Handling sequences with PyTorch

INTERMEDIATE DEEP LEARNING WITH PYTORCH

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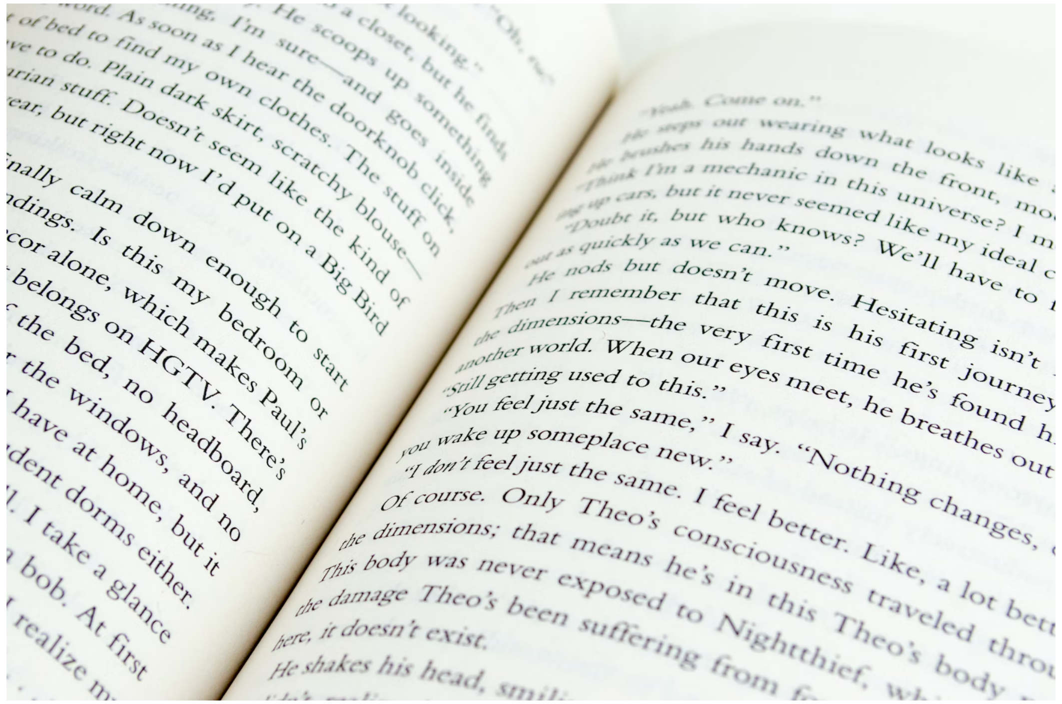
Sequential data

- Ordered in time or space
- Order of the data points contains dependencies between them
- Examples of sequential data:
  - Time series
  - Text
  - Audio waves



Electricity consumption prediction

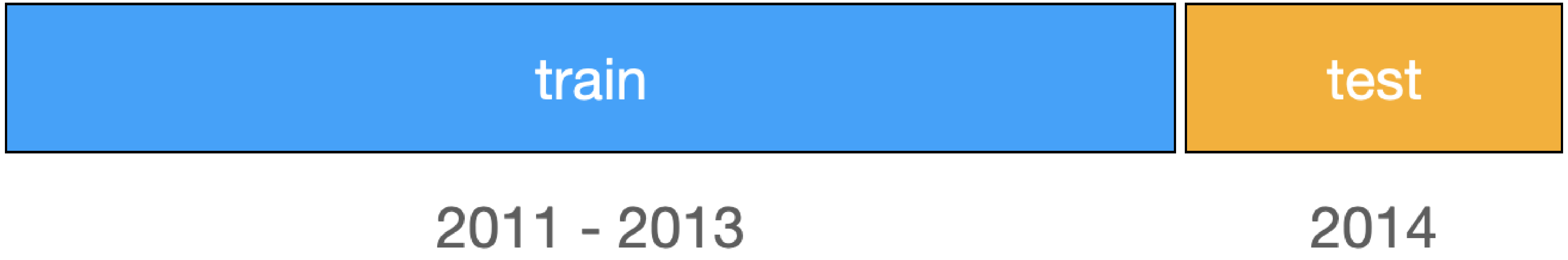
- Task: predict future electricity consumption based on past patterns
- Electricity consumption dataset:

```
                  timestamp  consumption
0       2011-01-01 00:15:00    -0.704319
1       2011-01-01 00:30:00    -0.704319
...                     ...          ...
140254  2014-12-31 23:45:00    -0.095751
140255  2015-01-01 00:00:00    -0.095751
```

[1] Trindade,Artur. (2015). ElectricityLoadDiagrams20112014. UCI Machine Learning Repository. https://doi.org/10.24432/C58C86.

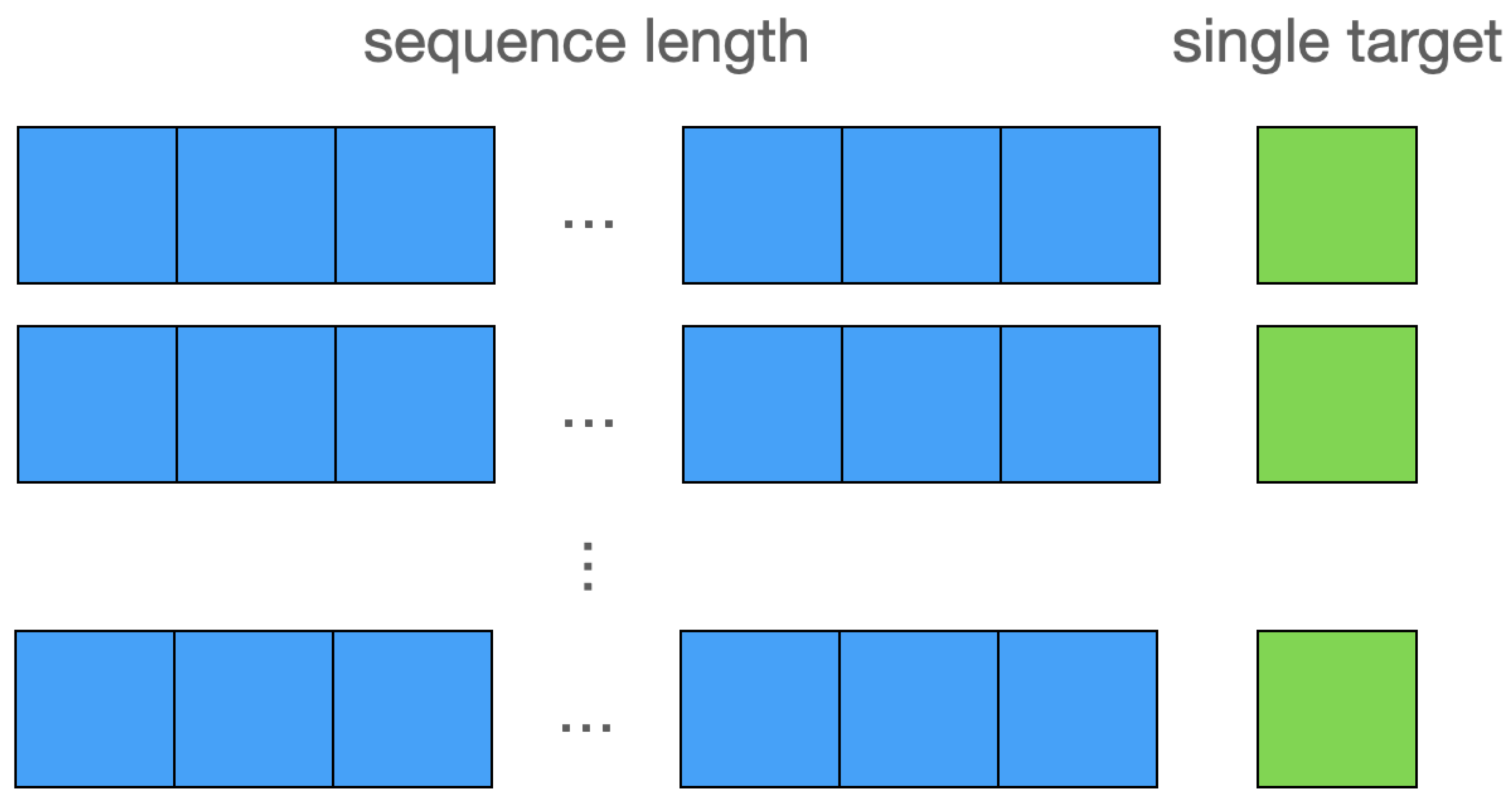
Train-test split

- No random splitting for time series!
- **Look-ahead bias:** model has info about the future
- Solution: split by time



Creating sequences

- Sequence length = number of data points in one training example
  - $24 \times 4 = 96$ -> consider last 24 hours
- Predict single next data point



Creating sequences in Python

```
import numpy as np

def create_sequences(df, seq_length):
    xs, ys = [], []
    for i in range(len(df) - seq_length):
        x = df.iloc[i:(i+seq_length), 1]
        y = df.iloc[i+seq_length, 1]
        xs.append(x)
        ys.append(y)
    return np.array(xs), np.array(ys)
```

- Take data and sequence length as inputs
- Initialize inputs and targets lists
- Iterate over data points
- Define inputs and target
- Append to pre-initialized lists
- Return inputs and targets as NumPy arrays

TensorDataset

Create training examples

```
X_train, y_train = create_sequences(train_data, seq_length)
print(X_train.shape, y_train.shape)
```

```
(34944, 96) (34944,)
```

Convert them to a Torch Dataset

```
from torch.utils.data import TensorDataset

dataset_train = TensorDataset(
    torch.from_numpy(X_train).float(),
    torch.from_numpy(y_train).float(),
)
```

Applicability to other sequential data

Same techniques are applicable to other sequences:

- Large Language Models
- Speech recognition

Let's practice!

INTERMEDIATE DEEP LEARNING WITH PYTORCH

Recurrent Neural Networks

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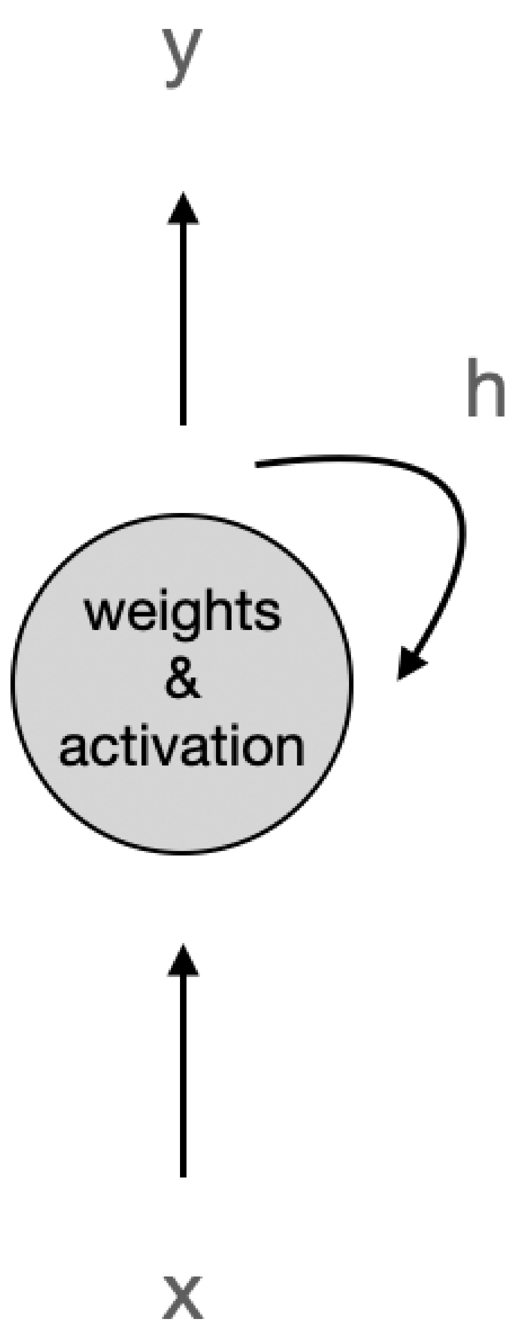
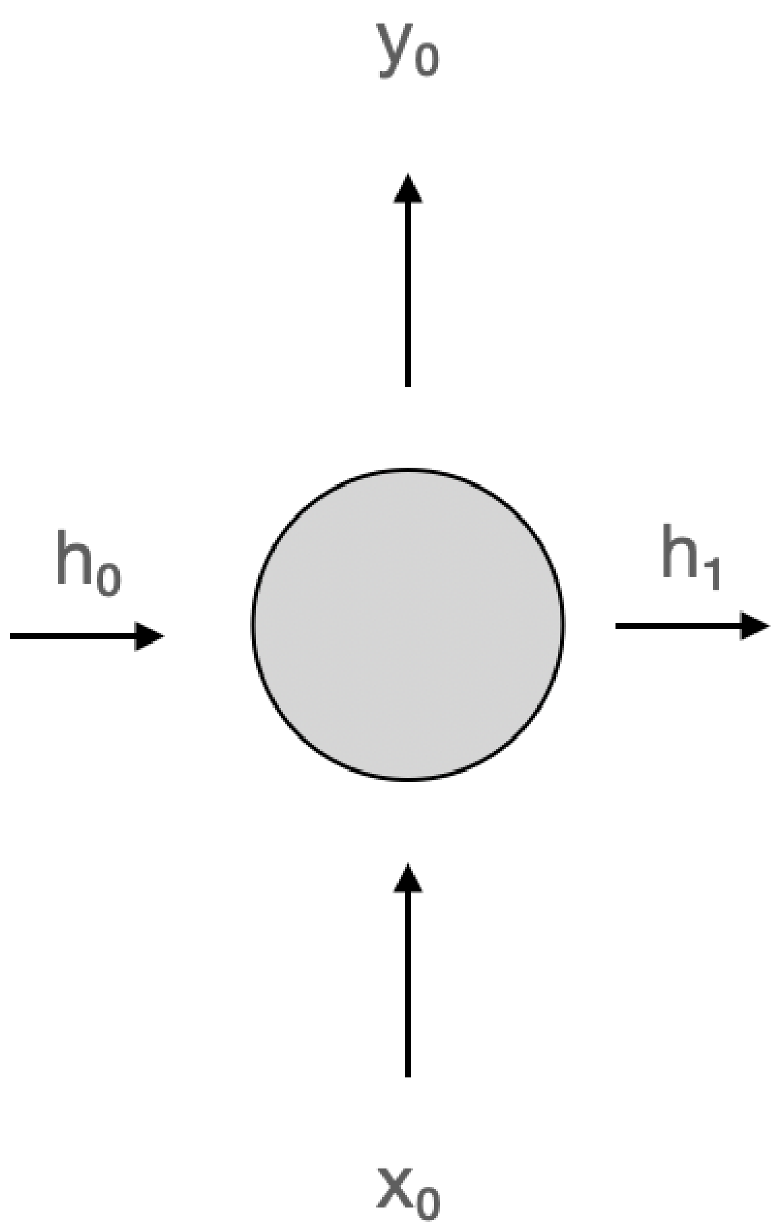
Recurrent neuron

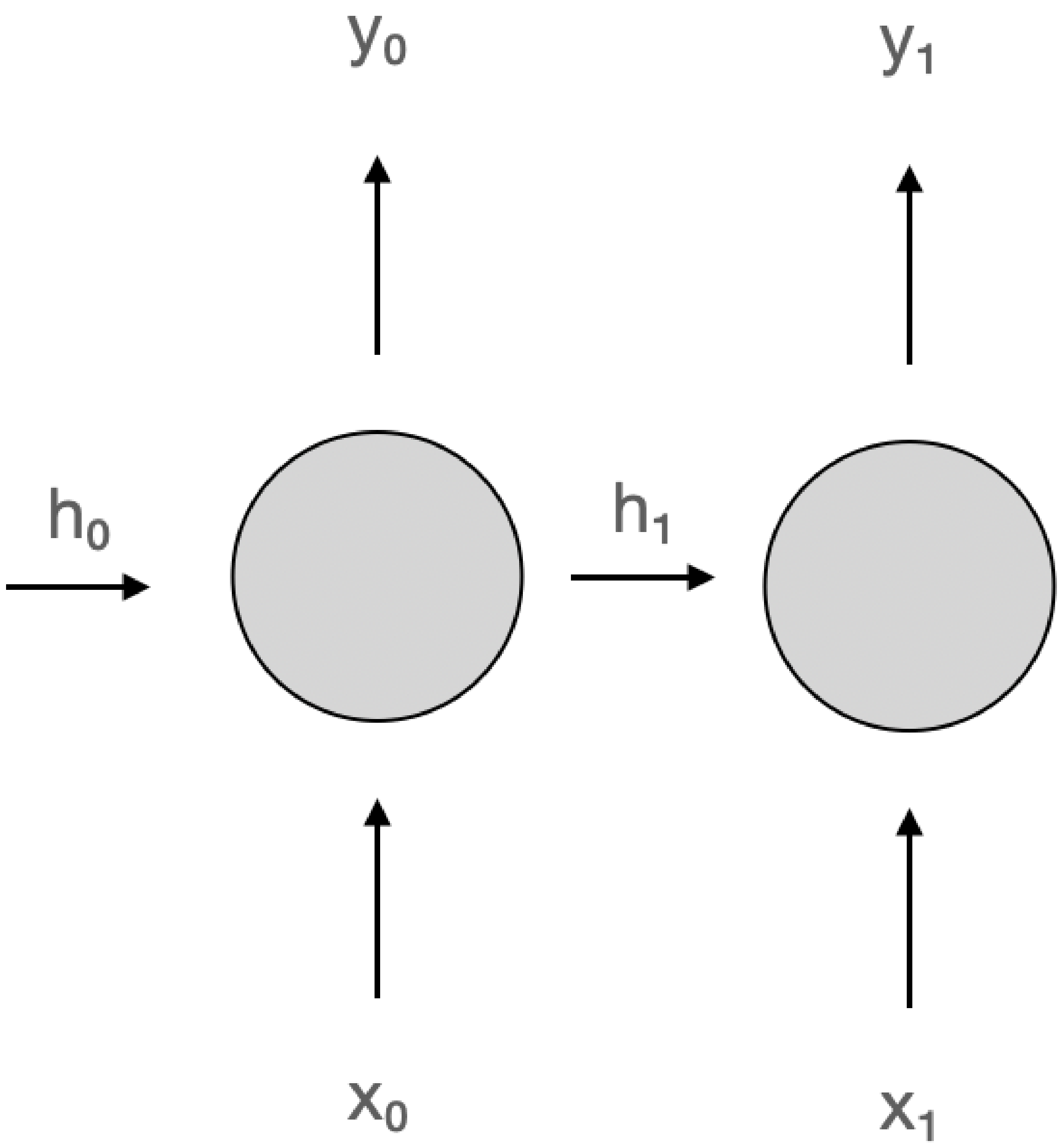
- Feed-forward networks
- **RNNs:** have connections pointing back
- Recurrent neuron:
  - Input `x`
  - Output `y`
  - Hidden state `h`
- In PyTorch: `nn.RNN()`



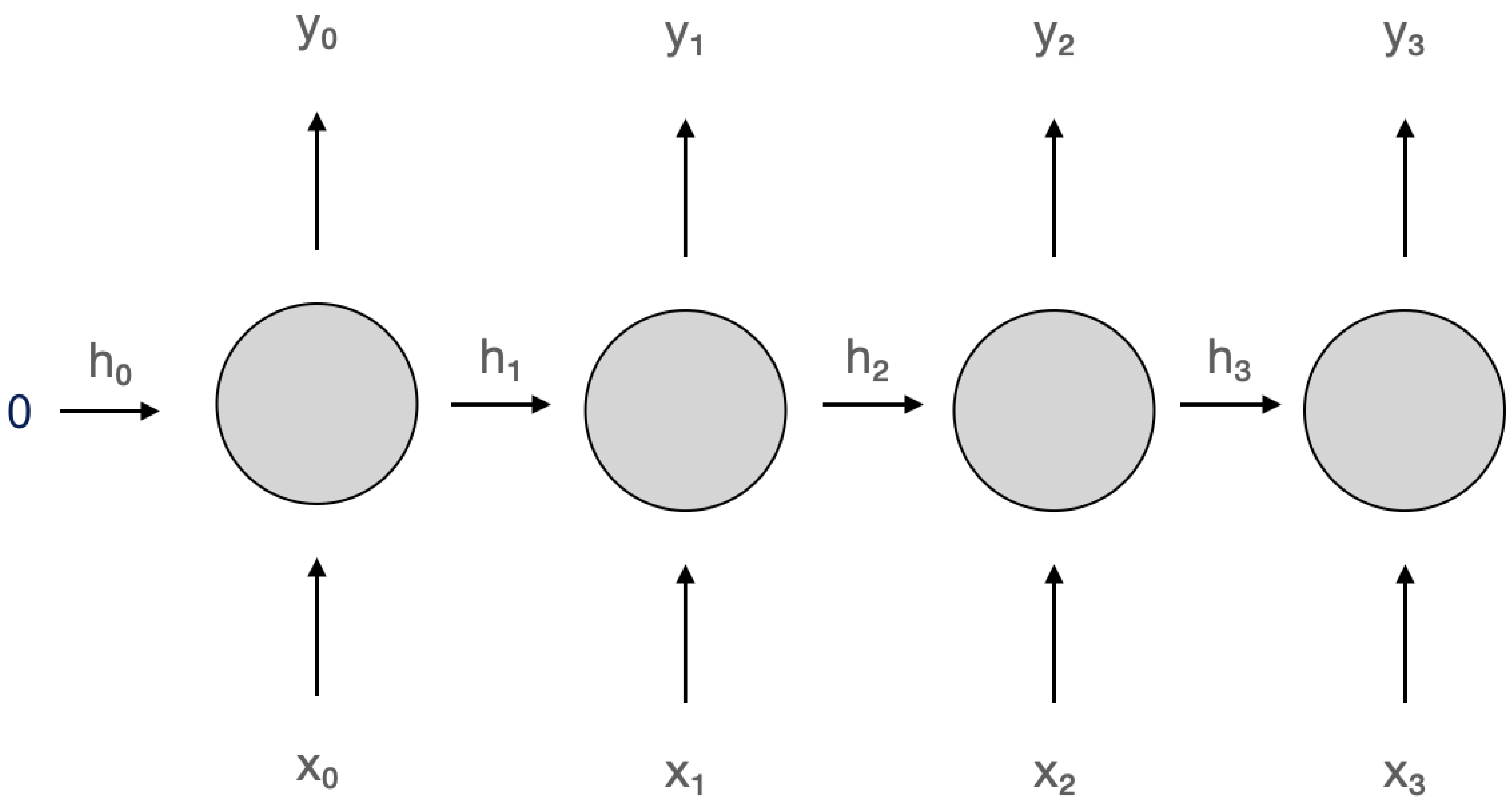
Unrolling recurrent neuron through time



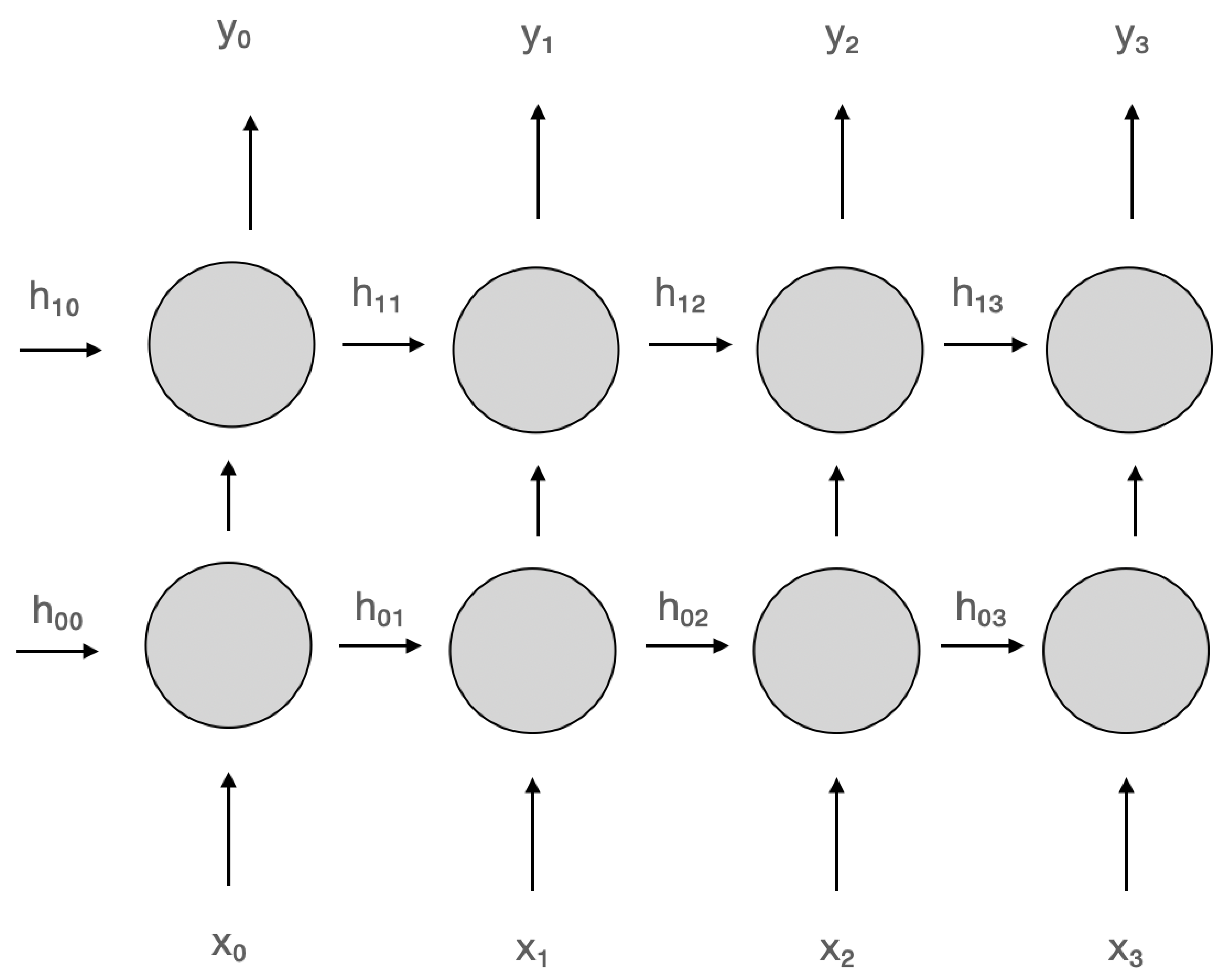
Unrolling recurrent neuron through time



Unrolling recurrent neuron through time

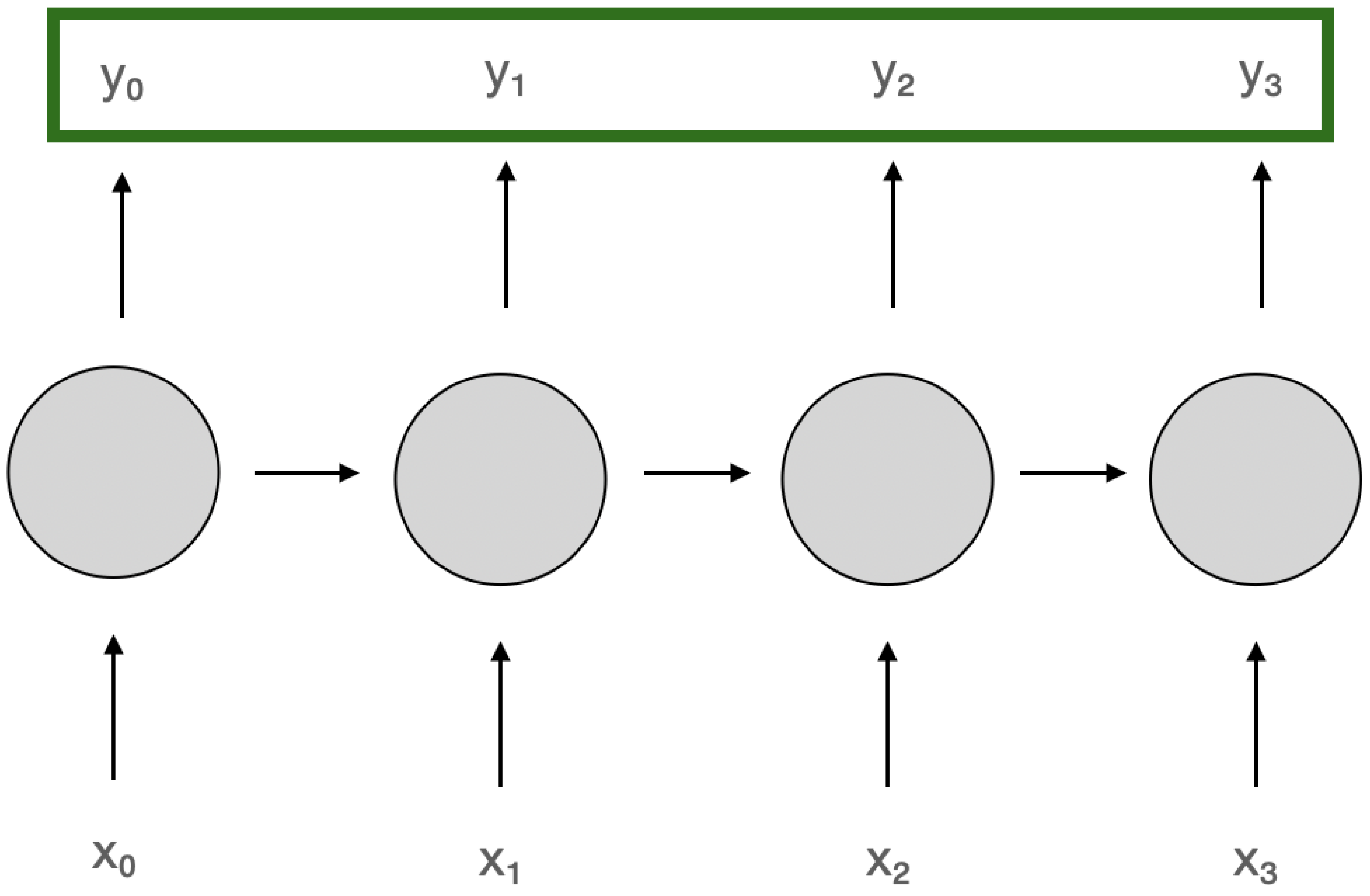


Deep RNNs



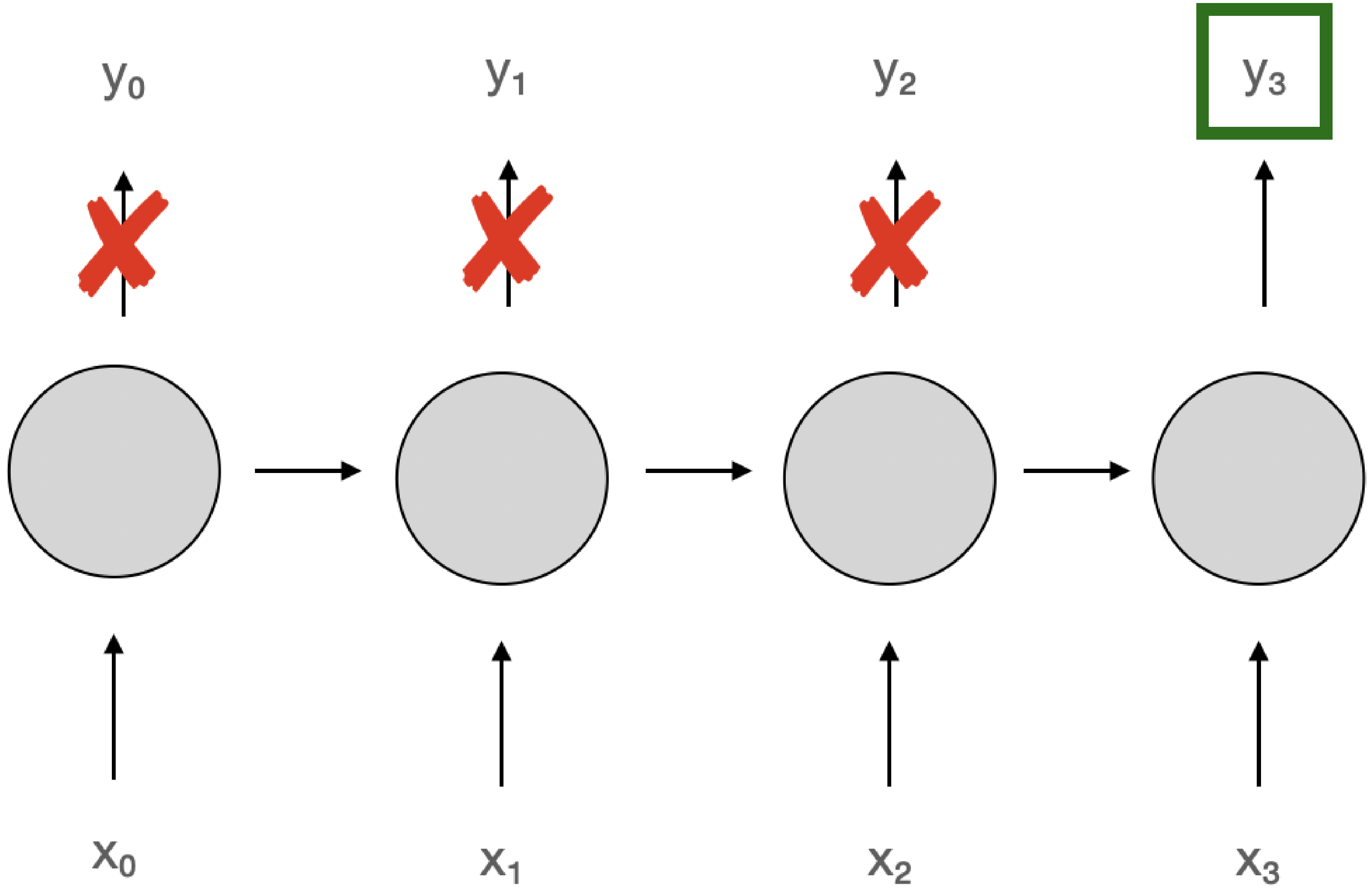
Sequence-to-sequence architecture

- Pass sequence as input, use the entire output sequence
- **Example:** Real-time speech recognition



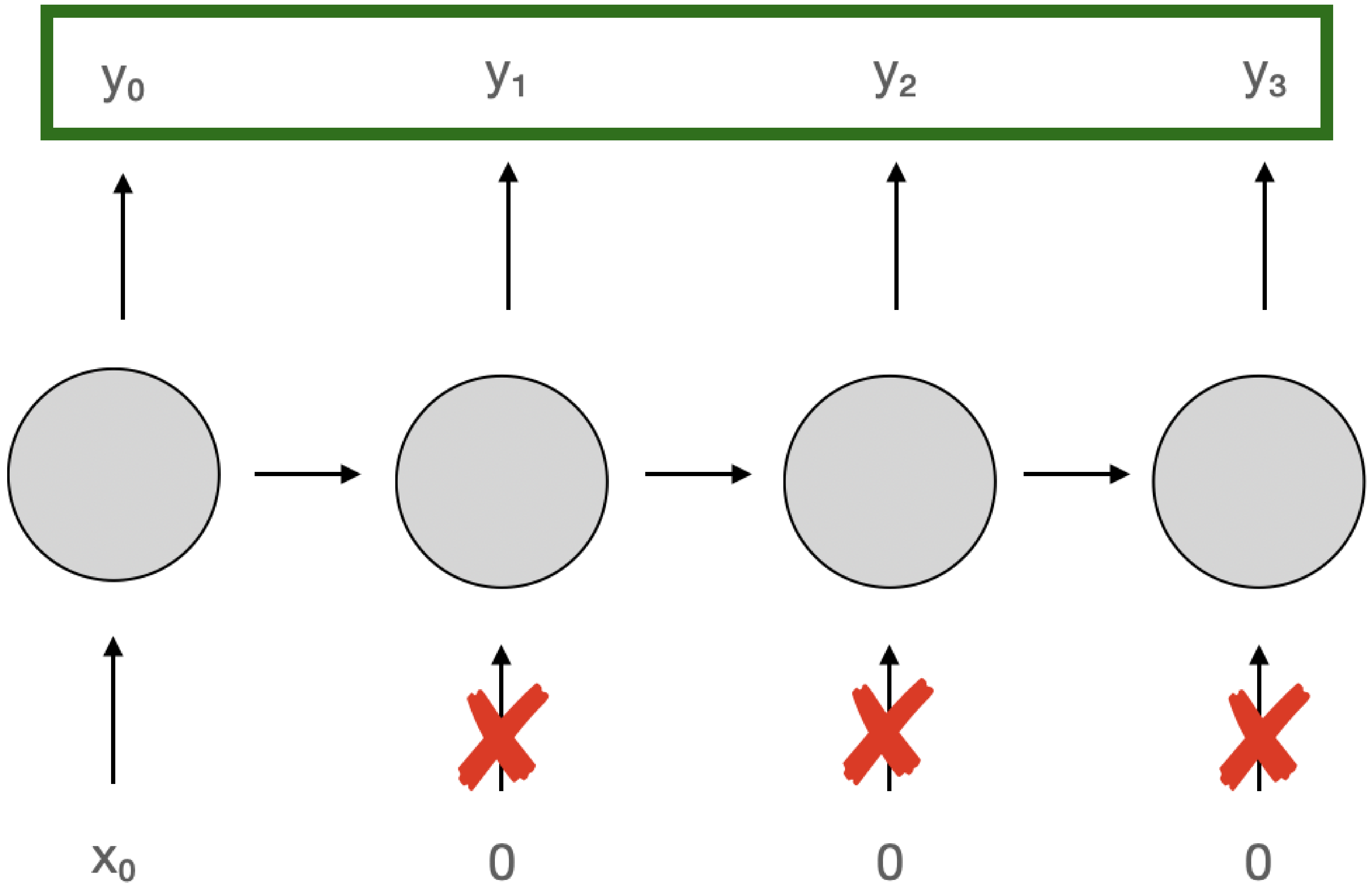
Sequence-to-vector architecture

- Pass sequence as input, use only the last output
- **Example:** Text topic classification



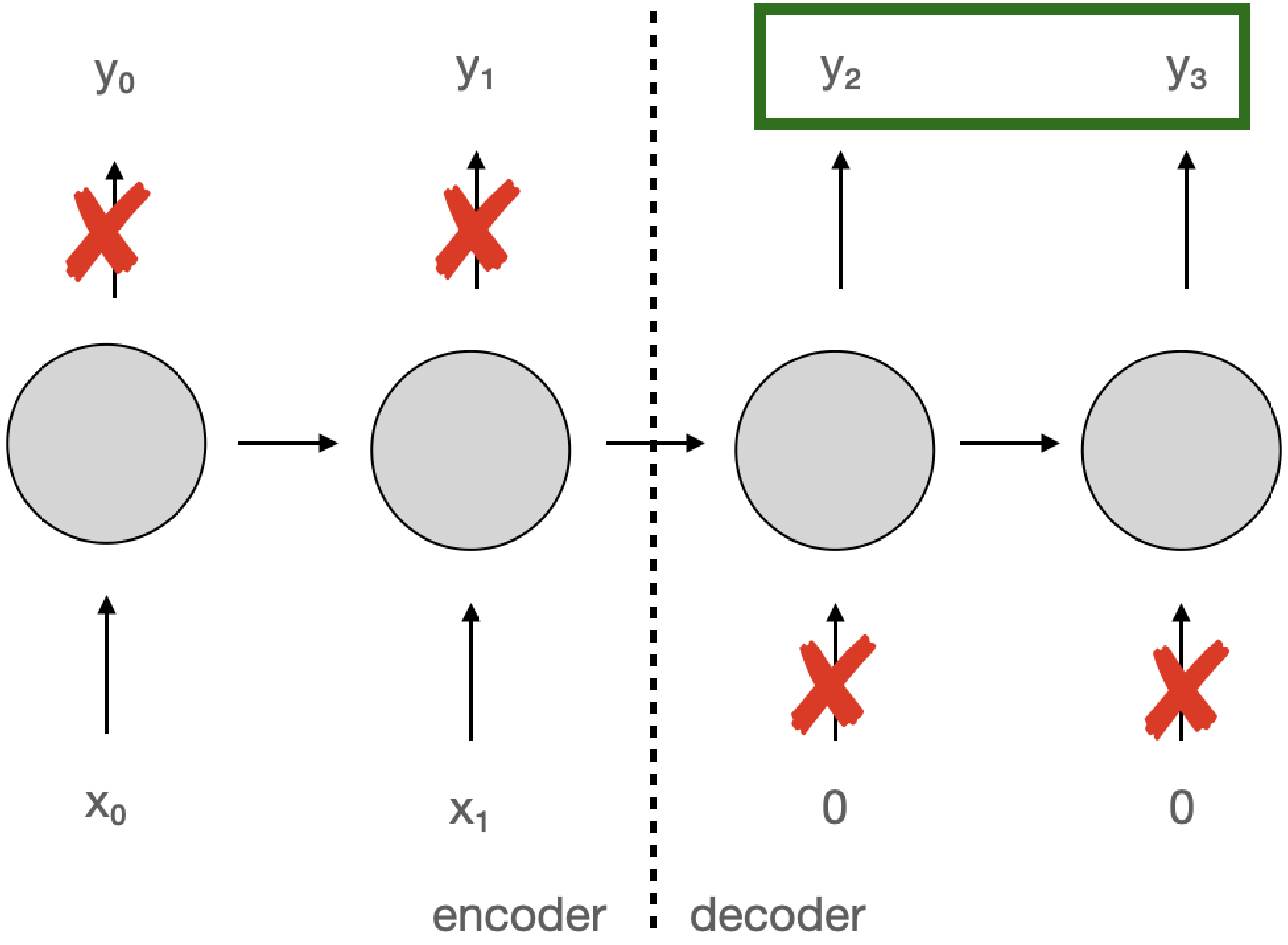
Vector-to-sequence architecture

- Pass single input, use the entire output sequence
- **Example:** Text generation



Encoder-decoder architecture

- Pass entire input sequence, only then start using output sequence
- **Example:** Machine translation



RNN in PyTorch

```
class Net(nn.Module):
    def __init__(self):
        super().__init__()
        self.rnn = nn.RNN(
            input_size=1,
            hidden_size=32,
            num_layers=2,
            batch_first=True,
        )
        self.fc = nn.Linear(32, 1)

    def forward(self, x):
        h0 = torch.zeros(2, x.size(0), 32)
        out, _ = self.rnn(x, h0)
        out = self.fc(out[:, -1, :])
        return out
```

- Define model class with `__init__` method
- Define recurrent layer, `self.rnn`
- Define linear layer, `fc`
- In `forward()`, initialize first hidden state to zeros
- Pass input and first hidden state through RNN layer
- Select last RNN's output and pass it through linear layer

Let's practice!

INTERMEDIATE DEEP LEARNING WITH PYTORCH

LSTM and GRU cells

INTERMEDIATE DEEP LEARNING WITH PYTORCH

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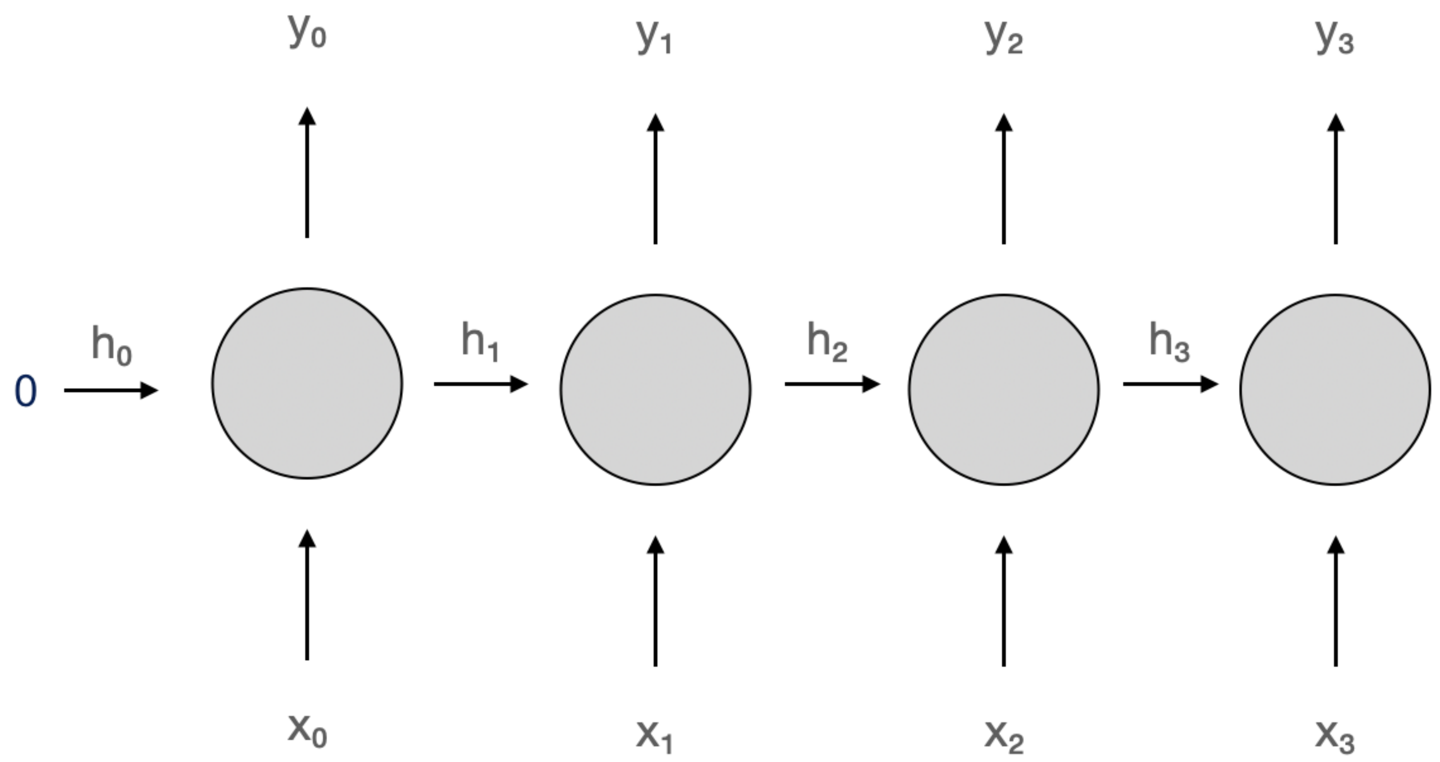
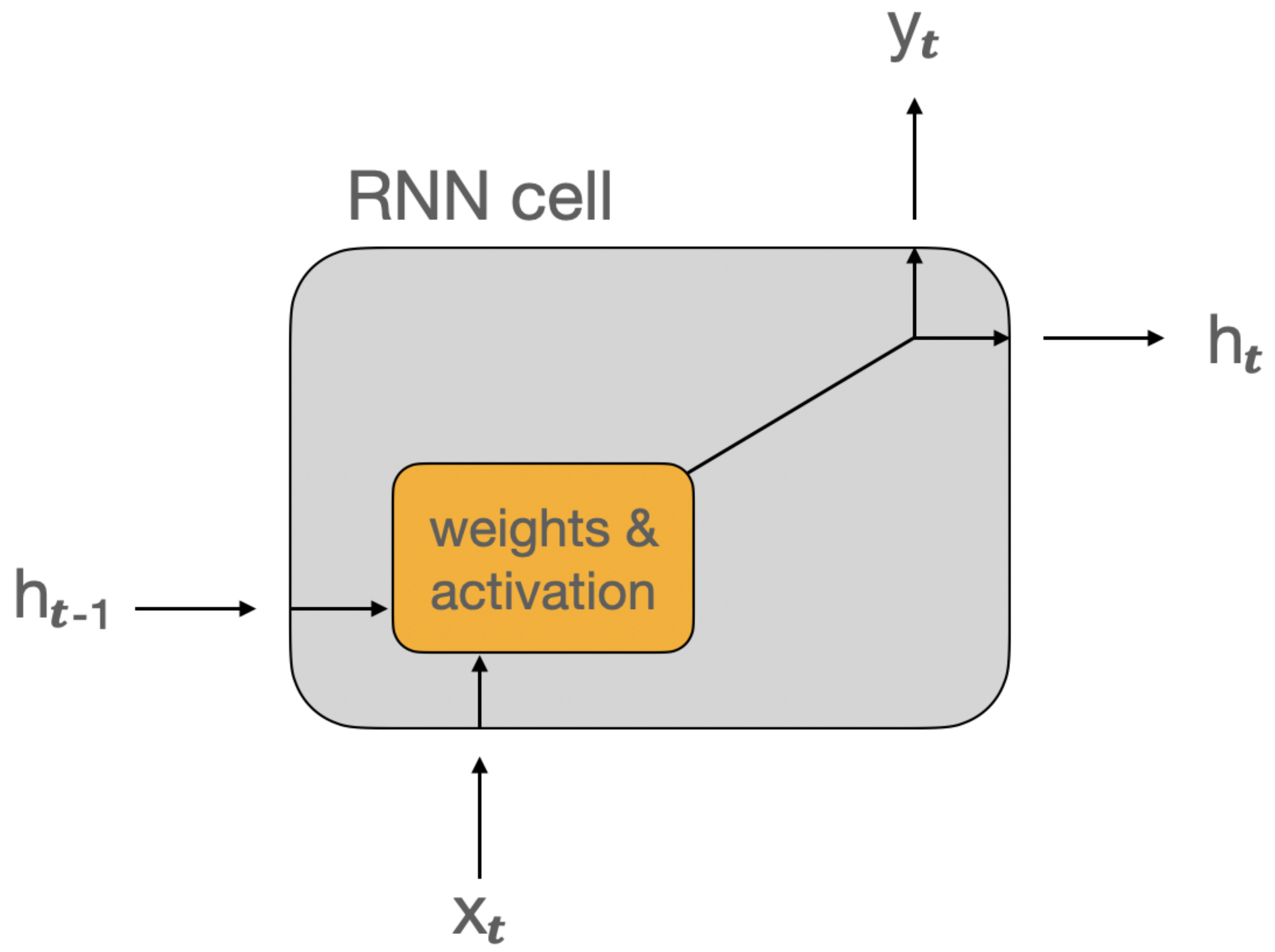
Short-term memory problem

- RNN cells maintain memory via hidden state
- This memory is very short-term
- Two more powerful cells solve the problem:
  - LSTM (Long Short-Term Memory) cell
  - GRU (Gated Recurrent Unit) cell

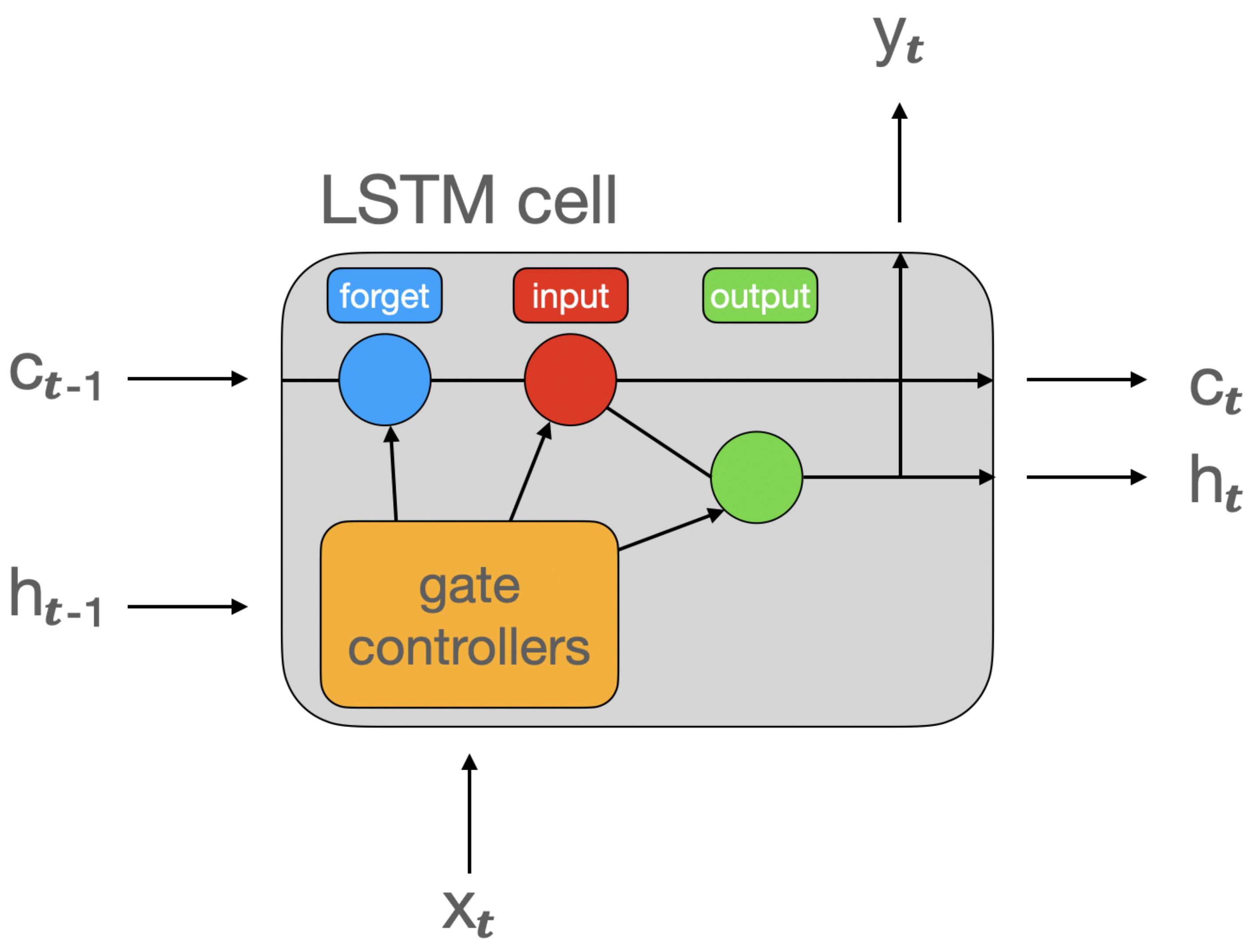


RNN cell



- Two inputs:
  - current input data `x`
  - previous hidden state `h`
- Two outputs:
  - current output `y`
  - next hidden state `h`

LSTM cell



- Three inputs and outputs (two hidden states):
  - `h` : short-term state
  - `c` : long-term state
- Three "gates":
  - **Forget gate:** what to remove from long-term memory
  - **Input gate:** what to save to long-term memory
  - **Output gate:** what to return at the current time step
- Outputs `h` and `y` are the same

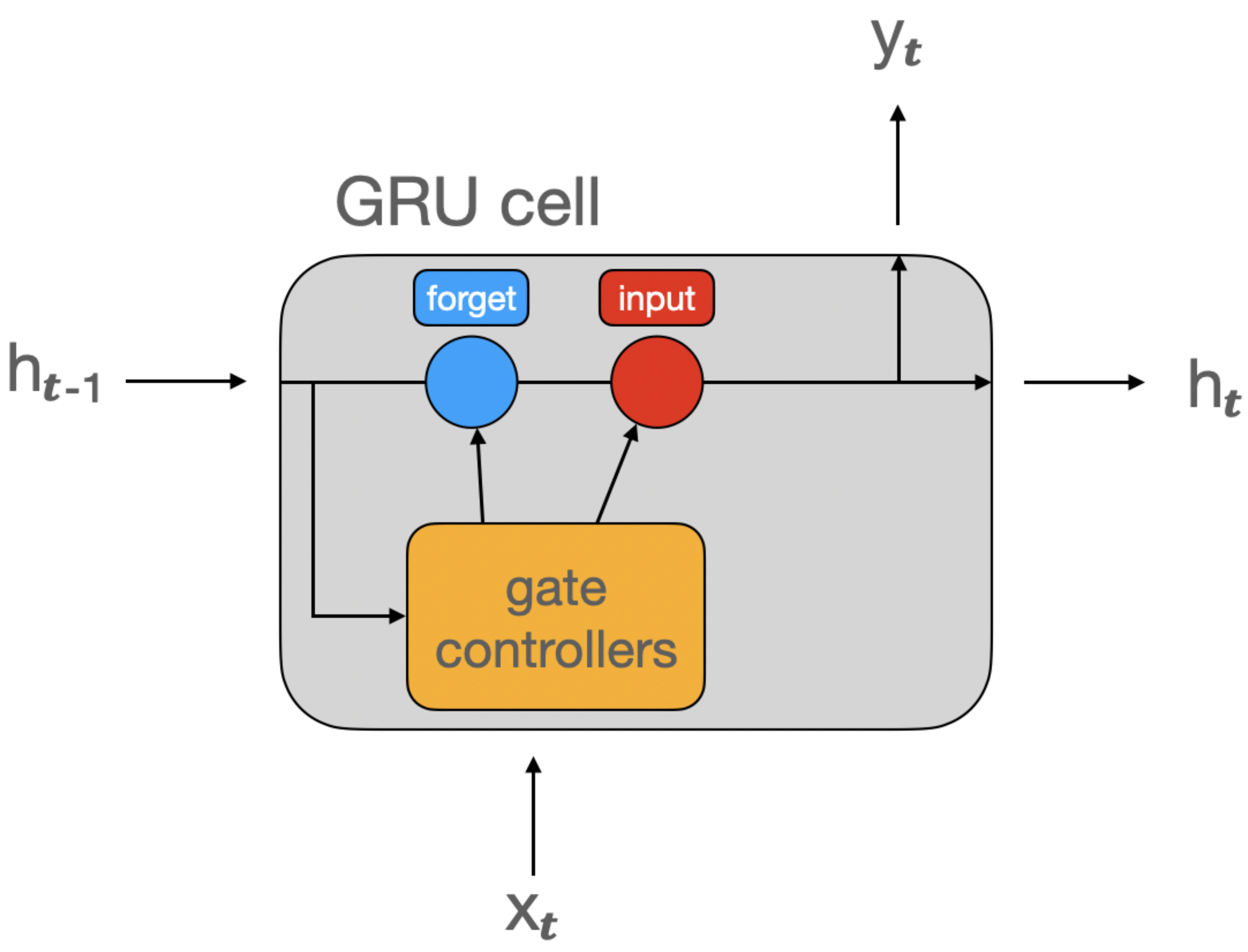
LSTM in PyTorch

```
class Net(nn.Module):
    def __init__(self, input_size):
        super().__init__()
        self.lstm = nn.LSTM(
            input_size=1,
            hidden_size=32,
            num_layers=2,
            batch_first=True,
        )
        self.fc = nn.Linear(32, 1)

    def forward(self, x):
        h0 = torch.zeros(2, x.size(0), 32)
        c0 = torch.zeros(2, x.size(0), 32)
        out, _ = self.lstm(x, (h0, c0))
        out = self.fc(out[:, -1, :])
        return out
```

- `__init__()` :
  - Replace `nn.RNN` with `nn.LSTM`
- `forward()` :
  - Add another hidden state `c`
  - Initialize `c` and `h` with zeros
  - Pass both hidden states to `lstm` layer

GRU cell



- Simplified version of LSTM cell
- Just one hidden state
- No output gate

GRU in PyTorch

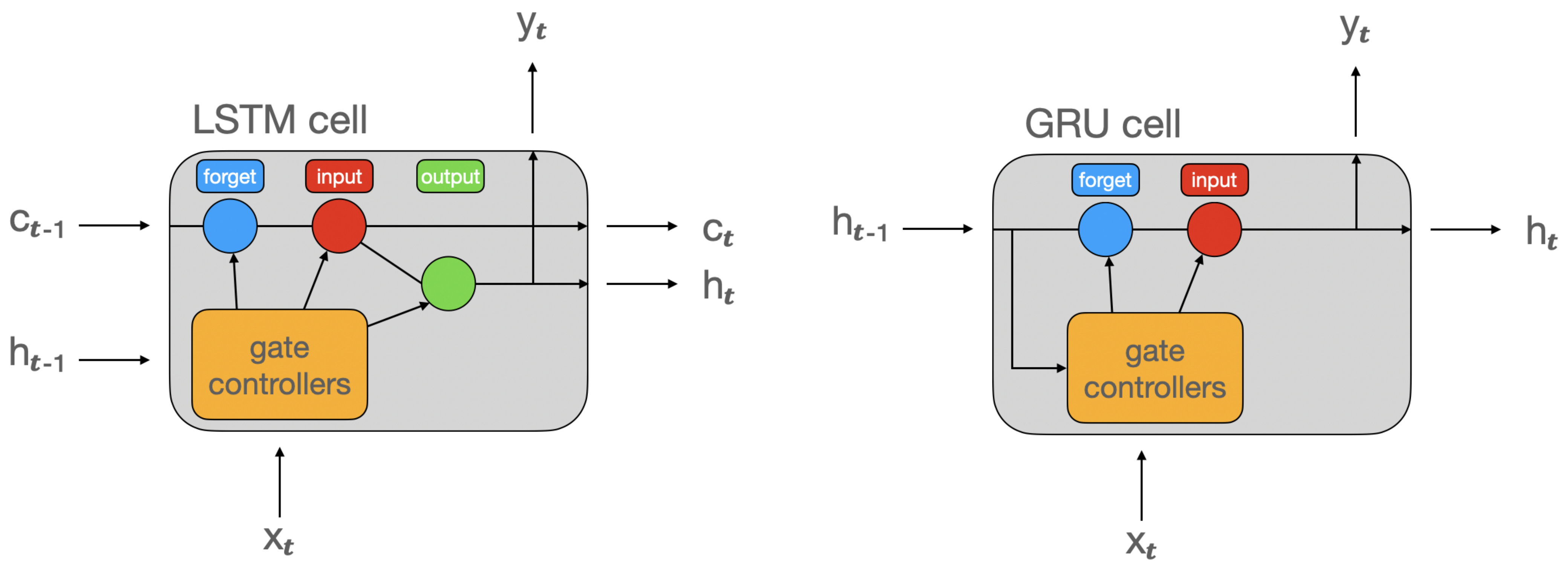
```
class Net(nn.Module):
    def __init__(self, input_size):
        super().__init__()
        self.gru = nn.GRU(
            input_size=1,
            hidden_size=32,
            num_layers=2,
            batch_first=True,
        )
        self.fc = nn.Linear(32, 1)

    def forward(self, x):
        h0 = torch.zeros(2, x.size(0), 32)
        out, _ = self.gru(x, h0)
        out = self.fc(out[:, -1, :])
        return out
```

- `__init__()`:
    - Replace `nn.RNN` with `nn.GRU`
- `forward()`:
    - Use the `gru` layer

Should I use RNN, LSTM, or GRU?

- RNN is not used much anymore
- GRU is simpler than LSTM = less computation
- Relative performance varies per use-case
- Try both and compare



Let's practice!

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Training and evaluating RNNs

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Mean Squared Error Loss

- Error:

$$prediction - target$$

- Squared Error:

$$(prediction - target)^2$$

- Mean Squared Error:

$$avg[(prediction - target)^2]$$

Squaring the error:

- Ensures positive and negative errors don't cancel out
- Penalizes large errors more
- In PyTorch:

```
criterion = nn.MSELoss()
```

Expanding tensors

- Recurrent layers expect input shape `(batch_size, seq_length, num_features)`
- We got `(batch_size, seq_length)`
- We must add one dimension at the end

```
for seqs, labels in dataloader_train:
    print(seqs.shape)
```

```
torch.Size([32, 96])
```

```
seqs = seqs.view(32, 96, 1)
print(seqs.shape)
```

```
torch.Size([32, 96, 1])
```

Squeezing tensors

- In evaluation loop, we need to revert the reshaping done in the training loop
- Labels are of shape `(batch_size)`

```
for seqs, labels in test_loader:
  print(labels.shape)
```

```
torch.Size([32])
```

- Model outputs are `(batch_size, 1)`

```
out = net(seqs)
```

```
torch.Size([32, 1])
```

- Shapes of model outputs and labels must match for the loss function
- We can drop the last dimension from model outputs

```
out = net(seqs).squeeze()
```

```
torch.Size([32])
```

Training loop

```
net = Net()
criterion = nn.MSELoss()
optimizer = optim.Adam(
  net.parameters(), lr=0.001
)

for epoch in range(num_epochs):
    for seqs, labels in dataloader_train:
        seqs = seqs.view(32, 96, 1)
        outputs = net(seqs)
        loss = criterion(outputs, labels)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()
```

- Instantiate model, define loss & optimizer
- Iterate over epochs and data batches
- Reshape input sequence
- The rest: as usual

Evaluation loop

```
mse = torchmetrics.MeanSquaredError()

net.eval()
with torch.no_grad():
    for seqs, labels in test_loader:
        seqs = seqs.view(32, 96, 1)
        outputs = net(seqs).squeeze()
        mse(outputs, labels)

print(f"Test MSE: {mse.compute()}")
```

```
Test MSE: 0.13292162120342255
```

- Set up MSE metric
- Iterate through test data with no gradients
- Reshape model inputs
- Squeeze model outputs
- Update the metric
- Compute final metric value

LSTM vs. GRU

- LSTM:

```
Test MSE: 0.13292162120342255
```

- GRU:

```
Test MSE: 0.12187089771032333
```

- GRU preferred: same or better results with less processing power

Let's practice!

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