Training Deep Feedforwards Networks

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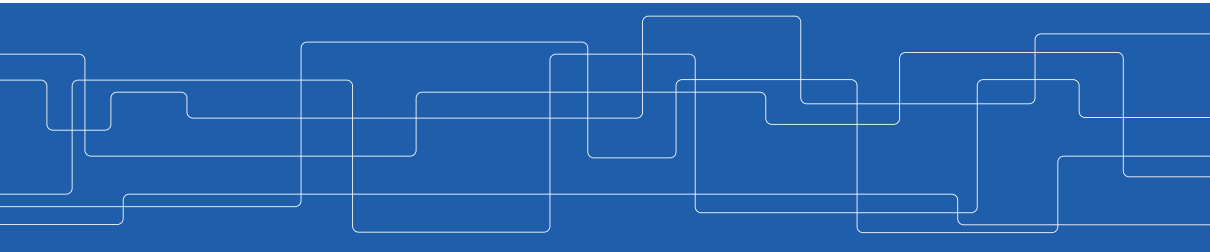
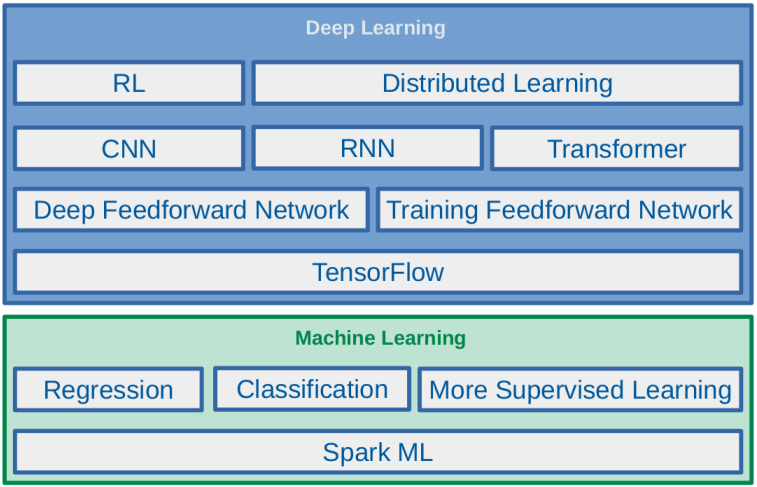


The Course Web Page

https://id2223kth.github.io

https://tinyurl.com/6s5jy46a

Where Are We?


Deep Learning
RL
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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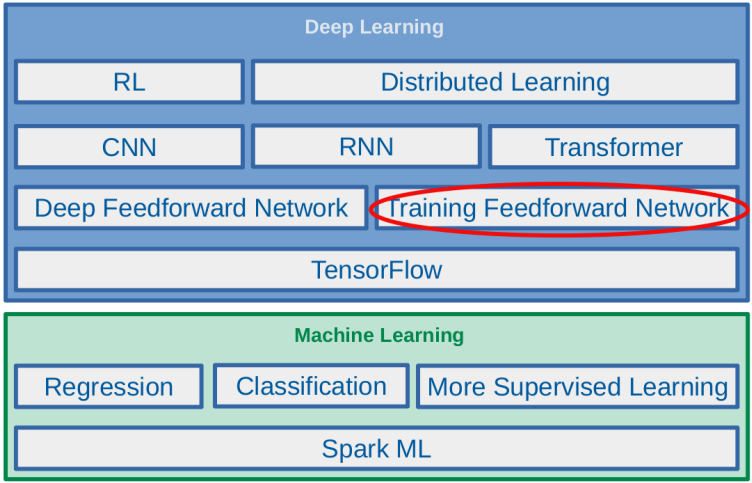
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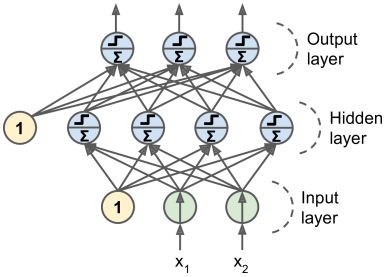
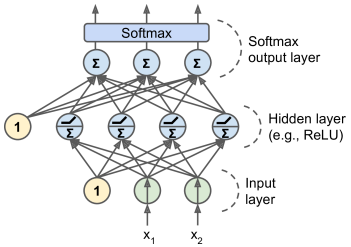
Feedforward Neural Network Architecture

- 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)
```

Challenges of Training Feedforward Neural Networks

- Challenges ...
- 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

High Degree of Freedom and Overfitting Problem

- With large number of parameters, a network has a high degree of freedom.
- It can fit a huge variety of complex datasets.
- This flexibility also means that it is prone to overfitting on training set.
- Let's reduce the degree of freedom a model.

Avoiding Overfitting

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

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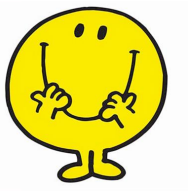
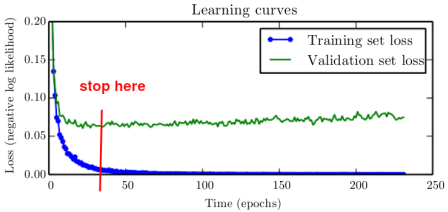


Early Stopping (1/2)

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

Avoiding Overfitting

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

/1 and /2 Regularization (1/3)

- Penalize large values of weights w_j.

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

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

/1 and /2 Regularization (2/3)

- /1 regression: $R(w) = \lambda \sum_{i=1}^{n} |w_i|$ is added to the cost function.

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

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

/1 and /2 Regularization (3/3)

- /2 regression: $R(w) = \lambda \sum_{i=1}^{n} w_i^2$ is added to the cost function.

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

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

Avoiding Overfitting

- Early stopping
- $l1$ and $l2$ regularization
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Max-Norm Regularization

- Max-norm regularization: constrains the weights w_j of the incoming connections for each neuron j.
  - Prevents them from getting too large.

- After each training step, clip w_j as below, if $||w_j||_2 > r$:

$$w_j \leftarrow w_j \frac{r}{||w_j||_2}$$

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

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

Avoiding Overfitting

- Early stopping
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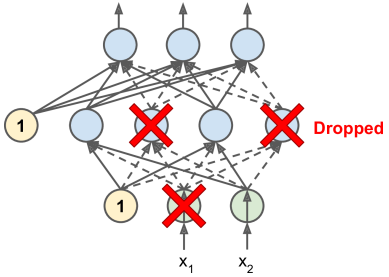
Dropout (1/4)

- 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?

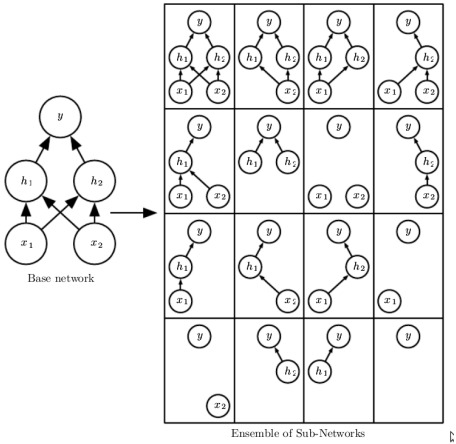
Dropout (2/4)

- At each training step, each neuron drops out temporarily with a probability p.
  - The hyperparameter p is called the dropout rate.
  - A neuron will be entirely ignored during this training step.
  - 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")
])
```

Avoiding Overfitting

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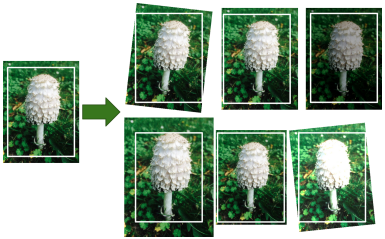
Data Augmentation

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

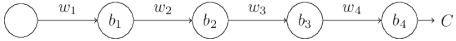
- The backpropagation goes from output to input layer, and propagates the error gradient on the way.

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

- 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.
- 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

- 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 ($\frac{\partial C}{\partial b_1}$).

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

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

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

Vanishing/Exploding Gradients Problem (4/4)

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

$$\frac{\partial C}{\partial b_3} = \frac{\partial C}{\partial a_4} \times \frac{\partial a_4}{\partial z_4} \times w_4 \times \frac{\partial a_3}{\partial z_3}$$

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

- 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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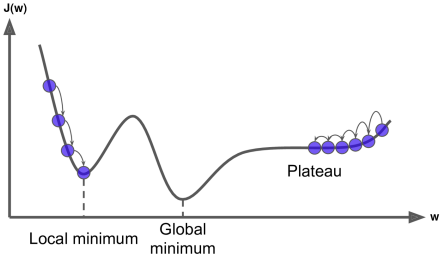
Parameter Initialization Strategies (1/4)

- The non-linearity of a neural network causes the cost functions to become non-convex.
- 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.



Parameter Initialization Strategies (2/4)

- The initial parameters need to break symmetry between different units.
- 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.

Parameter Initialization Strategies (3/4)

- We need the signals to flow properly in both directions.
- The Glorot and Bengio initialization proposed that:
  - The variance of the outputs of each layer to be equal to the variance of its inputs.
  - The gradients to have equal variance before and after flowing through a layer in the reverse direction.
- 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)

- $\texttt{fan}_{\texttt{in}}$ and $\texttt{fan}_{\texttt{out}}$ are the number of inputs and neurons for the layer whose weights are being initialized.
- $\texttt{fan}_{\texttt{avg}} = \frac{2}{\texttt{fan}_{\texttt{in}} + \texttt{fan}_{\texttt{out}}}$
- Glorot initialization, for none, logistic, sigmoid, and tanh: $\sigma^2 = \frac{1}{\texttt{fan}_{\texttt{avg}}}$
- He initialization, for ReLU: $\sigma^2 = \frac{2}{\texttt{fan}_{\texttt{in}}}$

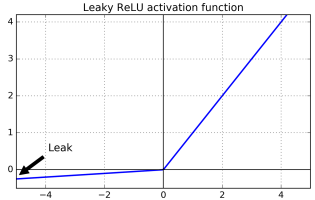
```
keras.layers.Dense(10, activation="relu", kernel_initializer="he_normal")
```

Overcoming the Vanishing Gradient

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

Nonsaturating Activation Functions (1/4)

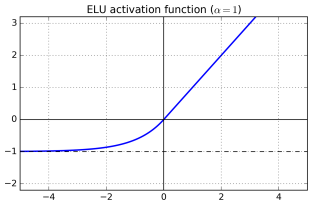
- $\texttt{ReLU}(z) = \max(0, z)$
- The dying ReLUs problem.
  - During training, some neurons stop outputting anything other than 0.
  - E.g., when the weighted sum of the neuron's inputs is negative, it starts outputting 0.
- Use leaky ReLU instead: $\texttt{LeakyReLU}_\alpha(z) = \max(\alpha z, z)$.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



Nonsaturating Activation Functions (2/4)

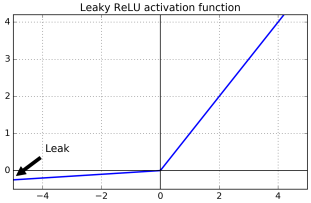
- Randomized Leaky ReLU (RReLU)
  - α is picked randomly during training, and it is fixed during testing.
- Parametric Leaky ReLU (PReLU)
  - Learn α during training (instead of being a hyperparameter).
- Exponential Linear Unit (ELU)

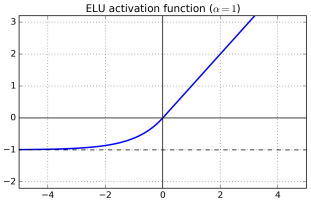
$$\mathrm{ELU}_\alpha(z) = \begin{cases} \alpha(\exp(z) - 1) & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$

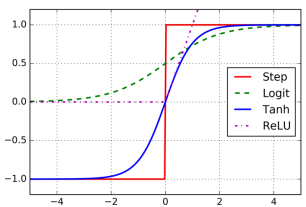


Nonsaturating Activation Functions (3/4)

- 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")
```

```
# 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")
])
```

Overcoming the Vanishing Gradient

- Parameter initiazlization strategies
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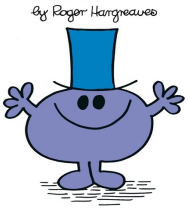
- Batch normalization
- Gradient clipping



Batch Normalization (1/4)

- The gradient tells how to update each parameter, under the assumption that the other layers do not change.
  - In practice, we update all of the layers simultaneously.
  - However, unexpected results can happen.
- 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.

Batch Normalization (2/4)

- It's zero-centering and normalizing the inputs, then scaling and shifting the result.
  - Estimates the inputs' mean and standard deviation of the current mini-batch.

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

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

- 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)

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

- $\hat{x}^{(i)}$: the zero-centered and normalized input.
- $z^{(i)}$: 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)

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

Overcoming the Vanishing Gradient

- Parameter initiazlization strategies
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Gradient Clipping

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

```
optimizer = keras.optimizers.SGD(clipvalue=1.0)
model.compile(loss="mse", optimizer=optimizer)
```

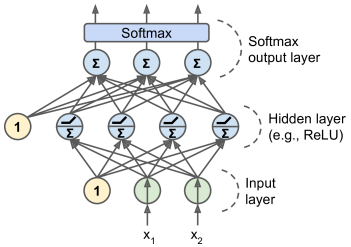
- Setting the `clipvalue` or `clipnorm` argument when creating an optimizer.
- `clipvalue=1.0` and `clipnorm=1.0`: values between -1.0 and 1.0.
- `clipvalue=1.0`: $[0.9, 100.0] \Rightarrow [0.9, 1.0]$
- `clipnorm=1.0`: $[0.9, 100.0] \Rightarrow [0.00899964, 0.9999595]$

Training Speed

Regular Gradient Descent Optimization (1/2)

- Gradient descent optimization algorithm
- It updates the weights $\mathtt{w}_{\mathtt{i}}^{(\mathtt{next})} = \mathtt{w}_{\mathtt{i}} - \eta \frac{\partial \mathtt{J}(\mathtt{w})}{\partial \mathtt{w}_{\mathtt{i}}}$
- 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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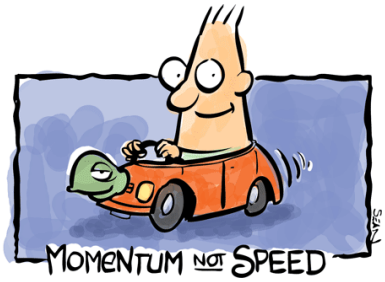
- Momentum
- Nesterov momentum
- AdaGrad
- RMSProp
- Adam optimization

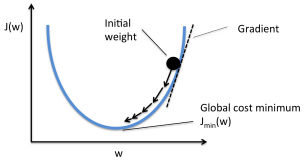
Momentum (1/3)

- 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.



Momentum (2/3)

- This is the very simple idea behind momentum optimization.
- We can see the change in the parameters w as motion: $\mathtt{w}_\mathtt{i}^{(\mathtt{next})} = \mathtt{w}_\mathtt{i} - \eta \frac{\partial \mathtt{J}(\mathtt{w})}{\partial \mathtt{w}_\mathtt{i}}$
- 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.



Momentum (3/3)

- Regular gradient descent optimization: $\mathtt{w}_\mathtt{i}^{(\mathtt{next})} = \mathtt{w}_\mathtt{i} - \eta \frac{\partial \mathtt{J}(\mathtt{w})}{\partial \mathtt{w}_\mathtt{i}}$
- Momentum optimization cares about what previous gradients were.
- At each iteration, it adds the local gradient to the momentum vector m.

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

$$\mathtt{w}_\mathtt{i}^{(\mathtt{next})} = \mathtt{w}_\mathtt{i} - \mathtt{m}_\mathtt{i}$$

- β is called momentum, ans it is between 0 and 1.

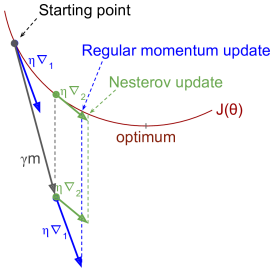
```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

Optimization Algorithms

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

Nesterov Momentum (1/2)

- 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 w, and $\nabla 2$ represents the gradient at the point located at $w + \beta m$.



Nesterov Momentum (2/2)

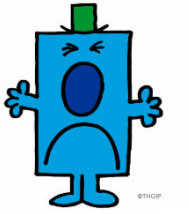
- Measure the gradient of the cost function slightly ahead in the direction of the momentum (not at the local position).

$$\mathtt{m}_i = \beta \mathtt{m}_i + \eta \frac{\partial J(\mathtt{w} + \beta \mathtt{m})}{\partial \mathtt{w}_i}$$
$$\mathtt{w}_i^{(\mathtt{next})} = \mathtt{w}_i - \mathtt{m}_i$$

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

Optimization Algorithms

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



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 w_i, we do the following steps:

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

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

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

Optimization Algorithms

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

RMSProp (1/2)

- AdaGrad often stops too early when training neural networks.
- 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 w_i, we do the following steps:

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

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

```
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.
- 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)

$$
\begin{aligned}
1.\ \mathbf{m}^{(\text{next})} &= \beta_1 \mathbf{m} + (1-\beta_1)\nabla_{\mathbf{w}} J(\mathbf{w}) \\
2.\ \mathbf{s}^{(\text{next})} &= \beta_2 \mathbf{s} + (1-\beta_2)\nabla_{\mathbf{w}} J(\mathbf{w}) \otimes \nabla_{\mathbf{w}} J(\mathbf{w}) \\
3.\ \mathbf{m}^{(\text{next})} &= \frac{\mathbf{m}}{1-\beta_1^T} \\
4.\ \mathbf{s}^{(\text{next})} &= \frac{\mathbf{s}}{1-\beta_2^T} \\
5.\ \mathbf{w}^{(\text{next})} &= \mathbf{w} - \eta \mathbf{m} \oslash \sqrt{\mathbf{s}+\epsilon}
\end{aligned}
$$

- $\otimes$ 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 $\mathbf{m}$ and $\mathbf{s}$ are initialized at 0, they will be biased toward 0 at the beginning of training, so these two steps will help boost $\mathbf{m}$ and $\mathbf{s}$ 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

Summary

- 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?