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# Imports
%matplotlib inline
%config InlineBackend.figure_formats = ['svg']

import itertools
import numpy as np  # Matrix and vector computation package
import matplotlib
import matplotlib.pyplot as plt  # Plotting library
import seaborn as sns  # Fancier plots

# Set seaborn plotting style
sns.set_style('darkgrid')
# Set the seed for reproducibility
np.random.seed(seed=1)
#

# Create dataset
nb_train = 2000  # Number of training samples
# Addition of 2 n-bit numbers can result in a n+1 bit number
sequence_len = 28  # Length of the binary sequence

def create_dataset(nb_samples, sequence_len):
    """Create a dataset for binary subtraction and
    return as input, targets."""
    max_int = 2**(sequence_len-1)  # Maximum integer that can be
    subtracted
    # Transform integer in binary format
    format_str = '{:0' + str(sequence_len) + 'b}'
    nb_inputs = 2  # Subtract 2 binary numbers
    nb_outputs = 1  # Result is 1 binary number
    # Input samples
    X = np.zeros((nb_samples, sequence_len, nb_inputs))
    # Target samples
    T = np.zeros((nb_samples, sequence_len, nb_outputs))
    # Fill up the input and target matrix
    for i in range(nb_samples):
        # Generate random numbers to subtract
        nb1 = np.random.randint(0, max_int)
        nb2 = np.random.randint(0, max_int)
        if nb1 < nb2:
            nb1, nb2 = nb2, nb1
        # Fill current input and target row.
        # Note that binary numbers are subtracted from right to left,
        # but our RNN reads from left to right, so reverse the
        sequence.
        X[i,:,0] = list(
            reversed([int(b) for b in format_str.format(nb1)]))
        X[i,:,1] = list(
            reversed([int(b) for b in format_str.format(nb2)]))
        T[i,:,0] = list(

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        reversed([int(b) for b in format_str.format(nb1-nb2)]))
    return X, T

# Create training samples
X_train, T_train = create_dataset(nb_train, sequence_len)
print(f'X_train tensor shape: {X_train.shape}')
print(f'T_train tensor shape: {T_train.shape}')
#
X_train tensor shape: (2000, 28, 2)
T_train tensor shape: (2000, 28, 1)

# Show an example input and target
def printSample(x1, x2, t, y=None):
    """Print a sample in a more visual way."""
    x1 = ''.join([str(int(d)) for d in x1])
    x1_r = int(''.join(reversed(x1)), 2)
    x2 = ''.join([str(int(d)) for d in x2])
    x2_r = int(''.join(reversed(x2)), 2)
    t = ''.join([str(int(d[0])) for d in t])
    t_r = int(''.join(reversed(t)), 2)
    if not y is None:
        y = ''.join([str(int(d[0])) for d in y])
    print(f'x1:    {x1:s}    {x1_r:2d}')
    print(f'x2: - {x2:s}    {x2_r:2d}')
    print(f'      -----  --')
    print(f't:   = {t:s}    {t_r:2d}')
    if not y is None:
        print(f'y:   = {y:s}')

# Print the first sample
printSample(X_train[0,:,0], X_train[0,:,1], T_train[0,:,:])
#
x1:    0110000110111101000101110000    15252870
x2: - 1001000010000110011100010000    9330953
      -----  --
t:   = 1011111000111010010110100000    5921917

# Define the linear tensor transformation layer
class TensorLinear(object):
    """The linear tensor layer applies a linear tensor dot product
    and a bias to its input."""
    def __init__(self, n_in, n_out, tensor_order, W=None, b=None):
        """Initialise the weight W and bias b parameters."""
        a = np.sqrt(6.0 / (n_in + n_out))
        self.W = (np.random.uniform(-a, a, (n_in, n_out))
                  if W is None else W)
        self.b = (np.zeros((n_out)) if b is None else b)
        # Axes summed over in backprop

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        self.bpAxes = tuple(range(tensor_order-1))

    def forward(self, X):
        """Perform forward step transformation with the help
        of a tensor product."""
        # Same as: Y[i,j,:] = np.dot(X[i,j,:], self.W) + self.b
        #             (for i,j in X.shape[0:1])
        # Same as: Y = np.einsum('ijk,kl->ijl', X, self.W) + self.b
        return np.tensordot(X, self.W, axes=((-1),(0))) + self.b

    def backward(self, X, gY):
        """Return the gradient of the parameters and the inputs of
        this layer."""
        # Same as: gW = np.einsum('ijk,ijl->kl', X, gY)
        # Same as: gW += np.dot(X[:,j,:].T, gY[:,j,:])
        #             (for i,j in X.shape[0:1])
        gW = np.tensordot(X, gY, axes=(self.bpAxes, self.bpAxes))
        gB = np.sum(gY, axis=self.bpAxes)
        # Same as: gX = np.einsum('ijk,kl->ijl', gY, self.W.T)
        # Same as: gX[i,j,:] = np.dot(gY[i,j,:], self.W.T)
        #             (for i,j in gY.shape[0:1])
        gX = np.tensordot(gY, self.W.T, axes=((-1),(0)))
        return gX, gW, gB

# Define the logistic classifier layer
class LogisticClassifier(object):
    """The logistic layer applies the logistic function to its
    inputs."""

    def forward(self, X):
        """Perform the forward step transformation."""
        return 1. / (1. + np.exp(-X))

    def backward(self, Y, T):
        """Return the gradient with respect to the loss function
        at the inputs of this layer."""
        # Average by the number of samples and sequence length.
        return (Y - T) / (Y.shape[0] * Y.shape[1])

    def loss(self, Y, T):
        """Compute the loss at the output."""
        return -np.mean((T * np.log(Y)) + ((1-T) * np.log(1-Y)))

# Define tanh layer
class TanH(object):
    """TanH applies the tanh function to its inputs."""

    def forward(self, X):
        """Perform the forward step transformation."""
        return np.tanh(X)

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def backward(self, Y, output_grad):
    """Return the gradient at the inputs of this layer."""
    gTanh = 1.0 - (Y**2)
    return (gTanh * output_grad)

# Define internal state update layer
class RecurrentStateUpdate(object):
    """Update a given state."""
    def __init__(self, nbStates, W, b):
        """Initialise the linear transformation and tanh transfer function."""
        self.linear = TensorLinear(nbStates, nbStates, 2, W, b)
        self.tanh = TanH()

    def forward(self, Xk, Sk):
        """Return state k+1 from input and state k."""
        return self.tanh.forward(Xk + self.linear.forward(Sk))

    def backward(self, Sk0, Sk1, output_grad):
        """Return the gradient of the parameters and the inputs of this layer."""
        gZ = self.tanh.backward(Sk1, output_grad)
        gSk0, gW, gB = self.linear.backward(Sk0, gZ)
        return gZ, gSk0, gW, gB

# Define layer that unfolds the states over time
class RecurrentStateUnfold(object):
    """Unfold the recurrent states."""
    def __init__(self, nbStates, nbTimesteps):
        """Initialise the shared parameters, the initial state and state update function."""
        a = np.sqrt(6. / (nbStates * 2))
        self.W = np.random.uniform(-a, a, (nbStates, nbStates))
        self.b = np.zeros((self.W.shape[0])) # Shared bias
        self.S0 = np.zeros(nbStates) # Initial state
        self.nbTimesteps = nbTimesteps # Timesteps to unfold
        self.stateUpdate = RecurrentStateUpdate(
            nbStates, self.W, self.b) # State update function

    def forward(self, X):
        """Iteratively apply forward step to all states."""
        # State tensor
        S = np.zeros((X.shape[0], X.shape[1]+1, self.W.shape[0]))
        S[:,0,:] = self.S0 # Set initial state
        for k in range(self.nbTimesteps):
            # Update the states iteratively
            S[:,k+1,:] = self.stateUpdate.forward(X[:,k,:], S[:,k,:])
        return S

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def backward(self, X, S, gY):
    """Return the gradient of the parameters and the inputs of
    this layer."""
    # Initialise gradient of state outputs
    gSk = np.zeros_like(gY[:,self.nbTimesteps-1,:])
    # Initialise gradient tensor for state inputs
    gZ = np.zeros_like(X)
    gWSum = np.zeros_like(self.W) # Initialise weight gradients
    gBSum = np.zeros_like(self.b) # Initialise bias gradients
    # Propagate the gradients iteratively
    for k in range(self.nbTimesteps-1, -1, -1):
        # Gradient at state output is gradient from previous state
        # plus gradient from output
        gSk += gY[:,k,:]
        # Propagate the gradient back through one state
        gZ[:,k,:], gSk, gW, gB = self.stateUpdate.backward(
            S[:,k,:], S[:,k+1,:], gSk)
        gWSum += gW # Update total weight gradient
        gBSum += gB # Update total bias gradient
    # Get gradient of initial state over all samples
    gS0 = np.sum(gSk, axis=0)
    return gZ, gWSum, gBSum, gS0

# Define the full network
class RnnBinaryAdder(object):
    """RNN to perform binary addition of 2 numbers."""
    def __init__(self, nb_of_inputs, nb_of_outputs, nb_of_states,
                  sequence_len):
        """Initialise the network layers."""
        # Input layer
        self.tensorInput = TensorLinear(nb_of_inputs, nb_of_states, 3)
        # Recurrent layer
        self.rnnUnfold = RecurrentStateUnfold(nb_of_states,
sequence_len)
        # Linear output transform
        self.tensorOutput = TensorLinear(nb_of_states, nb_of_outputs,
3)
        self.classifier = LogisticClassifier() # Classification
output

    def forward(self, X):
        """Perform the forward propagation of input X through all
        layers."""
        # Linear input transformation
        recIn = self.tensorInput.forward(X)
        # Forward propagate through time and return states
        S = self.rnnUnfold.forward(recIn)
        # Linear output transformation
        Z = self.tensorOutput.forward(S[:,1:sequence_len+1,:])
        Y = self.classifier.forward(Z) # Classification probabilities

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        # Return: input to recurrent layer, states, input to
classifier,
        # output
        return recIn, S, Z, Y

def backward(self, X, Y, recIn, S, T):
    """Perform the backward propagation through all layers.
    Input: input samples, network output, input to recurrent
    layer, states, targets."""
    gZ = self.classifier.backward(Y, T) # Get output gradient
    gRecOut, gWout, gBout = self.tensorOutput.backward(
        S[:,1:sequence_len+1,:], gZ)
    # Propagate gradient backwards through time
    gRnnIn, gWrec, gBrec, gS0 = self.rnnUnfold.backward(
        recIn, S, gRecOut)
    gX, gWin, gBin = self.tensorInput.backward(X, gRnnIn)
    # Return the parameter gradients of: linear output weights,
    # linear output bias, recursive weights, recursive bias, #
    # linear input weights, linear input bias, initial state.
    return gWout, gBout, gWrec, gBrec, gWin, gBin, gS0

def getOutput(self, X):
    """Get the output probabilities of input X."""
    recIn, S, Z, Y = self.forward(X)
    return Y

def getBinaryOutput(self, X):
    """Get the binary output of input X."""
    return np.around(self.getOutput(X))

def getParamGrads(self, X, T):
    """Return the gradients with respect to input X and
    target T as a list. The list has the same order as the
    get_params_iter iterator."""
    recIn, S, Z, Y = self.forward(X)
    gWout, gBout, gWrec, gBrec, gWin, gBin, gS0 = self.backward(
        X, Y, recIn, S, T)
    return [g for g in itertools.chain(
        np.nditer(gS0),
        np.nditer(gWin),
        np.nditer(gBin),
        np.nditer(gWrec),
        np.nditer(gBrec),
        np.nditer(gWout),
        np.nditer(gBout))]

def loss(self, Y, T):
    """Return the loss of input X w.r.t. targets T."""
    return self.classifier.loss(Y, T)

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def get_params_iter(self):
    """Return an iterator over the parameters.
    The iterator has the same order as get_params_grad.
    The elements returned by the iterator are editable in-
    place."""
    return itertools.chain(
        np.nditer(self.rnnUnfold.S0, op_flags=['readwrite']),
        np.nditer(self.tensorInput.W, op_flags=['readwrite']),
        np.nditer(self.tensorInput.b, op_flags=['readwrite']),
        np.nditer(self.rnnUnfold.W, op_flags=['readwrite']),
        np.nditer(self.rnnUnfold.b, op_flags=['readwrite']),
        np.nditer(self.tensorOutput.W, op_flags=['readwrite']),
        np.nditer(self.tensorOutput.b, op_flags=['readwrite']))

# Do gradient checking
# Define an RNN to test
RNN = RnnBinaryAdder(2, 1, 3, sequence_len)
# Get the gradients of the parameters from a subset of the data
backprop_grads = RNN.getParamGrads(
    X_train[0:100, :, :], T_train[0:100, :, :])

eps = 1e-7 # Set the small change to compute the numerical gradient
# Compute the numerical gradients of the parameters in all layers.
for p_idx, param in enumerate(RNN.get_params_iter()):
    grad_backprop = backprop_grads[p_idx]
    # + eps
    param += eps
    plus_loss = RNN.loss(
        RNN.getOutput(X_train[0:100, :, :], T_train[0:100, :, :])
    # - eps
    param -= 2 * eps
    min_loss = RNN.loss(
        RNN.getOutput(X_train[0:100, :, :], T_train[0:100, :, :])
    # reset param value
    param += eps
    # calculate numerical gradient
    grad_num = (plus_loss - min_loss) / (2*eps)
    # Raise error if the numerical grade is not close to the
    # backprop gradient
    if not np.isclose(grad_num, grad_backprop):
        raise ValueError((
            f'Numerical gradient of {grad_num:.6f} is not close '
            f'to the backpropagation gradient of {grad_backprop:.6f}!'
        ))
print('No gradient errors found')
#
No gradient errors found

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# Set hyper-parameters
lmbd = 0.5 # Rmsprop lambda
learning_rate = 0.05 # Learning rate
momentum_term = 0.80 # Momentum term
eps = 1e-6 # Numerical stability term to prevent division by zero
mb_size = 100 # Size of the minibatches (number of samples)

# Create the network
nb_of_states = 3 # Number of states in the recurrent layer
RNN = RnnBinaryAdder(2, 1, nb_of_states, sequence_len)
# Set the initial parameters
# Number of parameters in the network
nbParameters = sum(1 for _ in RNN.get_params_iter())
# Rmsprop moving average
maSquare = [0.0 for _ in range(nbParameters)]
Vs = [0.0 for _ in range(nbParameters)] # Momentum

# Create a list of minibatch losses to be plotted
ls_of_loss = [
    RNN.loss(RNN.getOutput(X_train[0:100,:,:]), T_train[0:100,:,:])]
# Iterate over some iterations
for i in range(5):
    # Iterate over all the minibatches
    for mb in range(nb_train // mb_size):
        X_mb = X_train[mb:mb+mb_size,:,:] # Input minibatch
        T_mb = T_train[mb:mb+mb_size,:,:] # Target minibatch
        V_tmp = [v * momentum_term for v in Vs]
        # Update each parameters according to previous gradient
        for pIdx, P in enumerate(RNN.get_params_iter()):
            P += V_tmp[pIdx]
        # Get gradients after following old velocity
        # Get the parameter gradients
        backprop_grads = RNN.getParamGrads(X_mb, T_mb)
        # Update each parameter seperately
        for pIdx, P in enumerate(RNN.get_params_iter()):
            # Update the Rmsprop moving averages
            maSquare[pIdx] = lmbd * maSquare[pIdx] + (
                1-lmbd) * backprop_grads[pIdx]**2
            # Calculate the Rmsprop normalised gradient
            pGradNorm = ((
                learning_rate * backprop_grads[pIdx]) / np.sqrt(
                    maSquare[pIdx])) + eps)
            # Update the momentum
            Vs[pIdx] = V_tmp[pIdx] - pGradNorm
            P -= pGradNorm # Update the parameter
        # Add loss to list to plot
        ls_of_loss.append(RNN.loss(RNN.getOutput(X_mb), T_mb))

# Plot the loss over the iterations
fig = plt.figure(figsize=(5, 3))

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plt.plot(ls_of_loss, 'b-')
plt.xlabel('minibatch iteration')
plt.ylabel('$\\xi$', fontsize=15)
plt.title('Decrease of loss over backprop iteration')
plt.xlim(0, 100)
fig.subplots_adjust(bottom=0.2)
plt.show()
#

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# Create test samples
nb_test = 5
Xtest, Ttest = create_dataset(nb_test, sequence_len)
# Push test data through network
Y = RNN.getBinaryOutput(Xtest)
Yf = RNN.getOutput(Xtest)

# Print out all test examples
for i in range(Xtest.shape[0]):
    printSample(Xtest[i,:,0], Xtest[i,:,1], Ttest[i,:,:], Y[i,:,:])
    print('')
#

```

| | | |
|-----|--------------------------------|-----------|
| x1: | 1011111101000100001100000110 | 101458685 |
| x2: | - 0101010001010011101111111000 | 33409578 |
| | ----- -- | |
| t: | = 1100101100011010011100000010 | 68049107 |
| y: | = 1100101100011010011100000010 | |
| | | |
| x1: | 1000011100011110110011100110 | 108230881 |
| x2: | - 101111111011010000111011010 | 95968253 |
| | ----- -- | |
| t: | = 0010011100111000110111010000 | 12262628 |

```

y:  = 0010011100111000110111010000
x1:  1111011110001010001101001110    120345071
x2:  - 0111101111010001000011100100    40930270
      -----
t:   = 1000100001100011110111010010    79414801
y:   = 1000100001100011110111010010
x1:  1011111011010000001001100110    107219837
x2:  - 1111001000001011110100110010    80465999
      -----
t:   = 0111010011011100000110011000    26753838
y:   = 0111010011011100000110011000
x1:  1001101110110100001000100110    105131481
x2:  - 1000101010111010010110100000    5922129
      -----
t:   = 0001000100001011100101111010    99209352
y:   = 0001000100001011100101111010

```