Desired Features of RNNs

- Have a mechanism for storing vital early information in a *memory cell*.
  - An early observation is highly significant for predicting all future observations.
  - Without such a mechanism, we will have to assign a very large gradient to this observation
- Handle situations where some symbols carry no pertinent information and have a mechanism for *skipping such symbols* in the latent state representation.
  - E.g. when parsing a web page there might be auxiliary HTML code that is irrelevant for the purpose of assessing the sentiment conveyed on the page.
- Have a mechanism of *resetting* our internal state representation.
  - When there is a logical break between parts of a sequence, e.g. a transition between chapters in a book.

LSTMs and GRUs

- The Long Short Term Memory (LSTM) is an Advanced RNN which can handle all of the above requirements.
- The Gated Recurrent Unit (GRU) is a simplied version of LSTM.
    - Due to its simplicity, we will start with the GRU.

Gated Recurrent Units (GRU)

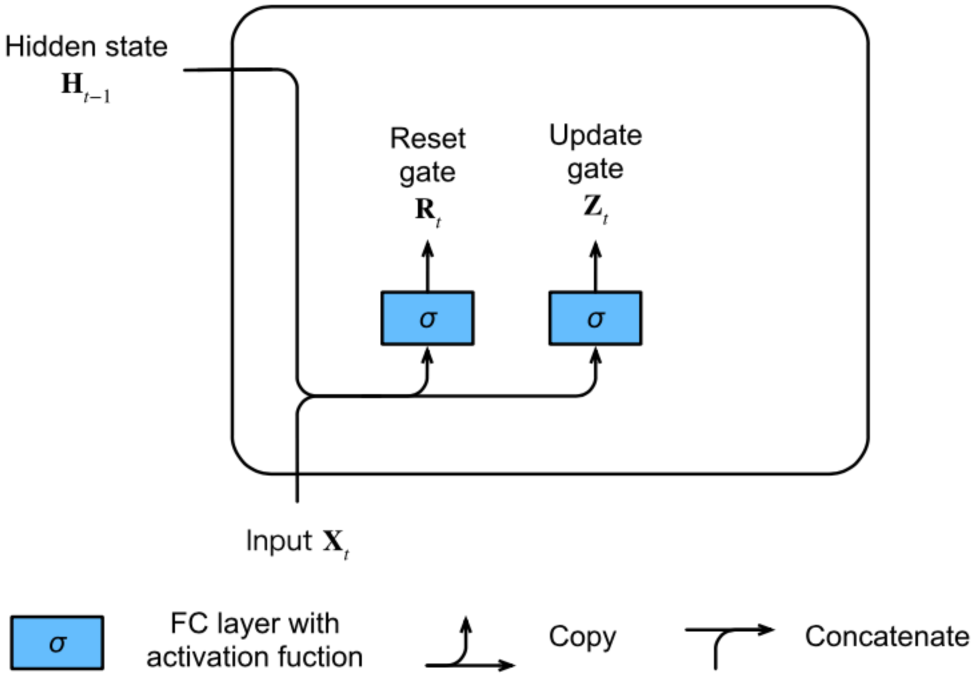
Gating the Hidden State

- The key distinction between regular RNNs and GRUs is that the latter support gating of the hidden state.
    - This means that we have dedicated mechanisms for when a hidden state should be updated and also when it should be reset.
- These mechanisms are learned:
    - E.g., if the first symbol is of great importance, it will learn not to update the hidden state after the first observation.
    - Likewise, it will learn to skip irrelevant temporary observations.
    - Last, it can learn to reset the latent state whenever needed.

Reset Gates and Update Gates

- The first thing we need to introduce are reset and update gates.
- A reset gate would allow us to control how much of the previous state we might still want to remember.
- An update gate would allow us to control how much of the new state is just a copy of the old state.
- We engineer them to be vectors with entries in $(0, 1)$.

- The following figure shows how the reset and update gates are computed a each time step:
    - They are functions of $\mathbf{X}_t$ and $\mathbf{H}_{t-1}$.
    - The function output is given by a fully connected layer with a sigmoid as its activation function.



- Assume, for a given time step t, the minibatch input is $\mathbf{X}_t \in \mathbb{R}^{n \times d}$ (number of examples: n, number of inputs: d) and the hidden state of the last time step is $\mathbf{H}_{t-1} \in \mathbb{R}^{n \times h}$ (number of hidden states: h).

- Then, the reset gate $\mathbf{R}_t \in \mathbb{R}^{n \times h}$ and update gate $\mathbf{Z}_t \in \mathbb{R}^{n \times h}$ are computed as follows:

$$
\begin{aligned}
\mathbf{R}_t &= \sigma(\mathbf{X}_t \mathbf{W}_{xr} + \mathbf{H}_{t-1} \mathbf{W}_{hr} + \mathbf{b}_r),\\
\mathbf{Z}_t &= \sigma(\mathbf{X}_t \mathbf{W}_{xz} + \mathbf{H}_{t-1} \mathbf{W}_{hz} + \mathbf{b}_z).
\end{aligned}
$$

- $\mathbf{W}_{xr}, \mathbf{W}_{xz} \in \mathbb{R}^{d \times h}$ and $\mathbf{W}_{hr}, \mathbf{W}_{hz} \in \mathbb{R}^{h \times h}$ are weight parameters and $\mathbf{b}_r, \mathbf{b}_z \in \mathbb{R}^{1 \times h}$ are biases.
- A sigmoid function is used to transform input values to the interval $(0, 1)$.

Reset Gates in Action

- In a conventional RNN, we would have an hidden state update of the form

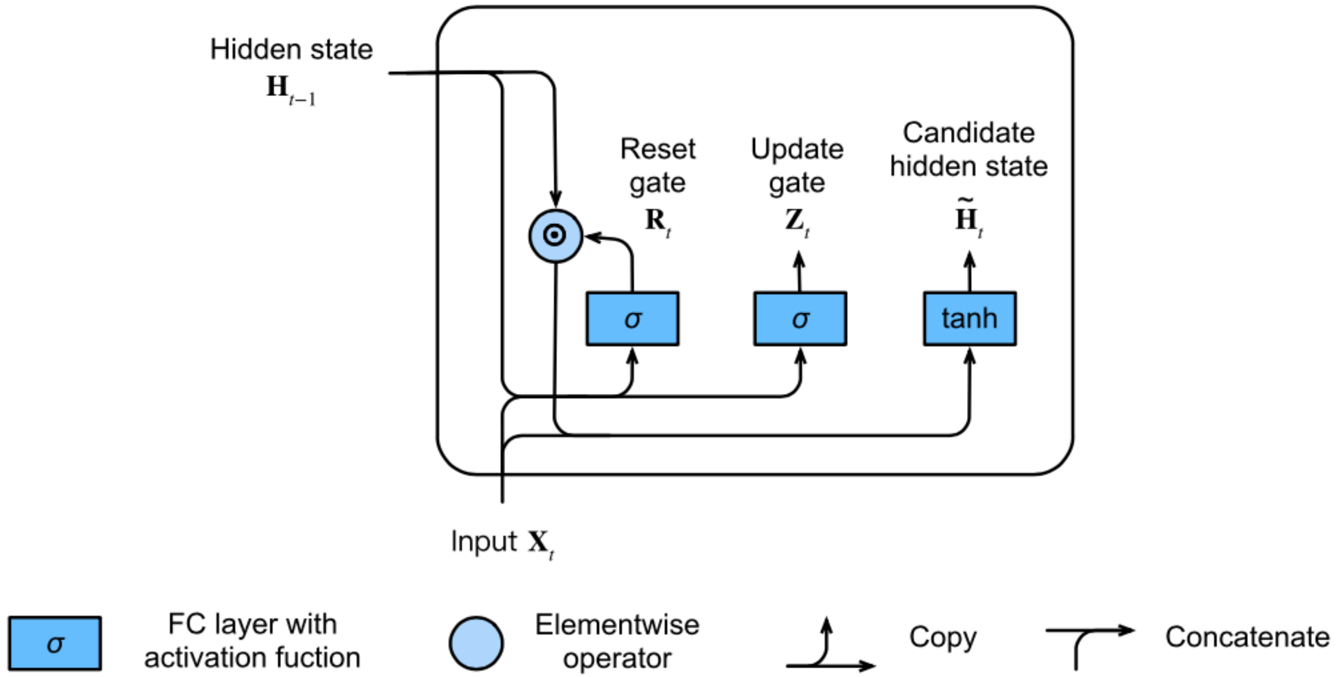
$$\mathbf{H}_t = \tanh(\mathbf{X}_t \mathbf{W}_{xh} + \mathbf{H}_{t-1} \mathbf{W}_{hh} + \mathbf{b}_h).$$

- If we want to reduce the influence of the previous states we can multiply $\mathbf{H}_{t-1}$ with $\mathbf{R}_t$ elementwise.
    - For all entries of $\mathbf{R}_t$ that are close to 1, we recover a conventional RNN.
    - For all entries of $\mathbf{R}_t$ that are close to 0, the pre-existing hidden state is reset to defaults.

- This leads to the following *candidate hidden state*:

$$\tilde{\mathbf{H}}_t = \tanh(\mathbf{X}_t \mathbf{W}_{xh} + \left(\mathbf{R}_t \odot \mathbf{H}_{t-1}\right) \mathbf{W}_{hh} + \mathbf{b}_h).$$

- The following figure illustrates the computational flow after applying the reset gate.
  - The symbol ⊙ indicates elementwise multiplication between tensors.



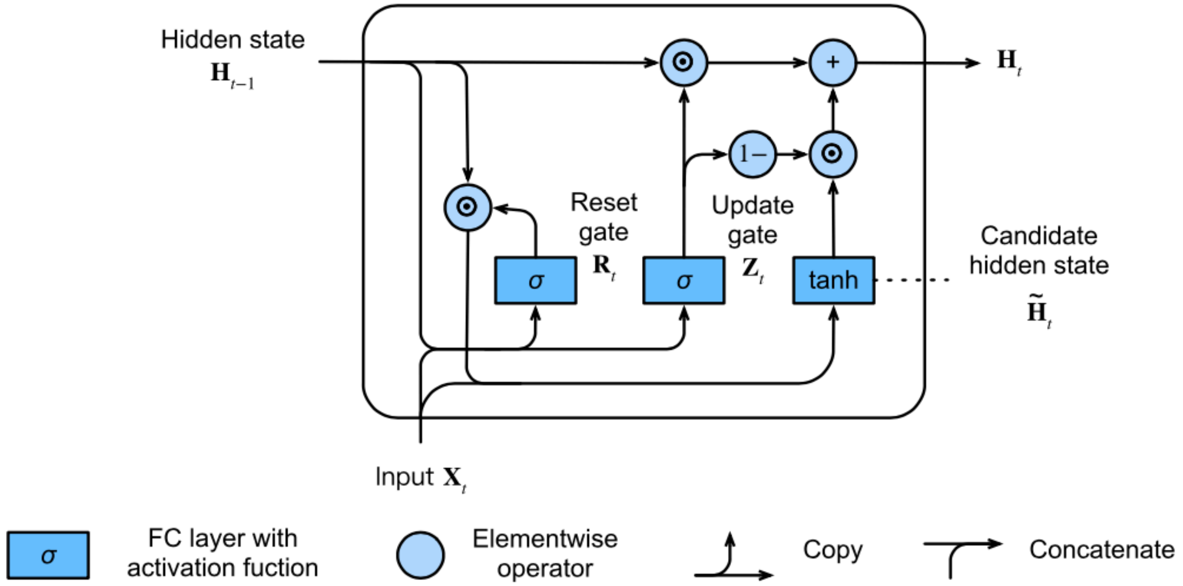
Update Gates in Action

- The update gate $\mathbf{Z}_t$, determines the extent to which the new state $\mathbf{H}_t$ is just the old state $\mathbf{H}_{t-1}$ and by how much the new candidate state $\tilde{\mathbf{H}}_t$ is used.
- This leads to the final update equation for the GRU:

$$\mathbf{H}_t = \mathbf{Z}_t \odot \mathbf{H}_{t-1} + (1 - \mathbf{Z}_t) \odot \tilde{\mathbf{H}}_t.$$

- Whenever $\mathbf{Z}_t$ is close to 1, we simply retain the old state.
    - In this case $\mathbf{X}_t$ is essentially ignored, effectively skipping time step t in the dependency chain.
- Whenever $\mathbf{Z}_t$ is close to 0, the new latent state $\mathbf{H}_t$ becomes the candidate latent state $\tilde{\mathbf{H}}_t$.

- Put everything together the GRU is shown in the following figure:



- In summary, GRUs have the following two distinguishing features:
  - Reset gates help capture short-term dependencies in time series.
  - Update gates help capture long-term dependencies in time series.
- These designs help with:
  - Cope with the vanishing gradient problem in RNNs
  - Better capture dependencies for time series with large time step distances.

Concise Implementation of GRU

Loading the Dataset

In [8]:
```
batch_size, num_steps = 32, 35
train_iter, vocab = mu.load_data_time_machine(batch_size, num_steps)
```

In [17]:

```python
# RNNModel class contains a complete RNN model.
# rnn_layer only contains the hidden recurrent layers, we need to create a separ
ate output layer.
class RNNModel(nn.Module):
    """The RNN model."""
    def __init__(self, rnn_layer, vocab_size):
        super(RNNModel, self).__init__()
        self.rnn = rnn_layer
        self.vocab_size = vocab_size
        self.num_hiddens = self.rnn.hidden_size
        self.linear = nn.Linear(self.num_hiddens, self.vocab_size)

    def forward(self, inputs, state):
        X = F.one_hot(inputs.T.long(), self.vocab_size)
        X = X.to(torch.float32)
        Y, state = self.rnn(X, state)
        #print(X.size()) # 35x32x28
        #print(Y.size()) # 35x32x256
        #print(state.size()) # 32x256
        Y1 = Y.reshape((-1, Y.shape[-1]))
        #print(Y1.size()) # 1120x256
        out = self.linear(Y1)
        #print(out.size()) # 1120x28
        return out, state

    def begin_state(self, batch_size=1):
        state = torch.zeros((self.rnn.num_layers, batch_size, self.num_hiddens))
        return state
```

In [25]:
```
def train_epoch_ch8(model, train_iter, loss, optimizer, use_random_iter):
    """Train a model for one epoch """
    state = None
    metric = mu.Accumulator(2)  # Sum of training loss, no. of tokens
    for X, Y in train_iter:
        # Initialize `state` when first iteration or using random sampling
        if state is None or use_random_iter:
            state = model.begin_state(batch_size=X.shape[0])
        else:
            if isinstance(model, nn.Module) and not isinstance(state, tuple):
            # `state` is a tensor for `nn.GRU`
                state.detach_()
        #print(X.size(), Y.size(), state.size()) # 32x35, 32x35, 32x256
        y = Y.T.reshape(-1)
        #print(y.size()) # 35x32 -> 1120
        y_hat, state = model(X, state)
        #print(y_hat.size()) # 1120x28
        l = loss(y_hat, y.long())
        optimizer.zero_grad()
        l.backward()
        mu.grad_clipping(model, 1)
        optimizer.step()

        metric.add(l * mu.size(y), mu.size(y))
    return math.exp(metric[0] / metric[1])
```

In [26]:

```
def train_ch8(model, train_iter, vocab, lr, num_epochs, use_random_iter=False):
    """Train a model for num_epochs"""
    animator = mu.Animator(xlabel='epoch', ylabel='perplexity', legend=['train']
, xlim=[1, num_epochs])
    loss = nn.CrossEntropyLoss()
    optimizer = torch.optim.SGD(model.parameters(), lr)
    # Train and predict
    for epoch in range(num_epochs):
        ppl = train_epoch_ch8(model, train_iter, loss, optimizer, use_random_ite
r)
        if epoch % 10 == 0:
            print(predict_ch8('time traveller', 50, model, vocab))
            animator.add(epoch + 1, [ppl])
    print(f'perplexity {ppl:.1f}')
    print(predict_ch8('time traveller', 50, model, vocab))
    print(predict_ch8('traveller', 50, model, vocab))
```

In [27]:

```
def predict_ch8(prefix, num_preds, model, vocab):
    """Generate new characters following the `prefix`."""
    state = model.begin_state(batch_size=1)
    outputs = [vocab[prefix[0]]]
    get_input = lambda: mu.reshape(torch.tensor([outputs[-1]]), (1, 1))
    for y in prefix[1:]:  # Warm-up period
        _, state = model(get_input(), state)
        outputs.append(vocab[y])
    for _ in range(num_preds):  # Predict `num_preds` steps
        y, state = model(get_input(), state)
        outputs.append(int(y.argmax(dim=1).reshape(1)))
    return ''.join([vocab.idx_to_token[i] for i in outputs])
```

Training and Prediction

In [28]:

```
vocab_size, num_hiddens = len(vocab), 256
num_epochs, lr = 500, 1
num_inputs = vocab_size
gru_layer = nn.GRU(num_inputs, num_hiddens)
model = RNNModel(gru_layer, len(vocab))
train_ch8(model, train_iter, vocab, lr, num_epochs)
```

```
perplexity 1.0
time traveller  it s against reason said filby  what reason said
traveller  it s against reason said filby  what reason said
```