Deep Neural Networks

Prof. Gheith Abandah

Reference: *Hands-On Machine Learning with Scikit-Learn, Keras and TensorFlow* by Aurélien Géron (O'Reilly). 2019, 978-1-492-03264-9.

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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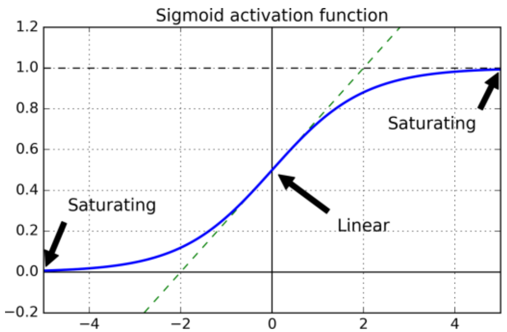
2. Vanishing/Exploding Gradients Problems

- **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**:

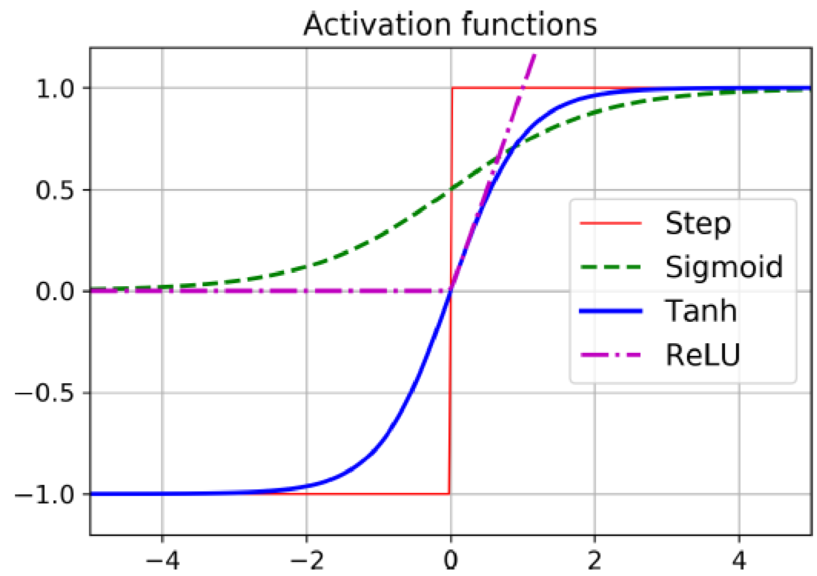
```
keras.layers.Dense(10, activation="relu",
      kernel_initializer="he_normal") # Or "he_uniform"
```

- **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.

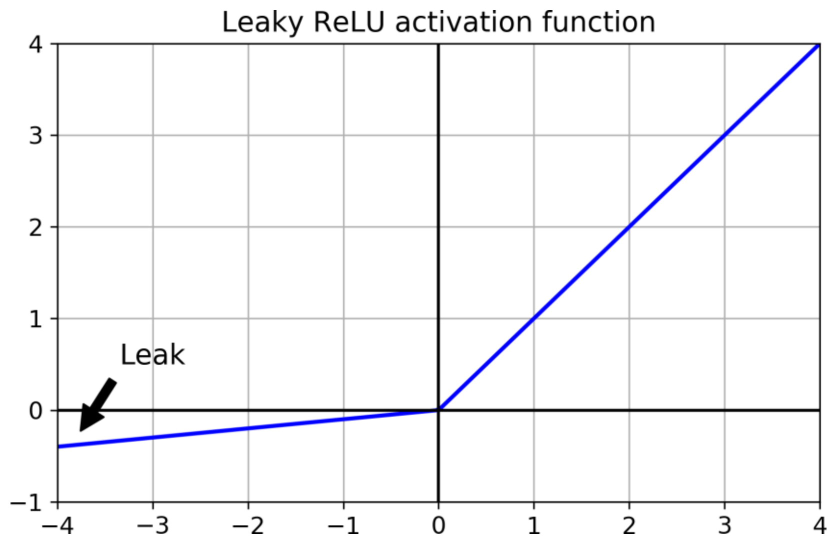


2.2 Nonsaturating Activation Functions

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

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

- **α** between 0.01 and 0.3

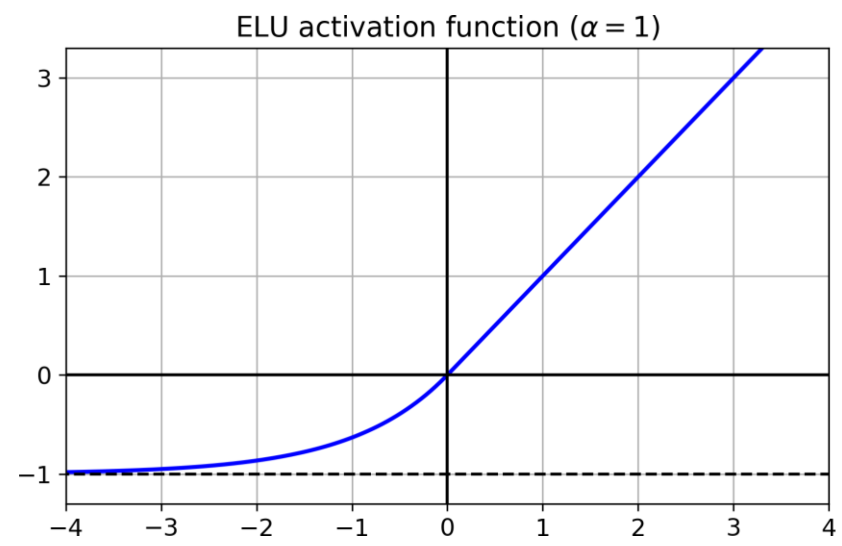



```
model = keras.models.Sequential([
    …
    keras.layers.Dense(10, kernel_initializer="he_normal"),
    keras.layers.LeakyReLU(alpha=0.2), # added as a layer
    …
])
```

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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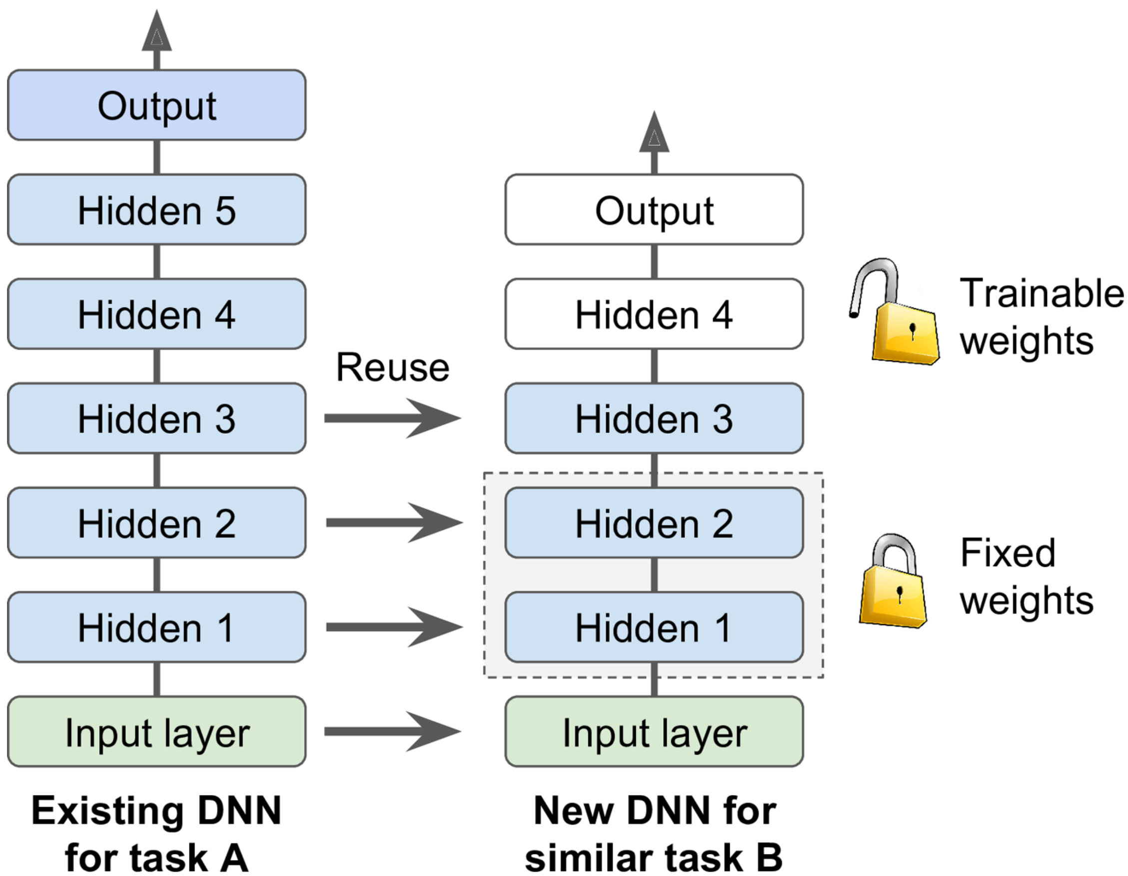
3. Reusing Pretrained Layers

- **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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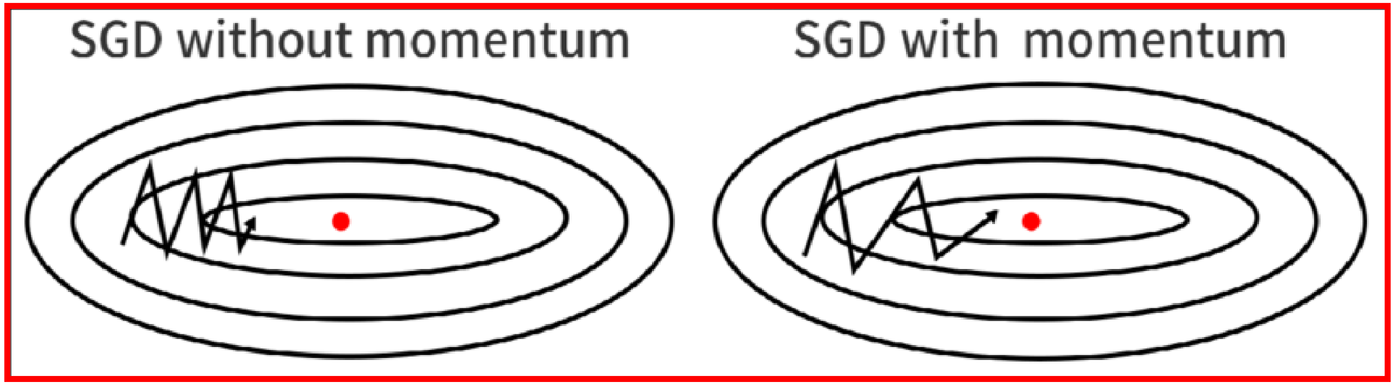
4. Faster Optimizers

- 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. $\theta \leftarrow \theta + \mathbf{m}$

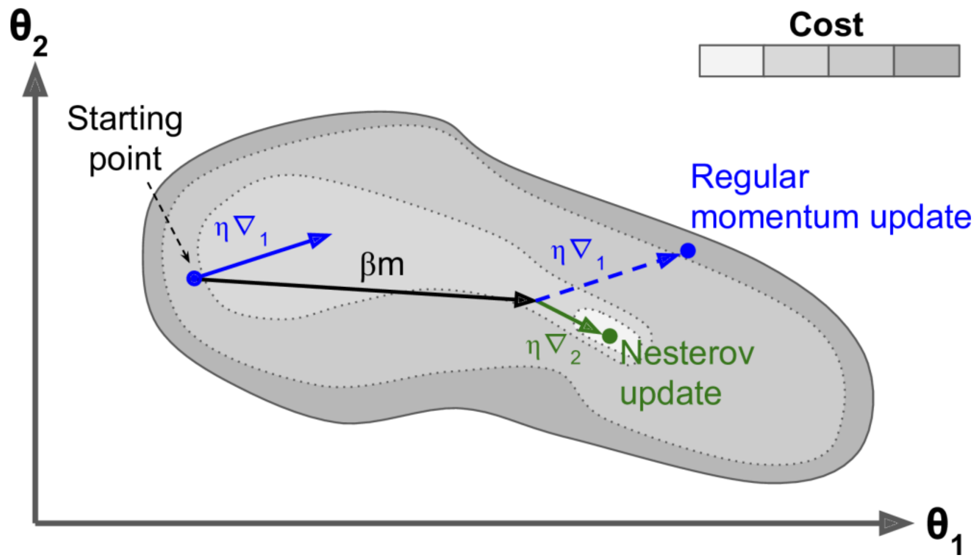
$\boxed{\beta}$

```
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 $\boldsymbol{\theta} + \beta\mathbf{m}$

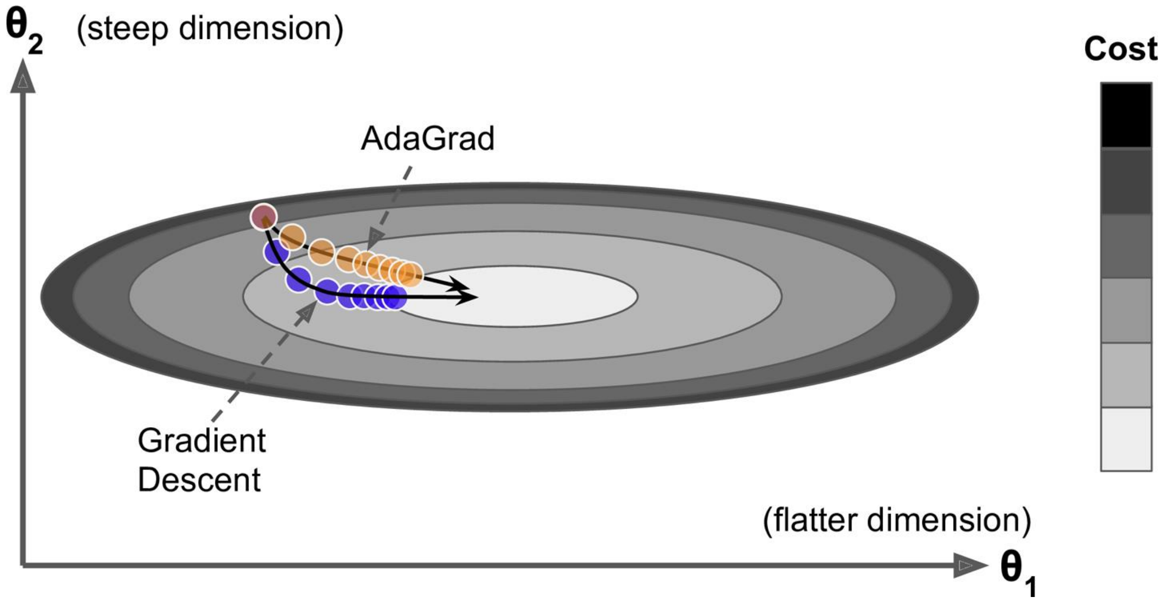
1. $\mathbf{m} \leftarrow \beta\mathbf{m} - \eta\nabla_{\boldsymbol{\theta}}J(\boldsymbol{\theta} + \beta\mathbf{m})$
2. $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \mathbf{m}$




```
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

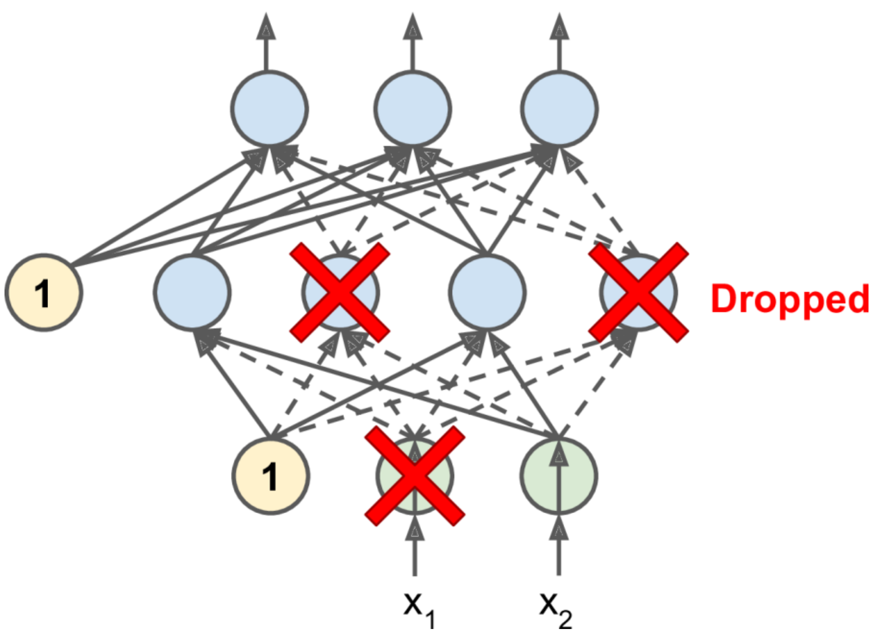
5.1 ℓ_1 and ℓ_2 Regularization

- Constrain a neural network's connection weights.
- ℓ_1: $$Cost\ function = Loss + \frac{\lambda}{2m} * \sum \|w\|$$
- ℓ_2: $$Cost\ function = Loss + \frac{\lambda}{2m} * \sum \|w\|^2$$

```
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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6. Summary

- 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

From Chapter 11, solve exercise:

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