# 实验3 循环神经网络实验

主讲教师：丛润民　　助教：张禹墨

北京交通大学　《深度学习》课程组

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# 序列数据处理

处理目标：将原始序列数据处理为方便模型运算的序列数据

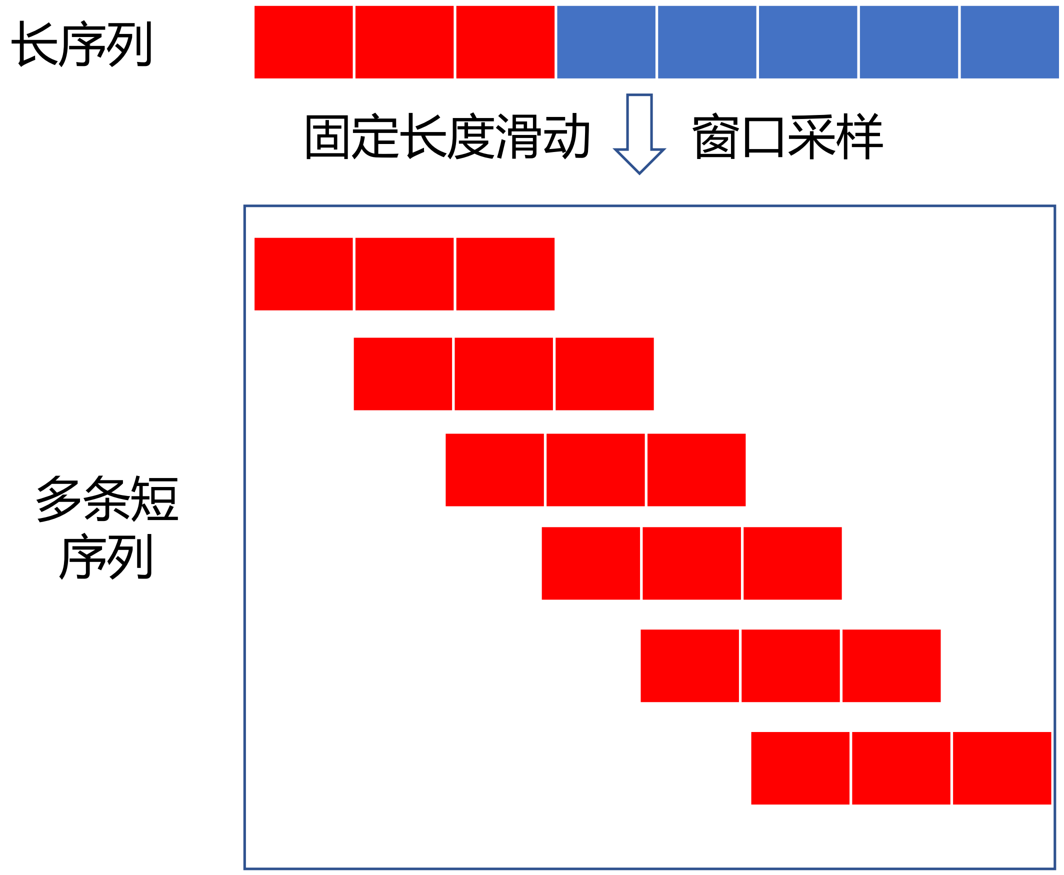
基本处理

- 固定长度滑动窗口
- 数据集划分注意事项

高级处理

- 固定时间跨度滑动窗口
- 不等长序列填充&打包
- 序列重采样

# 基本数据处理 - 固定长度滑动窗口




固定滑动窗口采样示意图

```
long_seq = raw_df.loc[2, '2017-01']['temperature'].dropna()
long_seq
```

打印长序列long_seq

```
UTC时间                 Temperature

2017-01-01 00:00:00    0.264706
2017-01-01 01:00:00    0.250000
2017-01-01 02:00:00    0.250000
2017-01-01 03:00:00    0.250000
2017-01-01 04:00:00    0.250000
                         ...
2017-01-31 19:00:00    0.294118
2017-01-31 20:00:00    0.294118
2017-01-31 21:00:00    0.279412
2017-01-31 22:00:00    0.294118
2017-01-31 23:00:00    0.279412
```

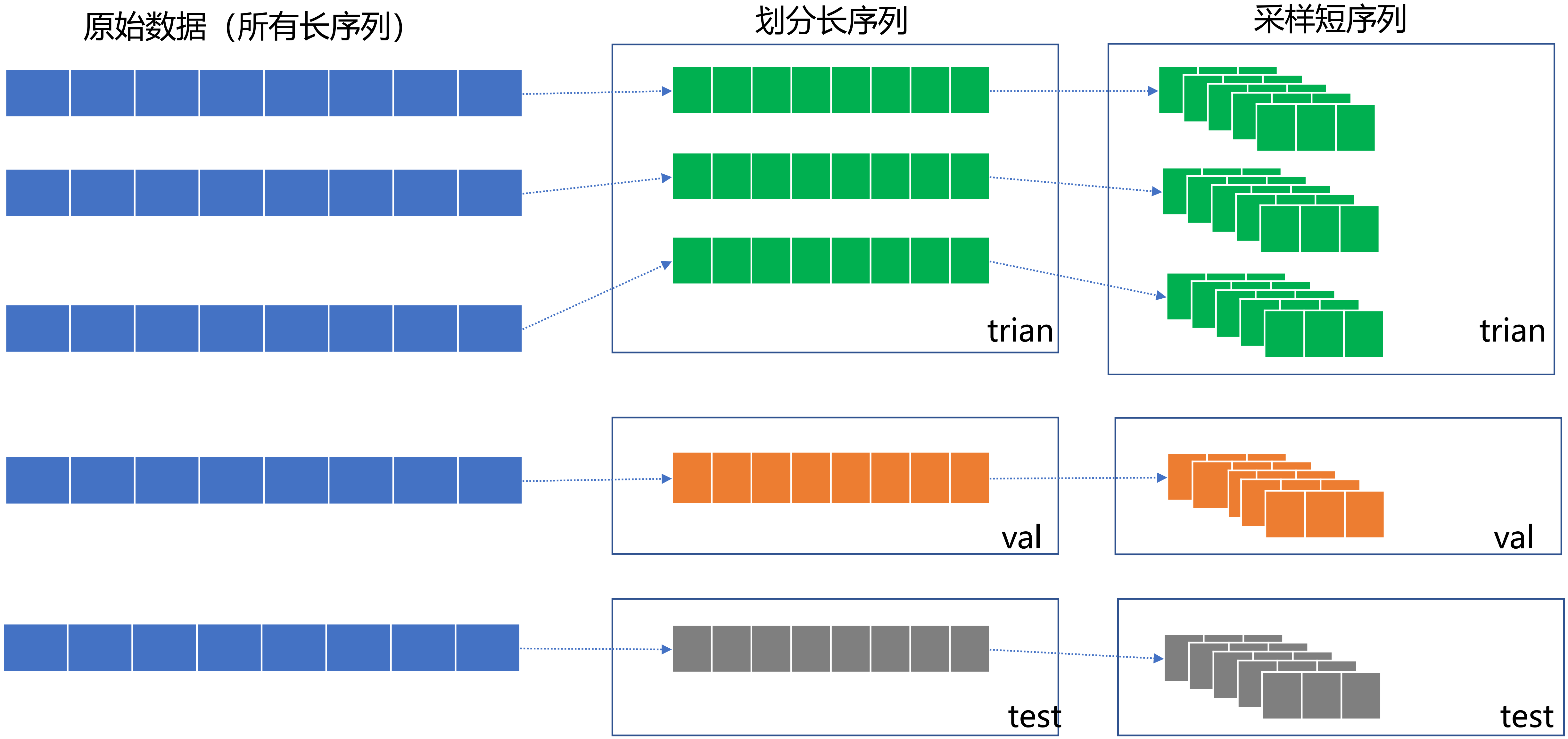
```
window_size = 12
short_seqs = []
for i in range(long_seq.shape[0] - window_size):
    short_seqs.append(long_seq.iloc[i:i+window_size].tolist())
short_seqs = np.array(short_seqs)
print(short_seqs.shape)
```

取长度窗口12，得到多条短序列

| | long_seq | window_size | short_seqs |
|---|---|---|---|
| shape | (1, 691) | 12 | (679, 12) |

# 基本数据处理 - 数据集划分注意事项

**先划分原始长序列，再采样短序列**



# 基本数据处理 – 数据集划分示例代码

```
train_set_proportion, val_set_proportion = 0.6, 0.2
total_len = long_seq.shape[0]
train_val_split = int(total_len * train_set_proportion)
val_test_split = int(total_len * (train_set_proportion + val_set_proportion))
train_seq, val_seq, test_seq = long_seq[:train_val_split],\
                               long_seq[train_val_split:val_test_split],\
                               long_seq[val_test_split:]

train_set = []
for i in range(train_seq.shape[0] - window_size):
    train_set.append(train_seq.iloc[i:i+window_size].tolist())
train_set = np.array(train_set)
print(train_set.shape)
```

```
(402, 12)
```

数据划分比例 trian：val：test = 6：2：2

划分长序列

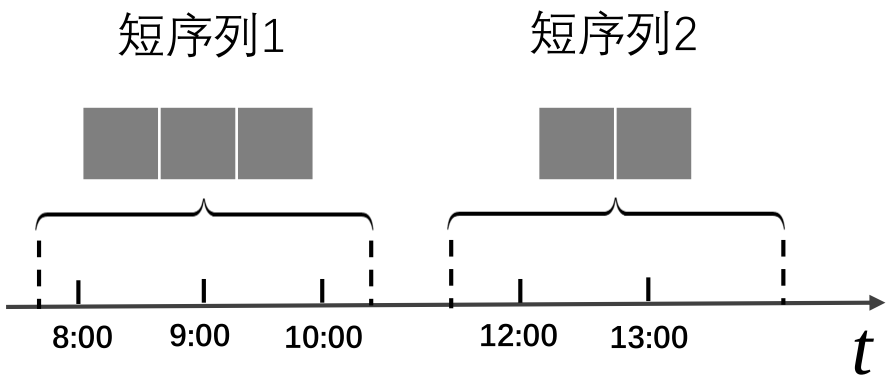
采样短序列

**注意**

✓ 首先对完整、有序的原始长序列按比例划分，再分别进行滑动窗口，采样短序列

✗ 首先用滑动窗口生成多条短序列，再划分短序列。

# 高级数据处理 – 固定时间窗口滑动




**固定时间窗口采样示意图**

注：固定时间窗口采样得到的序列的长度不一致，无法直接处理为Tensor，需要进行**填充**

```
long_seq = raw_df.loc[2, '2017-01']['temperature'].dropna()
long_seq
```

| UTC时间 | Temperature |
|---|---|
| 2017-01-01 00:00:00 | 0.264706 |
| 2017-01-01 01:00:00 | 0.250000 |
| 2017-01-01 02:00:00 | 0.250000 |
| 2017-01-01 03:00:00 | 0.250000 |
| 2017-01-01 04:00:00 | 0.250000 |
| | ... |
| 2017-01-31 19:00:00 | 0.294118 |
| 2017-01-31 20:00:00 | 0.294118 |
| 2017-01-31 21:00:00 | 0.279412 |
| 2017-01-31 22:00:00 | 0.294118 |
| 2017-01-31 23:00:00 | 0.279412 |

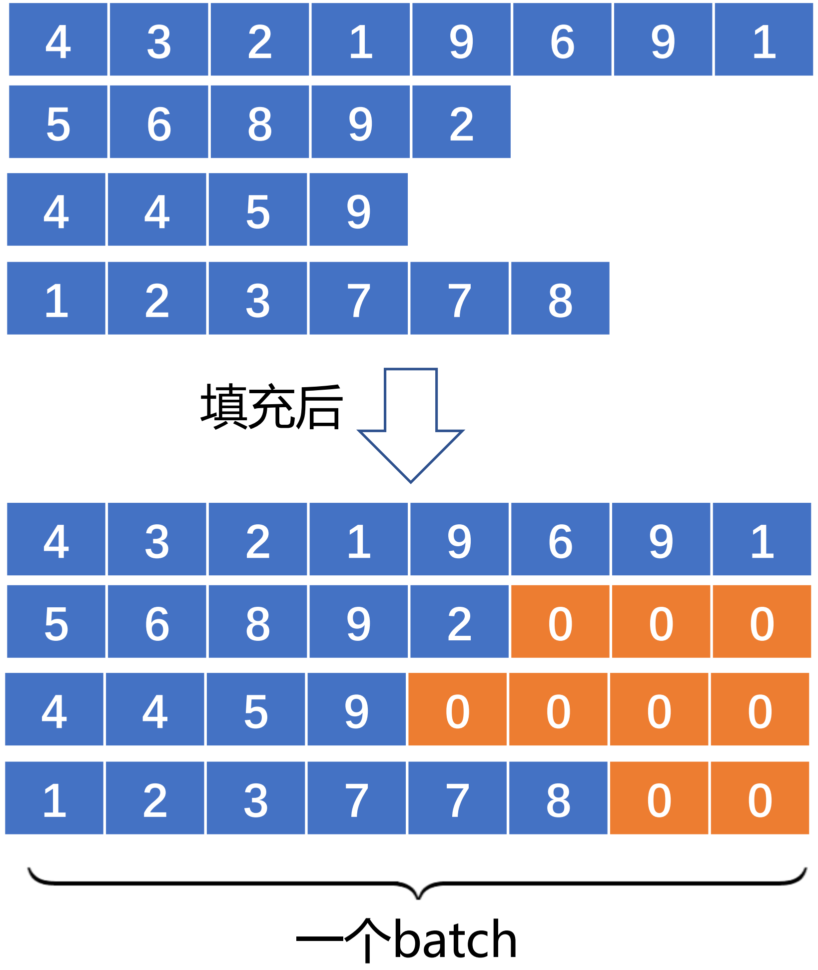
```
window_size = 12  # (小时)
short_seqs = []
start_time, end_time = long_seq.index.min(), long_seq.index.max() - pd.Timedelta(window_size, 'h')
cur_time = start_time
while cur_time < end_time:
    short_seqs.append(long_seq.loc[cur_time:cur_time + pd.Timedelta(window_size-1, 'h')].tolist())
    cur_time += pd.Timedelta(1, 'h')
```

取时间窗口12，得到多条短序列

| | long_seq | window_size | short_seqs |
|---|---|---|---|
| shape | (1, 663) | 12 | (659, 3~12) |

所有短序列中最短序列长度为3

# 高级数据处理 – 不等长序列填充&打包




**序列填充示意图**

## 序列填充

```python
from itertools import import zip_longest
```

```python
from itertools import zip_longest

padded_seqs = np.array(list(zip_longest(*short_seqs, fillvalue=0))).transpose()
padded_seqs.shape
```

```
(659, 12)
```

借助itertools中的zip_longest

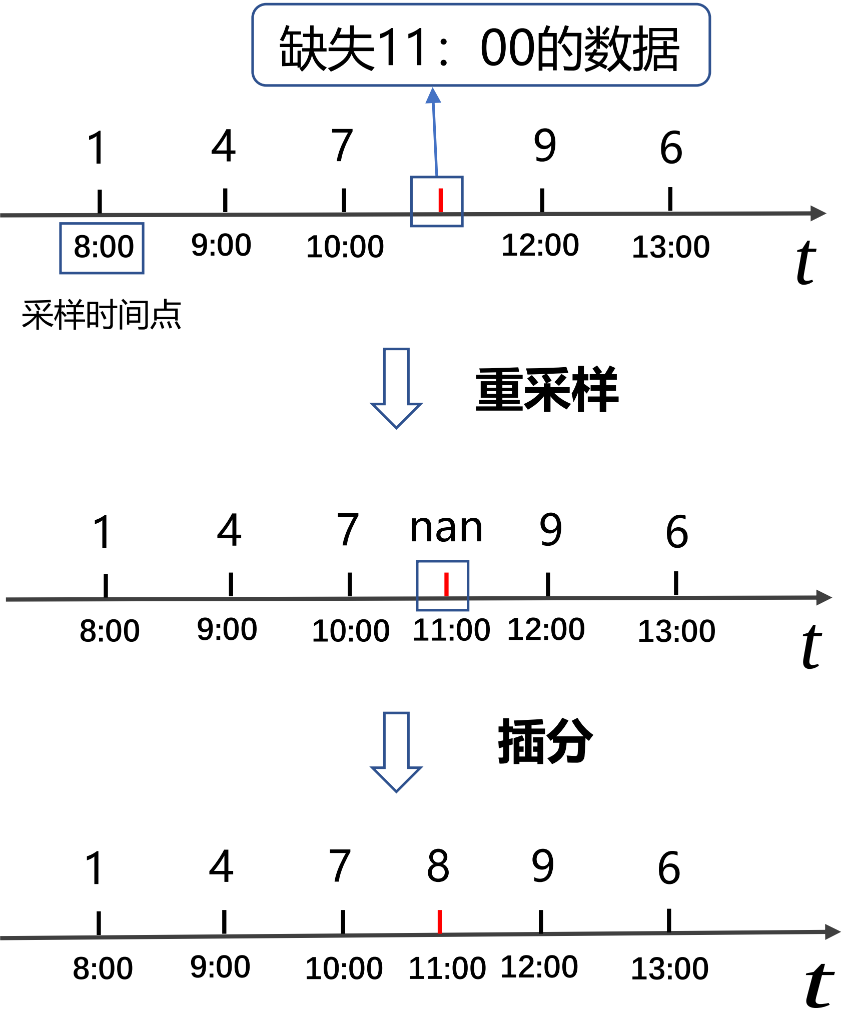
## 序列打包

```python
import torch
from torch.nn.utils.rnn import pack_padded_sequence

packed_seqs = pack_padded_sequence(torch.tensor(padded_seqs), seq_lengths,
                                   batch_first=True, enforce_sorted=False)
```

需要手动输入每条序列的长度

# 高级数据处理 – 序列重采样




**重采样+插分示意图**

## 重采样

```
start_time, end_time = long_seq.index.min(), long_seq.index.max() - pd.Timedelta(window_size, 'h')
full_index = pd.date_range(start_time, end_time, freq='h')
reindex_seq = long_seq.reindex(full_index)
```

将原始长序列中缺失的时间戳补全，
缺失时间点值被填充为nan

## 线性插分

```
inter_seq = reindex_seq.interpolate(method='linear', axis=0, limit=2, limit_direction='both')
```

将空缺的值补全，
使用interpolate进行线性插分

# 目录

# 循环神经网络 – 基本原理

- 循环神经网络能够处理**任意长度的时序数据**

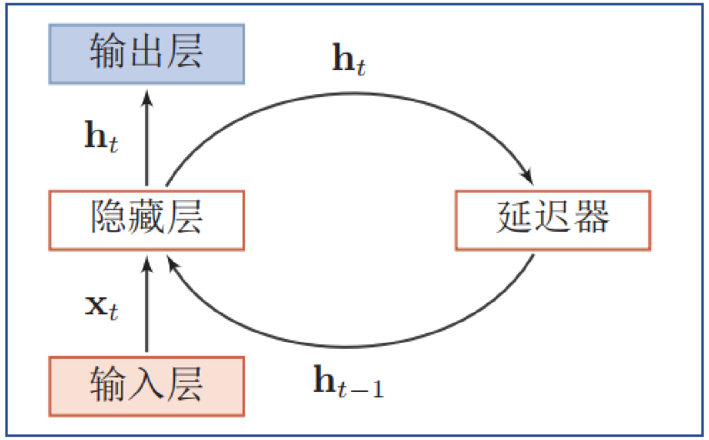
给定一个输入序列，$x_{1:T} = (x_1, x_2, \cdots, x_t, \cdots x_T)$ 其计算公式如下：

$$h_t = f(h_{t-1}, x_t),$$
$$y_t = g(h_t)$$

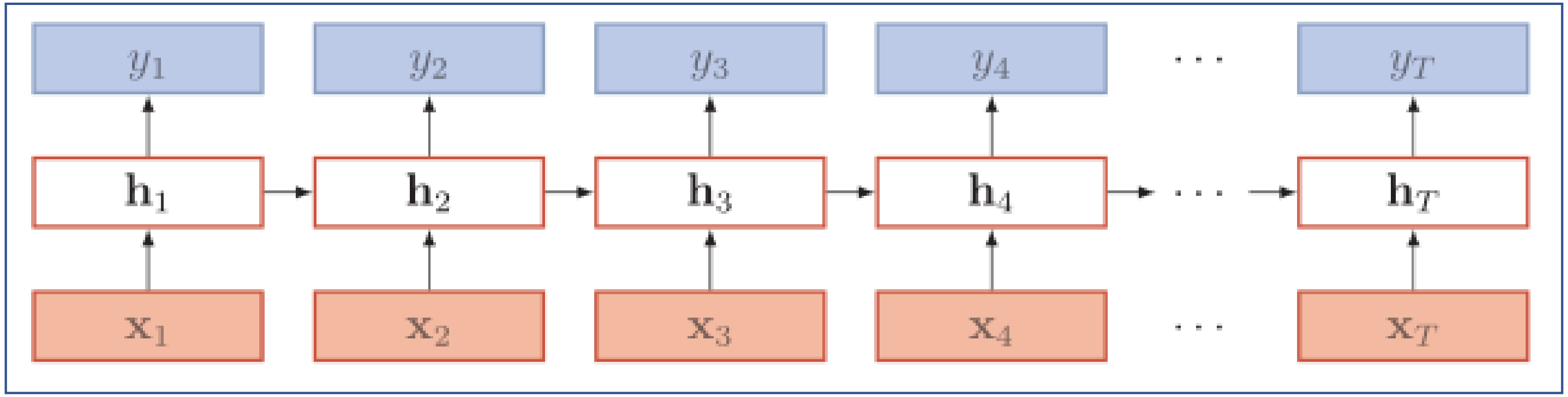
$f(\square), g(\square)$ 实例化

$$h_t = \sigma(W_h x_t + U_h h_{t-1} + b_h),$$
$$y_t = \sigma(W_y h_t + b_y)$$

激活函数可以替换，
如tanh、Relu




画法一




画法二

# 循环神经网络 – 模型实现 – 初始化参数

```
class MyRNN(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        """
        :param input_size: 指定输入数据的维度。例如，对于简单的时间序列预测问题，每一步的输入均为一个采样值，因此input_size=1.
        :param hidden_size: 指定隐藏状态的维度。这个值并不受输入和输出控制，但会影响模型的容量。
        :param output_size: 指定输出数据的维度。此值取决于具体的预测要求。例如，对简单的时间序列预测问题，output_size=1.
        """
        super().__init__()
        self.hidden_size = hidden_size

        # 可学习参数的维度设置，可以类比一下全连接网络的实现。其维度取决于输入数据的维度，以及指定的隐藏状态维度。
        self.w_h = nn.Parameter(torch.rand(input_size, hidden_size))
        self.u_h = nn.Parameter(torch.rand(hidden_size, hidden_size))
        self.b_h = nn.Parameter(torch.zeros(hidden_size))

        self.w_y = nn.Parameter(torch.rand(hidden_size, output_size))
        self.b_y = nn.Parameter(torch.zeros(output_size))

        # 准备激活函数。Dropout函数可选。
        self.tanh = nn.Tanh()
        self.leaky_relu = nn.LeakyReLU()

        # 可选：使用性能更好的参数初始化函数
        for param in self.parameters():
            if param.dim() > 1:
                nn.init.xavier_uniform_(param)
```

- **参数维度定义**
- **激活函数选取**
- **参数初始化**

# 循环神经网络 – 模型实现 – 隐状态更新

```python
def forward(self, x):
    """
    :param x: 输入序列。一般来说，此输入包含三个维度：batch，序列长度，以及每条数据的特征。
    """
    batch_size = x.size(0)
    seq_len = x.size(1)

    # 初始化隐藏状态，一般设为全0。由于是内部新建的变量，需要同步设备位置。
    h = torch.zeros(batch_size, self.hidden_size).to(x.device)
    # RNN实际上只能一步一步处理序列。因此需要用循环迭代。
    y_list = []
    for i in range(seq_len):
        h = self.tanh(torch.matmul(x[:, i, :], self.w_h) +
                          torch.matmul(h, self.u_h) + self.b_h)  # (batch_size, hidden_size)
        y = self.leaky_relu(torch.matmul(h, self.w_y) + self.b_y)  # (batch_size, output_size)
        y_list.append(y)
    # 一般来说，RNN的返回值为最后一步的隐藏状态，以及每一步的输出状态。
    return h, torch.stack(y_list, dim=1)
```

- **隐藏状态初始化**
- **循环迭代更新**
- **注意返回值**

# 循环神经网络 – 数据处理

数据情况

| | sensor_index | UTC time | temperature | humidity | pressure | pm1 | pm25 | pm10 |
|---|---|---|---|---|---|---|---|---|
| 395 | 0 | 2017-01-17 11:00:00 | 0.323529 | 0.971508 | 0.482360 | 0.068882 | 0.289673 | 0.186466 |
| 396 | 0 | 2017-01-17 12:00:00 | 0.294118 | 0.973699 | 0.484556 | 0.060778 | 0.264484 | 0.174436 |
| 397 | 0 | 2017-01-17 13:00:00 | 0.294118 | 0.973890 | 0.487776 | 0.035656 | 0.156171 | 0.117293 |
| 398 | 0 | 2017-01-17 14:00:00 | 0.279412 | 0.974271 | 0.491729 | 0.038898 | 0.171285 | 0.129323 |
| 399 | 0 | 2017-01-17 15:00:00 | 0.279412 | 0.974557 | 0.497731 | 0.040519 | 0.178841 | 0.133835 |

选择temperature这一列进行预测

```python
def sliding_window(seq, window_size):
    result = []
    for i in range(len(seq) - window_size):
        result.append(seq[i:i+window_size])
    return result

train_set, test_set = [], []
for sensor_index, group in raw_df.groupby('sensor_index'):
    full_seq = group['temperature'].interpolate(method='linear', limit=3, limit_area='outside')
    full_len = full_seq.shape[0]
    train_seq, test_seq = full_seq.iloc[:int(full_len * 0.8)].to_list(), \
                          full_seq.iloc[int(full_len * 0.8):].to_list()
    train_set += sliding_window(train_seq, window_size=13)
    test_set += sliding_window(test_seq, window_size=13)

# 即使使用了线性插分，依然可能会有缺失值。这里选择直接抛弃。
train_set, test_set = np.array(train_set), np.array(test_set)
train_set, test_set = (item[~np.isnan(item).any(axis=1)] for item in (train_set, test_set))
print(train_set.shape, test_set.shape)
```

- 固定长度滑动窗口

- 1）划分长序列
- 2）采样短序列

# 循环神经网络 – 模型训练

```
device = 'cuda:0'
model = MyRNN(input_size=1, hidden_size=32, output_size=1).to(device)

loss_func = nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=0.0005)
```

- 初始化模型、loss函数、优化器

```
def mape(y_true, y_pred):
    y_true, y_pred = np.array(y_true), np.array(y_pred)
    non_zero_index = (y_true > 0)
    y_true = y_true[non_zero_index]
    y_pred = y_pred[non_zero_index]

    mape = np.abs((y_true - y_pred) / y_true)
    mape[np.isinf(mape)] = 0
    return np.mean(mape) * 100
```

- 定义和实现指标函数
- 对于回归任务一般选取**RMSE, MAE, MAPE**
- Scikit-learn中提供了MAE和MSE
- RMSE由MSE求根得到
- **MAPE需要自己实现**

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}$$

Root Mean Square Error

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i|$$

Mean Absolute Error

$$MAPE = \frac{100\%}{n}\sum_{i=1}^{n}\left|\frac{\hat{y}_i - y_i}{y_i}\right|$$

Mean Absolute Percentage Error

# 循环神经网络 – 模型训练

训练函数

```python
from sklearn.utils import shuffle

loss_log = []
score_log = []
trained_batches = 0
for epoch in range(4):
    for batch in next_batch(shuffle(train_set), batch_size=64):
        batch = torch.from_numpy(batch).float().to(device)  # (b
        # 使用短序列的前12个值作为历史，最后一个值作为预测值。
        x, label = batch[:, :12], batch[:, -1]

        hidden, out = model(batch.unsqueeze(-1))
        prediction = out[:, -1, :].squeeze(-1)  # (batch)

        loss = loss_func(prediction, label)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
        loss_log.append(loss.detach().cpu().numpy().tolist())
        trained_batches += 1

        # 每训练一定数量的batch，就在测试集上测试模型效果。
        if trained_batches % 200 == 0:
```

测试函数

读取batch

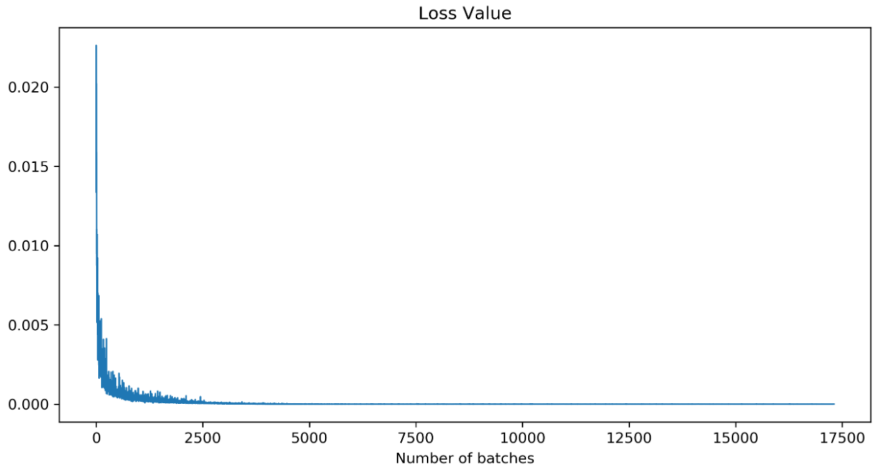
```python
def next_batch(data, batch_size):
    data_length = len(data)
    num_batches = math.ceil(data_length / batch_size)
    for batch_index in range(num_batches):
        start_index = batch_index * batch_size
        end_index = min((batch_index + 1) * batch_size, data_length)
        yield data[start_index:end_index]
```

测试函数

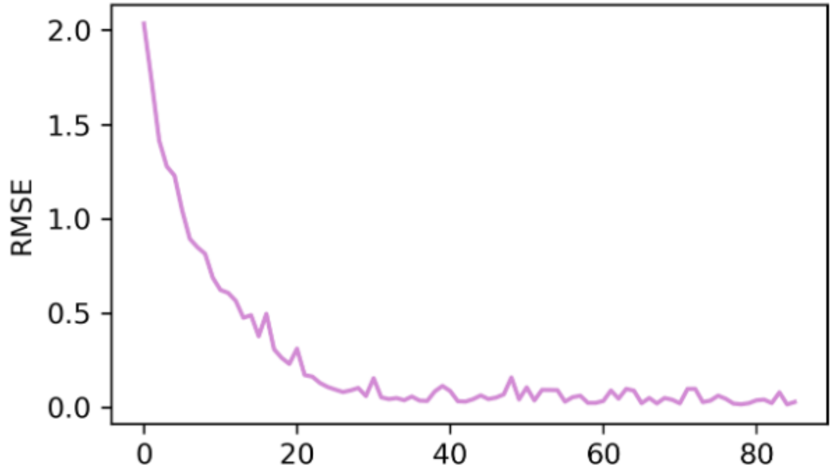
```python
for batch in next_batch(test_set, batch_size=64):
    batch = torch.from_numpy(batch).float().to(device)
    # (batch, seq_len)
    x, label = batch[:, :12], batch[:, -1]

    hidden, out = model(batch.unsqueeze(-1))
    prediction = out[:, -1, :].squeeze(-1)  # (batch)
    all_prediction.append(prediction.detach().cpu().numpy())
all_prediction = np.concatenate(all_prediction)
all_label = test_set[:, -1]
# 进行反归一化操作。
all_prediction = dataset.denormalize(all_prediction, 'temperature')
all_label = dataset.denormalize(all_label, 'temperature')
# 计算测试指标。
rmse_score = math.sqrt(mse(all_label, all_prediction))
mae_score = mae(all_label, all_prediction)
mape_score = mape(all_label, all_prediction)
score_log.append([rmse_score, mae_score, mape_score])
print('RMSE: %.4f, MAE: %.4f, MAPE: %.4f' %
      (rmse_score, mae_score, mape_score))
```

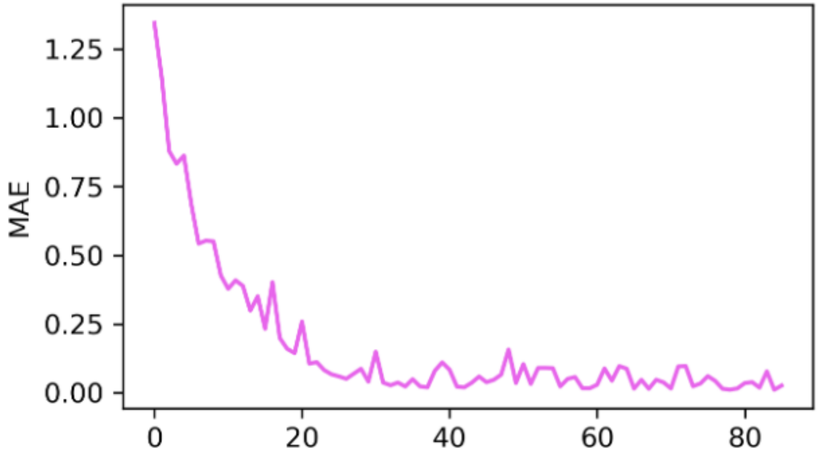
# 循环神经网络 – 训练结果可视化（使用自己实现的模型）



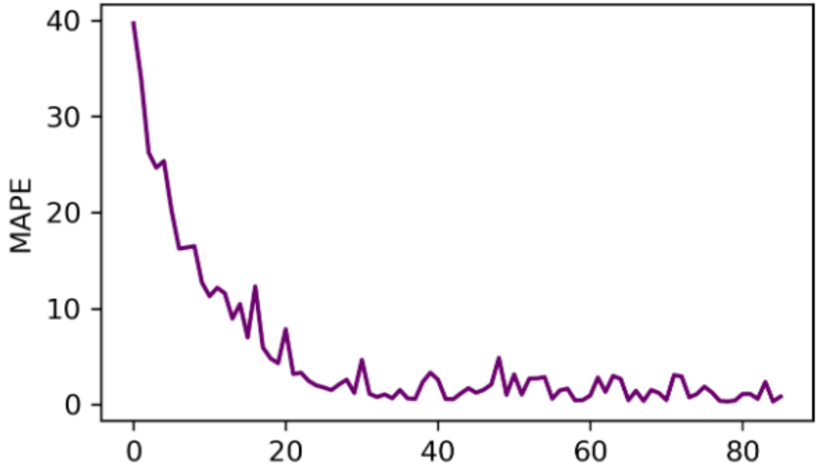

**Loss变化**




**RMSE变化**




**MAE变化**




**MAPE变化**

# 循环神经网络 – torch.nn.RNN

输入

Inputs: input, h_0

- **input** of shape (*seq_len, batch, input_size*): tensor containing the features of the input sequence. The input can also be a packed variable length sequence. See `torch.nn.utils.rnn.pack_padded_sequence()` or `torch.nn.utils.rnn.pack_sequence()` for details.
- **h_0** of shape (*num_layers*num_directions, batch, hidden_size*): tensor containing the initial hidden state for each element in the batch. Defaults to zero if not provided. If the RNN is bidirectional, num_directions should be 2, else it should be 1.

输出

Outputs: output, h_n

- **output** of shape (*seq_len, batch, num_directions*hidden_size*): tensor containing the output features ($h_t$) from the last layer of the RNN, for each $t$. If a `torch.nn.utils.rnn.PackedSequence` has been given as the input, the output will also be a packed sequence.
  For the unpacked case, the directions can be separated using `output.view(seq_len, batch, num_directions, hidden_size)`, with forward and backward being direction $0$ and $1$ respectively.
  Similarly, the directions can be separated in the packed case.
- **h_n** of shape (*num_layers*num_directions, batch, hidden_size*): tensor containing the hidden state for $t = seq\_len$.
  Like *output*, the layers can be separated using `h_n.view(num_layers, num_directions, batch, hidden_size)`.

# 循环神经网络 – torch.nn.RNN

**参数**

Parameters

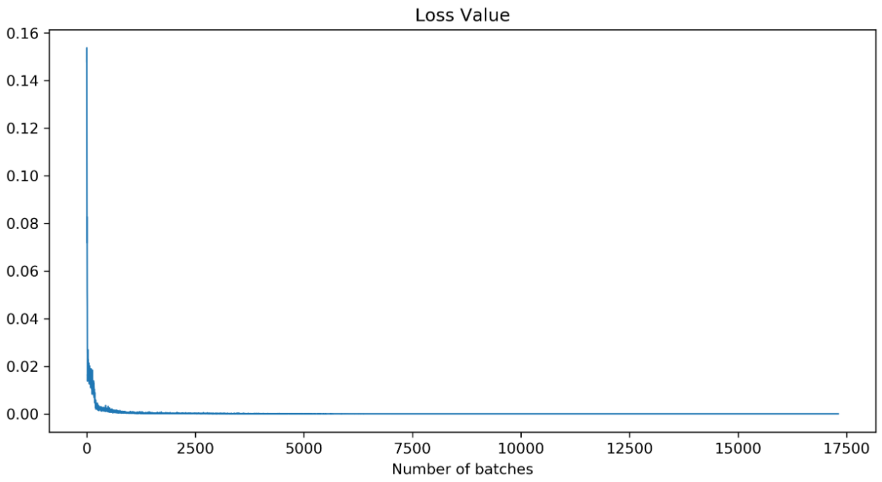
- **input_size** – The number of expected features in the input *x*
- **hidden_size** – The number of features in the hidden state *h*
- **num_layers** – Number of recurrent layers. E.g., setting `num_layers=2` would mean stacking two RNNs together to form a *stacked RNN*, with the second RNN taking in outputs of the first RNN and computing the final results. Default: 1
- **nonlinearity** – The non-linearity to use. Can be either `'tanh'` or `'relu'`. Default: `'tanh'`
- **bias** – If `False`, then the layer does not use bias weights *b_ih* and *b_hh*. Default: `True`
- **batch_first** – If `True`, then the input and output tensors are provided as *(batch, seq, feature)*. Default: `False`
- **dropout** – If non-zero, introduces a *Dropout* layer on the outputs of each RNN layer except the last layer, with dropout probability equal to `dropout`. Default: 0
- **bidirectional** – If `True`, becomes a bidirectional RNN. Default: `False`

**例子**

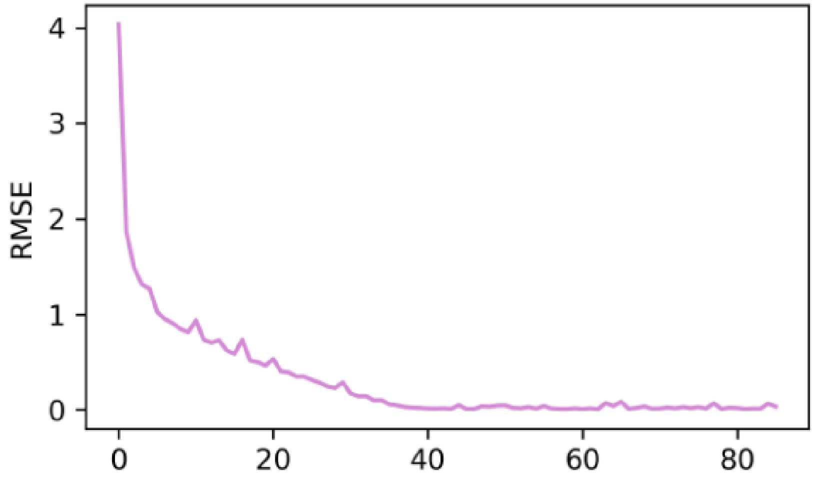
Examples:

```
>>> rnn = nn.RNN(10, 20, 2)
>>> input = torch.randn(5, 3, 10)
>>> h0 = torch.randn(2, 3, 20)
>>> output, hn = rnn(input, h0)
```

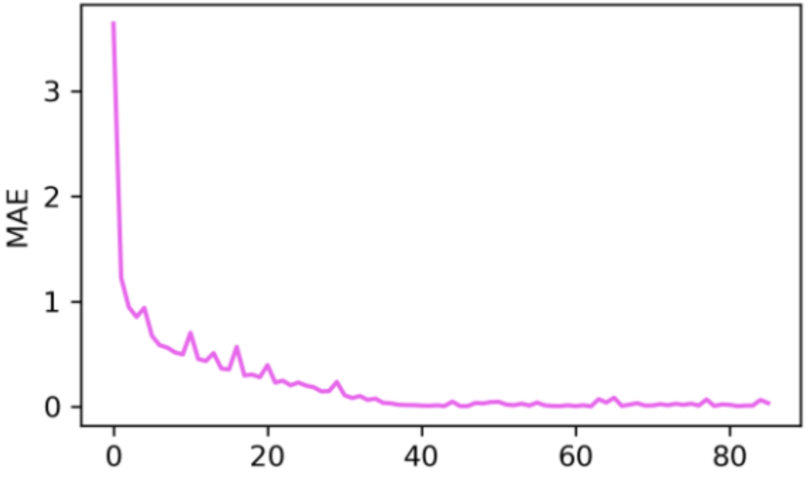
# 循环神经网络 – 训练结果可视化（使用Pytorch自带的模型）



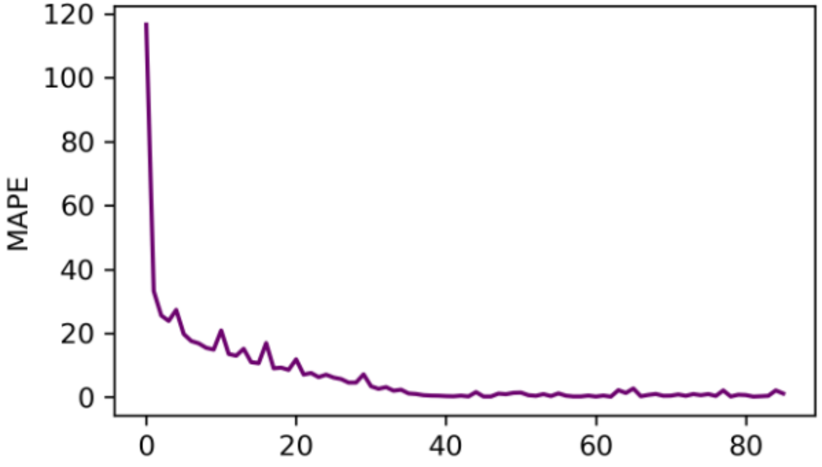

**Loss变化**




**RMSE变化**




**MAE变化**




**MAPE变化**

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- 基本原理
- 动手实现
- torch.nn.GRU

# 长短期记忆网络LSTM – 基本原理

**LSTM**：Long Short Term Memory networks

- 一种特殊形式的RNN
- 解决长程依赖问题

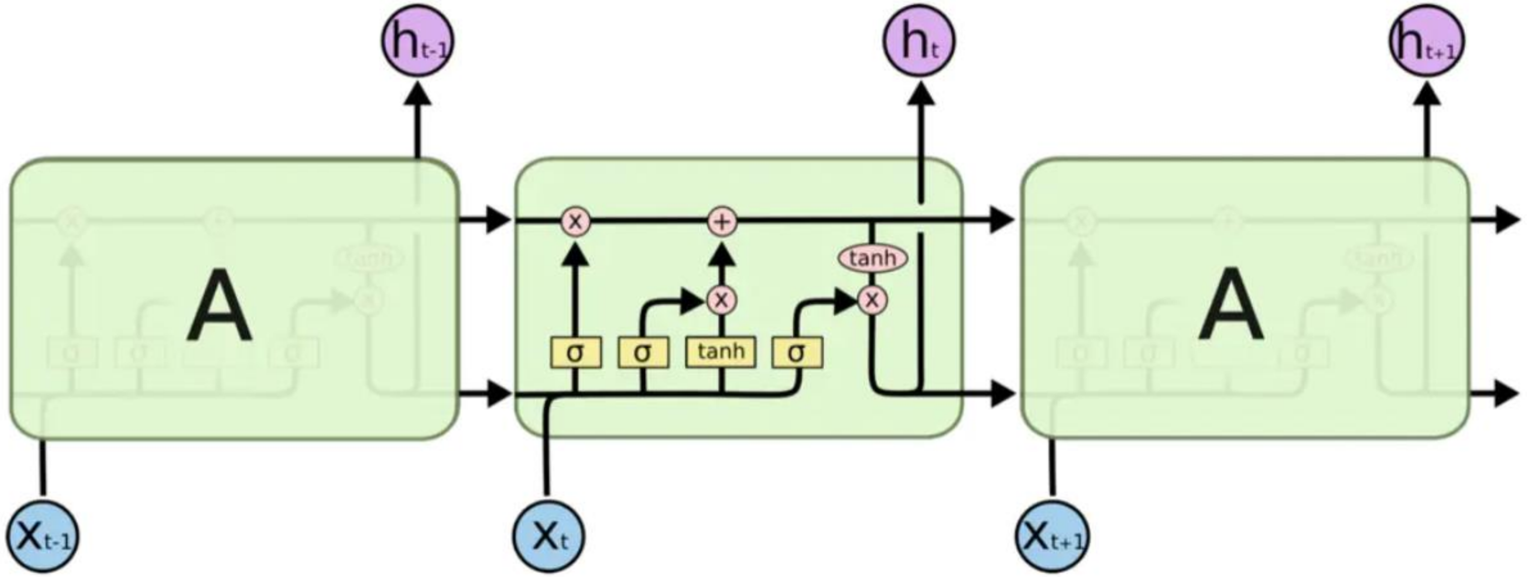
The clouds are in the ___. → 输入 → RNN → 预测 → The clouds are in the <u>sky</u>.

短程依赖，普通的RNN能够解决

I grew up in China…
I speak fluent ___. → 输入 → LSTM → 预测 → I grew up in China…
I speak fluent <u>Chinese</u>.

长程依赖，借助LSTM解决

# 长短期记忆网络 – 基本原理

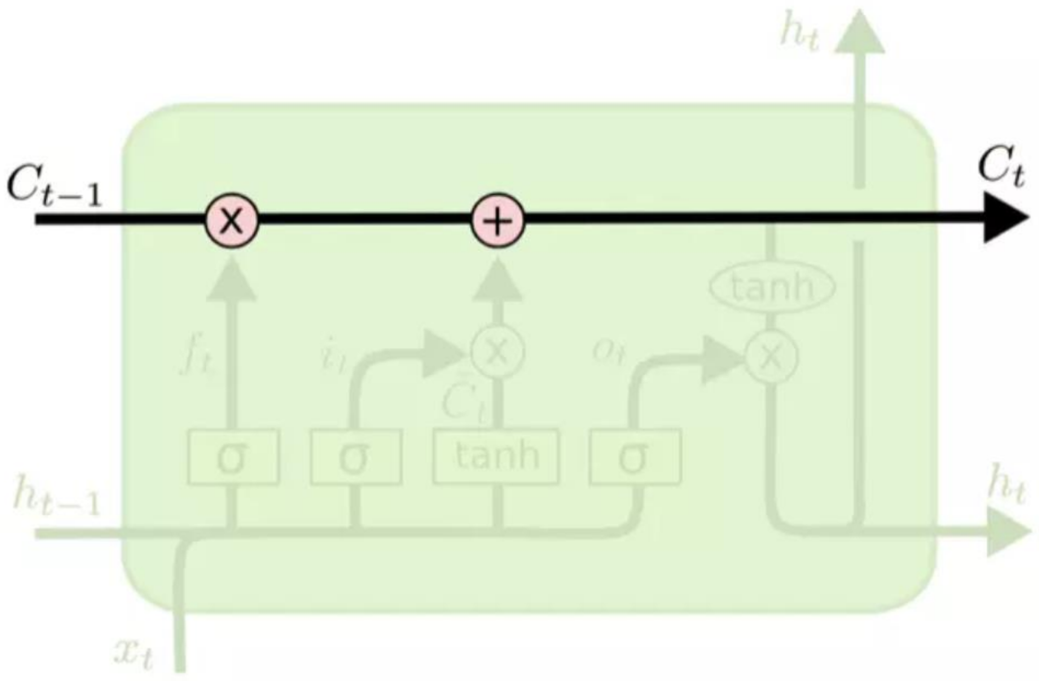



**LSTM结构**

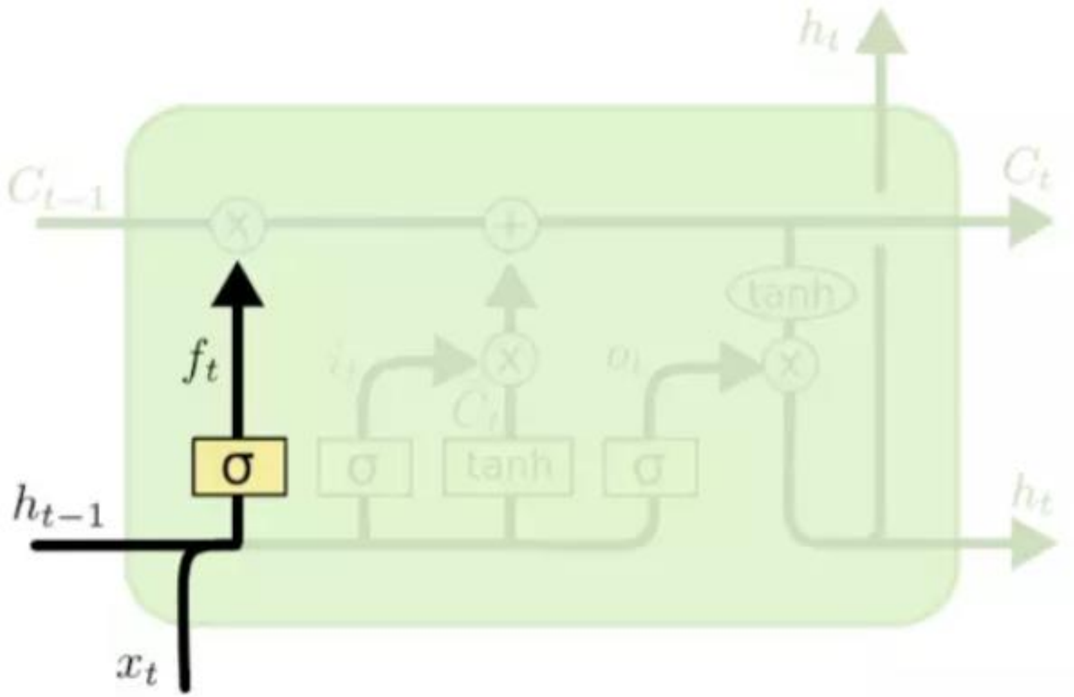
$$f_t = \sigma_g\left(W_f x_t + U_f h_{t-1} + b_f\right)$$
$$i_t = \sigma_g\left(W_i x_t + U_i h_{t-1} + b_i\right)$$
$$o_t = \sigma_g\left(W_o x_t + U_o h_{t-1} + b_o\right)$$
$$c_t = f_t \circ c_{t-1} + i_t \circ \sigma_c\left(W_c x_t + U_c h_{t-1} + b_c\right)$$
$$h_t = o_t \circ \sigma_h\left(c_t\right)$$

**LSTM公式**

# 长短期记忆网络 – 基本原理



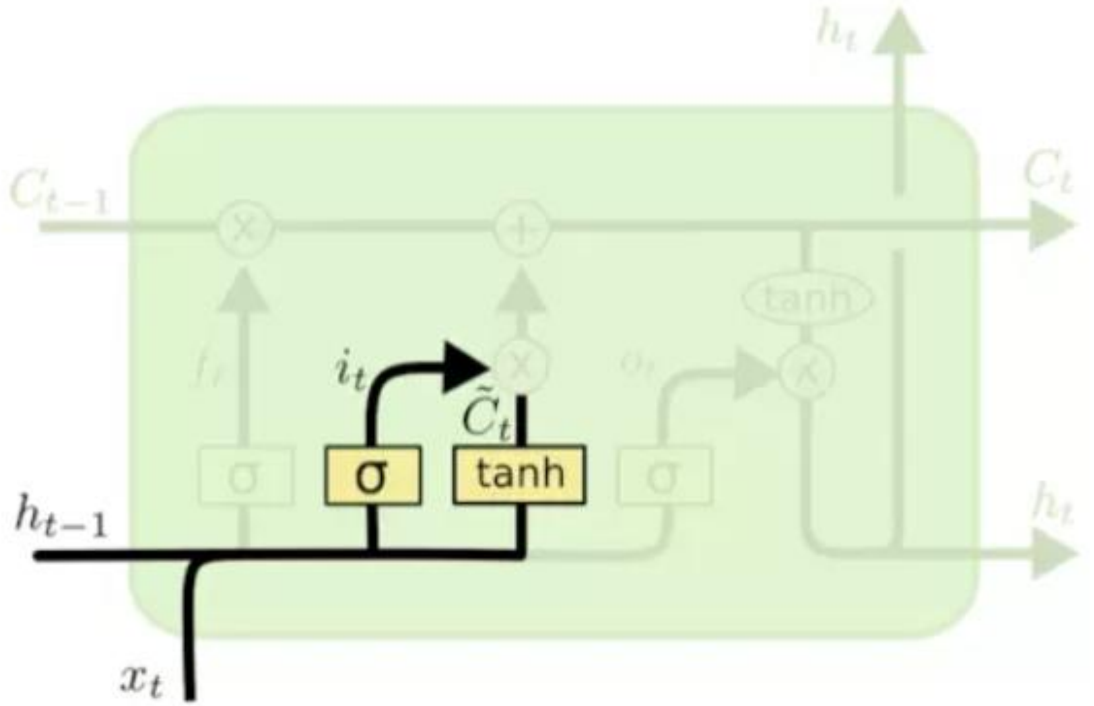

- LSTM的核心是细胞状态，用贯穿细胞的水平线表示




- 1）计算遗忘门，决定细胞状态需要舍弃哪部分无用信息

$$f_t = \sigma_g\left(W_f x_t + U_f h_{t-1} + b_f\right)$$

# 长短期记忆网络 – 基本原理

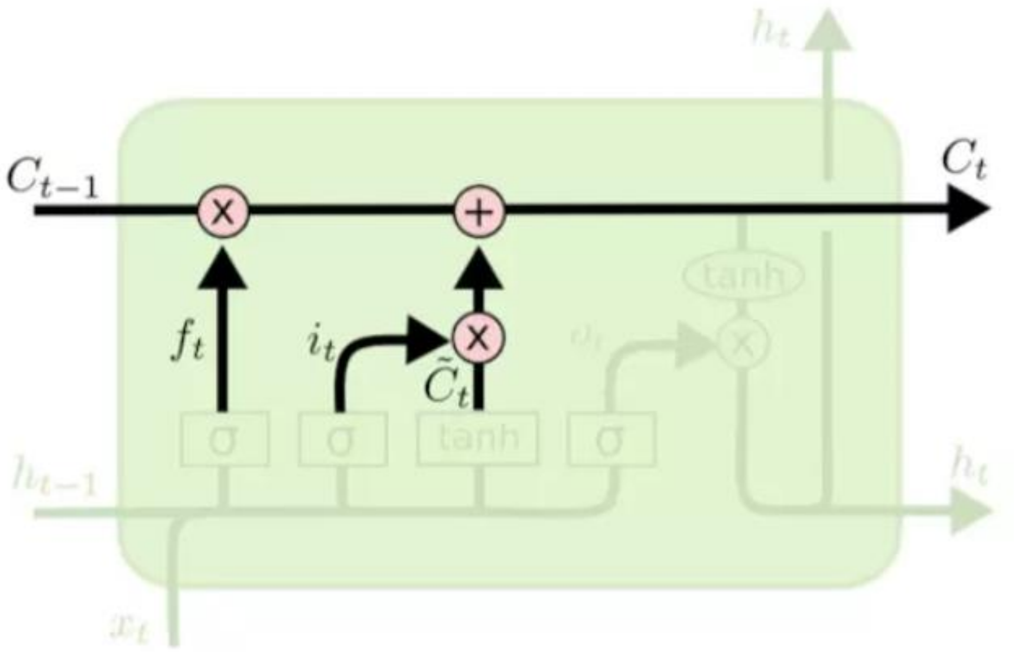



- 2）计算输入门，决定细胞状态需要添加哪些有用信息

$$i_t = \sigma_g\left(W_i x_t + U_i h_{t-1} + b_i\right)$$

- 3）计算候选细胞状态

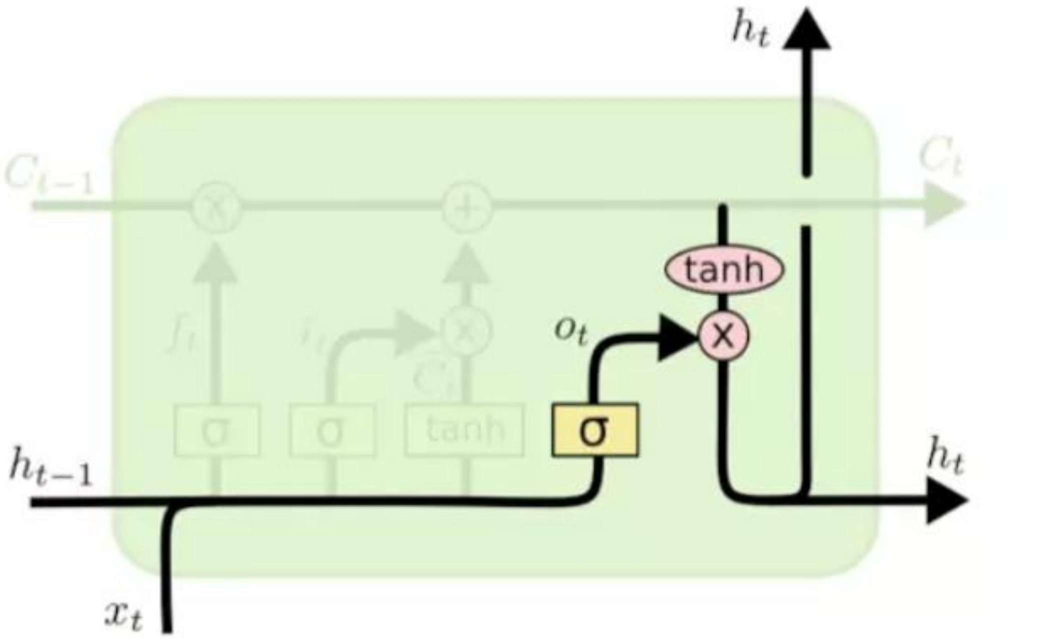
$$\tilde{c}_t = \sigma_c\left(W_c x_t + U_c h_{t-1} + b_c\right)$$




- 4）更新细胞状态

$$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$$

# 长短期记忆网络 – 基本原理




- 5）计算输出门，控制细胞状态中哪些信息被输出：

$$o_t = \sigma_g\left(W_o x_t + U_o h_{t-1} + b_o\right)$$

- 6）计算输出隐状态：

$$h_t = o_t \circ \sigma_h\left(c_t\right)$$

# 长短期记忆网络 – 模型实现 – 初始化参数

```python
class MyLegacyLSTM(nn.Module):
    def __init__(self, input_size, hidden_size):
        super().__init__()
        self.hidden_size = hidden_size

        self.w_f = nn.Parameter(torch.rand(input_size, hidden_size))
        self.u_f = nn.Parameter(torch.rand(hidden_size, hidden_size))
        self.b_f = nn.Parameter(torch.zeros(hidden_size))

        self.w_i = nn.Parameter(torch.rand(input_size, hidden_size))
        self.u_i = nn.Parameter(torch.rand(hidden_size, hidden_size))
        self.b_i = nn.Parameter(torch.zeros(hidden_size))

        self.w_o = nn.Parameter(torch.rand(input_size, hidden_size))
        self.u_o = nn.Parameter(torch.rand(hidden_size, hidden_size))
        self.b_o = nn.Parameter(torch.zeros(hidden_size))

        self.w_c = nn.Parameter(torch.rand(input_size, hidden_size))
        self.u_c = nn.Parameter(torch.rand(hidden_size, hidden_size))
        self.b_c = nn.Parameter(torch.zeros(hidden_size))

        self.sigmoid = nn.Sigmoid()
        self.tanh = nn.Tanh()

        for param in self.parameters():
            if param.dim() > 1:
                nn.init.xavier_uniform_(param)
```

$$f_t = \sigma_g\left(W_f x_t + U_f h_{t-1} + b_f\right)$$

$$i_t = \sigma_g\left(W_i x_t + U_i h_{t-1} + b_i\right)$$

$$o_t = \sigma_g\left(W_o x_t + U_o h_{t-1} + b_o\right)$$

$$c_t = f_t \circ c_{t-1} + i_t \circ \sigma_c\left(W_c x_t + U_c h_{t-1} + b_c\right)$$

$$h_t = o_t \circ \sigma_h\left(c_t\right)$$

# 长短期记忆网络 – 模型实现

```python
def forward(self, x):
    batch_size = x.size(0)
    seq_len = x.size(1)

    # 需要初始化隐藏状态和细胞状态
    h = torch.zeros(batch_size, self.hidden_size).to(x.device)
    c = torch.zeros(batch_size, self.hidden_size).to(x.device)
    y_list = []
    for i in range(seq_len):
        forget_gate = self.sigmoid(torch.matmul(x[:, i, :], self.w_f) +
                                   torch.matmul(h, self.u_f) + self.b_f)
        # (batch_size, hidden_size)
        input_gate = self.sigmoid(torch.matmul(x[:, i, :], self.w_i) +
                                  torch.matmul(h, self.u_i) + self.b_i)
        output_gate = self.sigmoid(torch.matmul(x[:, i, :], self.w_o) +
                                   torch.matmul(h, self.u_o) + self.b_o)
        # 这里可以看到各个门的运作方式。
        # 三个门均通过hadamard积作用在每一个维度上。
        c = forget_gate * c + \
            input_gate * self.tanh(torch.matmul(x[:, i, :], self.w_c) +
                                   torch.matmul(h, self.u_c) +
                                   self.b_c)
        h = output_gate * self.tanh(c)
        y_list.append(h)
    return torch.stack(y_list, dim=1), (h, c)
```

$$f_t = \boxed{\sigma_g}\left(W_f x_t + U_f h_{t-1} + b_f\right)$$

$$i_t = \boxed{\sigma_g}\left(W_i x_t + U_i h_{t-1} + b_i\right)$$

$$o_t = \boxed{\sigma_g}\left(W_o x_t + U_o h_{t-1} + b_o\right)$$

$$c_t = f_t \circ c_{t-1} + i_t \circ \boxed{\sigma_c}\left(W_c x_t + U_c h_{t-1} + b_c\right)$$

$$h_t = o_t \circ \boxed{\sigma_h}\left(c_t\right)$$

- 初始化隐藏状态hidden_state 为全0向量
- 按照公式循环迭代更新hidden_state，计算输出
- 返回最后一步的隐藏状态和每一步的输出
- 注意不同地方的激活函数的选取

# 长短期记忆网络 – 优化模型实现思路

**核心思想：合并矩阵运算，提高并行性**

**1）各门控计算优化，以遗忘门为例：**

$$f_t = \sigma_g\left(W_f x_t + U_f h_{t-1} + b_f\right) = \sigma_g\left(W_f'\left(x_t \| h_{t-1}\right) + b_f\right)$$

遗忘门中的两个矩阵运算实际上可以合并为一个，$W_f' \in \mathbb{R}^{(\text{input\_size+hidden\_size}),\ \text{hidden\_size}}$

相当于拼合 $W_f \in \mathbb{R}^{\text{input\_size},\ \text{hidden\_size}}$ 和 $U_f \in \mathbb{R}^{\text{hidden\_size},\ \text{hidden\_size}}$， 此时，门的计算和全连接网络一致，可使用nn.Linear替代：

```
self.forget_gate = nn.Linear(input_size+hidden_size, hidden_size)
f_g = self.sigmoid(self.hidden_gate(torch.cat([x, h], dim=-1)))
```

**核心思想：合并矩阵运算，提高并行性**

**2）所有门控一起计算：**

- 三个门控单元和 $\tilde{C}_t$ 的计算公式高度一致

⇩

一步实现所有门的计算，再将结果拆分后进行激活

```
self.gates = nn.Linear(input_size+hidden_size, hidden_size * 4)
f_g, i_g, o_g, c_g = self.gates(torch.cat([x, h], dim=-1)).chunk(chunks=4, dim=-1)
```

# 长短期记忆网络 – 优化模型实现

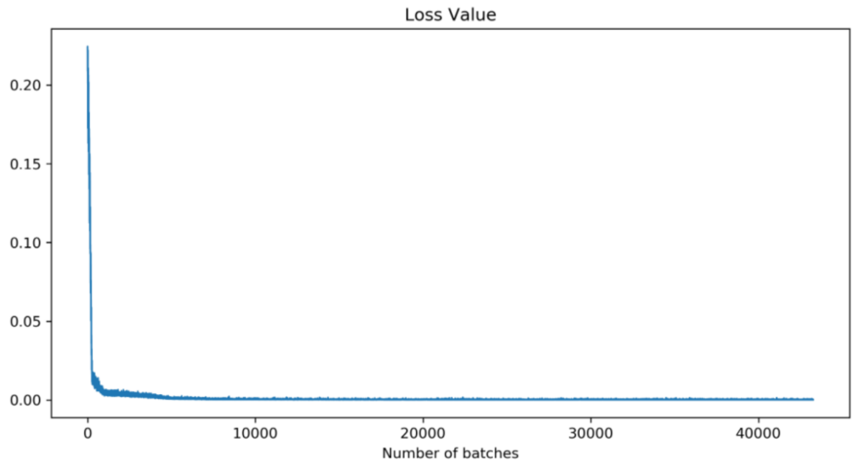
```
class MyLSTM(nn.Module):
    def __init__(self, input_size, hidden_size):
        super().__init__()
        self.hidden_size = hidden_size

        self.gates = nn.Linear(input_size+hidden_size, hidden_size * 4)
        self.sigmoid = nn.Sigmoid()
        self.tanh = nn.Tanh()

        for param in self.parameters():
            if param.dim() > 1:
                nn.init.xavier_uniform_(param)

    def forward(self, x):
        batch_size = x.size(0)
        seq_len = x.size(1)

        h, c = (torch.zeros(batch_size, self.hidden_size).to(x.device) for _ in range(2))
        y_list = []
        for i in range(seq_len):
            forget_gate, input_gate, \
            output_gate, candidate_cell = self.gates(torch.cat([x[:, i, :], h], dim=-1)).chunk(4, -1)
            forget_gate, input_gate, output_gate = (self.sigmoid(g)
                                                    for g in (forget_gate, input_gate, output_gate))
            c = forget_gate * c + input_gate * self.tanh(candidate_cell)
            h = output_gate * self.tanh(c)
            y_list.append(h)
        return torch.stack(y_list, dim=1), (h, c)
```

核心思想：

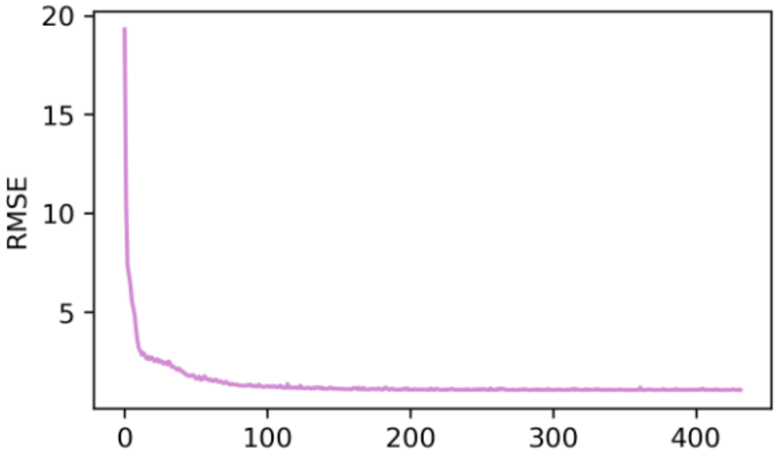
**提高并行性**

**合并矩阵运算**

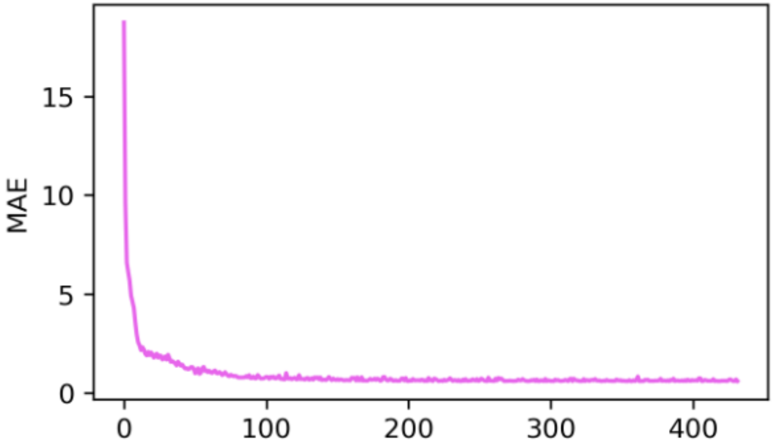
# 长短期记忆网络 – 训练结果可视化（使用自己实现的模型）



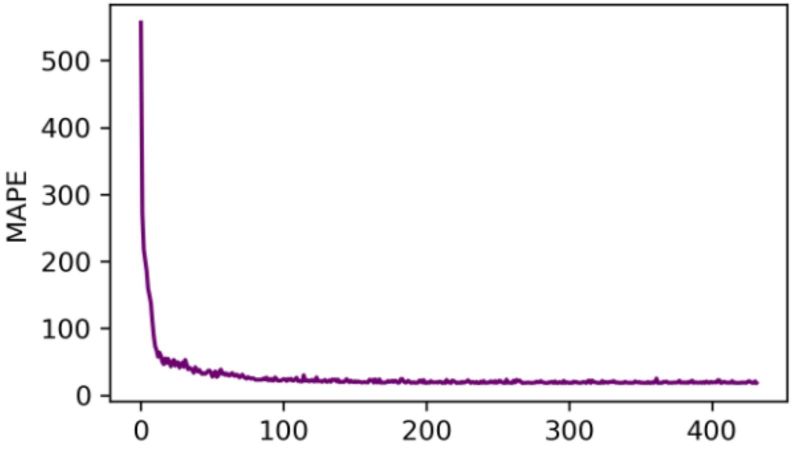

Loss变化




RMSE变化




MAE变化




MAPE变化

# 长短期记忆网络 – torch.nn.LSTM

**输入**

Inputs: input, (h_0, c_0)

- **input** of shape (*seq_len, batch, input_size*): tensor containing the features of the input sequence. The input can also be a packed variable length sequence. See `torch.nn.utils.rnn.pack_padded_sequence()` or `torch.nn.utils.rnn.pack_sequence()` for details.
- **h_0** of shape (*num_layers * num_directions, batch, hidden_size*): tensor containing the initial hidden state for each element in the batch. If the LSTM is bidirectional, num_directions should be 2, else it should be 1.
- **c_0** of shape (*num_layers * num_directions, batch, hidden_size*): tensor containing the initial cell state for each element in the batch.

  If (*h_0, c_0*) is not provided, both **h_0** and **c_0** default to zero.

**输出**

Outputs: output, (h_n, c_n)

- **output** of shape (*seq_len, batch, num_directions * hidden_size*): tensor containing the output features (*h_t*) from the last layer of the LSTM, for each *t*. If a `torch.nn.utils.rnn.PackedSequence` has been given as the input, the output will also be a packed sequence.

  For the unpacked case, the directions can be separated using `output.view(seq_len, batch, num_directions, hidden_size)`, with forward and backward being direction 0 and 1 respectively. Similarly, the directions can be separated in the packed case.
- **h_n** of shape (*num_layers * num_directions, batch, hidden_size*): tensor containing the hidden state for $t$ = *seq_len*.

  Like *output*, the layers can be separated using `h_n.view(num_layers, num_directions, batch, hidden_size)` and similarly for *c_n*.
- **c_n** of shape (*num_layers * num_directions, batch, hidden_size*): tensor containing the cell state for $t$ = *seq_len*.

# 长短期记忆网络 – torch.nn.LSTM

参数

Parameters

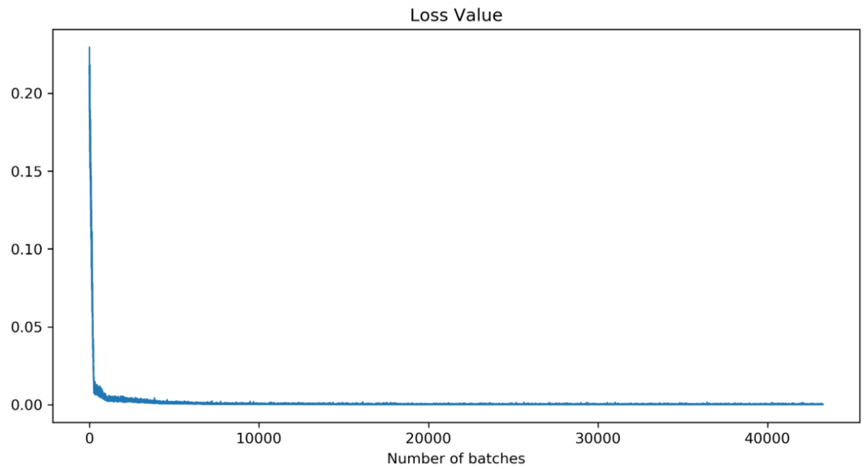
- **input_size** – The number of expected features in the input *x*
- **hidden_size** – The number of features in the hidden state *h*
- **num_layers** – Number of recurrent layers. E.g., setting `num_layers=2` would mean stacking two LSTMs together to form a *stacked LSTM*, with the second LSTM taking in outputs of the first LSTM and computing the final results. Default: 1
- **bias** – If `False`, then the layer does not use bias weights *b_ih* and *b_hh*. Default: `True`
- **batch_first** – If `True`, then the input and output tensors are provided as (batch, seq, feature). Default: `False`
- **dropout** – If non-zero, introduces a *Dropout* layer on the outputs of each LSTM layer except the last layer, with dropout probability equal to `dropout`. Default: 0
- **bidirectional** – If `True`, becomes a bidirectional LSTM. Default: `False`

例子

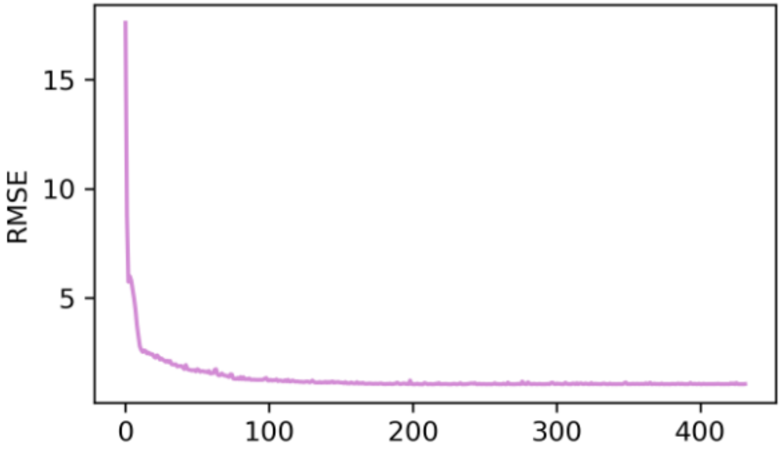
Examples:

```
>>> rnn = nn.LSTM(10, 20, 2)
>>> input = torch.randn(5, 3, 10)
>>> h0 = torch.randn(2, 3, 20)
>>> c0 = torch.randn(2, 3, 20)
>>> output, (hn, cn) = rnn(input, (h0, c0))
```

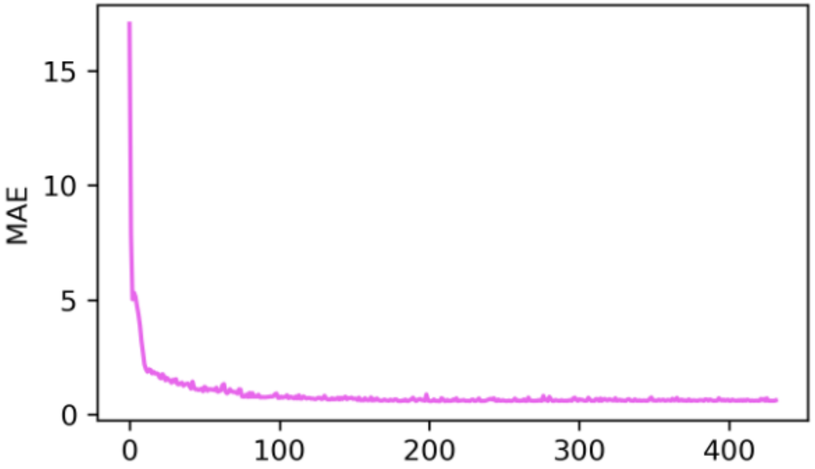
# 长短期记忆网络 – 训练结果可视化（使用Pytorch自带模型）



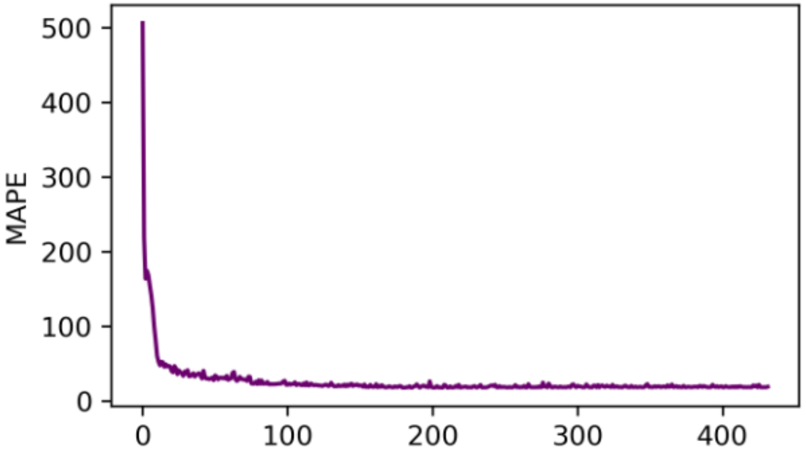

**Loss变化**




**RMSE变化**




**MAE变化**




**MAPE变化**

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## 4. 门控循环单元

- 基本原理
- 动手实现
- torch.nn.GRU

# 门控循环单元 – 基本原理

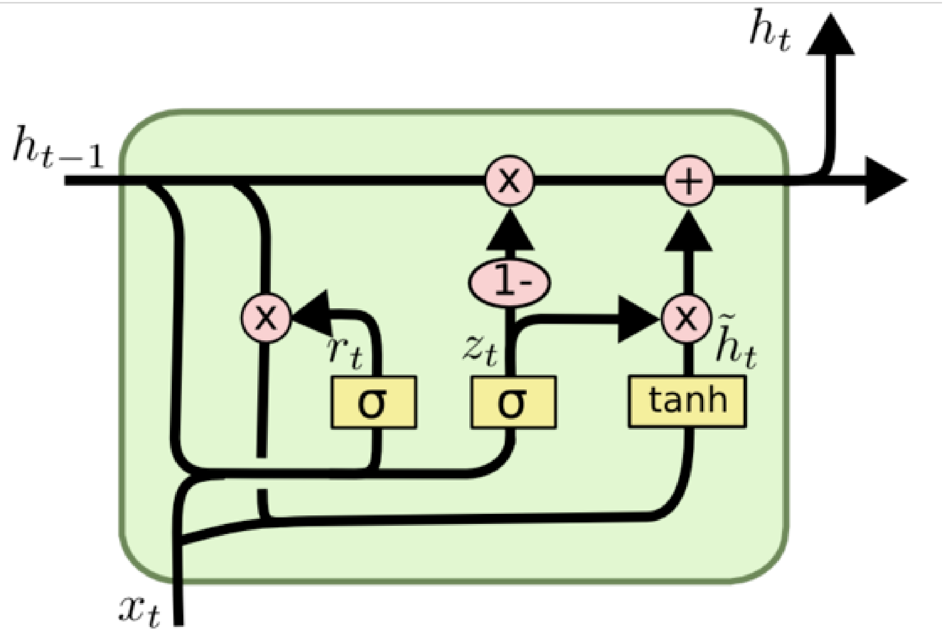
## GRU：Gate Recurrent Unit

- 一种特殊形式的RNN
- 相比LSTM，简化门控机制，提高计算效率
- 门控：
  - 重置门 $r_t$ ：控制遗忘多少之前时刻的信息
  - 更新门 $z_t$ ：控制保留多少当前时刻的信息

RNN —解决长期依赖→ LSTM

LSTM —提高计算效率→ GRU

# 门控循环单元 – 基本原理




**GRU结构**

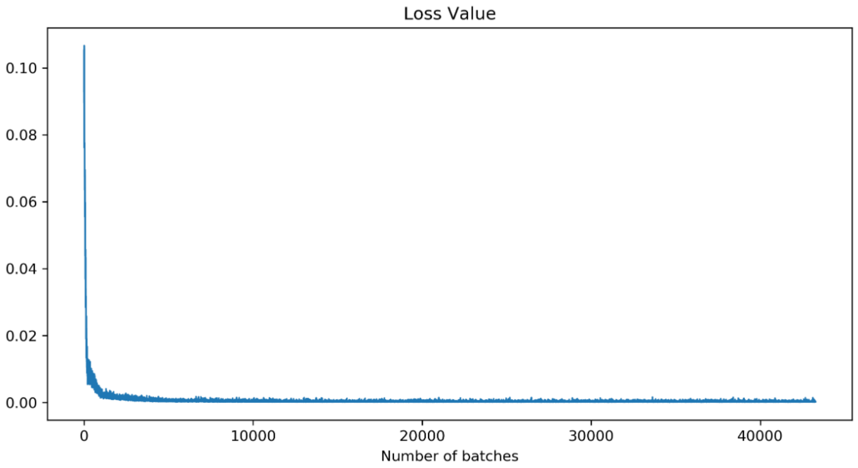
$$
\begin{aligned}
z_t &= \sigma_g(W_z x_t + U_z h_{t-1} + b_z) \\
r_t &= \sigma_g(W_r x_t + U_r h_{t-1} + b_r) \\
\hat{h}_t &= \phi_h(W_h x_t + U_h(r_t \odot h_{t-1}) + b_h) \\
h_t &= (1 - z_t) \odot h_{t-1} + z_t \odot \hat{h}_t
\end{aligned}
$$

**GRU公式**

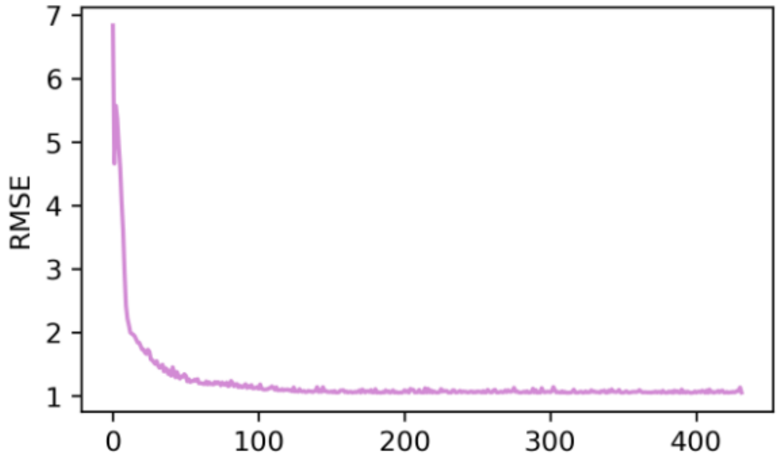
# 门控循环单元 – 模型实现（优化后）

```
class MyGRU(nn.Module):
    def __init__(self, input_size, hidden_size):
        super().__init__()
        self.hidden_size = hidden_size

        self.gates = nn.Linear(input_size+hidden_size, hidden_size*2)
        # 用于计算candidate hidden state
        self.hidden_transform = nn.Linear(input_size+hidden_size, hidden_size)

        self.sigmoid = nn.Sigmoid()
        self.tanh = nn.Tanh()

        for param in self.parameters():
            if param.dim() > 1:
                nn.init.xavier_uniform_(param)

    def forward(self, x):
        batch_size = x.size(0)
        seq_len = x.size(1)

        h = torch.zeros(batch_size, self.hidden_size).to(x.device)
        y_list = []
        for i in range(seq_len):
            update_gate, reset_gate = self.gates(torch.cat([x[:, i, :], h], dim=-1)).chunk(2, -1)
            update_gate, reset_gate = (self.sigmoid(gate) for gate in (update_gate, reset_gate))
            candidate_hidden = self.tanh(self.hidden_transform(torch.cat([x[:, i, :], reset_gate * h], dim=-1)))
            h = (1-update_gate) * h + update_gate * candidate_hidden
            y_list.append(h)
        return torch.stack(y_list, dim=1), h
```

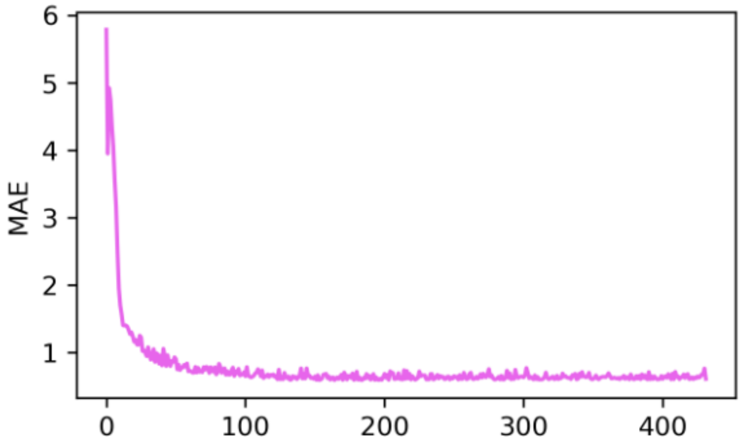
# 门控循环单元– 训练结果可视化（使用自己实现的GRU）



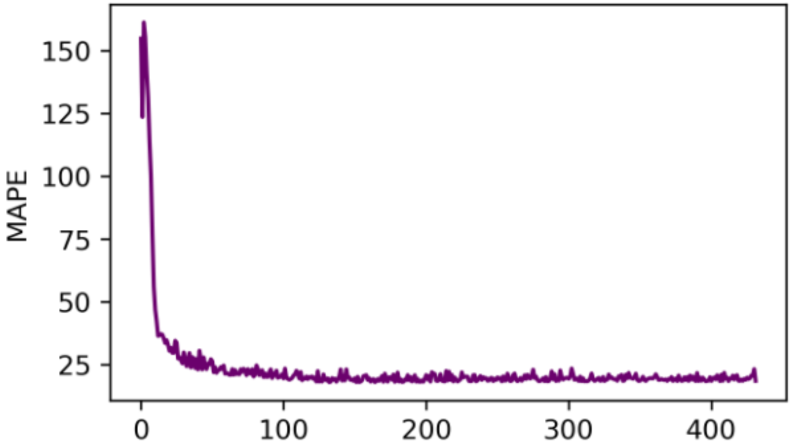

Loss变化




RMSE变化




MAE变化




MAPE变化

# 门控循环单元 – torch.nn.GRU

输入

Inputs: input, h_0

- **input** of shape (*seq_len, batch, input_size*): tensor containing the features of the input sequence. The input can also be a packed variable length sequence. See `torch.nn.utils.rnn.pack_padded_sequence()` for details.
- **h_0** of shape (*num_layers *num_directions, batch, hidden_size*): tensor containing the initial hidden state for each element in the batch. Defaults to zero if not provided. If the RNN is bidirectional, num_directions should be 2, else it should be 1.

输出

Outputs: output, h_n

- **output** of shape (*seq_len, batch, num_directions *hidden_size*): tensor containing the output features h_t from the last layer of the GRU, for each $t$. If a `torch.nn.utils.rnn.PackedSequence` has been given as the input, the output will also be a packed sequence. For the unpacked case, the directions can be separated using `output.view(seq_len, batch, num_directions, hidden_size)`, with forward and backward being direction *0* and *1* respectively.
  Similarly, the directions can be separated in the packed case.
- **h_n** of shape (*num_layers *num_directions, batch, hidden_size*): tensor containing the hidden state for $t$ = *seq_len*
  Like *output*, the layers can be separated using `h_n.view(num_layers, num_directions, batch, hidden_size)`.

# 门控循环单元 – torch.nn.GRU

参数

Parameters

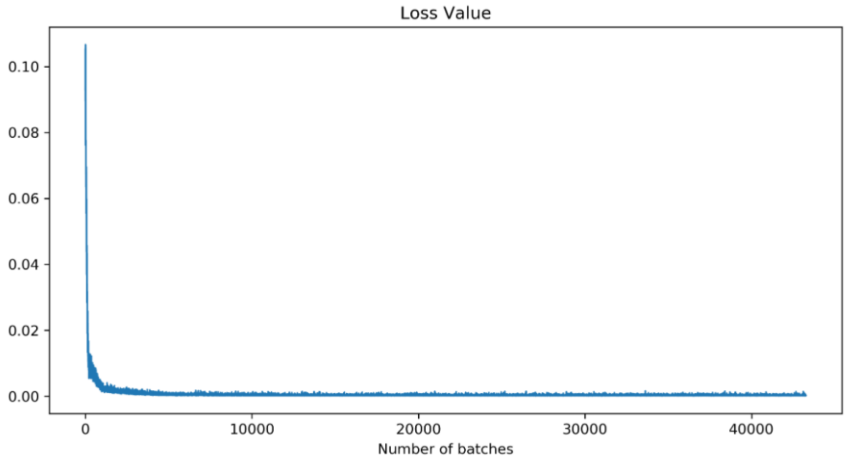
- **input_size** – The number of expected features in the input $x$
- **hidden_size** – The number of features in the hidden state $h$
- **num_layers** – Number of recurrent layers. E.g., setting `num_layers=2` would mean stacking two GRUs together to form a *stacked GRU*, with the second GRU taking in outputs of the first GRU and computing the final results. Default: 1
- **bias** – If `False`, then the layer does not use bias weights *b_ih* and *b_hh*. Default: `True`
- **batch_first** – If `True`, then the input and output tensors are provided as (batch, seq, feature). Default: `False`
- **dropout** – If non-zero, introduces a *Dropout* layer on the outputs of each GRU layer except the last layer, with dropout probability equal to `dropout`. Default: 0
- **bidirectional** – If `True`, becomes a bidirectional GRU. Default: `False`

例子

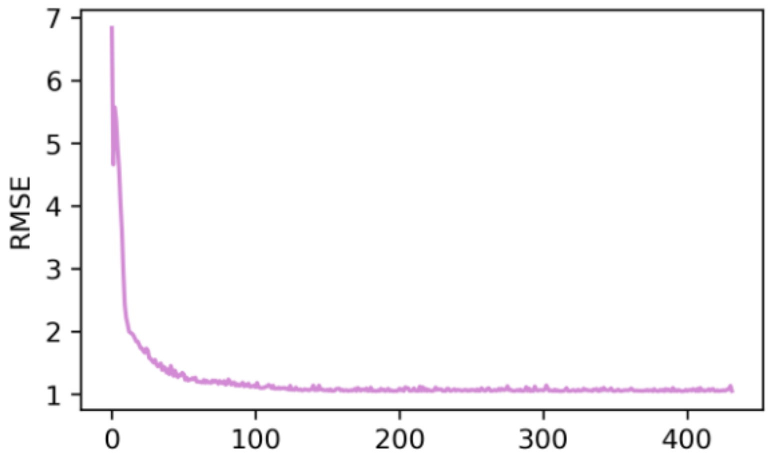
Examples:

```
>>> rnn = nn.GRU(10, 20, 2)
>>> input = torch.randn(5, 3, 10)
>>> h0 = torch.randn(2, 3, 20)
>>> output, hn = rnn(input, h0)
```

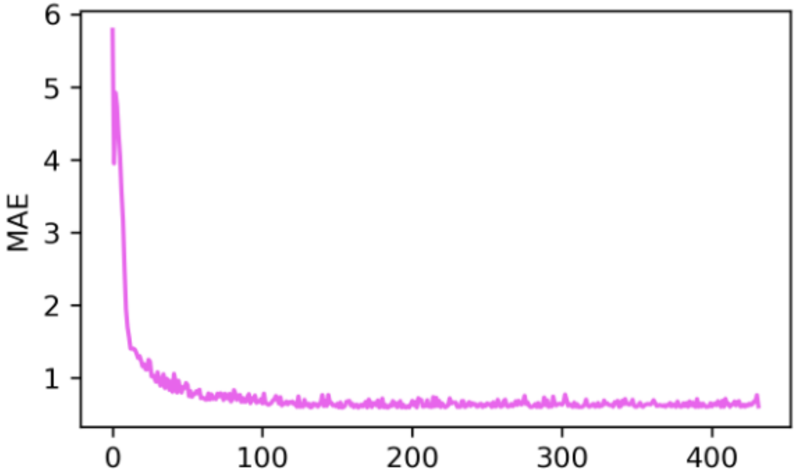
# 门控循环单元– 训练结果可视化（使用Pytorch自带GRU）



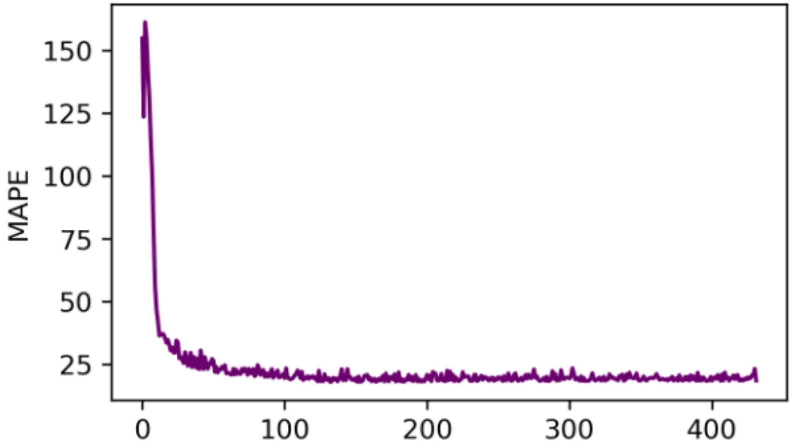

Loss变化




RMSE变化



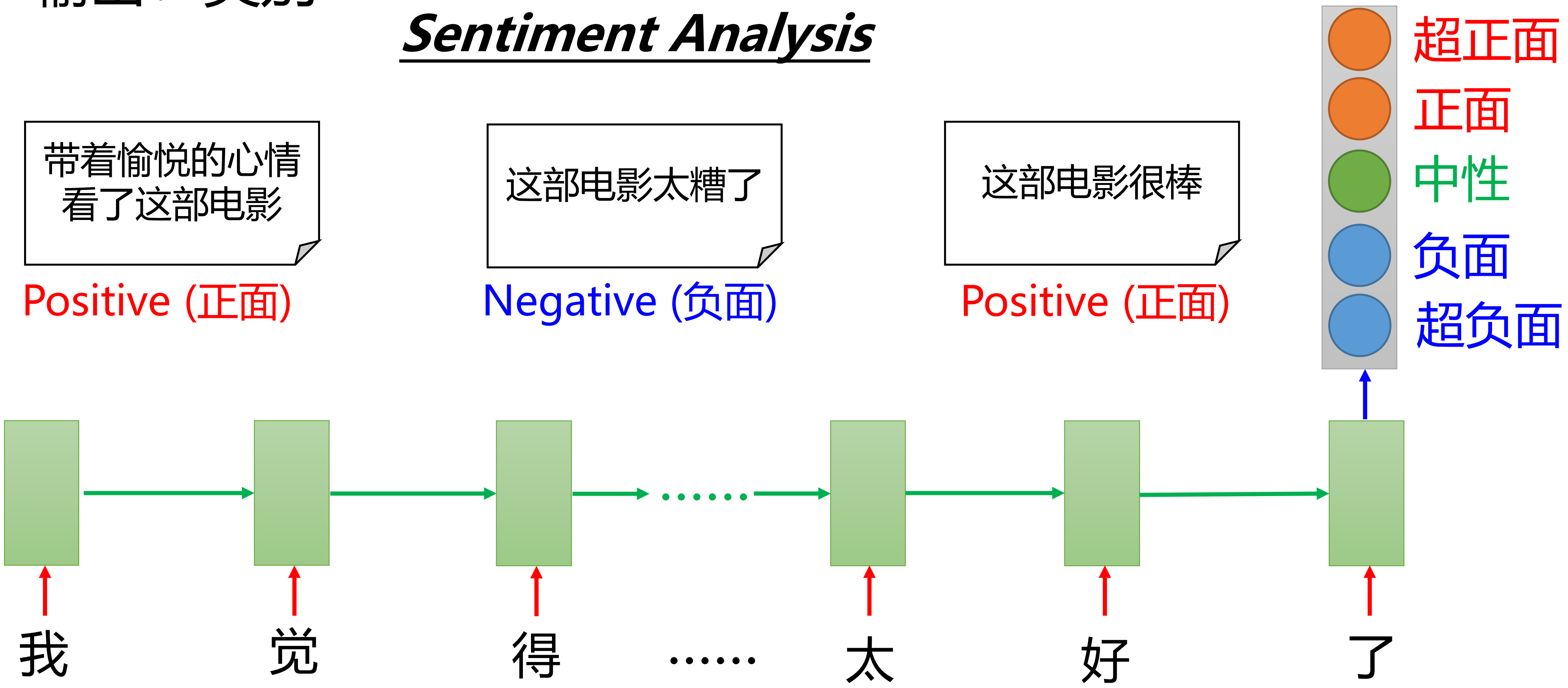

MAE变化




MAPE变化

# RNN的一些应用-序列到类别

- 输入：序列
- 输出：类别

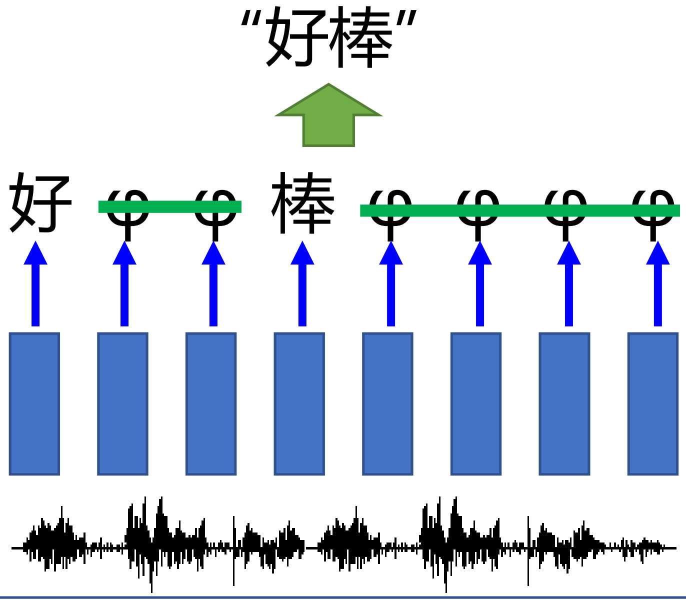


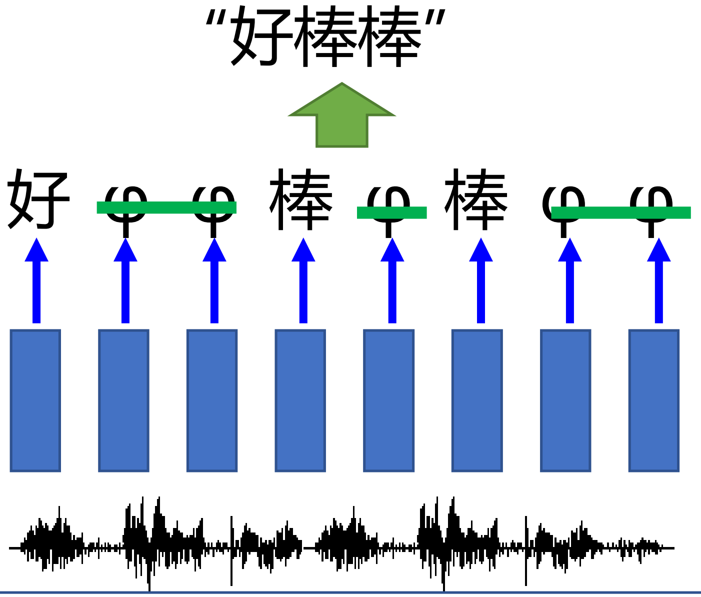
# RNN的一些应用-序列到序列

来源：李宏毅《1天搞懂深度学习》

语音识别

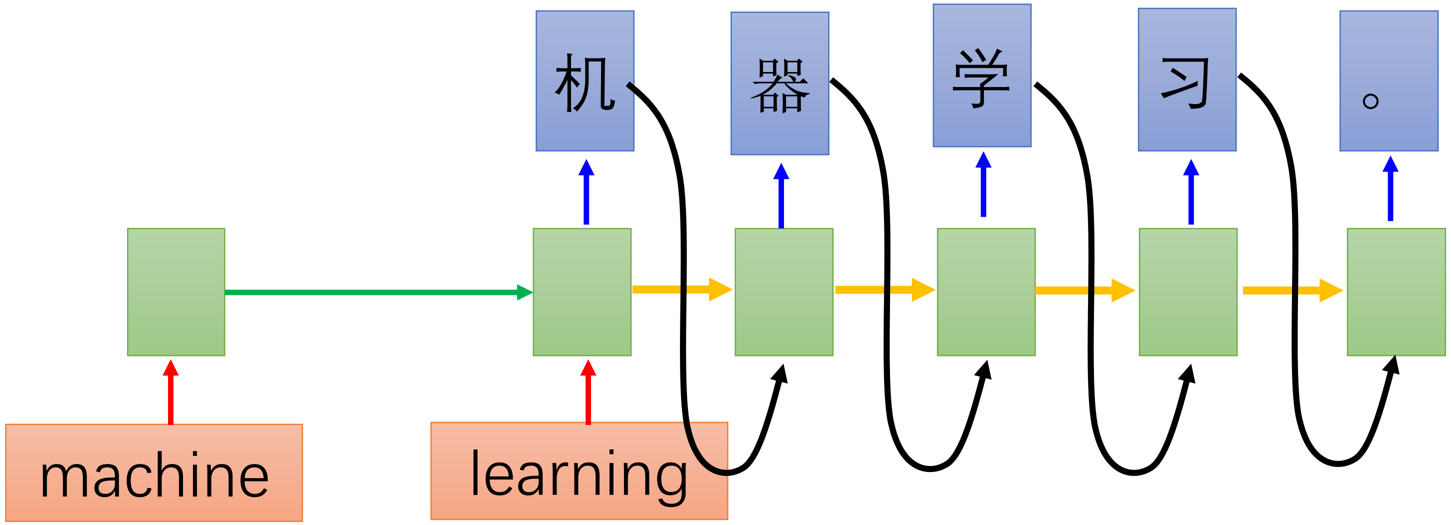
同步的序列到序列



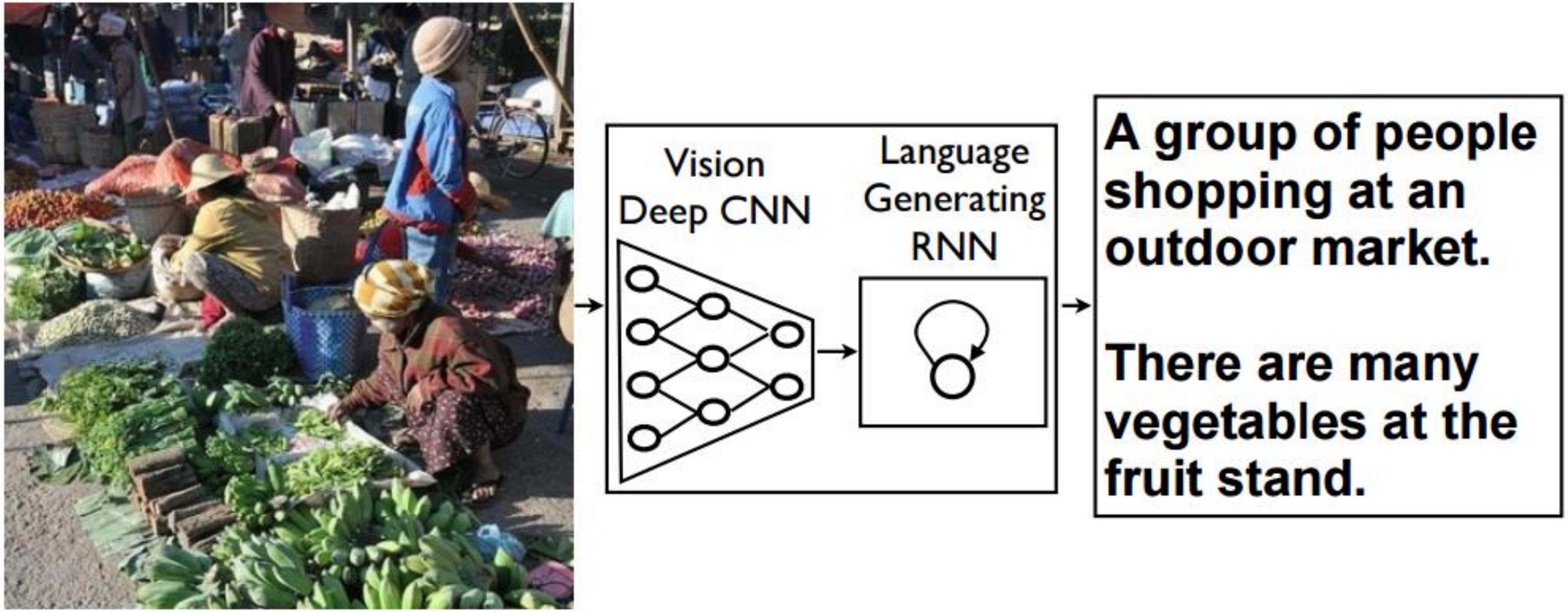




机器翻译

异步的序列到序列

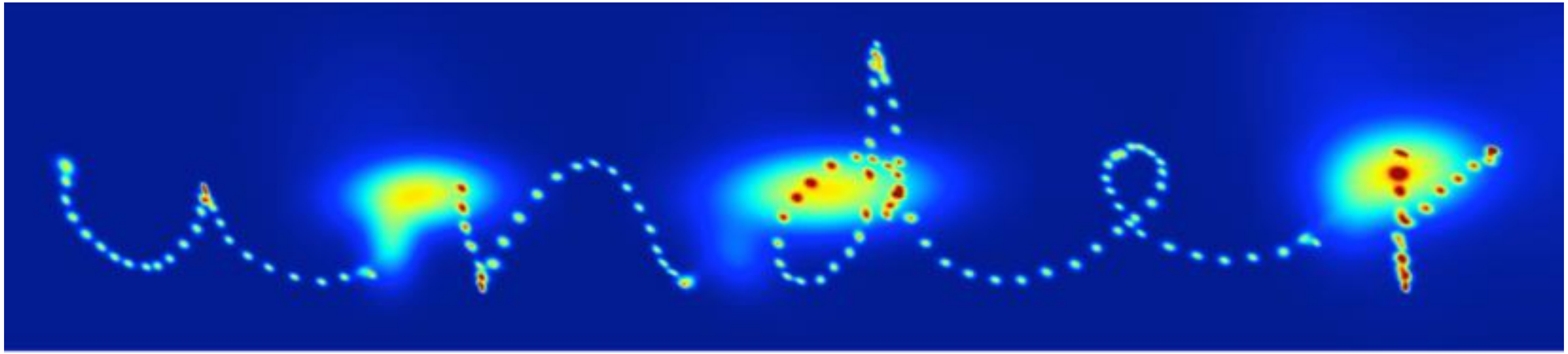


# RNN的一些应用 – 看图说话



# RNN的一些应用 – 写字、作诗

## 写字



## 作诗

| | |
|---|---|
| 白鹭窥鱼立, | 满怀风月一枝春, |
| Egrets stood, peeping fishes. | Budding branches are full of romance. |
| 青山照水开. | 未见梅花亦可人. |
| Water was still, reflecting mountains. | Plum blossoms are invisible but adorable. |
| 夜来风不动, | 不为东风无此客, |
| The wind went down by nightfall, | With the east wind comes Spring. |
| 明月见楼台. | 世间何处是前身. |
| as the moon came up by the tower. | Where on earth do I come from? |

# 实验要求

## 数据集介绍1

- 高速公路车流量数据
- PeMS是美国加利福尼亚州高速公路的实时车流量数据。
- 数据由铺设在道路上的检测线圈采集。
- 本实验中包含04和07两个地区的数据，分别储存在PEMS04.npz和PEMS07.npz两个文件中。
- 原始数据使用numpy二进制文件存储，可以使用numpy.load函数读取。
- 数据中的三个特征维度：车流量、拥挤程度和车速

| 列名 | 含义 |
|---|---|
| userId | 用户ID，不同用户的唯一标识符 |
| venueId | 地点ID，不同地点的唯一标识符 |
| venueCategoryId | 地点类别ID |
| venueCategory | 地点类别的名称 |
| latitude | 地点的纬度 |
| longitude | 地点的经度 |
| timezoneOffset | 所在时区相对于格林威治时间的时差(分钟) |
| utcTimestamp | 格林威治标准时间 |

# 实验要求

## 数据集介绍2

- 用户签到数据
- FourSquare是一个地点推荐网站，类似于国内的大众点评。
- 当用户到达某个地点时，可以通过手机App进行“签到”(check-in)。
- 将一个用户所有的签到记录按照时间顺序排序，就能得到此用户的行动轨迹
- 本实验中使用的数据包含纽约和东京两个城市的用户签到数据，分别存储在FS_NYC.csv和FS_TKY.csv两个文件中。

| 列名 | 含义 |
|---|---|
| userId | 用户ID，不同用户的唯一标识符 |
| venueId | 地点ID，不同地点的唯一标识符 |
| venueCategoryId | 地点类别ID |
| venueCategory | 地点类别的名称 |
| latitude | 地点的纬度 |
| longitude | 地点的经度 |
| timezoneOffset | 所在时区相对于格林威治时间的时差(分钟) |
| utcTimestamp | 格林威治标准时间 |

## 循环神经网络实验

- 手动实现循环神经网络RNN，并在至少一个数据集上进行实验，从训练时间、预测精度、Loss变化等角度分析实验结果（最好使用图表展示）

- 使用torch.nn.rnn实现循环神经网络，并在至少一个数据集上进行实验，从训练时间、预测精度、Loss变化等角度分析实验结果（最好使用图表展示）

- 不同超参数的对比分析（包括hidden_size、batchsize、lr等）选其中至少1-2个进行分析