FORNAX

Introduction to Deep Learning, part 1

Krzysztof Kolasiński, Rafał Cycoń - 30 March - 2017

Presentation outline

1. **A short motivation for DL**
2. **Mathematical model of neuron**
3. **DL - extreme crash course**

This talk:

- more technical, less practical
- we want to stress the importance of basic building blocks
- dense material, may be hard to follow
- non overlapping concepts
- assignment: try to understand covered concepts
- the feedback form

All slides and notebooks:
https://github.com/fornaxco/ai-tech-meetup

Why do we need DL?

A short motivation

Why do we need DL?

1. **DL is fun!**

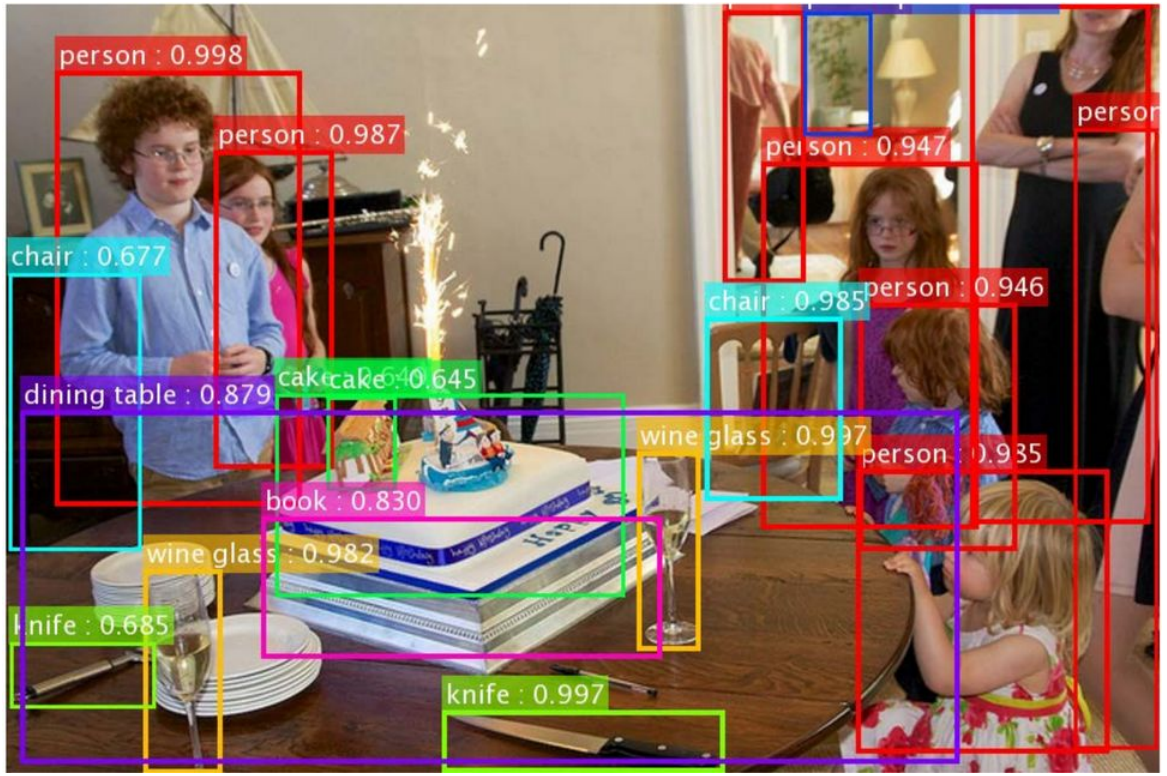
Deep dream

Neural style transfer

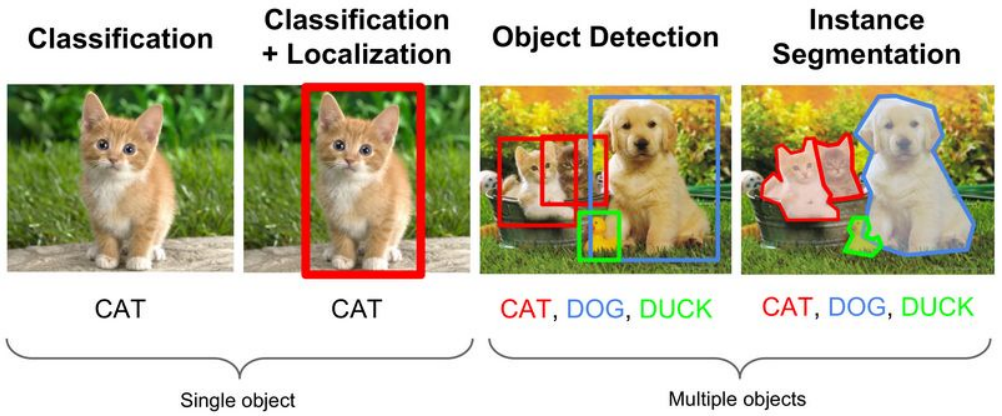
Why do we need DL?

2. DL is important

image segmentation



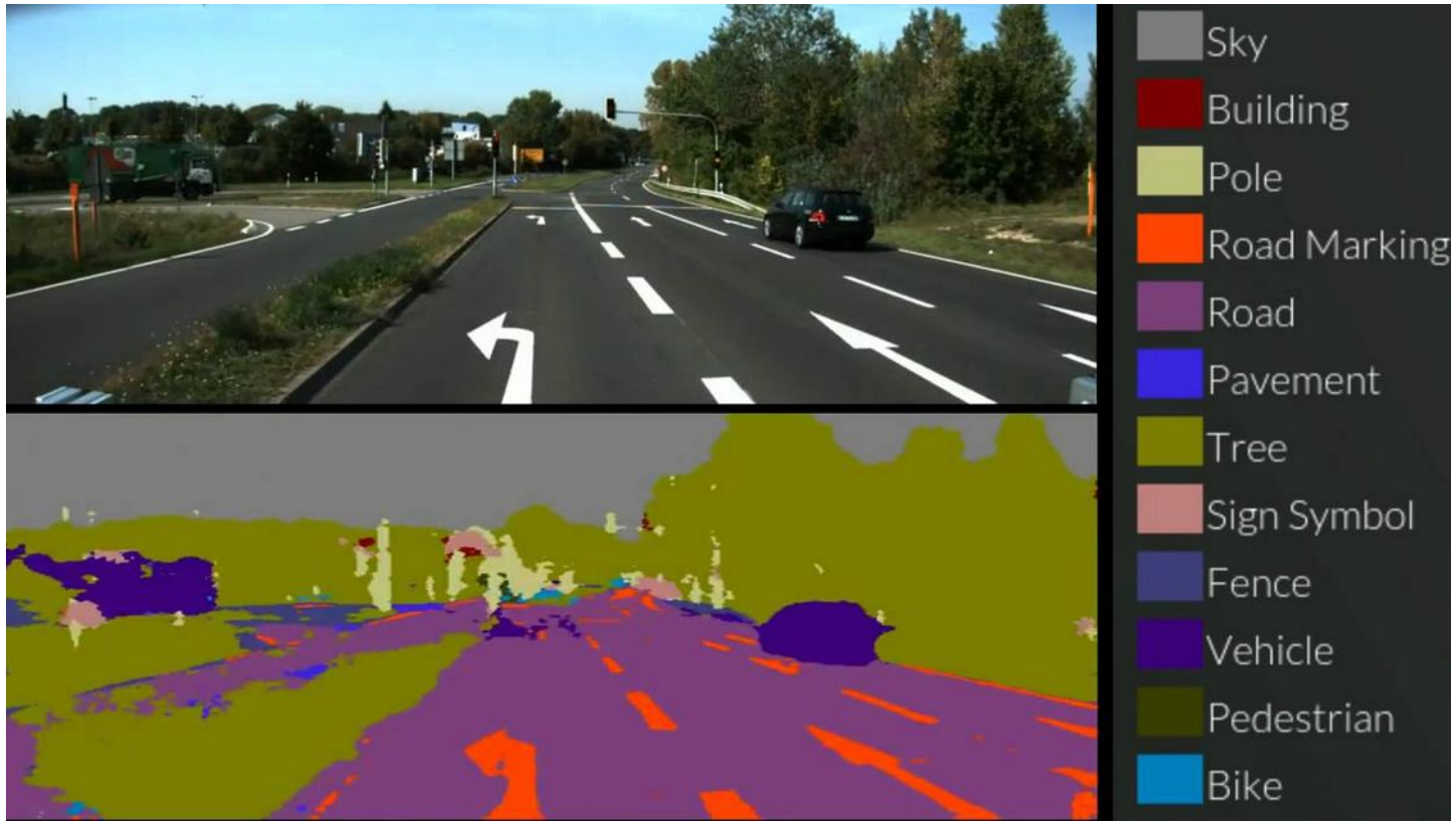
object detection



Source: CS231n (Stanford)

Why do we need DL?

2. DL is important



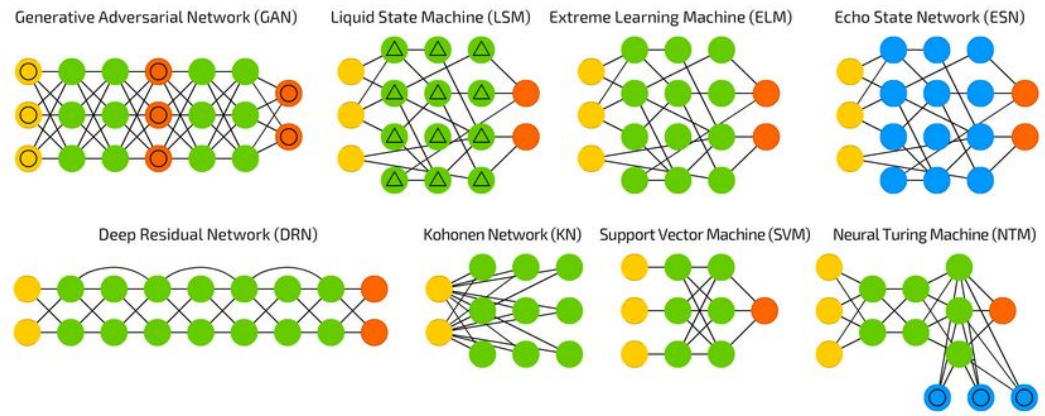
Application to self driving cars

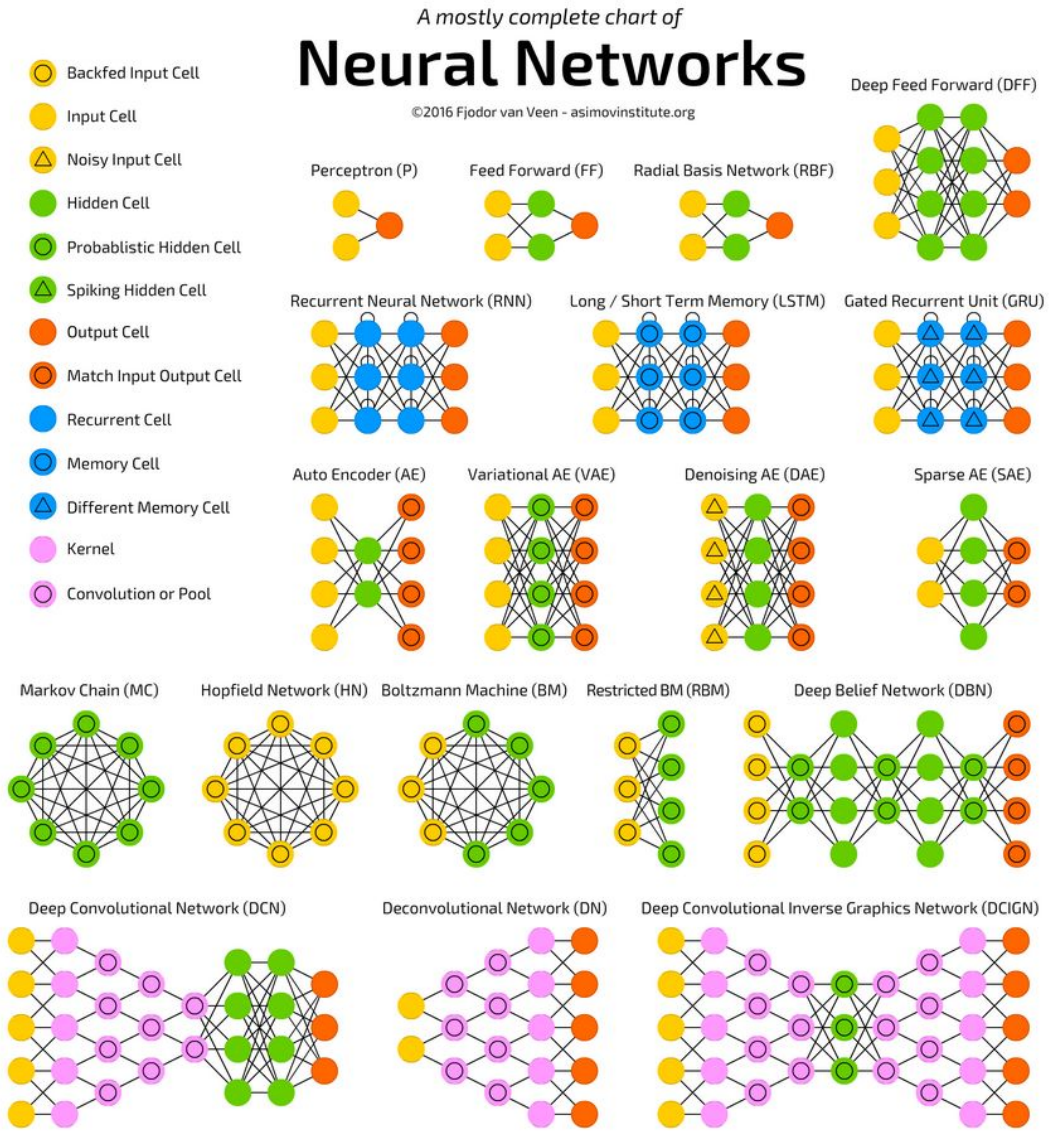
And many more…

The NN zoo

Understanding basic building blocks helps to create new and understand existing architectures

That NN family is growing up every day





http://www.asimovinstitute.org/neural-network-zoo/

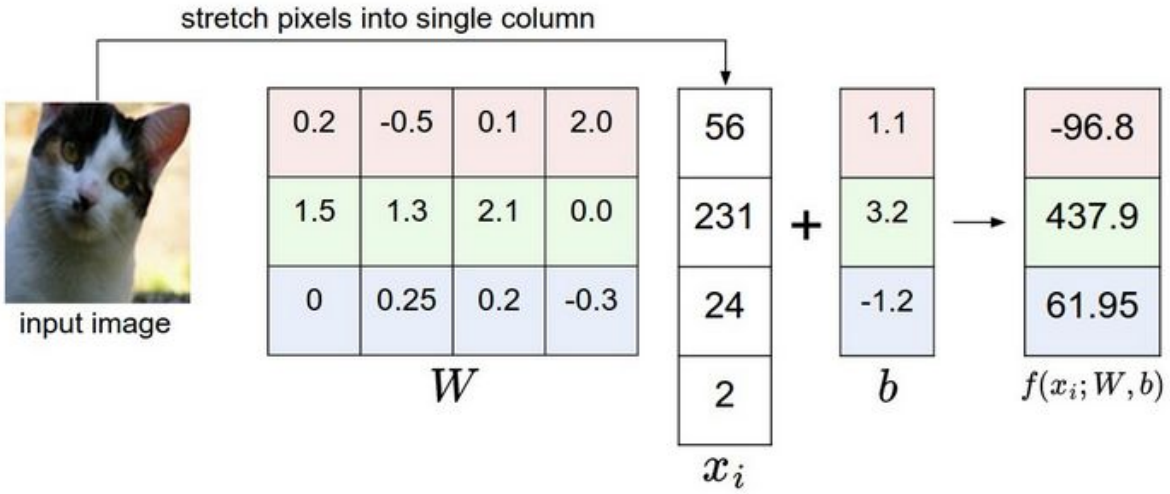
Prologue: The basics

The simple Neuron unit

Feed forward Neural Network

We define linear unit as

$$f(\mathbf{x}; \mathbf{W}, \mathbf{b}) = \mathbf{W}\mathbf{x} + \mathbf{b}$$

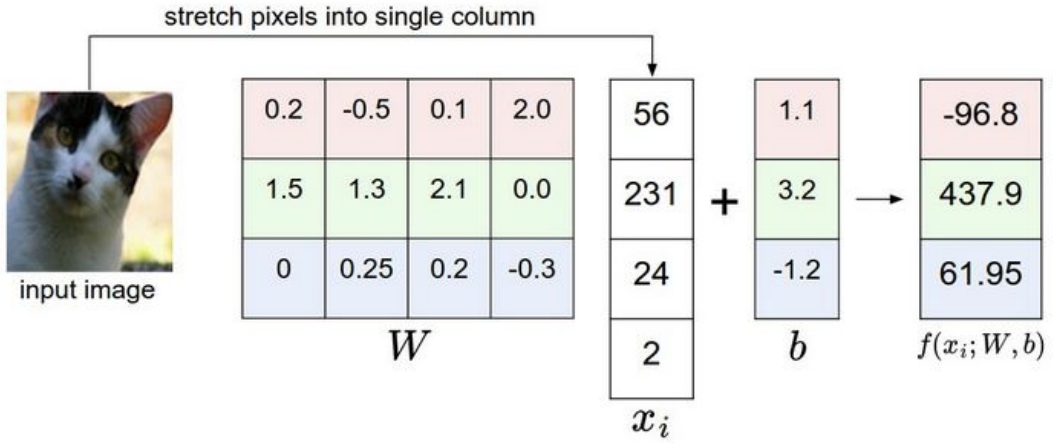


source: Stanford CS231 course

The simple Neuron unit

Linear classifier

$$f(\mathbf{x}; \mathbf{W}, \mathbf{b}) = \mathbf{W}\mathbf{x} + \mathbf{b}$$

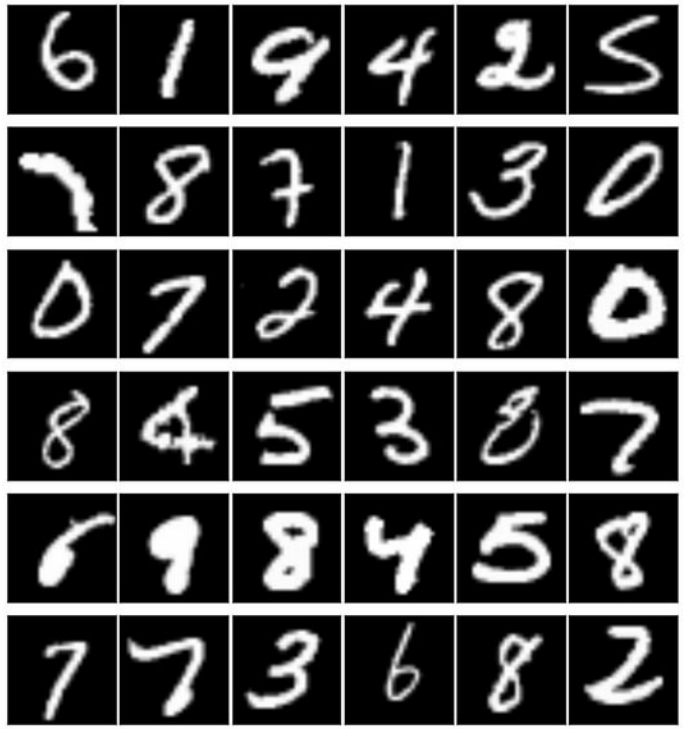


source: Stanford CS231 course

Case study: **MNIST** dataset and linear classifier

Steps:

1. Dataset consists of N images (28x28 pixels/gray scale) of handwritten digits between 0-9



The simple Neuron unit

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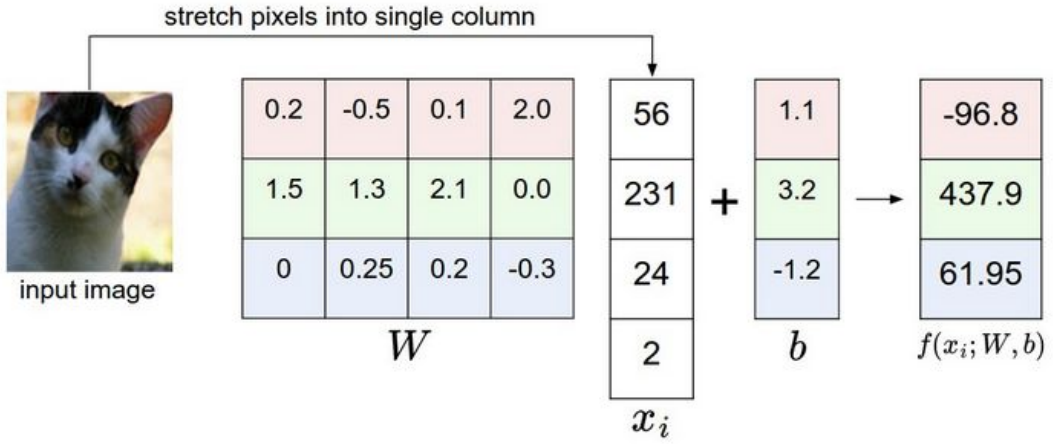

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Case study: **MNIST** dataset and linear classifier

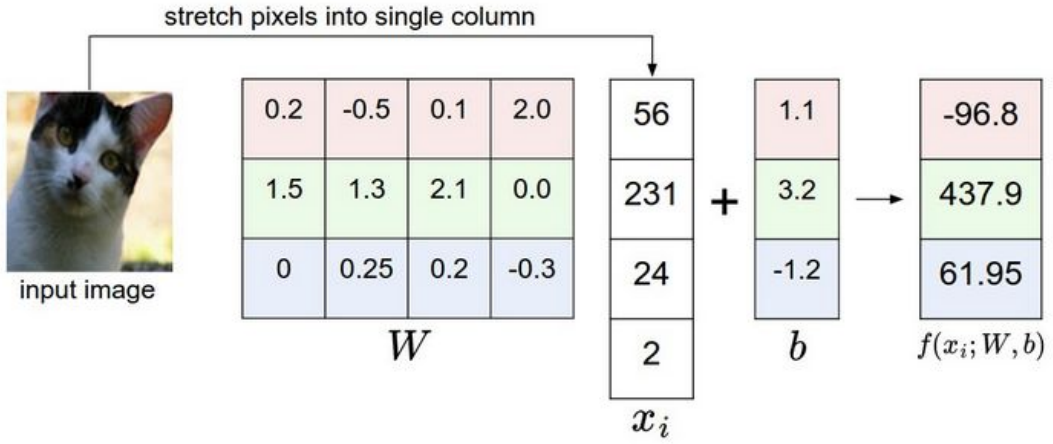
Steps:

1. Dataset consists of N images (28x28 pixels/gray scale) of handwritten digits between 0-9
2. The images are labeled (0-9)

The simple Neuron unit

Linear classifier

$$f(\mathbf{x}; \mathbf{W}, \mathbf{b}) = \mathbf{W}\mathbf{x} + \mathbf{b}$$



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Case study: **MNIST** dataset and linear classifier

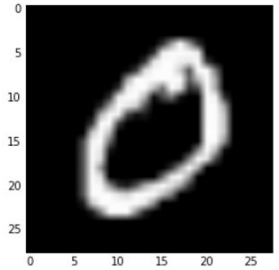
Steps:

1. Dataset consists of N images (28x28 pixels/gray scale) of handwritten digits between 0-9
2. The images are labeled (0-9)
3. Lets solve the simplest possible **supervised** task:

$$\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$$

model prediction

- We can compare this prediction with given label



$$\mathbf{y}_i = [0, \ldots, 1_i, \ldots, 0]$$

For example if the input image is **0** the label becomes

$$\mathbf{y}_i = [1, 0, \ldots]$$

The simple Neuron unit

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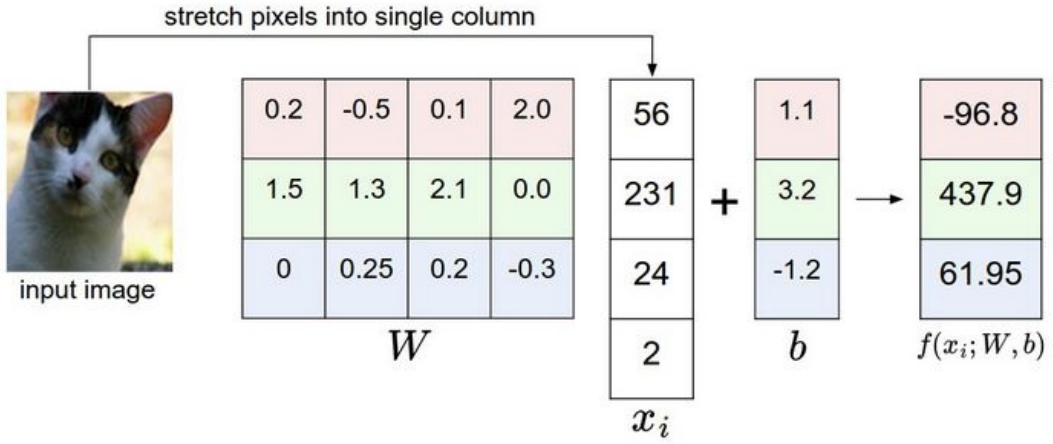

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3. Lets solve the simplest possible **supervised** task:

$$\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$$

- For each training example **i** we can define the loss function

$$\mathcal{L}_i \equiv l\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right)$$

In general lower loss == better prediction

The simple Neuron unit

Linear classifier

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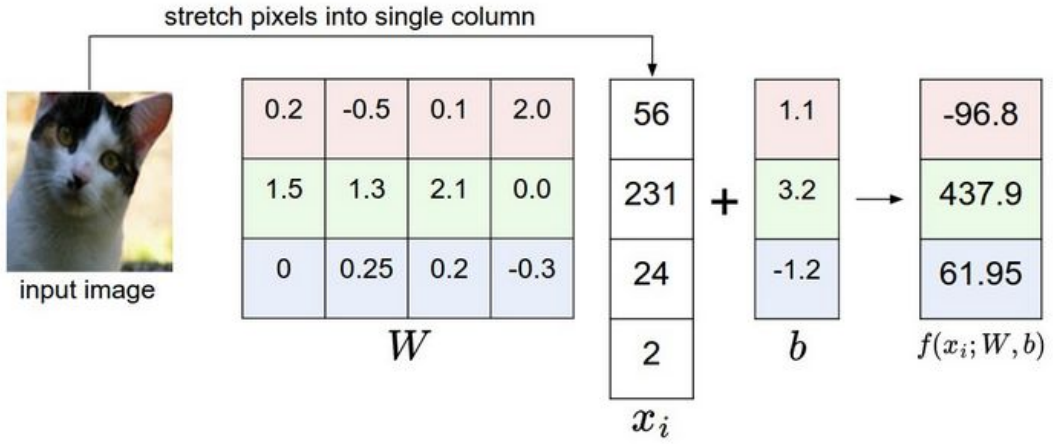

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- For simplicity we choose MSE loss

$$l\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) = MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) = \frac{1}{N_c}\sum_{j=1}^{N_c}(\hat{y}_{ij} - y_{ij})^2$$

The simple Neuron unit

Linear classifier

$$\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$$

prediction loss per one image

$$\mathcal{L}_i \equiv l\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) \qquad l\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) = MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) = \frac{1}{N_c}\sum_{j=1}^{N_c}(\hat{y}_{ij} - y_{ij})^2$$

The **MNIST** dataset (keras) consists of 60000 training images. Hence the total loss is given:

$$\mathcal{L}_{\text{total}} \equiv \frac{1}{N_s}\sum_{i=1}^{N_s} MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right)$$

Target: find **W** and **b** such that **loss** will be minimal

Solution: use gradient descent method to update model parameters:

$$\theta^{k+1} := \theta^k - \lambda \frac{\partial \mathcal{L}_{\text{total}}}{\partial \theta^k}$$

one has to compute gradient of loss w.r.t. model parameters

The simple Neuron unit

Linear classifier

$$\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$$

prediction loss per one image

$$\mathcal{L}_i \equiv l\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) \qquad l\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) = MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) = \frac{1}{N_c}\sum_{j=1}^{N_c}(\hat{y}_{ij} - y_{ij})^2$$

The **MNIST** dataset (keras) consists of 60000 training images. Hence the total loss is given:

It is more practical to use mini-batch approximation of gradients instead taking whole sum:

$$\mathcal{L}_{\text{total}} \equiv \frac{1}{N_s}\sum_{i=1}^{N_s} MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right) \quad \rightarrow \quad \mathcal{L}_{\text{mini-batch}} \equiv \frac{1}{N_{\text{MB}}}\sum_{i\in\text{MB}}^{N_{MB}} MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right)$$

mini-batch size

This lead to mini-batch **stochastic gradient descent** algorithm:

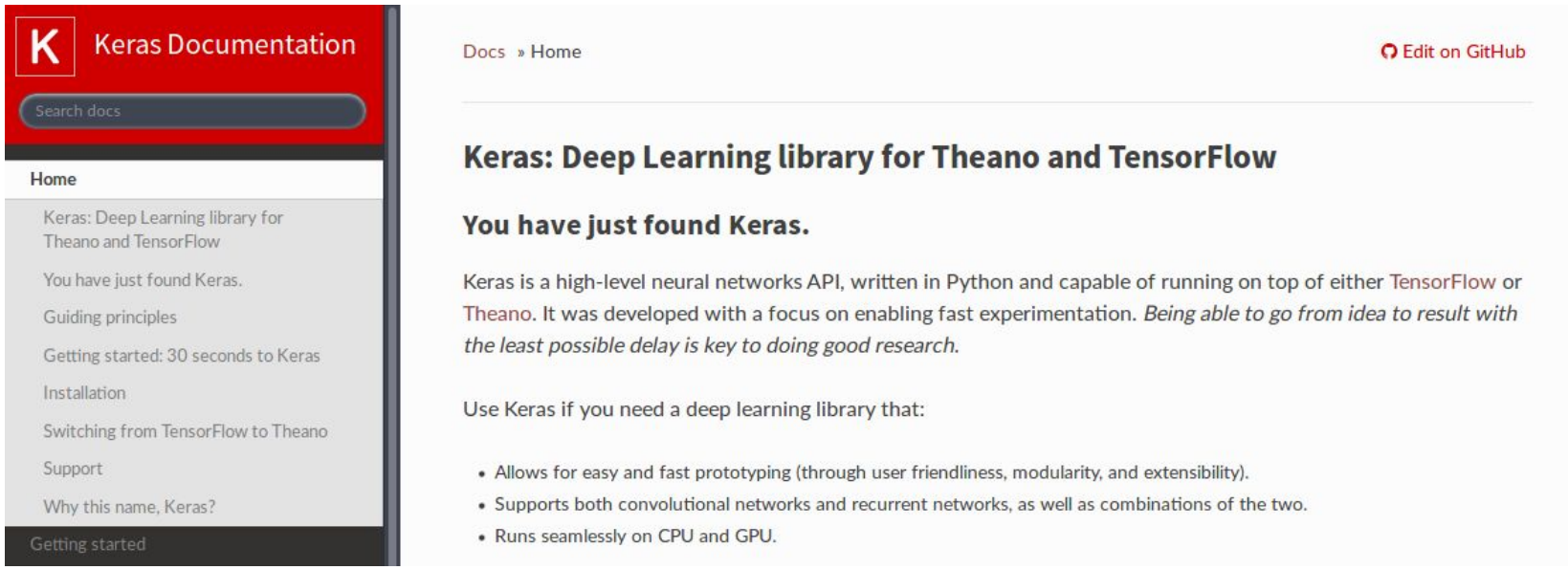
$$\theta^{k+1} := \theta^k - \lambda \left.\frac{\partial \mathcal{L}}{\partial \theta^k}\right|_{\text{mini-batch}}$$

The simple Neuron unit

Linear classifier - steps:

1. Define the model: $\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$
2. Define the objective: $\mathcal{L}_{\text{mini-batch}} \equiv \frac{1}{N_{\text{MB}}} \sum_{i \in \text{MB}}^{N_{MB}} MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right)$
3. Define parameter optimizer: $\theta^{k+1} := \theta^k - \lambda \left. \frac{\partial \mathcal{L}}{\partial \theta^k} \right|_{\text{mini-batch}}$

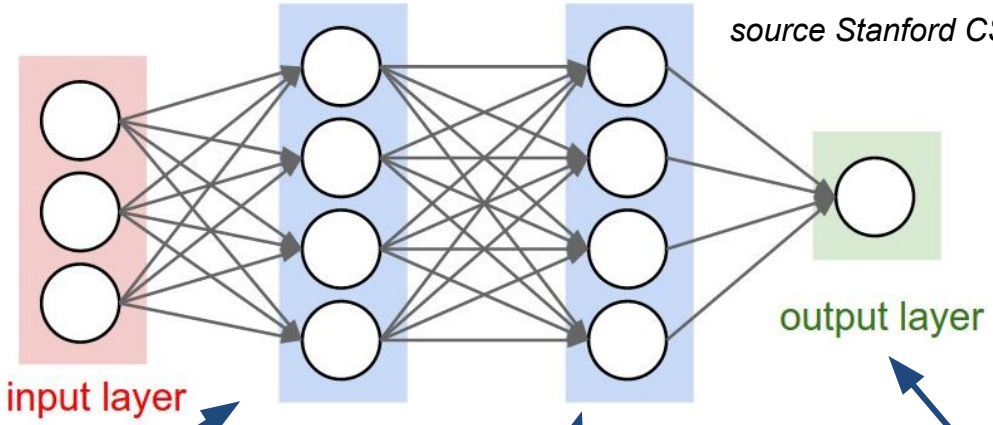
Example in [Keras]



The simple Neuron unit

Linear classifier gives 85% accuracy $\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$

Can we stack multiple **linear classifiers** to build something more powerful?



source Stanford CS231n

$$\mathbf{y}_i^{(1)} = \mathbf{W}^{(1)}\mathbf{x}_i + \mathbf{b}^{(1)}$$

$$\mathbf{y}_i^{(2)} = \mathbf{W}^{(2)}\mathbf{y}_i^{(1)} + \mathbf{b}^{(2)}$$

$$\hat{\mathbf{y}}_i = \mathbf{W}^{(3)}\mathbf{y}_i^{(2)} + \mathbf{b}^{(3)}$$

The simple Neuron unit

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Can we stack multiple **linear classifiers** to build something more powerful?

source Stanford CS231n

$$\mathbf{y}_i^{(1)} = \mathbf{W}^{(1)}\mathbf{x}_i + \mathbf{b}^{(1)}$$

$$\mathbf{y}_i^{(2)} = \mathbf{W}^{(2)}\mathbf{y}_i^{(1)} + \mathbf{b}^{(2)}$$

$$\hat{\mathbf{y}}_i = \mathbf{W}^{(3)}\mathbf{y}_i^{(2)} + \mathbf{b}^{(3)} \longrightarrow \hat{\mathbf{y}}_i = \mathbf{W}^{(3)}\left(\mathbf{W}^{(2)}\left(\mathbf{W}^{(1)}\mathbf{x}_i + \mathbf{b}^{(1)}\right) + \mathbf{b}^{(2)}\right) + \mathbf{b}^{(3)}$$

Lets

$$\hat{\mathbf{y}}_i = \mathbf{W}^{(3)}\mathbf{W}^{(2)}\mathbf{W}^{(1)}\mathbf{x}_i + \mathbf{W}^{(3)}\mathbf{W}^{(2)}\mathbf{b}^{(1)} + \mathbf{W}^{(3)}\mathbf{b}^{(2)} + \mathbf{b}^{(3)}$$

$$\hat{\mathbf{y}}_i = \mathbf{W}'\mathbf{x}_i + \mathbf{b}'$$

The model with multiple layers cannot be better than single layer case!

The simple Neuron unit

The definition of neuron

To obtain neuron (fully connected layer) we replace

$$\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$$

with

$$\hat{\mathbf{y}}_i = f\left(\mathbf{W}\mathbf{x}_i + \mathbf{b}\right)$$

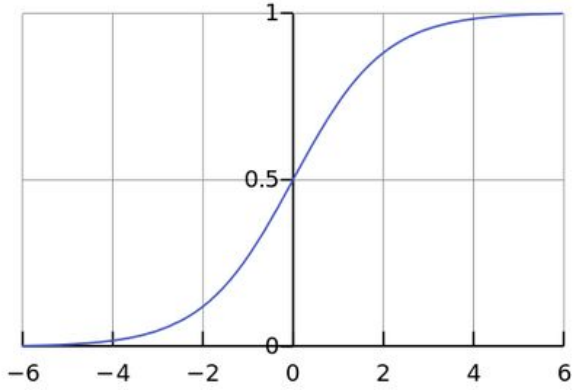
where **f(...)** is so-called activation function

f is a non linear function hence we cannot factorize multiple layers as before

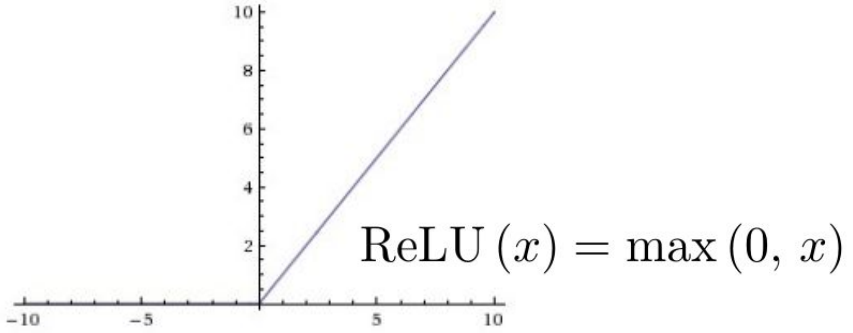
Some examples:

- sigmoid

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



- ReLU (Rectified Linear Unit)



The simple Neuron classifier revisited

We are going to solve the same problem as before lets add nonlinearity

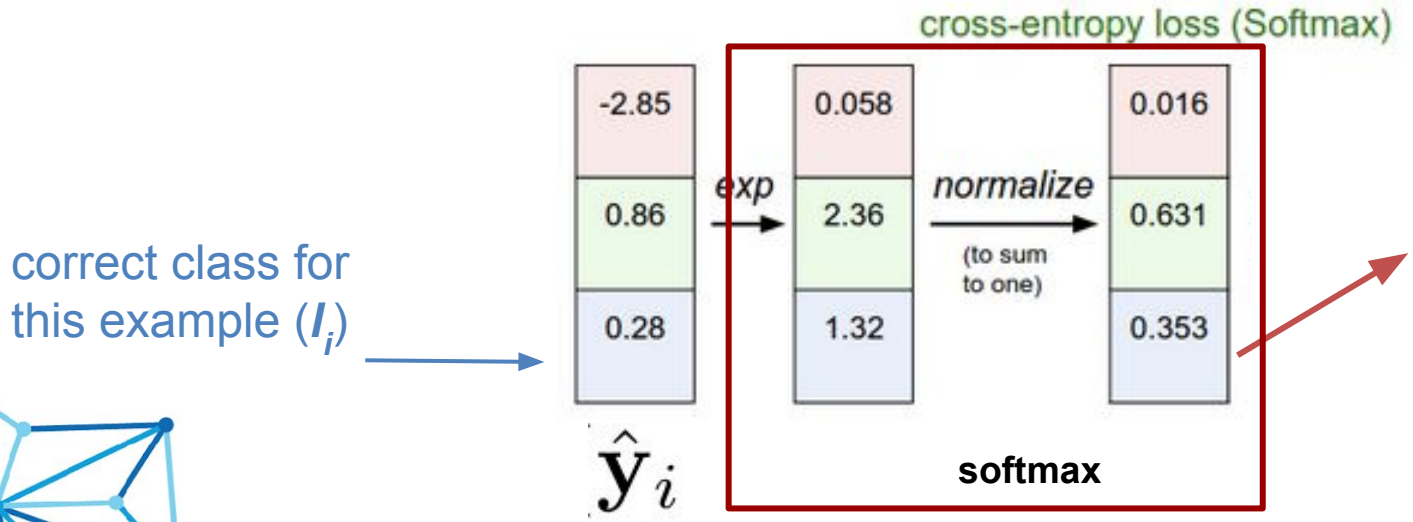
$$\hat{\mathbf{y}}_i = f\left(\mathbf{W}\mathbf{x}_i + \mathbf{b}\right)$$

The standard approach for last layer in classification problem is a softmax activation function for 10 classes:

$$f\left(\hat{\mathbf{y}}_i\right) = \frac{e^{\hat{y}_{il_i}}}{\sum_{k=1}^{10} e^{\hat{y}_{ik}}}$$

Note: In keras softmax activation returns vector of probabilities

Then the standard approach i to use cross-entropy loss function: $l_i = -\log(p(\hat{\mathbf{y}}_i))$



correct class for this example (l_i)

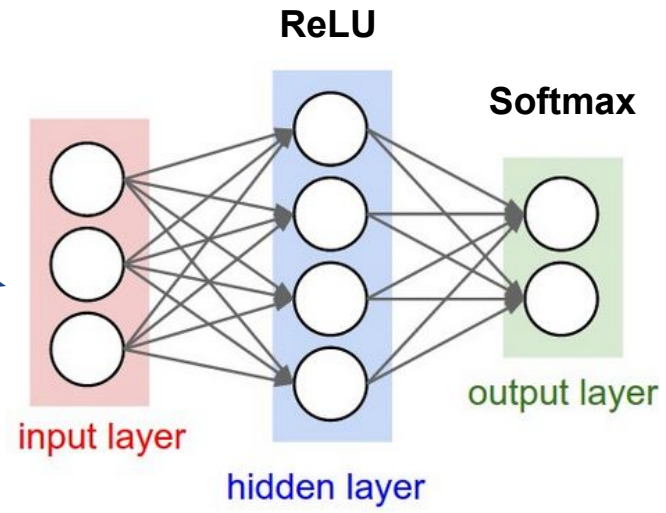
$$l_i = -\log(0.353) = 1.04$$

source: Stanford CS231 course

The simple Neuron classifier revisited

Examples in Keras:

- single layer with softmax: 0.9 accuracy!
- double layer with softmax

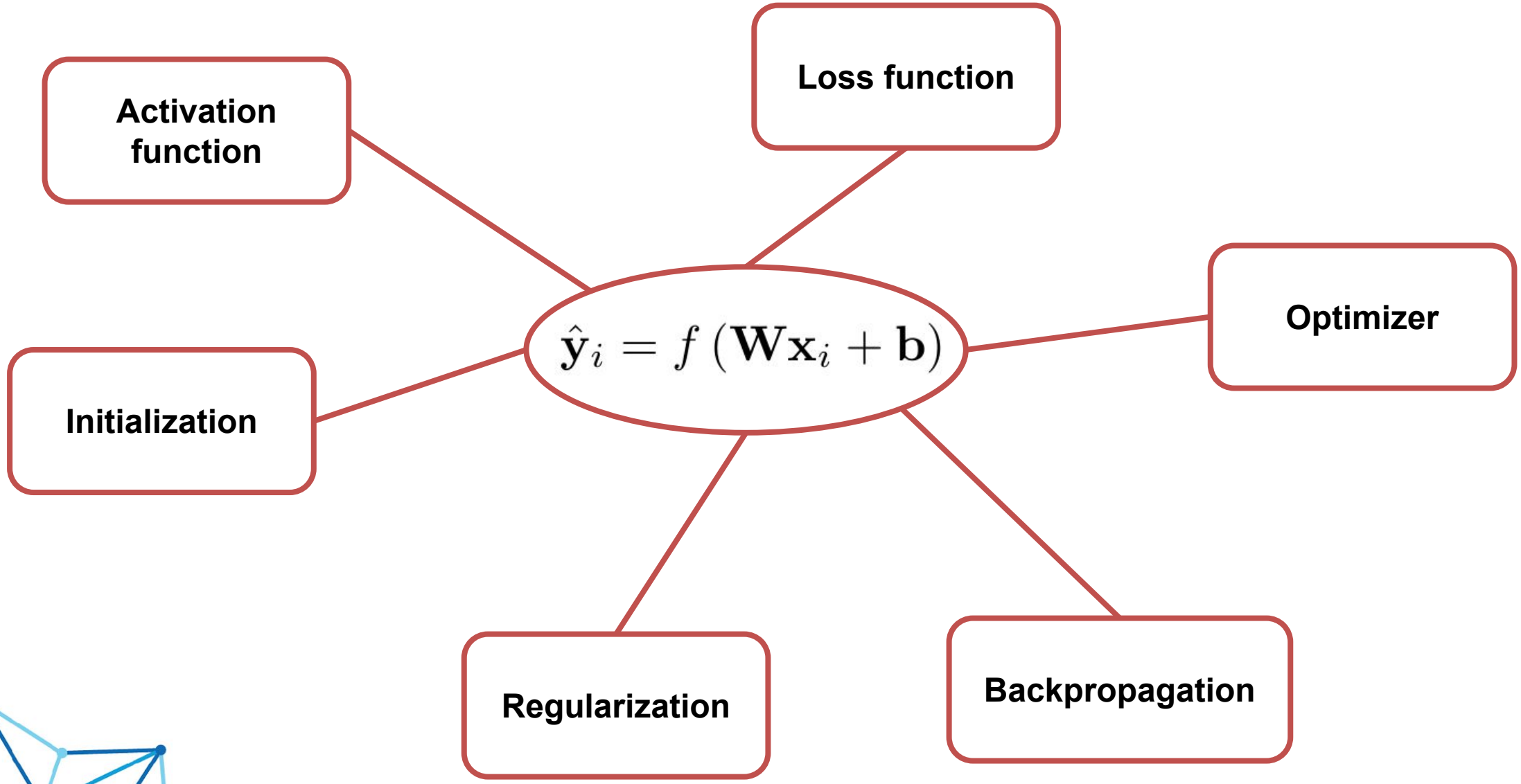


source: Stanford CS231 course

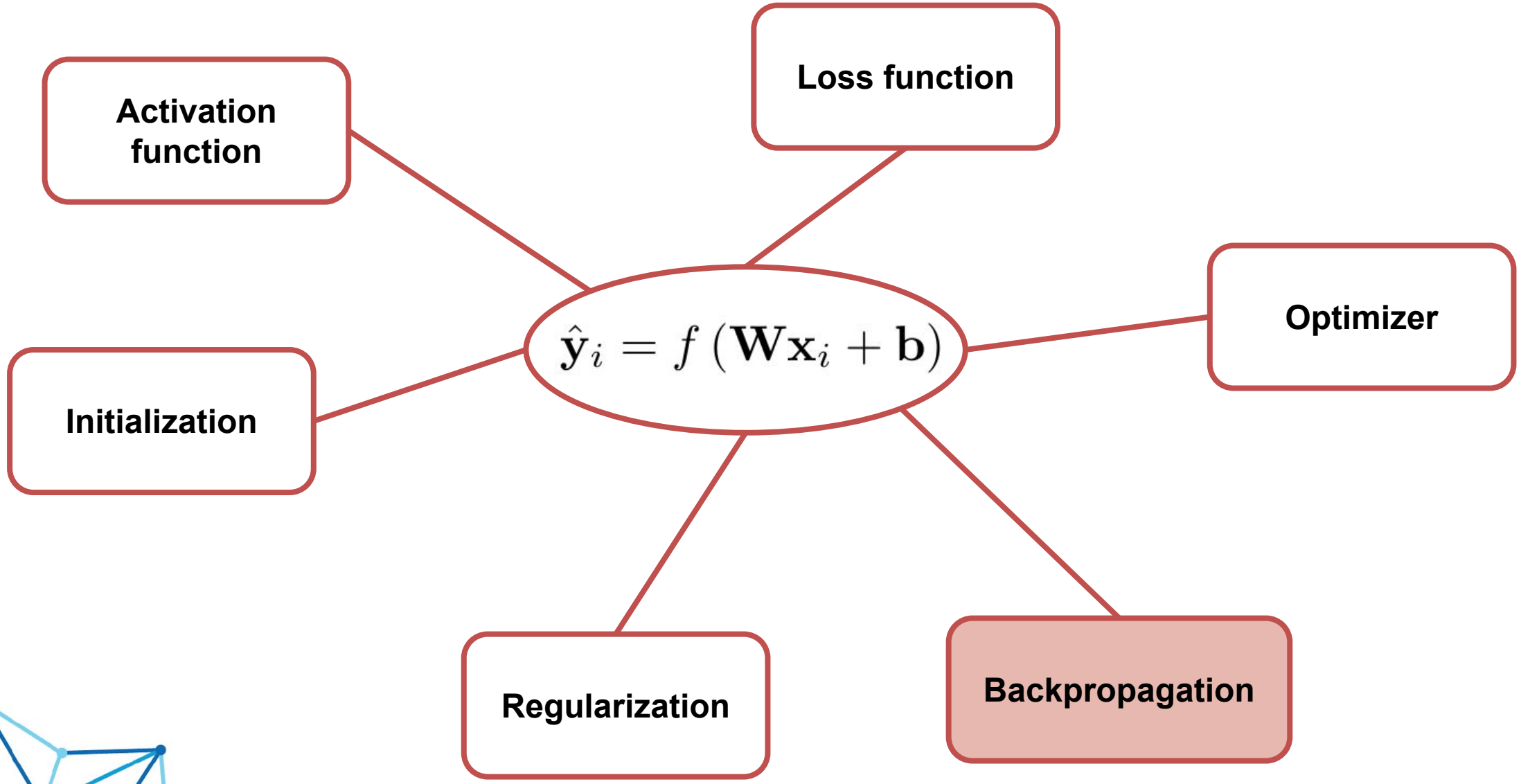
with double layer NN we get 0.98 accuracy!

NN extreme crash course

Neural Networks



Neural Networks



Backpropagation

Backpropagation is a pillar of deep learning

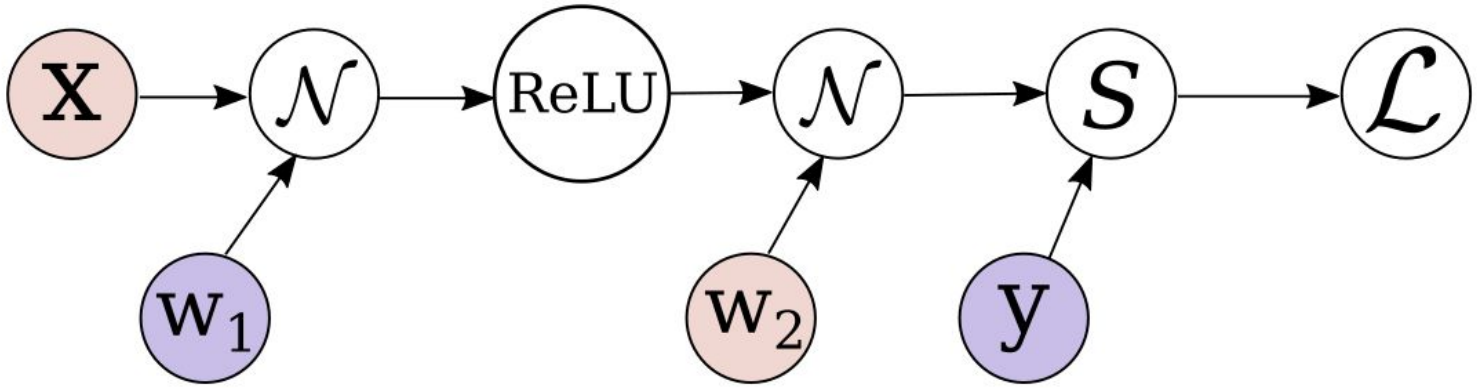
$$\theta^{k+1} := \theta^k - \lambda \left. \frac{\partial \mathcal{L}}{\partial \theta^k} \right|_{\text{mini-batch}}$$

$$\mathcal{L}_{\text{mini-batch}} \equiv \frac{1}{N_{\text{MB}}} \sum_{i \in \text{MB}}^{N_{MB}} MSE\left(\hat{\mathbf{y}}_i, \mathbf{y}_i\right)$$

Layer (type)	Output Shape	Param #
x (InputLayer)	(None, 784)	0
W1 (Dense)	(None, 100)	78500
W2 (Dense)	(None, 10)	1010

we need to compute gradient of loss with respect to model parameters

Lets come back to our two layer neural network



Backpropagation

Backpropagation of mini-batch

$$\theta^{k+1} := \theta^k - \lambda \left.\frac{\partial \mathcal{L}}{\partial \theta^k}\right|_{\text{mini-batch}}$$

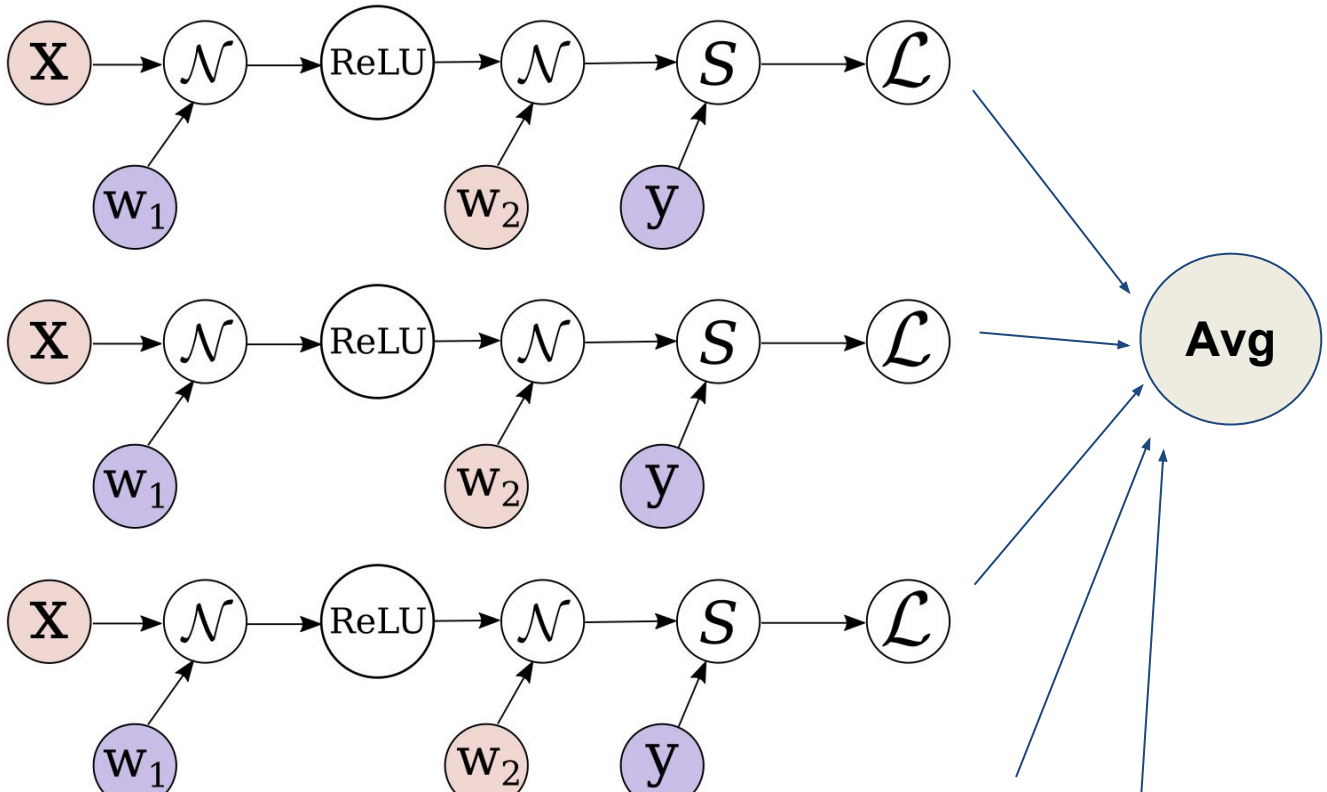
$$\mathcal{L}_{\text{mini-batch}} = \frac{1}{N_{MB}} \sum_{i \in MB}^{N_{MB}} \mathcal{L}_i$$

hence the gradient

$$\left.\frac{\partial \mathcal{L}}{\partial \theta}\right|_{\text{mini-batch}} = \frac{1}{N_{MB}} \sum_{i \in MB}^{N_{MB}} \boxed{\frac{\partial \mathcal{L}_i}{\partial \theta}}$$

1st example in MB

2nd example in MB

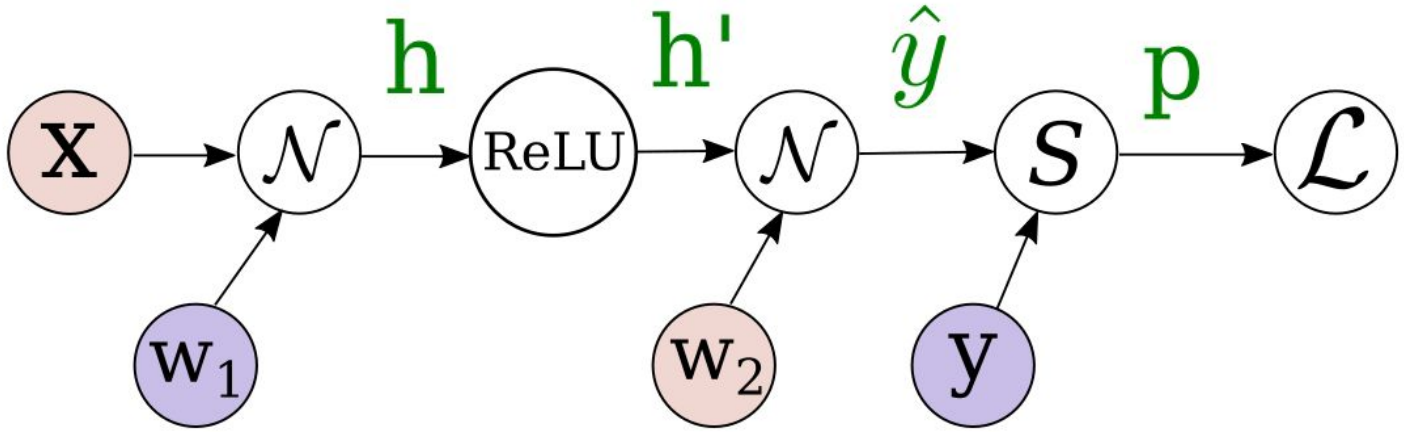


Avg - is a linear operation hence we can compute gradients for each example in mini-batch separately and then compute mean gradient on mini-batch

Backpropagation

$$\theta^{k+1} := \theta^k - \lambda \left. \frac{\partial \mathcal{L}}{\partial \theta^k} \right|_{\text{mini-batch}}$$

Forward pass



$$\mathcal{N}(x; w_1) = w_1 x$$

$$ReLU(x) = \max(0, x)$$

$$\mathcal{L}(x) = -\log(x)$$

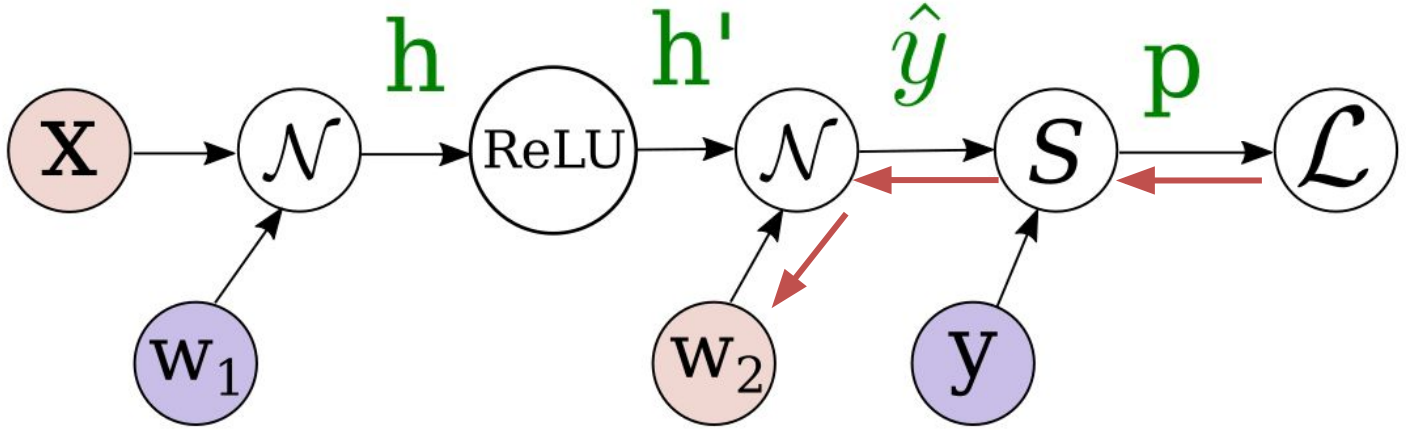
$$p(\hat{\mathbf{y}}_i) = \frac{e^{\hat{y}_{il_i}}}{\sum_{k=1}^{10} e^{\hat{y}_{ik}}}$$

In forward pass we have to define output value for each type node for given input vector

Backpropagation

$$\theta^{k+1} := \theta^k - \lambda \left. \frac{\partial \mathcal{L}}{\partial \theta^k} \right|_{\text{mini-batch}}$$

In backward pass we use chain rule to find gradients



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Chain rule for w_2

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial p} \frac{\partial p}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_2} = -\frac{1}{p} s \cdot h'^T$$

Each of the components can be computed easily e.g.:

$$\frac{\partial \mathcal{L}(p)}{\partial p} = -\frac{1}{p}$$

$$\frac{\partial p}{\partial \hat{y}} = s$$

$$\hat{y} = w_2 h' = \mathcal{N}(h'; w_2)$$

$$\frac{\partial \hat{y}}{\partial w_2} = h'^T$$

Backpropagation

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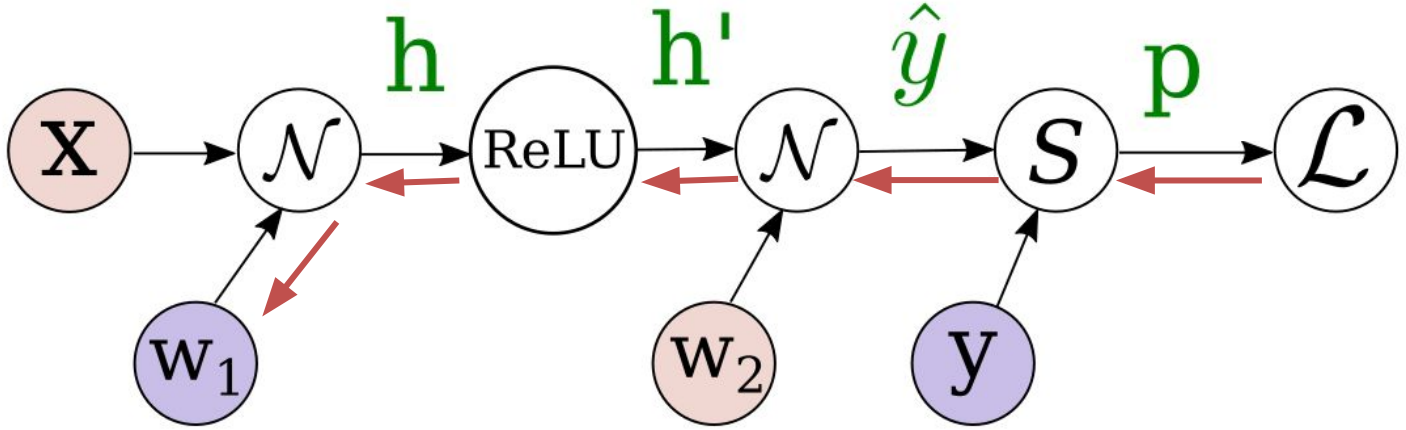

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$$p(\hat{\mathbf{y}}_i) = \frac{e^{\hat{y}_{il_i}}}{\sum_{k=1}^{10} e^{\hat{y}_{ik}}}$$

Chain rule for w_2

$$\frac{\partial \mathcal{L}}{\partial w_2} = \frac{\partial \mathcal{L}}{\partial p} \frac{\partial p}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_2}$$

Chain rule for w_1

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial p} \frac{\partial p}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial h'} \frac{\partial h'}{\partial h} \frac{\partial h}{\partial w_1}$$

Backpropagation

$$\theta^{k+1} := \theta^k - \lambda \left. \frac{\partial \mathcal{L}}{\partial \theta^k} \right|_{\mathrm{mini-batch}}$$

What we can learn from that:

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial p} \frac{\partial p}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial h'} \frac{\partial h'}{\partial h} \frac{\partial h}{\partial w_1}$$

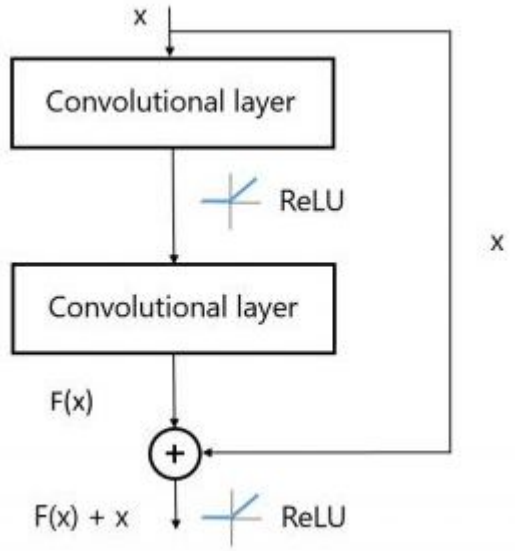
- if one of the factors is close to zero, gradient vanishes, hence no update
- oppositely, many multiplication of large numbers may lead to exploding gradients problem

Backpropagation

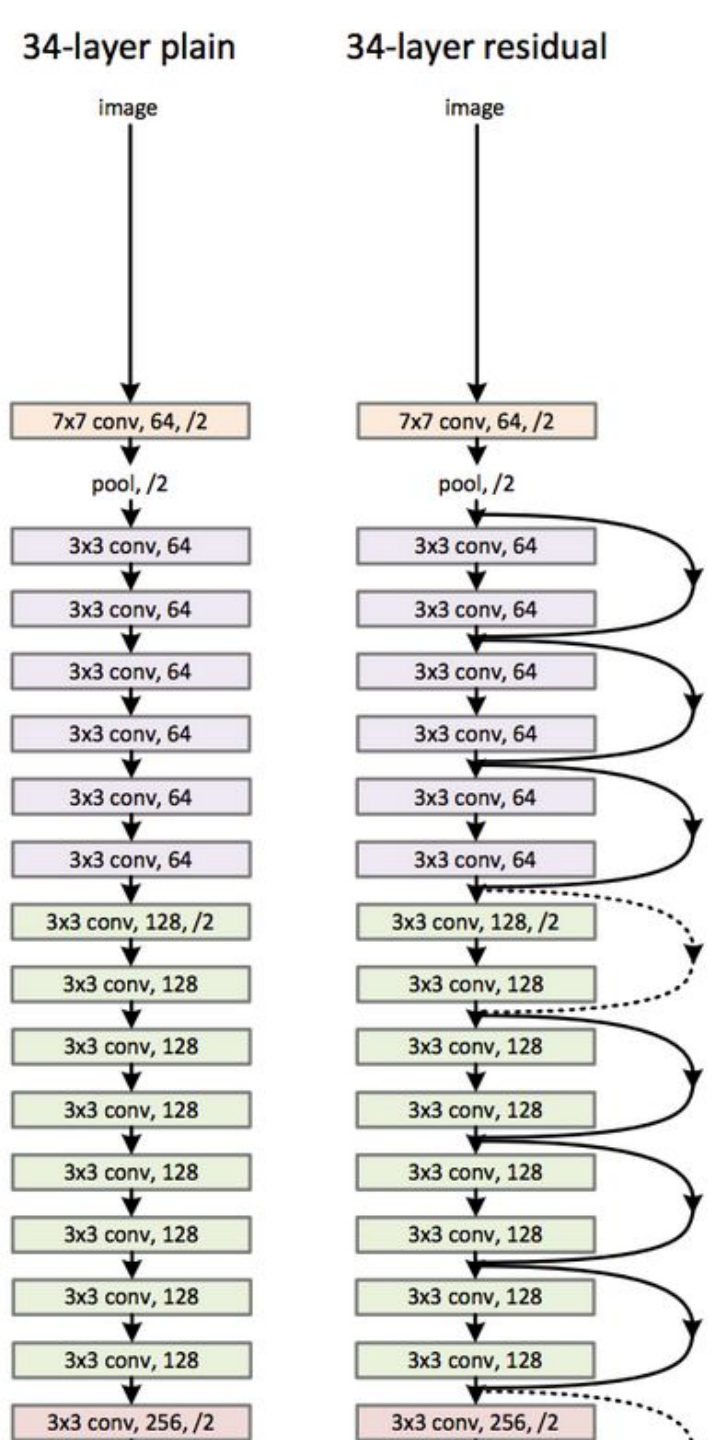
What we can learn from that:

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial p}\frac{\partial p}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial h'}\frac{\partial h'}{\partial h}\frac{\partial h}{\partial w_1}$$

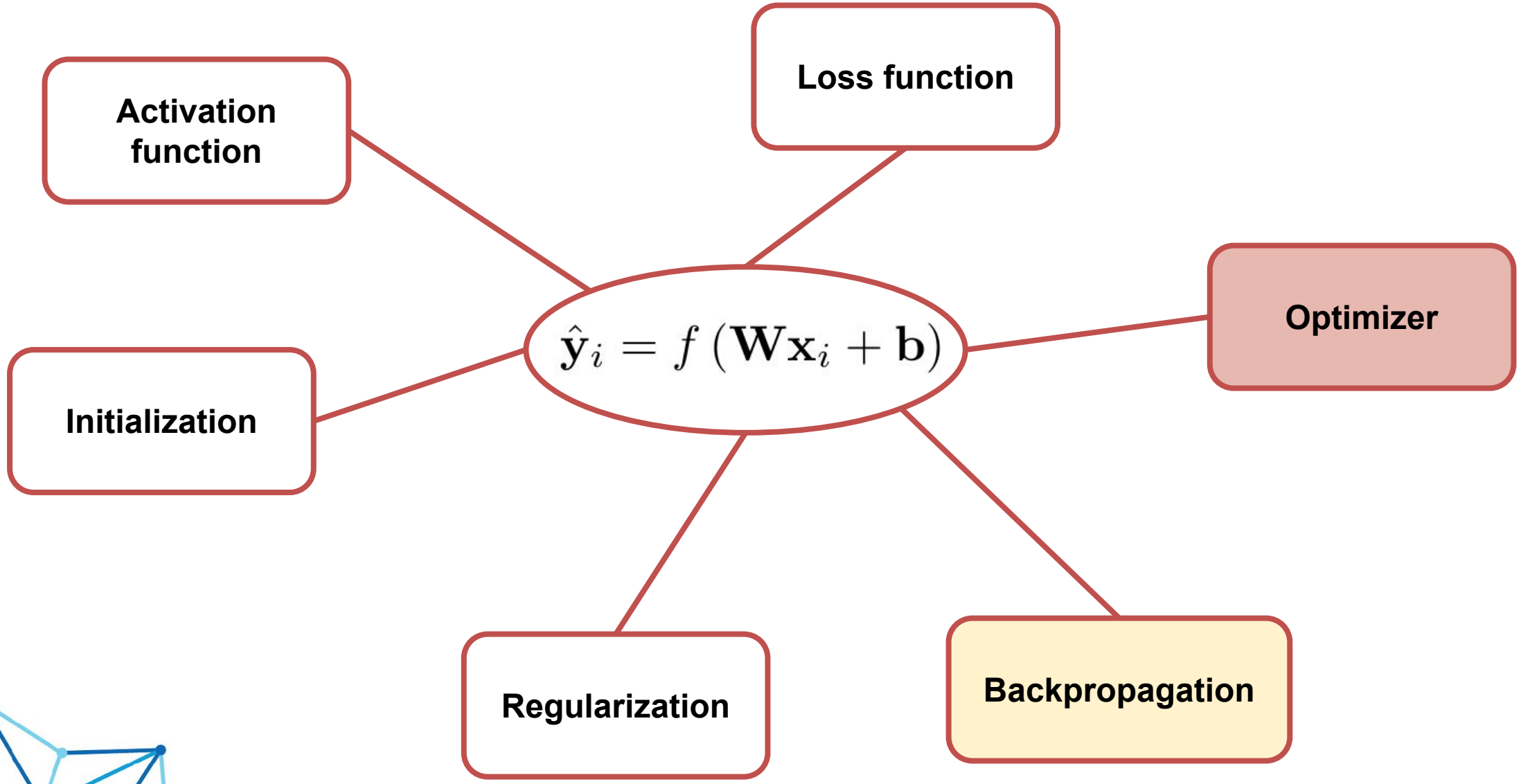
- We problem of vanishing gradients can be solve with skip connections: ResNet architecture
- ImageNet 2015 winning solution



in such case the gradient can propagate by two branches



Neural Networks



Optimizer

We know how the gradients are computed - backpropagation i.e. chain rule

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial p}\frac{\partial p}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial h'}\frac{\partial h'}{\partial h}\frac{\partial h}{\partial w_1}$$

gradients are used to update model parameters:

$$\theta^{k+1} := \theta^k - \lambda \left.\frac{\partial \mathcal{L}}{\partial \theta^k}\right|_{\mathrm{mini-batch}}$$

- **Batch gradient descent** - the simplest and the slowest one, compute gradients for all data

$$\theta = \theta - \eta \cdot \nabla_\theta J(\theta)$$

source: S. Ruder post

Optimizer

We know how the gradients are computed - backpropagation i.e. chain rule

$$\frac{\partial \mathcal{L}}{\partial w_1} = \frac{\partial \mathcal{L}}{\partial p}\frac{\partial p}{\partial \hat{y}}\frac{\partial \hat{y}}{\partial h'}\frac{\partial h'}{\partial h}\frac{\partial h}{\partial w_1}$$

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- **Stochastic gradient descent (SGD)** - (mini-batch version) - compute gradients for set of examples, typically ~10 to ~100 examples in batch

source: S. Ruder post

Optimizer

- **Batch gradient descent** - the simplest and the slowest one, compute gradients for all data
- **Stochastic gradient descent (SGD)** - (mini-batch version) - compute gradients for set of examples, typically ~10 to ~100 examples in batch
- **Momentum** - improves SGD by adding velocity term which accumulates gradient vector during training

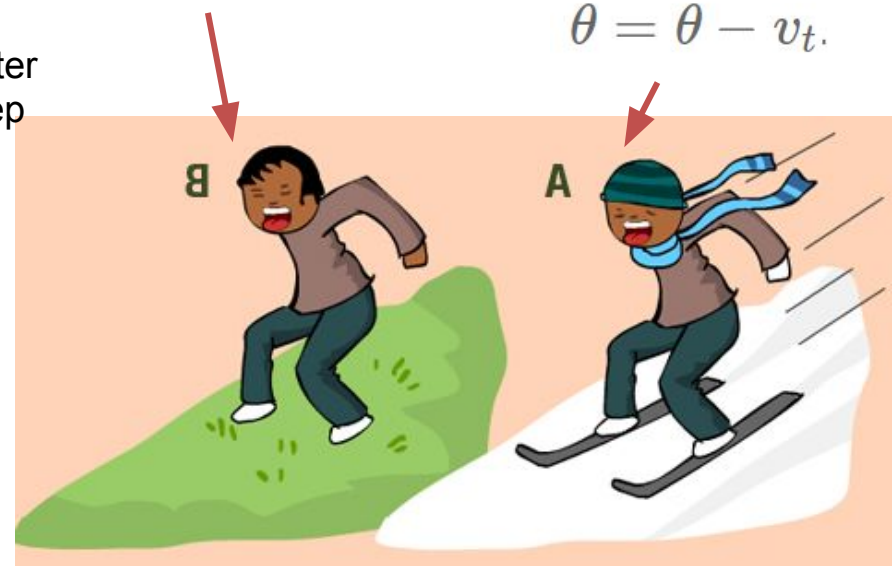
$$\theta = \theta - \eta \cdot \nabla_\theta J(\theta)$$

$$v_t = \gamma v_{t-1} + \eta \nabla_\theta J(\theta).$$

$$\theta = \theta - v_t.$$

gamma - momentum term, usually 0.9, when 0 we recover SGD

SGD
stops after each step



It simulates Newton dynamics problem with gradient being the force

Note: Momentum equal 1 means no friction, the movement will never stop

source: S. Ruder post

Optimizer

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- **Nesterov accelerated gradient (NAG)** - extension to the momentum method, compute gradient by approximating position in the next step

$$v_t = \gamma v_{t-1} + \eta \nabla_\theta J(\theta).$$

$$\theta = \theta - v_t.$$

$$v_t = \gamma v_{t-1} + \eta \nabla_\theta J(\theta - \gamma v_{t-1}).$$

$$\theta = \theta - v_t.$$

source: S. Ruder post

Optimizer

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- **Adagrad** (Duchi, J 2011)- performs adaptive tuning of learning rate based on model parameters

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \odot \nabla_\theta J(\theta_i)$$

Gt is a sum of square gradients accumulated over all time steps

```
dLdw_cache += dLdw**2
W += - learning_rate * dLdw / (np.sqrt(dLdw_cache) + eps)
```

source: S. Ruder post

Optimizer

- **Batch gradient descent** - the simplest and the slowest one, compute gradients for all data
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- **Adadelta** (Zeiler, M. D. (2012)), **RMSprop** (G. Hinton) - extensions to Adagrad, reduces the problem with monotonically decreasing learning rate by

```
dLdw_cache =  dLdw_cache*decay_rate +  dLdw**2*(1 - decay_rate)
W += - learning_rate * dLdw / (np.sqrt(dLdw_cache) + eps)
```

RMSprop implementation: decay_rate is usually 0.9

source: S. Ruder post

Optimizer

- **Batch gradient descent** - the simplest and the slowest one, compute gradients for all data
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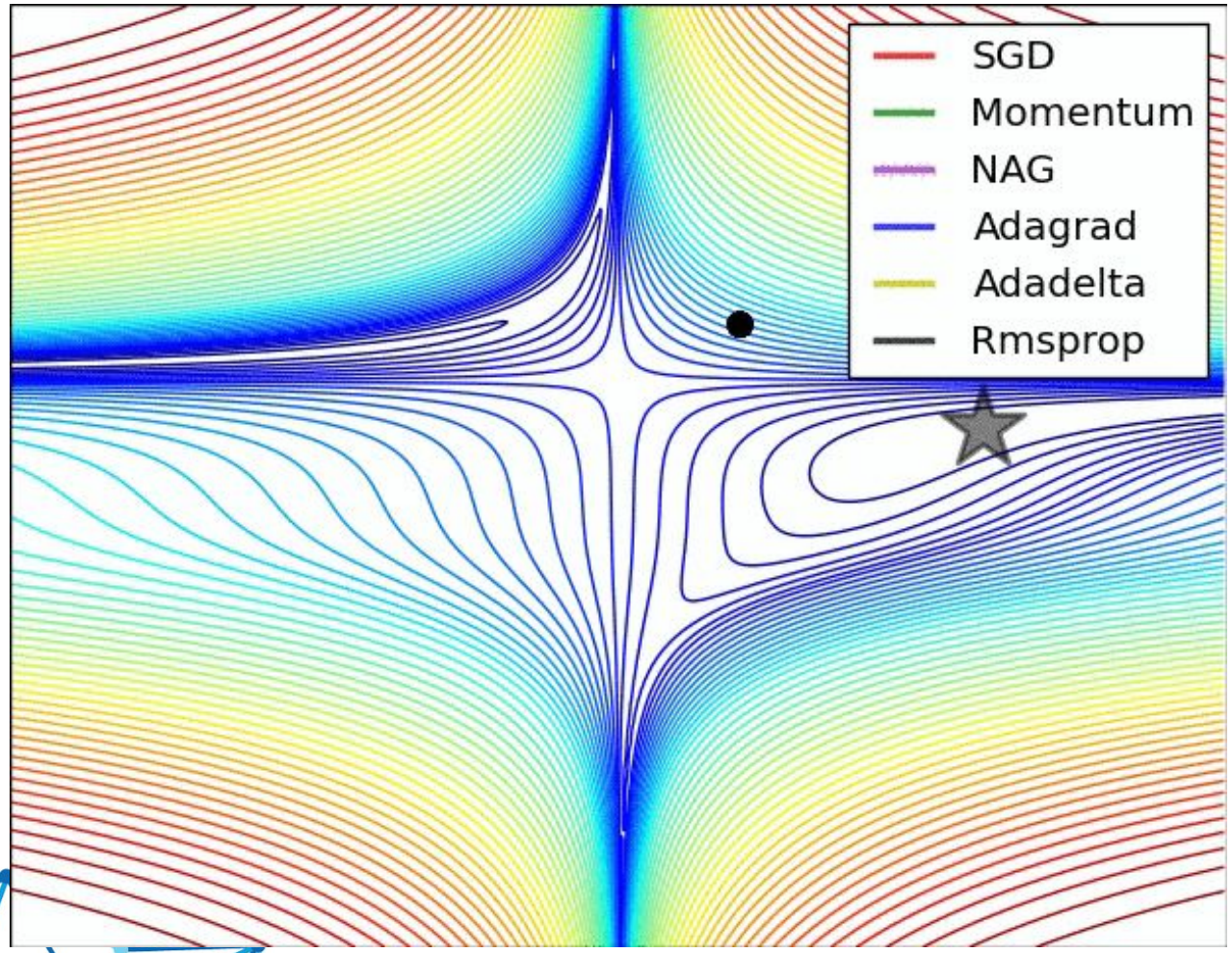
- **Adam** (Adaptive Moment Estimation) (Kingma, D. P., & Ba, J. L. (2015)) - a marriage of **momentum** and **RMSprop** methods

source: S. Ruder post

Optimizer

Comparison of different optimizers



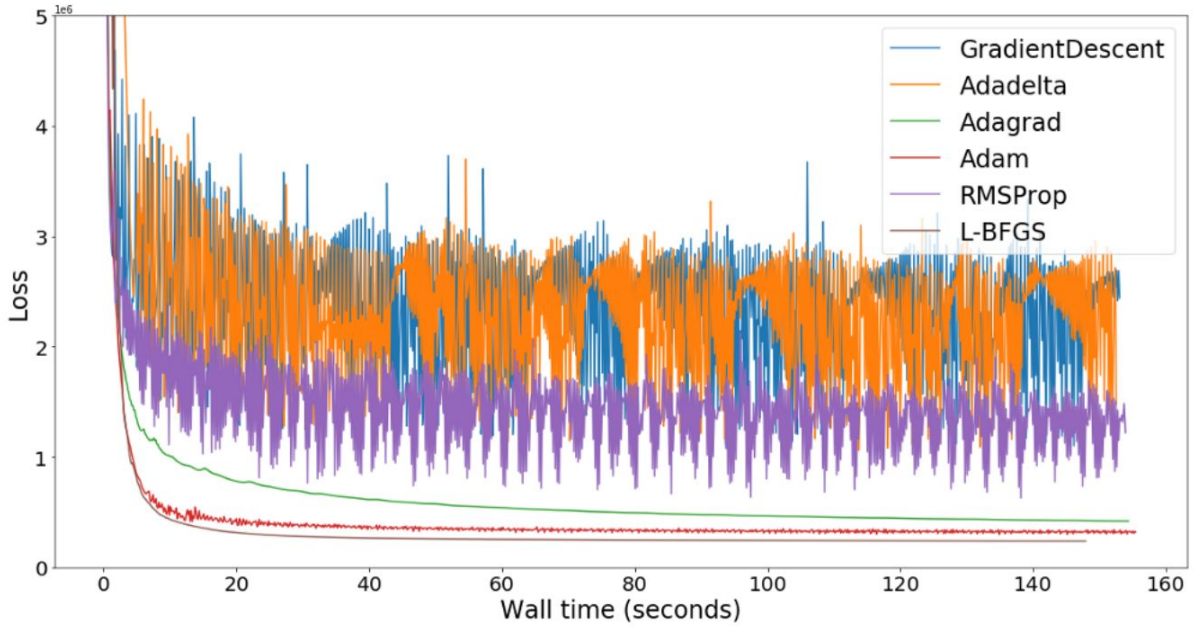
Now it is recommended to use Adam, Adadelta, RMSprop

Images credit: Alec Radford.

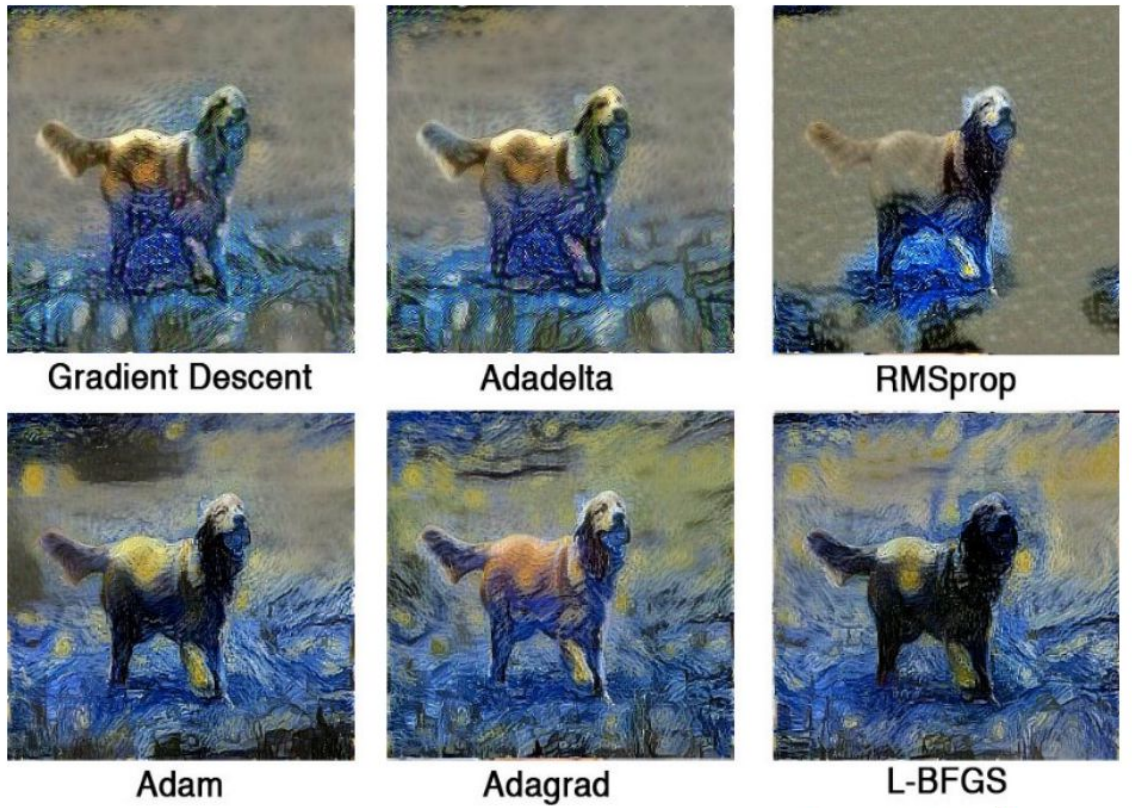
Optimizer

The choice of the optimizer may significantly affect model predictions

Landscape (content) + Scream (style)



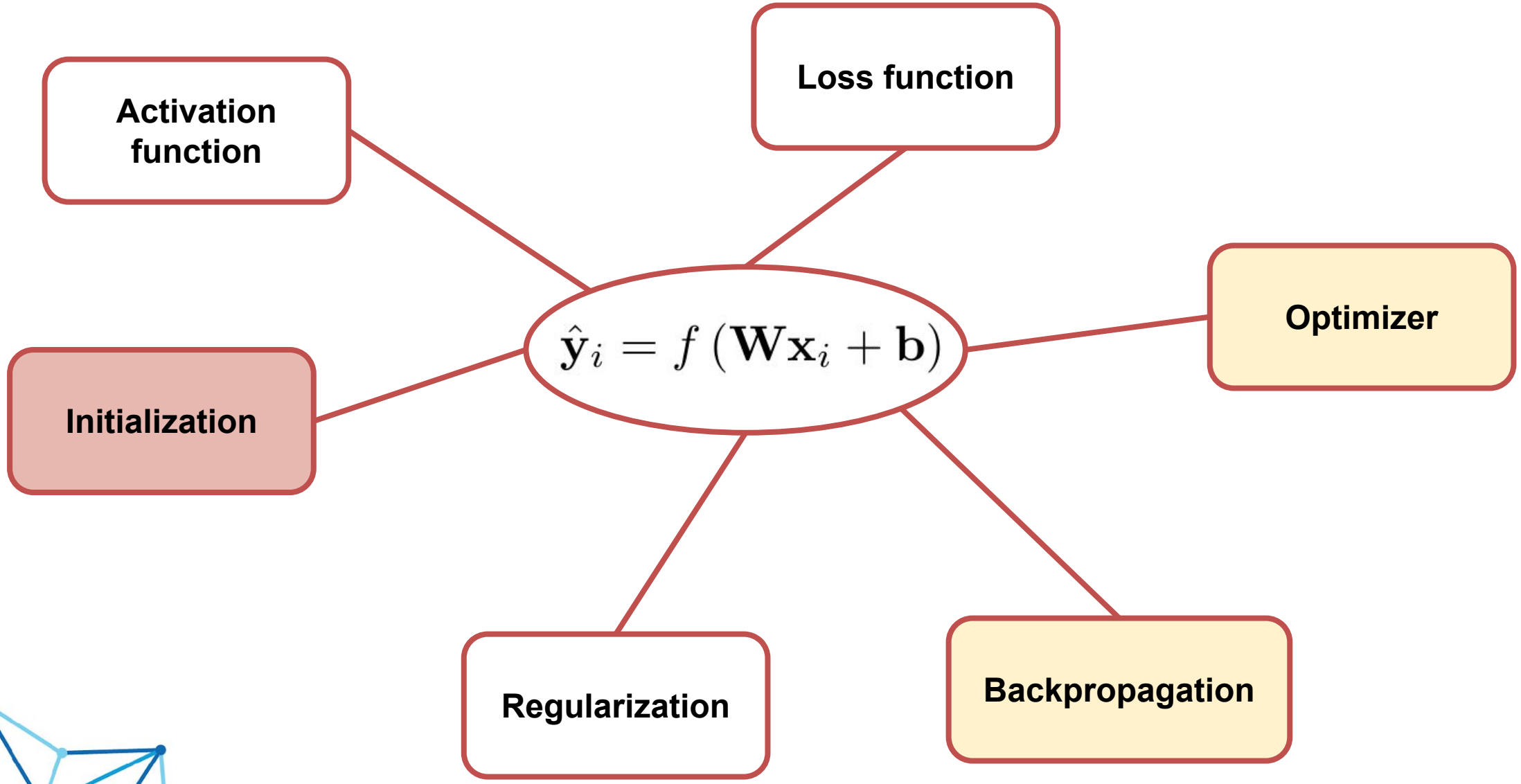
Style transfer: which optimizer choose to get the best results?



$$x \leftarrow x - [Hf(x)]^{-1} \nabla f(x)$$

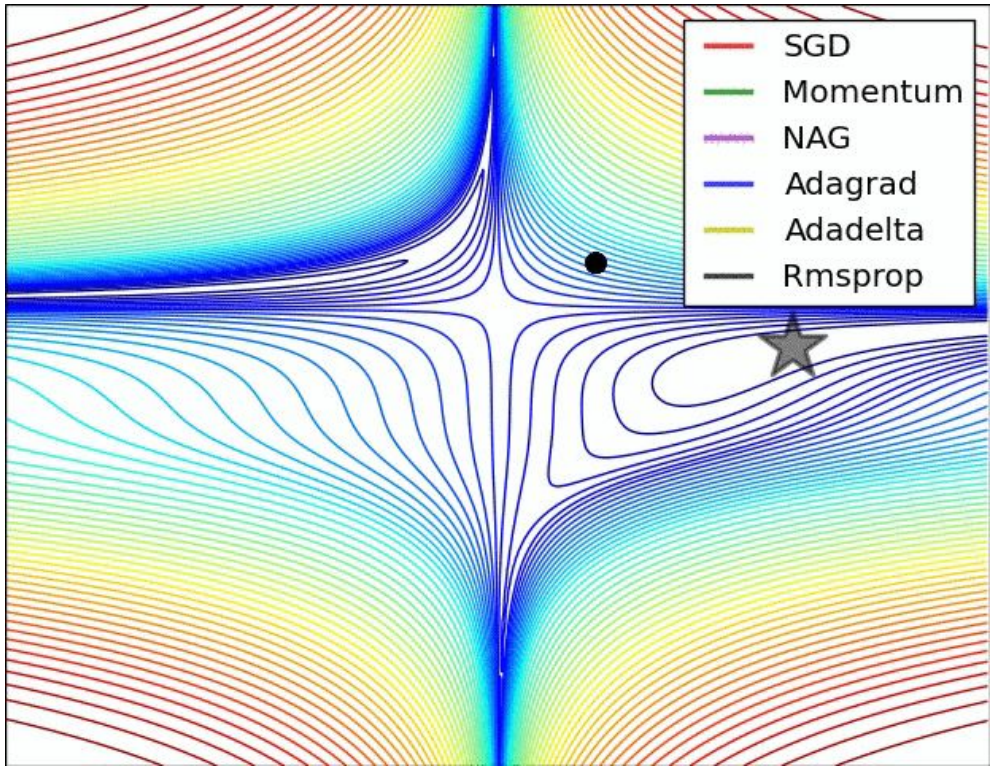
source: [Slav Ivanov blog post]

Neural Networks



Initialization

We've seen the performance of each methods on the convergence:



Images credit: Alec Radford.

- One of the biggest problems in DL was improper initialization of system parameters
- Mostly solved thanks to normalization techniques (**discussed later in the talk**)

- We initialize weights with some small random numbers
- This helps to break symmetries in our model

Probably the most popular is **Glorot**, **Bengio (2010)** initialization:

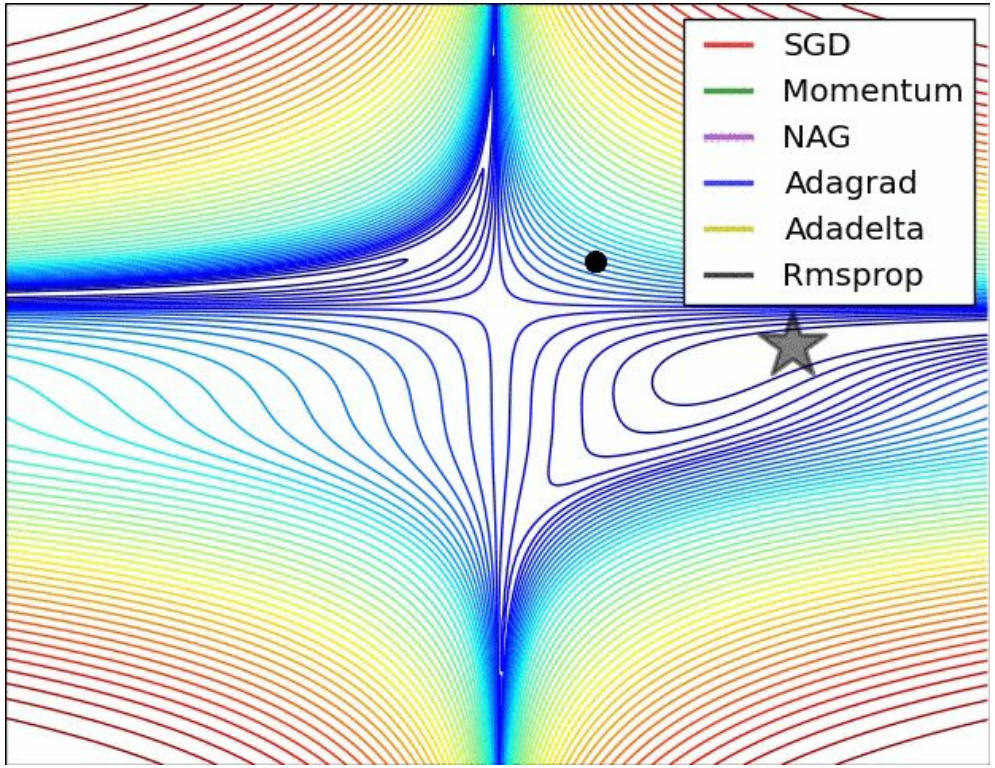
$$W_{i,j} \sim U\left(-\frac{6}{\sqrt{m+n}}, \frac{6}{\sqrt{m+n}}\right)$$

m/n - number of input.output units

We usually initialize bias vector with zero

Initialization

We've seen the performance of each methods on the convergence:



Images credit: Alec Radford.

- One of the biggest problems in DL was improper initialization of system parameters
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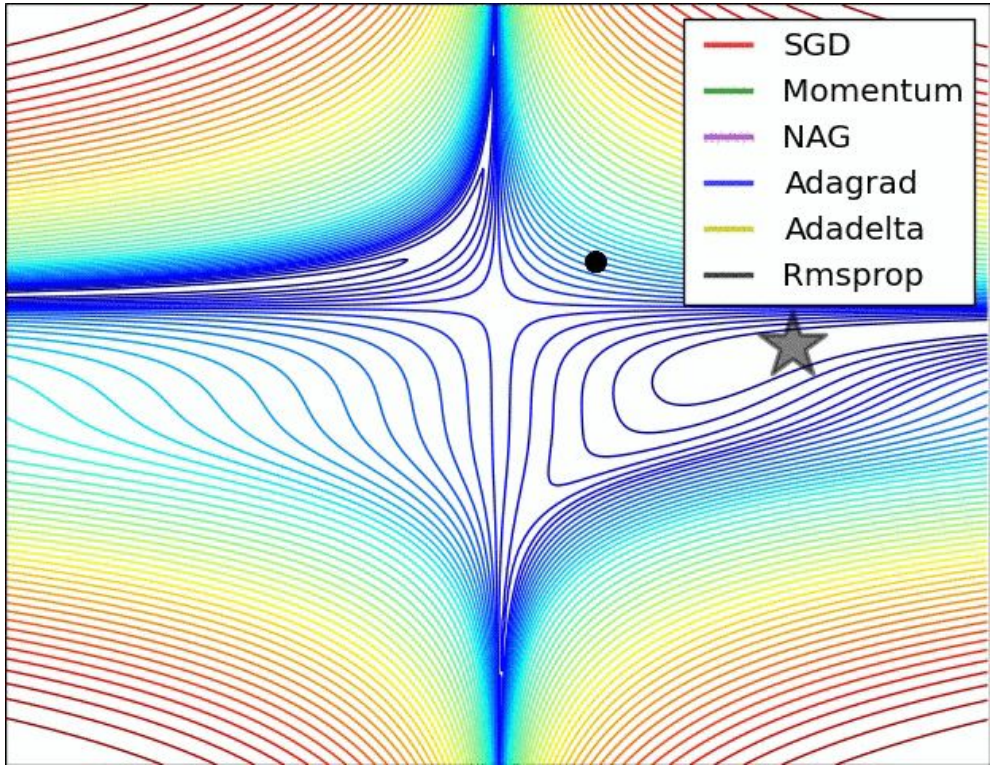
Less popular but worth to try: **orthogonal initialization (Saxe et al. (2013))**: orthogonal matrices preserve the norm, hence we can mostly avoid the vanishing and exploding gradients.

Initialization

We've seen the performance of each methods on the convergence:



Images credit: Alec Radford.

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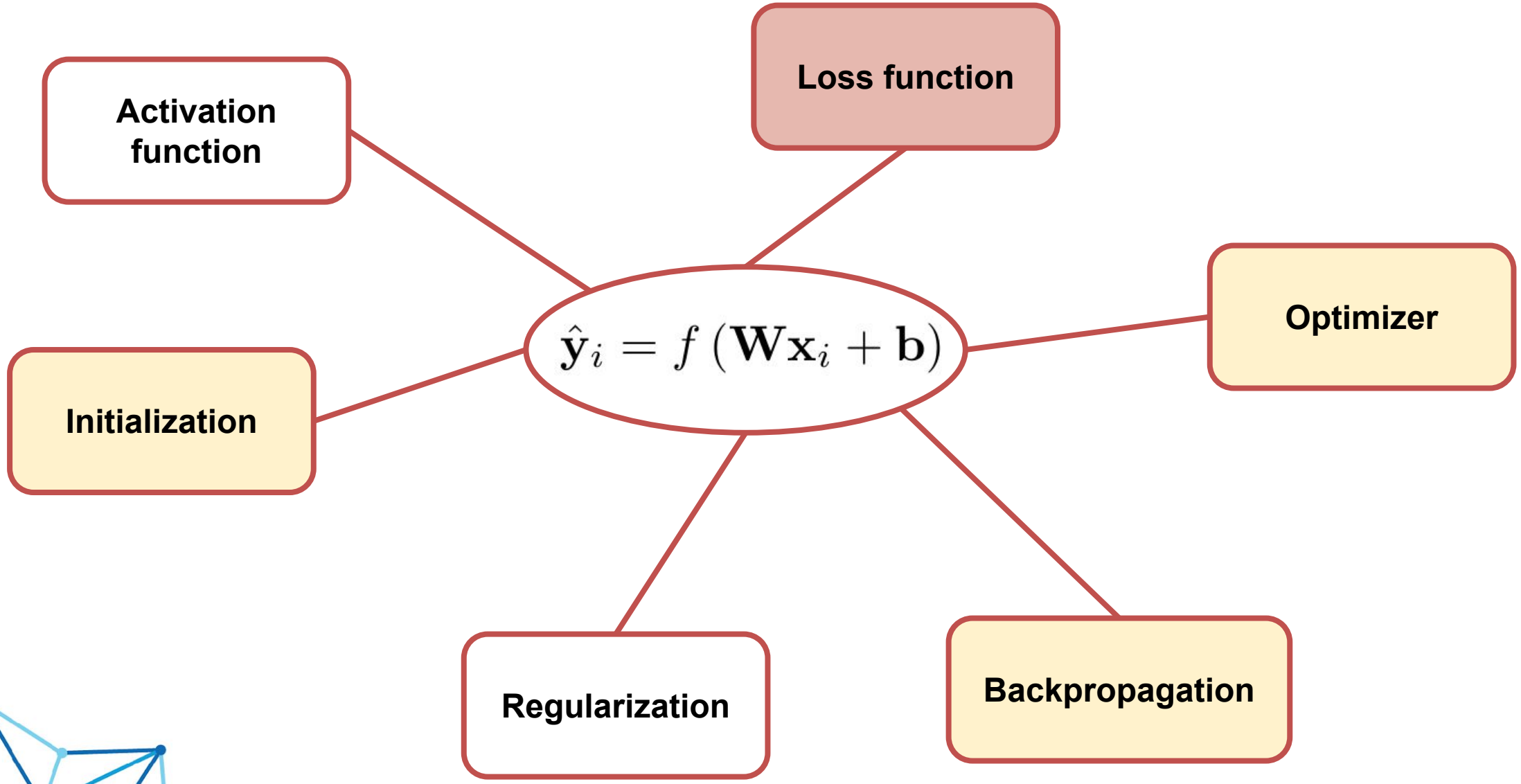
Sparse initialization (Martens (2010)) - each unit is initialized to have k non-zero weights

Neural Networks



Loss function

By choosing loss function we shape the gradient flow in the network

$$\frac{\partial \mathcal{L}}{\partial w_1} = \boxed{\frac{\partial \mathcal{L}}{\partial p}} \frac{\partial p}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial h'} \frac{\partial h'}{\partial h} \frac{\partial h}{\partial w_1}$$

The type of used loss function will depend on the type of problem we want to solve

Classification problem:

$$L_i = \sum_{j \neq y_i} \max(0, f_j - f_{y_i} + 1)$$

hinge loss

also squared hinge loss

$$L_i = -\log\left(\frac{e^{f_{y_i}}}{\sum_j e^{f_j}}\right)$$

softmax loss

Loss function

Regression problem: prediction of real valued quantities (e.g. average price)

$$L_i = \|f - y_i\|_2^2$$

squared L2 norm

$$L_i = \|f - y_i\|_1 = \sum_j |f_j - (y_i)_j|$$

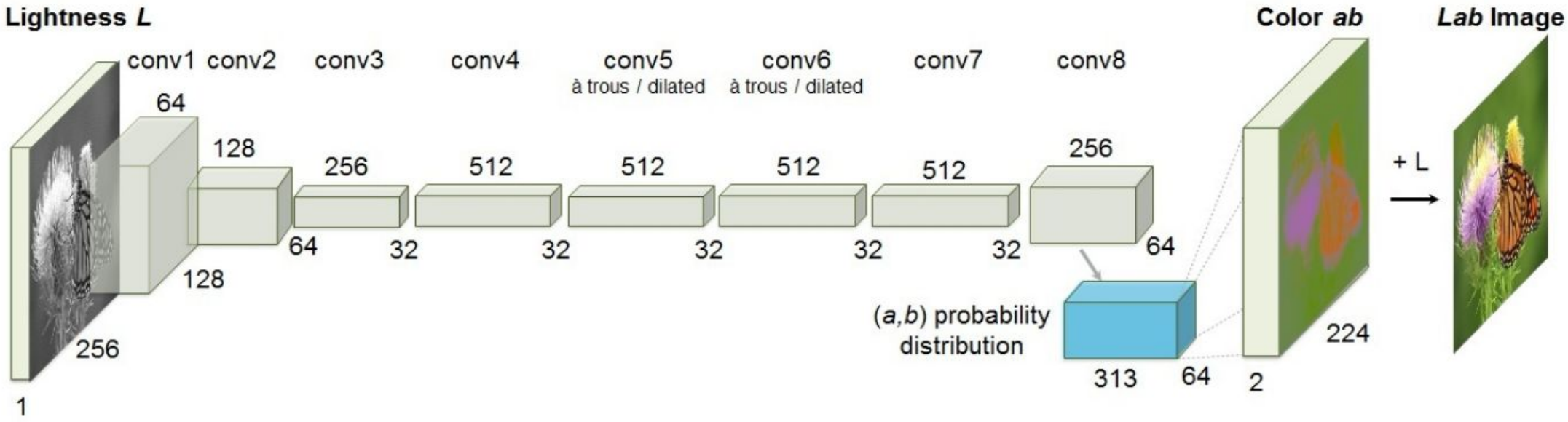
L1 norm

and many others: cosine proximity, KL divergence, ...

Loss function

Choosing loss function may have very serious consequences on model accuracy

Task: Given the input image in grayscale predict its pixel color:



Zhang, Isola, Efros. Colorful Image Colorization. ECCV, 2016.

Given an input lightness channel $\mathbf{X} \in \mathbb{R}^{H \times W \times 1}$, our objective is to learn a mapping $\widehat{\mathbf{Y}} = \mathcal{F}(\mathbf{X})$ to the two associated color channels $\mathbf{Y} \in \mathbb{R}^{H \times W \times 2}$, where H, W are image dimensions.

Loss function

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$$\mathrm{L}_2(\widehat{\mathbf{Y}}, \mathbf{Y}) = \frac{1}{2} \sum_{h,w} \|\mathbf{Y}_{h,w} - \widehat{\mathbf{Y}}_{h,w}\|_2^2$$

A natural choice of loss function could be L2 norm

Instead of they use multinomial classification problem on ab color

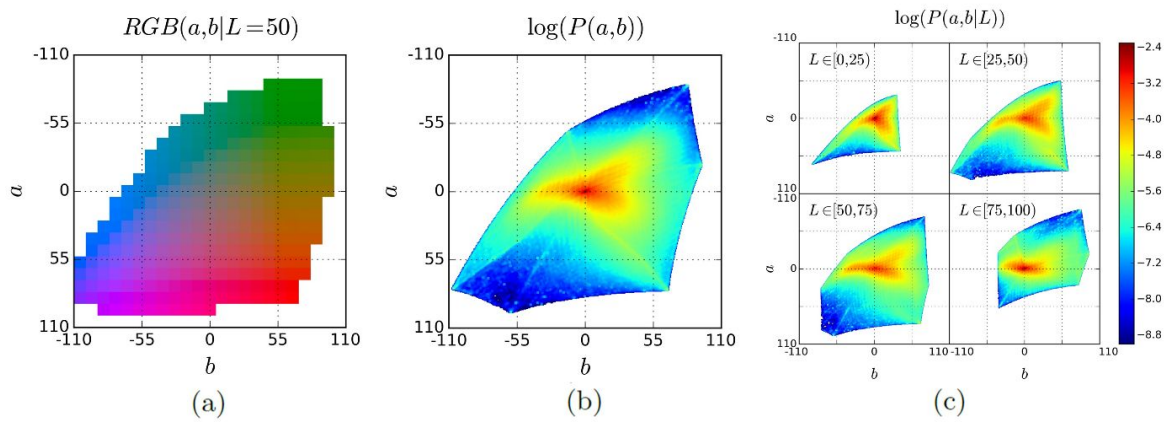


Fig. 3. (a) Quantized ab color space with a grid size of 10. A total of 313 ab pairs are in gamut. (b) Empirical probability distribution of ab values, shown in log scale. (c) Empirical probability distribution of ab values, conditioned on L, shown in log scale.

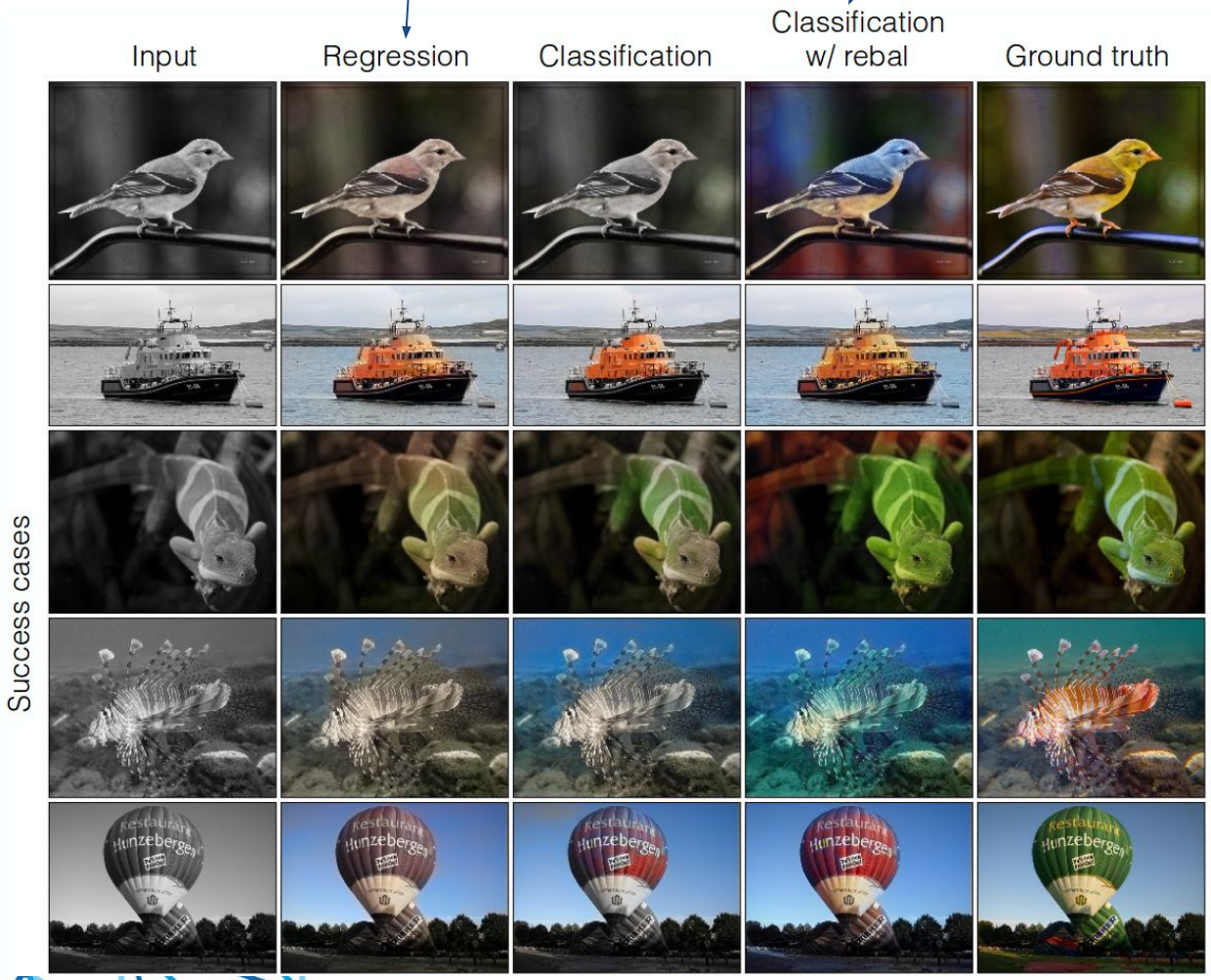
$$\mathrm{L}_{cl}(\widehat{\mathbf{Z}}, \mathbf{Z}) = -\sum_{h,w} v(\mathbf{Z}_{h,w}) \sum_{q} \mathbf{Z}_{h,w,q} \log(\widehat{\mathbf{Z}}_{h,w,q})$$

Weighted cross-entropy loss

Loss function

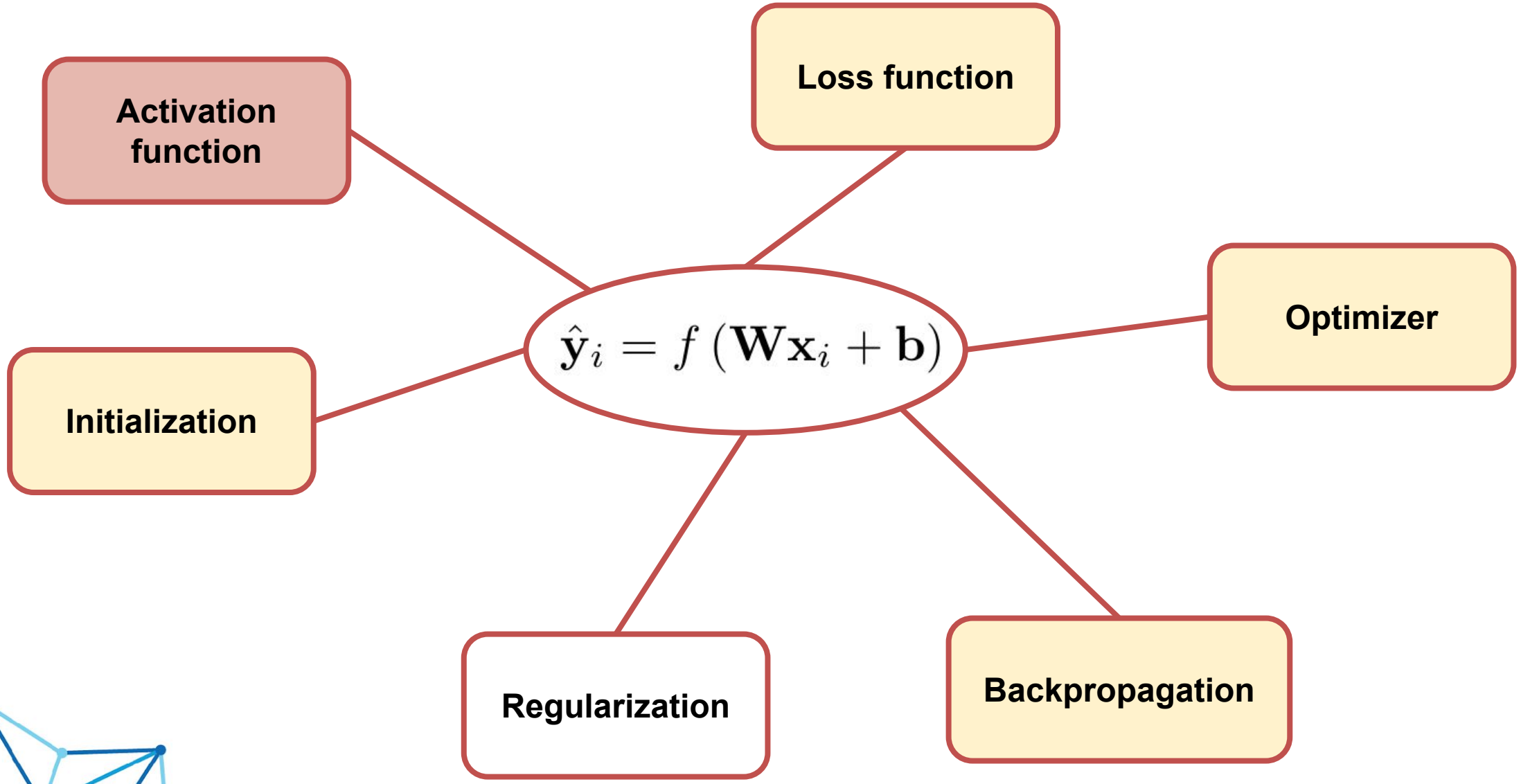
Choosing loss function may have very serious consequences on model accuracy

$$\mathrm{L}_2(\widehat{\mathbf{Y}}, \mathbf{Y}) = \frac{1}{2}\sum_{h,w} \|\mathbf{Y}_{h,w} - \widehat{\mathbf{Y}}_{h,w}\|_2^2 \qquad \mathrm{L}_{cl}(\widehat{\mathbf{Z}}, \mathbf{Z}) = -\sum_{h,w} v(\mathbf{Z}_{h,w}) \sum_{q} \mathbf{Z}_{h,w,q} \log(\widehat{\mathbf{Z}}_{h,w,q})$$



Colorization of old and out of the dataset images:

Neural Networks



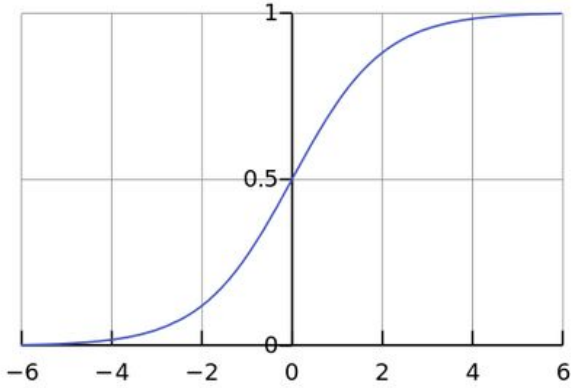
Activation functions - zoo

Activation function is a necessary building block which introduces nonlinearity to increase capacity of neural network

$$\hat{\mathbf{y}}_i = f\left(\mathbf{W}\mathbf{x}_i + \mathbf{b}\right)$$

We have already seen some of them:

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

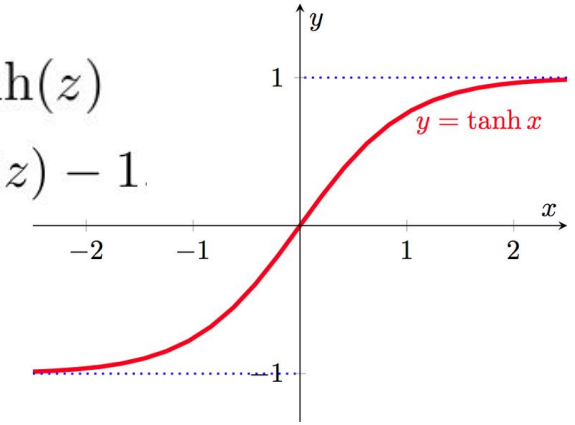


hard to train because of saturated gradient

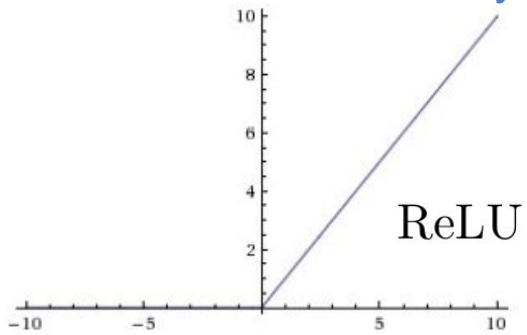
Hyperbolic tangent:

$$g(z) = \tanh(z)$$

$$\tanh(z) = 2\sigma(2z) - 1$$

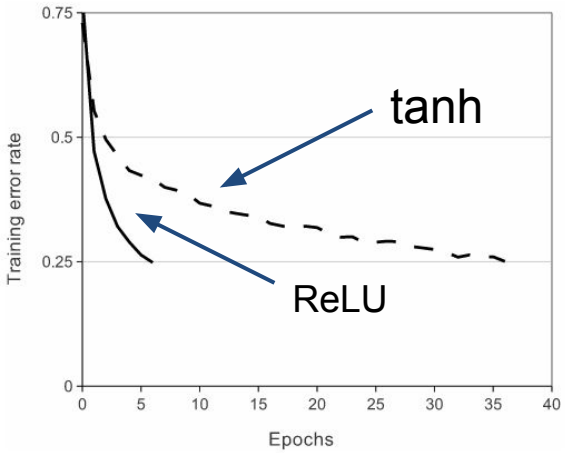


most common and easy to optimize



$$\mathrm{ReLU}\,(x) = \max\,(0,\, x)$$

2012 - It was shown that network with ReLU learnt several times faster with ReLU units

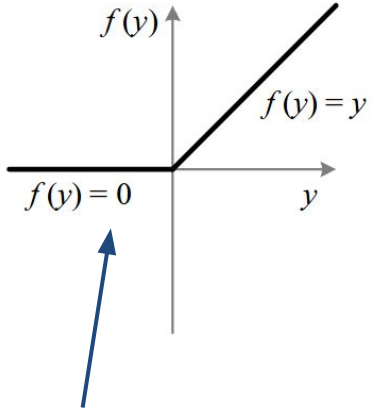


Krizhevsky, A. 2012
ImageNet
winning solution

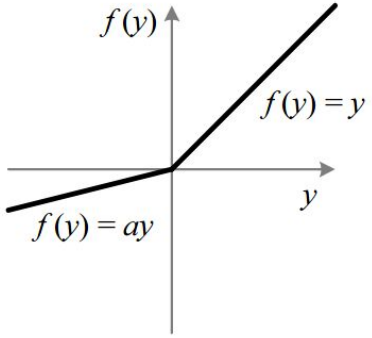
Activation functions - zoo

Activation function is a necessary building block which introduces nonlinearity to increase capacity of neural network

$$\hat{\mathbf{y}}_i = f\left(\mathbf{W}\mathbf{x}_i + \mathbf{b}\right)$$



dying gradients problem

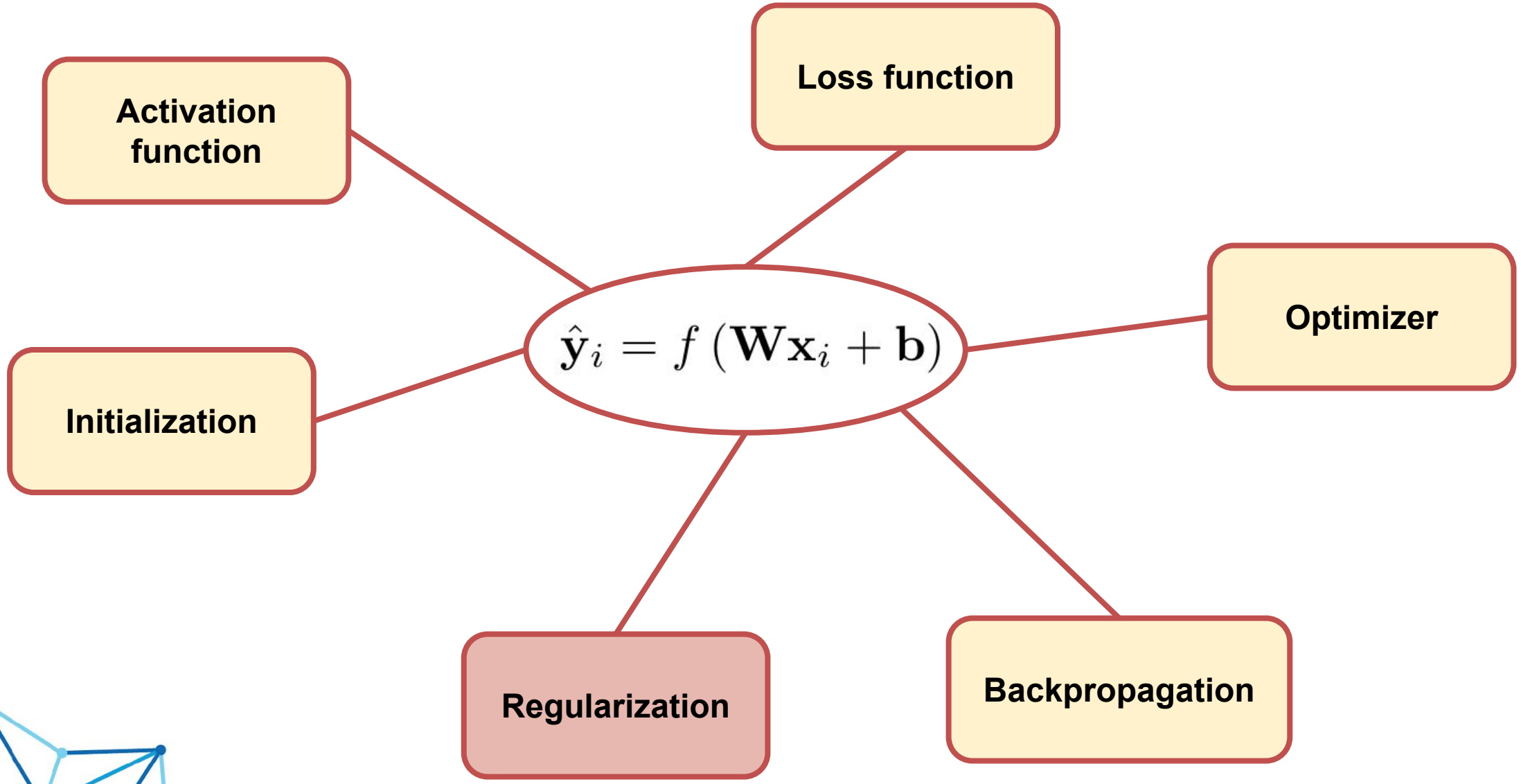


- ReLU
- Leaky ReLU - allows for small negative values
- Parametric ReLU - alpha is learned
- maxout - as a generalization of ReLUs family

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

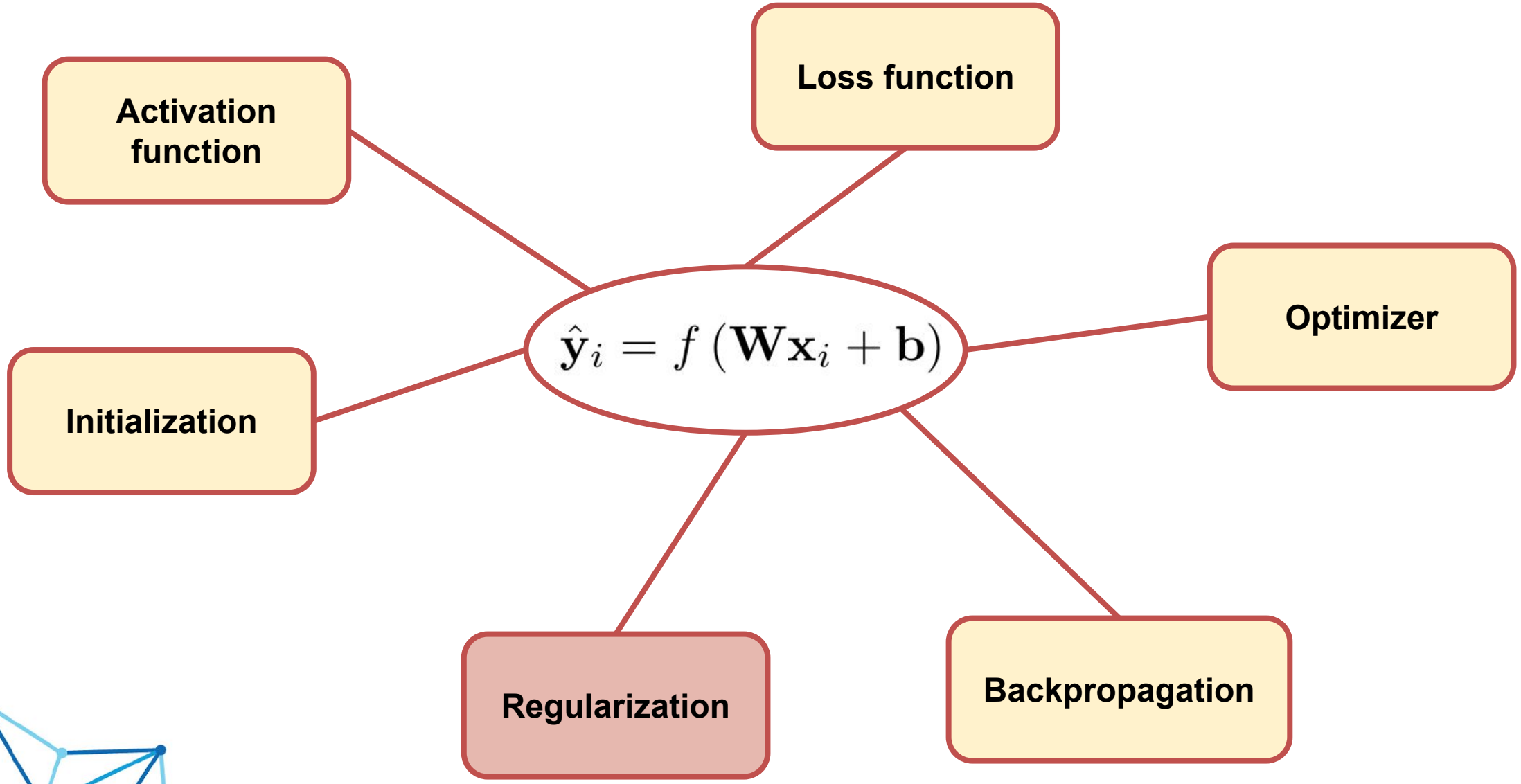
It is worth to try all activations from ReLU family, but probably one will end up with the simplest one.

Neural Networks



Short break

Neural Networks



Regularization

Regularization is a way to preventing our model from overfitting

Overfitting is when our model learn to remember data instead to understanding them

Keras overfitting example

Regularization - zoo

Parameter norm penalties

$$\hat{\mathbf{y}}_i = f\left(\mathbf{W}\mathbf{x}_i + \mathbf{b}\right)$$

we want to put penalties on our model parameters in order to prevent overfitting

Add second term which penalizes special values of model parameters

$$\mathcal{L}_{\text{total}}\left(\theta; \mathbf{y}, \hat{\mathbf{y}}\right) = \mathcal{L}_{\text{objective}}\left(\theta; \mathbf{y}, \hat{\mathbf{y}}\right) + \mathcal{L}_{\theta}\left(\theta\right)$$

- **L2 regularization** $\mathcal{L}\left(\mathbf{W}; \lambda\right) = \frac{1}{2}\lambda \left\|\mathbf{W}\right\|_2^2$ with gradient $\frac{\partial \mathcal{L}\left(\mathbf{W}; \lambda\right)}{\partial \mathbf{W}} = \lambda \mathbf{W}$

usually small number, model hyperparameter

- L2 works as soft constraint on the values of the W matrix, large values are forbidden since they lead to large loss

Regularization - zoo

Parameter norm penalties

- **L2 regularization** $\mathcal{L}(\mathbf{W};\lambda) = \frac{1}{2}\lambda \|\mathbf{W}\|_2^2$ with gradient $\frac{\partial \mathcal{L}(\mathbf{W};\lambda)}{\partial \mathbf{W}} = \lambda \mathbf{W}$

Regularization has smoothing effect on model predictions:
consider following task: separate green dots from red

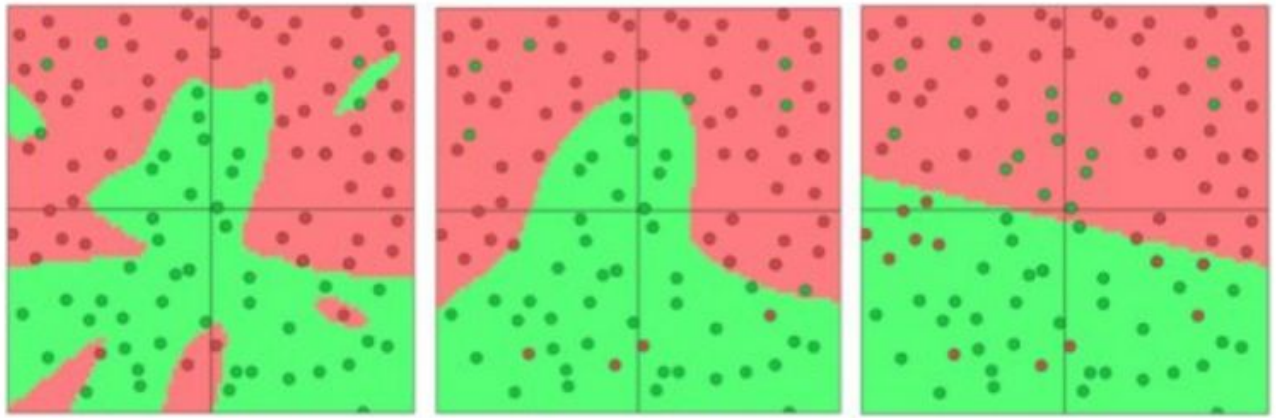


Fig 5. Separating green dots vs red dots, L2 regularization strengths of 0.01, 0.1, and 1

source: kdnuggets.com

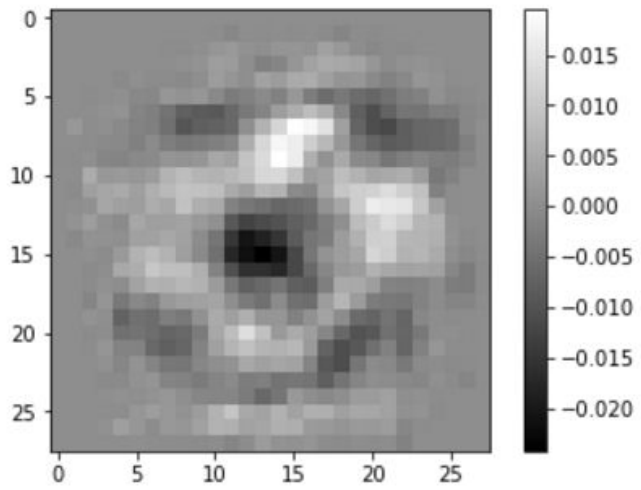
Regularization - zoo

Parameter norm penalties

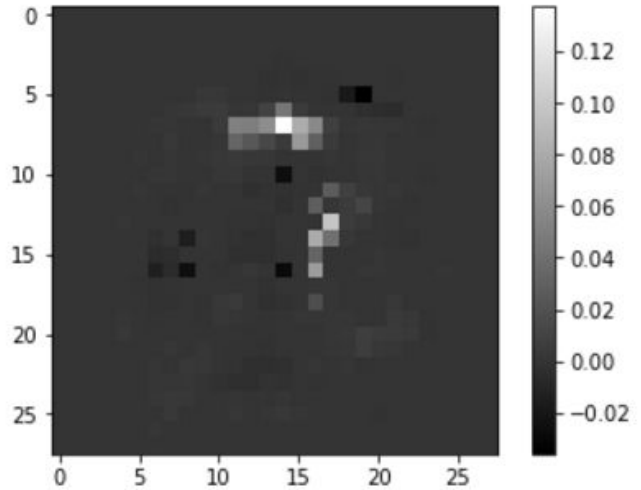
- **L2 regularization** $\mathcal{L}(\mathbf{W};\lambda) = \frac{1}{2}\lambda \|\mathbf{W}\|_2^2$ with gradient $\frac{\partial \mathcal{L}(\mathbf{W};\lambda)}{\partial \mathbf{W}} = \lambda \mathbf{W}$

- **L1 regularization** $\mathcal{L}(\mathbf{W};\lambda) = \lambda |\mathbf{W}|$ with gradient $\frac{\partial \mathcal{L}(\mathbf{W};\lambda)}{\partial \mathbf{W}} = \lambda \text{sign}(\mathbf{W})$

the L1 regularization leads to a sparse matrices



first “W image” with L2



first “W image” with L1

In practice L2 can be expected to overperform L1 regularization

Regularization - zoo

Constraints regularizers

- max norm constraint - $\|\vec{w}\|_2 < c$
- non negativity constraint - *each element of the W matrix must be positive*
- unit norm - *enforces the matrix to have unit norm along the last axis*

in keras we can do it easily:

```
from keras.constraints import maxnorm
model.add(Dense(64, kernel_constraint=max_norm(2.)))
```

Regularization - zoo

Data augmentation = *more data better generalization => generate more data based on existing ones*

- for images one may apply translations, rotations, stretching, shearing, distortion

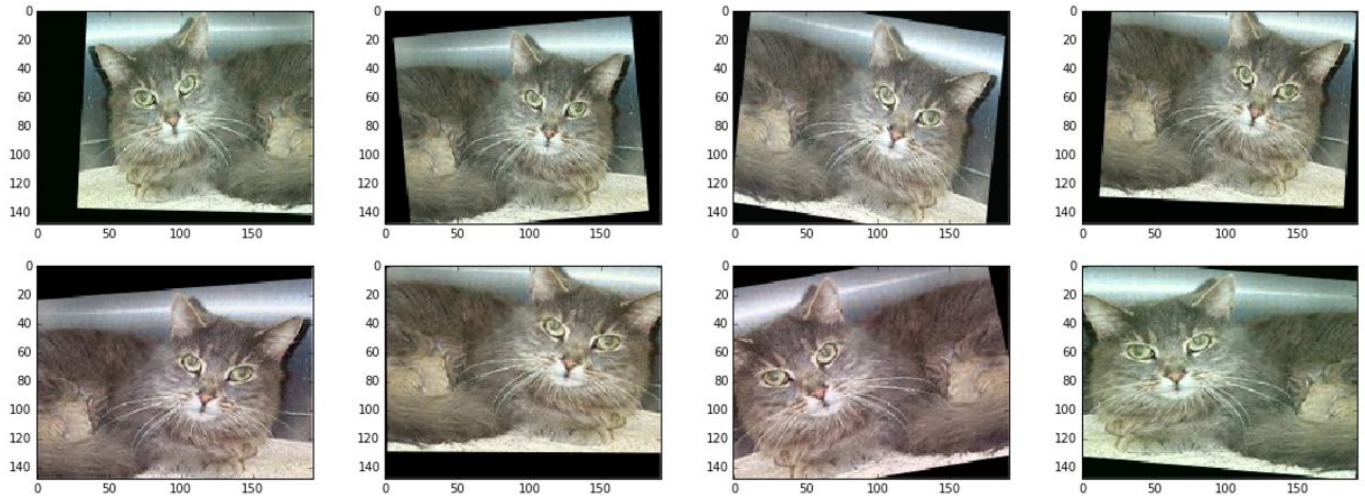
Keras has cool Image generator class which allows for online augmentation during training

```
(X_train, y_train), (X_test, y_test) = cifar10.load_data()
Y_train = np_utils.to_categorical(y_train, num_classes)
Y_test = np_utils.to_categorical(y_test, num_classes)

datagen = ImageDataGenerator(
    featurewise_center=True,
    featurewise_std_normalization=True,
    rotation_range=20,
    width_shift_range=0.2,
    height_shift_range=0.2,
    horizontal_flip=True)

# compute quantities required for featurewise normalization
# (std, mean, and principal components if ZCA whitening is applied)
datagen.fit(X_train)

# fits the model on batches with real-time data augmentation:
model.fit_generator(datagen.flow(X_train, Y_train, batch_size=32),
                    steps_per_epoch=len(X_train), epochs=epochs)
```



whenever you can, use it !

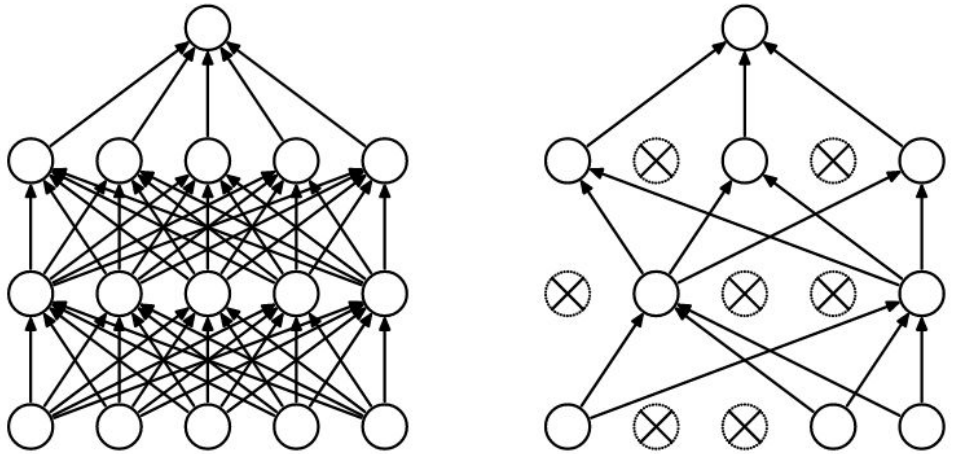
Regularization - zoo

Dropout - 2014

Dropout: A Simple Way to Prevent Neural Networks from Overfitting

Nitish Srivastava NITISH@CS.TORONTO.EDU
Geoffrey Hinton HINTON@CS.TORONTO.EDU
Alex Krizhevsky KRIZ@CS.TORONTO.EDU
Ilya Sutskever ILYA@CS.TORONTO.EDU
Ruslan Salakhutdinov RSALAKHU@CS.TORONTO.EDU

The idea behind the dropout



(a) Standard Neural Net (b) After applying dropout.

Figure 1: Dropout Neural Net Model. **Left**: A standard neural net with 2 hidden layers. **Right**: An example of a thinned net produced by applying dropout to the network on the left. Crossed units have been dropped.

Standard Neuron:

$$z_i^{(l+1)} = \mathbf{w}_i^{(l+1)} \mathbf{y}^l + b_i^{(l+1)},$$
$$y_i^{(l+1)} = f(z_i^{(l+1)}),$$

Standard Neuron with dropout:

$$r_j^{(l)} \sim \text{Bernoulli}(p),$$
$$\tilde{\mathbf{y}}^{(l)} = \mathbf{r}^{(l)} * \mathbf{y}^{(l)},$$
$$z_i^{(l+1)} = \mathbf{w}_i^{(l+1)} \tilde{\mathbf{y}}^l + b_i^{(l+1)},$$
$$y_i^{(l+1)} = f(z_i^{(l+1)}).$$

binary mask created with probability p

source: Srivastava, 2014

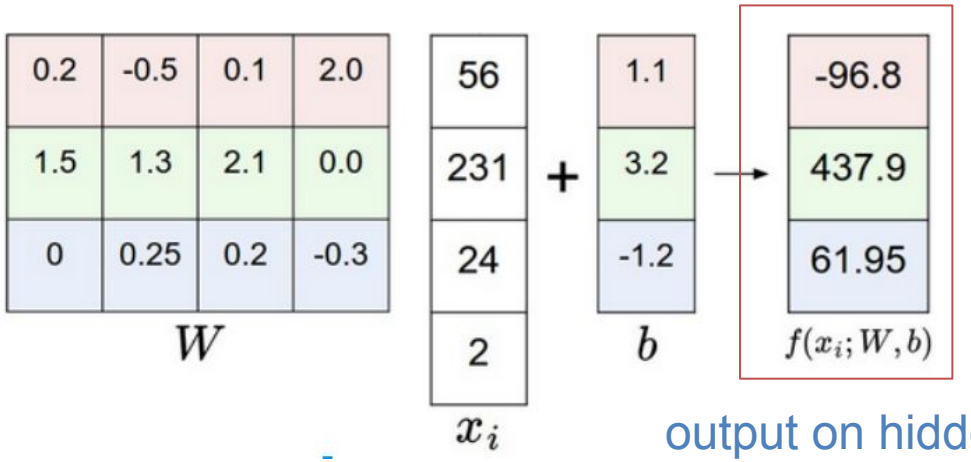
Example in keras

Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner

Normalize the inputs of hidden layer using mini-batch statistic



output on hidden unit for a single example

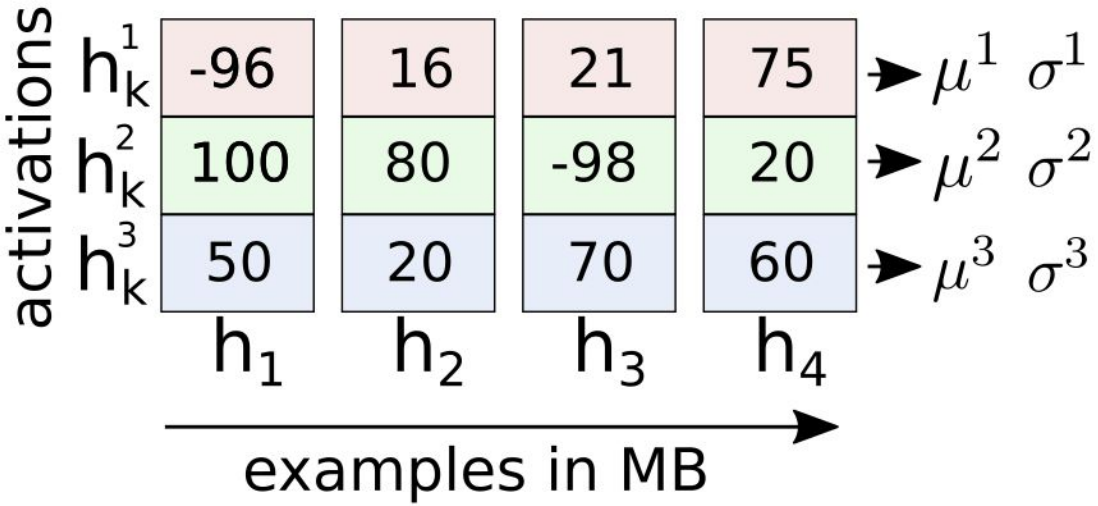
$$\hat{\mathbf{y}}_i = \mathbf{W}\mathbf{x}_i + \mathbf{b}$$

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift

Sergey Ioffe
Google Inc., *sioffe@google.com*

Christian Szegedy
Google Inc., *szegedy@google.com*

In mini-batch we have many examples



Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner

Normalize the inputs of hidden layer using mini-batch statistic

The NB algorithm (per particular activation)

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma^2_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

source: BN - paper

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift

Sergey Ioffe
Google Inc., *sioffe@google.com*

Christian Szegedy
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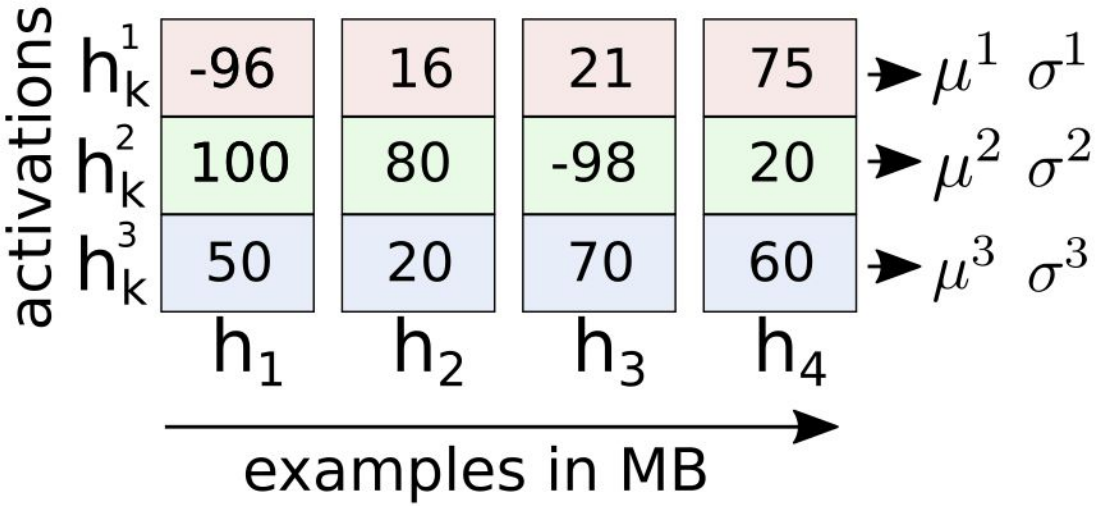
In mini-batch we have many examples



Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner

With batch normalization one may:

- increase learning rate
- in some cases remove Dropout
- reduce L2 regularization

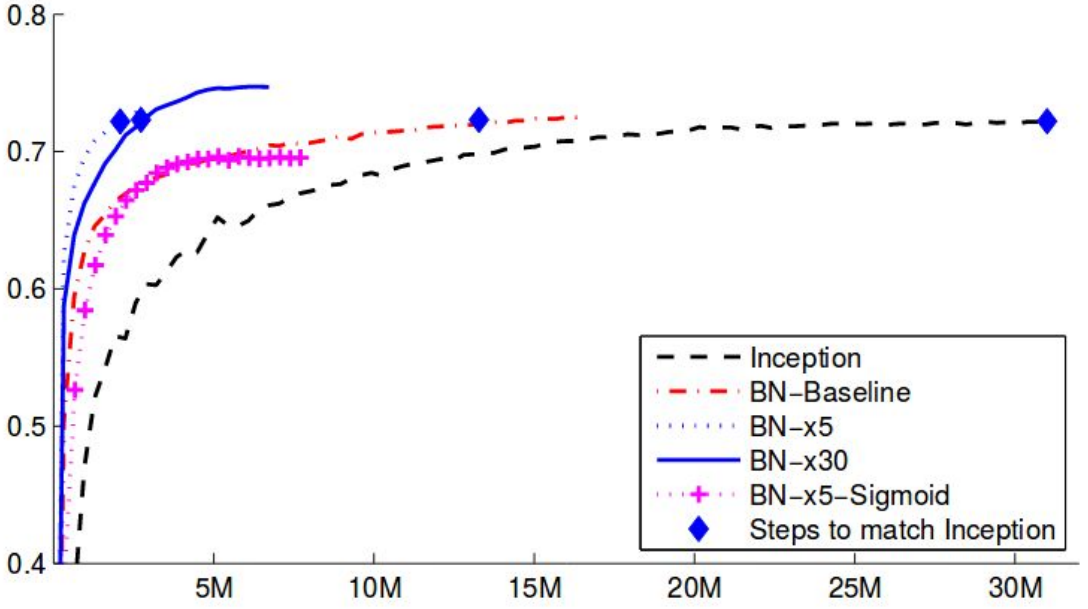


Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner
- **Layer normalization (2016)** - normalize hidden activation per example in mini-batch (paper)

Batch normalization has problems with RNNs, here the normalization depends only on current step hence it can be applied to normalize RNNs networks

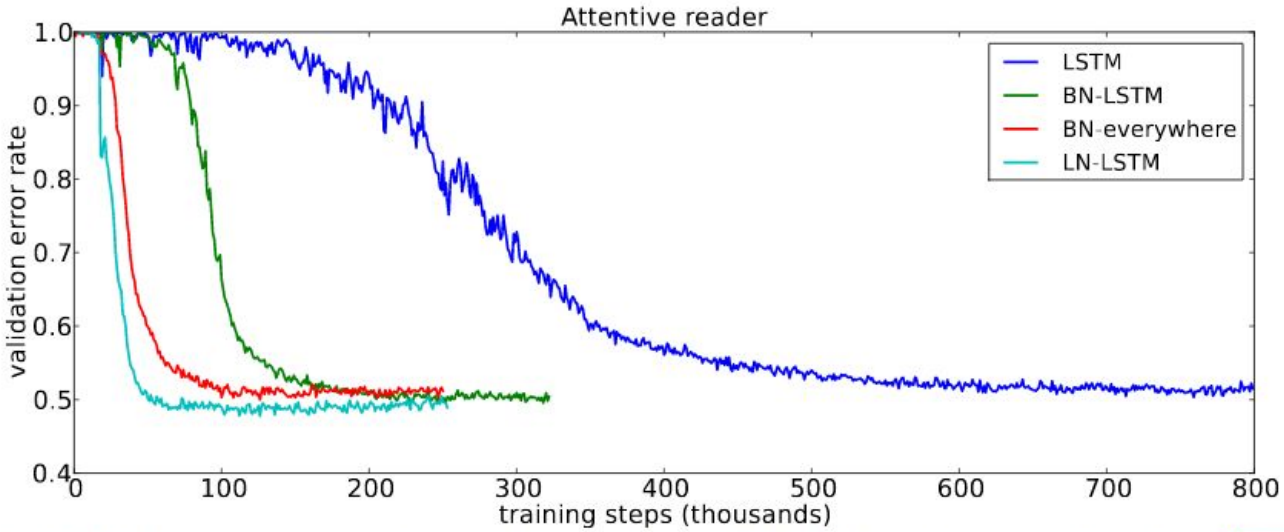


Figure 2: Validation curves for the attentive reader model. BN results are taken from [Cooijmans et al., 2016].

Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner
- **Layer normalization (2016)** - normalize hidden activation per example in mini-batch (paper)
- **Weight normalization (2016)** - normalize weight matrix instead of activations: replace **w** with **v** and g (paper), can be applied to RNNs

$$\mathbf{w} = \frac{g}{||\mathbf{v}||}\mathbf{v}$$

Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner
- **Layer normalization (2016)** - normalize hidden activation per example in mini-batch (paper)
- **Weight normalization (2016)** - normalize weight matrix instead of activations: replace **w** with **v** and g (paper), can be applied to RNNs
- **Batch renormalization (Feb 2017!)** - quite promising, extension to the original BN paper. Its done by introducing additional learnable parameters which fix the difference between train and test inference, learning is quite tricky and demands hand tuning.

Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner
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- **Orthogonalization regularization (Feb 2017!)** - make you matrix to be an orthogonal one! Cool - it preserves the norm and make gradients more stable (Neural Photo Editing with Introspective Adversarial Networks)

$$\mathcal{L}_{ortho} = \Sigma(|WW^T - I|)$$

Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Batch normalization (2015) -** introduces normalization operation in a differentiable manner
- **Layer normalization (2016)** - normalize hidden activation per example in mini-batch (paper)
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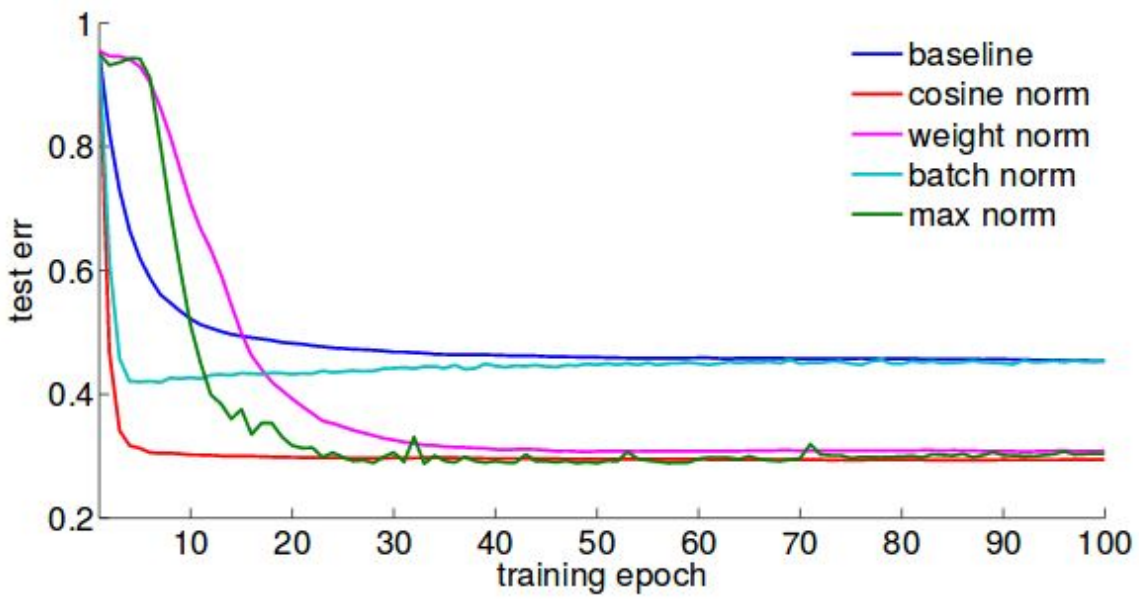
- **Batch renormalization (Feb 2017!)** - quite promising, extension to the original BN paper. Its done by introducing additional learnable parameters which fix the difference between train and test inference, learning is quite tricky and demands hand tuning (paper)
- **Orthogonalization regularization (Feb 2017!)** - make you matrix to be an orthogonal one! Cool - it preserves the norm and make gradients more stable (Neural Photo Editing with Introspective Adversarial Networks)
- **Cosine normalization (Feb 2017!)** - replace dot product with cosine similarity (paper)

Regularization - zoo

Normalization layers family - prevent overfitting and speed up training

- **Cosine normalization (Feb 2017!)** - replace dot product with cosine similarity

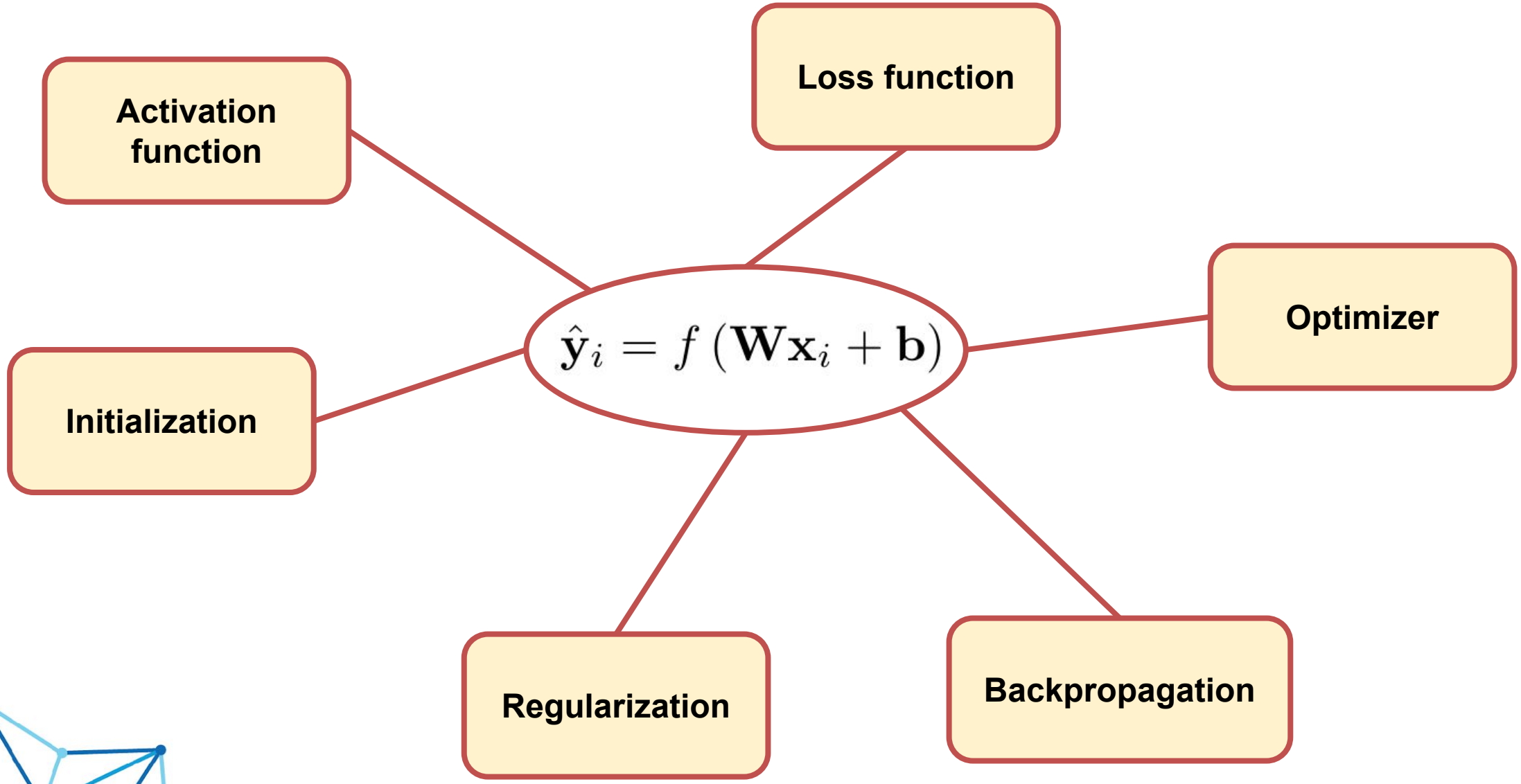
instead this: $\vec{w} \cdot \vec{x}$ use this: $\frac{\vec{w} \cdot \vec{x}}{|\vec{w}|\,|\vec{x}|}$



- easy to implement
- faster learning
- better accuracy
- can be applied to RNNs

Figure 6. The 20NEWS test err of networks trained with differ-

Neural Networks



Thank you for your attention

Krzysztof Kolasiński krzysztof.kolasinski@fornax.ai

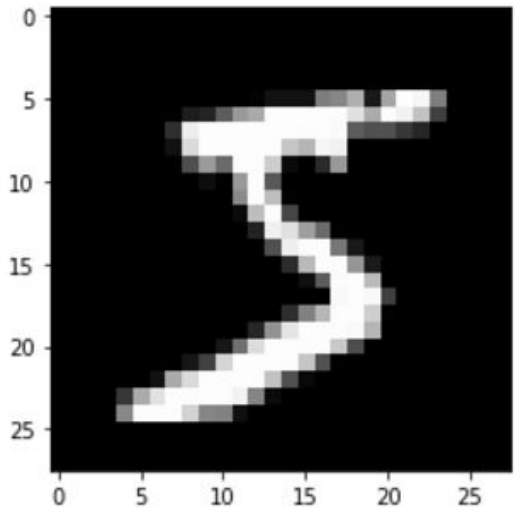
Appendix

FORNAX

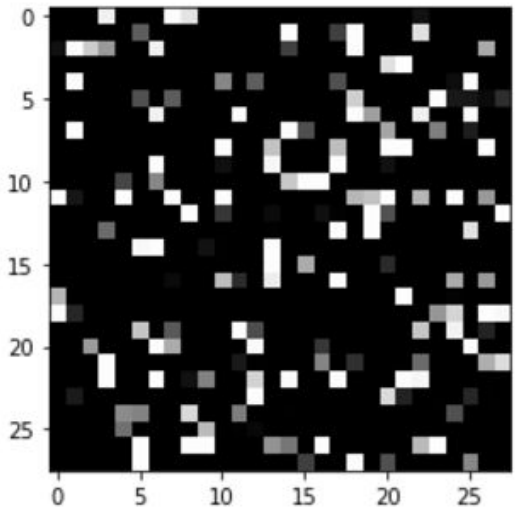
WWW.FORNAX.CO

Epilogue: The neural nets “paradox”

Given the input image:



We permute every pixel:



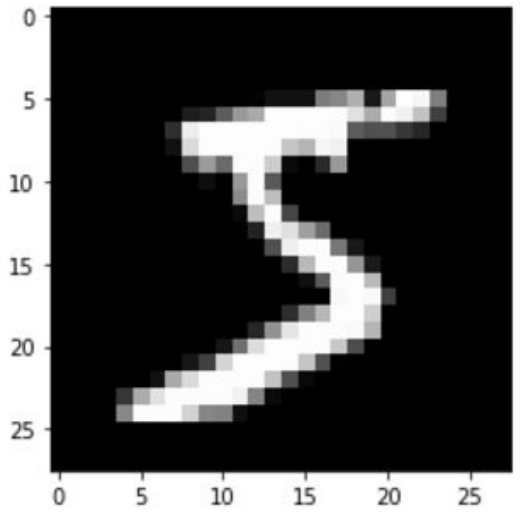
Then apply the same permutation for every image in dataset
and train Neural Network

What NN network will learn? Will it perform better or worse ?

It will learn exactly the same (in terms of accuracy)!

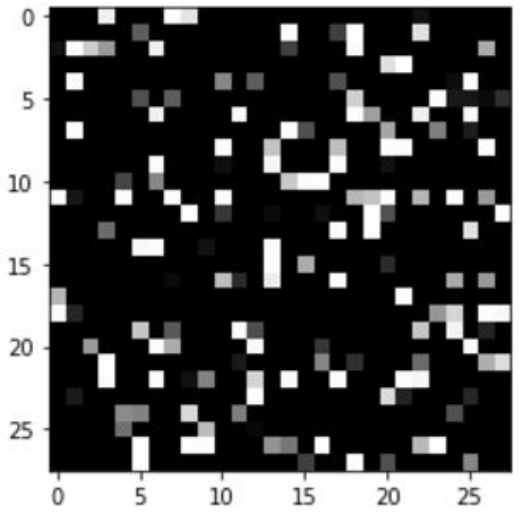
Epilogue: The neural nets “paradox”

Given the input image:



$\mathbf{x}_i$

We permute every pixel:



$\mathbf{x}_i' = \mathbf{R}\mathbf{x}_i$

Explanation:

- we notice that permutation is a rotation operation

$$\mathbf{x}_i' = \mathbf{R}\mathbf{x}_i \qquad \mathbf{R}^T\mathbf{R} = 1$$

- we work with single layer NN (before permutation)

$$\hat{\mathbf{y}}_i = f\left(\mathbf{W}\mathbf{x}_i + \mathbf{b}\right)$$

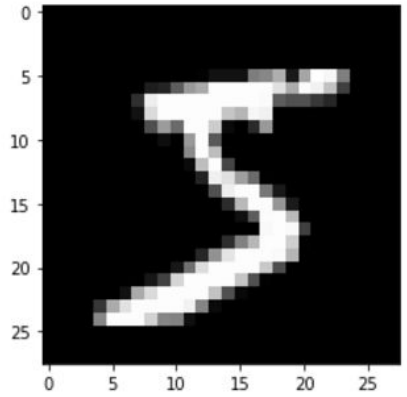
- and after permutation

$$\hat{\mathbf{y}}_i' = f\left(\mathbf{W}'\mathbf{x}_i' + \mathbf{b}'\right)$$

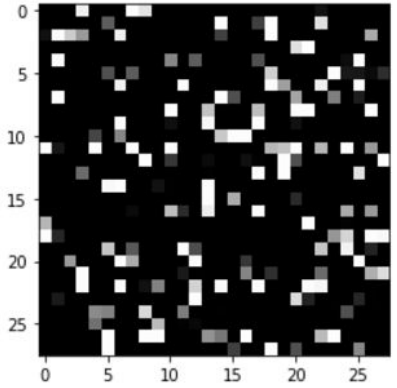
We assume (with primes) that our model will learn different parameters

Epilogue: The neural nets “paradox”

Given the input image: $\mathbf{x}_i$



$\mathbf{x}_i' = \mathbf{R}\mathbf{x}_i$



$$\mathbf{x}_i' = \mathbf{R}\mathbf{x}_i$$

- we don’t permute labels hence our predictions must be the same
- we ask then if this is possible

$$\hat{\mathbf{y}}_i' = \hat{\mathbf{y}}_i$$

- we get condition to satisfy

softmax

$$f\left(\mathbf{W}'\mathbf{x}_i' + \mathbf{b}'\right) = f\left(\mathbf{W}\mathbf{x}_i + \mathbf{b}\right)$$

$$\mathbf{W}'\mathbf{x}_i' + \mathbf{b}' = \mathbf{W}\mathbf{x}_i + \mathbf{b} \quad + \texttt{const}$$

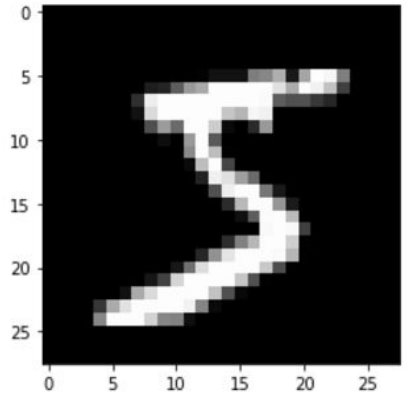
$$\mathbf{W}'\mathbf{R}\mathbf{x}_i + \mathbf{b}' = \mathbf{W}\mathbf{x}_i + \mathbf{b} \quad + \texttt{const}$$

- hence both sides are equal when

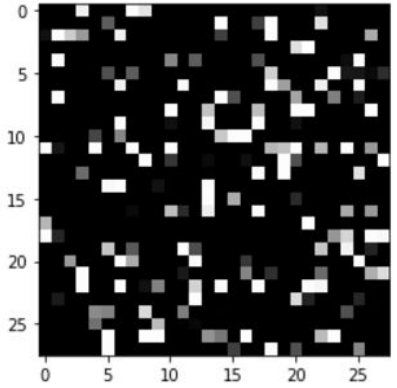
$$\mathbf{W} = \mathbf{W}'\mathbf{R} \Rightarrow \mathbf{W}' = \mathbf{W}\mathbf{R}^T \qquad \mathbf{b} = \mathbf{b}' - \texttt{const}$$

Epilogue: The neural nets “paradox”

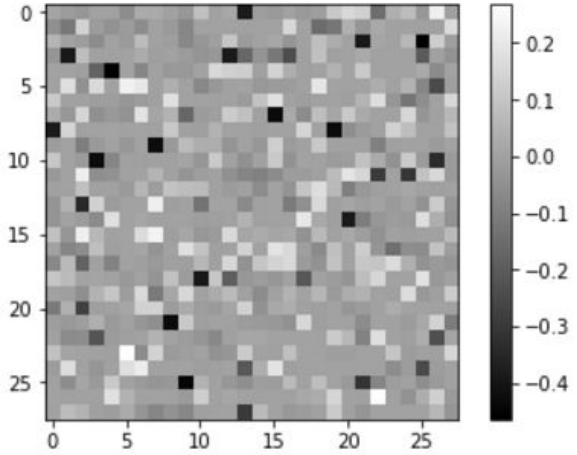
Given the input image: $\mathbf{x}_i$



$\mathbf{x}_i' = \mathbf{R}\mathbf{x}_i$

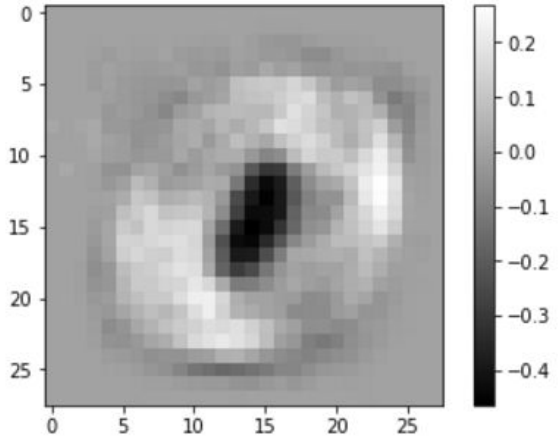


Let’s check it in Keras: $\mathbf{W} = \mathbf{W}'\mathbf{R} \Rightarrow \mathbf{W}' = \mathbf{W}\mathbf{R}^T$



Learned weights do not correspond to anything intuitive (for humans)

$\mathbf{W}'$

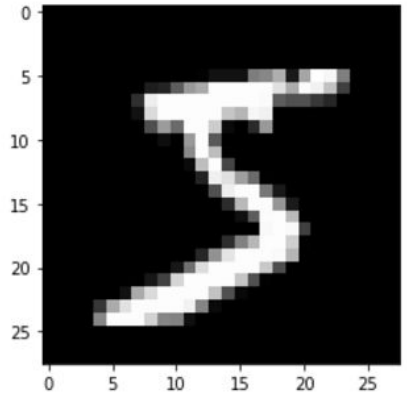


After rotation!

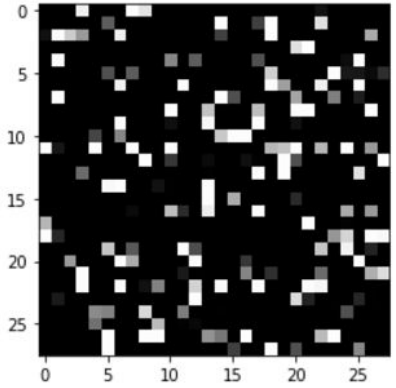
$\mathbf{W} = \mathbf{W}'\mathbf{R}$

Epilogue: The neural nets “paradox”

Given the input image: $\mathbf{x_i}$



$\mathbf{x_i' = Rx_i}$



Ok, but what we can learn from that?

- NNs do not capture spatial correlations in data
- NNs are not translational and rotational invariant, small shift in the image is enough to get wrong predictions
- The same with scaling

Ok, how we can solve those problems?

- For images use CNNs! Next talk :)

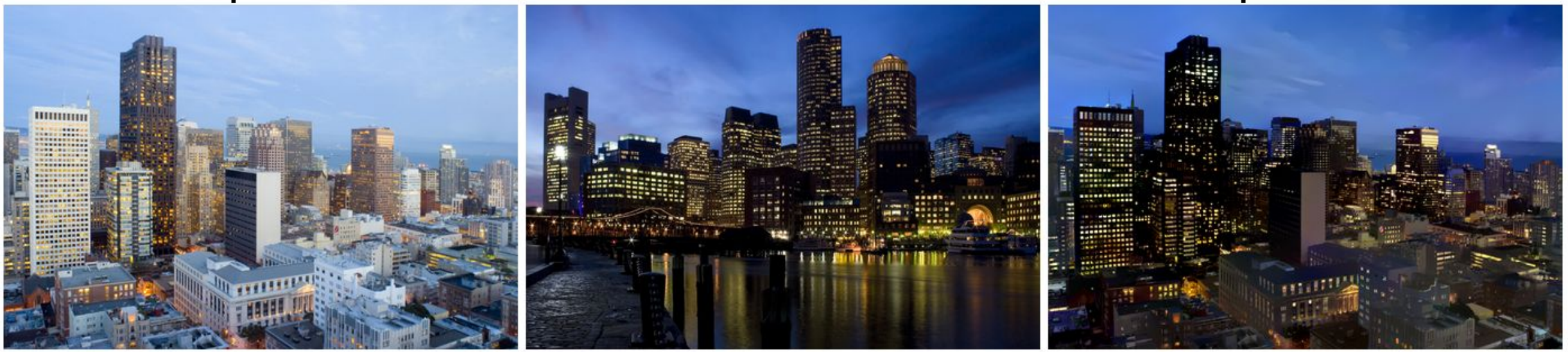
References

- http://uvadlc.github.io/lectures/lecture1.pdf
- https://chaosmail.github.io/deeplearning/2016/10/22/intro-to-deep-learning-for-computer-vision/
- http://karpathy.github.io/2016/05/31/rl/
- https://culurciello.github.io/tech/2016/06/04/nets.html
- http://www.asimovinstitute.org/neural-network-zoo/
- https://blog.acolyer.org/2017/03/24/a-miscellany-of-fun-deep-learning-papers/ importance of loss function
- http://cs231n.github.io/linear-classify/
- http://sebastianruder.com/optimizing-gradient-descent/

Why do we need DL?

1. **DL is fun!**

Input | **Reference** | **Output**



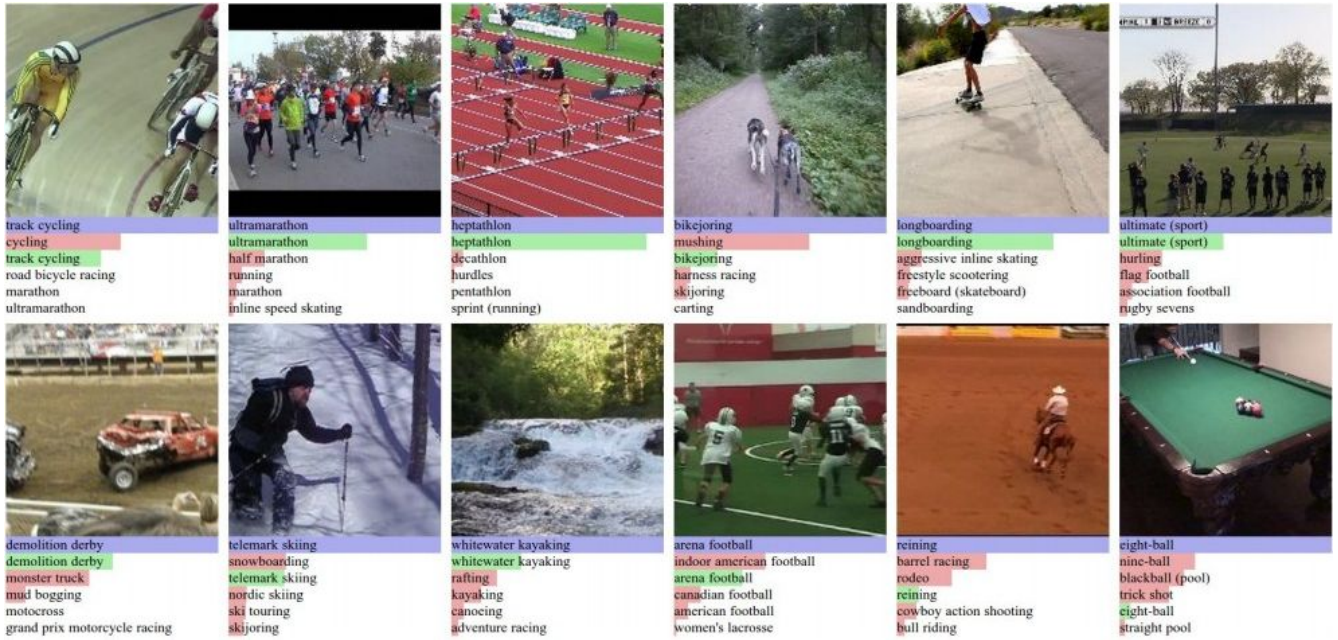
[Deep Photo Style Transfer] paper from 22 March 2017 !
Project page: https://github.com/luanfujun/deep-photo-styletransfer

Learning process

Learning is a mathematical process of tuning our DL architecture to achieve some desired target

We can distinguish few types of learning strategies:

- **supervised learning** (today's workshop!) - neural networks, CNNs
- unsupervised learning - Autoencoders, RBMs
- semi-supervised learning - mix of above
- reinforcement learning - agents must act to maximize the rewards



Regularization - zoo

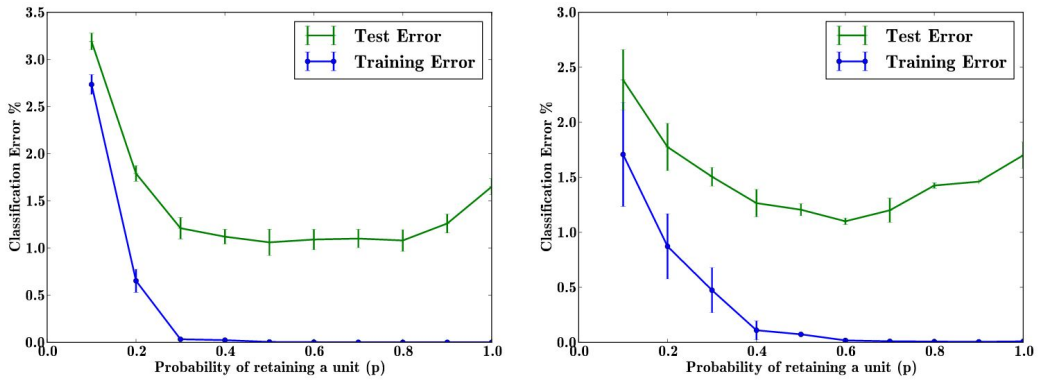
Dropout - 2014

Dropout: A Simple Way to Prevent Neural Networks from Overfitting

Nitish Srivastava NITISH@CS.TORONTO.EDU
Geoffrey Hinton HINTON@CS.TORONTO.EDU
Alex Krizhevsky KRIZ@CS.TORONTO.EDU
Ilya Sutskever ILYA@CS.TORONTO.EDU
Ruslan Salakhutdinov RSALAKHU@CS.TORONTO.EDU

Method	Test Classification error %
L2	1.62
L2 + L1 applied towards the end of training	1.60
L2 + KL-sparsity	1.55
Max-norm	1.35
Dropout + L2	1.25
Dropout + Max-norm	**1.05**

Table 9: Comparison of different regularization methods on MNIST.



(a) Keeping n fixed. (b) Keeping pn fixed.

Figure 9: Effect of changing dropout rates on MNIST

Standard Neuron:

$$z_i^{(l+1)} = \mathbf{w}_i^{(l+1)} \mathbf{y}^l + b_i^{(l+1)},$$
$$y_i^{(l+1)} = f(z_i^{(l+1)}),$$

Standard Neuron with dropout:

binary mask created with probability p

$$r_j^{(l)} \sim \text{Bernoulli}(p),$$
$$\tilde{\mathbf{y}}^{(l)} = \mathbf{r}^{(l)} * \mathbf{y}^{(l)},$$
$$z_i^{(l+1)} = \mathbf{w}_i^{(l+1)} \tilde{\mathbf{y}}^l + b_i^{(l+1)},$$
$$y_i^{(l+1)} = f(z_i^{(l+1)}).$$

Example in keras

Why do we need DL?

2. DL is important

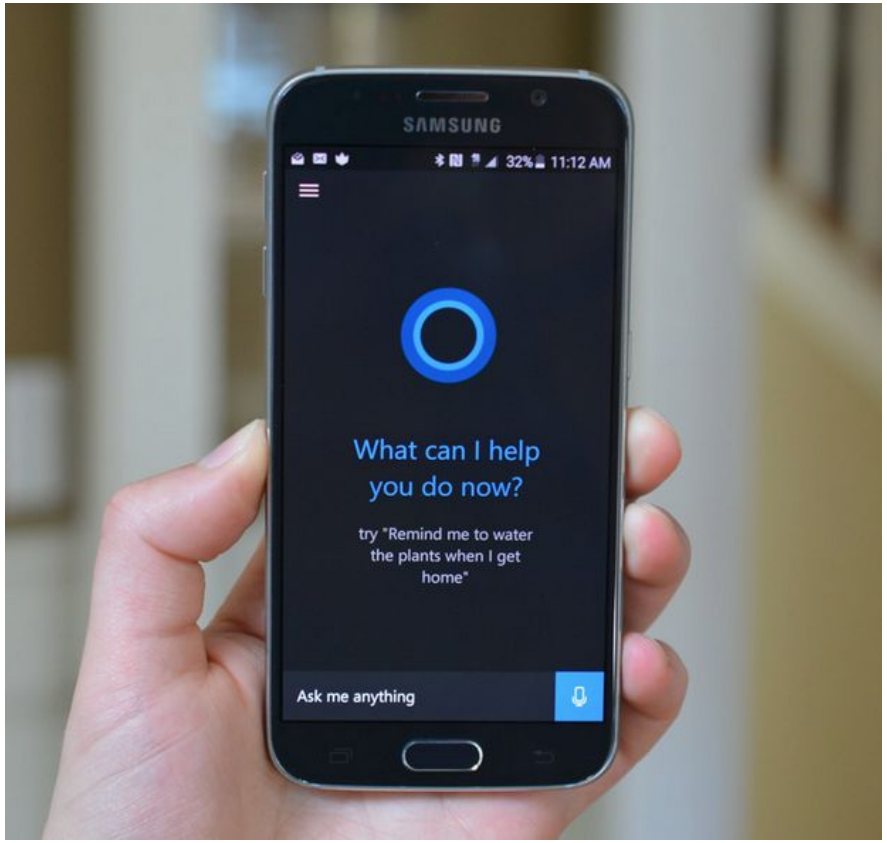
LETTER

doi:10.1038/nature14236

Human-level control through deep reinforcement learning

Volodymyr Mnih[1]*, Koray Kavukcuoglu[1]*, David Silver[1]*, Andrei A. Rusu[1], Joel Veness[1], Marc G. Bellemare[1], Alex Graves[1], Martin Riedmiller[1], Andreas K. Fidjeland[1], Georg Ostrovski[1], Stig Petersen[1], Charles Beattie[1], Amir Sadik[1], Ioannis Antonoglou[1], Helen King[1], Dharshan Kumaran[1], Daan Wierstra[1], Shane Legg[1] & Demis Hassabis[1]

"DQN achieved human-level performance in almost half of the 50 games to which it was applied"



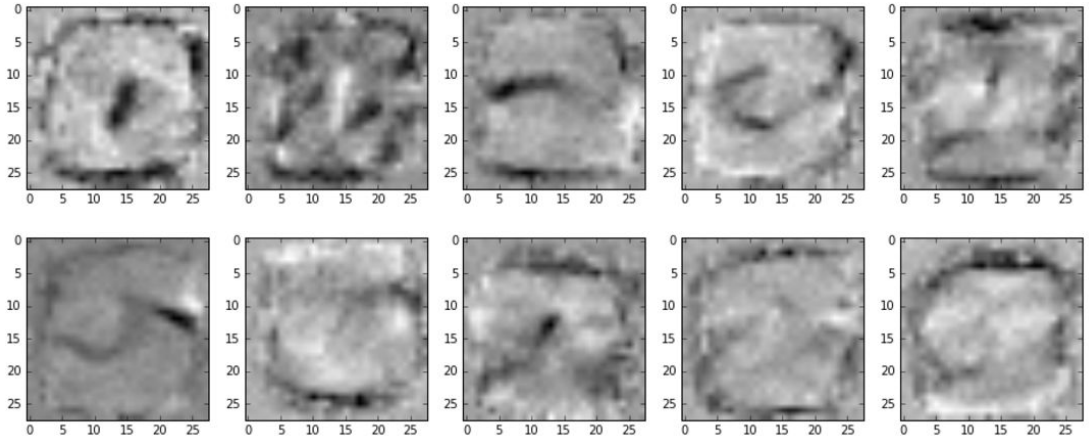
Natural Language Processing e.g. speech recognition task

Regularization - zoo

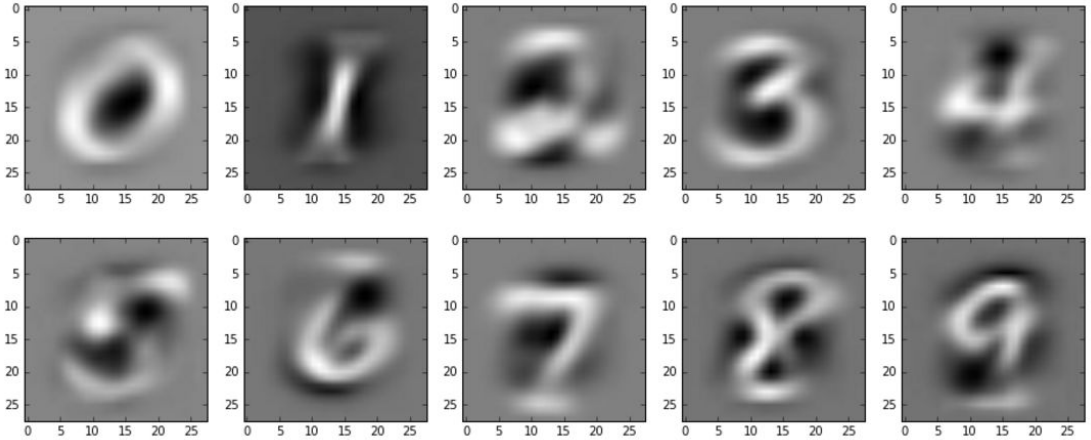
Parameter norm penalties

- **L2 regularization** $\mathcal{L}(\mathbf{W};\lambda) = \frac{1}{2}\lambda \|\mathbf{W}\|_2^2$ with gradient $\frac{\partial \mathcal{L}(\mathbf{W};\lambda)}{\partial \mathbf{W}} = \lambda \mathbf{W}$

Regularization has smoothing effect on model parameters:



before regularization



after adding L2 regularization

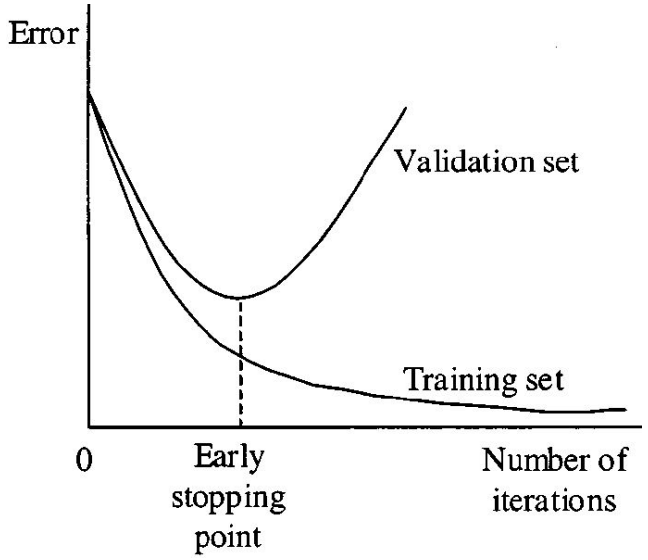
source: *Sam's Research Blog*

Regularization - zoo

Noise regularizers

- add noise with infinitesimal variance to input of the model
- add noise to hidden activations

Early stopping: *stop training before overfitting of model with large capacity*



Algorithm:

- Monitor your training and validation loss
- Stop training when the validation loss starts to increase

In keras we can use callbacks

EarlyStopping [source]

```
keras.callbacks.EarlyStopping(monitor='val_loss', min_delta=0, patience=0, verbose=0, mode='auto')
```

Stop training when a monitored quantity has stopped improving.

Regularization - zoo

Noise regularizers

- add noise with infinitesimal variance to input of the model
- add noise to hidden activations

Early stopping: *stop training before overfitting of model with large capacity*

Ensembling and bagging methods, etc …

Backpropagation

$$\theta^{k+1} := \theta^k - \lambda \left. \frac{\partial \mathcal{L}}{\partial \theta^k} \right|_{\text{mini-batch}}$$

Everything is a graph...