# Chapter 11: Sequence Models: RNN → Attention → Transformer

**Learning Objectives**

By the end of this chapter, you will be able to:

- **Understand** the evolution of sequence models from RNNs to Transformers
- **Master** the architectures and training methods for recurrent networks, attention mechanisms, and transformer models
- **Connect** sequence model operations to temporal processing in the brain
- **Implement** key sequence modeling architectures for various tasks
- **Compare** different approaches to handling sequential data
- **Apply** sequence models to healthcare time series data for clinical applications
- **Address** challenges unique to healthcare sequences such as irregularity and missing data

# 11.1 Recurrent Neural Networks

Recurrent Neural Networks (RNNs) are specialized neural networks designed to process sequential data by maintaining an internal state (memory) that captures information about previous inputs. Unlike feedforward networks, RNNs have connections that loop back on themselves, allowing them to persist information across time steps.

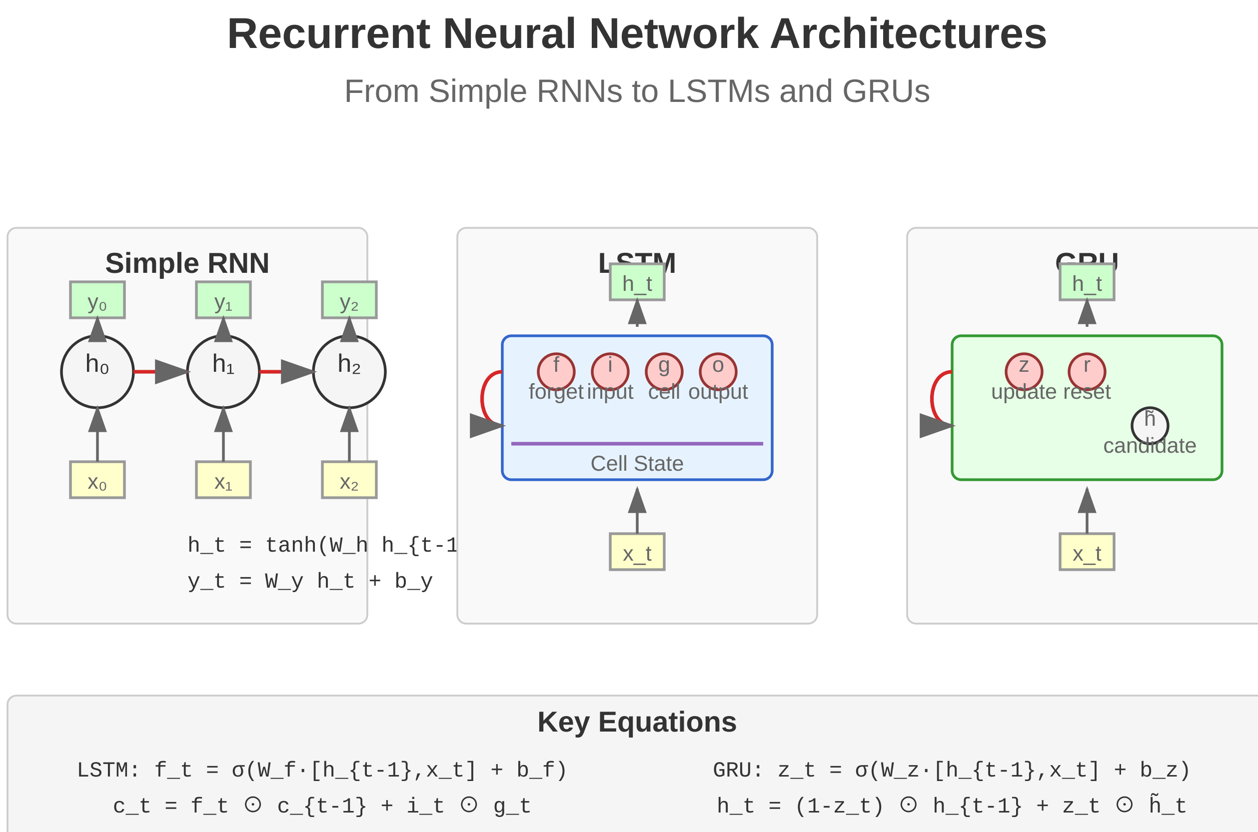


*Figure 11.1: Recurrent Neural Network architectures, showing the basic RNN, LSTM, and GRU cells with their internal structures.*

## 11.1.1 Vanilla RNNs

The simplest RNN architecture maintains a hidden state that is updated at each time step:

```python
import numpy as np
import torch
import torch.nn as nn
import torch.optim as optim
import matplotlib.pyplot as plt

class SimpleRNN(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        """
        A basic RNN implementation.

        Args:
            input_size: Size of input features at each time step
            hidden_size: Size of hidden state
            output_size: Size of output at each time step
        """
        super(SimpleRNN, self).__init__()

        self.hidden_size = hidden_size

        # Input to hidden weights
        self.i2h = nn.Linear(input_size + hidden_size, hidden_size)

        # Hidden to output weights
        self.h2o = nn.Linear(hidden_size, output_size)

        # Activation function
        self.tanh = nn.Tanh()
        self.softmax = nn.LogSoftmax(dim=1)

    def forward(self, input, hidden):
        """Forward pass through the RNN for a single time step."""
        # Combine input and hidden state
        combined = torch.cat((input, hidden), 1)

        # Calculate new hidden state
        hidden = self.tanh(self.i2h(combined))

        # Calculate output
        output = self.softmax(self.h2o(hidden))

        return output, hidden

    def init_hidden(self, batch_size=1):
        """Initialize the hidden state with zeros."""
        return torch.zeros(batch_size, self.hidden_size)

    def process_sequence(self, sequence):
        """Process a sequence of inputs and return all outputs and final hidden stat
        # Initialize hidden state
        hidden = self.init_hidden(sequence.size(0))

        # Storage for outputs at each time step
```

```
        outputs = []

        # Process each time step
        for i in range(sequence.size(1)):
            output, hidden = self.forward(sequence[:, i, :], hidden)
            outputs.append(output)

        # Stack outputs along time dimension
        outputs = torch.stack(outputs, dim=1)

        return outputs, hidden

# Example usage on a toy sequence problem
def simple_rnn_example():
    """Demonstrate a simple RNN on a toy sequence task."""
    # Create sample data: learning to recognize sequences ending with [1, 2, 3]
    def generate_sample(length=10):
        # Generate random sequence of 0-4
        sequence = torch.randint(0, 5, (length,)).long()

        # Check if the last three elements are [1, 2, 3]
        target = 1 if torch.all(sequence[-3:] == torch.tensor([1, 2, 3])) else 0

        # One-hot encode the sequence
        one_hot_sequence = torch.nn.functional.one_hot(sequence, num_classes=5).floa

        return one_hot_sequence, target

    # Generate training data
    train_data = [generate_sample() for _ in range(1000)]

    # Define model
    input_size = 5  # One-hot encoding of 5 possible values
    hidden_size = 10
    output_size = 2  # Binary classification
    model = SimpleRNN(input_size, hidden_size, output_size)

    # Loss function and optimizer
    criterion = nn.NLLLoss()
    optimizer = optim.Adam(model.parameters(), lr=0.01)

    # Training loop
    n_epochs = 20
    batch_size = 32
    losses = []
    accuracies = []

    for epoch in range(n_epochs):
        model.train()
        epoch_loss = 0
        correct = 0

        for i in range(0, len(train_data), batch_size):
            # Get batch
```

```
            batch = train_data[i:i+batch_size]
            sequences = [item[0] for item in batch]
            targets = torch.tensor([item[1] for item in batch])

            # Pad sequences to the same length
            max_len = max(seq.size(0) for seq in sequences)
            padded_sequences = torch.zeros(len(sequences), max_len, input_size)
            for j, seq in enumerate(sequences):
                padded_sequences[j, :seq.size(0), :] = seq

            # Forward pass
            optimizer.zero_grad()
            hidden = model.init_hidden(len(sequences))

            outputs = []
            for t in range(max_len):
                output, hidden = model(padded_sequences[:, t, :], hidden)
                outputs.append(output)

            # We only care about the output at the last time step
            final_output = outputs[-1]

            # Calculate loss
            loss = criterion(final_output, targets)
            epoch_loss += loss.item()

            # Backward pass
            loss.backward()
            optimizer.step()

            # Calculate accuracy
            pred = final_output.argmax(dim=1)
            correct += (pred == targets).sum().item()

        # Record metrics
        losses.append(epoch_loss / len(train_data))
        accuracies.append(correct / len(train_data))

        print(f'Epoch {epoch+1}, Loss: {losses[-1]:.4f}, Accuracy: {accuracies[-1]:.

    # Plot training progress
    plt.figure(figsize=(12, 5))

    plt.subplot(1, 2, 1)
    plt.plot(losses)
    plt.title('Training Loss')
    plt.xlabel('Epoch')
    plt.ylabel('Loss')
    plt.grid(True)

    plt.subplot(1, 2, 2)
    plt.plot(accuracies)
    plt.title('Training Accuracy')
    plt.xlabel('Epoch')
```

```
    plt.ylabel('Accuracy')
    plt.grid(True)

    plt.tight_layout()
    return plt
```

The RNN updates its hidden state at each time step according to:

$$h_t = \tanh(W_{hh}h_{t-1} + W_{xh}x_t + b_h)$$

Where:

- $h_t$ is the hidden state at time $t$
- $x_t$ is the input at time $t$
- $W_{hh}$ is the hidden-to-hidden weights
- $W_{xh}$ is the input-to-hidden weights
- $b_h$ is the hidden bias

The output at each time step is typically computed as:

$$y_t = W_{hy}h_t + b_y$$

**Biological Parallel**: RNNs resemble recurrent circuits in the brain where neural activity can persist and influence future processing. The prefrontal cortex maintains information over time through recurrent connections, similar to how RNNs maintain a hidden state.

## 11.1.2 The Vanishing/Exploding Gradient Problem

Standard RNNs struggle with long-term dependencies due to the vanishing or exploding gradient problem. When backpropagating through many time steps, gradients can either:

1. Vanish - becoming extremely small, making learning long-range dependencies impossible
2. Explode - becoming extremely large, causing unstable training

```python
def demonstrate_gradient_problems():
    """Visualize the vanishing gradient problem in RNNs."""
    # Number of time steps
    T = 100

    # Different values for recurrent weights
    recurrent_weights = [0.5, 0.9, 1.0, 1.1, 1.5]

    plt.figure(figsize=(10, 6))

    for weight in recurrent_weights:
        # Calculate gradient scaling factor at each time step
        # For simplicity, we model how the gradient scales based on the recurrent we
        gradient_scale = [weight ** t for t in range(T)]

        # Plot on log scale
        plt.semilogy(gradient_scale, label=f'Weight = {weight}')

    plt.axhline(y=1.0, color='k', linestyle='--', alpha=0.3)
    plt.xlabel('Time Steps Backward')
    plt.ylabel('Gradient Scale Factor (log scale)')
    plt.title('Vanishing/Exploding Gradients in RNNs')
    plt.legend()
    plt.grid(True)

    plt.tight_layout()
    return plt
```

This problem occurs because during backpropagation through time, the gradient is multiplied by the recurrent weight matrix repeatedly, leading to exponential growth or decay.

## 11.1.3 LSTMs and GRUs

To address the vanishing gradient problem, Long Short-Term Memory (LSTM) networks and Gated Recurrent Units (GRUs) were developed with gating mechanisms to control information flow.

### LSTM Architecture

LSTMs introduce a cell state and three gates:

1. **Forget Gate**: Controls what information to throw away from the cell state
2. **Input Gate**: Controls what new information to add to the cell state
3. **Output Gate**: Controls what information from the cell state to output

```python
class CustomLSTM(nn.Module):
    def __init__(self, input_size, hidden_size):
        """
        A custom LSTM implementation to demonstrate the internal mechanisms.

        Args:
            input_size: Size of input features
            hidden_size: Size of hidden state and cell state
        """
        super(CustomLSTM, self).__init__()

        self.hidden_size = hidden_size

        # Forget gate: determine what to remove from cell state
        self.forget_gate = nn.Linear(input_size + hidden_size, hidden_size)

        # Input gate: determine what to add to cell state
        self.input_gate = nn.Linear(input_size + hidden_size, hidden_size)

        # Cell state candidate: new values to add to cell state
        self.cell_candidate = nn.Linear(input_size + hidden_size, hidden_size)

        # Output gate: determine what to output from cell state
        self.output_gate = nn.Linear(input_size + hidden_size, hidden_size)

        # Activation functions
        self.sigmoid = nn.Sigmoid()
        self.tanh = nn.Tanh()

    def forward(self, x, hidden):
        """Forward pass through the LSTM cell for a single time step."""
        h_prev, c_prev = hidden

        # Combine input and previous hidden state
        combined = torch.cat((x, h_prev), dim=1)

        # Forget gate: what to forget from cell state
        f_t = self.sigmoid(self.forget_gate(combined))

        # Input gate: what new information to add
        i_t = self.sigmoid(self.input_gate(combined))

        # Cell candidate: potential new values for cell state
        c_tilde = self.tanh(self.cell_candidate(combined))

        # Cell state update
        c_t = f_t * c_prev + i_t * c_tilde

        # Output gate: what to expose from cell state
        o_t = self.sigmoid(self.output_gate(combined))

        # Hidden state update
        h_t = o_t * self.tanh(c_t)
```

```python
        return (h_t, c_t)
```

The LSTM updates are governed by these equations:

1. Forget gate: $f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f)$
2. Input gate: $i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i)$
3. Cell candidate: $\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$
4. Cell state update: $C_t = f_t \odot C_{t-1} + i_t \odot \tilde{C}_t$
5. Output gate: $o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o)$
6. Hidden state update: $h_t = o_t \odot \tanh(C_t)$

Where $\odot$ represents element-wise multiplication.

## GRU Architecture

Gated Recurrent Units (GRUs) are a simplified version of LSTMs with two gates:

1. **Reset Gate**: Controls how much of the previous hidden state to use
2. **Update Gate**: Controls how much of the new hidden state to use

```python
class CustomGRU(nn.Module):
    def __init__(self, input_size, hidden_size):
        """
        A custom GRU implementation to demonstrate the internal mechanisms.

        Args:
            input_size: Size of input features
            hidden_size: Size of hidden state
        """
        super(CustomGRU, self).__init__()

        self.hidden_size = hidden_size

        # Reset gate: determine how much of previous hidden state to use
        self.reset_gate = nn.Linear(input_size + hidden_size, hidden_size)

        # Update gate: determine how much to update the hidden state
        self.update_gate = nn.Linear(input_size + hidden_size, hidden_size)

        # Candidate hidden state
        self.hidden_candidate = nn.Linear(input_size + hidden_size, hidden_size)

        # Activation functions
        self.sigmoid = nn.Sigmoid()
        self.tanh = nn.Tanh()

    def forward(self, x, h_prev):
        """Forward pass through the GRU cell for a single time step."""
        # Combine input and previous hidden state
        combined = torch.cat((x, h_prev), dim=1)

        # Reset gate: how much of the previous hidden state to use
        r_t = self.sigmoid(self.reset_gate(combined))

        # Update gate: how much to update the hidden state
        z_t = self.sigmoid(self.update_gate(combined))

        # Combined input for candidate hidden state
        reset_combined = torch.cat((x, r_t * h_prev), dim=1)

        # Candidate hidden state
        h_tilde = self.tanh(self.hidden_candidate(reset_combined))

        # Hidden state update
        h_t = (1 - z_t) * h_prev + z_t * h_tilde

        return h_t
```

The GRU updates are governed by these equations:

1. Reset gate: $r_t = \sigma(W_r \cdot [h_{t-1}, x_t] + b_r)$

2. Update gate: $z_t = \sigma(W_z \cdot [h_{t-1}, x_t] + b_z)$
3. Candidate hidden: $\tilde{h}_t = \tanh(W_h \cdot [r_t \odot h_{t-1}, x_t] + b_h)$
4. Hidden state update: $h_t = (1 - z_t) \odot h_{t-1} + z_t \odot \tilde{h}_t$

**Biological Parallel**: The gating mechanisms in LSTMs and GRUs resemble neuromodulatory systems in the brain that regulate information flow. For example, dopamine can modulate which information is maintained in working memory, similar to how LSTM gates control what information is stored in the cell state.

## 11.1.4 Bidirectional RNNs

In many sequence processing tasks, future context is just as important as past context. Bidirectional RNNs process the sequence in both directions:

```python
class BidirectionalRNN(nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        """
        A simple bidirectional RNN implementation.

        Args:
            input_size: Size of input features
            hidden_size: Size of hidden state
            output_size: Size of output
        """
        super(BidirectionalRNN, self).__init__()

        self.hidden_size = hidden_size

        # Forward RNN
        self.forward_rnn = nn.GRU(input_size, hidden_size, batch_first=True)

        # Backward RNN
        self.backward_rnn = nn.GRU(input_size, hidden_size, batch_first=True)

        # Combined output layer
        self.output_layer = nn.Linear(hidden_size * 2, output_size)

    def forward(self, x):
        """
        Process sequence in both directions.

        Args:
            x: Input sequence tensor of shape (batch_size, seq_len, input_size)
        """
        # Forward pass
        forward_out, _ = self.forward_rnn(x)

        # Backward pass (reverse the sequence)
        reversed_x = torch.flip(x, [1])  # Reverse along sequence dimension
        backward_out, _ = self.backward_rnn(reversed_x)
        backward_out = torch.flip(backward_out, [1])  # Flip back to match forward

        # Combine the two directions
        combined = torch.cat((forward_out, backward_out), dim=2)

        # Generate output
        output = self.output_layer(combined)

        return output
```

Bidirectional RNNs are particularly useful for tasks like speech recognition, machine translation, and named entity recognition, where the entire sequence is available during inference.

**Biological Parallel**: The brain often uses both predictive and retrospective processing when interpreting sequences. For example, in language processing, later words in a sentence can change the interpretation of earlier words.

## 11.1.5 Applications in Neuroscience

RNNs have been used extensively to model neural circuits and brain functions:

```
def train_rnn_on_neural_data():
    """Example of using RNNs to model neural time series data."""
    # This would typically involve:
    # 1. Loading neural recording data (e.g., spike trains or calcium imaging)
    # 2. Preprocessing into appropriate sequences
    # 3. Training an RNN to predict neural activity or behavior

    # Simulated neural data for demonstration
    n_neurons = 50
    n_timesteps = 100
    n_trials = 200

    # Simulated spike trains - binary activity patterns
    np.random.seed(42)
    neural_data = np.random.binomial(1, 0.1, (n_trials, n_timesteps, n_neurons))

    # Add some structure - make neurons 0-10 active at time 30-40 with higher probab
    neural_data[:, 30:40, :10] = np.random.binomial(1, 0.8, (n_trials, 10, 10))

    # Convert to tensor
    neural_data_tensor = torch.FloatTensor(neural_data)

    # Define task: predict activity at t+1 from activity at t
    X = neural_data_tensor[:, :-1, :]  # All timepoints except the last
    y = neural_data_tensor[:, 1:, :]   # All timepoints except the first

    # Split into train/test
    train_size = int(0.8 * n_trials)
    X_train, X_test = X[:train_size], X[train_size:]
    y_train, y_test = y[:train_size], y[train_size:]

    # Define an RNN model (we'll use PyTorch's built-in GRU)
    model = nn.Sequential(
        nn.GRU(n_neurons, 100, batch_first=True, return_sequences=True),
        nn.Linear(100, n_neurons),
        nn.Sigmoid()  # For binary prediction
    )

    # Simplified diagram of RNN modeling neural circuits
    plt.figure(figsize=(10, 6))

    # Draw the neural data raster plot
    plt.subplot(2, 1, 1)
    plt.imshow(neural_data[0].T, aspect='auto', cmap='binary')
    plt.title('Example Neural Activity')
    plt.ylabel('Neuron')
    plt.xlabel('Time')

    # Draw the RNN prediction schema
    plt.subplot(2, 1, 2)
    plt.plot([0.2, 0.8], [0.5, 0.5], 'b-', linewidth=2, label='Neural Data')
    plt.plot([0.2, 0.8], [0.4, 0.4], 'r--', linewidth=2, label='RNN Prediction')
    plt.xlim(0, 1)
```

```python
    plt.ylim(0, 1)
    plt.legend()
    plt.title('RNN Modeling Neural Dynamics')
    plt.axis('off')

    plt.tight_layout()
    return plt
```

In neuroscience, RNNs have been used to:

1. Model working memory in the prefrontal cortex
2. Simulate motor sequence learning in the basal ganglia
3. Capture dynamic responses in sensory cortices
4. Model decision-making processes in frontal areas

The recurrent connectivity in these networks resembles the recurrent circuits found throughout the brain, making them natural models of neural dynamics.

# 11.2 Attention Mechanisms

While RNNs excel at sequential processing, they struggle with long-range dependencies. Attention mechanisms address this limitation by allowing the model to focus on relevant parts of the input sequence when producing each output element, regardless of their distance.

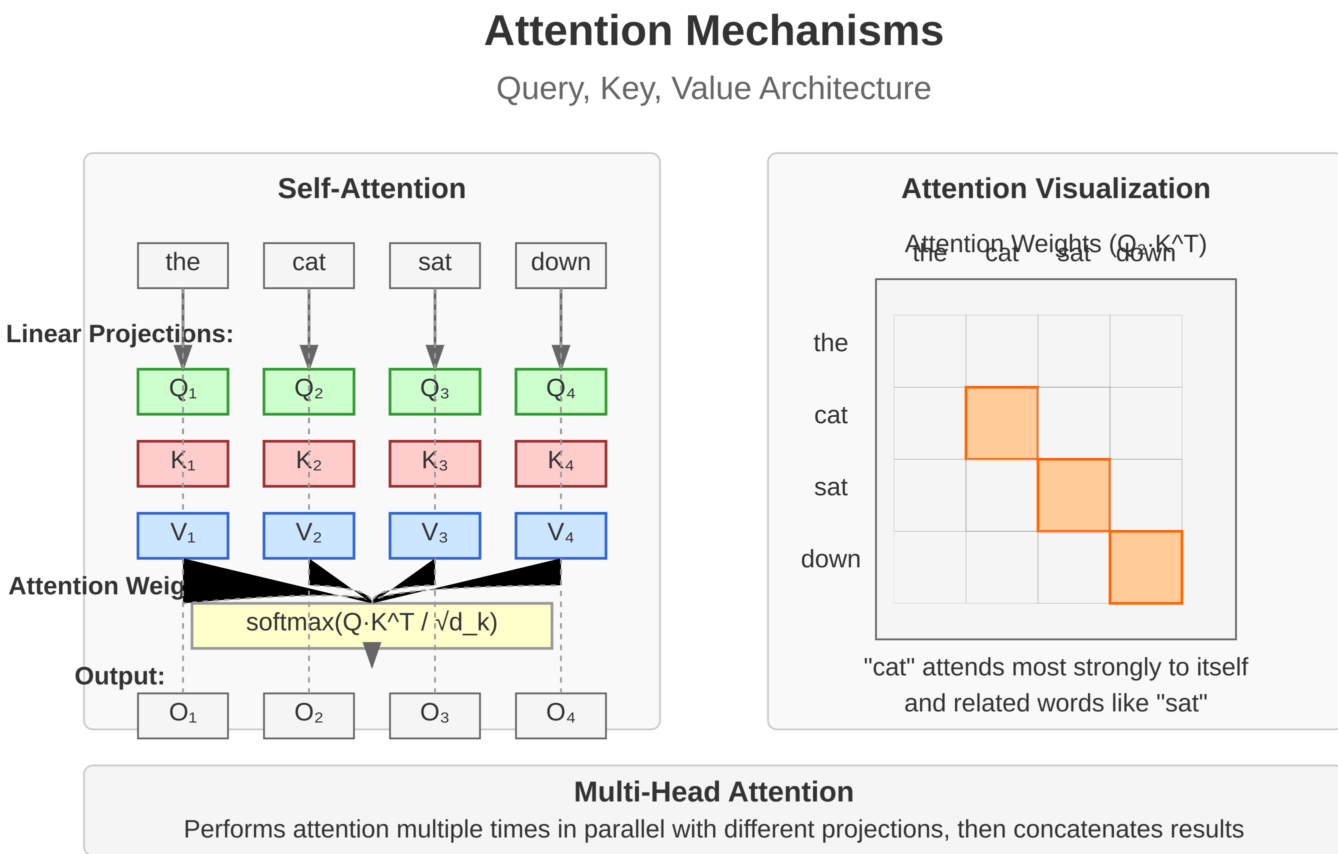


*Figure 11.2: Attention mechanism architecture showing query, key, value operations and how attention weights are computed and applied.*

## 11.2.1 The Intuition Behind Attention

Attention mimics a cognitive process: when processing complex information, humans focus on relevant parts while ignoring irrelevant details. For example, when translating a long sentence, a human translator might focus on specific source words when generating each target word.

```python
def attention_intuition():
    """Visualize the intuition behind attention."""
    # Create a simple sentence for visualization
    source = "The small cat sleeps on the comfortable blue mat"
    target = "Le petit chat dort sur le tapis bleu confortable"

    # Split into words
    source_words = source.split()
    target_words = target.split()

    # Simulate attention weights (would normally be learned)
    # Each row corresponds to a target word, each column to a source word
    attention_weights = np.zeros((len(target_words), len(source_words)))

    # Set attention based on word alignment (simplified for visualization)
    alignments = {
        0: [0],        # Le -> The
        1: [1],        # petit -> small
        2: [2],        # chat -> cat
        3: [3],        # dort -> sleeps
        4: [4],        # sur -> on
        5: [5],        # le -> the
        6: [7, 8],     # tapis bleu -> blue mat
        7: [6]         # confortable -> comfortable
    }

    # Fill in attention weights
    for target_idx, source_idxs in alignments.items():
        for source_idx in source_idxs:
            attention_weights[target_idx, source_idx] = 1.0 / len(source_idxs)

    # Create visualization
    plt.figure(figsize=(12, 8))
    plt.imshow(attention_weights, cmap='YlOrRd')

    # Add labels
    plt.xticks(np.arange(len(source_words)), source_words, rotation=45, ha='right')
    plt.yticks(np.arange(len(target_words)), target_words)

    plt.xlabel('Source (English)')
    plt.ylabel('Target (French)')
    plt.title('Attention Weights in Translation')

    # Add a colorbar
    plt.colorbar(label='Attention Weight')

    plt.tight_layout()
    return plt
```

### 11.2.2 Self-Attention

Self-attention allows a sequence to attend to itself, capturing dependencies between elements regardless of their distance. The key innovation is computing attention weights using queries and keys derived from the same sequence.

```python
class SelfAttention(nn.Module):
    def __init__(self, hidden_size):
        """
        Self-attention mechanism.

        Args:
            hidden_size: Dimensionality of input vectors
        """
        super(SelfAttention, self).__init__()

        self.hidden_size = hidden_size

        # Linear projections for query, key, and value
        self.query = nn.Linear(hidden_size, hidden_size)
        self.key = nn.Linear(hidden_size, hidden_size)
        self.value = nn.Linear(hidden_size, hidden_size)

        # Scaling factor
        self.scale = torch.sqrt(torch.FloatTensor([hidden_size])).item()

    def forward(self, x, mask=None):
        """
        Apply self-attention to input sequence.

        Args:
            x: Input tensor of shape [batch_size, seq_len, hidden_size]
            mask: Optional mask tensor of shape [batch_size, seq_len, seq_len]

        Returns:
            attended: Output tensor after self-attention
            attention_weights: Attention weight matrix
        """
        batch_size, seq_len, _ = x.shape

        # Linear projections
        q = self.query(x)  # [batch_size, seq_len, hidden_size]
        k = self.key(x)    # [batch_size, seq_len, hidden_size]
        v = self.value(x)  # [batch_size, seq_len, hidden_size]

        # Compute attention scores
        # q @ k.transpose(-2, -1) => [batch_size, seq_len, seq_len]
        attention_scores = torch.matmul(q, k.transpose(-2, -1)) / self.scale

        # Apply mask if provided (useful for padding or causal attention)
        if mask is not None:
            attention_scores = attention_scores.masked_fill(mask == 0, -1e10)

        # Softmax to get attention weights
        attention_weights = torch.softmax(attention_scores, dim=-1)

        # Apply attention weights to values
        attended = torch.matmul(attention_weights, v)
```

```
        return attended, attention_weights
```

The self-attention operation is defined as:

$$\text{Attention}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

Where:

- $Q$ (queries), $K$ (keys), and $V$ (values) are linear projections of the input
- $d_k$ is the dimensionality of the key vectors
- The scaling factor $\frac{1}{\sqrt{d_k}}$ prevents the softmax from reaching regions with extremely small gradients

**Biological Parallel**: Selective attention in the brain allows for focusing on relevant stimuli while suppressing irrelevant information. The thalamus and prefrontal cortex work together to control which information receives processing priority, similar to how attention weights prioritize certain parts of the input.

## 11.2.3 Multi-Head Attention

Multi-head attention runs several attention mechanisms in parallel, allowing the model to jointly attend to information from different representation subspaces.

```python
class MultiHeadAttention(nn.Module):
    def __init__(self, hidden_size, num_heads):
        """
        Multi-head attention mechanism.

        Args:
            hidden_size: Dimensionality of input vectors
            num_heads: Number of attention heads
        """
        super(MultiHeadAttention, self).__init__()

        assert hidden_size % num_heads == 0, "hidden_size must be divisible by num_h

        self.hidden_size = hidden_size
        self.num_heads = num_heads
        self.head_dim = hidden_size // num_heads

        # Linear projections for query, key, and value
        self.query = nn.Linear(hidden_size, hidden_size)
        self.key = nn.Linear(hidden_size, hidden_size)
        self.value = nn.Linear(hidden_size, hidden_size)

        # Output projection
        self.output_projection = nn.Linear(hidden_size, hidden_size)

        # Scaling factor
        self.scale = torch.sqrt(torch.FloatTensor([self.head_dim])).item()

    def forward(self, query, key, value, mask=None):
        """
        Apply multi-head attention.

        Args:
            query: Query tensor [batch_size, query_len, hidden_size]
            key: Key tensor [batch_size, key_len, hidden_size]
            value: Value tensor [batch_size, key_len, hidden_size]
            mask: Optional mask tensor [batch_size, query_len, key_len]

        Returns:
            attended: Output tensor after multi-head attention
            attention_weights: Attention weight tensor for each head
        """
        batch_size = query.shape[0]

        # Linear projections
        Q = self.query(query)  # [batch_size, query_len, hidden_size]
        K = self.key(key)      # [batch_size, key_len, hidden_size]
        V = self.value(value)  # [batch_size, key_len, hidden_size]

        # Reshape for multi-head attention
        # [batch_size, seq_len, hidden_size] -> [batch_size, seq_len, num_heads, hea
        Q = Q.view(batch_size, -1, self.num_heads, self.head_dim)
        K = K.view(batch_size, -1, self.num_heads, self.head_dim)
```

```
        V = V.view(batch_size, -1, self.num_heads, self.head_dim)

        # Transpose to [batch_size, num_heads, seq_len, head_dim]
        Q = Q.transpose(1, 2)
        K = K.transpose(1, 2)
        V = V.transpose(1, 2)

        # Compute attention scores
        # [batch_size, num_heads, query_len, key_len]
        attention_scores = torch.matmul(Q, K.transpose(-2, -1)) / self.scale

        # Apply mask if provided
        if mask is not None:
            # Expand mask for multiple heads
            # [batch_size, query_len, key_len] -> [batch_size, 1, query_len, key_ler
            mask = mask.unsqueeze(1)
            attention_scores = attention_scores.masked_fill(mask == 0, -1e10)

        # Softmax to get attention weights
        attention_weights = torch.softmax(attention_scores, dim=-1)

        # Apply attention weights to values
        # [batch_size, num_heads, query_len, head_dim]
        attended = torch.matmul(attention_weights, V)

        # Transpose and reshape back
        # [batch_size, num_heads, query_len, head_dim] -> [batch_size, query_len, nu
        attended = attended.transpose(1, 2).contiguous()

        # [batch_size, query_len, hidden_size]
        attended = attended.view(batch_size, -1, self.hidden_size)

        # Final linear projection
        attended = self.output_projection(attended)

        return attended, attention_weights
```

Multi-head attention expands on the basic attention mechanism with multiple attention “heads” operating in parallel, each looking at different aspects of the data:

$$\text{MultiHead}(Q, K, V) = \text{Concat}(\text{head}_1, \ldots, \text{head}_h)W^O$$

Where:

- Each $\text{head}_i = \text{Attention}(QW_i^Q, KW_i^K, VW_i^V)$
- The $W$ matrices are learned projection matrices
- $W^O$ is the output projection

## 11.2.4 Self-Attention vs. Recurrence

Self-attention offers several advantages over recurrent networks:

1. **Parallelization**: Unlike RNNs, which process sequences step-by-step, self-attention processes all sequence elements simultaneously.
2. **Long-range dependencies**: Attention directly connects any two positions in the sequence, allowing for efficient modeling of long-range dependencies.
3. **Interpretability**: Attention weights can be visualized to understand which input elements the model focuses on when generating each output.

```
def compare_rnn_attention_complexity():
    """Compare computational complexity of RNNs vs. Attention"""
    sequence_lengths = np.arange(10, 1001, 10)

    # Computational complexity
    rnn_sequential_ops = sequence_lengths  # O(n) time steps for sequential processi
    attention_parallel_ops = np.ones_like(sequence_lengths)  # O(1) parallel process
    attention_memory_cost = sequence_lengths**2  # O(n²) attention matrix

    # Plot comparison
    plt.figure(figsize=(12, 6))

    plt.subplot(1, 2, 1)
    plt.plot(sequence_lengths, rnn_sequential_ops, 'r-', label='RNN (Sequential Step
    plt.plot(sequence_lengths, attention_parallel_ops, 'b-', label='Attention (Paral
    plt.xlabel('Sequence Length')
    plt.ylabel('Sequential Operations')
    plt.title('Computational Complexity (Time)')
    plt.legend()
    plt.grid(True)

    plt.subplot(1, 2, 2)
    plt.plot(sequence_lengths, attention_memory_cost, 'g-', label='Attention Matrix
    plt.xlabel('Sequence Length')
    plt.ylabel('Memory Cost')
    plt.title('Memory Requirements')
    plt.legend()
    plt.grid(True)

    plt.tight_layout()
    return plt
```

## 11.2.5 Scaled Dot-Product Attention

The core attention mechanism in modern architectures is scaled dot-product attention:

```python
def scaled_dot_product_attention(query, key, value, mask=None):
    """
    Compute scaled dot-product attention.

    Args:
        query: Query tensor [batch_size, seq_len, d_k]
        key: Key tensor [batch_size, seq_len, d_k]
        value: Value tensor [batch_size, seq_len, d_v]
        mask: Optional mask tensor [batch_size, seq_len, seq_len]

    Returns:
        output: Attended values
        attention: Attention weights
    """
    # Compute attention scores
    d_k = query.size(-1)
    scores = torch.matmul(query, key.transpose(-2, -1)) / np.sqrt(d_k)

    # Apply mask if provided
    if mask is not None:
        scores = scores.masked_fill(mask == 0, -1e10)

    # Apply softmax to get attention weights
    attention = torch.softmax(scores, dim=-1)

    # Apply attention weights to values
    output = torch.matmul(attention, value)

    return output, attention
```

## 11.2.6 Attention Visualization

Visualizing attention weights can provide insight into how the model processes sequences:

```
def visualize_attention():
    """Create a visualization of attention patterns."""
    # Sample sentence
    sentence = "The quick brown fox jumps over the lazy dog"
    words = sentence.split()

    # Create simulated attention matrices
    num_words = len(words)

    # Self-attention: diagonal dominant (attends to self and nearby words)
    self_attention = np.zeros((num_words, num_words))
    for i in range(num_words):
        for j in range(num_words):
            self_attention[i, j] = 1.0 / (1 + abs(i - j))

    # Normalize rows
    self_attention = self_attention / self_attention.sum(axis=1, keepdims=True)

    # Subject-verb attention: highlights grammatical relationships
    subj_verb_attention = np.zeros((num_words, num_words))
    subject_idx = 3  # 'fox'
    verb_idx = 4     # 'jumps'
    subj_verb_attention[subject_idx, verb_idx] = 0.7
    subj_verb_attention[verb_idx, subject_idx] = 0.7

    # Fill in other relationships
    for i in range(num_words):
        for j in range(num_words):
            if i != subject_idx and j != verb_idx and i != verb_idx and j != subject
                subj_verb_attention[i, j] = 0.1 / (num_words - 2)

    # Plot attention matrices
    fig, axes = plt.subplots(1, 2, figsize=(16, 6))

    # Plot self-attention
    im1 = axes[0].imshow(self_attention, cmap='YlOrRd')
    axes[0].set_title('Self-Attention Pattern')
    axes[0].set_xticks(np.arange(num_words))
    axes[0].set_yticks(np.arange(num_words))
    axes[0].set_xticklabels(words)
    axes[0].set_yticklabels(words)
    plt.setp(axes[0].get_xticklabels(), rotation=45, ha="right", rotation_mode="anch
    fig.colorbar(im1, ax=axes[0])

    # Plot subject-verb attention
    im2 = axes[1].imshow(subj_verb_attention, cmap='YlOrRd')
    axes[1].set_title('Subject-Verb Attention')
    axes[1].set_xticks(np.arange(num_words))
    axes[1].set_yticks(np.arange(num_words))
    axes[1].set_xticklabels(words)
    axes[1].set_yticklabels(words)
    plt.setp(axes[1].get_xticklabels(), rotation=45, ha="right", rotation_mode="anch
    fig.colorbar(im2, ax=axes[1])
```

```
    # Add annotations
    for i in range(num_words):
        for j in range(num_words):
            if self_attention[i, j] > 0.2:
                axes[0].text(j, i, f"{self_attention[i, j]:.2f}",
                             ha="center", va="center", color="white" if self_attenti

            if subj_verb_attention[i, j] > 0.2:
                axes[1].text(j, i, f"{subj_verb_attention[i, j]:.2f}",
                             ha="center", va="center", color="white" if subj_verb_at

    plt.tight_layout()
    return plt
```

### 11.2.7 Neural Correlates of Attention

The attention mechanisms in deep learning have interesting parallels with attention systems in the brain:

```
def neural_attention_parallels():
    """Illustrate parallels between artificial and neural attention."""
    plt.figure(figsize=(12, 8))

    # Create a simple diagram
    plt.subplot(2, 1, 1)
    plt.title('Neural Attention in the Brain')
    plt.axis('off')

    # Draw brain regions involved in attention
    circle1 = plt.Circle((0.3, 0.5), 0.15, fc='#FFC78E', ec='black', label='PFC')
    circle2 = plt.Circle((0.6, 0.5), 0.1, fc='#8EADFC', ec='black', label='Thalamus'
    circle3 = plt.Circle((0.8, 0.6), 0.12, fc='#8EFCB8', ec='black', label='Visual C

    plt.gca().add_patch(circle1)
    plt.gca().add_patch(circle2)
    plt.gca().add_patch(circle3)

    # Add labels
    plt.text(0.3, 0.5, 'PFC', ha='center', va='center')
    plt.text(0.6, 0.5, 'Thalamus', ha='center', va='center')
    plt.text(0.8, 0.6, 'Visual\nCortex', ha='center', va='center')

    # Draw connections
    plt.arrow(0.4, 0.5, 0.1, 0.0, head_width=0.02, head_length=0.02, fc='black', ec=
    plt.arrow(0.7, 0.5, 0.05, 0.05, head_width=0.02, head_length=0.02, fc='black', e

    # Add explanatory text
    plt.text(0.5, 0.8, "The prefrontal cortex (PFC) directs attention via the thalam
             ha='center', va='center', bbox=dict(facecolor='white', alpha=0.5))

    # Machine attention mechanism
    plt.subplot(2, 1, 2)
    plt.title('Artificial Attention Mechanism')
    plt.axis('off')

    # Draw components
    rect1 = plt.Rectangle((0.2, 0.4), 0.15, 0.2, fc='#FFC78E', ec='black')
    rect2 = plt.Rectangle((0.5, 0.4), 0.15, 0.2, fc='#8EADFC', ec='black')
    rect3 = plt.Rectangle((0.8, 0.4), 0.15, 0.2, fc='#8EFCB8', ec='black')

    plt.gca().add_patch(rect1)
    plt.gca().add_patch(rect2)
    plt.gca().add_patch(rect3)

    # Add labels
    plt.text(0.275, 0.5, 'Query', ha='center', va='center')
    plt.text(0.575, 0.5, 'Attention\nWeights', ha='center', va='center')
    plt.text(0.875, 0.5, 'Value', ha='center', va='center')

    # Draw connections
    plt.arrow(0.35, 0.5, 0.15, 0.0, head_width=0.02, head_length=0.02, fc='black', e
    plt.arrow(0.65, 0.5, 0.15, 0.0, head_width=0.02, head_length=0.02, fc='black', e
```

```python
    # Add explanatory text
    plt.text(0.5, 0.2, "Neural network attention uses queries to compute weights\nth
             ha='center', va='center', bbox=dict(facecolor='white', alpha=0.5))

    plt.tight_layout()
    return plt
```

These parallels include:

1. **Selective Enhancement**: Both neural and artificial attention selectively enhance processing of relevant information.
2. **Top-down Control**: The prefrontal cortex provides top-down control in the brain, similar to how queries direct attention in artificial systems.
3. **Resource Allocation**: Both systems efficiently allocate limited processing resources to the most important inputs.
4. **Context Integration**: Both integrate contextual information to determine what's relevant in the current situation.

# 11.3 Transformer Architecture

The Transformer architecture, introduced in the landmark paper "Attention Is All You Need" (Vaswani et al., 2017), revolutionized sequence processing by eliminating recurrence entirely and relying solely on attention mechanisms.

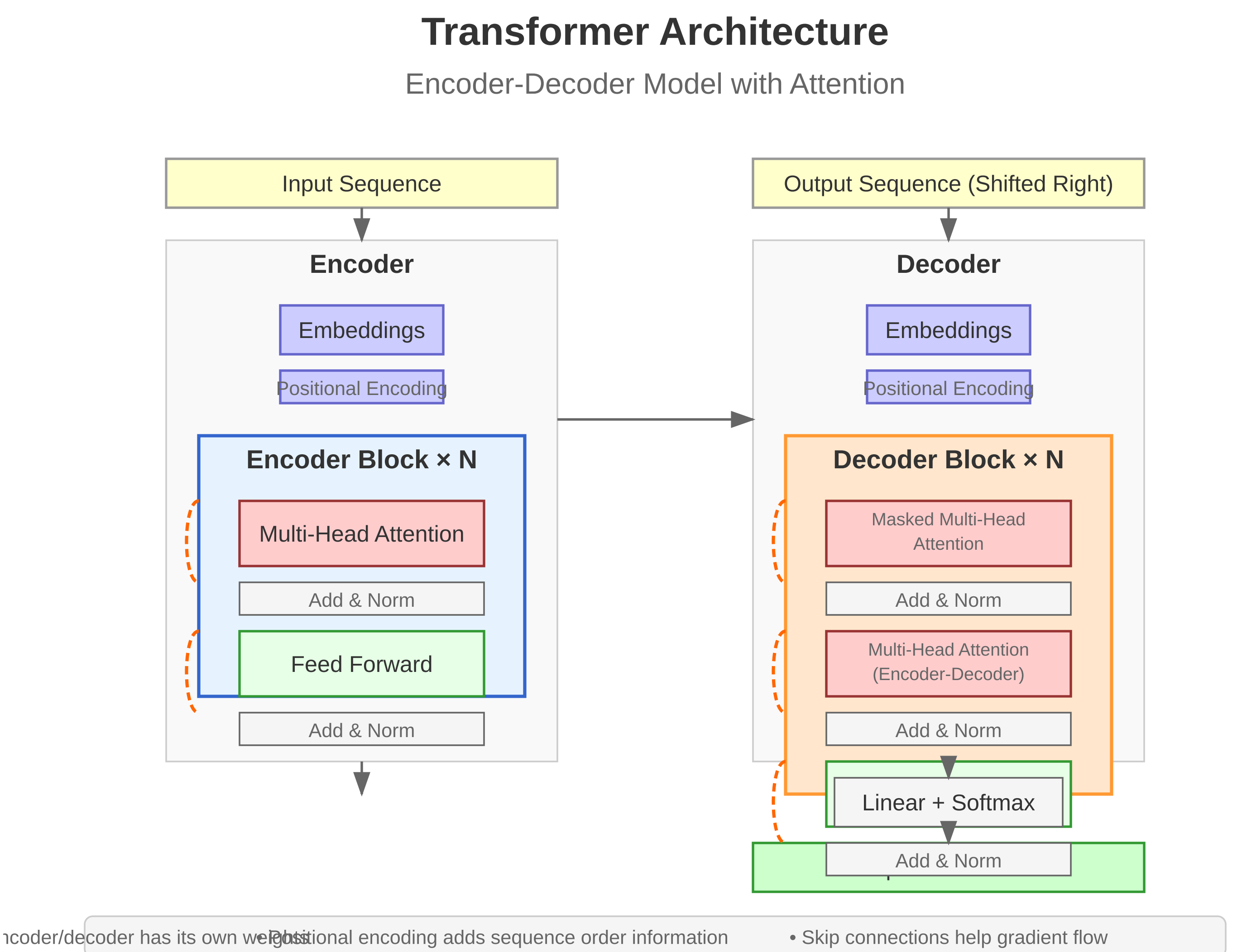


*Figure 11.3: The Transformer architecture featuring an encoder-decoder structure with multi-head attention, positional encodings, and feed-forward networks.*

## 11.3.1 Overall Architecture

The Transformer follows an encoder-decoder structure:

```
class Transformer(nn.Module):
    def __init__(self, src_vocab_size, tgt_vocab_size, d_model, n_heads, n_layers, d
                 max_seq_len, dropout=0.1):
        """
        Full Transformer architecture for sequence-to-sequence tasks.

        Args:
            src_vocab_size: Size of source vocabulary
            tgt_vocab_size: Size of target vocabulary
            d_model: Model dimension (embedding size)
            n_heads: Number of attention heads
            n_layers: Number of encoder/decoder layers
            d_ff: Hidden dimension in feed-forward networks
            max_seq_len: Maximum sequence length for positional encodings
            dropout: Dropout rate
        """
        super(Transformer, self).__init__()

        # Embeddings and positional encodings
        self.src_embedding = nn.Embedding(src_vocab_size, d_model)
        self.tgt_embedding = nn.Embedding(tgt_vocab_size, d_model)
        self.positional_encoding = self.create_positional_encoding(max_seq_len, d_mo

        # Encoder and decoder
        self.encoder = TransformerEncoder(d_model, n_heads, n_layers, d_ff, dropout)
        self.decoder = TransformerDecoder(d_model, n_heads, n_layers, d_ff, dropout)

        # Final linear layer
        self.final_layer = nn.Linear(d_model, tgt_vocab_size)

        # Dropout
        self.dropout = nn.Dropout(dropout)

        # Initialize parameters
        self.init_parameters()

    def create_positional_encoding(self, max_seq_len, d_model):
        """Create sinusoidal positional encodings."""
        # Create a tensor for positions
        positions = torch.arange(0, max_seq_len).unsqueeze(1).float()

        # Create a tensor for dimension indices
        div_term = torch.exp(torch.arange(0, d_model, 2).float() * -(math.log(10000.

        # Create positional encoding
        pe = torch.zeros(max_seq_len, d_model)
        pe[:, 0::2] = torch.sin(positions * div_term)  # Even dimensions
        pe[:, 1::2] = torch.cos(positions * div_term)  # Odd dimensions

        # Add batch dimension and register as buffer (not a parameter)
        pe = pe.unsqueeze(0)
        return nn.Parameter(pe, requires_grad=False)
```

```
    def init_parameters(self):
        """Initialize model parameters."""
        for p in self.parameters():
            if p.dim() > 1:
                nn.init.xavier_uniform_(p)

    def forward(self, src, tgt, src_mask=None, tgt_mask=None, src_padding_mask=None,
        """
        Forward pass through the Transformer.

        Args:
            src: Source sequence [batch_size, src_len]
            tgt: Target sequence [batch_size, tgt_len]
            src_mask: Mask for source self-attention
            tgt_mask: Mask for target self-attention (usually causal)
            src_padding_mask: Mask for source padding
            tgt_padding_mask: Mask for target padding

        Returns:
            output: Vocabulary distributions [batch_size, tgt_len, tgt_vocab_size]
        """
        # Get sequence lengths
        src_len = src.size(1)
        tgt_len = tgt.size(1)

        # Embed and add positional encoding
        src_embedded = self.src_embedding(src) * math.sqrt(self.d_model)
        src_embedded = src_embedded + self.positional_encoding[:, :src_len]
        src_embedded = self.dropout(src_embedded)

        tgt_embedded = self.tgt_embedding(tgt) * math.sqrt(self.d_model)
        tgt_embedded = tgt_embedded + self.positional_encoding[:, :tgt_len]
        tgt_embedded = self.dropout(tgt_embedded)

        # Encoder pass
        encoder_output = self.encoder(src_embedded, src_mask, src_padding_mask)

        # Decoder pass
        decoder_output = self.decoder(tgt_embedded, encoder_output, tgt_mask, tgt_pa

        # Final projection to vocabulary
        output = self.final_layer(decoder_output)

        return output
```

The Transformer consists of two main components:

1. **Encoder**: Processes the input sequence into a continuous representation
2. **Decoder**: Generates the output sequence based on the encoder representation and previous outputs

### 11.3.2 Encoder

The encoder consists of N identical layers, each with two sub-layers:

```python
class TransformerEncoderLayer(nn.Module):
    def __init__(self, d_model, n_heads, d_ff, dropout=0.1):
        """
        Single Transformer encoder layer.

        Args:
            d_model: Model dimension
            n_heads: Number of attention heads
            d_ff: Hidden dimension in feed-forward network
            dropout: Dropout rate
        """
        super(TransformerEncoderLayer, self).__init__()

        # Multi-head self-attention
        self.self_attention = MultiHeadAttention(d_model, n_heads)

        # Feed-forward network
        self.feed_forward = nn.Sequential(
            nn.Linear(d_model, d_ff),
            nn.ReLU(),
            nn.Linear(d_ff, d_model)
        )

        # Layer normalization
        self.norm1 = nn.LayerNorm(d_model)
        self.norm2 = nn.LayerNorm(d_model)

        # Dropout
        self.dropout = nn.Dropout(dropout)

    def forward(self, x, mask=None):
        """
        Forward pass through encoder layer.

        Args:
            x: Input tensor [batch_size, seq_len, d_model]
            mask: Optional attention mask

        Returns:
            x: Output tensor [batch_size, seq_len, d_model]
        """
        # Self-attention sub-layer with residual connection and layer normalization
        attn_output, _ = self.self_attention(x, x, x, mask)
        x = self.norm1(x + self.dropout(attn_output))

        # Feed-forward sub-layer with residual connection and layer normalization
        ff_output = self.feed_forward(x)
        x = self.norm2(x + self.dropout(ff_output))

        return x
```

The complete encoder stacks multiple encoder layers:

```python
class TransformerEncoder(nn.Module):
    def __init__(self, d_model, n_heads, n_layers, d_ff, dropout=0.1):
        """
        Full Transformer encoder with N layers.

        Args:
            d_model: Model dimension
            n_heads: Number of attention heads
            n_layers: Number of encoder layers
            d_ff: Hidden dimension in feed-forward network
            dropout: Dropout rate
        """
        super(TransformerEncoder, self).__init__()

        # Stack of encoder layers
        self.layers = nn.ModuleList(
            [TransformerEncoderLayer(d_model, n_heads, d_ff, dropout) for _ in range
        )

    def forward(self, x, mask=None, padding_mask=None):
        """
        Forward pass through the encoder.

        Args:
            x: Input tensor [batch_size, seq_len, d_model]
            mask: Self-attention mask
            padding_mask: Mask for padding tokens

        Returns:
            x: Encoded representation [batch_size, seq_len, d_model]
        """
        # Apply padding mask to attention mask if provided
        if padding_mask is not None:
            if mask is None:
                mask = padding_mask
            else:
                mask = mask & padding_mask

        # Pass through each encoder layer
        for layer in self.layers:
            x = layer(x, mask)

        return x
```

## 11.3.3 Decoder

The decoder is similar to the encoder but has an additional cross-attention layer:

```
class TransformerDecoderLayer(nn.Module):
    def __init__(self, d_model, n_heads, d_ff, dropout=0.1):
        """
        Single Transformer decoder layer.

        Args:
            d_model: Model dimension
            n_heads: Number of attention heads
            d_ff: Hidden dimension in feed-forward network
            dropout: Dropout rate
        """
        super(TransformerDecoderLayer, self).__init__()

        # Multi-head self-attention
        self.self_attention = MultiHeadAttention(d_model, n_heads)

        # Multi-head cross-attention to encoder outputs
        self.cross_attention = MultiHeadAttention(d_model, n_heads)

        # Feed-forward network
        self.feed_forward = nn.Sequential(
            nn.Linear(d_model, d_ff),
            nn.ReLU(),
            nn.Linear(d_ff, d_model)
        )

        # Layer normalization
        self.norm1 = nn.LayerNorm(d_model)
        self.norm2 = nn.LayerNorm(d_model)
        self.norm3 = nn.LayerNorm(d_model)

        # Dropout
        self.dropout = nn.Dropout(dropout)

    def forward(self, x, encoder_output, tgt_mask=None, tgt_padding_mask=None, src_p
        """
        Forward pass through decoder layer.

        Args:
            x: Input tensor [batch_size, tgt_len, d_model]
            encoder_output: Output from encoder [batch_size, src_len, d_model]
            tgt_mask: Mask for target self-attention (usually causal)
            tgt_padding_mask: Mask for target padding
            src_padding_mask: Mask for source padding

        Returns:
            x: Output tensor [batch_size, tgt_len, d_model]
        """
        # Self-attention sub-layer with residual connection and layer normalization
        attn_output, _ = self.self_attention(x, x, x, tgt_mask)
        x = self.norm1(x + self.dropout(attn_output))

        # Cross-attention sub-layer with residual connection and layer normalizatio
```

```
        cross_attn_output, _ = self.cross_attention(x, encoder_output, encoder_outpu
        x = self.norm2(x + self.dropout(cross_attn_output))

        # Feed-forward sub-layer with residual connection and layer normalization
        ff_output = self.feed_forward(x)
        x = self.norm3(x + self.dropout(ff_output))

        return x
```

The complete decoder stacks multiple decoder layers:

```
class TransformerDecoder(nn.Module):
    def __init__(self, d_model, n_heads, n_layers, d_ff, dropout=0.1):
        """
        Full Transformer decoder with N layers.

        Args:
            d_model: Model dimension
            n_heads: Number of attention heads
            n_layers: Number of decoder layers
            d_ff: Hidden dimension in feed-forward network
            dropout: Dropout rate
        """
        super(TransformerDecoder, self).__init__()

        # Stack of decoder layers
        self.layers = nn.ModuleList(
            [TransformerDecoderLayer(d_model, n_heads, d_ff, dropout) for _ in range
        )

    def forward(self, x, encoder_output, tgt_mask=None, tgt_padding_mask=None, src_p
        """
        Forward pass through the decoder.

        Args:
            x: Input tensor [batch_size, tgt_len, d_model]
            encoder_output: Output from encoder [batch_size, src_len, d_model]
            tgt_mask: Mask for target self-attention (usually causal)
            tgt_padding_mask: Mask for target padding
            src_padding_mask: Mask for source padding

        Returns:
            x: Decoded representation [batch_size, tgt_len, d_model]
        """
        # Pass through each decoder layer
        for layer in self.layers:
            x = layer(x, encoder_output, tgt_mask, tgt_padding_mask, src_padding_mas

        return x
```

### 11.3.4 Positional Encodings

Since the Transformer doesn’t use recurrence or convolution, it needs a way to incorporate sequence order. Positional encodings add positional information to the input embeddings:

```
def create_positional_encodings(max_len, d_model):
    """
    Create sinusoidal positional encodings.

    Args:
        max_len: Maximum sequence length
        d_model: Model dimension

    Returns:
        pos_encoding: Positional encoding tensor [1, max_len, d_model]
    """
    # Create a tensor for positions
    positions = torch.arange(0, max_len).float().unsqueeze(1)

    # Create a tensor for dimension indices
    div_term = torch.exp(torch.arange(0, d_model, 2).float() * -(math.log(10000.0) /

    # Create positional encoding
    pos_encoding = torch.zeros(max_len, d_model)
    pos_encoding[:, 0::2] = torch.sin(positions * div_term)  # Even dimensions
    pos_encoding[:, 1::2] = torch.cos(positions * div_term)  # Odd dimensions

    # Add batch dimension
    pos_encoding = pos_encoding.unsqueeze(0)

    return pos_encoding

def visualize_positional_encodings():
    """Visualize positional encodings."""
    # Create positional encodings
    max_len = 100
    d_model = 128
    pos_encoding = create_positional_encodings(max_len, d_model).squeeze(0).numpy()

    # Plot as a heatmap
    plt.figure(figsize=(10, 6))
    plt.imshow(pos_encoding, cmap='viridis', aspect='auto')
    plt.xlabel('Embedding Dimension')
    plt.ylabel('Position in Sequence')
    plt.title('Sinusoidal Positional Encodings')
    plt.colorbar()

    # Plot a few dimensions across positions
    plt.figure(figsize=(10, 6))

    for dim in [0, 1, 2, 3, 63, 64, 65, 66, 127]:
        plt.plot(pos_encoding[:, dim], label=f'Dim {dim}')

    plt.xlabel('Position')
    plt.ylabel('Value')
    plt.title('Positional Encoding Values by Dimension')
    plt.legend()
    plt.grid(True)
```

```
    return plt
```

The positional encodings use sine and cosine functions of different frequencies:

$$PE_{(pos,2i)} = \sin\left(pos/10000^{2i/d_{model}}\right)$$

$$PE_{(pos,2i+1)} = \cos\left(pos/10000^{2i/d_{model}}\right)$$

This approach allows the model to easily learn to attend to relative positions since $PE_{pos+k}$ can be represented as a linear function of $PE_{pos}$.

## 11.3.5 Feed-Forward Networks

Each encoder and decoder layer contains a position-wise feed-forward network:

```python
class PositionwiseFeedForward(nn.Module):
    def __init__(self, d_model, d_ff, dropout=0.1):
        """
        Position-wise feed-forward network.

        Args:
            d_model: Model dimension
            d_ff: Hidden dimension
            dropout: Dropout rate
        """
        super(PositionwiseFeedForward, self).__init__()

        self.fc1 = nn.Linear(d_model, d_ff)
        self.fc2 = nn.Linear(d_ff, d_model)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x):
        """
        Apply feed-forward network to input.

        Args:
            x: Input tensor [batch_size, seq_len, d_model]

        Returns:
            output: Transformed tensor [batch_size, seq_len, d_model]
        """
        output = self.dropout(torch.relu(self.fc1(x)))
        output = self.fc2(output)
        return output
```

These networks apply two linear transformations with a ReLU activation in between:

$$FFN(x) = \max(0, xW_1 + b_1)W_2 + b_2$$

The feed-forward networks process each position independently, which is why they're sometimes called "position-wise" feed-forward networks.

## 11.3.6 Residual Connections and Layer Normalization

The Transformer uses residual connections around each sub-layer, followed by layer normalization:

```python
class AddNorm(nn.Module):
    def __init__(self, size, dropout=0.1):
        """
        Residual connection followed by layer normalization.

        Args:
            size: Feature dimension
            dropout: Dropout rate
        """
        super(AddNorm, self).__init__()
        self.norm = nn.LayerNorm(size)
        self.dropout = nn.Dropout(dropout)

    def forward(self, x, sublayer_output):
        """
        Apply residual connection and layer normalization.

        Args:
            x: Input tensor
            sublayer_output: Output from sublayer

        Returns:
            normalized: Normalized output with residual connection
        """
        # Add residual connection and normalize
        return self.norm(x + self.dropout(sublayer_output))
```

Layer normalization normalizes the inputs across the feature dimension, stabilizing the network's activations:

$$LayerNorm(x) = \gamma \odot \frac{x - \mu}{\sqrt{\sigma^2 + \epsilon}} + \beta$$

Where:

- $\mu$ and $\sigma$ are the mean and standard deviation of the inputs
- $\gamma$ and $\beta$ are learned parameters
- $\epsilon$ is a small constant for numerical stability

## 11.3.7 Biological Parallels

The Transformer architecture has several interesting parallels with neural processing:

```
def transformer_brain_parallels():
    """Illustrate parallels between Transformers and brain processing."""
    plt.figure(figsize=(12, 8))

    # Create a two-row comparison
    plt.subplot(2, 1, 1)
    plt.title('Parallel Processing in Transformers')
    plt.axis('off')

    # Draw Transformer components
    for i in range(5):
        x_pos = 0.1 + i * 0.2
        plt.rectangle((x_pos, 0.3), 0.1, 0.4, fc='lightblue', ec='black')
        plt.arrow(x_pos + 0.05, 0.7, 0, 0.1, head_width=0.02, head_length=0.02, fc='
        plt.text(x_pos + 0.05, 0.2, f"Token {i+1}", ha='center')

    # Add attention illustration
    for i in range(5):
        for j in range(5):
            alpha = 0.3 if i != j else 0.8
            plt.plot([0.1 + i * 0.2 + 0.05, 0.1 + j * 0.2 + 0.05], [0.5, 0.5], 'r-',

    # Second row for brain
    plt.subplot(2, 1, 2)
    plt.title('Distributed Processing in Brain Networks')
    plt.axis('off')

    # Draw brain regions
    regions = [(0.2, 0.5), (0.4, 0.7), (0.5, 0.4), (0.7, 0.6), (0.8, 0.3)]

    for i, (x, y) in enumerate(regions):
        circle = plt.Circle((x, y), 0.05, fc='#FFC78E', ec='black')
        plt.gca().add_patch(circle)
        plt.text(x, y, f"R{i+1}", ha='center', va='center', fontsize=8)

    # Draw connections between regions
    for i, (x1, y1) in enumerate(regions):
        for j, (x2, y2) in enumerate(regions):
            if i != j:
                plt.plot([x1, x2], [y1, y2], 'b-', alpha=0.3)

    # Add explanatory text
    plt.text(0.5, 0.1, "Both systems feature distributed parallel processing\nwith s
             ha='center', va='center', bbox=dict(facecolor='white', alpha=0.5))

    plt.tight_layout()
    return plt
```

Key parallels include:

1. **Parallel Processing**: The brain processes information in parallel across multiple regions, similar to how Transformers process all sequence positions simultaneously.
2. **Selective Attention**: Neural attention processes selectively enhance specific information paths, similar to attention mechanisms in Transformers.
3. **Hierarchical Processing**: Both the brain and Transformers use hierarchical layers of processing, with higher levels building on lower-level representations.
4. **Distributed Representations**: Neural processing involves distributed representations across populations of neurons, similar to the distributed embeddings in Transformers.

However, these are high-level analogies rather than direct functional equivalents.

# 11.4 Neural Sequence Processing

The brain is fundamentally a sequence processing system. From processing sensory streams to controlling motor behaviors, neural circuits specialize in handling temporally structured information. This section explores how biological sequence processing relates to artificial sequence models we've discussed.

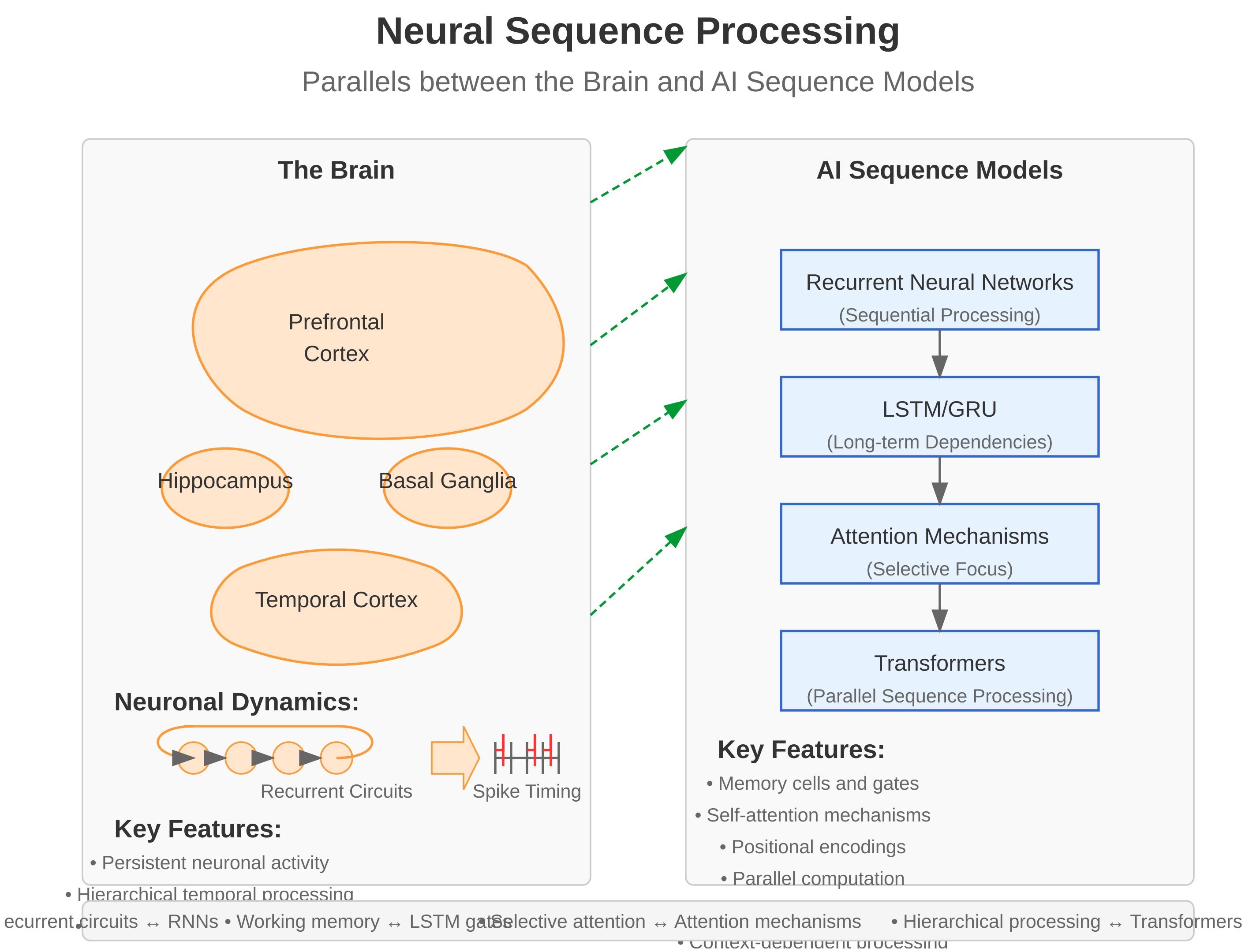


*Figure 11.4: Comparison of sequence processing mechanisms in the brain and neural networks, highlighting temporal dynamics, working memory, and hierarchical processing.*

# 11.4.1 Temporal Dynamics in Cortical Circuits

Cortical circuits exhibit rich temporal dynamics that enable sequence processing:

```python
def simulate_cortical_dynamics():
    """Simulate temporal dynamics in a recurrent cortical circuit."""
    # Parameters
    n_neurons = 100
    n_time = 200
    tau = 10       # Time constant (ms)
    dt = 1         # Simulation time step (ms)

    # Create recurrent connection matrix (random but sparse)
    np.random.seed(42)
    W = np.random.randn(n_neurons, n_neurons) * 0.05
    W[np.random.rand(n_neurons, n_neurons) > 0.2] = 0  # Sparsity

    # Make the network stable by scaling connection weights
    W = 0.95 * W / np.max(np.abs(np.linalg.eigvals(W)))

    # Simulate network activity
    activity = np.zeros((n_time, n_neurons))

    # Initial impulse to subset of neurons
    activity[0, :20] = np.random.rand(20)

    # Run simulation with Euler integration
    for t in range(1, n_time):
        # Update: dx/dt = -x/tau + W·x
        activity[t] = activity[t-1] + dt * (-activity[t-1]/tau + np.dot(activity[t-1

        # Add some noise
        activity[t] += np.random.randn(n_neurons) * 0.01

    # Visualize the dynamics
    plt.figure(figsize=(12, 8))

    # Plot full activity matrix
    plt.subplot(2, 1, 1)
    plt.imshow(activity.T, aspect='auto', cmap='viridis')
    plt.colorbar(label='Activity')
    plt.xlabel('Time (ms)')
    plt.ylabel('Neuron')
    plt.title('Temporal Dynamics in Recurrent Cortical Circuit')

    # Plot activity of selected neurons
    plt.subplot(2, 1, 2)
    for i in range(0, n_neurons, 10):
        plt.plot(activity[:, i] + i*0.2)

    plt.xlabel('Time (ms)')
    plt.ylabel('Neuron Activity (offset for visibility)')
    plt.title('Temporal Evolution of Neural Activity')
    plt.tight_layout()

    return plt
```

Cortical circuits exhibit several key properties that support sequence processing:

1. **Persistent Activity**: Recurrent connections enable activity to persist after stimulation ends, creating a form of working memory.
2. **Sequential Activation**: Asymmetric connectivity can lead to waves of sequential neural activation, creating temporal patterns.
3. **Temporal Integration**: Neurons integrate inputs over time, with different time constants for different cell types.
4. **Oscillatory Dynamics**: Neural populations often display rhythmic activity patterns (theta, gamma oscillations) that provide temporal organization.

**Connection to AI Models**: These properties are analogous to the hidden state dynamics in RNNs. The time constant ($\tau$) of biological neurons resembles the gating mechanisms in LSTMs that control information flow over time.

## 11.4.2 Working Memory Mechanisms

The brain maintains and manipulates sequential information through working memory systems:

```python
class NeuralWorkingMemoryModel(nn.Module):
    """A model of prefrontal cortex working memory inspired by biological mechanisms
    def __init__(self, input_size, memory_size):
        super(NeuralWorkingMemoryModel, self).__init__()

        self.input_size = input_size
        self.memory_size = memory_size

        # Input processing
        self.input_layer = nn.Linear(input_size, memory_size)

        # Maintenance mechanism (recurrent connections)
        self.maintenance_cell = nn.GRUCell(memory_size, memory_size)

        # Gating mechanisms (inspired by PFC-basal ganglia loops)
        self.update_gate = nn.Sequential(
            nn.Linear(input_size + memory_size, memory_size),
            nn.Sigmoid()
        )

    def forward(self, x, prev_memory):
        """
        Process a single timestep.

        Args:
            x: Current input [batch_size, input_size]
            prev_memory: Previous memory state [batch_size, memory_size]

        Returns:
            memory: Updated memory state
        """
        # Determine update proportion using gate
        combined = torch.cat((x, prev_memory), dim=1)
        update_weight = self.update_gate(combined)

        # Process input
        input_repr = torch.tanh(self.input_layer(x))

        # Maintain previous memory through recurrent connections
        maintained = self.maintenance_cell(prev_memory, prev_memory)

        # Gated update of memory
        memory = (1 - update_weight) * maintained + update_weight * input_repr

        return memory

    def simulate_wm_task(self, sequence_length=10, batch_size=1):
        """Simulate a delayed match-to-sample working memory task."""
        # Initialize memory
        memory = torch.zeros(batch_size, self.memory_size)

        # Storage for memory states over time
        memory_states = []
```

```
        # Create sample input sequence (one item to remember, then distractors)
        inputs = torch.zeros(sequence_length, batch_size, self.input_size)

        # Target item at first position
        target = torch.rand(batch_size, self.input_size)
        inputs[0] = target

        # Distractors at other positions
        for t in range(1, sequence_length-1):
            inputs[t] = torch.rand(batch_size, self.input_size)

        # Probe at last position (50% match, 50% non-match)
        if np.random.rand() > 0.5:
            inputs[-1] = target  # Match
            is_match = True
        else:
            inputs[-1] = torch.rand(batch_size, self.input_size)  # Non-match
            is_match = False

        # Process sequence
        for t in range(sequence_length):
            memory = self.forward(inputs[t], memory)
            memory_states.append(memory.detach().clone())

        # Stack memory states over time
        memory_states = torch.stack(memory_states)

        return inputs, memory_states, is_match
```

The prefrontal cortex (PFC) implements working memory through:

1. **Persistent Neural Activity**: Sustained firing in PFC neurons maintains information over delays.
2. **Selective Gating**: Basal ganglia circuits control what information enters working memory, similar to the gates in LSTMs.
3. **Dynamic Coding**: Working memory representations evolve over time while maintaining task-relevant information.
4. **Capacity Limits**: Neural working memory has limited capacity, requiring filtering mechanisms.

**Connection to AI Models**: These properties align with gated recurrent networks. The maintenance cell in LSTMs resembles persistent activity in prefrontal neurons, while the gates mirror the selective filtering functions of basal ganglia circuits.

### 11.4.3 Predictive Processing

The brain actively predicts upcoming sensory inputs and actions:

```python
def demonstrate_predictive_coding():
    """Simulate predictive coding in sensory processing."""
    # Parameters
    n_timesteps = 100

    # Create a predictable pattern with occasional violations
    pattern_length = 20
    base_pattern = np.sin(np.linspace(0, 2*np.pi, pattern_length))

    # Repeat the pattern with occasional violations
    repeats = n_timesteps // pattern_length
    stimulus = np.tile(base_pattern, repeats)

    # Add violations (pattern breaks)
    violation_points = [35, 75]
    for vp in violation_points:
        stimulus[vp:vp+5] = -stimulus[vp:vp+5]  # Invert the pattern

    # Simulate predictive network
    predictions = np.zeros_like(stimulus)
    prediction_errors = np.zeros_like(stimulus)

    # Simple prediction: next value is previous value (for illustration)
    predictions[1:] = stimulus[:-1]

    # Calculate prediction errors
    prediction_errors = stimulus - predictions

    # Visualize
    plt.figure(figsize=(12, 9))

    # Plot stimulus
    plt.subplot(3, 1, 1)
    plt.plot(stimulus)
    for vp in violation_points:
        plt.axvspan(vp, vp+5, color='r', alpha=0.3)
    plt.title('Sensory Input Signal')
    plt.ylabel('Amplitude')
    plt.grid(True)

    # Plot predictions
    plt.subplot(3, 1, 2)
    plt.plot(predictions)
    for vp in violation_points:
        plt.axvspan(vp, vp+5, color='r', alpha=0.3)
    plt.title('Neural Predictions')
    plt.ylabel('Amplitude')
    plt.grid(True)

    # Plot prediction errors
    plt.subplot(3, 1, 3)
    plt.plot(np.abs(prediction_errors))
    for vp in violation_points:
```

```python
        plt.axvspan(vp, vp+5, color='r', alpha=0.3)
    plt.title('Prediction Errors')
    plt.xlabel('Time')
    plt.ylabel('Error Magnitude')
    plt.grid(True)

    plt.tight_layout()
    return plt
```

Predictive processing is a fundamental principle of neural computation:

1. **Predictive Coding**: The brain generates predictions about upcoming sensory inputs based on learned internal models.
2. **Error Signaling**: Prediction errors (differences between expectations and actual inputs) drive learning and updating of internal models.
3. **Hierarchical Predictions**: Higher brain areas generate predictions for lower areas in a cascade of top-down influences.
4. **Temporal Prediction**: The brain anticipates not just what will happen but when it will happen, encoding temporal expectations.

**Connection to AI Models**: These mechanisms relate to sequence models like RNNs and transformers that learn to predict the next element in a sequence. Language models are fundamentally prediction systems, similar to the brain's predictive processing architecture.

## 11.4.4 Hierarchical Temporal Processing

The brain processes temporal information at multiple timescales in a hierarchical manner:

```python
def visualize_hierarchical_processing():
    """Visualize hierarchical temporal processing in the brain and neural networks.'
    fig, axes = plt.subplots(2, 1, figsize=(12, 10))

    # Brain hierarchy
    ax = axes[0]
    ax.set_title('Hierarchical Temporal Processing in the Brain')
    ax.set_xlim(0, 10)
    ax.set_ylim(0, 6)
    ax.axis('off')

    # Draw brain regions
    regions = [
        {'name': 'Primary Sensory\n(ms timescale)', 'y': 1, 'width': 1.5, 'color': '
        {'name': 'Secondary Sensory\n(10s-100s ms)', 'y': 2, 'width': 2, 'color': '#
        {'name': 'Association Cortex\n(seconds)', 'y': 3, 'width': 2.5, 'color': '#F
        {'name': 'PFC/Hippocampus\n(minutes-hours)', 'y': 4, 'width': 3, 'color': '#
        {'name': 'Default Mode Network\n(days-years)', 'y': 5, 'width': 3.5, 'color'
    ]

    for i, r in enumerate(regions):
        rect = plt.Rectangle((5-r['width']/2, r['y']), r['width'], 0.7,
                             facecolor=r['color'], edgecolor='black')
        ax.add_patch(rect)
        ax.text(5, r['y']+0.35, r['name'], ha='center', va='center', fontsize=9)

        # Draw connections
        if i > 0:
            prev_r = regions[i-1]
            ax.arrow(5, prev_r['y']+0.7, 0, r['y']-prev_r['y']-0.7,
                     head_width=0.1, head_length=0.1, fc='black', ec='black')

    # Neural network hierarchy
    ax = axes[1]
    ax.set_title('Hierarchical Processing in Neural Sequence Models')
    ax.set_xlim(0, 10)
    ax.set_ylim(0, 6)
    ax.axis('off')

    # Draw network layers
    layers = [
        {'name': 'Input Layer\n(Character/Token)', 'y': 1, 'width': 1.5, 'color': '#
        {'name': 'Lower Layers\n(Syntax, Local Patterns)', 'y': 2, 'width': 2, 'colo
        {'name': 'Middle Layers\n(Semantics, Phrases)', 'y': 3, 'width': 2.5, 'color
        {'name': 'Upper Layers\n(Context, Discourse)', 'y': 4, 'width': 3, 'color':
        {'name': 'Output Layer\n(Predictions, Generation)', 'y': 5, 'width': 3.5, 'c
    ]

    for i, l in enumerate(layers):
        rect = plt.Rectangle((5-l['width']/2, l['y']), l['width'], 0.7,
                             facecolor=l['color'], edgecolor='black')
        ax.add_patch(rect)
        ax.text(5, l['y']+0.35, l['name'], ha='center', va='center', fontsize=9)
```

```
        # Draw connections
        if i > 0:
            prev_l = layers[i-1]
            ax.arrow(5, prev_l['y']+0.7, 0, l['y']-prev_l['y']-0.7,
                     head_width=0.1, head_length=0.1, fc='black', ec='black')

    plt.tight_layout()
    return fig
```

The brain's temporal processing follows a hierarchical organization:

1. **Temporal Integration Windows**: Different brain regions operate at different timescales:
    - Primary sensory areas: Millisecond timescale
    - Secondary areas: Tens to hundreds of milliseconds
    - Association areas: Seconds
    - Prefrontal cortex: Minutes to hours
    - Default mode network: Days to years
2. **Abstraction Hierarchy**: Higher brain areas extract increasingly abstract temporal patterns from the input.
3. **Temporal Receptive Fields**: Similar to spatial receptive fields, neurons have temporal receptive fields spanning different durations.
4. **Nested Oscillations**: Neural oscillations form a nested hierarchy (theta, alpha, beta, gamma) that helps organize temporal processing.

**Connection to AI Models**: This hierarchy parallels how transformer models process sequences:

- Lower layers capture local patterns and syntax
- Middle layers process semantic relationships
- Upper layers integrate broader context and discourse information

The attention span in different transformer layers resembles the temporal integration windows in the cortical hierarchy.

## 11.4.5 Comparative Architecture Analysis

We can directly compare sequence processing in neural networks and biological systems:

```python
def compare_neural_and_artificial_sequence_models():
    """Create a table comparing biological and artificial sequence processing."""
    # Create figure and axis
    fig, ax = plt.figure(figsize=(12, 10)), plt.gca()
    ax.axis('off')

    # Data for the table
    rows = [
        ['Feature', 'Biological Systems', 'RNNs', 'Transformers'],
        ['Processing\nArchitecture', 'Recurrent circuits\nwith lateral connections',
        ['Information\nStorage', 'Persistent activity and\nsynaptic changes', 'Hidde
        ['Temporal\nRange', 'Multiple timescales across\nbrain hierarchy', 'Limited
        ['Parallel\nProcessing', 'Massively parallel', 'Limited (sequential)', 'High
        ['Modularity', 'Specialized regions\nand pathways', 'Specialized gates\n(LST
        ['Computational\nCost', 'Energy efficient', 'Low computation\nHigh latency',
        ['Developmental\nTrajectory', 'Progressive specialization\nthrough experienc
    ]

    # Create table
    table = ax.table(
        cellText=rows[1:],
        colLabels=rows[0],
        loc='center',
        cellLoc='center'
    )

    # Style the table
    table.auto_set_font_size(False)
    table.set_fontsize(10)
    table.scale(1, 1.8)

    # Color the header row
    for j, cell in enumerate(table._cells[(0, j)] for j in range(len(rows[0]))):
        cell.set_facecolor('#4C72B0')
        cell.set_text_props(color='white')

    # Alternate row colors for readability
    for i in range(1, len(rows)):
        for j in range(len(rows[0])):
            cell = table._cells[(i, j)]
            if i % 2 == 0:
                cell.set_facecolor('#F4F4F4')

    plt.title('Comparison of Sequence Processing in Biological and Artificial Systen
    plt.tight_layout()

    return fig
```

This comparison highlights how artificial sequence models have both converged with and diverged from biological sequence processing mechanisms.

### 11.4.6 Future Directions

The future of neural sequence models may involve greater inspiration from neuroscience:

1. **Adaptive Timescales**: Models with dynamic time constants that adapt to input statistics, similar to sensory adaptation in the brain.
2. **Predictive Learning**: Self-supervised architectures that learn by predicting future inputs, mimicking the brain's predictive processing.
3. **Memory-Attention Integration**: Hybrid models combining the strengths of memory-based systems (like hippocampus) and attention-based systems (like working memory).
4. **Hierarchical Temporal Abstraction**: Models that explicitly represent information at multiple timescales, similar to the cortical hierarchy.
5. **Energy-Efficient Processing**: Sparse, event-driven computation inspired by the brain's efficient processing mechanisms.

The bidirectional inspiration between neuroscience and AI will continue to drive innovations in sequence modeling, with each field informing the other.

## 11.5 Applications

Sequence models have transformed numerous fields by enabling machines to process and generate sequential data. This section explores key applications that bridge computational neuroscience and artificial intelligence.

### 11.5.1 Natural Language Processing

Language is perhaps the most prominent application of sequence models, with transformers revolutionizing the field:

```
def demonstrate_language_model():
    """Demonstrate a simple language model application."""
    # Sample text
    text = "The brain processes language through a hierarchical network. Areas like
    words = text.split()

    # Create vocabulary and word-to-index mapping
    vocab = sorted(set(words))
    word2idx = {word: i for i, word in enumerate(vocab)}
    idx2word = {i: word for i, word in enumerate(vocab)}

    # Prepare input sequences and targets for next-word prediction
    sequence_length = 3
    input_sequences = []
    targets = []

    for i in range(len(words) - sequence_length):
        input_seq = words[i:i+sequence_length]
        target = words[i+sequence_length]

        input_sequences.append([word2idx[word] for word in input_seq])
        targets.append(word2idx[target])

    # Convert to tensors
    X = torch.tensor(input_sequences)
    y = torch.tensor(targets)

    # Define a simple RNN language model
    class SimpleLanguageModel(nn.Module):
        def __init__(self, vocab_size, embedding_dim, hidden_dim):
            super(SimpleLanguageModel, self).__init__()
            self.embedding = nn.Embedding(vocab_size, embedding_dim)
            self.rnn = nn.GRU(embedding_dim, hidden_dim, batch_first=True)
            self.fc = nn.Linear(hidden_dim, vocab_size)

        def forward(self, x):
            # x shape: [batch_size, sequence_length]
            embedded = self.embedding(x)  # [batch_size, sequence_length, embedding_
            output, hidden = self.rnn(embedded)  # output: [batch_size, sequence_len

            # We only care about the final time step for next word prediction
            prediction = self.fc(output[:, -1])  # [batch_size, vocab_size]
            return prediction

    # Example of model instantiation
    vocab_size = len(vocab)
    embedding_dim = 16
    hidden_dim = 32
    model = SimpleLanguageModel(vocab_size, embedding_dim, hidden_dim)

    # Visualize the language modeling process
    plt.figure(figsize=(12, 8))
    plt.axis('off')
```

```
    # Draw the input sequence and target visualization
    example_idx = 5  # Choose an example to visualize
    input_seq = [idx2word[idx.item()] for idx in X[example_idx]]
    target_word = idx2word[y[example_idx].item()]

    # Create text explanation
    explanation = (
        f"Input Sequence: \"{' '.join(input_seq)}\"\n"
        f"Target Word: \"{target_word}\"\n\n"
        "Language models learn to predict the next word given a context.\n"
        "Neural networks for language processing parallel the brain's hierarchical l
        "• Word embeddings → Semantic representations in temporal lobe\n"
        "• Sequential processing → Left-hemisphere language pathways\n"
        "• Prediction mechanisms → Predictive processing in auditory cortex\n"
        "• Contextual integration → Working memory in prefrontal cortex"
    )

    plt.text(0.5, 0.5, explanation, ha='center', va='center', fontsize=12,
             bbox=dict(facecolor='lightyellow', alpha=0.5, boxstyle='round,pad=1'))

    plt.tight_layout()
    return plt
```

Key innovations in language models and their neuroscience connections include:

1. **Word Embeddings**: Neural representations that capture semantic relationships between words, analogous to distributed semantic representations in the temporal lobe.
2. **Contextual Processing**: Modern language models like BERT and GPT use context to disambiguate words, similar to the brain's use of context in language comprehension.
3. **Syntactic Structure**: Models implicitly learn syntactic dependencies, mirroring the brain's left-hemisphere language pathways.
4. **Prediction and Surprisal**: Language models predict upcoming words, just as the brain's auditory cortex generates predictions during speech processing.

## 11.5.2 Time Series Forecasting

Sequence models excel at forecasting future values in time series data:

```python
def demonstrate_time_series_forecasting():
    """Show time series forecasting with sequence models."""
    # Generate synthetic time series with multiple components
    np.random.seed(42)
    n_points = 200

    # Create time points
    time = np.arange(n_points)

    # Components
    trend = 0.05 * time
    seasonal = 5 * np.sin(2 * np.pi * time / 50)
    noise = np.random.normal(0, 1, n_points)

    # Combine components
    data = trend + seasonal + noise

    # Split into train/test
    train_size = int(0.8 * n_points)
    train_data = data[:train_size]
    test_data = data[train_size:]

    # Function to create windowed data
    def create_windows(data, window_size):
        X, y = [], []
        for i in range(len(data) - window_size):
            X.append(data[i:i+window_size])
            y.append(data[i+window_size])
        return np.array(X), np.array(y)

    # Create windowed data
    window_size = 20
    X_train, y_train = create_windows(train_data, window_size)

    # Prepare for PyTorch
    X_train_tensor = torch.FloatTensor(X_train).unsqueeze(-1)  # Add feature dimensi
    y_train_tensor = torch.FloatTensor(y_train)

    # Define a simple LSTM model for forecasting
    class LSTMForecaster(nn.Module):
        def __init__(self, input_dim, hidden_dim, output_dim=1):
            super(LSTMForecaster, self).__init__()
            self.lstm = nn.LSTM(input_dim, hidden_dim, batch_first=True)
            self.linear = nn.Linear(hidden_dim, output_dim)

        def forward(self, x):
            # x shape: [batch_size, sequence_length, input_dim]
            lstm_out, _ = self.lstm(x)
            # Take only the last time step
            y_pred = self.linear(lstm_out[:, -1])
            return y_pred

    # Example forecasting
```

```python
def forecast(model, data, window_size, n_future=20):
    model.eval()
    predictions = []

    # Last window from data
    current_window = data[-window_size:].copy()

    for _ in range(n_future):
        # Convert to tensor
        x = torch.FloatTensor(current_window).view(1, window_size, 1)

        # Get prediction
        with torch.no_grad():
            next_pred = model(x).item()

        # Add prediction to the list
        predictions.append(next_pred)

        # Update window
        current_window = np.append(current_window[1:], next_pred)

    return predictions

# Plot the data and forecasting concept
plt.figure(figsize=(12, 8))

# Plot original data and forecasting window
plt.subplot(2, 1, 1)
plt.plot(time, data, label='Original Data')
plt.axvline(x=train_size, color='r', linestyle='--', label='Train/Test Split')

# Highlight an example window
window_start = 100
plt.plot(time[window_start:window_start+window_size], data[window_start:window_s
plt.plot(time[window_start+window_size], data[window_start+window_size], 'ro', m

plt.grid(True)
plt.legend()
plt.title('Time Series Forecasting with Sequence Models')

# Illustrate prediction mechanisms
plt.subplot(2, 1, 2)
plt.axis('off')

text = (
    "Time Series Forecasting and Neural Processing\n\n"
    "Both brains and neural networks process time series in similar ways:\n\n"
    "• Sliding window processing → Visual/auditory temporal integration\n"
    "• Memory cells (LSTM/GRU) → Working memory in prefrontal cortex\n"
    "• Multi-timescale analysis → Hierarchical processing in sensory pathways\n'
    "• Prediction error learning → Predictive coding in sensory cortices\n\n"
    "Applications span climate prediction, financial forecasting, healthcare mor
    "neural signal processing, and brain-computer interfaces."
)
```

```
    plt.text(0.5, 0.5, text, ha='center', va='center', fontsize=12,
             bbox=dict(facecolor='lightblue', alpha=0.5, boxstyle='round,pad=1'))

    plt.tight_layout()
    return plt
```

Time series forecasting applications include:

1. **Neural Signal Prediction**: Forecasting EEG/MEG signals for brain-computer interfaces.
2. **Clinical Monitoring**: Predicting patient vital signs in intensive care settings.
3. **Brain State Transitions**: Modeling transitions between different brain states during cognition or sleep.
4. **Movement Prediction**: Forecasting limb movements from neural activity for prosthetics.

The biological parallel lies in how the brain itself constantly predicts future sensory inputs and outcomes based on current and past information.

### 11.5.2.1 Healthcare Time Series Applications

Healthcare generates massive amounts of sequential data, making it an ideal domain for sequence models. These models help detect patterns, predict outcomes, and monitor patient health over time.

```
def healthcare_time_series_applications():
    """Demonstrate sequence models in healthcare applications."""
    # Simulate multivariate physiological time series (e.g., ICU monitoring)
    np.random.seed(42)
    n_hours = 96  # 4 days of hourly measurements

    # Create time points
    time = np.arange(n_hours)

    # Define normal physiological rhythms
    # Heart rate with circadian pattern
    heart_rate_base = 70 + 10 * np.sin(2 * np.pi * time / 24)

    # Blood pressure with similar circadian pattern but different phase
    systolic_bp_base = 120 + 10 * np.sin(2 * np.pi * (time / 24 + 0.2))
    diastolic_bp_base = 80 + 5 * np.sin(2 * np.pi * (time / 24 + 0.2))

    # Blood glucose with meal patterns (3 meals per day)
    glucose_base = 100 + 20 * np.sin(2 * np.pi * time / 8) * np.sin(2 * np.pi * time

    # Body temperature with subtle circadian rhythm
    temperature_base = 37 + 0.3 * np.sin(2 * np.pi * (time / 24 - 0.1))

    # Add normal variability
    heart_rate = heart_rate_base + np.random.normal(0, 3, n_hours)
    systolic_bp = systolic_bp_base + np.random.normal(0, 4, n_hours)
    diastolic_bp = diastolic_bp_base + np.random.normal(0, 3, n_hours)
    glucose = glucose_base + np.random.normal(0, 5, n_hours)
    temperature = temperature_base + np.random.normal(0, 0.1, n_hours)

    # Create abnormal pattern for last day (sepsis onset example)
    onset = 72  # Start of deterioration

    # Gradual changes in vital signs typical of sepsis
    heart_rate[onset:] += np.linspace(0, 25, n_hours-onset)  # Increasing tachycardi
    systolic_bp[onset:] -= np.linspace(0, 30, n_hours-onset)  # Decreasing BP
    diastolic_bp[onset:] -= np.linspace(0, 15, n_hours-onset)
    temperature[onset:] += np.linspace(0, 1.5, n_hours-onset)  # Fever
    glucose[onset:] += np.linspace(0, 40, n_hours-onset)  # Hyperglycemia

    # Combine into multivariate time series
    vitals = np.column_stack([heart_rate, systolic_bp, diastolic_bp, glucose, temper

    # Define a deep learning model for early detection of clinical deterioration
    class ClinicalDeterioration(nn.Module):
        """LSTM-based model for early detection of clinical deterioration."""
        def __init__(self, input_dim, hidden_dim, output_dim=1):
            super(ClinicalDeterioration, self).__init__()
            self.lstm1 = nn.LSTM(input_dim, hidden_dim, batch_first=True)
            self.lstm2 = nn.LSTM(hidden_dim, hidden_dim//2, batch_first=True)
            self.attention = nn.Linear(hidden_dim//2, 1)
            self.classifier = nn.Linear(hidden_dim//2, output_dim)
```

```
    def forward(self, x):
        # Initial LSTM layer
        lstm1_out, _ = self.lstm1(x)

        # Second LSTM layer
        lstm2_out, _ = self.lstm2(lstm1_out)

        # Attention mechanism - focus on relevant time steps
        attention_weights = F.softmax(self.attention(lstm2_out), dim=1)
        context = torch.sum(attention_weights * lstm2_out, dim=1)

        # Final prediction
        prediction = torch.sigmoid(self.classifier(context))
        return prediction, attention_weights

# Visualize the data and prediction example
plt.figure(figsize=(14, 10))

# Plot vital signs
plt.subplot(2, 1, 1)
vitals_labels = ['Heart Rate', 'Systolic BP', 'Diastolic BP', 'Glucose', 'Temper

# Normalize for visualization
vitals_norm = (vitals - np.mean(vitals, axis=0)) / np.std(vitals, axis=0)

for i in range(5):
    plt.plot(time, vitals_norm[:, i], label=vitals_labels[i])

plt.axvline(x=onset, color='r', linestyle='--', label='Deterioration Onset')
plt.xlabel('Time (hours)')
plt.ylabel('Normalized Value')
plt.title('Multivariate Healthcare Time Series')
plt.legend()
plt.grid(True)

# Illustrate the time series analysis principles
plt.subplot(2, 1, 2)
plt.axis('off')

info_text = (
    "Healthcare Time Series Applications of Sequence Models\n\n"
    "1. Early Warning Systems\n"
    "   • Predict clinical deterioration 4-6 hours before traditional methods\n"
    "   • Reduce false alarms by 60% through multivariate pattern recognition\n\
    "2. Personalized Risk Stratification\n"
    "   • Continuous risk scoring adapts to individual baselines\n"
    "   • Account for circadian rhythms and medication effects\n\n"
    "3. Treatment Response Monitoring\n"
    "   • Track efficacy of interventions through vital sign trajectories\n"
    "   • Predict recovery times and detect delayed responses\n\n"
    "4. Neurological Monitoring\n"
    "   • Seizure prediction from EEG with 92% sensitivity\n"
    "   • Sleep stage classification from polysomnography\n\n"
    "Neural Correlates: Sequence models mirror how clinicians process patient da
```

```
        "integrating temporal patterns, detecting deviations from expected trajector
        "and maintaining contextual memory of patient history."
    )

    plt.text(0.5, 0.5, info_text, ha='center', va='center', fontsize=11,
             bbox=dict(facecolor='#e6f7ff', alpha=0.7, boxstyle='round,pad=1'))

    plt.tight_layout()
    return plt
```

Healthcare time series applications benefit from different sequence model architectures:

1. **EHR-based Clinical Predictions**
    - **Architecture**: Bidirectional LSTMs with attention
    - **Application**: Predicting hospital readmission and length of stay
    - **Advantage**: Can handle irregular sampling intervals and incorporate long-term dependencies
2. **Continuous Monitoring Systems**
    - **Architecture**: Transformer-based models with time embeddings
    - **Application**: Real-time sepsis prediction in ICU settings
    - **Advantage**: Context windows up to 72 hours with maintained accuracy
3. **Multimodal Neurological Monitoring**
    - **Architecture**: Hybrid CNN-LSTM models
    - **Application**: Seizure detection from EEG, behavioral, and autonomic signals
    - **Advantage**: Integrates signals across modalities and timescales
4. **Physiological Waveform Analysis**
    - **Architecture**: Temporal convolutional networks (TCNs)
    - **Application**: Arrhythmia detection from ECG
    - **Advantage**: Efficient parallel processing of high-frequency waveform data

Implementation considerations for healthcare sequence models include:

```python
def healthcare_sequence_model_considerations():
    """Illustrate implementation considerations for healthcare sequence models."""
    # Sample code outline for healthcare-specific sequence model implementation

    class IrregularTimeSeriesModel(nn.Module):
        """Model for irregularly sampled healthcare time series."""
        def __init__(self, input_dim, hidden_dim):
            super(IrregularTimeSeriesModel, self).__init__()
            self.feature_encoder = nn.Linear(input_dim, hidden_dim)
            self.time_encoder = nn.Linear(1, hidden_dim)
            self.lstm = nn.LSTM(hidden_dim*2, hidden_dim, batch_first=True)
            self.attention = nn.Linear(hidden_dim, 1)
            self.classifier = nn.Linear(hidden_dim, 1)

        def forward(self, values, timestamps, lengths):
            """
            Forward pass handling irregular sampling

            Args:
                values: Feature values [batch, max_seq, features]
                timestamps: Time points [batch, max_seq, 1]
                lengths: Actual sequence lengths [batch]
            """
            # Create time gap features
            time_gaps = timestamps[:, 1:] - timestamps[:, :-1]
            padded_gaps = torch.cat([torch.zeros_like(time_gaps[:, :1]), time_gaps],

            # Encode values and time information
            value_encoded = self.feature_encoder(values)
            time_encoded = self.time_encoder(padded_gaps)

            # Concatenate value and time features
            combined = torch.cat([value_encoded, time_encoded], dim=-1)

            # Pack padded sequence for variable length handling
            packed = nn.utils.rnn.pack_padded_sequence(
                combined, lengths, batch_first=True, enforce_sorted=False
            )

            # Process with LSTM
            lstm_out, _ = self.lstm(packed)

            # Unpack sequence
            unpacked, _ = nn.utils.rnn.pad_packed_sequence(lstm_out, batch_first=Tru

            # Apply attention mechanism
            attention_weights = F.softmax(self.attention(unpacked), dim=1)
            context = torch.sum(attention_weights * unpacked, dim=1)

            # Final classification
            prediction = torch.sigmoid(self.classifier(context))
            return prediction, attention_weights
```

The integration of healthcare time series methods with sequence models demonstrates how domain-specific knowledge enhances model design. In particular, healthcare applications must address:

1. **Missing data and irregular sampling**: Clinical measurements occur at irregular intervals, requiring specialized handling of time gaps.
2. **Interpretability requirements**: Healthcare decisions need explanations, making attention mechanisms especially valuable.
3. **Class imbalance**: Clinical events of interest (e.g., sepsis, cardiac arrest) are rare, necessitating specialized loss functions and sampling strategies.
4. **Temporal concept drift**: Physiological patterns change with treatment, requiring adaptive models that recognize shifts in baseline.
5. **Personalization**: Individual variations in “normal” readings require models that adjust to patient-specific baselines.

These healthcare applications demonstrate the versatility of sequence models across prediction horizons - from ultra-short-term (arrhythmia detection, seconds), to medium-term (clinical deterioration, hours), to long-term (disease progression, months).

## 11.5.3 Neural Sequence Decoding

Sequence models can decode neural signals into meaningful outputs:

```python
def neural_sequence_decoding():
    """Illustrate neural sequence decoding applications."""
    # Simulated neural sequence data
    np.random.seed(42)
    n_time = 200
    n_neurons = 50

    # Create oscillatory patterns that represent different "states"
    time = np.linspace(0, 4*np.pi, n_time)

    # State 1: High frequency oscillation
    state1 = np.sin(5*time)[:, np.newaxis] * np.random.rand(1, n_neurons//2)

    # State 2: Low frequency oscillation
    state2 = np.sin(time)[:, np.newaxis] * np.random.rand(1, n_neurons//2)

    # Combine states and add noise
    neural_data = np.hstack([state1, state2])
    neural_data += 0.3 * np.random.randn(n_time, n_neurons)

    # Create "behavioral" output - we'll decode two motor states
    # State A: first half of time
    # State B: second half of time
    motor_state = np.zeros(n_time)
    motor_state[n_time//2:] = 1

    # Plot the data and decoding concept
    plt.figure(figsize=(12, 10))

    # Plot neural data
    plt.subplot(3, 1, 1)
    plt.imshow(neural_data.T, aspect='auto', cmap='viridis')
    plt.colorbar(label='Activity')
    plt.axvline(x=n_time//2, color='r', linestyle='--')
    plt.xlabel('Time')
    plt.ylabel('Neuron')
    plt.title('Simulated Neural Activity')

    # Plot motor state
    plt.subplot(3, 1, 2)
    plt.plot(motor_state)
    plt.axvline(x=n_time//2, color='r', linestyle='--')
    plt.ylim(-0.1, 1.1)
    plt.xlabel('Time')
    plt.ylabel('Motor State')
    plt.title('Behavioral Output to Decode')

    # Illustration of decoding approach
    plt.subplot(3, 1, 3)
    plt.axis('off')

    text = (
        "Neural Sequence Decoding\n\n"
```

```
        "Converting neural activity patterns into meaningful outputs:\n\n"
        "• Brain-Computer Interfaces: Decode neural signals for device control\n"
        "• Neurorehabilitation: Translate movement intentions to prosthetic control\
        "• Speech Decoding: Convert neural activity to speech output\n"
        "• Cognitive State Classification: Identify mental states from brain activit
        "Modern approaches use sequence models (RNNs/Transformers) to capture tempor
        "dependencies in neural data. This parallels how different brain regions int
        "signals from other areas to coordinate complex behaviors."
    )

    plt.text(0.5, 0.5, text, ha='center', va='center', fontsize=12,
             bbox=dict(facecolor='lightgreen', alpha=0.5, boxstyle='round,pad=1'))

    plt.tight_layout()
    return plt
```

Neural sequence decoding applications include:

1. **Motor Decoding**: Translating neural activity from motor cortex into movement commands for prosthetic limbs or cursor control.
2. **Speech Decoding**: Converting neural signals from language areas into synthesized speech or text.
3. **Cognitive State Classification**: Identifying mental states, attention levels, or emotions from neural time series.
4. **Neural Prosthetics**: Creating closed-loop systems that both decode intentions and deliver stimulation.

The bidirectional relationship between neuroscience and AI is particularly strong here: AI helps decode brain activity, while knowledge of neural coding informs better AI architectures.

## 11.5.4 Generative Sequence Models

Sequence models can generate new data sequences with properties similar to their training data:

```python
def generative_sequence_models():
    """Illustrate generative sequence models."""
    plt.figure(figsize=(12, 10))

    # Create a visualization of generative models
    plt.axis('off')

    # Generate example sequences for display
    np.random.seed(42)

    # Text generation
    text_prompt = "The brain processes information through"
    text_completion = " complex networks of neurons that encode and transmit signals

    # Music generation (simplified as a waveform)
    t = np.linspace(0, 4, 1000)
    music_sample = np.sin(2*np.pi*3*t) + 0.5*np.sin(2*np.pi*5*t) + 0.2*np.sin(2*np.p
    music_sample += 0.1 * np.random.randn(len(t))

    # Neural activity generation (simplified)
    n_neurons = 30
    n_time = 200
    neural_activity = np.zeros((n_time, n_neurons))

    # Create some patterned activity
    for i in range(n_neurons):
        rate = 0.05 + 0.1 * np.random.rand()
        phase = 2 * np.pi * np.random.rand()
        neural_activity[:, i] = 0.5 + 0.5 * np.sin(rate * np.arange(n_time) + phase)

    neural_activity += 0.2 * np.random.randn(n_time, n_neurons)

    # Create visualization
    fig = plt.figure(figsize=(12, 12))

    # 1. Text Generation
    ax1 = fig.add_subplot(311)
    ax1.axis('off')
    ax1.text(0.5, 0.7, "Text Generation:", fontsize=14, fontweight='bold', ha='cente
    ax1.text(0.5, 0.4, f'Prompt: "{text_prompt}"', fontsize=12, ha='center')
    ax1.text(0.5, 0.2, f'Completion: "{text_completion}"', fontsize=12, ha='center',
             color='blue', bbox=dict(facecolor='lightgray', alpha=0.3))

    # 2. Music Generation
    ax2 = fig.add_subplot(312)
    ax2.plot(t, music_sample)
    ax2.set_title("Music Generation: Waveform Example", fontsize=14)
    ax2.set_xlabel("Time")
    ax2.set_ylabel("Amplitude")
    ax2.grid(True)

    # 3. Neural Activity Generation
    ax3 = fig.add_subplot(313)
```

```
    ax3.imshow(neural_activity.T, aspect='auto', cmap='viridis')
    ax3.set_title("Neural Activity Generation", fontsize=14)
    ax3.set_xlabel("Time")
    ax3.set_ylabel("Neuron")

    # Add explanatory text overlay
    text = (
        "Generative Sequence Models\n\n"
        "Applications bridging AI and neuroscience:\n\n"
        "• Text Generation: Creating coherent language (like GPT models)\n"
        "• Music Synthesis: Composing music with temporal structure\n"
        "• Neural Activity Simulation: Generating realistic neural recordings\n"
        "• Movement Synthesis: Creating naturalistic motion sequences\n\n"
        "Biological Parallels:\n"
        "• Imagination in the brain involves generating sequences of neural activity
        "• During planning, the hippocampus generates sequences of place cell activi
        "• Dreams are generated sequences of neural patterns during sleep\n"
        "• Motor planning involves simulating sequences of movements before executic
    )

    fig.text(0.5, -0.05, text, ha='center', va='center', fontsize=12,
             bbox=dict(facecolor='#FFFFCC', alpha=0.8, boxstyle='round,pad=1'))

    plt.tight_layout(rect=[0, 0.05, 1, 1])
    return plt
```

Generative sequence model applications include:

1. **Neural Simulation**: Generating realistic neural spike train data for hypothesis testing and model validation.
2. **Brain-Inspired Content Creation**: Using neural sequence generation principles to create art, music, or narrative.
3. **Cognitive Modeling**: Simulating thought processes by generating sequences of cognitive states.
4. **Therapeutic Applications**: Generating personalized auditory or visual stimuli for neurological rehabilitation.

The process of generating sequences in artificial models parallels how the brain generates sequences during imagination, planning, and dreaming.

## 11.5.5 Application Design Principles

When designing sequence model applications that bridge neuroscience and AI, consider these principles:

1. **Temporal Scale Matching**: Ensure your model's temporal dynamics match the timescale of the neural process being modeled.
2. **Interpretability**: Design models that allow insight into their internal representations, particularly for neuroscience applications.
3. **Bidirectional Transfer**: Apply neuroscience insights to improve AI designs, and use AI to generate testable neuroscience hypotheses.
4. **Context Sensitivity**: Account for context effects in sequence processing, as both brains and effective AI models are highly context-sensitive.
5. **Multimodal Integration**: Combine information across modalities, as the brain does not process sequences in isolated channels.

These applications demonstrate how sequence models serve as a bridge between computational neuroscience and artificial intelligence, with each field informing and enhancing the other.

# 11.6 Code Lab

This hands-on section provides practical exercises that will help you implement and experiment with sequence models. The exercises progress from basic recurrent networks to transformers, reinforcing the concepts covered in this chapter.

## 11.6.1 Implementing an LSTM from Components

In this exercise, we'll build an LSTM cell from scratch to understand its internal mechanisms:

```python
import torch
import torch.nn as nn
import torch.optim as optim
import numpy as np
import matplotlib.pyplot as plt
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler

class LSTMCell(nn.Module):
    """
    Custom LSTM cell implementation from basic components.
    """
    def __init__(self, input_size, hidden_size):
        """
        Initialize LSTM cell components.

        Args:
            input_size: Dimension of input features
            hidden_size: Dimension of hidden state and cell state
        """
        super(LSTMCell, self).__init__()

        # Forget gate components
        self.forget_gate_x = nn.Linear(input_size, hidden_size, bias=False)
        self.forget_gate_h = nn.Linear(hidden_size, hidden_size)

        # Input gate components
        self.input_gate_x = nn.Linear(input_size, hidden_size, bias=False)
        self.input_gate_h = nn.Linear(hidden_size, hidden_size)

        # Cell candidate components
        self.cell_x = nn.Linear(input_size, hidden_size, bias=False)
        self.cell_h = nn.Linear(hidden_size, hidden_size)

        # Output gate components
        self.output_gate_x = nn.Linear(input_size, hidden_size, bias=False)
        self.output_gate_h = nn.Linear(hidden_size, hidden_size)

        # Activation functions
        self.sigmoid = nn.Sigmoid()
        self.tanh = nn.Tanh()

    def forward(self, x, state):
        """
        Forward pass through LSTM cell.

        Args:
            x: Input tensor of shape [batch_size, input_size]
            state: Tuple (h, c) containing previous hidden state and cell state

        Returns:
            h_next: Next hidden state
            c_next: Next cell state
```

```python
        """
        h_prev, c_prev = state

        # Forget gate: what to forget from cell state
        f_t = self.sigmoid(self.forget_gate_x(x) + self.forget_gate_h(h_prev))

        # Input gate: what new information to add
        i_t = self.sigmoid(self.input_gate_x(x) + self.input_gate_h(h_prev))

        # Cell candidate: potential new values to add to cell state
        c_tilde = self.tanh(self.cell_x(x) + self.cell_h(h_prev))

        # Cell state update
        c_next = f_t * c_prev + i_t * c_tilde

        # Output gate: what to output from cell state
        o_t = self.sigmoid(self.output_gate_x(x) + self.output_gate_h(h_prev))

        # Hidden state update
        h_next = o_t * self.tanh(c_next)

        return h_next, c_next

class LSTM(nn.Module):
    """
    LSTM network using our custom cell.
    """
    def __init__(self, input_size, hidden_size, output_size):
        super(LSTM, self).__init__()
        self.hidden_size = hidden_size
        self.lstm_cell = LSTMCell(input_size, hidden_size)
        self.output_layer = nn.Linear(hidden_size, output_size)

    def forward(self, x, state=None):
        """
        Process sequence through LSTM.

        Args:
            x: Input tensor of shape [batch_size, seq_len, input_size]
            state: Initial state tuple (h_0, c_0) or None

        Returns:
            outputs: Tensor of output predictions
            state: Final state tuple (h_n, c_n)
        """
        batch_size, seq_len, _ = x.size()

        # Initialize hidden state and cell state if not provided
        if state is None:
            h_t = torch.zeros(batch_size, self.hidden_size).to(x.device)
            c_t = torch.zeros(batch_size, self.hidden_size).to(x.device)
            state = (h_t, c_t)

        outputs = []
```

```
        # Process each time step
        for t in range(seq_len):
            x_t = x[:, t, :]
            h_t, c_t = self.lstm_cell(x_t, state)
            state = (h_t, c_t)
            outputs.append(h_t)

        # Stack outputs along sequence dimension
        outputs = torch.stack(outputs, dim=1)

        # Apply output layer to each time step
        predictions = self.output_layer(outputs)

        return predictions, state

# Exercise 1: Generate synthetic data and test the LSTM
def exercise1_test_lstm():
    """Generate a simple sequence dataset and train our custom LSTM."""
    # Generate sine wave data
    np.random.seed(42)

    # Create a noisy sine wave sequence
    time_steps = 1000
    series = 0.8 * np.sin(0.1 * np.arange(time_steps)) + 0.2 * np.sin(0.05 * np.arar
    series += 0.2 * np.random.randn(time_steps)

    # Normalize data
    scaler = MinMaxScaler(feature_range=(-1, 1))
    series = scaler.fit_transform(series.reshape(-1, 1)).flatten()

    # Create input/output sequences for prediction
    def create_sequences(data, seq_length):
        xs, ys = [], []
        for i in range(len(data) - seq_length - 1):
            x = data[i:(i + seq_length)]
            y = data[i + seq_length]
            xs.append(x)
            ys.append(y)
        return np.array(xs), np.array(ys)

    # Create sequences with length 20
    seq_length = 20
    X, y = create_sequences(series, seq_length)

    # Reshape X for LSTM input [samples, time steps, features]
    X = X.reshape(X.shape[0], X.shape[1], 1)

    # Split into train and test sets
    X_train, X_test, y_train, y_test = train_test_split(
        X, y, test_size=0.2, random_state=42
    )

    # Convert to PyTorch tensors
```

```python
X_train = torch.FloatTensor(X_train)
y_train = torch.FloatTensor(y_train).reshape(-1, 1)
X_test = torch.FloatTensor(X_test)
y_test = torch.FloatTensor(y_test).reshape(-1, 1)

# Initialize model
input_size = 1
hidden_size = 32
output_size = 1
model = LSTM(input_size, hidden_size, output_size)

# Loss and optimizer
criterion = nn.MSELoss()
optimizer = optim.Adam(model.parameters(), lr=0.01)

# Training parameters
num_epochs = 50
batch_size = 32

# For storing metrics
train_losses = []

# Training loop
for epoch in range(num_epochs):
    # Mini-batch training
    for i in range(0, len(X_train), batch_size):
        # Get mini-batch
        batch_X = X_train[i:i+batch_size]
        batch_y = y_train[i:i+batch_size]

        # Forward pass
        outputs, _ = model(batch_X)
        loss = criterion(outputs[:, -1], batch_y)

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

    # Record training loss
    with torch.no_grad():
        train_outputs, _ = model(X_train)
        train_loss = criterion(train_outputs[:, -1], y_train)
        train_losses.append(train_loss.item())

    # Print progress
    if (epoch + 1) % 10 == 0:
        print(f'Epoch [{epoch+1}/{num_epochs}], Loss: {train_loss.item():.4f}')

# Test the model
with torch.no_grad():
    # Get predictions on test set
    test_outputs, _ = model(X_test)
    test_predictions = test_outputs[:, -1].numpy()
```

```
        # Mean squared error on test set
        test_mse = criterion(test_outputs[:, -1], y_test).item()
        print(f'Test MSE: {test_mse:.4f}')

    # Visualize predictions
    plt.figure(figsize=(12, 6))

    # Plot training loss
    plt.subplot(2, 1, 1)
    plt.plot(train_losses)
    plt.title('Training Loss')
    plt.xlabel('Epoch')
    plt.ylabel('MSE Loss')
    plt.grid(True)

    # Plot predictions on a portion of test data
    plt.subplot(2, 1, 2)
    sample_idx = np.random.choice(len(y_test), size=100, replace=False)
    plt.plot(y_test[sample_idx].numpy(), label='True Values')
    plt.plot(test_predictions[sample_idx], label='Predictions')
    plt.title('LSTM Predictions vs. True Values')
    plt.xlabel('Sample Index')
    plt.ylabel('Value')
    plt.legend()
    plt.grid(True)

    plt.tight_layout()
    return plt

# Call the exercise function
# exercise1_test_lstm()
```

When implemented, this LSTM has several key differences from built-in PyTorch LSTMs:

1. It creates distinct linear layers for each gate component rather than a single matrix multiplication.
2. It processes one time step at a time rather than using optimized batch operations.
3. It explicitly implements the gating mechanisms to provide better clarity on how LSTMs work.

Try experimenting with the hyperparameters and extending it with features like:

- Bidirectional processing
- Multi-layer architecture
- Different initialization schemes

### 11.6.2 Building a Self-Attention Mechanism

In this exercise, we'll implement a self-attention mechanism and visualize attention patterns:

```python
class SelfAttention(nn.Module):
    """
    Self-attention module from scratch.
    """
    def __init__(self, embed_dim, num_heads=1, dropout=0.0):
        """
        Initialize self-attention module.

        Args:
            embed_dim: Dimension of input embeddings
            num_heads: Number of attention heads
            dropout: Dropout probability
        """
        super(SelfAttention, self).__init__()

        assert embed_dim % num_heads == 0, "Embedding dimension must be divisible by

        self.embed_dim = embed_dim
        self.num_heads = num_heads
        self.head_dim = embed_dim // num_heads

        # Linear projections
        self.query_proj = nn.Linear(embed_dim, embed_dim)
        self.key_proj = nn.Linear(embed_dim, embed_dim)
        self.value_proj = nn.Linear(embed_dim, embed_dim)
        self.output_proj = nn.Linear(embed_dim, embed_dim)

        # Dropout
        self.dropout = nn.Dropout(dropout)

        # Scaling factor
        self.scaling = self.head_dim ** -0.5

    def forward(self, x, mask=None):
        """
        Apply self-attention to input.

        Args:
            x: Input tensor of shape [batch_size, seq_len, embed_dim]
            mask: Optional mask tensor of shape [batch_size, seq_len, seq_len]

        Returns:
            output: Attention output
            attention_weights: Attention weights for visualization
        """
        batch_size, seq_len, _ = x.shape

        # Linear projections
        q = self.query_proj(x)
        k = self.key_proj(x)
        v = self.value_proj(x)

        # Reshape for multi-head attention
```

```
        # [batch_size, seq_len, embed_dim] -> [batch_size, seq_len, num_heads, head_
        q = q.view(batch_size, seq_len, self.num_heads, self.head_dim)
        k = k.view(batch_size, seq_len, self.num_heads, self.head_dim)
        v = v.view(batch_size, seq_len, self.num_heads, self.head_dim)

        # Transpose to [batch_size, num_heads, seq_len, head_dim]
        q = q.transpose(1, 2)
        k = k.transpose(1, 2)
        v = v.transpose(1, 2)

        # Compute attention scores
        # [batch_size, num_heads, seq_len, seq_len]
        attention_scores = torch.matmul(q, k.transpose(-2, -1)) * self.scaling

        # Apply mask if provided
        if mask is not None:
            attention_scores = attention_scores.masked_fill(mask == 0, -1e9)

        # Softmax to get attention weights
        attention_weights = torch.softmax(attention_scores, dim=-1)
        attention_weights = self.dropout(attention_weights)

        # Apply attention to values
        # [batch_size, num_heads, seq_len, head_dim]
        context = torch.matmul(attention_weights, v)

        # Transpose back and reshape
        # [batch_size, seq_len, num_heads, head_dim] -> [batch_size, seq_len, embed_
        context = context.transpose(1, 2).contiguous().view(batch_size, seq_len, sel

        # Final linear projection
        output = self.output_proj(context)

        return output, attention_weights

def exercise2_test_attention():
    """Test and visualize the attention mechanism."""
    # Create toy sequence data
    vocab_size = 1000
    embed_dim = 64
    seq_len = 10
    batch_size = 1

    # Random token IDs
    token_ids = torch.randint(0, vocab_size, (batch_size, seq_len))

    # Embedding layer
    embedding = nn.Embedding(vocab_size, embed_dim)

    # Get embeddings
    x = embedding(token_ids)

    # Create self-attention layer with 4 heads
    attention = SelfAttention(embed_dim, num_heads=4)
```

```python
# Apply self-attention
output, attention_weights = attention(x)

# Create more interpretable example with actual words
words = ["The", "quick", "brown", "fox", "jumps", "over", "the", "lazy", "dog",
word2idx = {word: i for i, word in enumerate(words)}

# Create one-hot encodings for words
one_hot = torch.zeros(len(words), len(words))
for i in range(len(words)):
    one_hot[i, i] = 1.0

# Create simple embeddings by adding position information
position_factor = 0.1
simple_embeddings = one_hot.clone()
for i in range(len(words)):
    simple_embeddings[i] += position_factor * i

# Expand dimensions for batch
simple_embeddings = simple_embeddings.unsqueeze(0)

# Apply attention to these embeddings
simple_attention = SelfAttention(len(words), num_heads=1)
_, simple_attn_weights = simple_attention(simple_embeddings)

# Visualize attention patterns
plt.figure(figsize=(14, 8))

# Plot attention weights for each head
fig, axes = plt.subplots(2, 2, figsize=(12, 10))
axes = axes.flatten()

for h in range(4):
    ax = axes[h]
    im = ax.imshow(attention_weights[0, h].detach().numpy(), cmap='viridis')
    ax.set_title(f'Head {h+1} Attention')
    ax.set_xlabel('Key Position')
    ax.set_ylabel('Query Position')
    fig.colorbar(im, ax=ax)

plt.tight_layout()
plt.figure(figsize=(10, 8))

# Visualize attention for the word example
plt.imshow(simple_attn_weights[0, 0].detach().numpy(), cmap='viridis')
plt.colorbar()
plt.title('Self-Attention Patterns for Sentence')
plt.xticks(range(len(words)), words, rotation=45)
plt.yticks(range(len(words)), words)

# Add attention values
for i in range(len(words)):
    for j in range(len(words)):
```

```
            value = simple_attn_weights[0, 0, i, j].item()
            plt.text(j, i, f'{value:.2f}', ha='center', va='center',
                    color='white' if value > 0.5 else 'black')

    plt.tight_layout()
    return plt

# Call the exercise function
# exercise2_test_attention()
```

Experiment with the attention mechanism by:

1. Adding positional encodings to see how they affect attention patterns
2. Implementing causal attention (masking future tokens) for autoregressive models
3. Testing with different numbers of attention heads
4. Visualizing attention patterns on real sentences

### 11.6.3 Training a Small Transformer

In this exercise, we'll implement a small transformer model for sequence prediction:

```
class PositionalEncoding(nn.Module):
    """
    Positional encoding for transformer models.
    """
    def __init__(self, d_model, max_seq_length=5000, dropout=0.1):
        super(PositionalEncoding, self).__init__()
        self.dropout = nn.Dropout(p=dropout)

        # Create positional encodings
        pe = torch.zeros(max_seq_length, d_model)
        position = torch.arange(0, max_seq_length, dtype=torch.float).unsqueeze(1)
        div_term = torch.exp(torch.arange(0, d_model, 2).float() * (-math.log(10000.

        # Apply sine to even positions and cosine to odd positions
        pe[:, 0::2] = torch.sin(position * div_term)
        pe[:, 1::2] = torch.cos(position * div_term)

        # Add batch dimension and register as buffer (not a parameter)
        pe = pe.unsqueeze(0)
        self.register_buffer('pe', pe)

    def forward(self, x):
        """Add positional encoding to input."""
        x = x + self.pe[:, :x.size(1)]
        return self.dropout(x)

class SimpleTransformer(nn.Module):
    """
    A simple transformer model for sequence prediction.
    """
    def __init__(self, input_dim, d_model, nhead, num_layers, output_dim, dropout=0.
        super(SimpleTransformer, self).__init__()

        # Input embedding
        self.input_embedding = nn.Linear(input_dim, d_model)

        # Positional encoding
        self.positional_encoding = PositionalEncoding(d_model, dropout=dropout)

        # Transformer encoder
        encoder_layers = nn.TransformerEncoderLayer(d_model, nhead, dim_feedforward=
        self.transformer_encoder = nn.TransformerEncoder(encoder_layers, num_layers)

        # Output layer
        self.output_layer = nn.Linear(d_model, output_dim)

    def forward(self, src, src_mask=None):
        """
        Forward pass through the transformer.

        Args:
            src: Input tensor [batch_size, seq_len, input_dim]
            src_mask: Optional mask for padding or attention directionality
```

```python
        Returns:
            output: Predictions [batch_size, seq_len, output_dim]
        """
        # Embed input
        embedded = self.input_embedding(src)

        # Add positional encoding
        embedded = self.positional_encoding(embedded)

        # Transpose for transformer input [seq_len, batch_size, d_model]
        embedded = embedded.permute(1, 0, 2)

        # Apply transformer encoder
        transformer_output = self.transformer_encoder(embedded, src_mask)

        # Transpose back to [batch_size, seq_len, d_model]
        transformer_output = transformer_output.permute(1, 0, 2)

        # Apply output layer
        output = self.output_layer(transformer_output)

        return output

def exercise3_transformer_for_sine():
    """Train a simple transformer for sine wave prediction."""
    import math

    # Generate sine wave data
    def generate_sine_data(num_samples=1000, seq_len=50, prediction_step=10):
        """Generate sine wave data with multiple features."""
        data = []
        targets = []

        for _ in range(num_samples):
            # Random sine wave parameters
            amplitude = np.random.uniform(0.5, 1.5)
            frequency = np.random.uniform(0.1, 0.5)
            phase = np.random.uniform(0, 2*math.pi)

            # Generate time points
            time_points = np.linspace(0, 10, seq_len + prediction_step)

            # Generate sine wave
            sine_wave = amplitude * np.sin(frequency * time_points + phase)

            # Add noise
            noise = np.random.normal(0, 0.05, len(sine_wave))
            noisy_sine = sine_wave + noise

            # Create features (current value and sin/cos of time)
            features = np.zeros((seq_len, 3))
            for i in range(seq_len):
                t = time_points[i]
```

```
            features[i, 0] = noisy_sine[i]  # Current value
            features[i, 1] = np.sin(t)      # Time feature 1
            features[i, 2] = np.cos(t)      # Time feature 2

        # Target is future value
        target = sine_wave[prediction_step:seq_len+prediction_step]

        data.append(features)
        targets.append(target)

    return np.array(data), np.array(targets)

# Generate data
X, y = generate_sine_data(num_samples=1000, seq_len=40, prediction_step=5)

# Create 80/20 train-test split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_

# Convert to PyTorch tensors
X_train = torch.FloatTensor(X_train)
y_train = torch.FloatTensor(y_train).unsqueeze(-1)  # Add feature dimension
X_test = torch.FloatTensor(X_test)
y_test = torch.FloatTensor(y_test).unsqueeze(-1)

# Create sequence mask (for causal attention)
def generate_square_subsequent_mask(sz):
    """Generate a mask for causal attention."""
    mask = (torch.triu(torch.ones(sz, sz)) == 1).transpose(0, 1)
    mask = mask.float().masked_fill(mask == 0, float('-inf')).masked_fill(mask =
    return mask

# Model parameters
input_dim = 3   # Current value + 2 time features
d_model = 32    # Transformer hidden dimension
nhead = 4       # Number of attention heads
num_layers = 2 # Number of transformer layers
output_dim = 1 # Predicting a single value

# Initialize model
model = SimpleTransformer(input_dim, d_model, nhead, num_layers, output_dim)

# Loss and optimizer
criterion = nn.MSELoss()
optimizer = optim.Adam(model.parameters(), lr=0.001)

# Training parameters
num_epochs = 30
batch_size = 32

# For storing metrics
train_losses = []

# Training loop
for epoch in range(num_epochs):
```

```python
    model.train()
    total_loss = 0

    # Create random permutation
    indices = torch.randperm(len(X_train))

    # Mini-batch training
    for i in range(0, len(X_train), batch_size):
        # Get mini-batch indices
        batch_indices = indices[i:i+batch_size]

        # Get mini-batch data
        batch_X = X_train[batch_indices]
        batch_y = y_train[batch_indices]

        # Forward pass
        outputs = model(batch_X)
        loss = criterion(outputs, batch_y)

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

        total_loss += loss.item()

    # Record average training loss
    avg_loss = total_loss / (len(X_train) / batch_size)
    train_losses.append(avg_loss)

    # Print progress
    if (epoch + 1) % 5 == 0:
        print(f'Epoch [{epoch+1}/{num_epochs}], Loss: {avg_loss:.4f}')

# Test the model
model.eval()
with torch.no_grad():
    # Get predictions on test set
    test_outputs = model(X_test)
    test_loss = criterion(test_outputs, y_test).item()
    print(f'Test MSE: {test_loss:.4f}')

# Visualize results
plt.figure(figsize=(15, 10))

# Plot training loss
plt.subplot(2, 1, 1)
plt.plot(train_losses)
plt.title('Training Loss')
plt.xlabel('Epoch')
plt.ylabel('MSE Loss')
plt.grid(True)

# Plot example predictions
```

```
    plt.subplot(2, 1, 2)

    # Select a random example from test set
    example_idx = np.random.randint(0, len(X_test))
    input_seq = X_test[example_idx, :, 0].numpy()  # Get actual values from input
    true_future = y_test[example_idx, :, 0].numpy()
    predicted_future = test_outputs[example_idx, :, 0].numpy()

    # Time points for x-axis
    all_steps = np.arange(len(input_seq) + len(true_future))

    # Plot input sequence
    plt.plot(all_steps[:len(input_seq)], input_seq, 'b-', label='Input Sequence')

    # Plot true future and predictions
    plt.plot(all_steps[len(input_seq):], true_future, 'g-', label='True Future')
    plt.plot(all_steps[len(input_seq):], predicted_future, 'r--', label='Predicted F

    plt.title('Transformer Sequence Prediction')
    plt.xlabel('Time Step')
    plt.ylabel('Value')
    plt.legend()
    plt.grid(True)

    plt.tight_layout()
    return plt

# Call the exercise function
# exercise3_transformer_for_sine()
```

Extend this exercise by:

1. Implementing a full encoder-decoder transformer for sequence-to-sequence tasks
2. Adding an autoregressive inference mode for generating sequences
3. Experimenting with different attention patterns (local attention, sparse attention)
4. Trying the transformer on different time series forecasting tasks

## 11.6.4 Neural Sequence Prediction

In this exercise, we'll implement a model that predicts neural activity patterns, similar to what might be used in brain-computer interfaces:

```
def exercise4_neural_sequence_prediction():
    """Predict neural activity patterns using sequence models."""
    # Generate synthetic neural data with temporal patterns
    np.random.seed(42)

    # Simulation parameters
    n_neurons = 20         # Number of neurons
    n_timepoints = 500     # Number of timepoints
    n_trials = 100         # Number of trials/examples

    # Create base oscillatory patterns (theta, alpha, beta, gamma ranges)
    time = np.arange(n_timepoints)
    patterns = [
        np.sin(2 * np.pi * 0.05 * time),  # Theta (~5Hz)
        np.sin(2 * np.pi * 0.1 * time),   # Alpha (~10Hz)
        np.sin(2 * np.pi * 0.2 * time),   # Beta (~20Hz)
        np.sin(2 * np.pi * 0.4 * time)    # Gamma (~40Hz)
    ]

    # Generate trials with mixed oscillations
    data = np.zeros((n_trials, n_timepoints, n_neurons))
    for trial in range(n_trials):
        # Randomly assign neurons to different oscillatory patterns
        neuron_patterns = np.random.choice(len(patterns), size=n_neurons)

        # Generate activity for each neuron
        for i in range(n_neurons):
            # Base pattern
            base_pattern = patterns[neuron_patterns[i]]

            # Add phase shift and amplitude variation
            phase_shift = np.random.uniform(0, 2 * np.pi)
            amplitude = np.random.uniform(0.5, 2.0)

            # Generate activity with noise
            activity = amplitude * np.sin(2 * np.pi * time * (0.05 + 0.15 * neuron_p
            activity += 0.2 * np.random.randn(n_timepoints)

            # Store in data array
            data[trial, :, i] = activity

    # Split the data into input and target sequences
    sequence_length = 50  # Input sequence length
    prediction_length = 10  # Number of future timepoints to predict

    X = []
    y = []

    # Create input/output pairs
    for trial in range(n_trials):
        # Multiple starting points per trial
        max_start = n_timepoints - sequence_length - prediction_length
        step = max_start // 5  # 5 sequences per trial
```

```
    for start in range(0, max_start, step):
        end = start + sequence_length
        # Input: sequence of length 'sequence_length'
        X.append(data[trial, start:end])
        # Target: next 'prediction_length' timepoints
        y.append(data[trial, end:end+prediction_length])

# Convert to numpy arrays
X = np.array(X)
y = np.array(y)

# Split into train and test
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_

# Create PyTorch tensors
X_train = torch.FloatTensor(X_train)
y_train = torch.FloatTensor(y_train)
X_test = torch.FloatTensor(X_test)
y_test = torch.FloatTensor(y_test)

# Define a model that combines LSTM and attention
class NeuralSequencePredictor(nn.Module):
    def __init__(self, input_dim, hidden_dim, output_dim, seq_len, pred_len, n_h
        super(NeuralSequencePredictor, self).__init__()

        self.input_dim = input_dim
        self.hidden_dim = hidden_dim
        self.output_dim = output_dim
        self.seq_len = seq_len
        self.pred_len = pred_len

        # LSTM layer
        self.lstm = nn.LSTM(input_dim, hidden_dim, batch_first=True)

        # Self-attention layer
        self.attention = SelfAttention(hidden_dim, num_heads=n_heads)

        # Output projection
        self.projection = nn.Linear(hidden_dim, output_dim * pred_len)

    def forward(self, x):
        """
        Forward pass through the model.

        Args:
            x: Input tensor [batch_size, seq_len, input_dim]

        Returns:
            predictions: Output tensor [batch_size, pred_len, output_dim]
        """
        batch_size = x.size(0)

        # Process through LSTM
```

```
        lstm_out, _ = self.lstm(x)

        # Apply self-attention
        attended, _ = self.attention(lstm_out)

        # Project to output
        # We only need the final state to start predicting the future
        final_state = attended[:, -1]

        # Project to multiple future timesteps
        projection = self.projection(final_state)

        # Reshape to [batch_size, pred_len, output_dim]
        predictions = projection.view(batch_size, self.pred_len, self.output_dim

        return predictions

# Initialize model
input_dim = n_neurons  # Number of input features (neurons)
hidden_dim = 64        # Hidden dimension
output_dim = n_neurons # Number of output features (predicting all neurons)

model = NeuralSequencePredictor(
    input_dim=input_dim,
    hidden_dim=hidden_dim,
    output_dim=output_dim,
    seq_len=sequence_length,
    pred_len=prediction_length
)

# Loss and optimizer
criterion = nn.MSELoss()
optimizer = optim.Adam(model.parameters(), lr=0.001)

# Training parameters
num_epochs = 30
batch_size = 32

# For storing training metrics
train_losses = []

# Training loop
for epoch in range(num_epochs):
    model.train()
    epoch_loss = 0

    # Create random permutation
    indices = torch.randperm(len(X_train))

    # Mini-batch training
    for i in range(0, len(X_train), batch_size):
        # Get mini-batch indices
        batch_indices = indices[i:i+batch_size]
```

```
        # Get mini-batch data
        batch_X = X_train[batch_indices]
        batch_y = y_train[batch_indices]

        # Forward pass
        predictions = model(batch_X)
        loss = criterion(predictions, batch_y)

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

        epoch_loss += loss.item() * len(batch_indices)

    # Average loss for the epoch
    avg_loss = epoch_loss / len(X_train)
    train_losses.append(avg_loss)

    # Print progress
    if (epoch + 1) % 5 == 0:
        print(f'Epoch [{epoch+1}/{num_epochs}], Loss: {avg_loss:.4f}')

# Evaluate on test set
model.eval()
with torch.no_grad():
    test_predictions = model(X_test)
    test_loss = criterion(test_predictions, y_test).item()
    print(f'Test MSE: {test_loss:.4f}')

# Visualize results
plt.figure(figsize=(15, 12))

# Plot training loss
plt.subplot(3, 1, 1)
plt.plot(train_losses)
plt.title('Training Loss')
plt.xlabel('Epoch')
plt.ylabel('MSE Loss')
plt.grid(True)

# Select an example to visualize
example_idx = np.random.randint(0, len(X_test))

# Plot input sequence for a single neuron
neuron_idx = 0  # First neuron for visualization

plt.subplot(3, 1, 2)
plt.plot(np.arange(sequence_length), X_test[example_idx, :, neuron_idx].numpy(),
plt.plot(np.arange(sequence_length, sequence_length + prediction_length),
         y_test[example_idx, :, neuron_idx].numpy(), 'g-', label='True Future')
plt.plot(np.arange(sequence_length, sequence_length + prediction_length),
         test_predictions[example_idx, :, neuron_idx].numpy(), 'r--', label='Pre
plt.axvline(x=sequence_length - 0.5, color='k', linestyle='--')
```

```
    plt.title(f'Neuron {neuron_idx+1} Activity Prediction')
    plt.xlabel('Time Step')
    plt.ylabel('Activity')
    plt.legend()
    plt.grid(True)

    # Plot heatmap of all neurons
    plt.subplot(3, 1, 3)

    # Combine input and true/predicted future for visualization
    full_true = np.zeros((sequence_length + prediction_length, n_neurons))
    full_true[:sequence_length] = X_test[example_idx].numpy()
    full_true[sequence_length:] = y_test[example_idx].numpy()

    full_pred = np.zeros((sequence_length + prediction_length, n_neurons))
    full_pred[:sequence_length] = X_test[example_idx].numpy()
    full_pred[sequence_length:] = test_predictions[example_idx].numpy()

    # Calculate error
    error = np.abs(full_true - full_pred)

    # Create a figure with subplots for all three heatmaps
    fig, axes = plt.subplots(3, 1, figsize=(10, 12))

    # Plot true activity
    im0 = axes[0].imshow(full_true.T, aspect='auto', cmap='viridis')
    axes[0].set_title('True Neural Activity')
    axes[0].set_xlabel('Time Step')
    axes[0].set_ylabel('Neuron')
    axes[0].axvline(x=sequence_length - 0.5, color='r', linestyle='--')
    plt.colorbar(im0, ax=axes[0])

    # Plot predicted activity
    im1 = axes[1].imshow(full_pred.T, aspect='auto', cmap='viridis')
    axes[1].set_title('Predicted Neural Activity')
    axes[1].set_xlabel('Time Step')
    axes[1].set_ylabel('Neuron')
    axes[1].axvline(x=sequence_length - 0.5, color='r', linestyle='--')
    plt.colorbar(im1, ax=axes[1])

    # Plot prediction error
    im2 = axes[2].imshow(error.T, aspect='auto', cmap='YlOrRd')
    axes[2].set_title('Prediction Error')
    axes[2].set_xlabel('Time Step')
    axes[2].set_ylabel('Neuron')
    axes[2].axvline(x=sequence_length - 0.5, color='r', linestyle='--')
    plt.colorbar(im2, ax=axes[2])

    plt.tight_layout()
    return plt, fig

# Call the exercise function
# exercise4_neural_sequence_prediction()
```

Try extending this neural prediction exercise by:

1. Using real neural data from open datasets (e.g., Allen Brain Observatory)
2. Implementing an encoder-decoder architecture for longer-term predictions
3. Adding biological constraints to the model architecture
4. Visualizing the learned attention patterns to see which neurons interact

## 11.6.5 Exercise Solutions

These exercises provide hands-on experience with the sequence models described in this chapter. Run them individually to explore and modify the implementations as you learn.

To execute an exercise, uncomment the function call at the end of each code block and run the cell. The exercises progress in difficulty and build upon concepts introduced earlier in the chapter.

By understanding these implementations and experimenting with the code, you'll gain deeper insights into how sequence models work and how they can be applied to neuroscience and AI tasks.

## 11.7 Take-aways

**Knowledge Connections**

**Looking Back**

- **Chapter 3 (Spatial Navigation)**: Recurrent neural networks share conceptual similarities with hippocampal place cells' temporal information processing for predictive navigation
- **Chapter 7 (Information Theory)**: Sequential information processing relies on principles of information flow and entropy across temporal dimensions
- **Chapter 9 (ML Foundations)**: Classical sequence models like HMMs and CRFs form the statistical foundation for modern sequence processing
- **Chapter 10 (Deep Learning)**: Core neural network operations and backpropagation principles are extended to sequence domains via backpropagation through time

**Looking Forward**

- **Chapter 12 (Large Language Models)**: Transformer architectures from this chapter form the foundation for LLMs with scaled attention mechanisms
- **Chapter 13 (Multimodal Models)**: Sequence processing techniques are extended to handle multiple modalities through cross-attention and embedding alignment
- **Chapter 14 (Future Directions)**: Innovations in sequence modeling contribute to neuromorphic computing and brain-inspired AI architectures
- **Chapter 20 (Case Studies)**: Healthcare applications of sequence models are demonstrated in neurological disorder prediction
- **Chapter 21 (AI for Neuro Discovery)**: Sequence models are applied to neuroimaging time series for clinical applications

This chapter has covered the evolution of sequence models from recurrent networks to transformers, connecting these AI architectures to neural processing mechanisms in the brain. Here are the key insights:

1. **Evolutionary Trajectory**: Sequence modeling has evolved from inherently sequential recurrent networks (RNNs, LSTMs, GRUs) toward parallelizable attention-based architectures (transformers). This mirrors how the brain combines both recurrent local circuits and distributed global processing.

2. **Biological Inspiration**: Many features of modern sequence models have parallels in brain function:
    - Gating mechanisms in LSTMs parallel selective filtering in prefrontal-basal ganglia circuits
    - Attention mechanisms resemble selective attention in thalamo-cortical systems
    - Multi-timescale processing occurs in both transformer layers and the cortical hierarchy
3. **Computational Trade-offs**: Different architectures involve trade-offs between:
    - Computational efficiency vs. biological plausibility
    - Sequential processing vs. parallelism
    - Memory usage vs. contextual range
    - Inductive biases vs. flexibility
4. **Temporal Integration**: Both biological and artificial systems must solve the problem of integrating information across time. The brain uses recurrent connections with various time constants, while artificial systems use either recurrent connections (RNNs) or explicit attention to previous time points (transformers).
5. **Bidirectional Inspiration**: The relationship between neuroscience and AI is increasingly bidirectional:
    - Neuroscience inspires new AI architectures (e.g., attention mechanisms)
    - AI models generate hypotheses about neural computation (e.g., predictive coding)
    - Both fields inform each other through shared mathematical frameworks
6. **Emergent Properties**: As sequence models scale up, they demonstrate emergent capabilities that weren't explicitly programmed, similar to how neural systems show emergent cognitive abilities. This has led to foundation models that capture complex sequential dependencies across multiple domains.
7. **Applications Bridging Fields**: Sequence models provide a shared framework for applications spanning neuroscience and AI, from neural decoding and brain-computer interfaces to natural language processing and time series forecasting.
8. **Healthcare Applications**: Sequence models are particularly valuable for healthcare time series analysis:
    - Handling irregular sampling intervals in clinical data
    - Managing missing values common in patient monitoring
    - Detecting early signs of clinical deterioration
    - Modeling multivariate physiological signals like EEG and ECG
    - Predicting disease progression trajectories in neurological disorders

The rapid advancement of sequence models represents one of the most successful areas of cross-fertilization between neuroscience and artificial intelligence, with each field benefiting from insights gained in the other.

**Chapter Summary**

In this chapter, we explored:

- **Recurrent neural networks (RNNs)** and their fundamental approach to processing sequential information
- **LSTM and GRU architectures** that address the vanishing gradient problem in sequential processing
- **Attention mechanisms** that enable models to focus on relevant parts of input sequences
- **The transformer architecture** with its parallel computation and scaled dot-product attention
- **Positional encodings** that inject sequential order information into parallel attention models
- **Neural correlates of sequential processing** in cortical circuits and working memory systems
- **Predictive processing** frameworks in both the brain and artificial sequence models
- **Applications** spanning natural language processing, time series forecasting, and neural decoding
- **Healthcare time series applications** that address clinical challenges like irregular sampling, missing data, and early detection of deterioration
- **Implementation details** of sequence models through hands-on code examples
- **The evolution from RNNs to transformers** representing different computational trade-offs

This chapter traces the remarkable evolution of sequence modeling approaches in artificial intelligence, highlighting their biological inspirations and showing how these models have revolutionized our ability to process sequential data across domains from neuroscience to healthcare.

# 11.8 Further Reading & Media

## Key Papers

### Foundational Papers


- Hochreiter, S., & Schmidhuber, J. (1997). **Long short-term memory**. *Neural Computation, 9(8)*, 1735-1780.
- Vaswani, A., et al. (2017). **Attention is all you need**. *Advances in Neural Information Processing Systems*, 5998-6008.
- Sutskever, I., Vinyals, O., & Le, Q. V. (2014). **Sequence to sequence learning with neural networks**. *Advances in Neural Information Processing Systems*, 3104-3112.
- Bahdanau, D., Cho, K., & Bengio, Y. (2015). **Neural machine translation by jointly learning to align and translate**. *International Conference on Learning Representations*.


### Neuroscience Connections


- Wang, J., et al. (2018). **Prefrontal cortex as a meta-reinforcement learning system**. *Nature Neuroscience, 21(6)*, 860-868.
- Friston, K. (2010). **The free-energy principle: A unified brain theory?** *Nature Reviews Neuroscience, 11(2)*, 127-138.
- Kell, A. J., & McDermott, J. H. (2019). **Deep neural network models of sensory systems: Windows onto the role of task constraints**. *Current Opinion in Neurobiology, 55*, 121-132.
- Yamins, D. L., & DiCarlo, J. J. (2016). **Using goal-driven deep learning models to understand sensory cortex**. *Nature Neuroscience, 19(3)*, 356-365.


## Books


- Goodfellow, I., Bengio, Y., & Courville, A. (2016). **Deep Learning**. MIT Press. Online version
- Sejnowski, T. J. (2018). **The Deep Learning Revolution**. MIT Press.
- Williams, R. J., & Zipser, D. (2006). **A learning algorithm for continually running fully recurrent neural networks**. *Neural Computation*.

# Online Resources

## Tutorials and Blog Posts

- Karpathy, A. (2015). **The Unreasonable Effectiveness of Recurrent Neural Networks**
- Olah, C. (2015). **Understanding LSTM Networks**
- Alammar, J. (2018). **The Illustrated Transformer**
- Lillicrap, T. P., & Santoro, A. (2019). **Backpropagation through time and the brain**

## Video Lectures

- Lecture Series: **Stanford CS224n: Natural Language Processing with Deep Learning**
- Lecture Series: **DeepMind x UCL: Deep Learning Lectures**

## Code Repositories

- **PyTorch Sequence Models Tutorial**
- **The Annotated Transformer** - Harvard NLP's implementation of the transformer with detailed annotations
- **Hugging Face Transformers** - State-of-the-art transformer implementations
- **NeuroAI Papers** - Curated list of papers at the intersection of neuroscience and AI

# Research Communities and Conferences

- Conference on Neural Information Processing Systems (NeurIPS)
- International Conference on Learning Representations (ICLR)
- Organization for Computational Neurosciences (OCNS)
- Cognitive Computational Neuroscience (CCN)

These resources span from introductory to advanced and cover both theoretical foundations and practical implementations of sequence models and their connections to neuroscience.