Lecture 6: Neural Networks II

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Deep Learning Course, Fall 2021

Today's Roadmap

Last lecture was about neural networks:

- From perceptron to multi-layer perceptron
- Feed-forward neural networks
- Activation funcions: sigmoid, tanh, relu, ...
- Activation maps: softmax, sparsemax, ...
- Non-convex optimization and local minima
- Universal approximation theorem
- Gradient backpropagation

Today: autodiff, regularization, tricks of the trade.

Outline

Outline

Recap: Forward Propagation

Now assume $L \geq 1$ hidden layers:

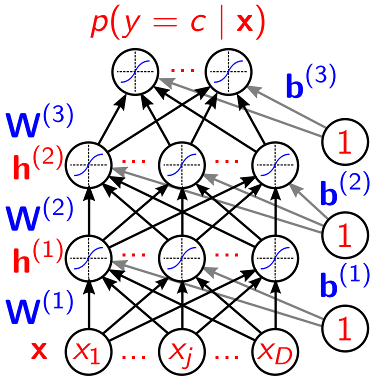
- **Hidden layer pre-activation** (define $\boldsymbol{h}^{(0)} = \boldsymbol{x}$ for convenience):

$$\boldsymbol{z}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{W}^{(\ell)}\boldsymbol{h}^{(\ell-1)} + \boldsymbol{b}^{(1)},$$

with $\boldsymbol{W}^{(\ell)} \in \mathbb{R}^{K_\ell \times K_{\ell-1}}$ and $\boldsymbol{b}^{(\ell)} \in \mathbb{R}^{K_\ell}$.

- **Hidden layer activation:**

$$\boldsymbol{h}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{z}^{(\ell)}(\boldsymbol{x})).$$



- **Output layer activation:**

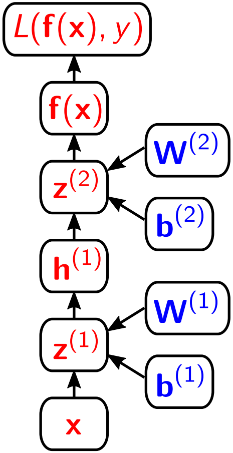
$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{o}(\boldsymbol{z}^{(L+1)}(\boldsymbol{x})) = \boldsymbol{o}(\boldsymbol{W}^{(L+1)}\boldsymbol{h}^{(L)} + \boldsymbol{b}^{(L+1)}).$$

Recap: Gradient Backpropagation

```
Compute output gradient (before activation):
    $\nabla_{\boldsymbol{z}^{(L+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = -(\mathbf{1}_y - \boldsymbol{f}(\boldsymbol{x}))$

for $\ell$ from $L+1$ to 1 do
    Compute gradients of hidden layer parameters:
        $\nabla_{\boldsymbol{W}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)\, \boldsymbol{h}^{(\ell-1)\top}$
        $\nabla_{\boldsymbol{b}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$

    Compute gradient of hidden layer below:
        $\nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \boldsymbol{W}^{(\ell+1)\top} \nabla_{\boldsymbol{z}^{(\ell+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$

    Compute gradient of hidden layer below (before activation):
        $\nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \odot \boldsymbol{g}'(\boldsymbol{z}^{(\ell)})$

end for
```

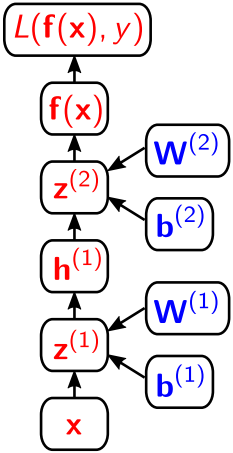
Computation Graph

- Forward propagation can be represented as a DAG
- Allows to implement forward propagation in a modular way
- Each box can be an object with a `fprop` method, that computes the value of the box given its children
- Calling the `fprop` method of each box in the right order (after a topological sort) yields forward propagation


$$\begin{tikzcd}
 & L(\mathbf{f}(\mathbf{x}), y) & \\
 & \mathbf{f}(\mathbf{x}) \arrow[u] & \mathbf{W}^{(2)} \arrow[dl] \\
 & \mathbf{z}^{(2)} \arrow[u] & \mathbf{b}^{(2)} \arrow[l] \\
 & \mathbf{h}^{(1)} \arrow[u] & \mathbf{W}^{(1)} \arrow[dl] \\
 & \mathbf{z}^{(1)} \arrow[u] & \mathbf{b}^{(1)} \arrow[l] \\
 & \mathbf{x} \arrow[u] &
\end{tikzcd}$$

Automatic Differentiation

- ... Also allows to implement backpropagation in a modular way
- Each box can also have a `bprop` method, that computes the loss gradient with respect to its children, given the loss gradient with respect to the output
- Can make use of cached computation done during the `fprop` method
- By calling the `bprop` method in reverse order, we get backpropagation (only need to reach the parameters)



Several Autodiff Strategies

Symbol-to-number differentiation (Caffe, Torch, Pytorch, Dynet, ...)

- Take a computational graph and a set of numerical inputs, then return a set of numerical values describing the gradient at those input values
- Advantage: simpler to implement and to debug
- Disadvantage: only works for first-order derivatives

Symbol-to-symbol differentiation (Theano, Tensorflow, ...)

- Take a computational graph and add additional nodes to the graph that provide a symbolic description of the desired derivatives (i.e. the derivatives are just another computational graph)
- Advantage: generalizes automatically to higher-order derivatives
- Disadvantage: harder to implement and to debug

Many Software Toolkits for Neural Networks

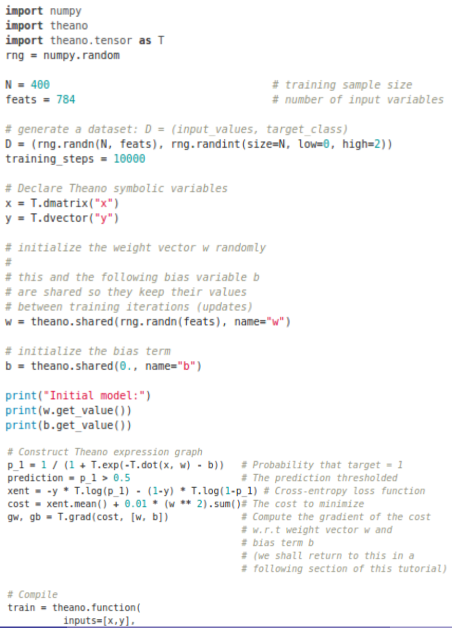
- Theano
- Tensorflow
- Torch, Pytorch
- MXNet
- Keras
- Caffe
- DyNet
- ...

All implement automatic differentiation.

We will have a Pytorch practical class this week

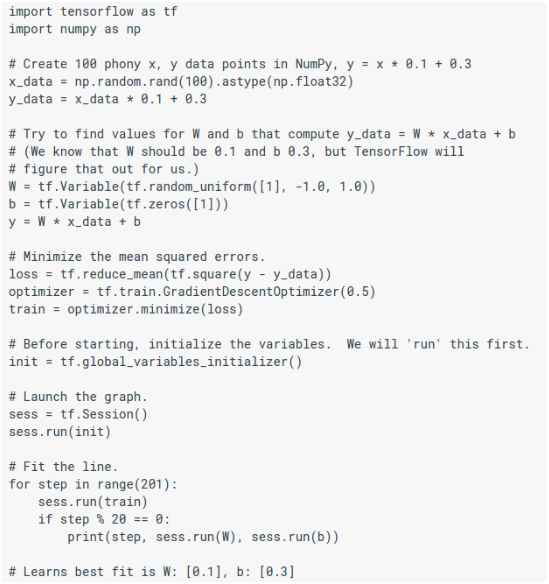
You may bring your laptops if you want to try it out!

Some Theano Code (Logistic Regression)



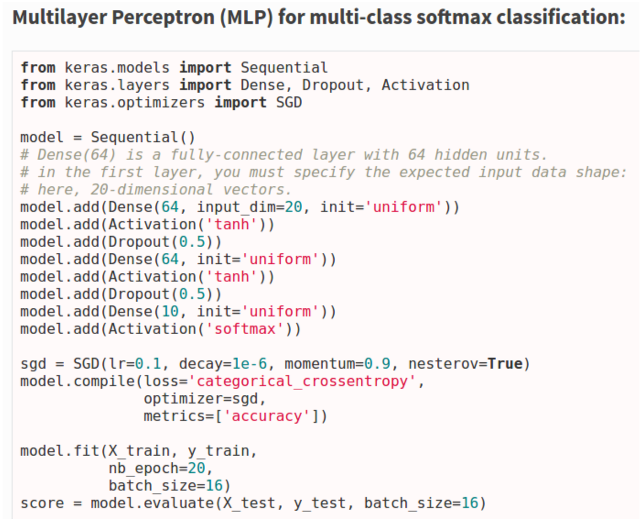
```
import numpy
import theano
import theano.tensor as T
rng = numpy.random

N = 400                                   # training sample size
feats = 784                               # number of input variables

# generate a dataset: D = (input_values, target_class)
D = (rng.randn(N, feats), rng.randint(size=N, low=0, high=2))
training_steps = 10000

# Declare Theano symbolic variables
x = T.dmatrix("x")
y = T.dvector("y")

# initialize the weight vector w randomly
#
# this and the following bias variable b
# are shared so they keep their values
# between training iterations (updates)
w = theano.shared(rng.randn(feats), name="w")

# initialize the bias term
b = theano.shared(0., name="b")

print("Initial model:")
print(w.get_value())
print(b.get_value())

# Construct Theano expression graph
p_1 = 1 / (1 + T.exp(-T.dot(x, w) - b))   # Probability that target = 1
prediction = p_1 > 0.5                    # The prediction thresholded
xent = -y * T.log(p_1) - (1-y) * T.log(1-p_1) # Cross-entropy loss function
cost = xent.mean() + 0.01 * (w ** 2).sum()# The cost to minimize
gw, gb = T.grad(cost, [w, b])             # Compute the gradient of the cost
                                          # w.r.t weight vector w and
                                          # bias term b
                                          # (we shall return to this in a
                                          # following section of this tutorial)


# Compile
train = theano.function(
          inputs=[x,y],
```

Some Code in Tensorflow (Linear Regression)



```
import tensorflow as tf
import numpy as np

# Create 100 phony x, y data points in NumPy, y = x * 0.1 + 0.3
x_data = np.random.rand(100).astype(np.float32)
y_data = x_data * 0.1 + 0.3

# Try to find values for W and b that compute y_data = W * x_data + b
# (We know that W should be 0.1 and b 0.3, but TensorFlow will
# figure that out for us.)
W = tf.Variable(tf.random_uniform([1], -1.0, 1.0))
b = tf.Variable(tf.zeros([1]))
y = W * x_data + b

# Minimize the mean squared errors.
loss = tf.reduce_mean(tf.square(y - y_data))
optimizer = tf.train.GradientDescentOptimizer(0.5)
train = optimizer.minimize(loss)

# Before starting, initialize the variables.  We will 'run' this first.
init = tf.global_variables_initializer()

# Launch the graph.
sess = tf.Session()
sess.run(init)

# Fit the line.
for step in range(201):
    sess.run(train)
    if step % 20 == 0:
        print(step, sess.run(W), sess.run(b))

# Learns best fit is W: [0.1], b: [0.3]
```

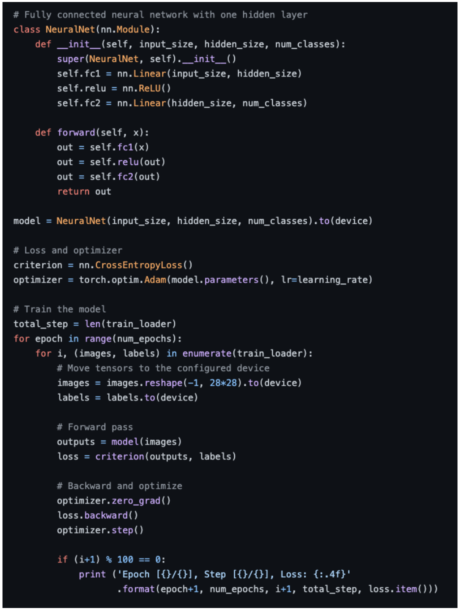
Some Code in Keras (Multi-Layer Perceptron)



Multilayer Perceptron (MLP) for multi-class softmax classification:

```
from keras.models import Sequential
from keras.layers import Dense, Dropout, Activation
from keras.optimizers import SGD

model = Sequential()
# Dense(64) is a fully-connected layer with 64 hidden units.
# in the first layer, you must specify the expected input data shape:
# here, 20-dimensional vectors.
model.add(Dense(64, input_dim=20, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(64, init='uniform'))
model.add(Activation('tanh'))
model.add(Dropout(0.5))
model.add(Dense(10, init='uniform'))
model.add(Activation('softmax'))

sgd = SGD(lr=0.1, decay=1e-6, momentum=0.9, nesterov=True)
model.compile(loss='categorical_crossentropy',
              optimizer=sgd,
              metrics=['accuracy'])

model.fit(X_train, y_train,
          nb_epoch=20,
          batch_size=16)
score = model.evaluate(X_test, y_test, batch_size=16)
```

Some Code in Pytorch (Multi-Layer Perceptron)



```python
# Fully connected neural network with one hidden layer
class NeuralNet(nn.Module):
    def __init__(self, input_size, hidden_size, num_classes):
        super(NeuralNet, self).__init__()
        self.fc1 = nn.Linear(input_size, hidden_size)
        self.relu = nn.ReLU()
        self.fc2 = nn.Linear(hidden_size, num_classes)

    def forward(self, x):
        out = self.fc1(x)
        out = self.relu(out)
        out = self.fc2(out)
        return out

model = NeuralNet(input_size, hidden_size, num_classes).to(device)

# Loss and optimizer
criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

# Train the model
total_step = len(train_loader)
for epoch in range(num_epochs):
    for i, (images, labels) in enumerate(train_loader):
        # Move tensors to the configured device
        images = images.reshape(-1, 28*28).to(device)
        labels = labels.to(device)

        # Forward pass
        outputs = model(images)
        loss = criterion(outputs, labels)

        # Backward and optimize
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

        if (i+1) % 100 == 0:
            print ('Epoch [{}/{}], Step [{}/{}], Loss: {:.4f}'
                   .format(epoch+1, num_epochs, i+1, total_step, loss.item()))
```

Reminder: The Key Ingredients of SGD

In sum, we need the following ingredients:

- The loss function $L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$;
- A procedure for computing the gradients $\nabla_{\boldsymbol{\theta}} L(f(\boldsymbol{x}_i; \boldsymbol{\theta}), y_i)$
- The regularizer $\Omega(\boldsymbol{\theta})$ and its gradient – next!

Outline

Regularization

Recall that we're minimizing the following objective function:

$$\mathcal{L}(\boldsymbol{\theta}) := \lambda\Omega(\boldsymbol{\theta}) + \frac{1}{N}\sum_{n=1}^{N} L(\boldsymbol{f}(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i)$$

It remains to define the regularizer and its gradient

We'll talk about:

- ℓ_2 regularization
- ℓ_1 regularization
- dropout regularization

ℓ_2 Regularization

- Gaussian prior on the weights
- **Note:** only the weights are regularized (not the biases)

$$\Omega(\boldsymbol{\theta}) = \frac{1}{2}\sum_{\ell} \|\boldsymbol{W}^{(\ell)}\|^2$$

- Gradient is:

$$\nabla_{\boldsymbol{W}^{(\ell)}}\Omega(\boldsymbol{\theta}) = \boldsymbol{W}^{(\ell)}$$

- This has the effect of a weight decay:

$$\begin{aligned}
\boldsymbol{W}^{(\ell)} &\leftarrow \boldsymbol{W}^{(\ell)} - \eta\nabla_{\boldsymbol{W}^{(\ell)}}\mathcal{L}_i(\boldsymbol{\theta}) \\
&= \boldsymbol{W}^{(\ell)} - \eta(\lambda\nabla_{\boldsymbol{W}^{(\ell)}}\Omega(\boldsymbol{\theta}) + \nabla_{\boldsymbol{W}^{(\ell)}}L(f(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i)) \\
&= (1-\eta\lambda)\boldsymbol{W}^{(\ell)} - \eta\nabla_{\boldsymbol{W}^{(\ell)}}L(f(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i)
\end{aligned}$$

ℓ_1 Regularization

- Laplacian prior on the weights
- **Note:** only the weights are regularized (not the biases)

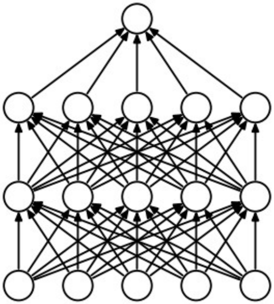
$$\Omega(\boldsymbol{\theta}) = \sum_{\ell} \|\boldsymbol{W}^{(\ell)}\|_1$$

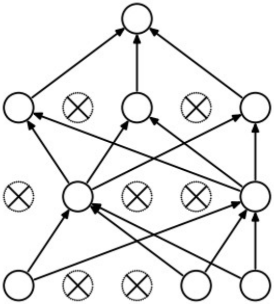
- Gradient is:

$$\nabla_{\boldsymbol{W}^{(\ell)}} \Omega(\boldsymbol{\theta}) = \mathrm{sign}(\boldsymbol{W}^{(\ell)})$$

- Promotes sparsity of the weights

Dropout Regularization (Srivastava et al., 2014)


(a) Standard Neural Net


(b) After applying dropout.

Idea: During training, remove some hidden units stochastically

Dropout Regularization (Srivastava et al., 2014)

- Each hidden unit's output is set to 0 with probability p (e.g. $p = 0.5$)
- This prevents hidden units to co-adapt to other units, forcing them to be more generally useful
- At test time, keep all units, but multiply their outputs by $1 - p$
- Shown to be a form of adaptive regularization (Wager et al., 2013)
- Note: many software packages implement another variant, inverted dropout, where at training time the output of the units that were not dropped is divided by $1 - p$ and requires no change at test time

Implementation of Dropout

- This is usually implemented using random binary masks
- The hidden layer activations become (for $\ell = 1, \ldots, L$):

$$\boldsymbol{h}^{(\ell)}(\boldsymbol{x}) = \boldsymbol{g}(\boldsymbol{z}^{(\ell)}(\boldsymbol{x})) \odot \boldsymbol{m}^{(\ell)}$$

- Beats regular backpropagation on many datasets (Hinton et al., 2012)
- Other variants, e.g. DropConnect (Wan et al., 2013), Stochastic Pooling (Zeiler and Fergus, 2013)

Backpropagation with Dropout

```
Compute output gradient (before activation):
    $$\nabla_{\boldsymbol{z}^{(L+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = -(\mathbf{1}_y - \boldsymbol{f}(\boldsymbol{x}))$$
for $\ell$ from $L+1$ to 1 do
    Compute gradients of hidden layer parameters:
        $$\nabla_{\boldsymbol{W}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \underbrace{\boldsymbol{h}^{(\ell-1)^\top}}_{\text{includes } \boldsymbol{m}^{(\ell-1)}}$$
        $$\nabla_{\boldsymbol{b}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$$
    Compute gradient of hidden layer below:
        $$\nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \boldsymbol{W}^{(\ell+1)^\top} \nabla_{\boldsymbol{z}^{(\ell+1)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y)$$
    Compute gradient of hidden layer below (before activation):
        $$\nabla_{\boldsymbol{z}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) = \nabla_{\boldsymbol{h}^{(\ell)}} L(\boldsymbol{f}(\boldsymbol{x};\boldsymbol{\theta}), y) \odot \boldsymbol{g}'(\boldsymbol{z}^{(\ell)}) \odot \boldsymbol{m}^{(\ell-1)}$$
end for
```

Outline

Initialization

Initialize all biases to zero

For weights:

- Cannot initialize to zero with **tanh** activation (the gradients would also be zero and we would reach a saddle point)
- Cannot initialize the weights to the same value (need to break the symmetry)
- Random initialization (Gaussian, uniform), sampling around 0 to break symmetry
- For ReLU activations, the mean should be a small positive number
- Variance cannot be too high, otherwise all neuron activations will be saturated

“Glorot Initialization”

- Recipe from Glorot and Bengio (2010):

$$\boldsymbol{W}_{i,j}^{(\ell)} \sim U[-t, t], \text{ with } t = \frac{\sqrt{6}}{\sqrt{K^{(\ell)} + K^{(\ell-1)}}}$$

- Works well in practice with **tanh** and sigmoid activations

Training, Validation, and Test Sets

Split datasets in training, validation, and test partitions.

- Training set serves to train the model
- Validation set serves to tune hyperparameters (learning rate, number of hidden units, regularization coefficient, dropout probability, best epoch, etc.)
- Test set serves to estimate the generalization performance

Hyperparameter Tuning: Grid Search, Random Search

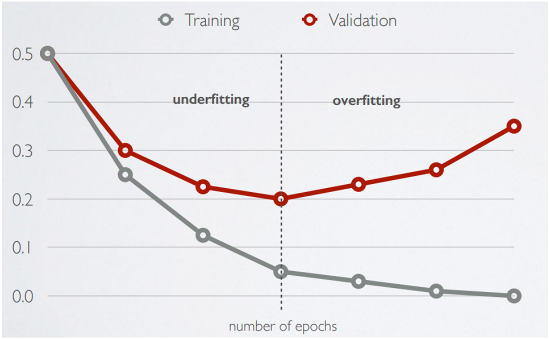
Search for the best configuration of the hyperparameters:

- Grid search: specify a set of values we want to test for each hyperparameter, and try all configurations of these values
- Random search: specify a distribution over the values of each hyper-parameter (e.g. uniform in some range) and sample independently each hyper-parameter to get configurations
- Bayesian optimization and learning to learn (Snoek et al., 2012)

We can always go back and fine-tune the grid/distributions if necessary

Early Stopping

- To select the number of epochs, stop training when validation error increases (with some look ahead)
- One common strategy (with SGD) is to halve the learning rate for every epoch where the validation error increases



(Image credit: Hugo Larochelle)

Tricks of the Trade

- Normalization of the data
- Decaying the learning rate
- Mini-batches
- Adaptive learning rates
- Gradient checking
- Debugging on a small dataset

Normalization of the Data

- For each input dimension: subtract the training set mean and divide by the training set standard deviation
- This makes each input dimension have zero mean, unit variance
- This can speed up training (in number of epochs)
- Doesn't work for sparse inputs (destroys sparsity)

Decaying the Learning Rate

In SGD, as we get closer to a local minimum, it makes sense to take smaller update steps (to avoid diverging)

- Start with a large learning rate (say 0.1)
- Keep it fixed while validation error keeps improving
- Divide by 2 and go back to the previous step

Mini-Batches

- Instead of updating after a single example, can aggregate a mini-batch of examples (e.g. 50–200 examples) and compute the averaged gradient for the entire mini-batch
- Less noisy than vanilla SGD
- Can leverage matrix-matrix computations (or tensor computations)
- Large computational speed-ups in GPUs (since computation is trivially parallelizable accross the mini-batch and we can exhaust the GPU memory)

Adaptive Learning Rates

Instead of using the same step size for all parameters, have one learning rate per parameter

- Adagrad (Duchi et al., 2011): learning rates are scaled by the square root of the cumulative sum of squared gradients

$$\eta^{(t)} = \eta^{(t-1)} + (\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y))^2, \qquad \bar{\nabla}_{\boldsymbol{\theta}}^{(t)} = \frac{\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y)}{\sqrt{\eta^{(t)} + \epsilon}}$$

- RMSprop (Tieleman and Hinton, 2012): instead of cumulative sum, use exponential moving average

$$\eta^{(t)} = \beta\eta^{(t-1)} + (1-\beta)(\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y))^2, \qquad \bar{\nabla}_{\boldsymbol{\theta}}^{(t)} = \frac{\nabla_{\boldsymbol{\theta}} L(\boldsymbol{f}(\boldsymbol{x}), y)}{\sqrt{\eta^{(t)} + \epsilon}}$$

- Adam (Kingma and Ba, 2014): combine RMSProp with momentum

Gradient Checking

- If the training loss is not decreasing even with a very small learning rate, there's likely a bug in the gradient computation
- To debug your implementation of `fprop`/`bprop`, compute the "numeric gradient," a finite difference approximation of the true gradient:

$$\frac{\partial f(x)}{\partial x} \approx \frac{f(x+\epsilon) - f(x-\epsilon)}{2\epsilon}$$

Debugging on a Small Dataset

- Extract a small subset of your training set (e.g. 50 examples)
- Monitor your training loss in this set
- You should be able to overfit in this small training set
- If not, see if some units are saturated from the very first iterations (if they are, reduce the initialization variance or properly normalize your inputs)
- If the training error is bouncing up and down, decrease the learning rate

Outline

Conclusions

- Multi-layer perceptrons are universal function approximators
- However, they need to be trained
- Stochastic gradient descent is an effective training algorithm
- This is possible with the gradient backpropagation algorithm (an application of the chain rule of derivatives)
- Most current software packages represent a computation graph and implement automatic differentiation
- Dropout regularization is effective to avoid overfitting

Thank you!

Questions?

References I

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