CEE 616: Probabilistic Machine Learning

M2 Deep Neural Networks: Neural Networks for Structured Data II

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Tue, Oct 21, 2025

Outline

1. Backpropagation
2. Training
3. Summary

Forward mode differentiation

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Let us think of a simple feedforward with inputs $\boldsymbol{x} = \boldsymbol{x}_1 \in \mathbb{R}^{D=4}$, 3 hidden layers with $m_1 = 8$, $m_2 = 6$, and $m_3 = 4$ neurons, and outputs $\boldsymbol{o} \in \mathbb{R}^2$:

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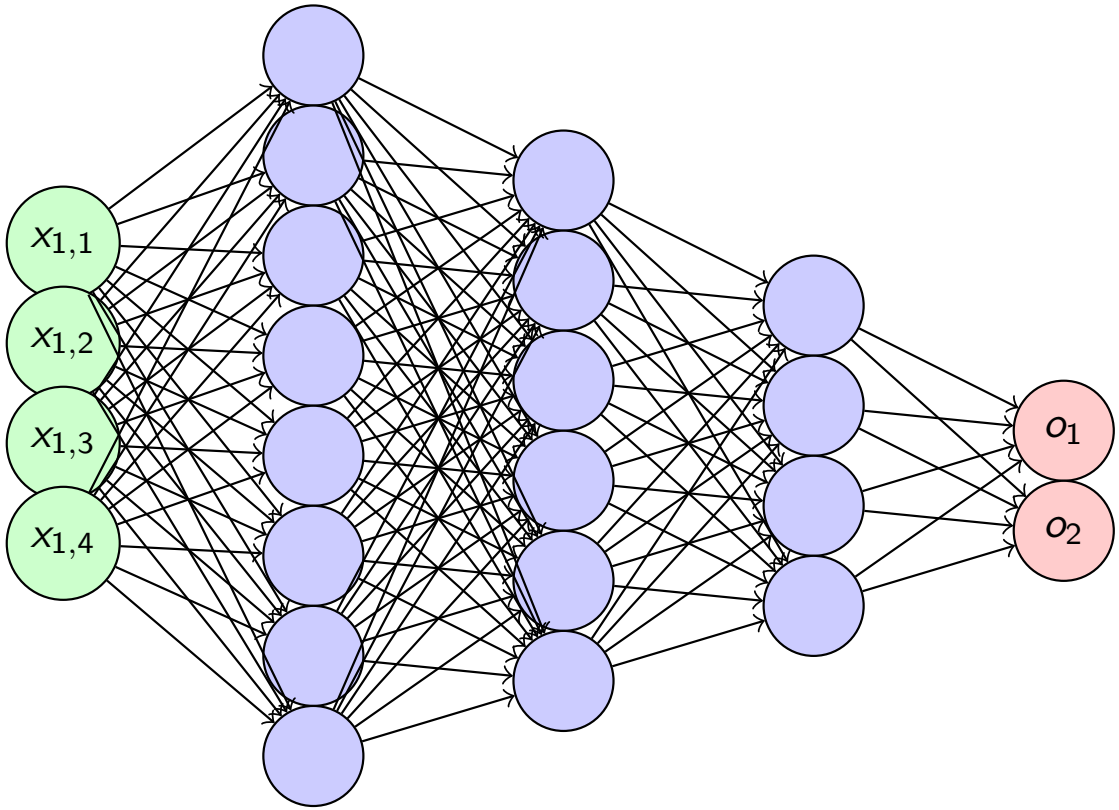

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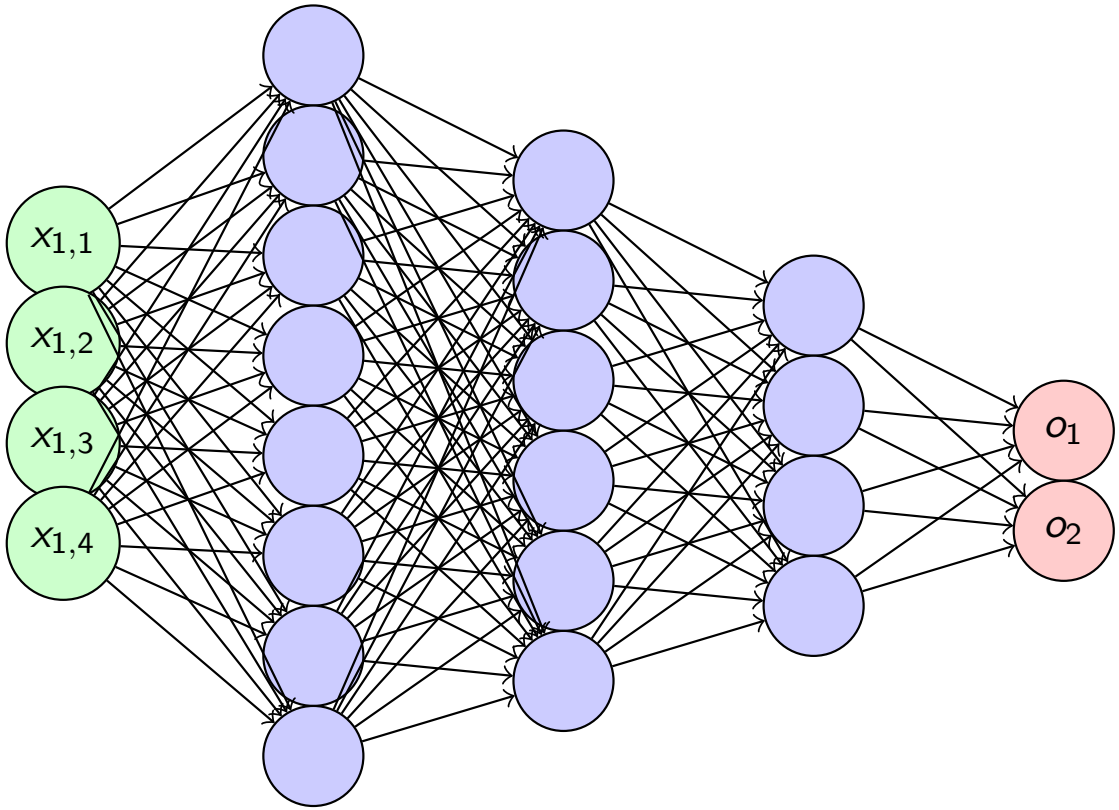

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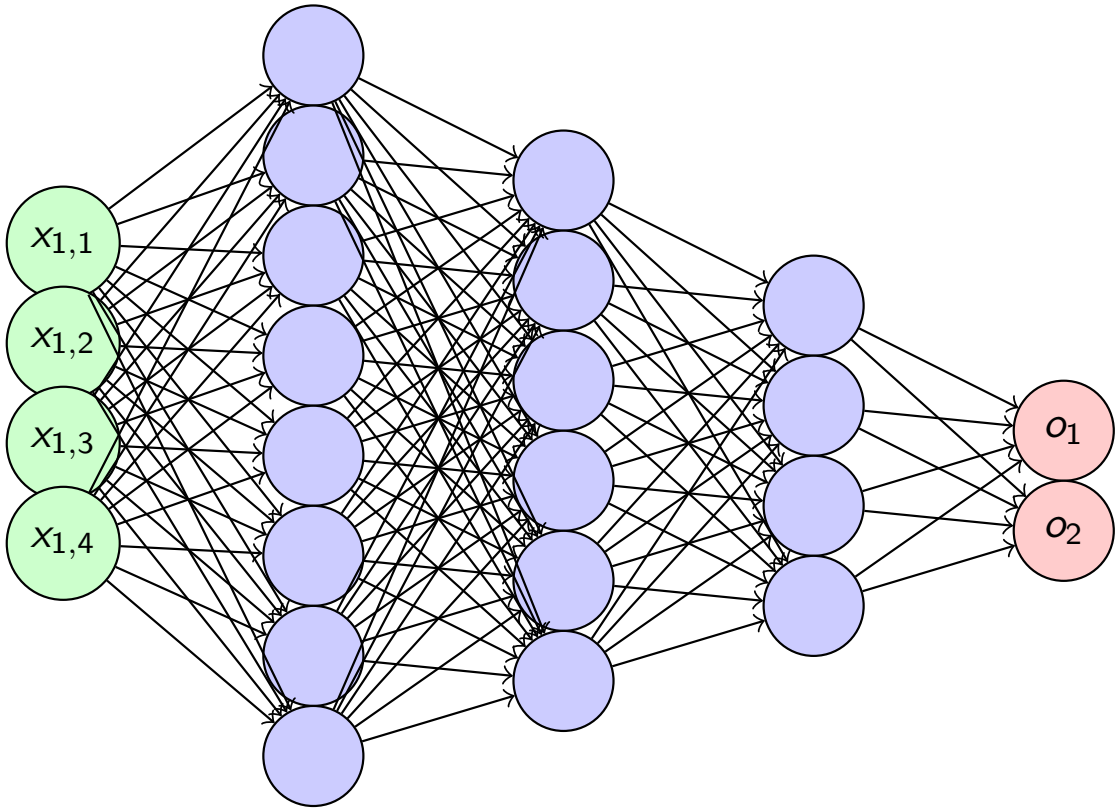

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where

$$\boldsymbol{f} = \boldsymbol{f}_4 \circ \boldsymbol{f}_3 \circ \boldsymbol{f}_2 \circ \boldsymbol{f}_1 \tag{2}$$

and thus

$$\boldsymbol{o} = \boldsymbol{f}_4(\boldsymbol{f}_3(\boldsymbol{f}_2(\boldsymbol{f}_1(\boldsymbol{x})))) \tag{3}$$

and

$$\begin{aligned}
\boldsymbol{x}_2 &= \boldsymbol{f}_1(\boldsymbol{x}_1), \quad \boldsymbol{f}_1 : \mathbb{R}^4 \to \mathbb{R}^8 \\
\boldsymbol{x}_3 &= \boldsymbol{f}_2(\boldsymbol{x}_2), \quad \boldsymbol{f}_2 : \mathbb{R}^8 \to \mathbb{R}^6 \\
\boldsymbol{x}_4 &= \boldsymbol{f}_3(\boldsymbol{x}_3), \quad \boldsymbol{f}_3 : \mathbb{R}^6 \to \mathbb{R}^4 \\
\boldsymbol{o} &= \boldsymbol{f}_4(\boldsymbol{x}_4), \quad \boldsymbol{f}_4 : \mathbb{R}^4 \to \mathbb{R}^2
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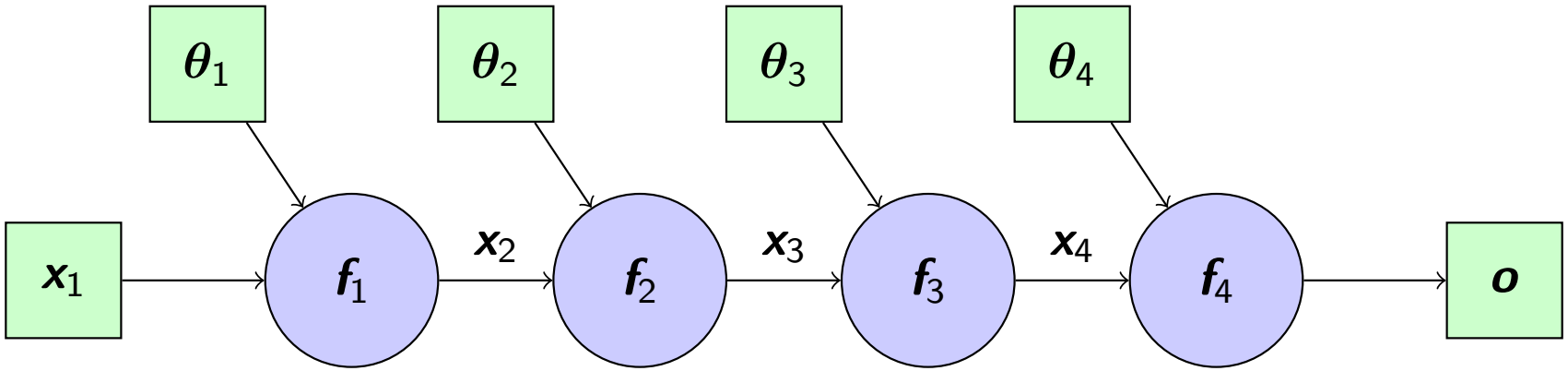

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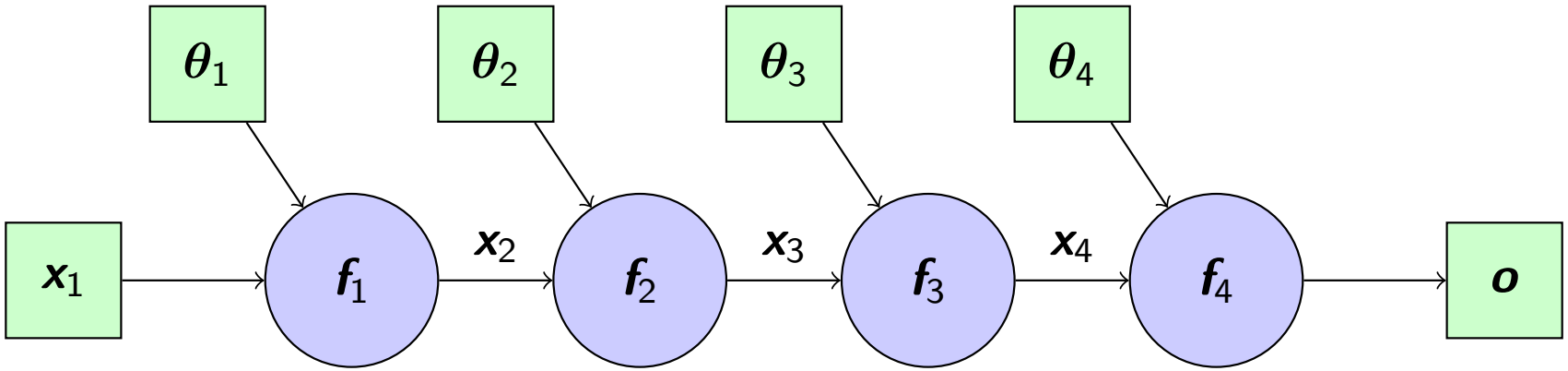

where θ_ℓ are the parameters (weights and biases) of layer ℓ.

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$$\frac{\partial \boldsymbol{o}}{\partial \boldsymbol{x}} = \frac{\partial \boldsymbol{f}_4(\boldsymbol{x}_4)}{\partial \boldsymbol{x}_4} \cdot \frac{\partial \boldsymbol{f}_3(\boldsymbol{x}_3)}{\partial \boldsymbol{x}_3} \cdot \frac{\partial \boldsymbol{f}_2(\boldsymbol{x}_2)}{\partial \boldsymbol{x}_2} \cdot \frac{\partial \boldsymbol{f}_1(\boldsymbol{x}_1)}{\partial \boldsymbol{x}_1} \tag{4}$$

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- i'th row: $\nabla f_i(\boldsymbol{x})^\top \in \mathbb{R}^{1 \times D}$ gradient of the i'th output w.r.t. all inputs
- j'th column: $\frac{\partial \boldsymbol{f}}{\partial x_j} \in \mathbb{R}^M$ gradient of all outputs w.r.t. the j'th input

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Thus:

$$\nabla \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{J}_{\boldsymbol{f}}(\boldsymbol{x})^\top = (\nabla f_1(\boldsymbol{x}), \nabla f_2(\boldsymbol{x}), \ldots, \nabla f_M(\boldsymbol{x})) \tag{8}$$

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- If $\boldsymbol{u} \in \mathbb{R}^M$ is a one-hot vector with 1 at index i and 0 elsewhere, e.g.

$$\boldsymbol{u} = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} = \boldsymbol{e}_i \tag{10}$$

then the VJP $\boldsymbol{e}_i^\top \boldsymbol{J_f}(\boldsymbol{x})$ extracts the i'th row from $\boldsymbol{J_f}(\boldsymbol{x})$, which is the gradient of the i'th output with respect to all inputs, $\nabla f_i(\boldsymbol{x})^\top$.

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- If $\boldsymbol{v} \in \mathbb{R}^D$ is a one-hot vector with 1 at index j and 0 elsewhere, e.g.

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then the JVP $\boldsymbol{J_f}(\boldsymbol{x})\boldsymbol{e}_j$ extracts the j'th column from $\boldsymbol{J_f}(\boldsymbol{x})$, which is the gradient of all outputs with respect to the j'th input, $\frac{\partial \boldsymbol{f}}{\partial x_j}$.

Computing the Jacobian

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- The Jacobian can be computed by performing either M JVPs (one per input dimension) or D VJPs (one per output dimension)
- If $D < M$, it is more efficient to compute the Jacobian via JVPs for each column j:

$$\boldsymbol{J_f}(\boldsymbol{x})(\boldsymbol{v}) = \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_4}_{M \times M_3} \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_3}_{M_3 \times M_2} \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_2}_{M_2 \times M_1} \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_1}_{M_1 \times D} \underbrace{\boldsymbol{v}}_{D \times 1} \tag{13}$$

  in a right-to-left fashion (**forward mode differentiation**)
- If $M < D$, it is more efficient to compute the Jacobian via VJPs for each row i:

$$\boldsymbol{u}^\top \boldsymbol{J_f}(\boldsymbol{x}) = \underbrace{\boldsymbol{u}^\top}_{1 \times M} \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_4}_{M \times M_3} \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_3}_{M_3 \times M_2} \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_2}_{M_2 \times M_1} \underbrace{\boldsymbol{J_f}(\boldsymbol{x})_1}_{M_1 \times D} \tag{14}$$

  in a left-to-right fashion (**reverse mode differentiation**)
- In neural networks, the number of outputs M is often much smaller than the number of inputs D
- Thus, backpropagation typically employs VJPs to compute the gradients efficiently

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\mathcal{L} &= \boldsymbol{f}_4(\boldsymbol{x}_4, \boldsymbol{y}) = \frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}_4||_2^2 && (20)
\end{aligned}$$

and $\mathcal{L} : \mathbb{R}^D \to \mathbb{R}$.

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$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}_1} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{x}_4} \frac{\partial \boldsymbol{x}_4}{\partial \boldsymbol{x}_3} \frac{\partial \boldsymbol{x}_3}{\partial \boldsymbol{x}_2} \frac{\partial \boldsymbol{x}_2}{\partial \boldsymbol{\theta}_1} \tag{23}$$

Note:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}_k} = (\nabla_{\boldsymbol{\theta}_k} \mathcal{L})^\top \tag{24}$$

is a d_k-dimensional gradient row vector, where d_k is the number of parameters in layer k

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Using the chain rule, We can express the gradient of the loss wrt the parameters in each layer as:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}_3} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{x}_4}\frac{\partial \boldsymbol{x}_4}{\partial \boldsymbol{\theta}_3} \tag{21}$$

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}_2} = \frac{\partial \mathcal{L}}{\partial \boldsymbol{x}_4}\frac{\partial \boldsymbol{x}_4}{\partial \boldsymbol{x}_3}\frac{\partial \boldsymbol{x}_3}{\partial \boldsymbol{\theta}_2} \tag{22}$$

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Note:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}_k} = (\nabla_{\boldsymbol{\theta}_k} \mathcal{L})^\top \tag{24}$$

is a d_k-dimensional gradient row vector, where d_k is the number of parameters in layer k and can be computed recursively as VJPs:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}_k} = \boldsymbol{u}_{k+1}^\top \frac{\partial \boldsymbol{f}_k(\boldsymbol{x}_k, \boldsymbol{\theta}_k)}{\partial \boldsymbol{\theta}_k} \tag{25}$$

where $\boldsymbol{x}_{k+1} = \boldsymbol{f}_k(\boldsymbol{x}_k, \boldsymbol{\theta}_k)$, $\boldsymbol{u}_k^\top = \boldsymbol{u}_{k+1}^\top \frac{\partial \boldsymbol{f}_k(\boldsymbol{x}_k, \boldsymbol{\theta}_k)}{\partial \boldsymbol{x}_k}$ and $\boldsymbol{u}_{K+1} = 1$.

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This procedure is also known as **online learning**

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   Thus, for each iteration, average the gradient over a *mini-batch* of B randomly selected observations
3. Repeat step 2 until convergence

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- Cost function C is nonlinear and nonconvex; other optimization approaches (e.g. conjugate gradient) can provide faster convergence compared to stochastic gradient descent

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