Deep Learning (BEV033DLE)
Lecture 13 Recurrent Neural Networks

Czech Technical University in Prague

- Recurrent models
- Special cases and recurrent back propagation
- Error back propagation through time
- Gated recurrent units, GRU and LSTM networks

Recurrent networks

Recurrent models in a nutshell

- input sequence $x = (x_1, \ldots, x_t, \ldots, x_T)$, $x_t \in \mathbb{R}^n$, output sequence $y = (y_1, \ldots, y_T)$, $y_t \in \mathcal{Y}$ and sequence of hidden states $h = (h_1, \ldots, h_T)$, $h_t \in \mathbb{R}^d$.
- recurrent (dynamic) system with outputs

$$
\begin{aligned}
h_t &= f(x_t, h_{t-1}, w) \\
y_t &= g(h_t, v)
\end{aligned}
$$

  where w and v are parameters. The model defines sequence-to-sequence mappings $h = F_w(x)$ and $y = G_v(h)$.
- loss function $\ell(y, y')$, often locally additive $\ell(y, y') = \sum_t \ell_t(y_t, y'_t)$

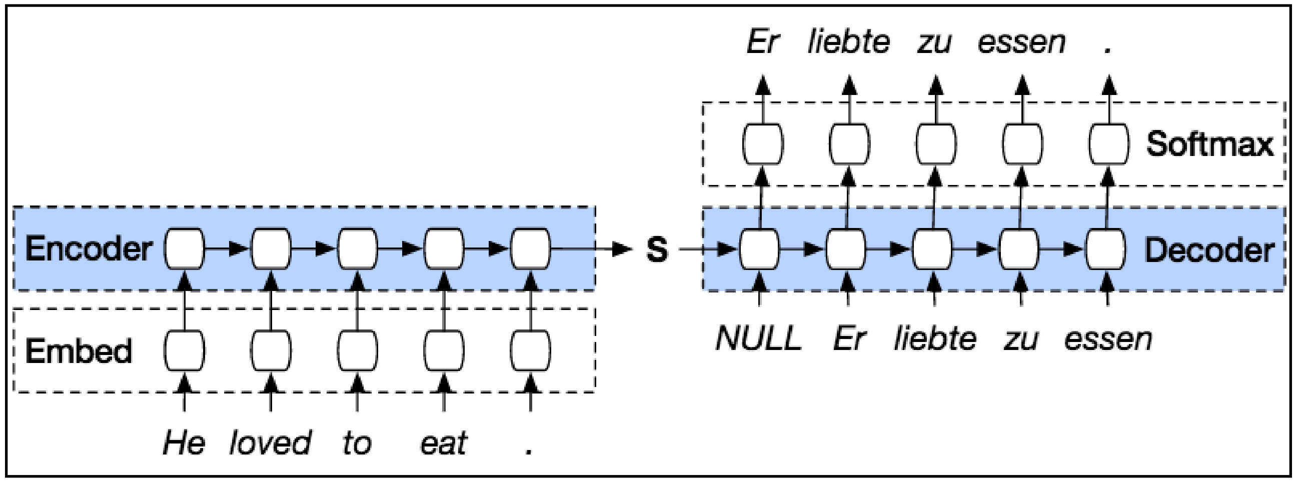
Training goal: given training data $\mathcal{T} = \big\{(x^j, y^j) \mid j = 1, \ldots, m\big\}$, learn the model parameters w, v by solving

$$
\frac{1}{m} \sum_{(x,y) \in \mathcal{T}} \ell\big(y, (G_v \circ F_w)(x)\big) \to \min_{w,v}
$$

Recurrent networks

Incarnations of recurrent models and related tasks

- Deep neural network for classification with additional feedback connections: x_t - constant input, y_t - output of the network, h_t -states of all hidden layers. The loss function depends on the last output y_T only.
- "infinite state automata": the output space is sufficient for keeping the history, thus h and y can be identified, i.e. $y_t = f(x_t, y_{t-1}, w)$.
  Example: Earth observation, landcover type monitoring x_t - sequence of spectral satellite measurements, y_t - sequence of states (e.g. coniferous forest, broadleaf forest, clearcut, bark beetle degradation etc.)
- general sequence-to-sequence segmentation: hidden states h_t are needed for keeping track of longer past and are latent.
  Example: NLP translation:



Learning RNNs special cases: infinite state automata

Learning RNNs is particularly simple in the case that

- h and y can be identified, i.e. $y_t = f(x_t, y_{t-1}, w)$ and
- the loss is locally additive $\sum_t \ell(y_t, y_t')$

Split each sequence $(x,y) \in \mathcal{T}^m$ into triplets (y_{t-1}, x_t, y_t) and train f from

$$\frac{1}{m} \sum_{(x,y)\in\mathcal{T}} \sum_t \ell\big(y_t, f(x_t, y_{t-1}, w)\big) \to \min_w$$

Neither forward nor backward propagation through the sequence are needed.

Learning RNNs special cases: Recurrent backpropagation

Recurrent backpropagation: (Almeida, 1987), (Pineda, 1987)

Learning approach for classifier/regression networks with *feedback connections*.

the network input $x_t = x$ is constant, y_t and h_t denote the network output and all hidden layers.

$$h_t = f(x, h_{t-1}, w) \quad \text{and} \quad y_t = g(h_t, v)$$

Assumptions:

- the network configuration h_t converges to a fixpoint h^* if we clamp its input to $x_t = x$
- the loss depends on the final output $y^* = g(h^*, v)$ only.

Computing $\nabla_v \ell(y^*, y)$ poses no problem if ℓ and g are differentiable. What about $\nabla_w \ell(y^*, y)$?

We have (implicit function theorem)

$$\frac{\partial h^*}{\partial w} = \big[I - J_f(h^*)\big]^{-1} \frac{\partial f}{\partial w},$$

where $J_f(h^*) = \frac{\partial f(x,w,h^*)}{\partial h}$ is the Jacobian of f w.r.t. h.

Learning RNNs special cases: Recurrent backpropagation

Now, let us consider the gradient of the loss w.r.t. w.

$$\partial_w \ell = \partial_y \ell(y^*)\, \partial_h g(h^*)\, \big[I - J_f(h^*)\big]^{-1} \partial_w f(x, w, h^*)$$

Applying this directly would require to compute $\big[I - J_f(h^*)\big]^{-1}$.

Introduce the (column) vector z defined by

$$z = \big[I - J_f(h^*)\big]^{-T} \big(\partial_y \ell(y^*)\, \partial_h g(h^*)\big)^T$$

Multiplying both sides by $\big[I - J_f(h^*)\big]^T$, we get

$$z = J_f(h^*)^T z + \big(\partial_y \ell(y^*)\, \partial_h g(h^*)\big)^T .$$

This is a fixpoint equation for z and can be solved by fixpoint iteration.

Learning RNNs special cases: Recurrent backpropagation

The resulting algorithm for computing the derivative $\frac{\partial \ell}{\partial w}$ is:

- fix x, run the network until convergence $\to h^*$
- start from z_0 and iterate

$$z_i = J_f(h^*)^T z_{i-1} + \big(\partial_y \ell(y^*)\, \partial_h g(h^*)\big)^T$$

  until convergence.
- Return

$$\frac{\partial \ell}{\partial w} = z^T \frac{\partial f(x, w, h^*)}{\partial h}$$

Learning RNNs general case: backpropagation through time

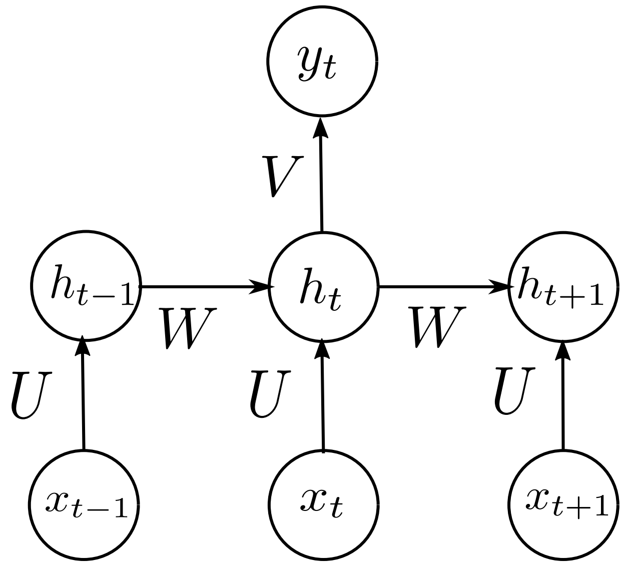
Assumptions:

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

The mappings f and g are implemented by neural networks and are differentiable w.r.t. their inputs and parameters. The loss function $\ell(y, y')$ is differentiable.

Example 1. Both mappings f and g are implemented by one layer networks

$$a_t = Wh_{t-1} + Ux_t + b \qquad h_t = \tanh(a_t)$$
$$o_t = Vh_t + c \qquad y_t = \mathrm{softmax}(o_t)$$



Learning RNNs general case: backpropagation through time

Computing the gradients: Unroll the network in time and apply backpropagation

Let us consider the loss for a single example (x, y^*) from the training data.

Computing the gradient w.r.t. v is easy (see Slide 4.). Let us consider the gradient w.r.t. w

$$\partial_w \ell(y, y^*) = \sum_{t=1}^{T} \partial_w \ell(y_t, y_t^*) = \sum_{t=1}^{T} \partial_{y_t} \ell(y_t, y_t^*) \, \partial_{h_t} g(h_t, v) \, \partial_w h_t$$

The first two derivatives are simple. For the last one we have the recurrent expression

$$\partial_w h_t = \partial_w f(x_t, h_{t-1}, w) + \partial_{h_{t-1}} f(x_t, h_{t-1}, w) \, \partial_w h_{t-1}$$

This gives

$$\partial_w h_t = \partial_w f(x_t, h_{t-1}, w) + \sum_{i=1}^{t-1} \Big[\prod_{j=i+1}^{t} \partial_{h_{j-1}} f(x_j, h_{j-1}, w) \Big] \partial_w f(x_i, h_{i-1}, w)$$

Learning RNNs general case: backpropagation through time

Problems:

- backpropagation through time is computationally expensive
- Exploding/vanishing gradients: consider for simplicity the linear recurrence $h_t = W h_{t-1}$. For τ steps we get $h_\tau = W^\tau h_0$. Suppose that we can write $W = U^{-1} \Lambda U$, where Λ is diagonal. We get
$$h_\tau = U^{-1} \Lambda^\tau U h_0.$$
Eigenvalues with magnitude less than one will decay and eigenvalues with magnitude greater than one will explode.
- We can not apply batch normalisation as simple remedy.
- We want the following model ability: events long in the past can trigger changes in conjunction with current measurements.

Possible solutions: skip connections? designate special nodes in h_t for keeping record of events long in the past?

RNNs with gated recurrent units

LSTM (Hochreiter, Schmidhuber, 1997), GRU (Cho et al., 2014), ...

Gated recurrent unit (simplified):

A cell consisting of a recurrent unit h_t and a gate unit $u_t \in [0,1]$

$$\begin{aligned} h_t &= u_{t-1} h_{t-1} + [1 - u_{t-1}] f(x_t, h_{t-1}, w) \\ u_t &= \mathrm{S}(x_t, h_t, v) \end{aligned}$$

The gate unit u_t has sigmoid nonlinearity and "decides" whether to copy h_t from h_{t-1} or to apply the recurrence with f.

RNNs with gated recurrent units

Gated recurrent unit (general):

- h is a state vector
- u is a vector of "update" gates
- r is a vector of "reset" gates

The update equations are

$$h_t = u_{t-1} \odot h_{t-1} + [1 - u_{t-1}] \odot \mathrm{S}\Big(U x_{t-1} + W r_{t-1} \odot h_{t-1}\Big)$$

where $\odot$ denotes the element-wise product of vectors. The gate unit outputs are given by

$$u_t = \mathrm{S}\big(U^u x_t + W^u h_t\big)$$
$$r_t = \mathrm{S}\big(U^r x_t + W^r h_t\big)$$

LSTM cells are somewhat more complicated – they have separate "forget" and "update" gates.