Deep Neural Networks

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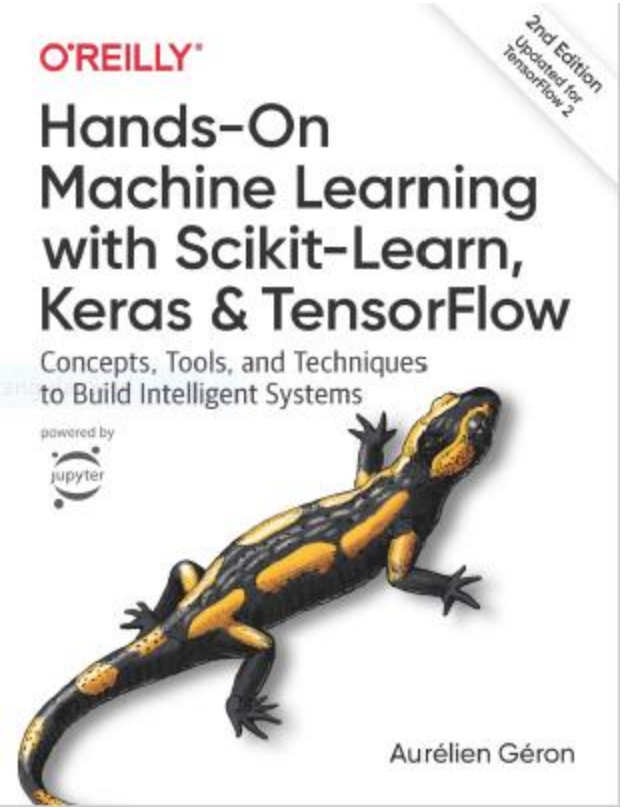
Reference

- Chapter 11: **Training Deep Neural Networks**



- Aurélien Géron, **Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow**, O'Reilly, 2nd Edition, 2019
  - Material: https://github.com/ageron/handson-ml2

Outline

1. Introduction
2. Vanishing/Exploding Gradients Problems
   - Glorot and He Initialization
   - Nonsaturating Activation Functions
   - Batch Normalization
   - Gradient Clipping
3. Reusing Pretrained Layers
4. Faster Optimizers
5. Avoiding Overfitting
   - ℓ_1 and ℓ_2 Regularization
   - Dropout
6. Summary
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1. Introduction

- Deep neural networks can solve **complex problems** and provide **end-to-end** solutions.
- When you train a deep network, you may face the following **problems**:
  - **Vanishing** or **exploding gradients**: The gradients grow smaller and smaller, or larger and larger.
  - **Not enough data**
  - **Long training time**
  - **Overfitting**

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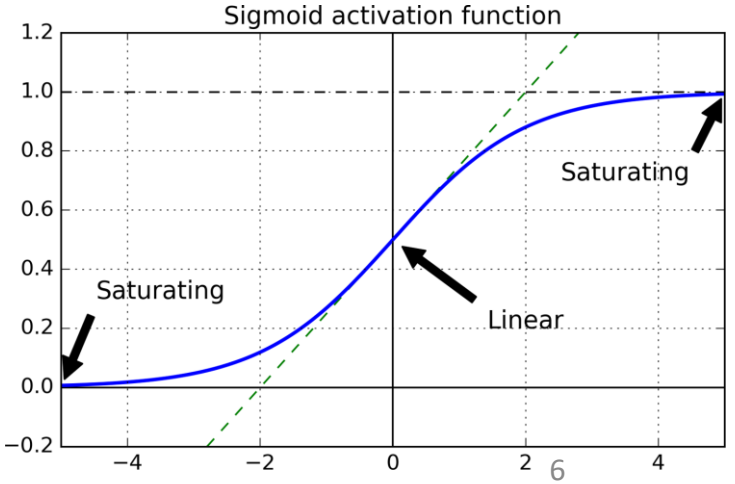
2. Vanishing/Exploding Gradients Problems

- **Vanishing Problem**: In the backpropagation algorithm, gradients often get smaller and smaller as the algorithm progresses down to the lower layers.
  - Lower layers' connection are left unchanged.
- **Exploding Problem**: the gradients can grow bigger and bigger.
  - Layers get very large weight updates and the algorithm diverges.
- **Main Reasons**: Using activation functions (logistic sigmoid) and weight initialization (normal distribution with 0-mean and 1-standard deviation).



2.1 Glorot and He Initialization

- **Glorot and Bengio**: In order for the signal not to die out, nor to explode and saturate, the variance of the outputs of each layer should be equal to the variance of its inputs.
- **Solution**: the connection weights of each layer must be initialized randomly as follows:

Normal distribution with mean 0 and variance $\sigma^2 = \frac{1}{\text{fan}_{\text{avg}}}$

Or a uniform distribution between $-r$ and $+r$, with $r = \sqrt{\frac{3}{\text{fan}_{\text{avg}}}}$

$$fan_{\text{avg}} = (fan_{\text{in}} + fan_{\text{out}})/2.$$

2.1 Glorot and He Initialization

- **Recommended** initialization parameters for each type of activation function.

Initialization	Activation functions	σ^2 (Normal)
Glorot	None, Tanh, Logistic, Softmax	$1 / fan_{avg}$
He	ReLU & variants	$2 / fan_{in}$
LeCun	SELU	$1 / fan_{in}$

- For the uniform distribution, use $r = \sqrt{3\sigma^2}$
- Keras uses **Glorot initialization** with a **uniform** distribution.

2.1 Glorot and He Initialization

- To change it to **He initialization**:

```
keras.layers.Dense(10, activation="relu",
     kernel_initializer="he_normal") # Or "he_uniform"
```

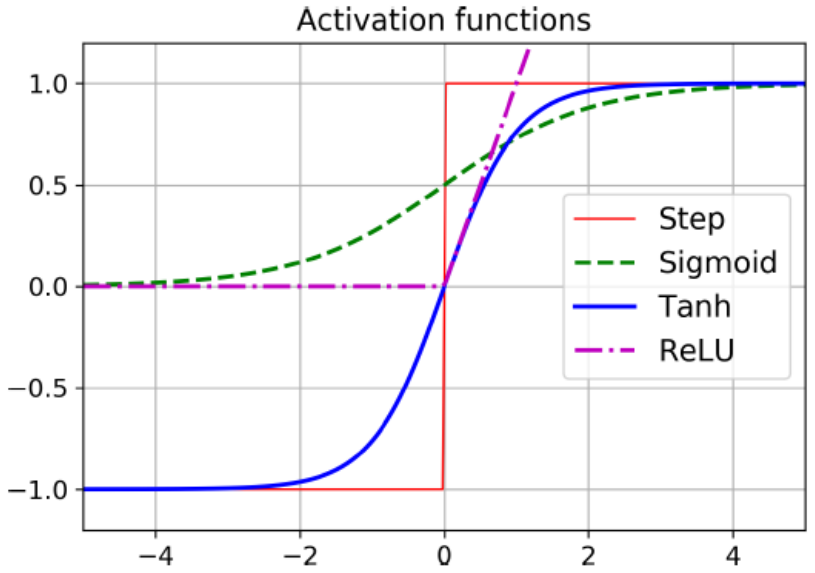
- **He initialization** with a **uniform** distribution but based on **fan_{avg}**:

```
he_avg_init = keras.initializers.VarianceScaling(scale=2.,
                                                 mode='fan_avg', distribution='uniform')

keras.layers.Dense(10, activation="sigmoid",
                   kernel_initializer=he_avg_init)
```

2.2 Nonsaturating Activation Functions

- **Step** does not work with the back propagation algorithm.
- **ReLU** is better than **sigmoid** because it does not saturate for positive values and is fast.
- **Dying ReLUs**: A neuron dies when its input is negative for all training instances.

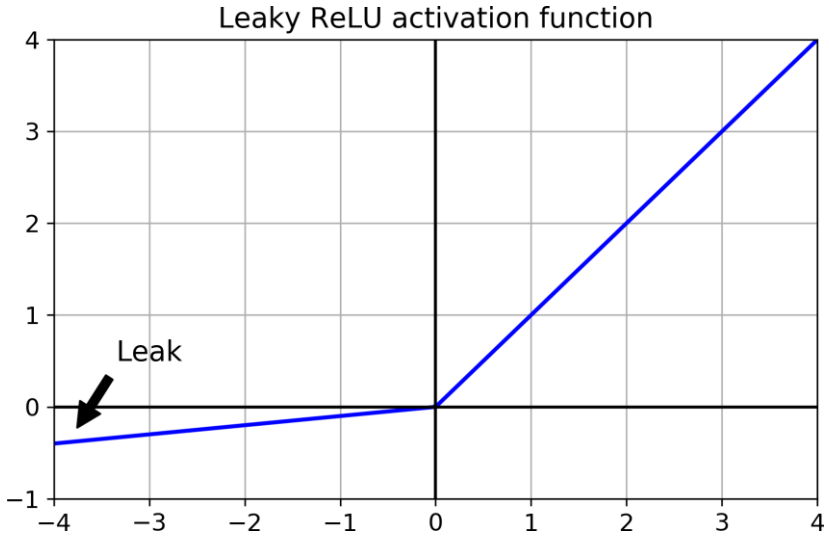


2.2 Nonsaturating Activation Functions

- **Leaky ReLU** performs better than ReLU.

$$\text{LeakyReLU}_{\alpha}(z) = \max(\alpha z, z)$$

- **α** between 0.01 and 0.3

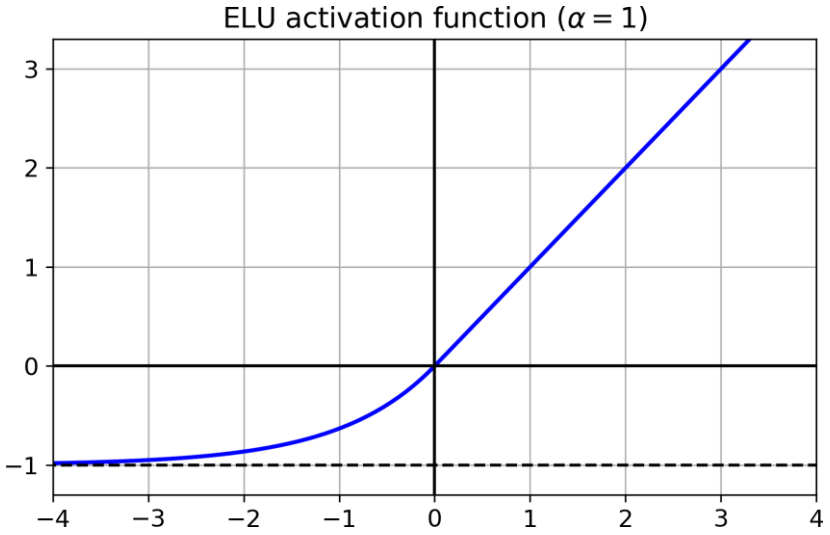



```
model = keras.models.Sequential([
    …
    keras.layers.Dense(10, kernel_initializer="he_normal"),
    keras.layers.LeakyReLU(alpha=0.2), # added as a layer
    …
])
```

2.2 Nonsaturating Activation Functions

- **Exponential linear unit (ELU)** also performs better than ReLU but is slower.
- **Scaled ELU (SELU)** performs best with dense and CNN, but must scale inputs and use **`lecun_normal`**.

$$\mathrm{ELU}_\alpha(z) = \begin{cases} \alpha(\exp(z) - 1) & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$




```
layer = keras.layers.Dense(10, activation="selu",
    kernel_initializer="lecun_normal")
```

2.2 Nonsaturating Activation Functions

- **Summary:**
  - SELU > ELU > leaky ReLU > ReLU > tanh > logistic
- If you cannot use SELU, use ELU.
- For fast response, use leaky ReLU or ReLU.

2.3 Batch Normalization

- The techniques in §2.1 and §2.2 can significantly reduce the vanishing/exploding gradients problems at the **beginning of training**, but don't guarantee that they won't **come back during training**.

- **Batch Normalization (BN)** zero-centers and normalizes each layer input using statistics from the mini batch (> 30).

- **Other benefits**: Works even without §2.1 and §2.2, allows using larger LR, and have regularization effect.

2.3 Batch Normalization

- Implementing batch normalization with Keras is easy.

```
model = keras.models.Sequential([
        keras.layers.Flatten(input_shape=[28, 28]),
        keras.layers.BatchNormalization(),
        keras.layers.Dense(300, activation="elu",
        kernel_initializer="he_normal"),
        keras.layers.BatchNormalization(),
        keras.layers.Dense(100, activation="elu",
        kernel_initializer="he_normal"),
        keras.layers.BatchNormalization(),
        keras.layers.Dense(10, activation="softmax")
])
```

2.4 Gradient Clipping

- Mitigates the exploding gradients problem by **clipping the gradients** during backpropagation so that they never exceed some threshold.
- Use it when you observe that the gradients are exploding during training. You can **track the size of the gradients** using TensorBoard.

```
optimizer = keras.optimizers.SGD(clipvalue=1.0)

model.compile(loss="mse", optimizer=optimizer)
```

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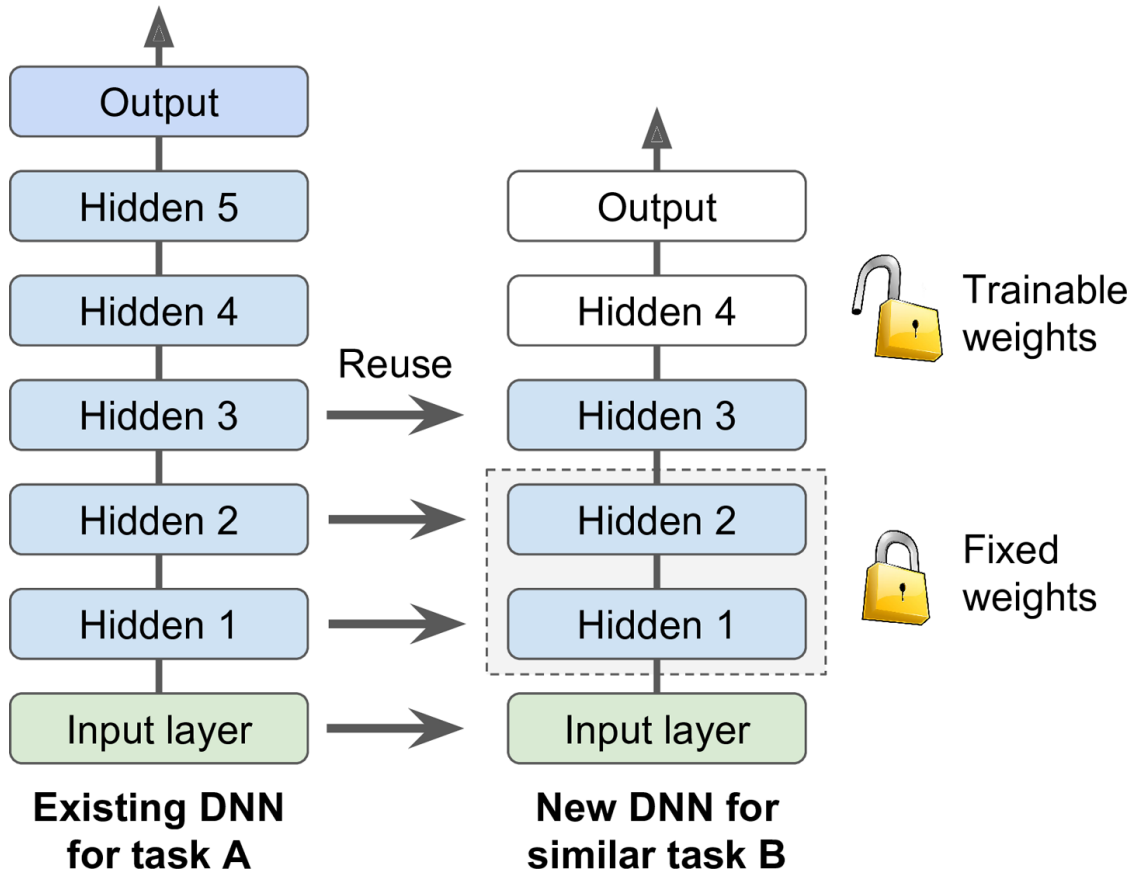
3. Reusing Pretrained Layers

- **Transfer Learning**: Using one NN developed for a certain task to solve another task.

- Useful to **shorten training time** or with **small datasets**.



Transfer Learning with Keras

```
# Load the ready model
model_A = keras.models.load_model("my_model_A.h5")
# Create a new model using all but the last layer
model_B_on_A = keras.models.Sequential(model_A.layers[:-1])
model_B_on_A.add(keras.layers.Dense(1, activation="sigmoid"))
# Freeze loaded layers then compile
for layer in model_B_on_A.layers[:-1]:
        layer.trainable = False

model_B_on_A.compile(loss="binary_crossentropy",
        optimizer="sgd", metrics=["accuracy"])
```

Transfer Learning with Keras

```
# Train the model for a few epochs
history = model_B_on_A.fit(X_train_B, y_train_B, epochs=4,
        validation_data=(X_valid_B, y_valid_B))
# Unreeze loaded layers
for layer in model_B_on_A.layers[:-1]:
        layer.trainable = True
# Compile with small learning rate (defalut = 1e-2)
optimizer = keras.optimizers.SGD(lr=1e-4)
model_B_on_A.compile(loss="binary_crossentropy",
        optimizer=optimizer, metrics=["accuracy"])
```

Transfer Learning with Keras

```
# Train the model for more epochs
history = model_B_on_A.fit(X_train_B, y_train_B, epochs=16,
        validation_data=(X_valid_B, y_valid_B))
```

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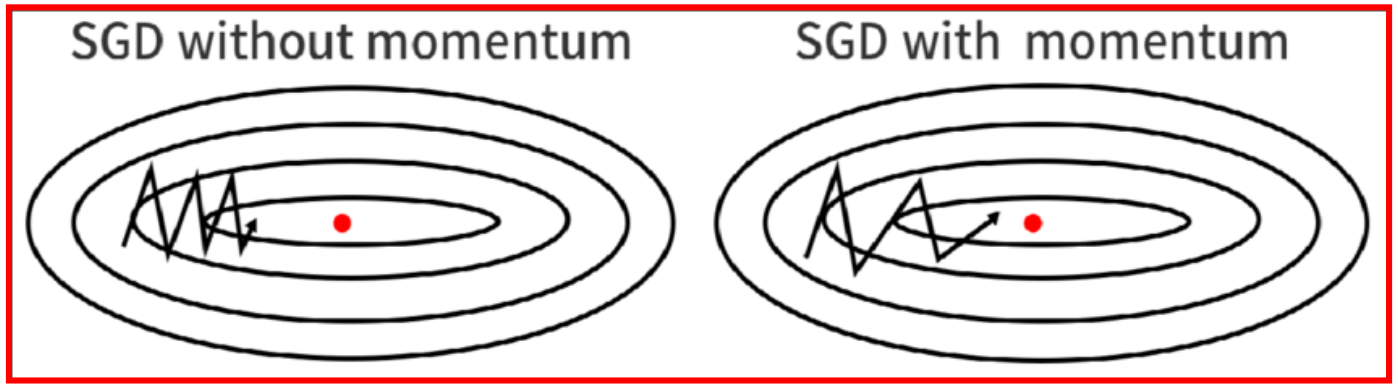
4. Faster Optimizers

- The SGD optimizer can be made faster using **momentum optimization**



$$\theta \leftarrow \theta - \eta \nabla_\theta J(\theta)$$

1. $\mathbf{m} \leftarrow \beta \mathbf{m} - \eta \nabla_\theta J(\theta)$
2. $\theta \leftarrow \theta + \mathbf{m}$

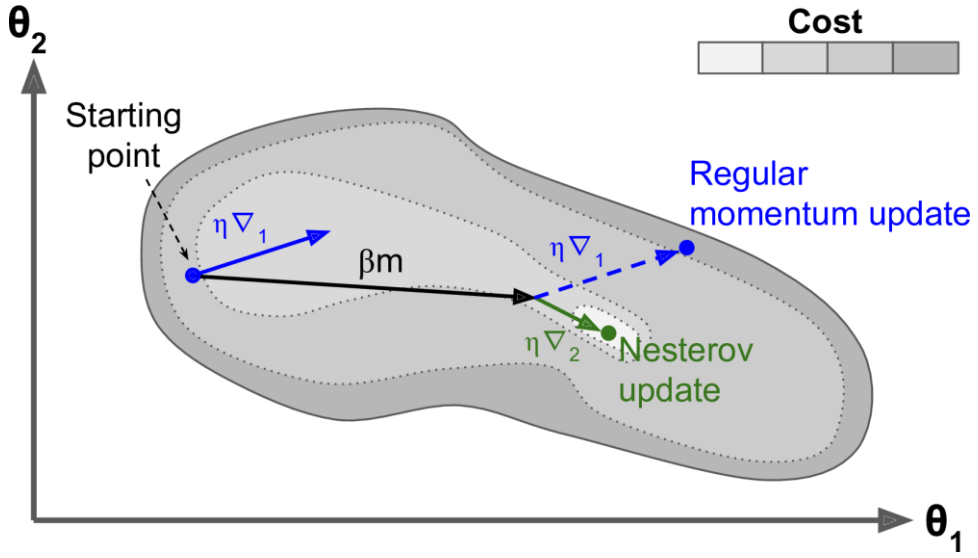
β

```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9)
```

4. Faster Optimizers

- **Nesterov momentum optimization** measures the gradient of the cost function not at the local position **θ** but slightly ahead in the direction of the momentum, at **θ** + β**m**

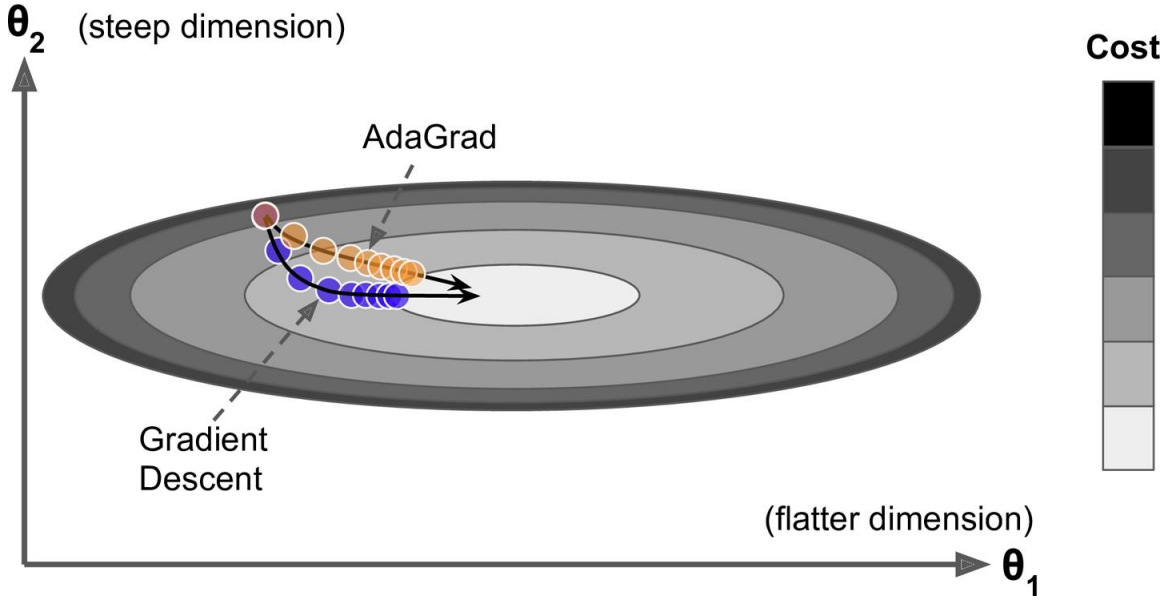
1. $\mathbf{m} \leftarrow \beta\mathbf{m} - \eta\nabla_{\theta}J(\theta + \beta\mathbf{m})$
2. $\theta \leftarrow \theta + \mathbf{m}$




```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9,
                                 nesterov=True)
```

4. Faster Optimizers

- The **adaptive optimizers** such as **AdaGrad**, **RMSProp**, **Adam**, and **Nadam** scale down the gradient vector along the steepest dimensions.




```
optimizer = keras.optimizers.RMSprop()
optimizer = keras.optimizers.Adam()
```

4. Faster Optimizers

- RMSProp, Adam and Nadam often **converge fast**. But they can give poor **generalization**.
- Solution: Use Nesterov accelerated gradient.

Class	Speed	Quality
SGD	*	***
SGD with momentum, Nestrov	**	***
Adagrad	***	*
RMSProp, Adam, Nadam, AdaMax	***	** or ***

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5. Avoiding Overfitting

- Deep neural networks typically have many parameters, giving them **ability to fit** a huge variety of complex datasets.

- **Useful regularization techniques**:
  - Early stopping
  - Batch normalization
  - ℓ_1 and ℓ_2 regularization
  - Dropout

5.1 ℓ_1 and ℓ_2 Regularization

- Constrain a neural network's connection weights.
- ℓ_1:
- ℓ_2:

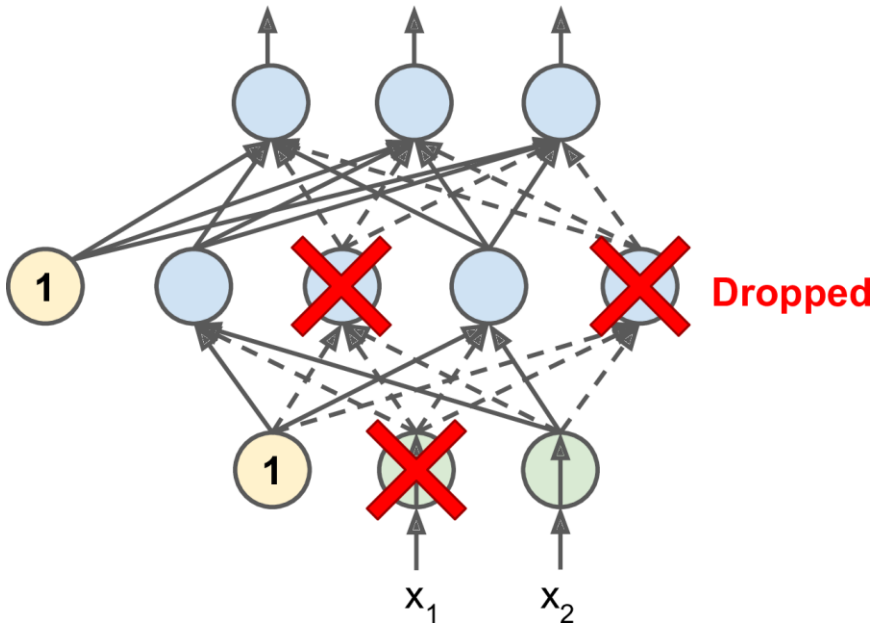
$$Cost\,function = Loss + \frac{\lambda}{2m} * \sum \|w\|$$

$$Cost\,function = Loss + \frac{\lambda}{2m} * \sum \|w\|^2$$

```
layer = keras.layers.Dense(100, activation="elu",
       kernel_initializer="he_normal",
       kernel_regularizer=keras.regularizers.l1(0.01))
# The other regularization functions:
keras.regularizers.l2(0.01)
keras.regularizers.l1_l2(l1=0.01, l2=0.01)
```

5.2 Dropout

- Popular technique to improve accuracy.
- At every training step, every neuron (excluding the output neurons) has a probability p of being temporarily **dropped out**.



5.2 Dropout

```
model = keras.models.Sequential([
        keras.layers.Flatten(input_shape=[28, 28]),
        keras.layers.Dropout(rate=0.2),
        keras.layers.Dense(300, activation="elu",
                kernel_initializer="he_normal"),
        keras.layers.Dropout(rate=0.2),
        keras.layers.Dense(100, activation="elu",
                kernel_initializer="he_normal"),
        keras.layers.Dropout(rate=0.2),
        keras.layers.Dense(10, activation="softmax")
])
```

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- **Recommended default DNN** configuration

Hyperparameter	Default value
Kernel initializer	He initialization
Activation function	ELU
Normalization	None if shallow; Batch Norm if deep
Regularization	Early stopping (+ℓ_2 reg. if needed)
Optimizer	Momentum optimization (or RMSProp or Nadam)
Learning rate schedule	1 cycle

6. Summary

- For a simple **stack of dense** or **CNN layers**.

Hyperparameter	Default value
Kernel initializer	LeCun initialization
Activation function	SELU
Normalization	None (self-normalization)
Regularization	Alpha dropout if needed
Optimizer	Momentum optimization (or RMSProp or Nadam)
Learning rate schedule	1 cycle

7. Exercise

11.8. Practice training a deep neural network on the **CIFAR10 image dataset**:

a) Build a DNN with 20 hidden layers of 100 neurons each (that's too many, but it's the point of this exercise). Use He initialization and the ELU activation function.

b) Using Nadam optimization and early stopping, train the network on the CIFAR10 dataset. You can load it with keras.datasets.cifar10.load_ data(). The dataset is composed of 60,000 32 × 32–pixel color images (50,000 for training, 10,000 for testing) with 10 classes, so you'll need a softmax output layer with 10 neurons. Remember to search for the right learning rate each time you change the model's architecture or hyperparameters.

c) Now try adding Batch Normalization and compare the learning curves: Is it converging faster than before? Does it produce a better model? How does it affect training speed?

d) Try replacing Batch Normalization with SELU, and make the necessary adjustments to ensure the network self-normalizes (i.e., standardize the input features, use LeCun normal initialization, make sure the DNN contains only a sequence of dense layers, etc.).

e) Try regularizing the model with alpha dropout. Then, without retraining your model, see if you can achieve better accuracy using MC Dropout.

f) Retrain your model using 1cycle scheduling and see if it improves training speed and model accuracy.