

CS6421: Deep Neural Networks

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Lecture 4: Mathematical Foundations

Based on notes from Marc Diesendorf

Overview

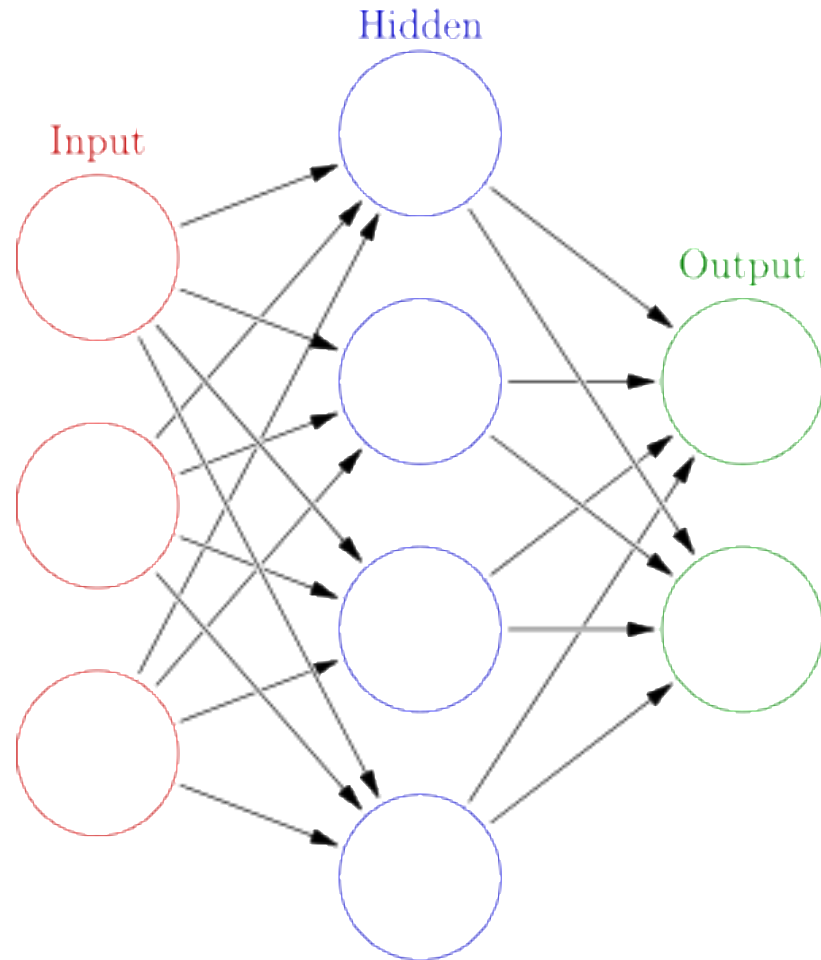
- Mathematical Basis of Deep Learning
- Linear Algebra
- Multivariate Calculus

Key Mathematical Concepts

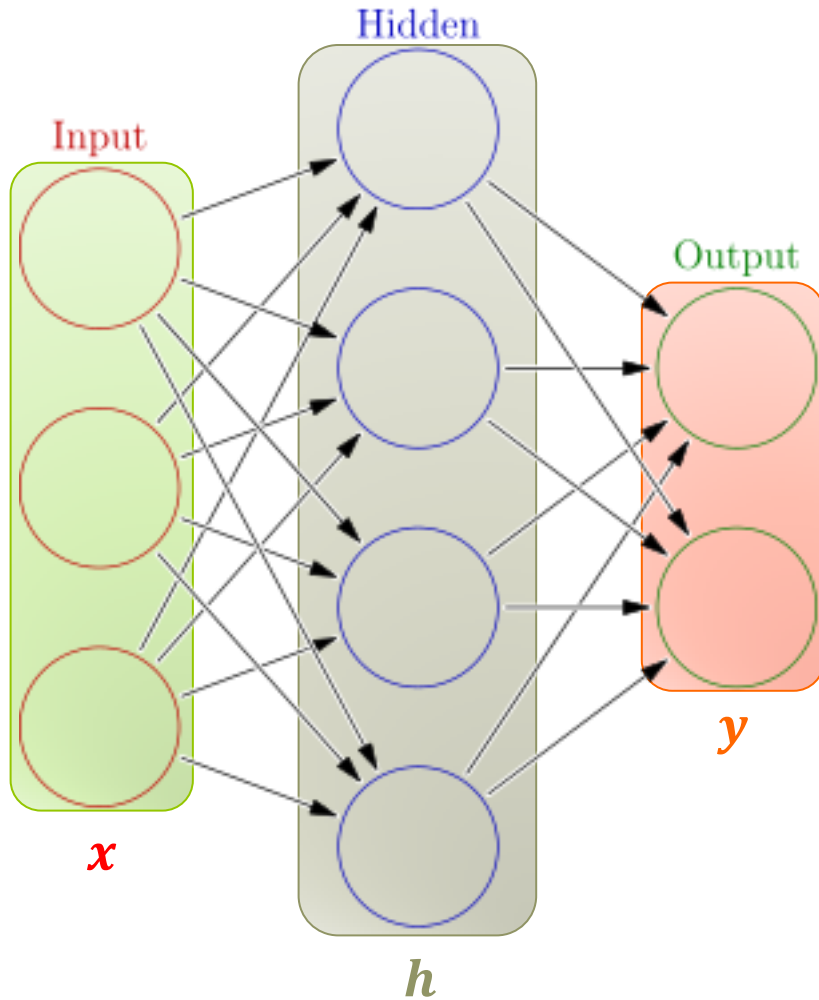
- Linear algebra and matrix decomposition
- **Differentiation**
- **Integration**
- Optimization
- Probability theory and Bayesian inference
- Functional analysis

Neural Networks Basics

- Operations
 - Forward prop: makes predictions
 - Backward prop: adjusts parameters



Neural Network: Definition



Weights

$$h = \sigma(W_1 x + b_1)$$
$$y = \sigma(W_2 h + b_2)$$

Activation functions

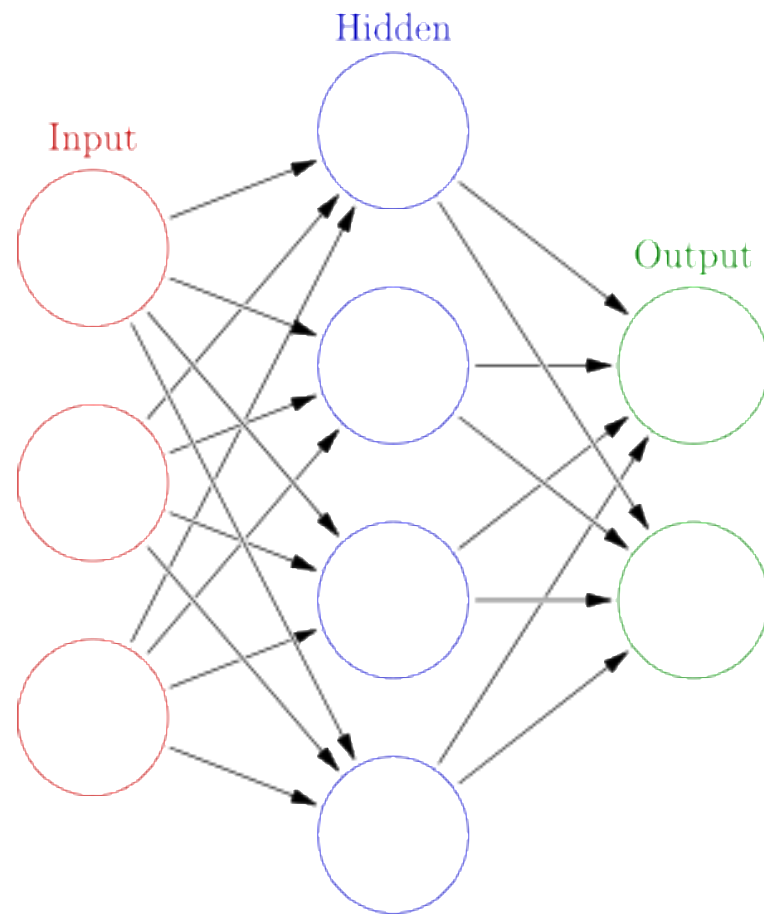
What are the underlying mathematical operations?

Forward Propagation

$$\vec{X} \rightarrow \vec{H} \rightarrow \hat{\vec{Y}}$$

$$\vec{H} = \text{relu} \left(\left([W] * \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \right) + [b] \right)$$

$$\hat{\vec{Y}} = \text{relu} \left(\left([U] * \begin{bmatrix} H_1 \\ H_2 \\ H_3 \\ H_4 \end{bmatrix} \right) + [c] \right)$$



Forward Propagation

$$\vec{H} = \text{relu} \left(\left([W] * \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \right) + [b] \right)$$

Matrix Multiplication

- Changes Dimensionality

$$(m * n) * (n * p) = (m * p)$$

$$(m * n) * (3 * 1) = (4 * 1)$$

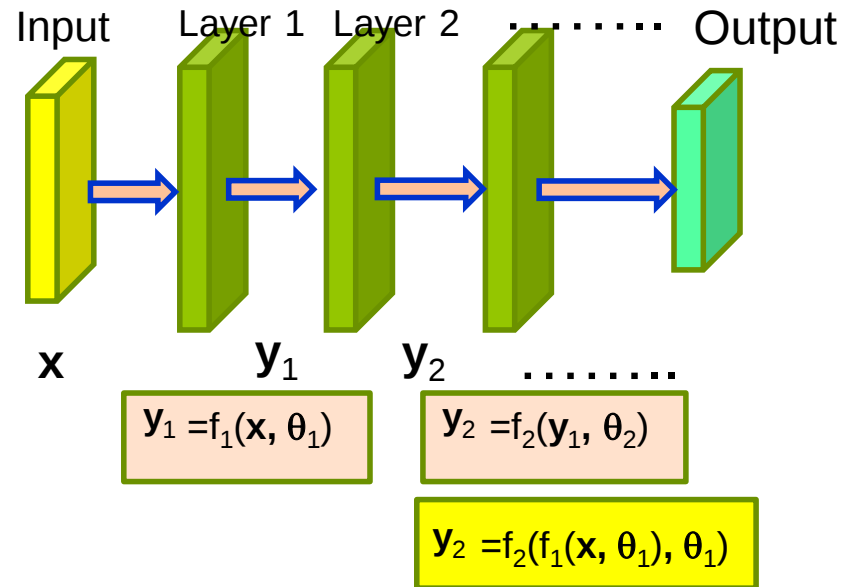
$$(4 * 3) * (3 * 1) = (4 * 1)$$

$$\vec{H} = \text{relu} \left(\left(\begin{bmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \\ W_{41} & W_{42} & W_{43} \end{bmatrix} * \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} \right) + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{bmatrix} \right)$$

Deep Network: Generic Definition

- A family of parametric, non-linear and hierarchical representation learning functions
 - massively optimized with stochastic gradient descent to encode domain knowledge, i.e. domain invariances, stationarity.
- $a^L(x; w^1, \dots, w^L) = h^L(h^{L-1} \dots h^1(x, w^1), w^{L-1}), w^L)$
 - x : input,
 - w^l : parameters for layer l ,
 - $a^l = h^l(x, w^l)$: (non-) linear function
- Given training corpus $\{X, Y\}$ find optimal parameters
 - $w^* \leftarrow \operatorname{argmin}_w \sum_{(x,y) \subseteq (X,Y)} L(y, a^L(x))$

Forward Propagation: Deep Network



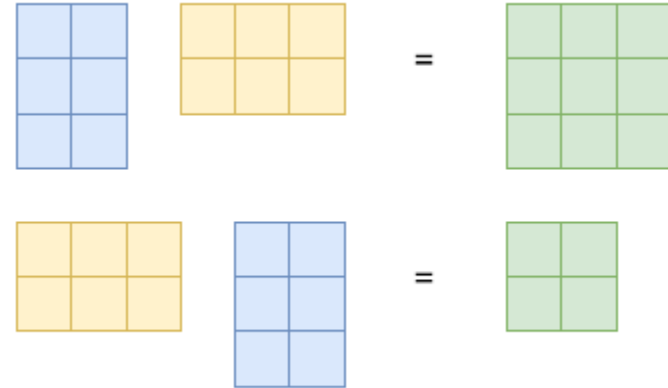
Deep Network: family of parametric, non-linear, hierarchical representations

$$y_N(x, \theta_1, \theta_2, \dots, \theta_N) = f_N(f_{N-1}(\dots(f_1(x, \theta_1), \theta_{N-1}), \theta_N)$$

Implemented as matrix/vector operations

Matrix Multiplication

- Matrix multiplication is not commutative, i.e., **$\mathbf{AB} \neq \mathbf{BA}$**
- When multiplying matrices, the “neighbouring” dimensions have to fit:



$$\underbrace{A}_{n \times k} \underbrace{B}_{k \times m} = \underbrace{C}_{n \times m}$$

$$y = Ax$$

$$y_i = \sum_j A_{ij} x_j$$

$$C = AB$$

$$C_{ij} = \sum_k A_{ik} B_{kj}$$

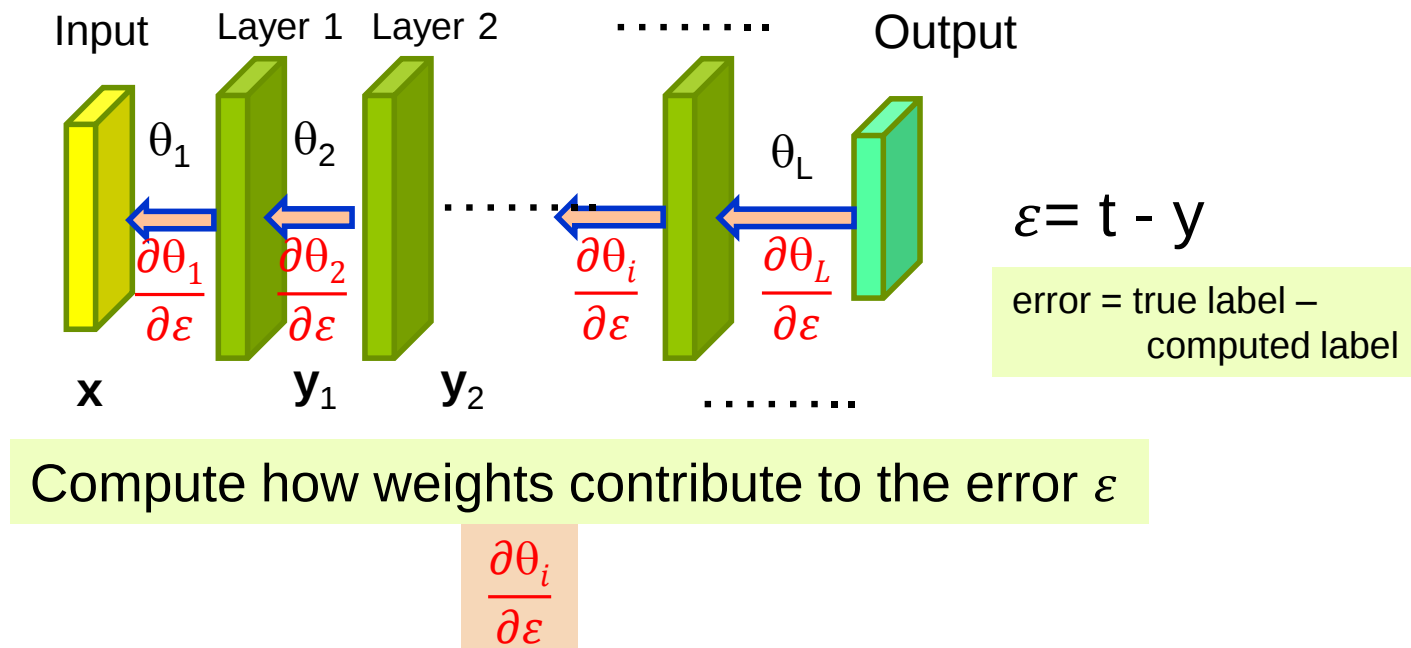
$$y = A.\text{dot}(x)$$

$$y = \text{np.einsum}('ij, j', A, x)$$

$$C = A.\text{dot}(B)$$

$$C = \text{np.einsum}('ik, kj', A, B)$$

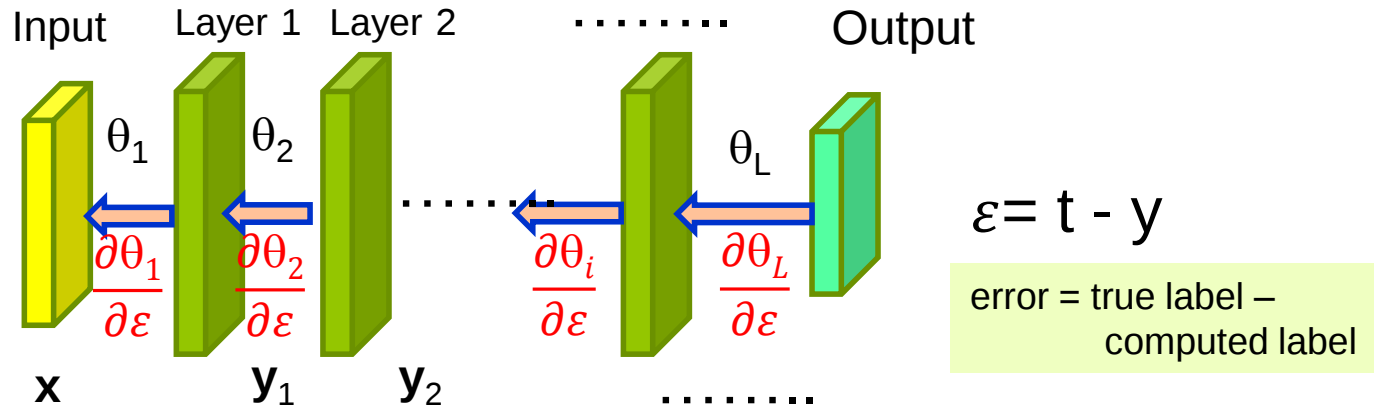
Back Propagation: Deep Network



Training: optimize network parameters to minimise loss over training set

$$\theta^* = \arg \min \sum_{(x,y) \in (X,Y)} J[y, f^L(x, \theta_1, \dots, \theta_L)]$$

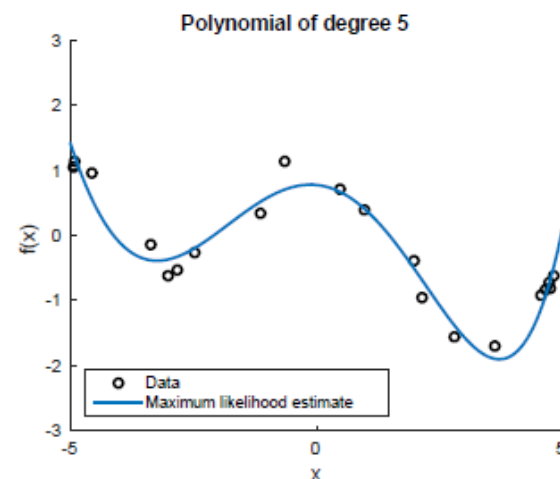
Training: Computes Derivatives



- Must use partial derivative plus chain rule
- Shows that backpropagation can be done layer by layer

Network Training

- ▶ Training data, e.g., N pairs (x_i, y_i) of inputs x_i and observations y_i
- ▶ **Training the model** means finding parameters θ^* , such that $f(x_i, \theta^*) \approx y_i$



- ▶ Define a **loss function**, e.g., $\sum_{i=1}^N (y_i - f(x_i, \theta))^2$, which we want to optimize
- ▶ Typically: Optimization based on some form of **gradient descent**
 - ▶▶ Differentiation required

Requirement for Differentiation

- Differentiate arbitrary formulae
 - Loss function: $L = \Psi(t-y)^2$
 - Activation function: $\tanh$
 - Algebraic operation: Wx
- Rules of differentiation must be used
 - Sum, product, chain, etc.

Differentiation: Rules

- ▶ Sum Rule

$$(f(x) + g(x))' = f'(x) + g'(x) = \frac{df}{dx} + \frac{dg}{dx}$$

- ▶ Product Rule

$$(f(x)g(x))' = f'(x)g(x) + f(x)g'(x) = \frac{df}{dx}g(x) + f(x)\frac{dg}{dx}$$

- ▶ Chain Rule

$$(g \circ f)'(x) = (g(f(x)))' = g'(f(x))f'(x) = \frac{dg}{df} \frac{df}{dx}$$

Example

$$(g \circ f)'(x) = (g(f(x)))' = g'(f(x))f'(x) = \frac{dg}{df} \frac{df}{dx}$$

$$g(z) = \tanh(z)$$

$$z = f(x) = x^n$$

$$(g \circ f)'(x) = \underbrace{(1 - \tanh^2(x^n))}_{dg/df} \underbrace{nx^{n-1}}_{df/dx}$$

Partial Derivatives

$$f : \mathbb{R}^N \rightarrow \mathbb{R}$$

$$y = f(\mathbf{x}), \quad \mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} \in \mathbb{R}^N$$

- ▶ **Partial derivative** (change one coordinate at a time):

$$\frac{\partial f}{\partial x_i} = \lim_{h \rightarrow 0} \frac{f(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_N) - f(\mathbf{x})}{h}$$

- ▶ **Jacobian** vector (**gradient**) collects all partial derivatives:

$$\frac{df}{d\mathbf{x}} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{1 \times N}$$

Note: This is a row vector.

Example

$$f : \mathbb{R}^2 \rightarrow \mathbb{R}$$

$$f(x_1, x_2) = x_1^2 x_2 + x_1 x_2^3 \in \mathbb{R}$$

- Partial derivatives:

$$\frac{\partial f(x_1, x_2)}{\partial x_1} = 2x_1 x_2 + x_2^3$$

$$\frac{\partial f(x_1, x_2)}{\partial x_2} = x_1^2 + 3x_1 x_2^2$$

- Gradient:

$$\frac{df}{d\mathbf{x}} = \left[\frac{\partial f(x_1, x_2)}{\partial x_1} \quad \frac{\partial f(x_1, x_2)}{\partial x_2} \right] = \left[2x_1 x_2 + x_2^3 \quad x_1^2 + 3x_1 x_2^2 \right] \in \mathbb{R}^{1 \times 2}.$$

Example: Chain Rule

- Consider the function

$$L(\mathbf{e}) = \frac{1}{2} \|\mathbf{e}\|^2 = \frac{1}{2} \mathbf{e}^\top \mathbf{e}$$

$$\mathbf{e} = \mathbf{y} - \mathbf{A}\mathbf{x}, \quad \mathbf{x} \in \mathbb{R}^N, \mathbf{A} \in \mathbb{R}^{M \times N}, \mathbf{e}, \mathbf{y} \in \mathbb{R}^M$$

- Compute $dL/d\mathbf{x}$. What is the dimension/size of $dL/d\mathbf{x}$?
- $dL/d\mathbf{x} \in \mathbb{R}^{1 \times N}$

$$\frac{dL}{d\mathbf{x}} = \frac{dL}{d\mathbf{e}} \frac{d\mathbf{e}}{d\mathbf{x}}$$

$$\frac{dL}{d\mathbf{e}} = \mathbf{e}^\top \in \mathbb{R}^{1 \times M}$$

$$\frac{d\mathbf{e}}{d\mathbf{x}} = -\mathbf{A} \in \mathbb{R}^{M \times N}$$

$$\Rightarrow \frac{dL}{d\mathbf{x}} = \mathbf{e}^\top (-\mathbf{A}) = -(\mathbf{y} - \mathbf{A}\mathbf{x})^\top \mathbf{A} \in \mathbb{R}^{1 \times N}$$

Jacobian Matrix

$$f : \mathbb{R}^N \rightarrow \mathbb{R}^M$$

$$\mathbf{y} = f(\mathbf{x}) \in \mathbb{R}^M, \quad \mathbf{x} \in \mathbb{R}^N$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\mathbf{x}) \\ \vdots \\ f_M(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} f_1(x_1, \dots, x_N) \\ \vdots \\ f_M(x_1, \dots, x_N) \end{bmatrix}$$

- **Jacobian** matrix (collection of all partial derivatives)

$$\begin{bmatrix} \frac{dy_1}{dx} \\ \vdots \\ \frac{dy_M}{dx} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{M \times N}$$

Example

$$f(\mathbf{x}) = \mathbf{A}\mathbf{x}, \quad f(\mathbf{x}) \in \mathbb{R}^M, \quad \mathbf{A} \in \mathbb{R}^{M \times N}, \quad \mathbf{x} \in \mathbb{R}^N$$

- ▶ Compute the gradient $d\mathbf{f}/d\mathbf{x}$

- ▶ Dimension of $d\mathbf{f}/d\mathbf{x}$:

Since $f : \mathbb{R}^N \rightarrow \mathbb{R}^M$, it follows that $d\mathbf{f}/d\mathbf{x} \in \mathbb{R}^{M \times N}$

- ▶ Gradient:

$$\begin{aligned} f_i &= \sum_{j=1}^N A_{ij}x_j \quad \Rightarrow \quad \frac{\partial f_i}{\partial x_j} = A_{ij} \\ \Rightarrow \frac{d\mathbf{f}}{d\mathbf{x}} &= \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MN} \end{bmatrix} = \mathbf{A} \end{aligned}$$

Example

- Consider $f : \mathbb{R}^2 \rightarrow \mathbb{R}$, $\mathbf{x} : \mathbb{R} \rightarrow \mathbb{R}^2$

$$f(\mathbf{x}) = f(x_1, x_2) = x_1^2 + 2x_2,$$

$$\mathbf{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \sin(t) \\ \cos(t) \end{bmatrix}$$

- The dimensions $df/d\mathbf{x}$ and $d\mathbf{x}/dt$ are 1×2 and 2×1 , respectively
- Compute the gradient df/dt using the chain rule.

$$\begin{aligned} \frac{df}{dt} &= \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix} \\ &= \begin{bmatrix} 2 \sin t & 2 \end{bmatrix} \begin{bmatrix} \cos t \\ -\sin t \end{bmatrix} \\ &= 2 \sin t \cos t - 2 \sin t = 2 \sin t (\cos t - 1) \end{aligned}$$

Derivatives with Matrices: Summary

- Re-cap: Gradient of a function $f : \mathbb{R}^D \rightarrow \mathbb{R}^E$ is an $E \times D$ -matrix:

target dimensions $\times$ # parameters

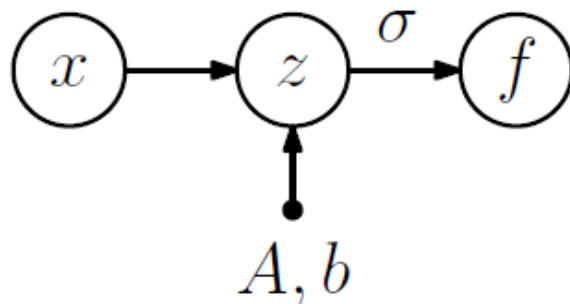
with

$$\frac{df}{d\mathbf{x}} \in \mathbb{R}^{E \times D}, \quad df[e, d] = \frac{\partial f_e}{\partial x_d}$$

- Generalization to cases, where the parameters (D) or targets (E) are matrices, apply immediately
- Assume $f : \mathbb{R}^{M \times N} \rightarrow \mathbb{R}^{P \times Q}$, then the gradient is a $(P \times Q) \times (M \times N)$ object (tensor) where

$$df[p, q, m, n] = \frac{\partial f_{pq}}{\partial X_{mn}}$$

Gradients of Single-Layer Network



$$f = \tanh(\underbrace{Ax + b}_{=: z \in \mathbb{R}^M}) \in \mathbb{R}^M, \quad x \in \mathbb{R}^N, A \in \mathbb{R}^{M \times N}, b \in \mathbb{R}^M$$

$$\frac{\partial f}{\partial b} = \underbrace{\frac{\partial f}{\partial z}}_{M \times M} \underbrace{\frac{\partial z}{\partial b}}_{M \times M} \in \mathbb{R}^{M \times M}$$

$$\frac{\partial f}{\partial A} = \underbrace{\frac{\partial f}{\partial z}}_{M \times M} \underbrace{\frac{\partial z}{\partial A}}_{M \times (M \times N)} \in \mathbb{R}^{M \times (M \times N)}$$

Example

$$f = \tanh(\underbrace{Ax + b}_{=: z \in \mathbb{R}^M}) \in \mathbb{R}^M, \quad x \in \mathbb{R}^N, A \in \mathbb{R}^{M \times N}, b \in \mathbb{R}^M$$

$$\frac{\partial f}{\partial b} = \underbrace{\frac{\partial f}{\partial z}}_{M \times M} \underbrace{\frac{\partial z}{\partial b}}_{M \times M} \in \mathbb{R}^{M \times M}$$

$$\frac{\partial f}{\partial z} = \text{diag}(1 - \tanh^2(z)) \in \mathbb{R}^{M \times M}$$

$$\frac{\partial z}{\partial b} = \mathbf{I} \in \mathbb{R}^{M \times M}$$

(5)

$$\frac{\partial f}{\partial b}[i, j] = \sum_{l=1}^M \frac{\partial f}{\partial z}[i, l] \frac{\partial z}{\partial b}[l, j]$$

```
dfdb = np.einsum('il, lj', dfdz, dzdb)
```

Example (continued)

$$f = \tanh(\underbrace{Ax + b}_{=:z \in \mathbb{R}^M}) \in \mathbb{R}^M, \quad x \in \mathbb{R}^N, A \in \mathbb{R}^{M \times N}, b \in \mathbb{R}^M$$

$$\frac{\partial f}{\partial A} = \underbrace{\frac{\partial f}{\partial z}}_{M \times M} \underbrace{\frac{\partial z}{\partial A}}_{M \times (M \times N)} \in \mathbb{R}^{M \times (M \times N)}$$

$$\frac{\partial f}{\partial z} = \text{diag}(1 - \tanh^2(z)) \in \mathbb{R}^{M \times M} \quad (6)$$

$\frac{\partial z}{\partial A} \gg \text{See (4)}$

$$\frac{\partial f}{\partial A}[i, j, k] = \sum_{l=1}^M \frac{\partial f}{\partial z}[i, l] \frac{\partial z}{\partial A}[l, j, k]$$

```
dfdA = np.einsum('il, ljk', dfdz, dzdA)
```

Summary: Single Layer NN

- Inputs x , observed outputs $y = f(z, \theta) + \epsilon, \epsilon \sim \mathcal{N}(\mathbf{0}, \Sigma)$
- Train single-layer neural network with

$$f(z, \theta) = \tanh(z), \quad z = Ax + b, \quad \theta = \{A, b\}$$

- Find A, b , such that the squared loss

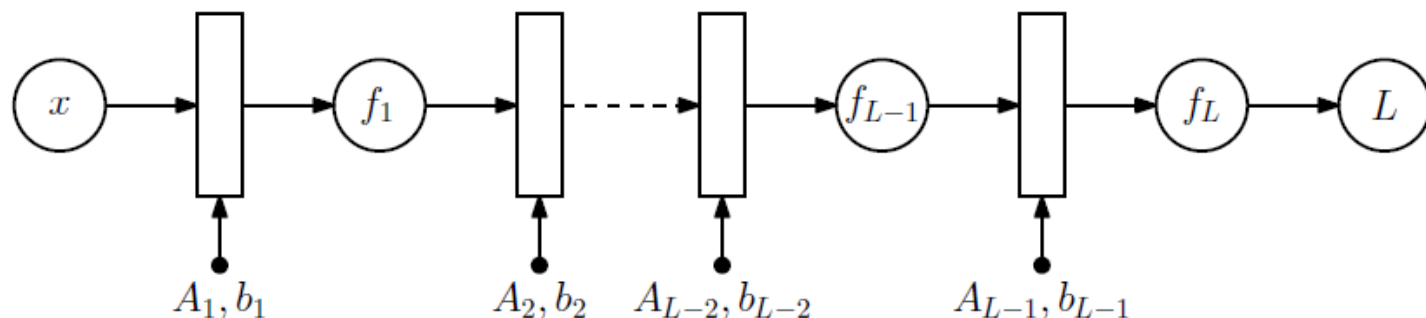
$$L(\theta) = \frac{1}{2} \|e\|^2, \quad e = y - f(z, \theta)$$

is minimized

- Partial derivatives:

$$\left. \begin{aligned} \frac{\partial L}{\partial A} &= \frac{\partial L}{\partial e} \frac{\partial e}{\partial f} \frac{\partial f}{\partial z} \frac{\partial z}{\partial A} \\ \frac{\partial L}{\partial b} &= \frac{\partial L}{\partial e} \frac{\partial e}{\partial f} \frac{\partial f}{\partial z} \frac{\partial z}{\partial b} \end{aligned} \right\} \begin{aligned} \frac{\partial L}{\partial e} &\gg (1) & \frac{\partial e}{\partial f} &\gg (2), (3) & \frac{\partial f}{\partial z} &\gg (6) \\ \frac{\partial z}{\partial A} &\gg (4) & \frac{\partial z}{\partial b} &\gg (5) \end{aligned}$$

Multi-Layer NN: Gradients



- Inputs x , observed outputs y
- Train multi-layer neural network with

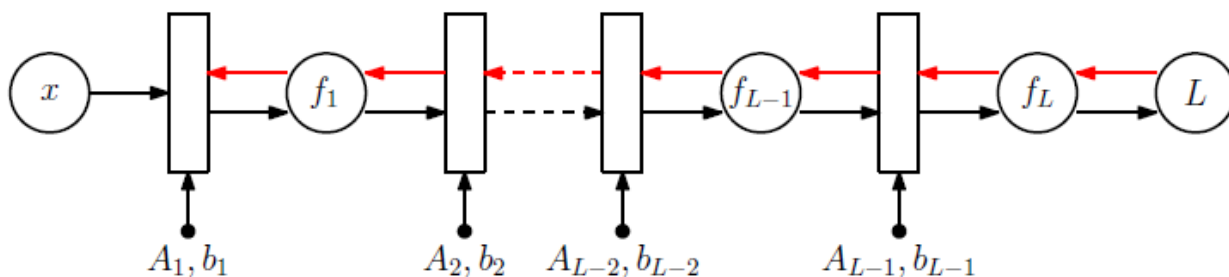
$$f_0 = x$$

$$f_i = \sigma_i(A_{i-1}f_{i-1} + b_{i-1}), \quad i = 1, \dots, L$$

- Find A_j, b_j for $j = 0, \dots, L-1$, such that the squared loss

$$L(\theta) = \|y - f_L(\theta, x)\|^2$$

is minimized, where $\theta = \{A_j, b_j\}$, $j = 0, \dots, L-1$



$$\frac{\partial L}{\partial \theta_{L-1}} = \frac{\partial L}{\partial f_L} \frac{\partial f_L}{\partial \theta_{L-1}}$$

$$\frac{\partial L}{\partial \theta_{L-2}} = \frac{\partial L}{\partial f_L} \left[\frac{\partial f_L}{\partial f_{L-1}} \frac{\partial f_{L-1}}{\partial \theta_{L-2}} \right]$$

$$\frac{\partial L}{\partial \theta_{L-3}} = \frac{\partial L}{\partial f_L} \frac{\partial f_L}{\partial f_{L-1}} \left[\frac{\partial f_{L-1}}{\partial f_{L-2}} \frac{\partial f_{L-2}}{\partial \theta_{L-3}} \right]$$

$$\frac{\partial L}{\partial \theta_i} = \frac{\partial L}{\partial f_L} \frac{\partial f_L}{\partial f_{L-1}} \dots \left[\frac{\partial f_{i+2}}{\partial f_{i+1}} \frac{\partial f_{i+1}}{\partial \theta_i} \right]$$

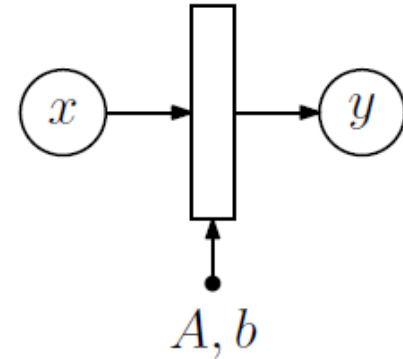
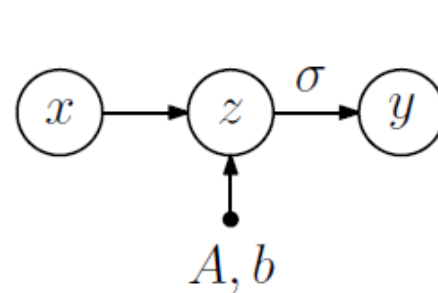
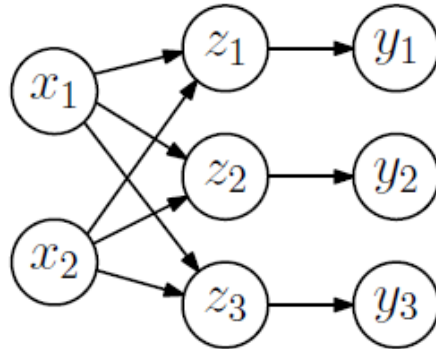
Summary

- **Deep Learning is based on core mathematical principles**
- **Review of**
 - **Linear algebra**
 - **Multivariable calculus (chain rule, etc.)**

Feed-Forward Neural Network

$$y = \sigma(z)$$

$$z = Ax + b$$



- Training a neural network means parameter optimization:
 - Typically via some form of gradient descent
- **Challenge 1: Differentiation.** Compute gradients of a loss function with respect to neural network parameters **A**, **b**
 - Computing statistics (e.g., means, variances) of predictions
- **Challenge 2: Integration.** Propagate uncertainty through a neural network