Machine Learning in Medicine

Sequence Generation with ONLY Numpy

Keywords : Sequence Models, Sequence Generation, Deep Learning, RNN, Numpy

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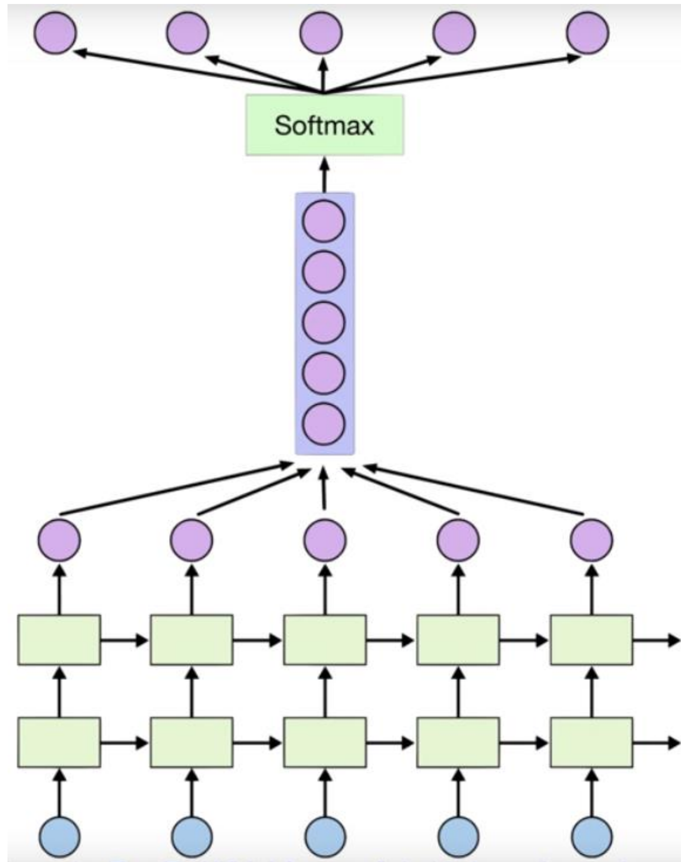
seq2seq - Numpy

Overview

< Sequence to Sequence >

Time-Series Data

Training



Generation

Time-Series Sequence

Language Generation
Signal Generation
...

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Source Code

- GitHub URL

https://github.com/mnchl-kim/seq2seq-Numpy

https://github.com/DHC5036/2019-fall-project-mnchl-kim

- **utils.py** : Includes several necessary function for running the other source code
- **model.py** : class RNN (stacked Recurrent Neural Networks) with ONLY Numpy
- **train.py** : Train data with RNN class
- **test.py** : Test file for live demo

To test the stacked RNN model, I used text data in online.

➡ character-level language generation.

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model.py

class RNN:

Stacked Recurrent Neural Networks with ONLY Numpy

The following parameters can be selected in the RNN class.

- input size
- output size
- hidden unit size
- time length
- depth size
- batch size
- dropout rate
- learning rate

Additional information for RNN class

- Weight initialization : Xavier initialization
- Weight update optimizer : Adagrad, RMSProp
- Dropout

class LSTM:

- ing…
- You can find out the source code at './models/lstm.py'

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Weight initialization

: Xavier initialization

We initialized the biases to be 0 and the weights W_{ij} at each layer with the following commonly used heuristic:

$$W_{ij} \sim U\left[-\frac{1}{\sqrt{n}}, \frac{1}{\sqrt{n}}\right], \qquad (1)$$

where $U[-a, a]$ is the uniform distribution in the interval $(-a, a)$ and n is the size of the previous layer (the number of columns of W).

```python
def initialize_xavier(first, second):
    """
    Xavier initialization

    Arguments:
        first -- first dimension size
        second -- second dimension size

    Returns:
        W -- Weight matrix initialized by Xavier method
    """

    sd = np.sqrt(2.0 / (first + second))
    W = np.random.randn(first, second) * sd

    return W
```

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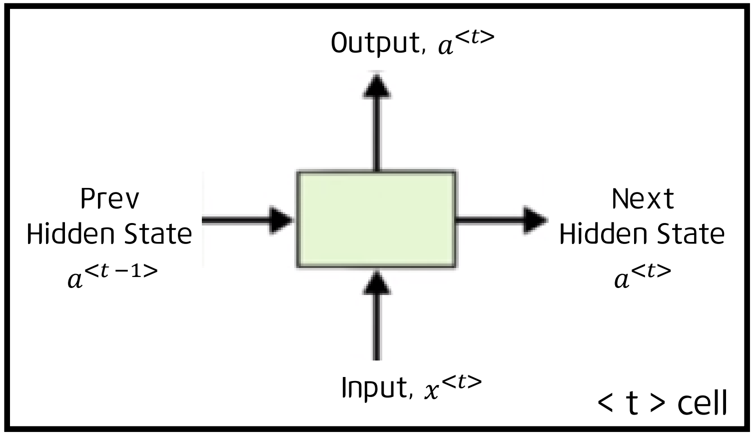
Stacked Recurrent Neural Networks



< Forward Propagation >

$$a^{\langle t\rangle} = \tanh(W_{ax}x^{\langle t\rangle} + W_{aa}a^{\langle t-1\rangle} + b_a)$$

At last layer,

$$\hat{y}^{\langle t\rangle} = soft\max(W_{ya}a^{\langle t\rangle} + b_y)$$

Multi-class Cross Entropy Loss

$$L(X_i, Y_i) = -\sum_{j=1}^{c} y_{ij} * \log(p_{ij})$$

$where\ \ Y_i\ is\ one-hot\ encoded\ target\ vector\ (y_{i1}, y_{i2}, \dots, y_{ic}),$

$$y_{ij} = \begin{cases} 1, & if\ i_{th}\ element\ is\ in\ class\ j \\ 0, & otherwise \end{cases}$$

$$p_{ij} = f(X_i) = Probability\ that\ i_{th}\ element\ is\ in\ class\ j$$

< Backward Propagation >

i) Derivative of Cross Entropy Loss, Softmax

$$P_k = \frac{e^{f_k}}{\sum_j e^{f_j}} \qquad L_i = -\sum_k p_{i,k} \log P_k \qquad f_m = (x_i W)_m$$

$$\text{when}\ \ k = m, \quad \frac{\partial P_k}{\partial f_m} = \frac{e^{f_k}\sum_j e^{f_j} - e^{f_k}\cdot e^{f_k}}{(\sum_j e^{f_j})^2} = P_k(1-P_k)$$

$$\text{when}\ \ k \neq m, \quad \frac{\partial P_k}{\partial f_m} = -\frac{e^{f_k}e^{f_m}}{(\sum_j e^{f_j})^2} = -P_k P_m$$

then:

$$\begin{aligned}
\frac{\partial L_i}{\partial f_m} &= -\sum_k p_{i,k}\frac{\partial \log P_k}{\partial f_m} \\
&= -\sum_k p_{i,k}\frac{1}{P_k}\frac{\partial P_k}{\partial f_m} \\
&= -\sum_{k=m} p_{i,k}\frac{1}{P_k}P_k(1-P_k) + \sum_{k\neq m} p_{i,k}\frac{1}{P_k}P_k P_m \\
&= \sum_{k\neq m} p_{i,k}P_m - \sum_{k=m} p_{i,k}(1-P_k) \\
&= \begin{cases} P_m & , \quad m \neq y_i \\ P_m - 1 & , \quad m = y_i \end{cases} \\
&= P_m - p_{i,m}
\end{aligned}$$

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Forward Propagation

```
def forward(self, X):
    self._loss = 0

    x, y_hat = [{} for d in range(self._depth_size + 1)], {}
    a = [{-1: np.copy(self._parameters['a'][d])} for d in range(self._depth_size)]
    dropout = [{} for d in range(self._depth_size)]

    for t in range(self._cell_length):
        x[0][t] = X[:, t, :, :].reshape(self._batch_size, self._input_size)

        for d in range(self._depth_size):
            dropout[d][t] = np.random.binomial(1, 1 - self._drop_rate, (1, self._hidden_size)) / (1 - self._drop_rate)
            a[d][t] = np.tanh(np.dot(x[d][t], self._parameters['W_xa'][d]) +
                              np.dot(a[d][t - 1], self._parameters['W_aa'][d]) +
                              self._parameters['b_a'][d])
            x[d + 1][t] = np.copy(a[d][t]) * dropout[d][t]

        z = np.dot(x[self._depth_size][t], self._parameters['W_ay'][0]) + self._parameters['b_y'][0]
        z = np.clip(z, -100, 100)
        y_hat[t] = np.array([softmax(z[b, :]) for b in range(self._batch_size)])

    cache = (x, a, y_hat, dropout)
    return cache
```

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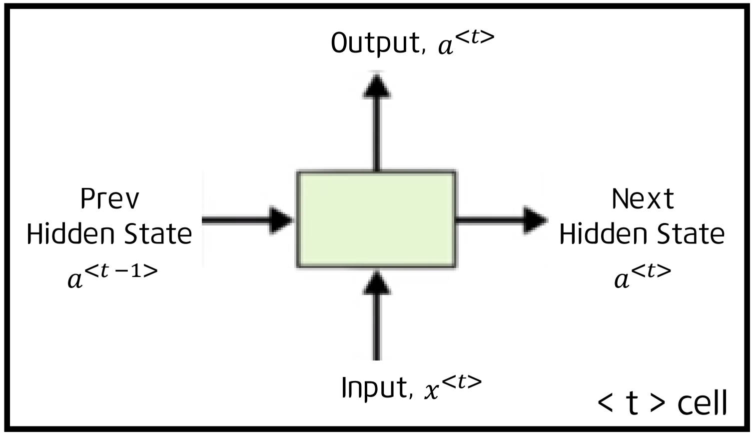
Stacked Recurrent Neural Networks



< Forward Propagation >

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At last layer,

$$\hat{y}^{\langle t\rangle} = soft\max(W_{ya}a^{\langle t\rangle} + b_y)$$

Multi-class Cross Entropy Loss

$$L(X_i, Y_i) = -\sum_{j=1}^{c} y_{ij} * \log(p_{ij})$$

where Y_i *is one* – *hot encoded target vector* $(y_{i1}, y_{i2}, \dots, y_{ic})$,

$$y_{ij} = \begin{cases} 1, & \text{if } i_{th} \text{ element is in class } j \\ 0, & \text{otherwise} \end{cases}$$

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< Backward Propagation >

ⅰ) Derivative of Softmax, Cross Entropy Loss

$$P_k = \frac{e^{f_k}}{\sum_j e^{f_j}} \qquad L_i = -\sum_k p_{i,k} \log P_k \qquad f_m = (x_i W)_m$$

$$\text{when } k = m, \quad \frac{\partial P_k}{\partial f_m} = \frac{e^{f_k}\sum_j e^{f_j} - e^{f_k}\cdot e^{f_k}}{(\sum_j e^{f_j})^2} = P_k(1-P_k)$$

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\end{aligned}$$

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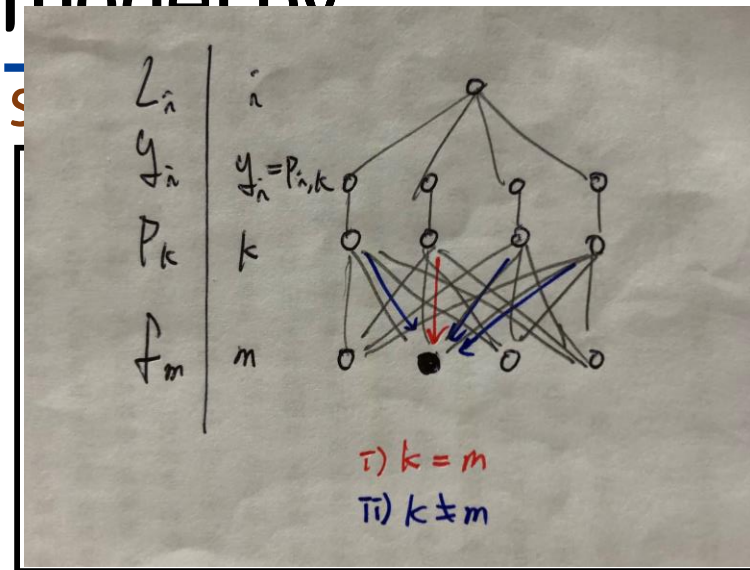

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\end{aligned}$$

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Forward Propagation

```
def cross_entropy(x, index):
    """
    Assumption: the ground truth vector contains only one non-zero component with a value of 1
    """

    loss = - np.log(x[index]) if x[index] > 0 else 0
    return loss


def cross_entropy_d(x, index):
    """
    Assumption: the ground truth vector contains only one non-zero component with a value of 1
    """

    x[index] -= 1
    return x
```

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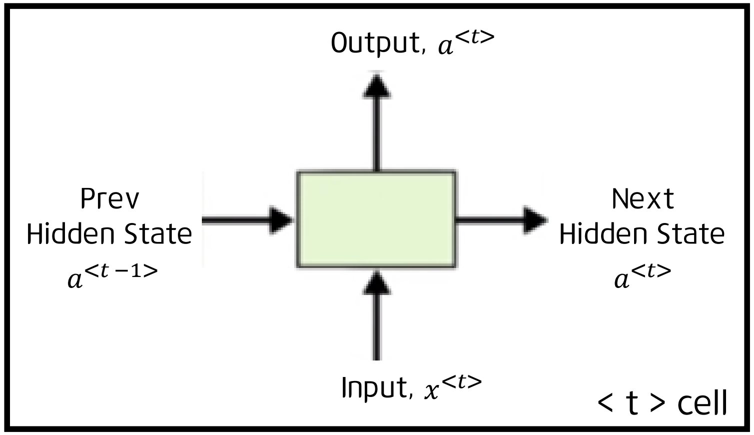
Stacked Recurrent Neural Networks



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At last layer,

$$\hat{y}^{\langle t\rangle} = soft\max(W_{ya}a^{\langle t\rangle} + b_y)$$

$$\frac{\partial L_i}{\partial W_k} = \frac{\partial L_i}{\partial f_m}\frac{\partial f_m}{\partial W_k} = x_i^T(P_m - p_{i,m})$$

< Backward Propagation >

ⅰ) Derivative of Softmax, Cross Entropy Loss

$$P_k = \frac{e^{f_k}}{\sum_j e^{f_j}} \qquad L_i = -\sum_k p_{i,k}\log P_k \qquad f_m = (x_i W)_m$$

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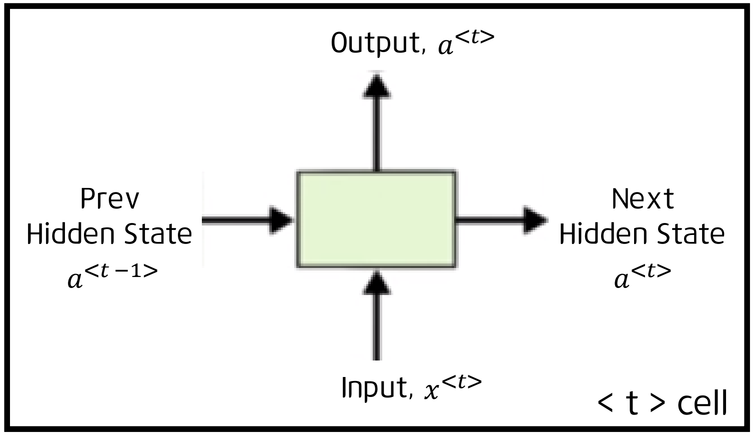
Stacked Recurrent Neural Networks



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At last layer,

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$$\frac{\partial L_i}{\partial W_k} = \frac{\partial L_i}{\partial f_m}\frac{\partial f_m}{\partial W_k} = x_i^{\ T}(P_m - p_{i,m})$$

< Backward Propagation >

ii) Derivative of $a^{<t>}$

$$a^{\langle t \rangle} = \tanh(W_{ax}x^{\langle t \rangle} + W_{aa}a^{\langle t-1 \rangle} + b)$$

$$\frac{\partial \tanh(x)}{\partial x} = 1 - \tanh(x)^2$$

$$\frac{\partial a^{\langle t \rangle}}{\partial W_{ax}} = (1 - \tanh(W_{ax}x^{\langle t \rangle} + W_{aa}a^{\langle t-1 \rangle} + b)^2) . x^{\langle t \rangle T}$$

$$\frac{\partial a^{\langle t \rangle}}{\partial W_{aa}} = (1 - \tanh(W_{ax}x^{\langle t \rangle} + W_{aa}a^{\langle t-1 \rangle} + b)^2) . a^{\langle t-1 \rangle T}$$

$$\frac{\partial a^{\langle t \rangle}}{\partial b} = \sum_{batch} (1 - \tanh(W_{ax}x^{\langle t \rangle} + W_{aa}a^{\langle t-1 \rangle} + b)^2)$$

$$\frac{\partial a^{\langle t \rangle}}{\partial x^{\langle t \rangle}} = W_{ax}^{\ \ T} . (1 - \tanh(W_{ax}x^{\langle t \rangle} + W_{aa}a^{\langle t-1 \rangle} + b)^2)$$

$$\frac{\partial a^{\langle t \rangle}}{\partial a^{\langle t-1 \rangle}} = W_{aa}^{\ \ T} . (1 - \tanh(W_{ax}x^{\langle t-1 \rangle} + W_{aa}a^{\langle t-1 \rangle} + b)^2)$$

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Backward Propagation

```
def backward(self, Y, cache):
    self._gradients = {key: [np.zeros_like(self._gradients[key][d]) for d in range(len(self._gradients[key]))] for key in self._gradients.keys()}
    (x, a, y_hat, dropout) = cache

    for t in reversed(range(self._cell_length)):
        self._loss += sum([cross_entropy(y_hat[t][b, :], Y[b, t]) for b in range(self._batch_size)]) / (self._cell_length * self._batch_size)
        dy = np.array([cross_entropy_d(y_hat[t][b, :], Y[b, t]) for b in range(self._batch_size)]) / (self._cell_length * self._batch_size)

        self._gradients['dW_ay'][0] += np.dot(x[self._depth_size][t].T, dy)
        self._gradients['db_y'][0] += dy.sum(axis=0)
        da = np.dot(dy, self._parameters['W_ay'][0].T)

        for d in reversed(range(self._depth_size)):
            da = (1 - a[d][t] ** 2) * (da * dropout[d][t] + self._gradients['da'][d])
            self._gradients['dW_xa'][d] += np.dot(x[d][t].T, da)
            self._gradients['dW_aa'][d] += np.dot(a[d][t - 1].T, da)
            self._gradients['db_a'][d] += da.sum(axis=0)
            self._gradients['da'][d] = np.dot(da, self._parameters['W_aa'][d].T)
            da = np.dot(da, self._parameters['W_xa'][d].T)

    self._parameters['a'] = [a[d][self._cell_length - 1] for d in range(self._depth_size)]
```

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model.py

Weight update

1. Adagrad (Adaptive Gradient)

$$G_t = G_{t-1} + (\nabla_\theta J(\theta_t))^2$$

$$\theta_{t+1} = \theta_t - \frac{\eta}{\sqrt{G_t + \epsilon}} \cdot \nabla_\theta J(\theta_t)$$

2. RMSProp

$$G = \gamma G + (1-\gamma)(\nabla_\theta J(\theta_t))^2$$

$$\theta = \theta - \frac{\eta}{\sqrt{G + \epsilon}} \cdot \nabla_\theta J(\theta_t)$$

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Weight update

```
def update_parameters(self, learning_rate=0.01):
    parameters = self._parameters['W_xa'] + self._parameters['W_aa'] + self._parameters['W_ay'] + self._parameters['b_a'] + self._parameters['b_y']
    gradients = self._gradients['dW_xa'] + self._gradients['dW_aa'] + self._gradients['dW_ay'] + self._gradients['db_a'] + self._gradients['db_y']
    momentums = self._momentums['dW_xa'] + self._momentums['dW_aa'] + self._momentums['dW_ay'] + self._momentums['db_a'] + self._momentums['db_y']

    for w, g, m in zip(parameters, gradients, momentums):
        np.clip(w, -1, 1, out=w)

        # Adagrad
        m += g ** 2
        w -= learning_rate * g / np.sqrt(m + 1e-8)

        # # RMSProp
        # m = 0.9 * m + 0.1 * g ** 2
        # w -= learning_rate * g / np.sqrt(m + 1e-8)
```

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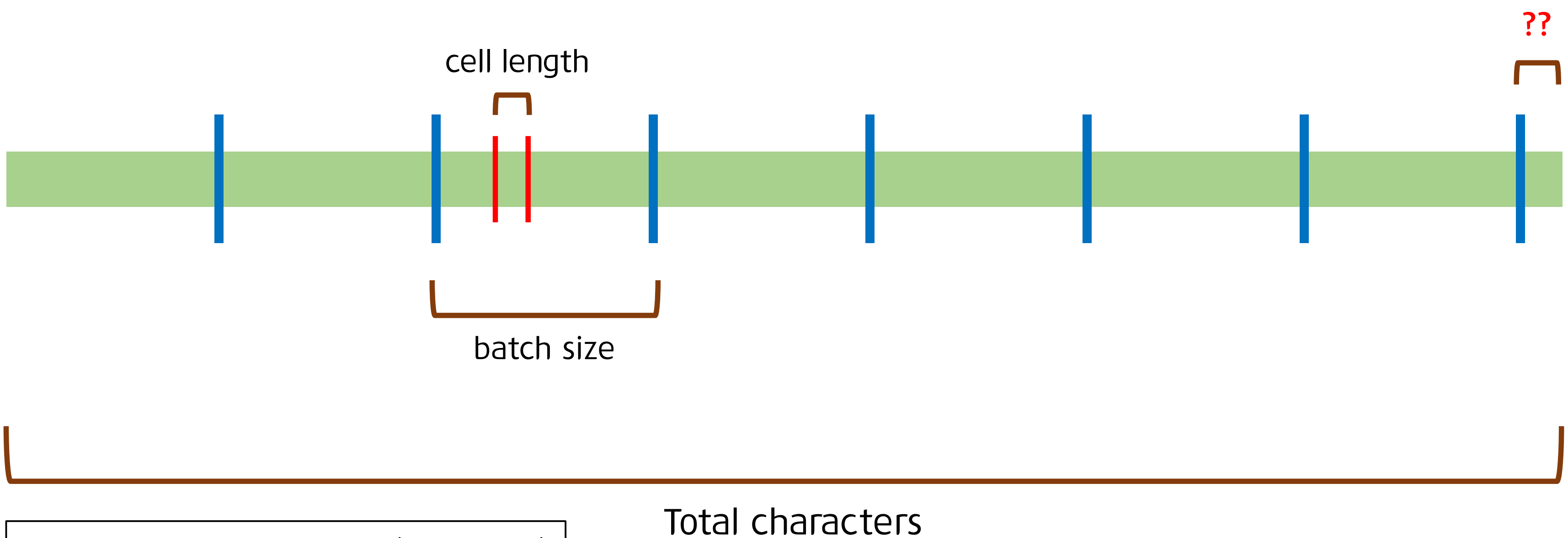
train.py

Input Data

Text Data (The Little Prince.txt)

- Total characters : 93,609
- Unique characters : 81

> Character-level language generation



mini_batch_X.shape : (b, t, x, 1)
mini_batch_Y.shape : (b, t, x, 1)

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train.py

Input Data

```
# Split text by mini-batch with batch_size
batch_length = data_size // batch_size
for i in range(0, batch_length - seq_length, seq_length):
    mini_batch_X, mini_batch_Y = [], []

    for j in range(0, data_size - batch_length + 1, batch_length):
        mini_batch_X.append(one_hot(data[j + i:j + i + seq_length], ch2ix))
        mini_batch_Y.append([ch2ix[ch] for ch in data[j + i + 1:j + i + seq_length + 1]])

    mini_batch_X = np.array(mini_batch_X)
    mini_batch_Y = np.array(mini_batch_Y)

    model.optimize(mini_batch_X, mini_batch_Y, learning_rate=learning_rate)
```

mini_batch_X.shape : (b, t, x, 1)
mini_batch_Y.shape : (b, t, x, 1)

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train.py

Training Process

- Total iteration : 3,000
- Input size : 81
- Output size : 81
- Hidden unit size : 256
- Time length : 100
- Depth size : 3
- Batch size : 10
- Dropout rate : 0.1
- Learning rate : 0.01
- Optimizer : Adagrad

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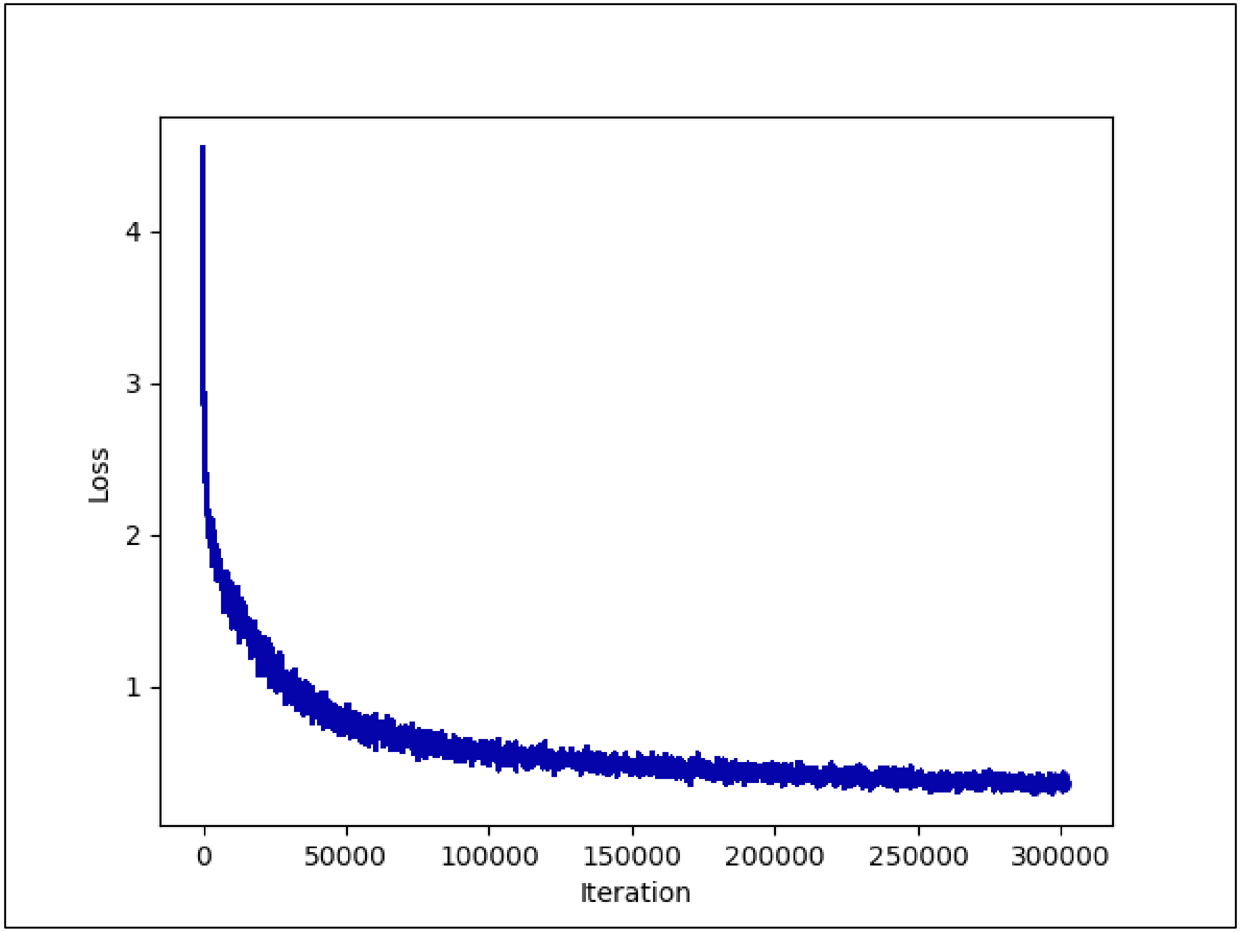
Training Process



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Training Process

```
######################################
Total iteration: 1
Iteration: 1
Loss: 4.621846
Time: 0.406110

### Starts Here ###

5i"?VT9H“\Y9R!Bxjn4OswaYuT?" KM
5!Zf'CK3M:3jByo435i–’0e–1o8‘3na
”95q1SIjeihz.hjh?–.Vf:fEAb$eMw"AI"s-:D6ij5A1GK8DW
"sDrybxIJK;C:-”‘YjyG

### Ends Here ###
######################################
```

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Training Process

```
######################################
Total iteration: 2944
Iteration: 273700
Loss: 0.386915
Time: 73135.271786

### Starts Here ###

N But his allies make..."

"I chilk nig to little man regrothing har jrapne..." And he lay down in the grass and cried.

It was then that the fox appeared.

"Good morning," said the fox. "Men

### Ends Here ###
######################################
```

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Discussion

It can be used for sequence generation.

- Language Generation
- Medical Signal Generation (Ex, ECG)
- Time-series prediction

Further Improvements

- Word Embedding
- LSTM, GRU
- Bidirectional RNN
- Attention
- Bert

Q&A?

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