Training Deep Feedforwards Networks

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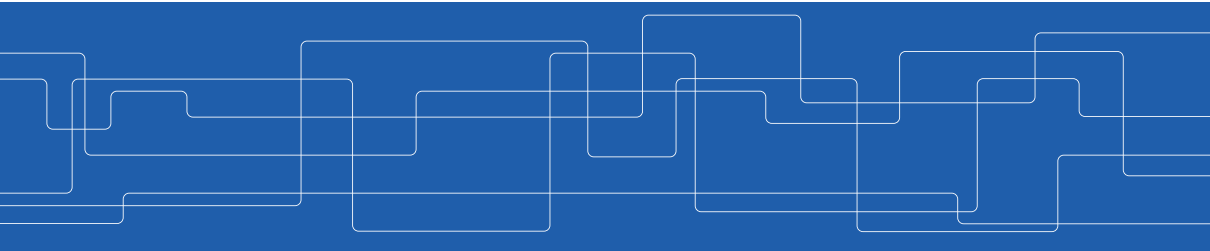
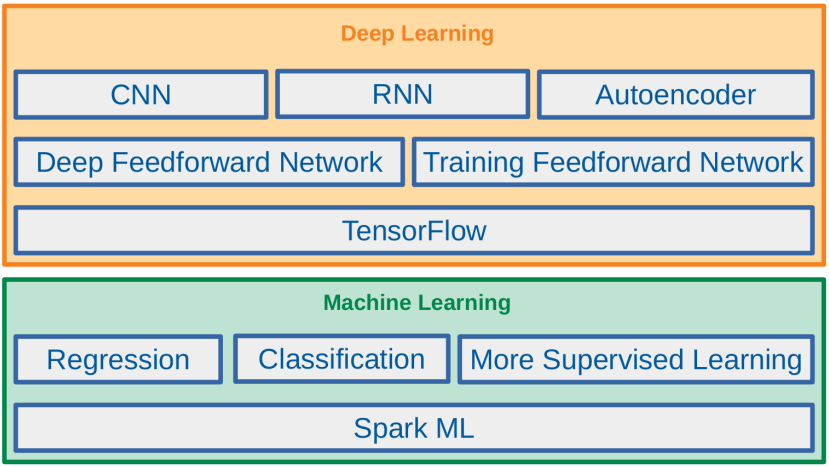


The Course Web Page

https://id2223kth.github.io

Where Are We?


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

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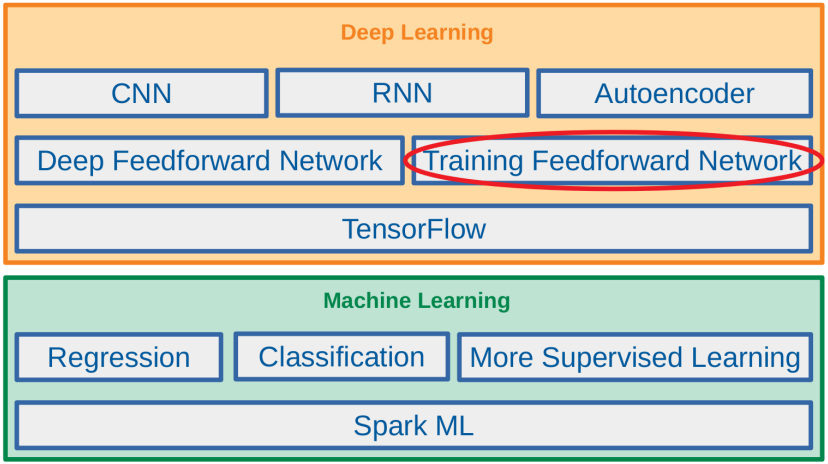
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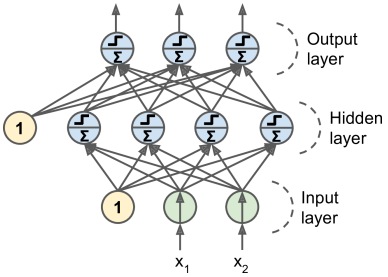
Feedforward Neural Network Architecture

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



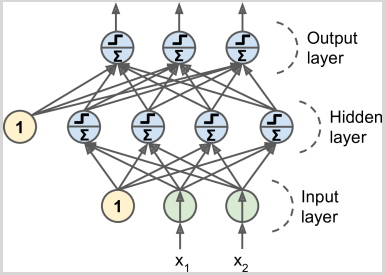
Feedforward Network in TensorFlow (1/2)

- `n_neurons_h`: number of neurons in the hidden layer.
- `n_neurons_out`: number of neurons in the output layer.
- `n_features`: number of features.

```
n_neurons_h = 4
n_neurons_out = 3
n_features = 2

# placeholder
X = tf.placeholder(tf.float32, shape=(None, n_features),
  name="X")
y_true = tf.placeholder(tf.int64, shape=(None),
  name="y")

# make the network
hidden = tf.layers.dense(X, n_neurons_h, name="hidden",
  activation=tf.sigmoid)
logit = tf.layers.dense(hidden, n_neurons_out, name="output") # logit = Wh + b
y_hat = tf.sigmoid(logit)
```



Feedforward Network in TensorFlow (2/2)

- Define the cost and the optimization, and execute the network.

```
# define the cost
cross_entropy = tf.nn.sigmoid_cross_entropy_with_logits(logit, y_true)
cost = tf.reduce_mean(cross_entropy)

# train the model
learning_rate = 0.1
optimizer = tf.train.GradientDescentOptimizer(learning_rate)
training_op = optimizer.minimize(cost)

# execute the model
init = tf.global_variables_initializer()

n_epochs = 100
with tf.Session() as sess:
    init.run()
    for epoch in range(n_epochs):
      sess.run(training_op, feed_dict={X: training_X, y_true: training_y})
```

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.
- Regularization: a way to reduce the risk of overfitting.
- It reduces the degree of freedom a model.

Avoiding Overfitting Through Regularization

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

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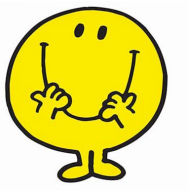
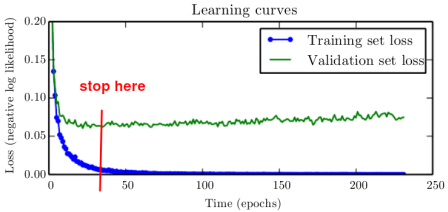


Early Stopping

- 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.



Avoiding Overfitting Through Regularization

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/1 and /2 Regularization (1/4)

- Penalize large values of weights $\mathtt{w_j}$.

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

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

/1 and /2 Regularization (2/4)

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

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

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

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

/1 and /2 Regularization (3/4)

- Manually implement it in TensorFlow.

```
# make the network
hidden = tf.layers.dense(X, n_neurons_h, activation=tf.sigmoid, name="hidden")
logit = tf.layers.dense(hidden, n_neurons_out, name="output")
```

```
# extract the weights of layers
W1 = tf.get_default_graph().get_tensor_by_name("hidden/kernel:0")
W2 = tf.get_default_graph().get_tensor_by_name("output/kernel:0")
```

```
# l1 regularization
reg_cost = tf.reduce_sum(tf.abs(W1)) + tf.reduce_sum(tf.abs(W2))
```

```
# define the cost
cross_entropy = tf.nn.sigmoid_cross_entropy_with_logits(logit, y_true)
base_cost = tf.reduce_mean(cross_entropy)

l1_param = 0.001
cost = base_cost + l1_param * reg_cost

# the rest is as before
```

/1 and /2 Regularization (5/5)

- Alternatively, we can pass a regularization function to the `tf.layers.dense()`.

```
# make the network
l1_param = 0.001 # l1 regularization hyperparameter

hidden = tf.layers.dense(X, n_neurons_h, activation=tf.sigmoid, name="hidden",
  kernel_regularizer=tf.contrib.layers.l1_regularizer(l1_param))
logit = tf.layers.dense(hidden, n_neurons_out, name="output",
  kernel_regularizer=tf.contrib.layers.l1_regularizer(l1_param))
```

```
# define the cost
cross_entropy = tf.nn.sigmoid_cross_entropy_with_logits(logit, y_true)

base_cost = tf.reduce_mean(cross_entropy)
reg_cost = tf.losses.get_regularization_loss()

cost = base_cost + reg_cost

# the rest is as before
```

Avoiding Overfitting Through Regularization

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Max-Norm Regularization (1/3)

- Max-norm regularization: constrains the weights $\mathbf{w}_j$ of the incoming connections for each neuron j.
  - Prevents them from getting too large.
- After each training step, clip $\mathbf{w}_j$ as below:

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

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

Max-Norm Regularization (2/3)

```
# make the network
hidden = tf.layers.dense(X, n_neurons_h, activation=tf.sigmoid, name="hidden")
logit = tf.layers.dense(hidden, n_neurons_out, name="output")
```

```
# define the cost
cross_entropy = tf.nn.sigmoid_cross_entropy_with_logits(logit, y_true)
cost = tf.reduce_mean(cross_entropy)

# define the optimizer
optimizer = tf.train.GradientDescentOptimizer(learning_rate)
training_op = optimizer.minimize(cost)
```

Max-Norm Regularization (3/3)

- Use `tf.clip_by_norm`.

```
# max-norm regularization - hidden layer
threshold = 1.0

weights = tf.get_default_graph().get_tensor_by_name("hidden/kernel:0")
clipped_weights = tf.clip_by_norm(weights, clip_norm=threshold, axes=1)
clip_weights = weights.assign(clipped_weights)
```

```
# executing the model
init = tf.global_variables_initializer()

with tf.Session() as sess:
  init.run()
  for epoch in range(n_epochs):
    sess.run(training_op, feed_dict={X: training_X, y_true: training_y})
    clip_weights.eval()
```

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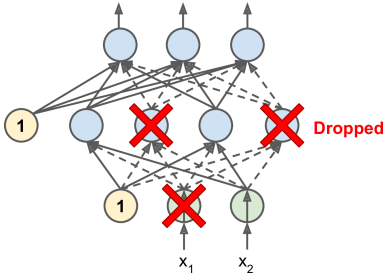
Dropout (1/4)

- 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?

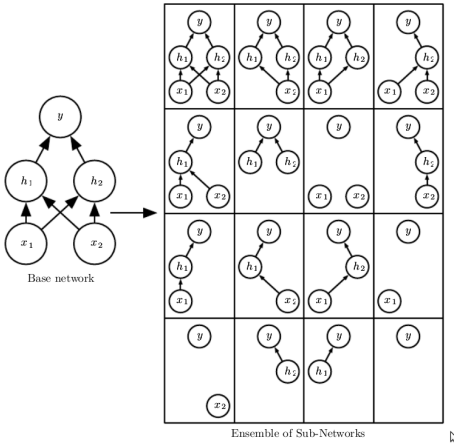
Dropout (2/4)

- 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)

- Use `tf.layers.dropout`: specify the dropout rate rather than the keep probability.

```
# make the network
dropout_rate = 0.5  # == 1 - keep_prob
training = tf.placeholder_with_default(False, shape=(), name="training")

X_drop = tf.layers.dropout(X, dropout_rate, training=training)
hidden = tf.layers.dense(X_drop, n_neurons_h, activation=tf.sigmoid, name="hidden")
hidden_drop = tf.layers.dropout(hidden, dropout_rate, training=training)
logit = tf.layers.dense(hidden_drop, n_neurons_out, name="output")
```

```
# executing the model
init = tf.global_variables_initializer()

with tf.Session() as sess:
  init.run()
  for epoch in range(n_epochs):
    sess.run(training_op, feed_dict={X: training_X, y_true: training_y, training: True})
```

Avoiding Overfitting Through Regularization

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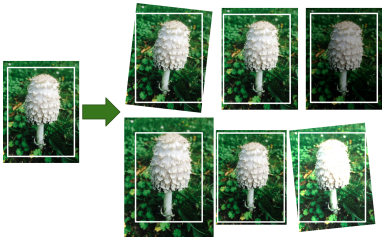
Data Augmentation

- 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)

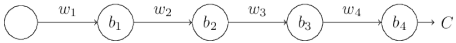
- The backpropagation goes from output to input layer, and propagates the error gradient on the way.

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

- 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)

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

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

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

$$\frac{\partial C}{\partial b_1} = \frac{\partial C}{\partial a_4} \times \sigma^{'}(z_4) \times w_4 \times \sigma^{'}(z_3) \times w_3 \times \sigma^{'}(z_2) \times \times w_2 \times \sigma^{'}(z_1) \times 1$$

Vanishing/Exploding Gradients Problem (4/4)

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

$$\frac{\partial C}{\partial b_3} = \frac{\partial C}{\partial a_4} \times \sigma'(z_4) \times w_4 \times \sigma'(z_3)$$

$$\frac{\partial C}{\partial b_1} = \frac{\partial C}{\partial a_4} \times \sigma'(z_4) \times w_4 \times \sigma'(z_3) \times w_3 \times \sigma'(z_2) \times w_2 \times \sigma'(z_1) \times 1$$

- Assume $w_3\sigma'(z_2) < \frac{1}{4}$ and $w_2\sigma'(z_1) < \frac{1}{4}$
  - 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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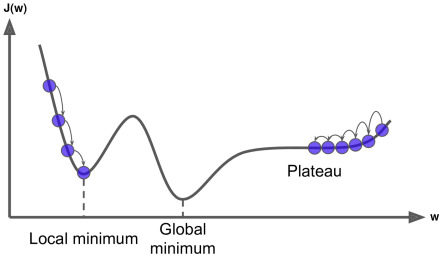
Parameter Initialization Strategies (1/5)

- 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 (2/5)

- 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 (3/5)

- We need the signals to flow properly in both directions.
- The Xavier 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.

Parameter Initialization Strategies (4/5)

- Based on the Xavier initialization, the weights are initialized using normal distribution with mean 0 and the following standard deviation.
  - For the sigmoid activation function:

$$\sigma = \sqrt{\frac{2}{\mathtt{n}_{\mathtt{inputs}} + \mathtt{n}_{\mathtt{outputs}}}}$$

  - For the ReLU activation function:

$$\sigma = \sqrt{2}\sqrt{\frac{2}{\mathtt{n}_{\mathtt{inputs}} + \mathtt{n}_{\mathtt{outputs}}}}$$

  - $\mathtt{n}_{\mathtt{inputs}}$ and $\mathtt{n}_{\mathtt{outputs}}$ are the number of input and output connections for the layer whose weights are being initialized.

Parameter Initialization Strategies (5/5)

- Use `tf.variance_scaling_initializer()`

```
# make the network
he_init = tf.variance_scaling_initializer()

hidden = tf.layers.dense(X, n_neurons_h, activation=tf.sigmoid, name="hidden",
    kernel_initializer=he_init)

logit = tf.layers.dense(hidden, n_neurons_out, name="output")
```

Overcoming the Vanishing Gradient

- Parameter initiazlization strategies
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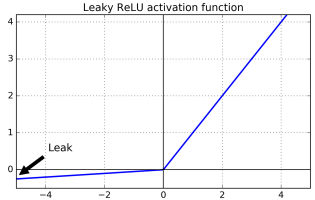
Nonsaturating Activation Functions (1/4)

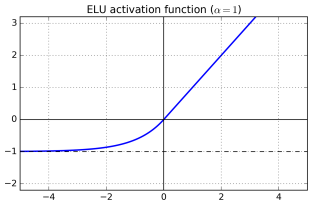
- $\texttt{ReLU}(z) = \max(0, z)$
- The dying ReLUs problem.
  - During training, some neurons stop outputting anything other than 0.
  - E.g., when the weighted sum of the neuron's inputs is negative, it starts outputting 0.
- Use leaky ReLU instead: $\texttt{LeakyReLU}_\alpha(z) = \max(\alpha z, z)$.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



Nonsaturating Activation Functions (2/4)

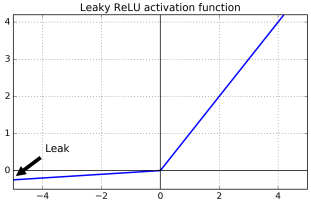
- Randomized Leaky ReLU (RReLU)
  - α is picked randomly during training, and it is fixed during testing.
- Parametric Leaky ReLU (PReLU)
  - Learn α during training (instead of being a hyperparameter).
- Exponential Linear Unit (ELU)

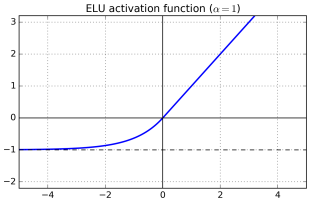
$$\mathrm{ELU}_\alpha(z) = \begin{cases} \alpha(\exp(z) - 1) & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$

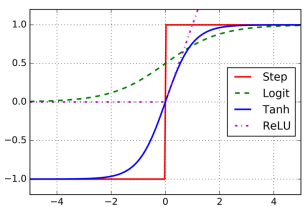


Nonsaturating Activation Functions (3/4)

- 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)

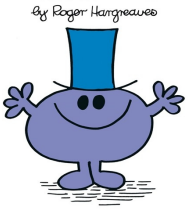
```
# leaky relu
def leaky_relu(z, name=None):
  alpha = 0.01
  return tf.maximum(alpha * z, z, name=name)

hidden = tf.layers.dense(X, n_neurons_h, activation=leaky_relu, name="hidden")
```

```
# elu
hidden = tf.layers.dense(X, n_neurons_h, activation=tf.nn.elu, name="hidden")
```

Overcoming the Vanishing Gradient

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



Batch Normalization (1/5)

- 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 (2/5)

- 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.

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

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

- 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 (3/5)

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

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

Batch Normalization (4/5)

- Use `tf.layers.batch_normalization`

```
# make the network
training = tf.placeholder_with_default(False, shape=(), name="training")

hidden = tf.layers.dense(X, n_neurons_h, name="hidden")
bn = tf.layers.batch_normalization(hidden, training=training)
bn_act = tf.sigmoid(bn)

logits_before_bn = tf.layers.dense(bn_act, n_outputs, name="output")
logits = tf.layers.batch_normalization(logits_before_bn, training=training)
```

```
# define the cost
cross_entropy = tf.nn.sparse_softmax_cross_entropy_with_logits(labels=y, logits=logits)
cost = tf.reduce_mean(cross_entropy)

# train the model
optimizer = tf.train.GradientDescentOptimizer(learning_rate)
training_op = optimizer.minimize(cost)
```

Batch Normalization (5/5)

- We need to explicitly run the extra update operations needed by batch normalization `sess.run([training_op, extra_update_ops], ...)`.

```
extra_update_ops = tf.get_collection(tf.GraphKeys.UPDATE_OPS)
init = tf.global_variables_initializer()

with tf.Session() as sess:
  init.run()
  for epoch in range(n_epochs):
    sess.run([training_op, extra_update_ops],
             feed_dict={X: training_X, y_true: training_y, training: True})
```

Overcoming the Vanishing Gradient

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

Gradient Clipping (1/2)

- Gradient clipping: clip the gradients during backpropagation so that they never exceed some threshold.
- In TensorFlow, the optimizer's `minimize()` function takes care of:
  1. Compute the gradients with `compute_gradients()`
  2. Apply the processed gradients with `apply_gradients()`
- To enable the gradient clipping, you must instead of calling `minimize()`, call:
  1. Compute the gradients with `compute_gradients()`
  2. Process the gradients as you wish.
  3. Apply the processed gradients with `apply_gradients()`

Gradient Clipping (2/2)

- Use `clip_by_value()`

```
# define the cost
cross_entropy = tf.nn.sparse_softmax_cross_entropy_with_logits(labels=y, logits=logits)
cost = tf.reduce_mean(cross_entropy)
```

```
# train the model
threshold = 1.0

optimizer = tf.train.GradientDescentOptimizer(learning_rate)

# returns a list of (gradient, variable) pairs
grads_and_vars = optimizer.compute_gradients(cost)

capped_gvs = [(tf.clip_by_value(grad, -threshold, threshold), var)
              for grad, var in grads_and_vars]

training_op = optimizer.apply_gradients(capped_gvs)
```

Training Speed

Regular Gradient Descent Optimization (1/2)

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

Regular Gradient Descent Optimization (2/2)

```
# define the cost
cross_entropy = tf.nn.sigmoid_cross_entropy_with_logits(z, y_true)
cost = tf.reduce_mean(cross_entropy)

# train the model
learning_rate = 0.1
optimizer = tf.train.GradientDescentOptimizer(learning_rate)
training_op = optimizer.minimize(cost)
```

Optimization Algorithms

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

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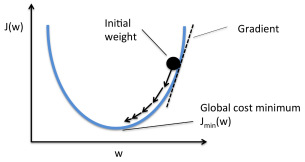
Momentum (1/4)

- 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 (2/4)

- This is the very simple idea behind momentum optimization.
- We can see the change in the parameters $\mathbf{w}$ as motion: $\mathtt{w}_\mathtt{i}^{(\mathtt{next})} = \mathtt{w}_\mathtt{i} - \eta \frac{\partial \mathtt{J}(\mathbf{w})}{\partial \mathtt{w}_\mathtt{i}}$
- 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 (3/4)

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

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

- β is called momentum, ans it is between 0 and 1.
- Updates the weights by subtracting this momentum vector.

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

Momentum (4/4)

```
# train the model

optimizer = tf.train.MomentumOptimizer(learning_rate=learning_rate, momentum=0.9)
```

Optimization Algorithms

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

Nesterov Momentum (1/3)

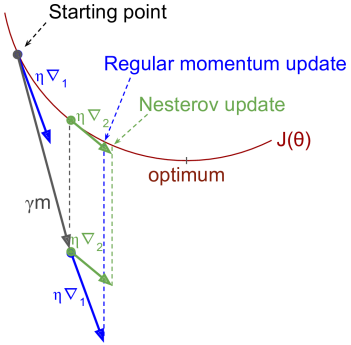
- Nesterov Momentum is a small variant to Momentum optimization.
- Faster than vanilla Momentum optimization.
- Measure the gradient of the cost function slightly ahead in the direction of the momentum (not at the local position).

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

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

Nesterov Momentum (2/3)

- $\nabla 1$ 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 $\mathbf{w} + \beta\mathbf{m}$.



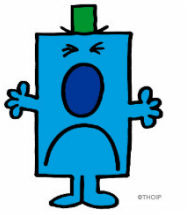
Nesterov Momentum (3/3)

```
# train the model

optimizer = tf.train.MomentumOptimizer(learning_rate=learning_rate, momentum=0.9,
  use_nesterov=True)
```

Optimization Algorithms

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



AdaGrad (1/3)

- AdaGrad keeps track of a learning rate for each parameter.
- Adapts the learning rate over time (adaptive learning rate).

AdaGrad (2/3)

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

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

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

- Parameters with large partial derivative of the cost have a rapid decrease in their learning rate.
- Parameters with small partial derivatives have a small decrease in their learning rate.

AdaGrad (3/3)

```
# train the model

optimizer = tf.train.AdagradOptimizer(learning_rate=learning_rate)
```

Optimization Algorithms

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

RMSProp (1/3)

- 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.

RMSProp (2/3)

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

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

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

RMSProp (3/3)

```
# train the model

optimizer = tf.train.RMSPropOptimizer(learning_rate=learning_rate, momentum=0.9,
  decay=0.9, epsilon=1e-10)
```

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 $\oslash$ represents the represents 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)

```
# train the model

optimizer = tf.train.AdamOptimizer(learning_rate=learning_rate)
```

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?