Training Deep Feedforwards Networks

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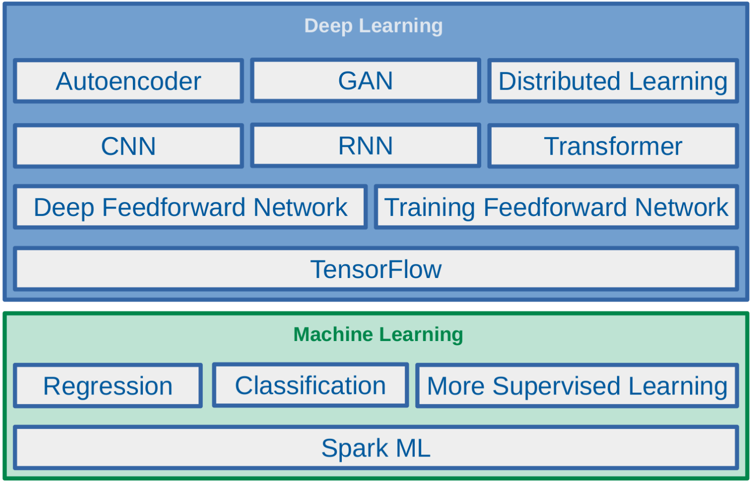
The Course Web Page

https://id2223kth.github.io

https://tinyurl.com/y6kcpmzy

Where Are We?


Deep Learning
Autoencoder
GAN
Distributed Learning
CNN
RNN
Transformer
Deep Feedforward Network
Training Feedforward Network
TensorFlow
Machine Learning
Regression
Classification
More Supervised Learning
Spark ML

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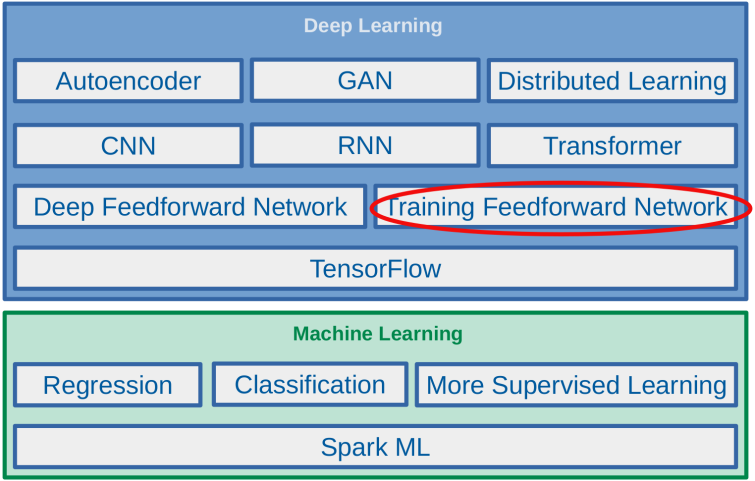

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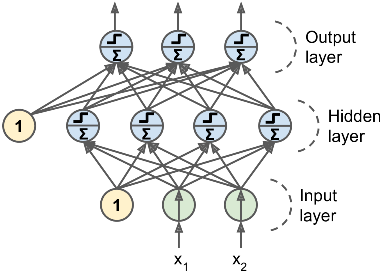
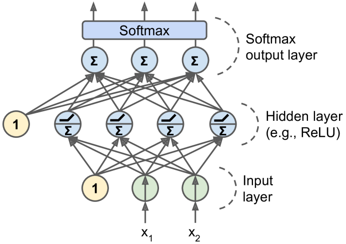
Feedforward Neural Network Architecture

- A feedforward neural network is composed of:
  - One input layer
  - One or more hidden layers
  - One final output layer



Feedforward Network in TensorFlow




```
n_output = 3
n_hidden = 4
n_features = 2

model = keras.models.Sequential()
model.add(keras.layers.Dense(n_hidden, input_shape=(n_features,), activation="relu"))
model.add(keras.layers.Dense(n_output, activation="softmax"))

model.compile(loss="sparse_categorical_crossentropy", optimizer="sgd", metrics=["accuracy"])
model.fit(X_train, y_train, epochs=30)
```

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- Overfitting: risk of overfitting a model with large number of parameters.
- Vanishing/exploding gradients: hard to train lower layers.
- Training speed: slow training with large networks.

Overfitting

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- Let's reduce the degree of freedom a model.

Avoiding Overfitting

- Early stopping
- $l1$ and $l2$ regularization
- Max-norm regularization
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- Data augmentation

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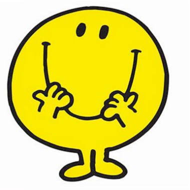
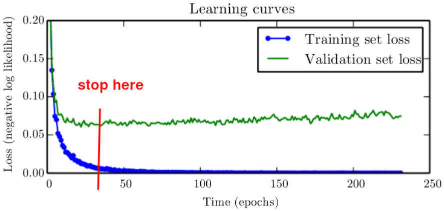


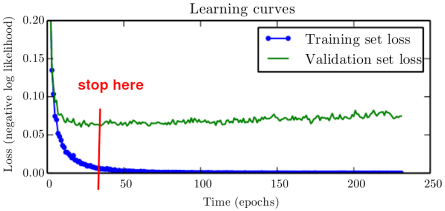
Early Stopping (1/2)

- As the training steps go by, its prediction error on the training/validation set naturally goes down.



Early Stopping (1/2)

- As the training steps go by, its prediction error on the training/validation set naturally goes down.
- After a while the validation error stops decreasing and starts to go back up.
    - The model has started to overfit the training data.



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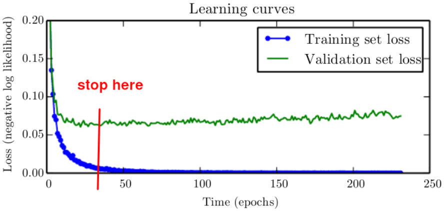
- As the training steps go by, its prediction error on the training/validation set naturally goes down.
- After a while the validation error stops decreasing and starts to go back up.
  - The model has started to overfit the training data.
- In the early stopping, we stop training when the validation error reaches a minimum.



Early Stopping (2/2)

```
from tensorflow.keras.callbacks import EarlyStopping

model = tf.keras.models.Sequential(...)

model.compile(optimizer='sgd', loss='sparse_categorical_crossentropy', metrics=['accuracy'])

earlystop_callback = EarlyStopping(monitor='accuracy', min_delta=0.05, patience=1)

model.fit(x_train, y_train, epochs=500, callbacks=[earlystop_callback])
```

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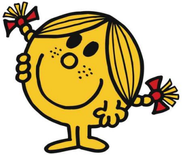

$l1$ and $l2$ Regularization (1/3)

- Penalize large values of weights w_j.

$$\tilde{J}(\mathbf{w}) = J(\mathbf{w}) + \lambda R(\mathbf{w})$$

- Two questions:
  1. How should we define $R(w)$?
  2. How do we determine λ?

$l1$ and $l2$ Regularization (2/3)

- *l1* regression: $\mathtt{R}(\mathbf{w}) = \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} |\mathtt{w}_\mathtt{i}|$ is added to the cost function.

$$\tilde{\mathtt{J}}(\mathbf{w}) = \mathtt{J}(\mathbf{w}) + \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} |\mathtt{w}_\mathtt{i}|$$

```
keras.layers.Dense(100, activation="relu", kernel_regularizer=keras.regularizers.l1(0.1))
```

$l1$ and $l2$ Regularization (3/3)

- *l*2 regression: $\mathtt{R}(\mathbf{w}) = \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} \mathtt{w}_{\mathtt{i}}^2$ is added to the cost function.

$$\tilde{\mathtt{J}}(\mathbf{w}) = \mathtt{J}(\mathbf{w}) + \lambda \sum_{\mathtt{i}=1}^{\mathtt{n}} \mathtt{w}_{\mathtt{i}}^2$$

```
keras.layers.Dense(100, activation="relu", kernel_regularizer=keras.regularizers.l2(0.01))
```

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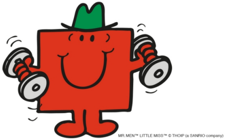

Max-Norm Regularization

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- After each training step, clip $\mathbf{w}_j$ as below, if $||\mathbf{w}_j||_2 > r$:

$$\mathbf{w}_j \leftarrow \mathbf{w}_j \frac{r}{||\mathbf{w}_j||_2}$$

  - r is the max-norm hyperparameter
  - $||\mathbf{w}_j||_2 = (\sum_i w_{i,j}^2)^{\frac{1}{2}} = \sqrt{w_{1,j}^2 + w_{2,j}^2 + \cdots + w_{n,j}^2}$

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```
keras.layers.Dense(100, activation="relu", kernel_constraint=keras.constraints.max_norm(1.))
```

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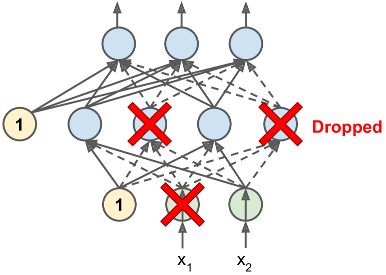
Dropout (1/4)

- Would a company perform better if its employees were told to toss a coin every morning to decide whether or not to go to work?

Dropout (2/4)

- At each training step, each neuron drops out temporarily with a probability p.



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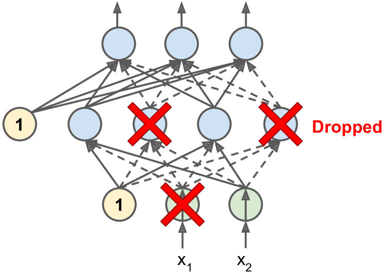

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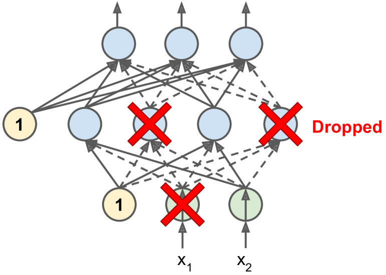

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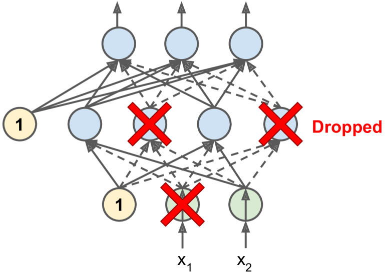

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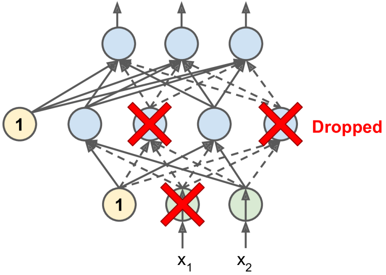
  - Exclude the output neurons.



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  - The hyperparameter p is called the dropout rate.
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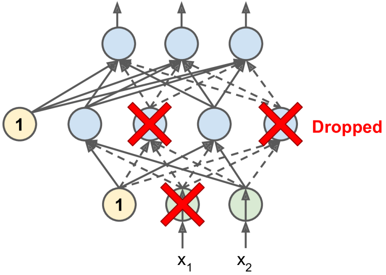
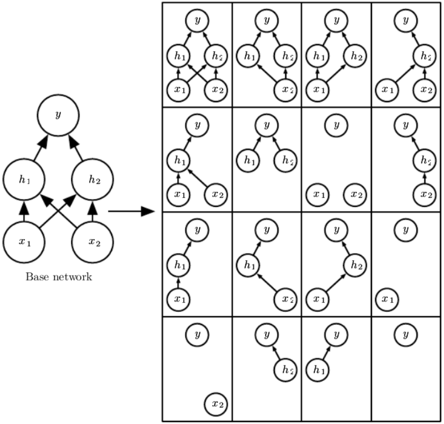
  - It may be active during the next step.
  - Exclude the output neurons.
- After training, neurons don't get dropped anymore.



Dropout (3/4)

- Each neuron can be either present or absent.
- 2^N possible networks, where N is the total number of droppable neurons.
  - $N = 4$ in this figure.



Dropout (4/4)

```
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dropout(rate=0.2),
    keras.layers.Dense(128, activation="relu"),
    keras.layers.Dropout(rate=0.2),
    keras.layers.Dense(10, activation="softmax")
])
```

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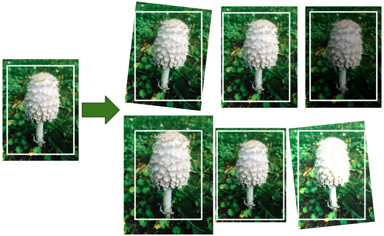
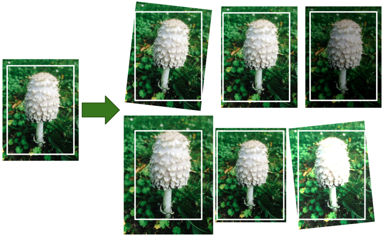
Data Augmentation

- One way to make a model generalize better is to train it on more data.
- This will reduce overfitting.



Data Augmentation

- One way to make a model generalize better is to train it on more data.
- This will reduce overfitting.
- Create fake data and add it to the training set.
  - E.g., in an image classification we can slightly shift, rotate and resize an image.
  - Add the resulting pictures to the training set.



Vanishing/Exploding Gradients

Vanishing/Exploding Gradients Problem (1/4)

- The backpropagation goes from output to input layer, and propagates the error gradient on the way.

$$\mathtt{w}^{(\mathtt{next})} = \mathtt{w} - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}}$$

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- Gradients often get smaller and smaller as the algorithm progresses down to the lower layers.
- As a result, the gradient descent update leaves the lower layer connection weights virtually unchanged.

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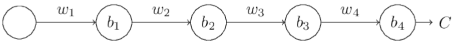
- This is called the vanishing gradients problem.

Vanishing/Exploding Gradients Problem (2/4)

- Assume a network with just a single neuron in each layer.



  - $w_1, w_2, \cdots$ are the weights
  - $b_1, b_2, \cdots$ are the biases
  - C is the cost function

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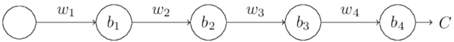

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- The output a_j from the jth neuron is $\sigma(z_j)$.
  - σ is the sigmoid activation function
  - $z_j = w_j a_{j-1} + b_j$
  - E.g., $a_4 = \sigma(z_4) = \mathtt{sigmoid}(w_4 a_3 + b_4)$

Vanishing/Exploding Gradients Problem (3/4)

- Lets compute the gradient associated to the first hidden neuron ($\frac{\partial C}{\partial b_1}$).

$$\frac{\partial C}{\partial b_1} = \frac{\partial C}{\partial a_4} \times \frac{\partial a_4}{\partial z_4} \times \frac{\partial z_4}{\partial a_3} \times \frac{\partial a_3}{\partial z_3} \times \frac{\partial z_3}{\partial a_2} \times \frac{\partial a_2}{\partial z_2} \times \frac{\partial z_2}{\partial a_1} \times \frac{\partial a_1}{\partial z_1} \times \frac{\partial z_1}{\partial b_1}$$

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$$\frac{\partial C}{\partial b_1} = \frac{\partial C}{\partial a_4} \times \frac{\partial a_4}{\partial z_4} \times \frac{\partial w_4 a_3 + b_4}{\partial a_3} \times \frac{\partial a_3}{\partial z_3} \times \frac{\partial w_3 a_2 + b_3}{\partial a_2} \times \frac{\partial a_2}{\partial z_2} \times \frac{\partial w_2 a_1 + b_2}{\partial a_1} \times \frac{\partial a_1}{\partial z_1} \times \frac{\partial w_1 a_0 + b_1}{\partial b_1}$$

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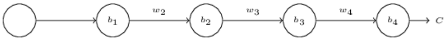
$$\frac{\partial C}{\partial b_1} = \frac{\partial C}{\partial a_4} \times \frac{\partial a_4}{\partial z_4} \times w_4 \times \frac{\partial a_3}{\partial z_3} \times w_3 \times \frac{\partial a_2}{\partial z_2} \times \times w_2 \times \frac{\partial a_1}{\partial z_1} \times 1$$

Vanishing/Exploding Gradients Problem (4/4)

- Now, consider $\frac{\partial C}{\partial b_3}$.



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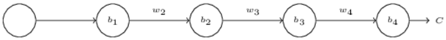

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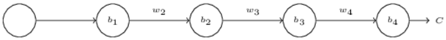

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- Assume $w_3 \times \frac{\partial a_2}{\partial z_2} < \frac{1}{4}$ and $w_2 \times \frac{\partial a_1}{\partial z_1} < \frac{1}{4}$
  - The gradient $\frac{\partial C}{\partial b_1}$ be a factor of 16 (or more) smaller than $\frac{\partial C}{\partial b_3}$.
  - This is the essential origin of the vanishing gradient problem.

Overcoming the Vanishing Gradient

- Parameter initialization strategies
- Nonsaturating activation function
- Batch normalization
- Gradient clipping

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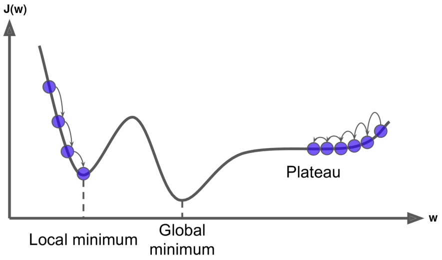

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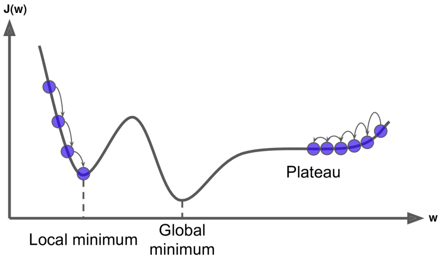

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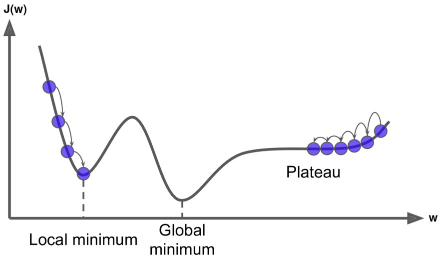
- The stochastic gradient descent on non-convex cost functions performs is sensitive to the values of the initial parameters.
- Designing initialization strategies is a difficult task.



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- Two hidden units with the same activation function connected to the same inputs, must have different initial parameters.

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- Two hidden units with the same activation function connected to the same inputs, must have different initial parameters.
  - The goal of having each unit compute a different function.
- It motivates random initialization of the parameters.
  - Typically, we set the biases to constants, and initialize only the weights randomly.

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- It is not possible to guarantee both unless each layer has an equal number of inputs and neurons.
- Based on the Xavier initialization, the weights are initialized using normal distribution with mean 0 and the following standard deviation.

Parameter Initialization Strategies (4/4)

- $\mathtt{fan}_{\mathtt{in}}$ and $\mathtt{fan}_{\mathtt{out}}$ are the number of inputs and neurons for the layer whose weights are being initialized.

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

Overcoming the Vanishing Gradient

- Parameter initiazlization strategies
- Nonsaturating activation function
- Batch normalization
- Gradient clipping

Nonsaturating Activation Functions (1/4)

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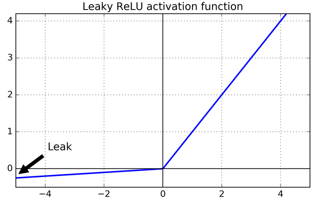
- The dying ReLUs problem.
  - During training, some neurons stop outputting anything other than 0.
  - E.g., when the weighted sum of the neuron's inputs is negative, it starts outputting 0.
- Use leaky ReLU instead: $\texttt{LeakyReLU}_{\alpha}(z) = \max(\alpha z, z)$.
  - α is the slope of the function for $z < 0$.



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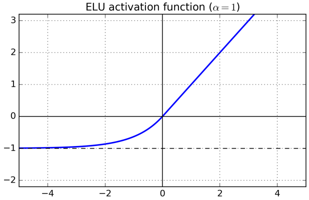
- Exponential Linear Unit (ELU)

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



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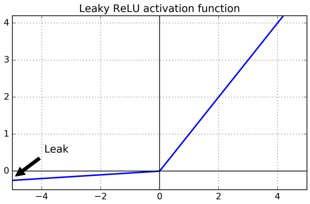
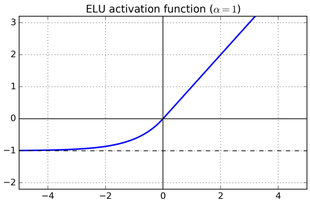
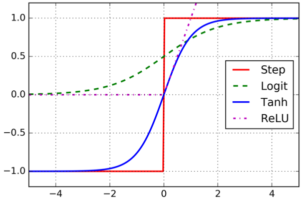
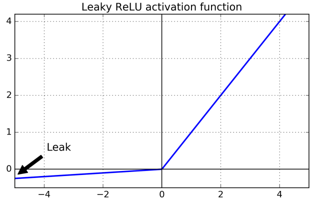


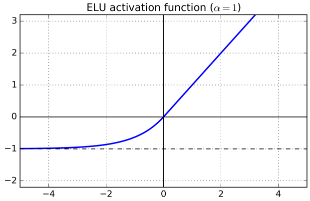


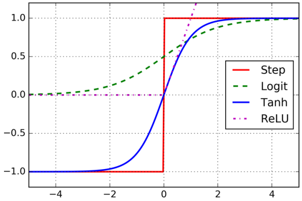


Nonsaturating Activation Functions (3/4)

- Which activation function should we use?
- In general logistic $<$ tanh $<$ ReLU $<$ leaky ReLU (and its variants) $<$ ELU
- If you care about runtime performance, then leaky ReLUs works better than ELUs.







Nonsaturating Activation Functions (4/4)

```
# elu
keras.layers.Dense(10, activation="elu")
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Nonsaturating Activation Functions (4/4)

```python
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```

```python
# leaky relu
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(128, kernel_initializer="he_normal"),
    keras.layers.LeakyReLU(),
    keras.layers.Dense(10, activation="softmax")
])
```

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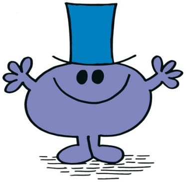

Batch Normalization (1/4)

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- Batch normalization makes the learning of layers in the network more independent of each other.
  - It is a technique to address the problem that the distribution of each layer's inputs changes during training, as the parameters of the previous layers change.
- The technique consists of adding an operation in the model just before the activation function of each layer.

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  - Estimates the inputs' mean and standard deviation of the current mini-batch.

$$\mu_B = \frac{1}{m_B} \sum_{i=1}^{m_B} \mathbf{x}^{(i)}$$

$$\sigma_B^2 = \frac{1}{m_B} \sum_{i=1}^{m_B} (\mathbf{x}^{(i)} - \mu_B)^2$$

- μ_B: the empirical mean, evaluated over the whole mini-batch B.
- σ_B: the empirical standard deviation, also evaluated over the whole mini-batch.
- m_B: the number of instances in the mini-batch.

Batch Normalization (3/4)

$$\hat{\mathbf{x}}^{(i)} = \frac{\mathbf{x}^{(i)} - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

$$\mathbf{z}^{(i)} = \gamma \hat{\mathbf{x}}^{(i)} + \beta$$

- $\hat{\mathbf{x}}^{(i)}$: the zero-centered and normalized input.
- $\mathbf{z}^{(i)}$: the output of the BN operation, which is a scaled and shifted version of the inputs.
- γ: the scaling parameter vector for the layer.
- β: the shifting parameter (offset) vector for the layer.
- ϵ: a tiny number to avoid division by zero.
- $\otimes$: represents the element-wise multiplication.

Batch Normalization (4/4)

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model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
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Gradient Clipping

- Gradient clipping: clip the gradients during backpropagation so that they never exceed some threshold.

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optimizer = keras.optimizers.SGD(clipvalue=1.0)
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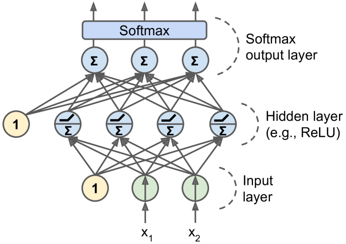
- `clipnorm=1.0`: $[0.9, 100.0] \Rightarrow [0.00899964, 0.9999595]$

Training Speed

Regular Gradient Descent Optimization (1/2)

- Gradient descent optimization algorithm
- It updates the weights $w_i^{(next)} = w_i - \eta \frac{\partial J(\mathbf{w})}{\partial w_i}$
- Better optimization algorithms to improve the training speed

Regular Gradient Descent Optimization (2/2)




```
n_output = 3
n_hidden = 4
n_features = 2

model = keras.models.Sequential()
model.add(keras.layers.Dense(n_hidden, input_shape=(n_features,), activation="relu"))
model.add(keras.layers.Dense(n_output, activation="softmax"))

model.compile(loss="sparse_categorical_crossentropy", optimizer="sgd", metrics=["accuracy"])
model.fit(X_train, y_train, epochs=30)
```

Optimization Algorithms

- Momentum
- Nesterov momentum
- AdaGrad
- RMSProp
- Adam Optimization

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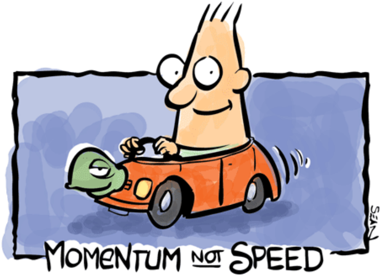
Momentum (1/3)

- Momentum is a concept from physics: an object in motion will have a tendency to keep moving.
- It measures the resistance to change in motion.
  - The higher momentum an object has, the harder it is to stop it.



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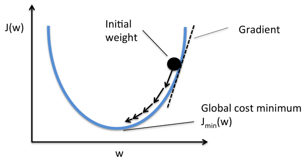

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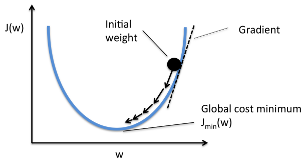
- We can thus use the concept of momentum to give the update process a tendency to keep moving in the same direction.



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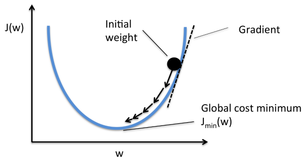
- We can thus use the concept of momentum to give the update process a tendency to keep moving in the same direction.
- It can help to escape from bad local minima pits.



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- Momentum optimization cares about what previous gradients were.
- At each iteration, it adds the local gradient to the momentum vector **m**.

$$\mathtt{m}_\mathtt{i} = \beta \mathtt{m}_\mathtt{i} + \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_\mathtt{i}}$$

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```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

Optimization Algorithms

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Nesterov Momentum (1/2)

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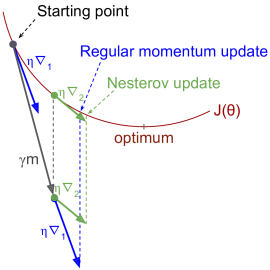
- Nesterov Momentum is a small variant to Momentum optimization.
- Faster than vanilla Momentum optimization.
- $\nabla 1$ represents the gradient of the cost function measured at the starting point $\mathbf{w}$, and $\nabla 2$ represents the gradient at the point located at $\mathbf{w} + \beta \mathbf{m}$.



Nesterov Momentum (2/2)

- Measure the gradient of the cost function slightly ahead in the direction of the momentum (not at the local position).

$$\mathtt{m_i} = \beta \mathtt{m_i} + \eta \frac{\partial \mathtt{J}(\mathbf{w} + \beta \mathbf{m})}{\partial \mathtt{w_i}}$$

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$$\mathtt{w_i^{(next)}} = \mathtt{w_i} - \mathtt{m_i}$$

```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9, nesterov=True)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

Optimization Algorithms

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AdaGrad (1/2)

- AdaGrad keeps track of a learning rate for each parameter.
- Adapts the learning rate over time (adaptive learning rate).
- Decays the learning rate faster for steep dimensions than for dimensions with gentler slopes.

AdaGrad (2/2)

- For each feature $\mathtt{w_i}$, we do the following steps:

$$\mathtt{s_i} = \mathtt{s_i} + \left(\frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w_i}}\right)^2$$

$$\mathtt{w_i}^{(\mathtt{next})} = \mathtt{w_i} - \frac{\eta}{\sqrt{\mathtt{s_i} + \epsilon}} \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w_i}}$$

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```
optimizer = keras.optimizers.Adagrad(lr=0.001)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

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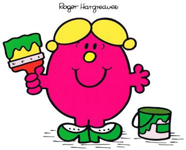

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- The learning rate gets scaled down so much that the algorithm ends up stopping entirely before reaching the global optimum.

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- The learning rate gets scaled down so much that the algorithm ends up stopping entirely before reaching the global optimum.
- The RMSProp fixed the AdaGrad problem.
- It is like the AdaGrad problem, but accumulates only the gradients from the most recent iterations (not from the beginning of training).

RMSProp (2/2)

- For each feature $\mathtt{w_i}$, we do the following steps:

$$\mathtt{s_i} = \beta \mathtt{s_i} + (1 - \beta)(\frac{\partial \mathtt{J(w)}}{\partial \mathtt{w_i}})^2$$

$$\mathtt{w_i^{(next)}} = \mathtt{w_i} - \frac{\eta}{\sqrt{\mathtt{s_i} + \epsilon}} \frac{\partial \mathtt{J(w)}}{\partial \mathtt{w_i}}$$

RMSProp (2/2)

- For each feature $\mathtt{w_i}$, we do the following steps:

$$\mathtt{s_i} = \beta \mathtt{s_i} + (1 - \beta)(\frac{\partial \mathtt{J}(\mathtt{w})}{\partial \mathtt{w_i}})^2$$

$$\mathtt{w_i^{(next)}} = \mathtt{w_i} - \frac{\eta}{\sqrt{\mathtt{s_i} + \epsilon}} \frac{\partial \mathtt{J}(\mathtt{w})}{\partial \mathtt{w_i}}$$

```
optimizer = keras.optimizers.RMSprop(lr=0.001, rho=0.9)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

Optimization Algorithms

- Momentum
- Nesterov momentum
- AdaGrad
- RMSProp
- Adam optimization

Adam Optimization (1/3)

- Adam (Adaptive moment estimation) combines the ideas of Momentum optimization and RMSProp.

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- Like Momentum optimization, it keeps track of an exponentially decaying average of past gradients.
- Like RMSProp, it keeps track of an exponentially decaying average of past squared gradients.

Adam Optimization (2/3)

$$1.\ \mathbf{m}^{(\texttt{next})} = \beta_1 \mathbf{m} + (1 - \beta_1)\nabla_{\mathbf{w}} \mathtt{J}(\mathtt{w})$$

$$2.\ \mathbf{s}^{(\texttt{next})} = \beta_2 \mathbf{s} + (1 - \beta_2)\nabla_{\mathbf{w}} \mathtt{J}(\mathtt{w}) \otimes \nabla_{\mathbf{w}} \mathtt{J}(\mathtt{w})$$

$$3.\ \mathbf{m}^{(\texttt{next})} = \frac{\mathbf{m}}{1 - \beta_1^{\mathrm{T}}}$$

$$4.\ \mathbf{s}^{(\texttt{next})} = \frac{\mathbf{s}}{1 - \beta_2^{\mathrm{T}}}$$

$$5.\ \mathbf{w}^{(\texttt{next})} = \mathbf{w} - \eta \mathbf{m} \oslash \sqrt{\mathbf{s} + \epsilon}$$

- $\otimes$ and $\oslash$ represent the element-wise multiplication and division.
- Steps 1, 2, and 5: similar to both Momentum optimization and RMSProp.
- Steps 3 and 4: since $\mathtt{m}$ and $\mathtt{s}$ are initialized at 0, they will be biased toward 0 at the beginning of training, so these two steps will help boost $\mathtt{m}$ and $\mathtt{s}$ at the beginning of training.

Adam Optimization (3/3)

```
optimizer = keras.optimizers.Adam(lr=0.001, beta_1=0.9, beta_2=0.999)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

Summary

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- Overfitting
  - Early stopping, $l1$ and $l2$ regularization, max-norm regularization
  - Dropout, data augmentation
- Vanishing gradient
  - Parameter initialization, nonsaturating activation functions
  - Batch normalization, gradient clipping
- Training speed
  - Momentum, nesterov momentum, AdaGrad
  - RMSProp, Adam optimization

Reference

- Ian Goodfellow et al., Deep Learning (Ch. 7, 8)
- Aurélien Géron, Hands-On Machine Learning (Ch. 11)

Questions?