Deep Learning

Linear Models

Linear models are a class of **regression** and **classification** models in which the prediction is a linear function of the input variables.

Linear Regression: $y = w^T x + b$

- w is a d-dimensional vector of **weights**;
- b is a **bias** - usually included in w as a constant feature $x_0 = 1$;
- Given **training data** $D = \{(x_n, y_n)\}_{n=1}^N$, we want to find the **best** w and b, so we use want to fit the model, i.e. find the best w and b, **minimizing the loss function** - usually, the **squared loss**: $\hat{w} = argmin_w \frac{1}{2} \sum_{n=1}^N (y_n - (w^T x_n + b))^2$;
  - $MSE = \frac{1}{N} \sum_{n=1}^N (y_n - \hat{y}_n)^2$;
- **Closed-form solution**: $w = (X^T X)^{-1} X^T y$, where $X = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{bmatrix}$ and $y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$;
- **Regularization** is a technique used to **reduce overfitting** by **constraining** the **weights** of the model;
  - If $X^T X$ is not invertible, we can add a regularization term to the loss function - **ridge regression**;
    - $L(w, b) = \sum_{n=1}^N (y_n - (w^T x_n + b))^2 + \lambda ||w||_2^2$;
    - **Closed-form solution**: $\hat{w_{ridge}} = (X^T X + \lambda I)^{-1} X^T y$;
    - l_2 regularization is also known as **weight decay**, or penalized least squares.

Reduce Overfitting

- **Regularization** is a technique used to **reduce overfitting** by **constraining** the **weights** of the model;
- **Early stopping** is a technique used to **reduce overfitting** by **stopping the training** when the **validation error** starts to **increase**;
- **Dropout** is a technique used to **reduce overfitting** by **randomly dropping neurons** during **training - ensemble** of **smaller networks - regularizes** the **network**;
- **Data augmentation** is a technique used to **reduce overfitting** by **increasing the size** of the **training set - artificially generate new data - regularizes** the **network**.

In case of **underfitting**, we can:

- **Increase the model capacity - increase the number of parameters**;
- **Decrease the regularization - decrease the regularization constant**;
- **Increase the training time - increase the number of epochs**.

Maximum A Posteriori Estimation

- A **Bayesian** approach to **linear regression**;
- Assume that the **weights** are **random variables** with a **prior distribution**: $w \sim \mathcal{N}(0, \tau^2 I)$;
- $\hat{w_{MAP}} = argmax_w p(w|y) = argmin_w \lambda ||w||_2^2 + \sum_{n=1}^{N} (y_n - w^T \phi(x_n))^2$;
  - $||w||_2^2$ is the **regularization term**;
  - $\sum_{n=1}^{N} (y_n - w^T \phi(x_n))^2$ is the **squared loss**.

Perceptron: $y = sign(w^T x + b)$

- **Binary classification** model - outputs $+1$ or -1 (**discrete**);
- **Discriminative** model - **directly** models $p(y|x)$;
- Bias b is included in w as a constant feature $x_0 = 1$;
- x can be represented as $\phi(x)$, where ϕ is a **feature map**;
- Algorithm:
  1. Initialize w to zero: $w_0 = 0$;

2. While not converged, for each (x_n, y_n) in D:
   (a) Predict: $\hat{y} = sign(w^T x_n)$;
   (b) If $\hat{y} \neq y_n$:
      i. Update: $w_{t+1} = w_t + y_n x_n$;
      ii. Go to step 2;

- **Perceptron convergence theorem**: if the **training data** is **linearly separable**, the **perceptron algorithm** will **converge** in a **finite number of steps**:
- It **cannot** be used for **non-linearly separable data** - XOR problem.

Logistic Regression: $y = \sigma(w^T x + b)$

- **Logistic regression** is a **linear model** for **binary classification** - differs from perceptron, because it uses a **sigmoid function (continuous)** instead of a **sign function (discrete)**;
- **Binary classification** model - outputs $[0, 1]$ (**continuous**);
- **Discriminative** model - **directly** models $p(y|x)$;
- No closed-form solution, so we use **gradient descent** to find the **best** w and b - **stochastic gradient descent** is usually used, because it is **faster**: $w_{t+1} = w_t - \eta \nabla_w L(w_t)$. The **learning rate** η is usually **small**;
  - Different than **gradient descent**: $w_{t+1} = w_t - \eta \nabla_w \sum_{n=1}^{N} L(w_t, x_n, y_n)$, which uses **all** the **training data** to compute the **gradient**.

Multi-class Classification

- **Multi-class classification** is a **classification** task with **more than two classes**, but there are several strategies to **reduce to binary classification**;
- Parametrized by a **weight matrix** $W \in \mathbb{R}^{d \times |Y|}$ and a **bias vector** $b \in \mathbb{R}^{|Y|}$;
- $\hat{y} = argmax_{y \in Y}(W\phi(x) + b)$;
- Multi-class perceptron algorithm:
  1. Initialize W to zero: $W_0 = 0$;
  2. While not converged, for each (x_n, y_n) in D:
     (a) Predict: $\hat{y} = argmax_{y \in Y}(W\phi(x_n))$;
     (b) If $\hat{y_n} \neq y_n$:
        i. Update: $W_{y_n}^{k+1} = W_{y_n}^{k} + \phi(x_n)$

ii. Update: $W_{\hat{y_n}}^{k+1} = W_{\hat{y_n}}^{k} - \phi(x_n)$;
iii. Go to step 2;

Neural Networks

- **Neural networks** are a class of **non-linear models** that are **inspired by the brain**;
- Consist of **neurons** that are **connected** to each other;
- **Pre-activation**: $z(x) = w^T x + b = \sum_{i=1}^{d} w_i x_i + b$;
- **Activation**: $h(x) = g(z(x))$; g can be:
  - **Linear**: $g(z) = z$ - linear regression;
    - Derivative: $\frac{d}{dz} linear(z) = 1$;
  - **Sigmoid**: $g(z) = \frac{1}{1+e^{-z}}$ - logistic regression;
    - Derivative: $\frac{d}{dz} sigmoid(z) = sigmoid(z)(1 - sigmoid(z))$;
  - **Rectified Linear Unit (ReLU)**: $g(z) = max(0, z)$ - most used because it is **fast** to compute;
    - Derivative: $\frac{d}{dz} ReLU(z) = \begin{cases} 1, & if z > 0 \\ 0, & if z \leq 0 \end{cases}$;
    - Mitigates the **vanishing gradient problem**;
  - **Hyperbolic Tangent (tanh)**: $g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$;
    - Derivative: $\frac{d}{dz} tanh(z) = 1 - tanh^2(z)$;
  - **Softmax**: $g(z) = \frac{e^{z_i}}{\sum_{j=1}^{k} e^{z_j}}$ - used for **multi-class classification**;
    - Derivative: $\frac{d}{dz} softmax(z)_i = softmax(z)_i(1 - softmax(z)_i)$;

  ReLUs are significantly simpler and have a much simpler derivative than the sigmoid, leading to faster computation times. Also, sigmoids are easy to saturate and, when that happens, the corresponding gradients are only residual, making learning slower. ReLUs saturate only for negative inputs, and have constant gradient for positive inputs, often exhibiting faster learning

Feed-forward Neural Networks

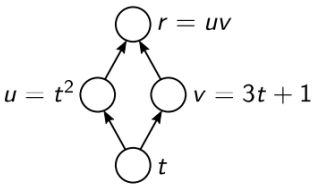
- A **feed-forward neural network** is a **neural network** where the **neurons** are **organized in layers** - there are **hidden layers** between the **input layer** and the **output layer**;

  - **Input layer**: x - vector of features;
  - **Hidden layers**: $h^{(1)}, h^{(2)}, \ldots, h^{(L)}$;
  - **Output layer**: y - vector of predictions;
  - **Weights**: $W^{(1)}, W^{(2)}, \ldots, W^{(L)}$ - each weight matrix is between two layers;
  - **Biases**: $b^{(1)}, b^{(2)}, \ldots, b^{(L)}$ - each bias vector is between two layers;
  - **Hidden layer pre-activation**: $z^{(l)}(x) = W^{(l)}h^{(l-1)}(x) + b^{(l)}$;
  - **Hidden layer activation**: $h^{(l)}(x) = g(z^{(l)}(x))$;
  - **Output layer activation**: $f(x) = h^{(L)}(x)$;
- **Universal approximation theorem**: a **feed-forward neural network** with a **single hidden layer** and **non-linear** activation can **approximate any function** - given enough **neurons**;

Training Neural Networks

- Training consists of **finding the best parameters** θ - weights and biases, that **minimize the loss function**: $L(\theta) := \lambda\omega(\theta) + \frac{1}{N}\sum_{n=1}^{N} L(f(x_n;\theta), y_n)$;
- λ is the **regularization constant**;
- $\omega(\theta)$ is the **regularization term**;
- $L(f(x_n;\theta), y_n)$ is the **loss function**;
  - **Mean squared error**: $L(f(x_n;\theta), y_n) = \frac{1}{2}(f(x_n;\theta) - y_n)^2$ - used for **regression**;
  - **Cross-entropy loss** (negative log-likelihood): $L(f(x_n;\theta), y_n) = -\sum_{i=1}^{k} y_{n,i} log(f(x_n;\theta)_i) = -log((softmax(z(x))_y))$ - used for **classification**, usually **logistic regression**;
- **Backpropagation** is a technique used to **compute the gradients** of the **loss function** with respect to the **parameters - chain rule**.

Recap: Chain Rule



$$\begin{aligned}\frac{\partial r(t)}{\partial t} &= \frac{\partial r(u)}{\partial u}\frac{\partial u(t)}{\partial t} + \frac{\partial r(v)}{\partial v}\frac{\partial v(t)}{\partial t} \\ &= 2tv + 3u \\ &= 2t(3t+1) + 3t^2 = 9t^2 + 2t.\end{aligned}$$

Automatic Differentiation

- **Automatic differentiation** is a **technique** for **computing derivatives** of **functions**;
  - Forward propagation can be represented as a **computation graph** - a **directed acyclic graph** (DAG) that represents the **computation** of the **function**;
    - Each box can be an object with a `fprop` method that computes the **forward pass**;
    - Calling the `fprop` method of each box in the **topological order** of the graph computes the **forward pass**;
  - **Backpropagation** is also implemented as a **computation graph** - a **directed acyclic graph** (DAG) that represents the **computation** of the **gradients**;
    - Each box can be an object with a `bprop` method that computes the **loss gradient** w.r.t. its parents, given the **loss gradient** w.r.t. to the output of the box;
    - Calling the `bprop` method of each box in the **reverse topological order** of the graph computes the **backward pass**.
  - There are several **Autodiff** strategies:
    - **Symbol-to-Number Differentiation**
      - Take a computational graph and numerical inputs;
      - Returns a set of numerical outputs describing the gradient at those inputs;
      - **Advantage**: simpler to implement and debug;
      - **Disadvantage**: only works for first-order derivatives;
      - **Example**: Caffe, Torch, PyTorch, ...
    - **Symbol-to-Symbol Differentiation**
      - Take a computational graph and add additional nodes to the graph that provide a symbolic description of the gradient;
      - **Advantage**: works for higher-order derivatives;
      - **Disadvantage**: more complex to implement and debug;
      - **Example**: Theano, TensorFlow, ...

Regularization

- **Regularization** is a technique used to **reduce overfitting** by **constraining** the **weights** of the model - $\Omega(\theta)$ is the **regularization term**;
  - **L2 regularization**: $\Omega(\theta) = \frac{1}{2} \sum_{li=1}^{L+1} ||W^{(l)}||^2$ - **weight decay** - penalizes **large weights**;
    - Equivalent to **Gaussian prior** on the weights;

- **L1 regularization**: $\Omega(\theta) = \sum_{li=1}^{L+1} ||W^{(l)}||$ - **sparse weights** - promotes **sparsity** of the weights;
  - Equivalent to **Laplace prior** on the weights;
- **Dropout**: randomly **drop** some **neurons** during **training** - **ensemble** of **smaller networks** - **regularizes** the **network**;
  - There is a dropout probability p for each neuron;
  - Usually implemented with random binary masks;
  - The hidden layer activations becomes: $h^{(\updownarrow)}(x) = g(z^{(\updownarrow)}(x)) \odot m^{(\updownarrow)}$, where $m^{(\updownarrow)} \in \{0,1\}^{K^{(\updownarrow)}}$ is a **random binary mask** with p probability of being 1;

Representing Learning - Auto-encoders

- **Auto-encoders** are feed-forward NNs trained to reproduce its input at its output layer;
  - Useful for **dimensionality reduction** and **unsupervised pre-training**;
- **Encoder** - maps input to a hidden representation : $h = g(Wx + b)$;
- **Decoder** - maps hidden representation to a reconstruction : $\hat{x} = W^T h(x) + c$;
- **Loss function** - $\mathcal{L}(\hat{x}, x) = \frac{1}{2}||\hat{x} - x||^2$;
- **Objective** - $\hat{W} = argmin_W \sum_i ||W^T g(Wx_i) - x_i||^2$ - drop the bias term b.

Auto-encoders are networks that are trained to learn the identify function, i.e., to reconstruct in the output what they see in the input. This is done by imposing some form of constraint in the hidden representations (e.g. lower dimensional or sparse). They are useful to learn good representations of data in an unsupervised manner, for example to capture a lower-dimensional manifold that approximately contains the data.

Single Value Decomposition (SVD)

- **SVD** is a matrix factorization method that decomposes a matrix $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ into the product of three matrices U, Σ and V such that $A = U\Sigma V^T$;
  - $U \in \mathbb{R}^{m \times m}$ - columns are an orthonormal basis of $R(A)$ (left singular vectors);

- $\Sigma \in \mathbb{R}^{m \times n}$ - diagonal matrix with singular values of A;
- $V \in \mathbb{R}^{n \times n}$ - columns are an orthonormal basis of $R(A^T)$ (right singular vectors);
- $sigma_1 \geq ... \geq \sigma_r$ - square roots of the eigenvalues of $A^T A$ or AA^T - **singular values** of A;
- $U^T U = I$ and $V^T V = I$.

Linear Auto-Encoder

- Let $X \in \mathbb{R}^{N \times D}$ be a data matrix with N samples and D features ($N > D$);
- Assume $W \in \mathbb{R}^{K \times D}$ ($K < D$);
- We want to minimize $\sum_{i=1}^{N} ||x_i - \hat{x}_i||_2^2 = ||X - XW^T W||_F^2$;
  - $|| \cdot ||_F^2$ - **Frobenius norm**;
  - $W^T W$ has rank K;
- From the **Eckart-Young theorem**, the minimizer is **truncated SVD** of X^T;
  - $\hat{X}^T = U_K \Sigma_K V_K^T$;
  - $W = U_K^T$;
- This is called **Principal Component Analysis (PCA)** - fits a **linear manifold** to the data - auto-encoder with **linear activations**.
- By using **non-linear activations**, we obtain more sophisticated codes (representations).

There are some variants of auto-encoders:

- **Sparse auto-encoders** - add a **sparsity penalty** $\Omega(h)$ to the loss function;
  - Typically the number of hidden units is larger than the number of inputs;
  - The sparsity penalty is a **regularization** term that encourages the hidden units to be **sparse**;
- **Stochastic auto-encoders** - encoder and decoder are **not deterministic**, but involve some **noise/randomness**;
  - Uses distribution $p_encoder(h|x)$ for the encoder and $p_decoder(x|h)$ for the decoder;
  - The auto-encoder can be trained to minimize $-log(p_decoder(x|h))$;

- **Denoising auto-encoders** - use a **perturbed version of the input** $\tilde{x} = x + n$, where n is a **random noise**;
  - Instead of minimizing $\frac{1}{2}||\hat{x} - x||^2$, we minimize $\frac{1}{2}||\hat{x} - \tilde{x}||^2$;
  - This is a form of implicit regularization that ensures **smoothness**: it forces the system to represent well not only the data points, but also their perturbations;
- **Stacked auto-encoders** - several layers of auto-encoders stacked together;
- Variational auto-encoders - learn a **latent variable model** of the data;
  - They maximize the **evidence lower bound (ELBO)** of the **data likelihood** - GANs do not.

Regularized Auto-Encoders

- We need some sort of **regularization** to avoid **overfitting**;
- To regularize auto-encoders, **regularization** is added to the loss function;
- The goal is then to minimize $\mathcal{L}(\hat{x}, x) + \Omega(h, x)$;
- For example:
  - Regularizing the code: $\Omega(h, x) = \lambda||h||^2$;
  - Regularizing the derivatives: $\Omega(h, x) = \lambda \sum_i ||\nabla_x h_i||^2$.

  One use of auto-encoders is **unsupervised pre-training** of **deep neural networks**.

Word Embeddings

- **Word embeddings** are a **representation** of a **word** in a **vector space - distributed representation**;
- **word2vec** is a **neural network** that learns **word embeddings - unsupervised** - considers a context window around each word in the sentence; it comes with two variantes:
  - **skip-gram**: given a word, predict the words around it;
  - **continuous bag-of-words (CBOW)**: given the words around a word, predict the word;
- **Global Vectors (GloVe)** is a **neural network** that learns **word embeddings - unsupervised** - considers the **co-occurrence matrix** of words in the corpus;
- **Contextualized word embeddings** are **word embeddings** that are **context-dependent - ELMo** and **BERT**.

Convolutional Neural Networks

- **Convolutional neural networks (CNNs)** are a class of **deep neural networks** that are **specialized** for **processing data** that has a **grid-like topology**, such as **images**;
- Equivalent to **translations** of the **input**;
- Convolutional and pooling layers exploit the fact that the same feature may appear in different **parts of the image**;
- Lower layers of a CNN learn **local features** (e.g. edges), while higher layers learn **global features** (e.g. objects);
- **Convolution layers** are alternated with **pooling layers** - **convolution** is a **linear operation** that **preserves the grid-like topology** of the input;
- **Activation maps** are the **output** of a **convolutional layer**;
- Image of size $N \times N \times D$ is represented as a **3D tensor**;
- **Filter/kernel** is a **small matrix** that is **convolved** with the **input** to produce an **activation map** - $F \times F \times D$;
- **Stride** is the **step size** of the **convolution** - S;
- **Padding** is the **number of zeros** added to the **input** - P;
  - A common padding size is $P = \frac{F-1}{2}$, which preserves the spatial size of the input $M = N$;
- **Number of channels** is the **number of filters** used in each layer - K;
- The **output** of a **convolutional layer** is of size $M \times M \times K$, where:
  - $M = \frac{N-F+2P}{S} + 1$;
- **Number of trainable parameters** in a **convolutional layer**: $K \times ((F \times F \times D) + 1)$;
- Properties of CNNs:
  - Pooling layers are **Invariant** - the output is **invariant** to **small translations** of the input;
  - Convolution layers provide **translation and scale equivariance** but not **rotation equivariance** - the output features appear in the same relative positions and scale as the input features;
  - **Locality** - the output is **only affected** by a **small region** of the input;

- **Sparse interactions** - each output value is the result of a **small number of interactions** with the input;
- **Parameter sharing** - the **same parameters** are used for **different parts** of the input.

```
nn.Sequential(
    nn.Conv2d(1, 5, kernel_size=3, stride=1, padding=1),
    nn.ReLU(),
    nn.MaxPool2d(kernel_size=2, stride=2),
    nn.Conv2d(5, 10, kernel_size=5, stride=1, padding=0),
    nn.ReLU(),
    nn.MaxPool2d(kernel_size=2, stride=2),
    nn.Conv2d(10, 20, kernel_size=2, stride=2, padding=0),
    nn.ReLU(),
    nn.MaxPool2d(kernel_size=5, stride=2),
    nn.Flatten(),
    nn.Linear(2800, 6))
```

Fill in the following table with the adequate values.

Layer	Output size	N. weights	N. biases
Input	$192 \times 256 \times 1$	0	0
1st conv. layer	$192 \times 256 \times 5$	45	5
1st pooling layer	$96 \times 128 \times 5$	0	0
2nd conv. layer	$92 \times 124 \times 10$	1250	10
2nd pooling layer	$46 \times 62 \times 10$	0	0
3rd conv. layer	$23 \times 31 \times 20$	800	20
3rd pooling layer	$10 \times 14 \times 20$	0	0
Output layer	6×1	$16,800$	6

For linear layers, the number of parameters is $input flat size \times outputs + outputs$.

Residual Networks (ResNets)

- **Residual networks** are a class of **neural networks** that **skip connections** - tend to lead to more stable learning;
- Key motivation: **mitigate the vanishing gradient problem**;
- With $H(x) = \mathcal{F}(x) + \lambda x$, the gradient backpropagation becomes:

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial H}\frac{\partial H}{\partial x} = \frac{\partial L}{\partial H}\left(\frac{\partial \mathcal{F}}{\partial x} + \lambda\right)$$

Recurrent Neural Networks

- RNNs allow to take advantage of **sequential data** - words in text, DNA sequences, sound waves, etc;
  - $h_t = g(Vx_t + Uh_{t-1} + c)$ - h_t is the **hidden state** at time t;
  - $\hat{y}_t = Wh_t + b$ - $\hat{y}_t$ is the **output** at time t;
- Used to generate, tag and classify sequences, and are trained using **back-propagation through time**;
  - Parameters V, U, W, c and b are **shared** across **time steps** - **parameter sharing**;
  - **Exploding gradients** are a problem - **gradient clipping** is used to avoid this problem;
  - **Vanishing gradients** are a problem - **LSTMs** and **GRUs** are used to avoid this problem;
    - Vanishing gradients problem of RNNs: the **gradient** of the **loss function** with respect to the **parameters vanishes** as the **sequence length** increases;
    - GRUs solve this problem by **skipping** the **hidden state** - **gating mechanism**;
    - LSTMs solve this problem by using **memory cells** (propagated additively) and **gating functions** that control how much information is propagated from the previous state to the current and how much input influences the current state.
- They have **unbounded memory** - **recurrent connections** allow information to persist - however, for long sequences, they have a tendency to remember less accurately the initial words they have generated;
- **Bidirectional RNNs** combine **left-to-right RNN** (encoder) and **right-to-left RNN** (decoder) - **encoder-decoder** architecture;
  - Used as sequence encoders, and their main advantage is that each state contains **contextual information coming from both sides**;
  - Unlike **standard RNNs**, they have the same focus on the beginning and the end of the input sequence.

Applications:

- **Sequence generation** - generate a sequence of words - **auto-regressive models**;
- **Sequence tagging** - assign a label to each element in a sequence;
- **Pooled classification** - classify a sequence as a whole;

Standard RNNs suffer from vanishing and exploding gradients - alternative parameterizations like **LSTMs** and **GRUs** are used to avoid this problem;

- **Gated Recurrent Units (GRUs)** are a type of **recurrent neural network** that are **simpler** than **LSTMs** and **perform better** than **standard RNNs** - idea is to create some **shortcuts** in the **standard RNN**;
  - $u_t = \sigma(V_u x_t + U_u h_{t-1} + b_u)$ - **update gate**;
  - $r_t = \sigma(V_r x_t + U_r h_{t-1} + b_r)$ - **reset gate**;
  - $\tilde{h}_t = tanh(v x_t + U(r_t \odot h_{t-1}) + b)$ - **candidate hidden state**;
  - $h_t = (1 - z_t) \odot h_{t-1} + z_t \odot \tilde{h}_t$ - **hidden state**;
- **Long Short-Term Memory (LSTM)** is a type of **recurrent neural network** that are **more complex** than **GRUs** and **perform better** than **standard RNNs** - idea is to use **memory cells** c_t to **store information**;
  - $i_t = \sigma(V_i x_t + U_i h_{t-1} + b_i)$ - **input gate**;
  - $f_t = \sigma(W_f x_t + U_f h_{t-1} + b_f)$ - **forget gate**;
  - $o_t = \sigma(W_o x_t + U_o h_{t-1} + b_o)$ - **output gate**;
  - $\tilde{c}_t = tanh(W_c x_t + U_c h_{t-1} + b)$ - **candidate cell state**;
  - $c_t = f_t \odot c_{t-1} + i_t \odot \tilde{c}_t$ - **cell state**;
  - $h_t = o_t \odot tanh(c_t)$ - **hidden state**.
  - A **Bidirectional LSTM (BiLSTM)** is a **recurrent neural network** that **processes** the **input sequence forward** and **backward** and **concatenates** the **outputs** - **encoder-decoder** architecture;
    - $h_t = \overrightarrow{h_t} \oplus \overleftarrow{h_t}$ - $\oplus$ is the **concatenation** operator;
    - $c_t = \overrightarrow{c_t} \oplus \overleftarrow{c_t}$ - $\oplus$ is the **concatenation** operator;
    - It is used for **sequence tagging** and **sequence classification**;
    - Better than **standard LSTMs** because they can **access future information**.

Sequence to Sequence Models

- **Sequence-to-sequence models** are a class of **neural networks** that are used to **map sequences** to **sequences** - **encoder-decoder** architecture;
  - Used for **machine translation**, **speech recognition**, **image captioning**, etc;
- A **Neural Machine Translation (NMT)** system is a **sequence-to-sequence model** that is used to **translate** a **sequence** in one **language** to a **sequence** in another **language** - **encoder-decoder** architecture;

  - **Encoder** RNN encodes source sentence into a **vector state** - $h_t = f(x_t, h_{t-1})$;
    * e.g. $h1 = relu(W_{hx}x_1 + W_{hh}h_0 + b_h)$, where $h_0 = 0$, W_{hx} is the **input weight matrix**, W_{hh} is the **hidden weight matrix** and b_h is the **bias vector**;
  - **Decoder** RNN decodes the **vector state** into a **target sentence** - $y_t = g(y_{t-1}, s_t)$;
    * e.g. $y_1 = argmax(W_{yh}h_1 + b_y)$, where W_{yh} is the **output weight matrix** and b_y is the **bias vector**;

- Representing the **input sequence** as a **single vector** is a **bottleneck** - **attention mechanisms** are used to **improve performance** - focus on different parts of the input;
- **Greedy decoding** is a **decoding strategy** that **greedily** picks the **most likely** output at each step;
- **Exposure bias** is the tendency of sequence-to-sequence models to be exposed only to correct target sequence prefixes at training time, and never to their own predictions. This makes them having trouble to recover from their own incorrect predictions at test time, if they are produced early on in the sequence. Exposure bias is caused by auto-regressive teacher forcing, where models are trained to maximize the probability of target sequences and are always assigned the previous target symbols as context;
- Sentences are **sorted** by **length** to **improve performance** - **batching**;
  - Within the same batch, all sequences must have the same length, and for this reason they must be padded with padding symbols for making them as long as the longest sentence in the batch. Since in NLP sentences can have very different lengths, if we don't sort sentences by length, we can end up with very unbalanced batches, where some sentences are very short and others are very long, which makes it necessary to add a lot of padding symbols. This process is inefficient and can make training more time consuming. For this reason, sentences are usually sorted by length, which makes each batch more balanced.

Attention Mechanisms and Transformers

- We want to **automatically weight** input relevance, to improve performance, reduce the number of parameters, faster training and inference (easy parallelization);

- Encoders/decoders can be RNNs, CNNs or **self-attention layers**;
- **Self-attention** is a **linear operation** that **maps** a **sequence** of **vectors** to a **sequence** of **vectors** - **encoder-decoder** architecture;
  - **Query** vector q_t - $Q = XW_q$ - W_q is the **query weight matrix**;
  - **Key** vectors $k_1, k_2, \ldots, k_n$ - $K = XW_k$ - W_k is the **key weight matrix**;
  - **Value** vectors $v_1, v_2, \ldots, v_n$ - $V = XW_v$ - W_v is the **value weight matrix**;
  - **Attention weights** $P = softmax(\frac{QK^T}{\sqrt{d_k}})$ - d_k is the **dimensionality** of the **query** and **key** vectors;
  - **Output** vector $Z = PV$;
  - Or it can be written without matrix multiplication:
    - $e_{i,j} = \frac{x_i^T x_j}{\sqrt{d_k}}$ - **score**;
    - $\alpha_{i,j} = \frac{exp(e_{i,j})}{\sum_{j=1}^{n} exp(e_{i,j})}$ - **attention weights**;
    - $z_i = \sum_{j=1}^{n} \alpha_{i,j} v_j$ - **output**;

  Self-attention encoders are better than RNN encoders, since they can better capture long-range relations between elements of a sequence, since information does not propagate sequentially, but in parallel. This makes them more efficient and easier to parallelize - faster training and inference.
- **Transformers**: **encoder-decoder** architecture with **self-attention** layers instead of **RNNs**;
  - **Encoder**: **self-attention** layers;
  - **Decoder**: **self-attention** layers (**masked needed**) + **encoder-decoder attention** layers;
    - They need **causal masking** at training time to avoid **cheating** - **mask** the **future** - reproduce test time conditions;
    - The difference between self-attention and masked self-attention is that in the latter the **attention weights** are **masked** to **avoid cheating** - **mask** the **future**;
  - *The self-attention in transformers allows any word to attend to any other word, both in the source and on the target. When the model is generating a sequence left-to-right it cannot attend at future words, which have not been generated yet. At training time, causal masking is needed in the decoder self-attention to mask future words, to reproduce test time conditions.*
- **Scaled dot-product attention** is a **self-attention** layer with **multiple heads**:

- **Scores** given by $z = \frac{Xq}{\sqrt{d_k}}$; d_k is the **dimensionality** of the **query** and **key** vectors;
- Apply **softmax** to get **attention probabilities**: $\alpha = softmax(z)$;
- The **output** vector is $c = X^T\alpha$;

- **Multi-head attention** is a **self-attention** layer with **multiple heads - parallel** self-attention layers;
  - **Query** vectors q_t - $Q = XW_q$ - W_q is the **query weight matrix**;
  - **Key** vectors $k_1, k_2, \ldots, k_n$ - $K = XW_k$ - W_k is the **key weight matrix**;
  - **Value** vectors $v_1, v_2, \ldots, v_n$ - $V = XW_v$ - W_v is the **value weight matrix**;
  - **Attention weights** $P = softmax(\frac{QK^T}{\sqrt{d_k}})$ - d_k is the **dimensionality** of the **query** and **key** vectors;
  - **Output** vector $Z = PV$;
  - Or it can be written without matrix multiplication:
    * $e_{i,j}^{(h)} = \frac{(W_q^{(h)}x_i)^T(W_k^{(h)}x_j)}{\sqrt{d_k}}$ - **score**;
    * $\alpha_{i,j}^{(h)} = \frac{exp(e_{i,j}^{(h)})}{\sum_{j=1}^{n} exp(e_{i,j}^{(h)})}$ - **attention weights**;
    * $z_i^{(h)} = \sum_{j=1}^{n} \alpha_{i,j}^{(h)}(W_v^{(h)}x_j)$ - **output**;
    * $z_i = concat(z_i^{(1)}, z_i^{(2)}, \ldots, z_i^{(H)})W_o$ - **output**;

- **Positional encoding** is a technique used to **encode the position** of each **word** in a **sequence**;
  - Without positional encodings, the self-attention in transformers is insensitive to the word positions being queried: permuting the words leads to a similar permutation in the self-attention responses. In order for transformers to be sensitive to the word order, each word embedding is augmented with a positional embedding

Self-attention vs. Multi-head attention

- **Self-attention** is a **linear operation** that **maps** a **sequence** of **vectors** to a **sequence** of **vectors** - **encoder-decoder** architecture;
- **Multi-head attention** is a **self-attention** layer with **multiple heads - parallel** self-attention layers;
- **Scaled dot-product attention** is a **self-attention** layer with **multiple heads**.

Self-Supervised Learning and Large Pretrained Models

- **Contextualized representations** are **embeddings** that **depend on the context**;
- Words can have different meanings depending on the context;
- **ELMo** is a model that learned **context-dependent embeddings**;
  - **E**mbeddings from **L**anguage **Mo**dels;
  - **ELMo** is a **bidirectional LSTM** model - BiLSTM;
  - Save all parameters at all layers;
  - Then, for your downstream task, tune a scalar parameter for each layer. and pass the entire sentence through this encoder.
- Pretraining large models and fine-tuning them to a specific task is a common practice in deep learning:
  - **Pretraining** is a technique used to **initialize** the **parameters** of a **neural network** - **self-supervised learning**;
  - **Fine-tuning** is a technique used to **adapt** the **parameters** of a **neural network** to a **specific task**;
- Models: ELMo, BERT, GPT, etc;
  - **GPT-3** - decoder-only transformer;
    - **Few-shot learning** - can be trained with **few examples**;
    - ChatGPT is a **chatbot** based on GPT-3;
    - Pretrained with causal language modeling;
  - **BERT (Bidirectional Encoder Representations from Transformers)** - encoder-only transformer, learn contextyualized word representations;
    - Pretrained on **masked language modeling** and **next sentence prediction**;
  - **T5** - encoder-decoder transformer;
    - Span corruption as an auxiliary task (replace a span of text with a mask token and train to predict the original span);
    - Suitable for classification and generation tasks;
- **Adapters** and **prompting** are other strategies more parameter-efficient than fine-tuning;

  - Adapters are small modules that are plugged into a pretrained model and trained on a specific task; their advantage over fine-tuning is that they require fewer parameters and less training time;
  - Prompting is usually done with models such as GPT, which are trained with a causal language modeling objective;
- Current models exhibit **few-shot learning** capabilities - can be trained with **few examples**.

Deep Generative Models

...

Derivatives and Gradients

- **Derivatives** are a **measure of how a function changes** when its **inputs change**;
- **Gradients** are a **generalization of derivatives** to **multiple dimensions - vector of partial derivatives**;
- **Partial derivatives** are the **derivatives** of a **function** with **respect to one variable**, while **holding the other variables constant**.

Derivative Rules

- $\frac{d}{dx}c = 0$;
- $\frac{d}{dx}x^n = nx^{n-1}$;
- $\frac{d}{dx}e^x = e^x$;
- $\frac{d}{dx}log(x) = \frac{1}{x}$;
- $\frac{d}{dx}sin(x) = cos(x)$;
- $\frac{d}{dx}cos(x) = -sin(x)$;
- $\frac{d}{dx}f(g(x)) = f'(g(x))g'(x)$;
- $\frac{d}{dx}f(x)g(x) = f'(x)g(x) + f(x)g'(x)$;
- $\frac{d}{dx}\frac{f(x)}{g(x)} = \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2}$;

- $\frac{d}{dx}\sum_{i=1}^{n} f_i(x) = \sum_{i=1}^{n} \frac{d}{dx} f_i(x)$;
- $\frac{d}{dx}\prod_{i=1}^{n} f_i(x) = \sum_{i=1}^{n} \frac{d}{dx} f_i(x) \prod_{j \neq i} f_j(x)$.

Chain Rule

- The **chain rule** is a **formula** for computing the **derivative** of the **composition** of **two or more functions**;
- If $y = f(u)$ and $u = g(x)$, then $\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx}$.

Gradient

- The **gradient** of a **scalar function** $f : \mathbb{R}^n \to \mathbb{R}$ is the **vector of partial derivatives** of f with respect to each of its **input variables**;
- $\nabla f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$;
- Rules:
- $\nabla_x c = 0$;
- $\nabla_x x^T A x = (A + A^T)x$;
- If A is **symmetric**, then $\nabla x^T A x = 2Ax$;
- Particular case: $f(x) = x^T x = ||x||^2$, then $\nabla f(x) = 2x$.
- If $f(x) = x^T b = b^T x$, then $\nabla f(x) = b$.
- If $g(x) = f(Ax), then \nabla g(x) = A^T \nabla f(Ax)$.
- If $g(x) = f(a \cdot x)$, then $\nabla g(x) = a \cdot \nabla f(a \cdot x)$.

Algorithmic Complexities

$M_1 \in \mathbb{R}^{N \times D}$ and $M_2 \in \mathbb{R}^{D \times M}$, so $M_1M_2 \in \mathbb{R}^{N \times M}$, has time complexity $O(NDM)$.

Inner Product or **Dot Product** is a matrix multiplication when vectors are expanded so that $M_1 \in \mathbb{R}^{1 \times D}$ and $M_2 \in \mathbb{R}^{D \times 1}$.

Outer product is a matrix multiplication when vectors are expanded so that $M_1 \in \mathbb{R}^{N \times 1}$ and $M_2 \in \mathbb{R}^{1 \times M}$.

$M^\top, M \in \mathbb{R}^{N \times D}$ has time complexity $O(ND)$.

$diag(M), M \in \mathbb{R}^{N \times M}$ has time complexity $O(min(N, M))$ for diagonal extraction and $O(NM)$ for diagonal matrix creation.

Hadamard product = elementwise multiplication $= M \odot N, M, N \in \mathbb{R}^{N \times M}$ has time complexity $O(NM)$.

All other elementwise operations, such as $exp(M)$ softmax(M), etc.. for $M \in \mathbb{R}^{N \times M}$ have time complexity $O(NM)$.