group['lr'], d_p) # update parameters
```

Dropout

How does dropout work?

- During training, we randomly "turn off" neurons,
  i.e. we randomly set elements of hidden layers z to 0

- During test, we do use the full network
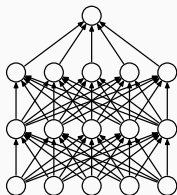
(a) Standard Neural Net   (b) After applying dropout.
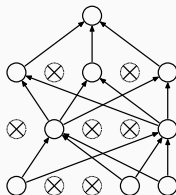
Intuition

- prevents co-adaptation between units

- equivalent to averaging different models that have different structure but
  share parameters
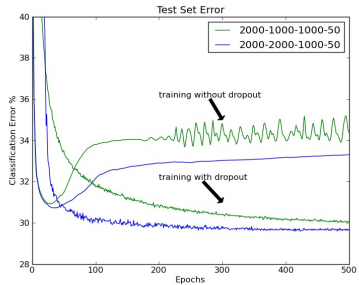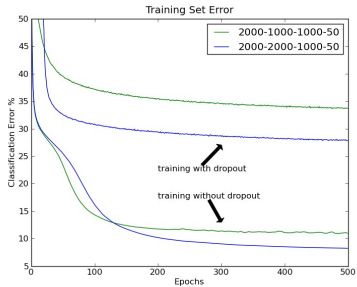
Dropout layer
A dropout layer is parameterized by the probability of "turning off" a neuron $p \in [0, 1]$:

$$z' = \text{Dropout}(z; p = 0.5)$$

Dropout 3/4

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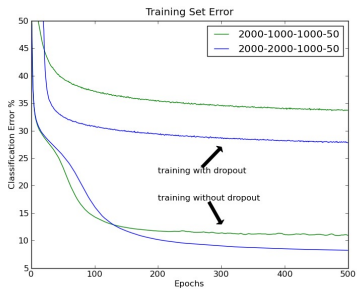
$$z' = \text{Dropout}(z; p = 0.5)$$

Implementation

- $z \in \mathbb{R}^n$: output of a hidden layer

- $p \in [0, 1]$: dropout probability

- $m \in \{0, 1\}^n$: mask vector

- z': hidden values after dropout application

The mask m is a vector of booleans stating if neurons z_i is kept ($m_i = 1$) or "turned off" ($m_i = 0$).

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Forward pass:

$$m \sim \text{Bernoulli}(1 - p)$$
$$z'_i = \frac{z_i * m_i}{1 - p}$$

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Backward pass:

$$\frac{\partial z'_i}{z_i} = \frac{m}{1 - p}$$

$\Rightarrow$ no gradient for "turned off" neurons.

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Dropout 4/4

Where do you apply dropout?

- On the input of the neural network x

- **After** activation functions ($sigmoid(0) \neq 0$)

- **Do not** apply dropout on the output logits

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Which dropout probability should you use?

- Empirical question: you have to test!

- Dropout probability at different layers can be different
  (especially input vs. hidden layers)

- Usually $0.1 \leq p \leq 0.5$

Dropout variants

Dropout can be applied differently for special neural network architectures
(e.g. convolutions, recurrent neural networks)

Optimizer

Stochastic Gradient Descent (SGD)

$$\Theta^{(t+1)} = \Theta^{(t)} - \epsilon^{(t)} \nabla_\Theta \mathcal{L}$$

Advantages

- Simple

- Single hyper-parameter: the step-size ϵ

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Advantages

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Downsides

- Forget information about previous updates

- Require to search for the best step-size strategy

- Require step-size annealing in practice: how? what scaling factor?

- Based on first-order information only
  (i.e. the curvature of the optimized function is ignored)

$\nabla_\Theta \mathcal{L}^{(t-2)}$

$\nabla_\Theta \mathcal{L}^{(t-1)}$
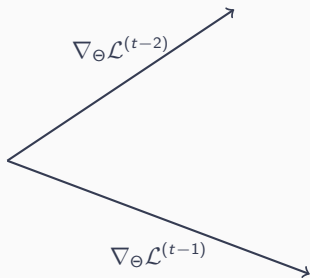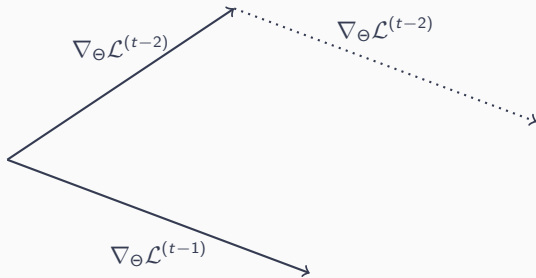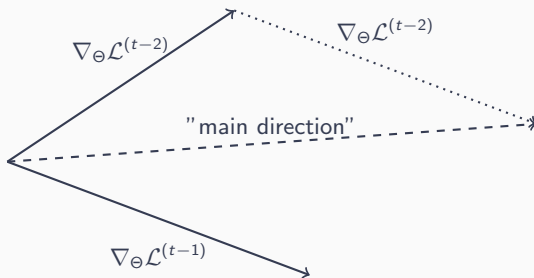
[Polyak, 1964]

- γ: velocity of parameters, i.e. cumulative information about past gradients

- $\mu \in [0, 1]$: momentum, i.e. how much information must be preserved?

$$\gamma^{(t+1)} = \mu\gamma^{(t)} + \nabla_\Theta \mathcal{L}$$
$$\Theta^{(t+1)} = \Theta^{(t)} - \epsilon\gamma^{(t+1)}$$

Variants

- Gradient dampening, i.e. diminish the contribution of the current gradient

- Nesterov's Accelerated Gradient [Sutskever et al., 2013]

Implementation from Pytorch (with minor modifications):

```
for group in self.param_groups:
  for p in group['params']:
    if p.grad is None:
      continue

    d_p = p.grad.data  # get the gradient
    if momentum != 0:
      param_state = self.state[p]
      if 'momentum_buffer' not in param_state:  # initialize velocity
          vector
        buf = param_state['momentum_buffer'] = torch.clone(d_p).detach()
      else:
        buf = param_state['momentum_buffer']  # retrieve velocity vector
        buf.mul_(momentum).add_(d_p)  # update velocity vector
      d_p = buf

    p.data.add_(-group['lr'], d_p)  # update parameters
```

Adaptive learning rates 1/2

Adagrad [Duchi et al., 2011]

- Replace global step-size with dynamic per parameter step-size + global learning rate

- The dynamic per parameter step-size is computed w.r.t. previous gradient l2-norm $\Rightarrow$ parameters with small (resp. large) gradient will have a large (resp. small) step-size

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Adadelta [Zeiler, 2012]

- Dynamic per parameter rate is computed with a fixed window of past gradients
- Approximate second-order information to incorporate curvature information $\Rightarrow$ less sensitive to the learning rate hyper-parameter!

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	SGD	MOMENTUM	ADAGRAD
$\epsilon = 1e^{0}$	**2.26%**	89.68%	43.76%
$\epsilon = 1e^{-1}$	2.51%	**2.03%**	2.82%
$\epsilon = 1e^{-2}$	7.02%	2.68%	**1.79%**
$\epsilon = 1e^{-3}$	17.01%	6.98%	5.21%
$\epsilon = 1e^{-4}$	58.10%	16.98%	12.59%

Table 1. MNIST test error rates after 6 epochs of training for various hyperparameter settings using SGD, MOMENTUM, and ADAGRAD.

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	$\rho = 0.9$	$\rho = 0.95$	$\rho = 0.99$
$\epsilon = 1e^{-2}$	2.59%	2.58%	2.32%
$\epsilon = 1e^{-4}$	2.05%	1.99%	2.28%
$\epsilon = 1e^{-6}$	1.90%	**1.83%**	2.05%
$\epsilon = 1e^{-8}$	2.29%	2.13%	2.00%

Table 2. MNIST test error rate after 6 epochs for various hyperparameter settings using ADADELTA.

Adam [Kingma and Ba, 2015]

- Combine dynamic per parameter learning rate and momentum

- Initialization bias correction

Convergence issue but works very well in practice [Reddi et al., 2018]
Variants: AdaMax, Nadam [Dozat, 2016], Radam [Liu et al., 2019], AMSGrad

Adaptive learning rate 2/2

Adam [Kingma and Ba, 2015]

- Combine dynamic per parameter learning rate and momentum

- Initialization bias correction

Convergence issue but works very well in practice [Reddi et al., 2018]
Variants: AdaMax, Nadam [Dozat, 2016], Radam [Liu et al., 2019], AMSGrad

Rule of thumb

- Optimizers based on adaptive learning rates usually work out of the box
  e.g. Adam is really popular in Natural Language Processing

- Fine-tuned SGD with step-size annealing can provide better results at the
  cost of expensive hyper-parameter tuning

Regularization issue
Weight decay is not equivalent to l2-norm when using adaptive learning rates!

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