Deep Learning in Practice

Wednesday, October 23, 2024 8:02 AM

Architecture choices:

- DAG: # layers, etc
- Activation functions (logistic, tanh, ReLU, ...)
- Error or log-loss functions
- Input preprocessing

Data choices: Train, validation, test, cross-validation, ...

Algorithm choices:

- Initialization of weights & biases
- Gradient descent, SGD, minibatches, line search, momentum, Adam, ...
- Stopping criterion, weight regularization, dropout, ...

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Weight Initialization (DL 8.4)

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- Recall that $\frac{\partial E}{\partial w_{lm}} \propto g'(x_m)$
- If $g'(x_m)$ is close to zero, it will be very difficult to change w_{lm}
  $\Rightarrow$ Initialize w's so $|g'(x_m)| > \epsilon$ ← Minimum derivative
- For $g = \tanh$, if we sample weights from a zero-mean distribution, then

$$E[x_m] = \sum_{i=1}^{m-1} E[w_{im}] E[g(x_i)] = 0 \quad (E[w_{im}] \to 0)$$

$$V[x_m] = \sum_{i=1}^{m-1} V[w_{im} g(x_i)] = \sum_{i=1}^{m-1} V[w_{im}] V[g(x_i)] \quad (V[g(x_i)] \leq 1)$$

$$\leq \sum_{i=1}^{m-1} V[w_{im}] = (\#\text{inputs to } x_m) \times V[w]$$

- So, sample w's with variance $= \frac{1}{\#\text{inputs}}$

Glorot & Bengio (DL 8.4)

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- Consider a fully connected layer with m inputs & n outputs

- Sample w's from $\text{Uniform}\left(-\sqrt{\frac{6}{m+n}}, \sqrt{\frac{6}{m+n}}\right)$

- Compromise between ensuring activation variance is the same across layers and all w's have same gradient variance

$$\text{Variance} \propto \frac{6}{m+n}$$

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Avoiding overfitting

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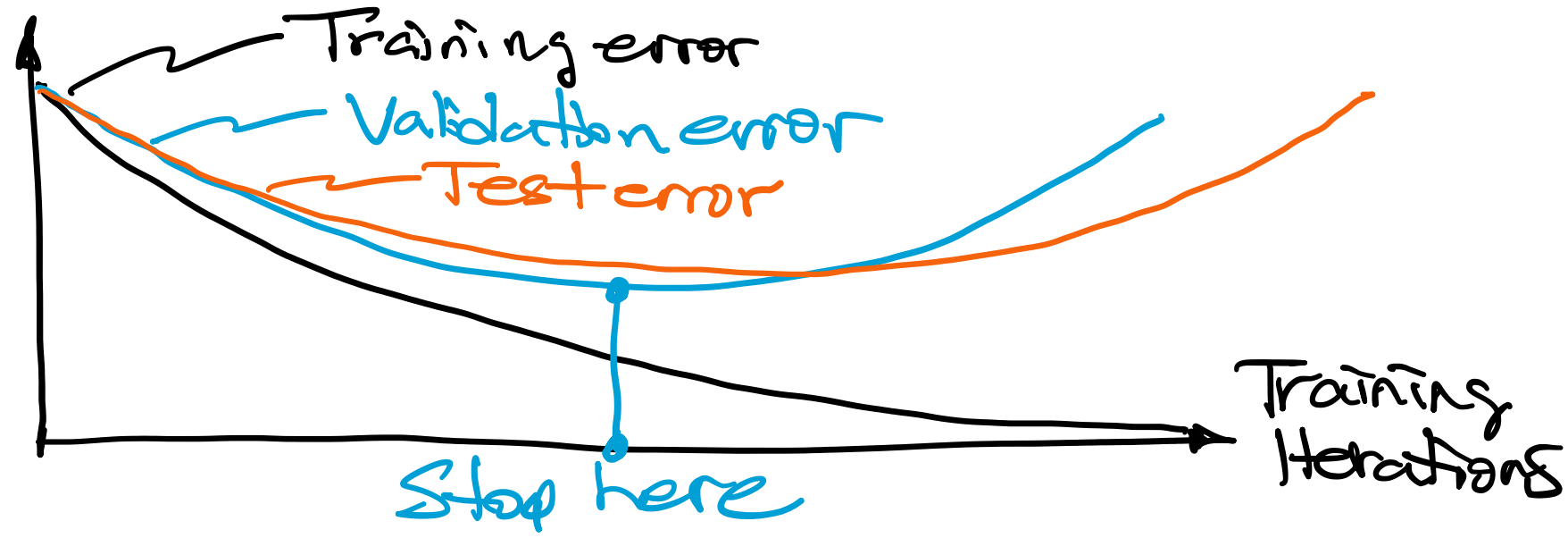
- Weight penalties (DL 7.1): Minimize $E(\text{Data}, w) + \lambda \|w\|$
  → Favors small weights & neural nets that make "smooth" predictions
- Early stopping (DL 7.8): Start with tiny weights monitor a validation set during training, and stop when the error increases



Avoiding overfitting

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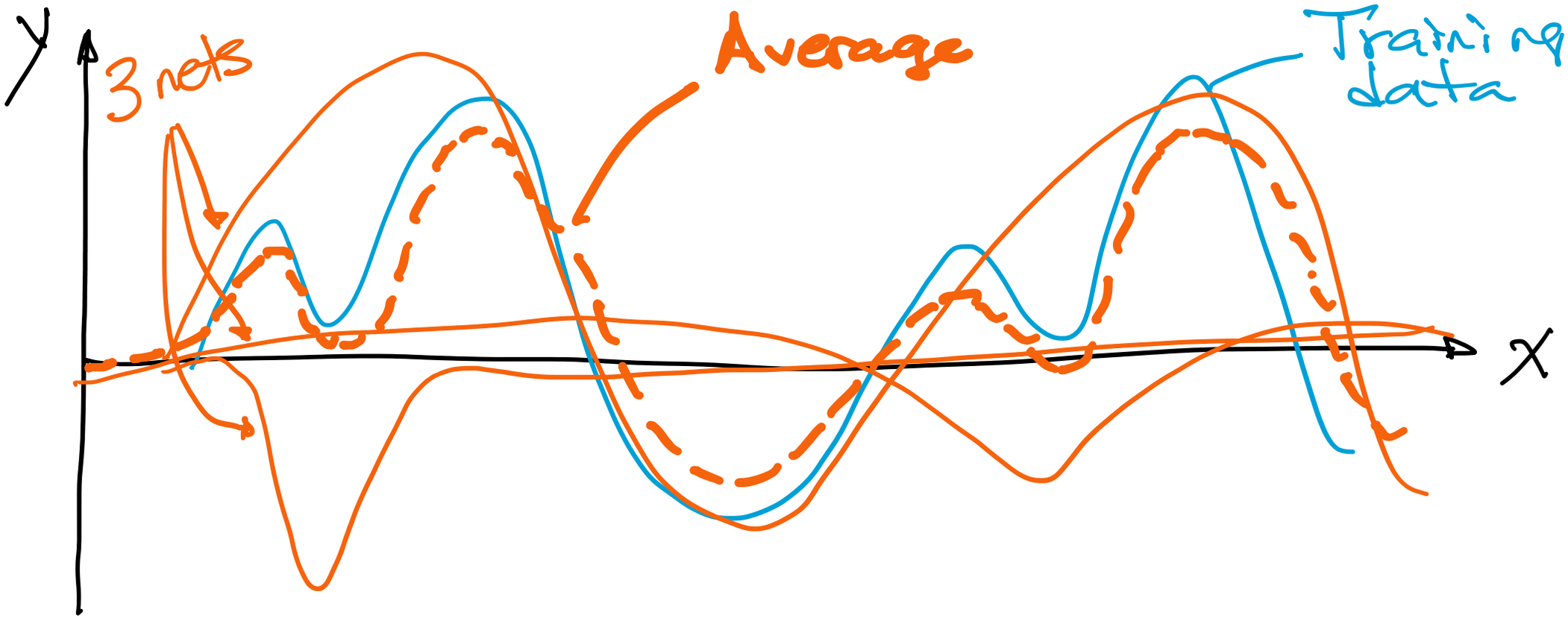
- Bagging (DL 7.11): Train many (eg, 10) neural nets, and allow them to overfit. To make a prediction for a ~~test~~ case, average the predictions from the ensemble of neural nets.



Wasted/stuck units

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- The main challenge for large neural nets is not just overfitting, but that most hidden units get <u>stuck where they aren't needed</u> & are thus <u>wasted</u>

- Weight regularization & early stopping don't help
- Bagging somewhat helps, but
  - The number of nets needed grows <u>rapidly</u> with the complexity of the data
- When training each net in the ensemble, most units still get stuck.

Example: Stuck units

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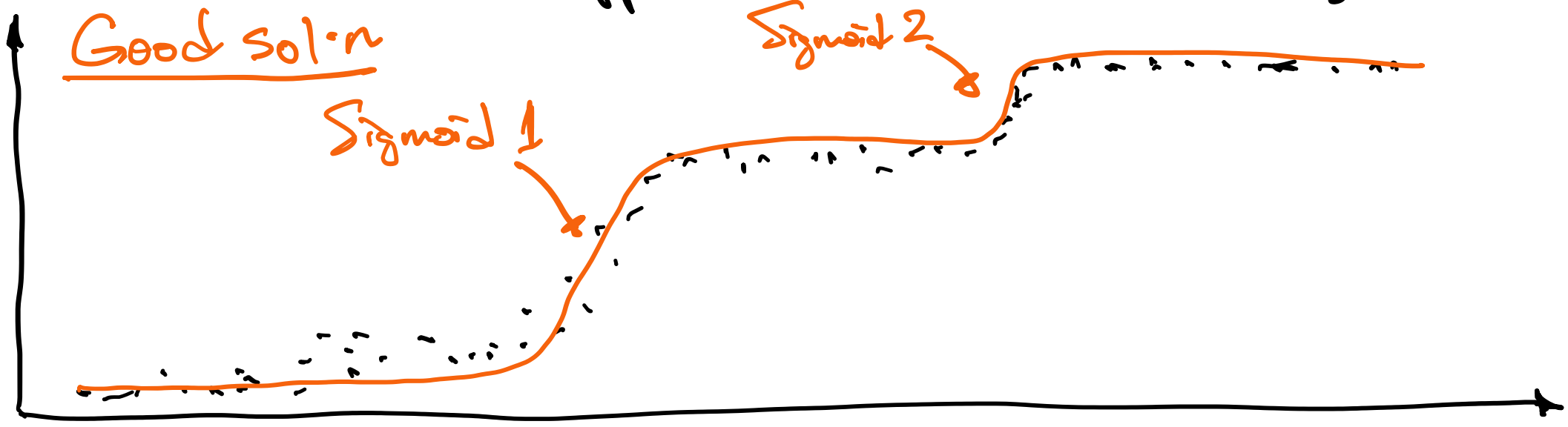
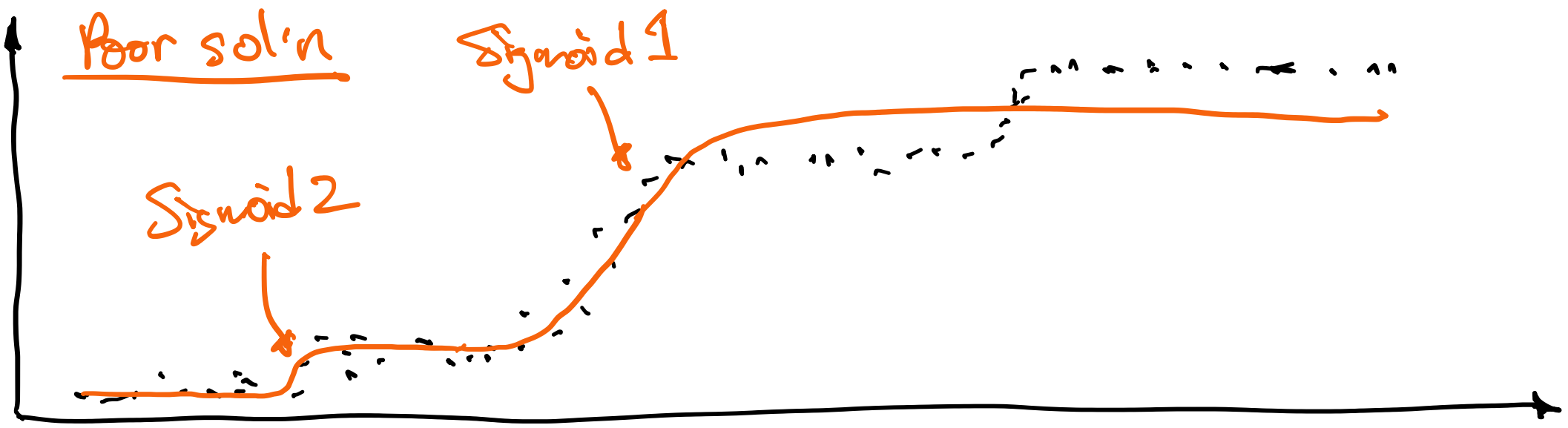
Consider function approximation using 2 logistic units



Here's a local minimum where sigmoid 2 is "stuck"



Dropout (DL 7.12)

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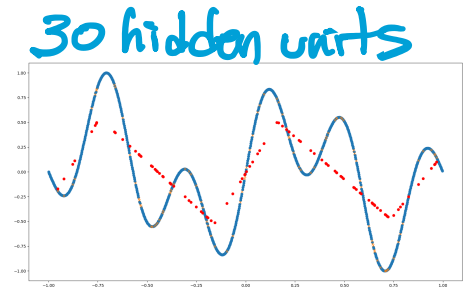
Eg, GPT-3 uses dropout

- Goal: Train very large networks while avoiding overfitting and wasting most hidden units

Recall the wasted hidden units for a simple task



- Method
  - Set dropout probabilities $\{\mu_i\}$, eg, for input units $\mu_i = 0.8$ & for hidden units $\mu_i = 0.5$.
  - During training, for each forward pass, set the activity of x_i to zero with probability $1-\mu_i$ & independent of other units
  - During testing, set $w_{ij} \leftarrow w_{ij} \cdot \mu_i \ \forall_{ij}$.

Dropout: Cooperation & exponential bagging (DL 7.12)

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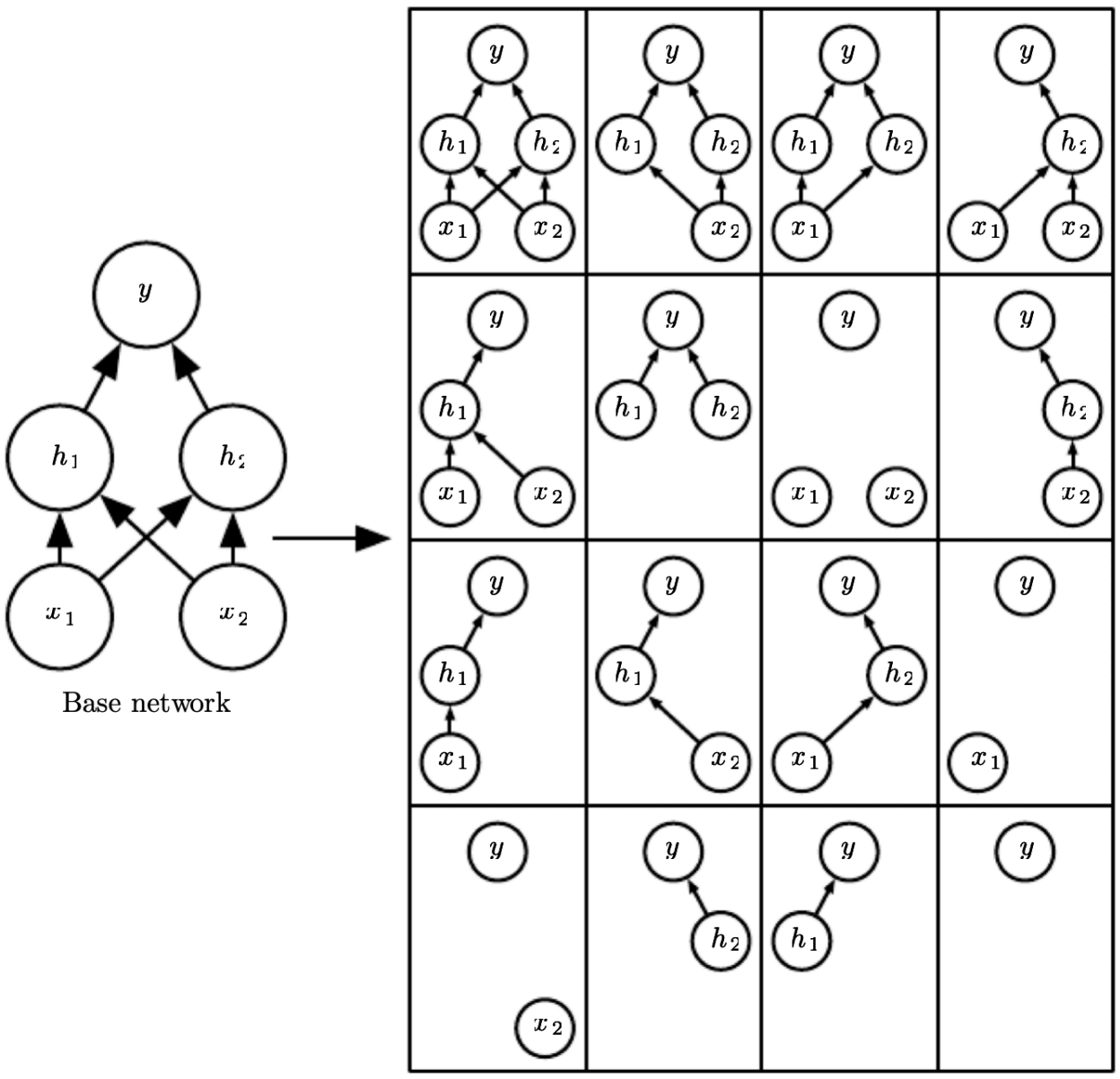

Base network

Ensemble of subnetworks

These are the nets that get sampled in the forward pass.

- Dropout simulates an exponential number of neural architectures
  → Exponential bagging.

- Because the weights are shared across all networks and they are trained jointly, the units can cooperate during training to get unstuck.

Dropout Example

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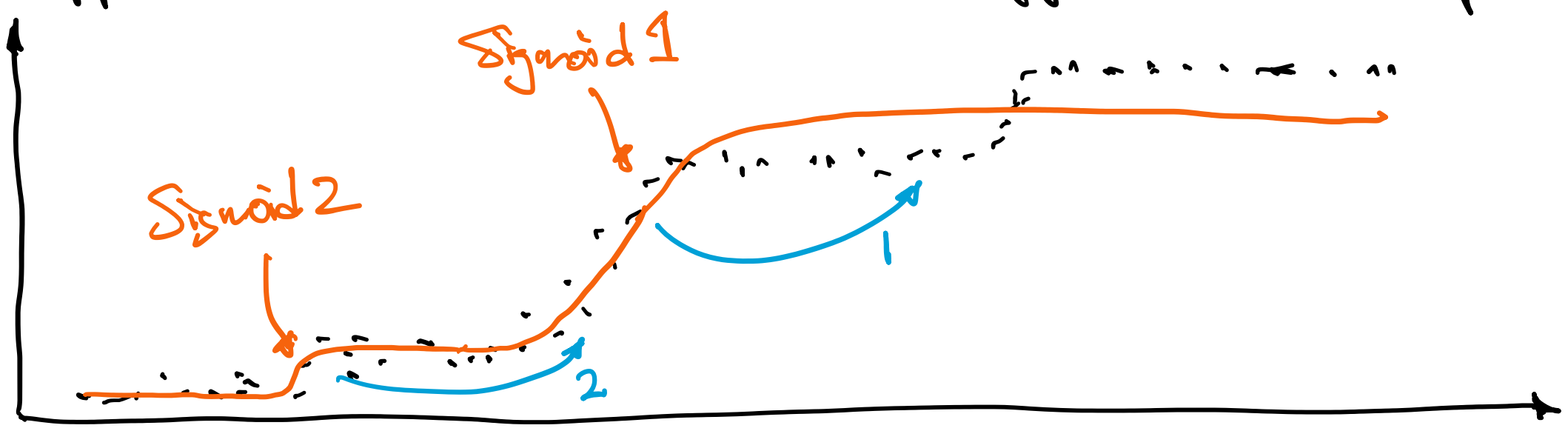
Suppose each hidden unit is dropped out with $p = 0.5$



- 1/4 of the time only sigmoid 2 is used to predict the output, so it will be pressured to take over for sigmoid 1, which can then capture the incline on the far right

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Convolutional neural nets (CNNs)

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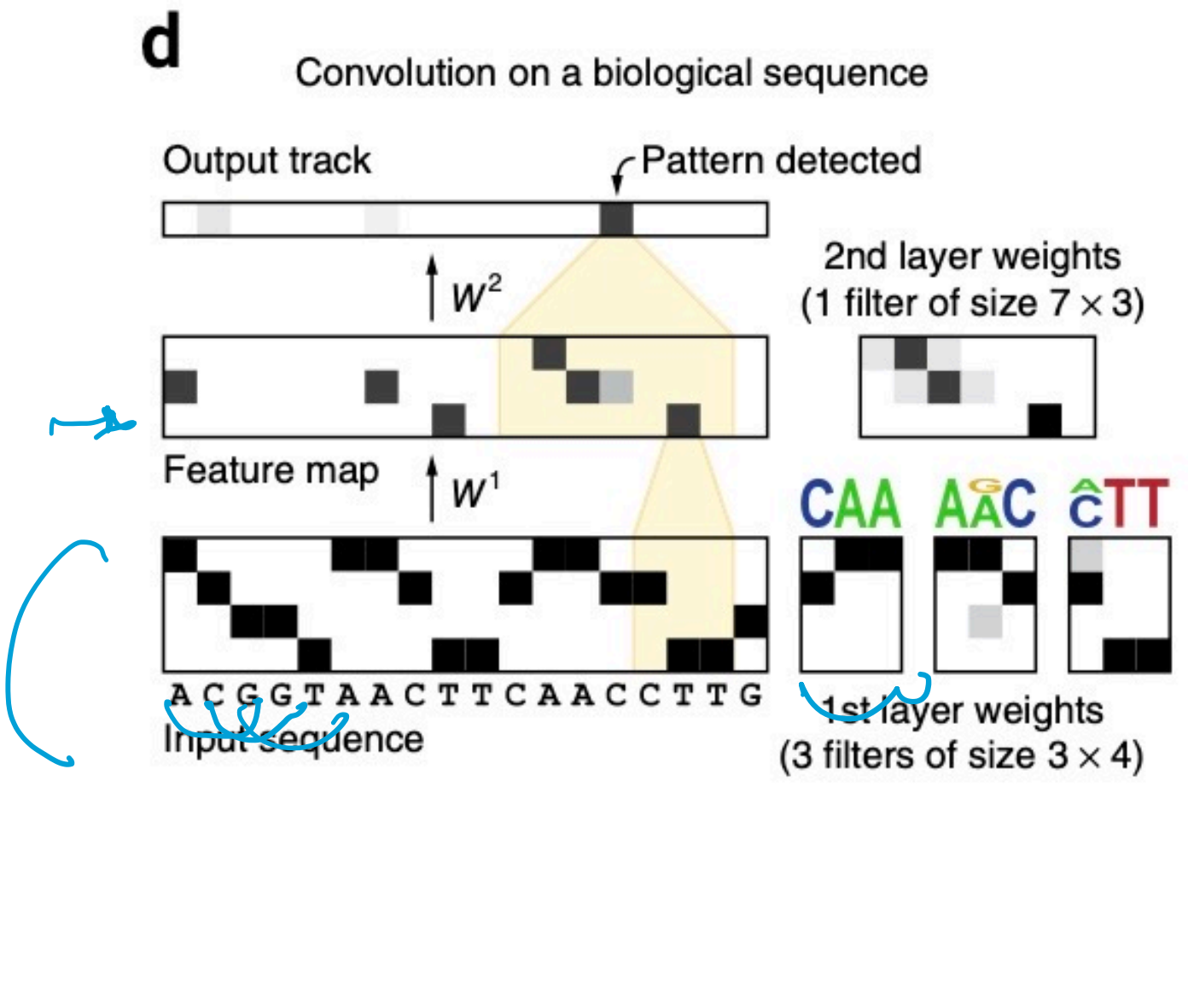
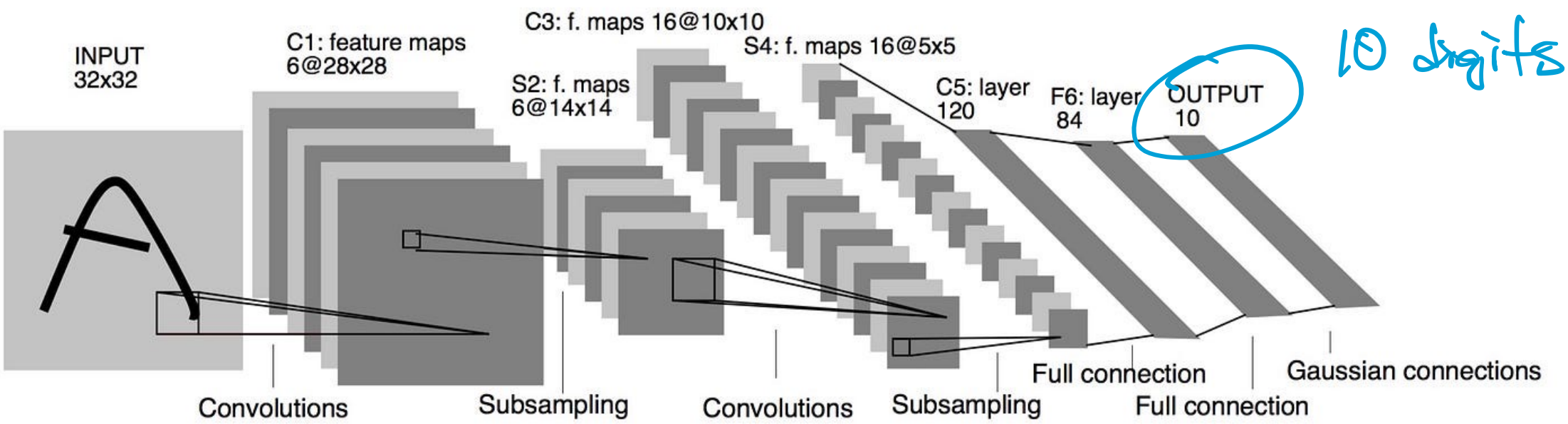
- To avoid overfitting and ensure cooperation of hidden units during training, employ <u>modularity</u>
- Use convolution modules: Recall from before:



LeCun, 1989

Saturday, November 2, 2024 6:02 PM

- Best result on handwritten digit recognition in 1989



10 digits

2-D convolutions

Weight sharing (DL 7.9)

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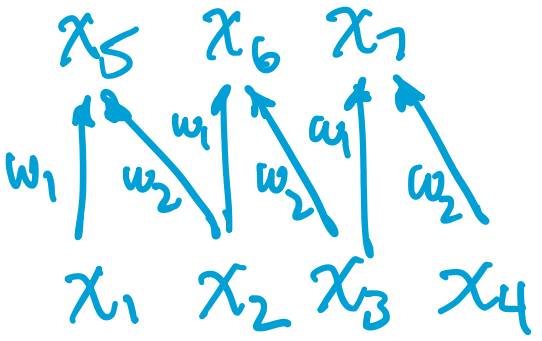
- In CNNs and other architectures we can have a situation where many connections share the same, single weight
- Let $K(i,j)$ be the index of the weight on connection $i \to j$. Instead of $x_j = \sum_{i=1}^{j-1} w_{ij}\, g_i(x_i)$ we have $x_j = \sum_{i=1}^{j-1} w_{K(i,j)}\, g_i(x_i)$
- Example



$K(1,5)=1,\ K(2,6)=1,\ K(3,7)=1$

$K(2,5)=2,\ K(3,6)=2,\ K(4,7)=2$

Weight sharing: Learning (DL 7.9)

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- Before, for $\partial E / \partial w_{lm}$, we had that w_{lm} influences E only via x_m, so $\frac{\partial E}{\partial w_{lm}} = \frac{\partial E}{\partial x_m}\frac{\partial x_m}{\partial w_{lm}} = \frac{\partial E}{\partial x_m} g_l(x_l)$

- Now, w_k influences E via all x_m s.t. $K(l,m) = k$, so

Use back prop to compute this

$$\frac{\partial E}{\partial w_k} = \sum_{\substack{l,m: \\ K(l,m)=k}} \frac{\partial E}{\partial x_m}\frac{\partial x_m}{\partial w_k} = \sum_{\substack{l,m: \\ K(l,m)=k}} \frac{\partial E}{\partial x_m} g_l(x_l)$$

- Algorithm
  - Forward & back propagation are same as before
  - The weight derivatives are computed as above.

Weight sharing: Learning (DL 7.9)

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Forward propagation: for $j = I+1 \dots M$, $x_j = \sum_{i=1}^{j-1} w_{K(i,j)} g_i(x_i)$

Output unit error derivatives:

For $m = M \dots M-O+1$: $\frac{\partial E}{\partial x_m} = -2(y_m - g_m(x_m))g'_m(x_m)$

Backpropagation:

For $m = M-O \dots M-O-H+1$: $\frac{\partial E}{\partial x_m} = \sum_{k=m+1}^{M} \frac{\partial E}{\partial x_k} w_{K(m,k)} g'_m(x_m)$

Weight derivatives:

For $l = 1 \dots M-O+1$, for $m = l+1 \dots M$

$$\frac{\partial E}{\partial w_k} = \sum_{l,m:} \frac{\partial E}{\partial x_m} g_l(x_l)$$

$K(l,m) = k$

Learning rate

$$w_{lm} \leftarrow w_{lm} - \eta \frac{\partial E}{\partial w_{lm}}$$

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Recurrent neural networks (RNN, DL 10.1-10.2)

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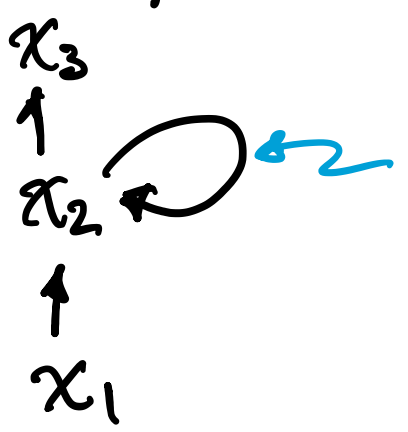
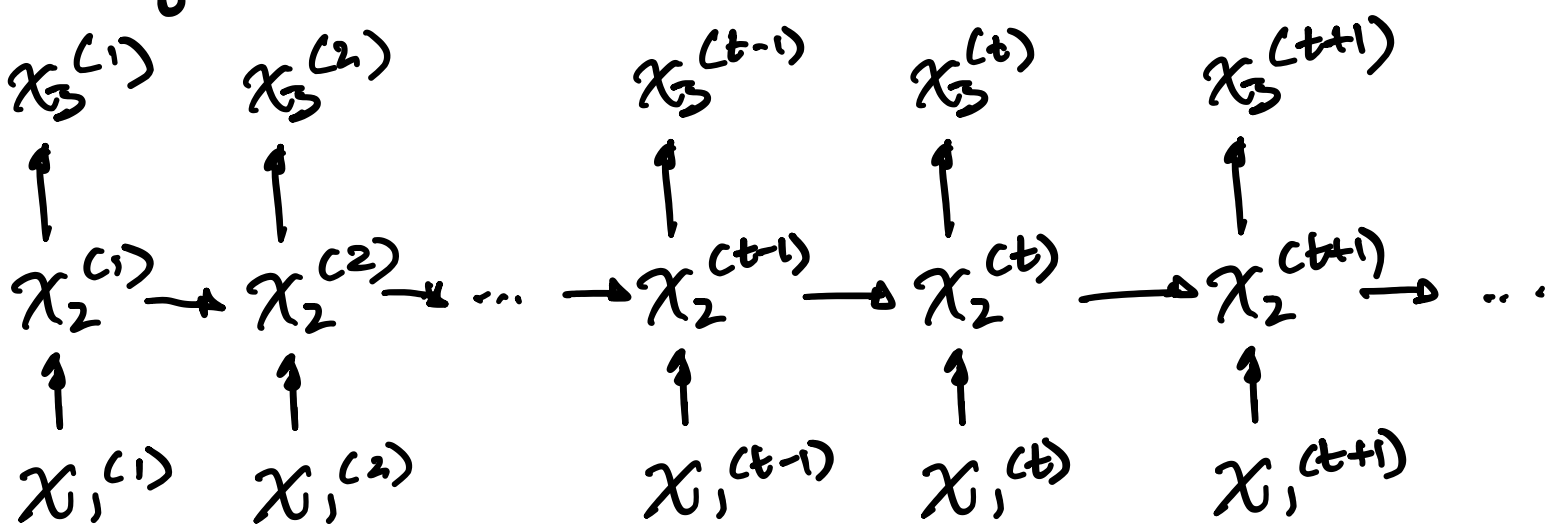
- Instead of a DAG, we allow cycles to denote signals feeding back <u>across time</u>:



x_2 at time t depends on x_2 at time $t-1$ and x_1 at time t.

- Unrolling an RNN



- Learning: This is <u>a DAG NN with weight sharing</u>, so we can use the method described previously.

Improving RNN as sequence generators (DL 10.2)

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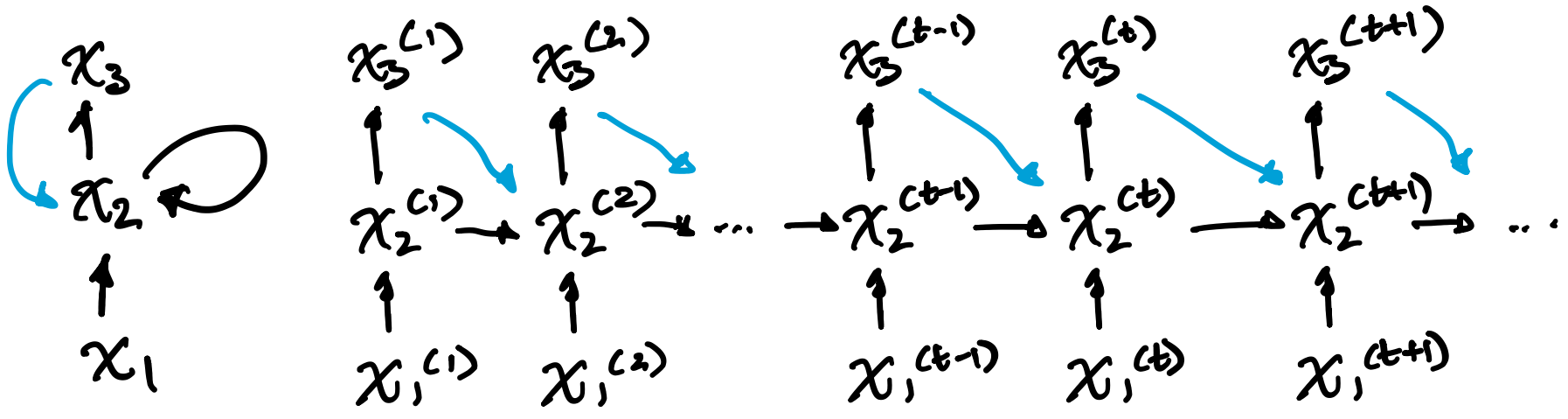
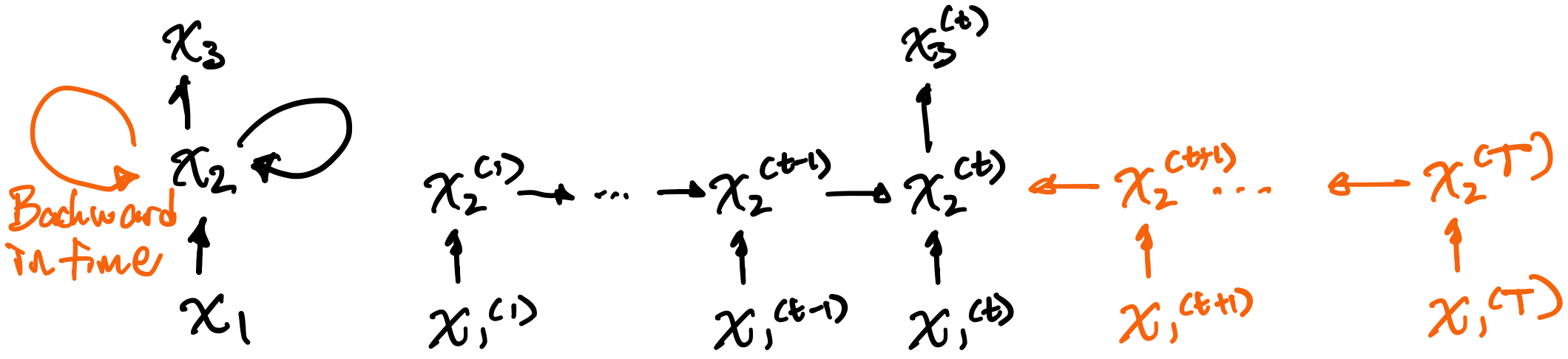
- **Conditional RNNs**: Output (t) "sees" outputs (1) ... (t-1)



- **Bidirectional RNN's**: Output (t) "sees" inputs (1) ... (T)



The problem of vanishing gradients

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- As gradients propagate through more hidden units, or through time, they get more and more suppressed (vanish) or amplified (explode)

- This makes it hard to learn RNNs with long sequences, or very deep NNs.

- A general approach is to add mechanisms that propagate derivatives directly across time, or layers.

LSTMs: Long short-term memory cells (SLP 8.5)

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- Create gates that can copy over the previous cell state to the next cell state

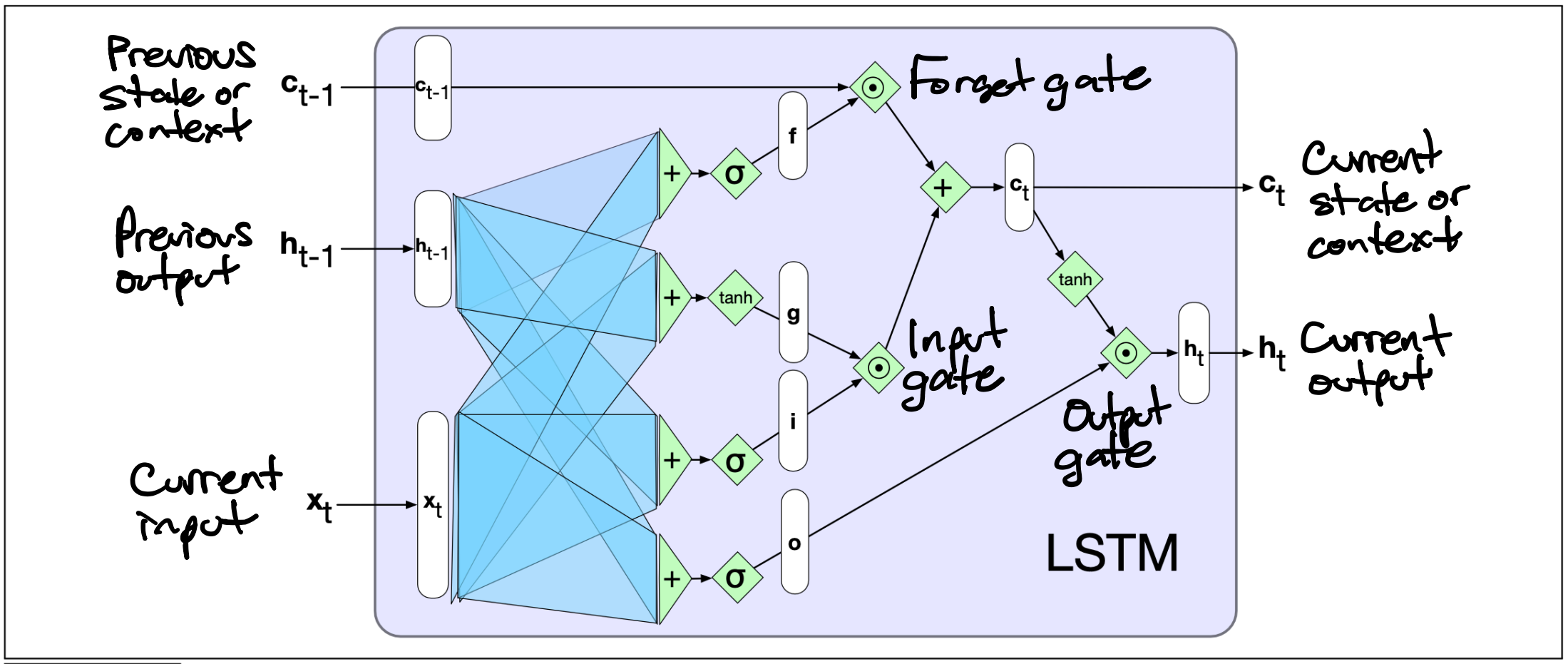

Figure 8.13 A single LSTM unit displayed as a computation graph. The inputs to each unit consists of the current input, x, the previous hidden state, h_{t-1}, and the previous context, c_{t-1}. The outputs are a new hidden state, h_t and an updated context, c_t.

* It's all differentiable!!!