

02456 Deep Learning
Cheat Sheet

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Vincent Van Schependom

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1 Basics & Feed Forward Networks

1.1 Multilayer Perceptron (MLP)

A feed-forward neural network (FNN) with multiple layers. The output of layer l is the input to layer $l + 1$. Notation follows the slides: superscripts denote layers, subscripts denote components.

Name	Symbol	Dimension	
Input Vector	$\mathbf{x} = \mathbf{h}^{(0)}$	$D^{(0)} \times 1$	Layer computation:
Weights (Layer l)	$\mathbf{W}^{(l)}$	$D^{(l)} \times D^{(l-1)}$	$\mathbf{z}^{(l)} = \mathbf{W}^{(l)} \mathbf{h}^{(l-1)} + \mathbf{b}^{(l)}$
Bias (Layer l)	$\mathbf{b}^{(l)}$	$D^{(l)} \times 1$	$\mathbf{h}^{(l)} = \sigma(\mathbf{z}^{(l)})$
Pre-activation (Layer l)	$\mathbf{z}^{(l)}$	$D^{(l)} \times 1$	Weight matrix:
Activation Function	$\sigma(\cdot)$		
Hidden State (Layer l)	$\mathbf{h}^{(l)}$	$D^{(l)} \times 1$	$\mathbf{W}^{(l)} = \begin{bmatrix} w_{1 \leftarrow 1}^{(l)} & w_{1 \leftarrow 2}^{(l)} & \cdots & w_{1 \leftarrow D^{(l-1)}}^{(l)} \\ \vdots & \vdots & \ddots & \vdots \\ w_{D^{(l)} \leftarrow 1}^{(l)} & w_{D^{(l)} \leftarrow 2}^{(l)} & \cdots & w_{D^{(l)} \leftarrow D^{(l-1)}}^{(l)} \end{bmatrix}$
Output	$\mathbf{y} = \mathbf{h}^{(L)}$	$D^{(L)} \times 1$	Here, $w_{j \leftarrow i}^{(l)}$ is the weight from input neuron i in layer $l - 1$ to output neuron j in layer l .
Number of Layers	L		
Neurons per Layer	D		
Distribution params	$\boldsymbol{\theta}$		
Model params	$\boldsymbol{\phi}$		

1.2 Full network

We predict the **distribution** (parameters $\boldsymbol{\theta}$) of the labels \mathbf{y} given the inputs \mathbf{x} using multi-output model $\mathbf{f}_\phi(\mathbf{x})$:

$$\boldsymbol{\theta} = \mathbf{f}_\phi(\mathbf{x}) \quad \rightsquigarrow \quad p(\mathbf{y}|\mathbf{f}_\phi(\mathbf{x})), \quad \boldsymbol{\phi} = \{\mathbf{W}^{(l)}, \mathbf{b}^{(l)}\}_{l=1}^L$$

We usually assume that all D outputs of $\mathbf{f}_\phi(\mathbf{x}) = [\mathbf{f}_{\phi,1}(\mathbf{x}), \dots, \mathbf{f}_{\phi,D}(\mathbf{x})]$ are independent:

$$p(\mathbf{y}|\mathbf{f}_\phi(\mathbf{x})) = \prod_{d=1}^D p(y_d|\mathbf{f}_{\phi,d}(\mathbf{x}))$$

Using these distribution parameters, we calculate the distributions:

- Regression (homo-/heteroscedastic):

$$p(\mathbf{y}|\mathbf{f}_\phi(\mathbf{x})) = p(\mathbf{y}|\mu_1, \dots, \mu_k, \sigma_1, \dots, \sigma_k) = \mathcal{N}(\mathbf{y}|\mu_1, \dots, \mu_k, \sigma_1, \dots, \sigma_k)$$

- Classification ($\mathbf{y} \in \{0, 1\}^K$ one-hot-encoded):

$$p(\mathbf{y}|\mathbf{f}_\phi(\mathbf{x})) = p(\mathbf{y}|\pi_1, \dots, \pi_K) \stackrel{\text{indep.}}{=} \prod_{d=1}^K p(y_d|\pi_d) = \prod_{d=1}^K \pi_d^{y_d}$$

1.3 Probabilistic Inference

For learned model parameters $\hat{\boldsymbol{\phi}}$, make predictions $\hat{\mathbf{y}}$ using $p(\mathbf{y}|\mathbf{f}_{\hat{\boldsymbol{\phi}}}(\mathbf{x}))$:

- Most probable value:

$$\hat{\mathbf{y}} = \arg \max_{\mathbf{y}} p(\mathbf{y}|\mathbf{f}_{\hat{\boldsymbol{\phi}}}(\mathbf{x}))$$

- Expected value:

$$\hat{\mathbf{y}} = \mathbb{E}_{\mathbf{y} \sim p(\mathbf{y}|f_{\phi}(\mathbf{x}))}[\mathbf{y}]$$

- Sample:

$$\hat{\mathbf{y}} \sim p(\mathbf{y}|f_{\phi}(\mathbf{x}))$$

1.4 Parameter Count

For a network with input dimension $D^{(0)}$, K hidden layers each with D neurons, and output dimension $D^{(L)}$:

$$D^{(0)} \cdot D + D + K \cdot (D \cdot D + D) + D \cdot D^{(L)} + D^{(L)}$$

Simplified for 1 input and 1 output:

$$3D + 1 + (K - 1)D(D + 1)$$

1.5 Activation Functions

Name	Formula	Layer Type
Sigmoid	$\sigma(z) = \frac{1}{1+e^{-z}}$	Hidden or output (binary classification)
Arc-tangent	$\sigma(z) = \arctan(z)$	Hidden
Hyperbolic tangent	$\sigma(z) = \tanh(z)$	Hidden
ReLU	$\sigma(z) = \max(0, z)$	Hidden
Leaky ReLU	$\sigma(z) = \max(\alpha z, z), \alpha \ll 1$	Hidden
Linear	$\sigma(z) = z$	Output
Softmax (Output)	$\sigma(z_d) = \pi_d = \frac{e^{z_d}}{\sum_d e^{z_d}}$	Output (multiclass classification)

1.6 Universal Approximation Theorem

A two-layer network with linear outputs can uniformly approximate any continuous function on a compact input domain (compact subset of \mathbb{R}^N) to arbitrary accuracy provided the network has sufficiently large number of hidden units.

This is because:

- Pre-activation = piecewise linear
- Number of **linear regions** for 1 input and D neurons = $D + 1$
- (only D of them are independent and 1 is either zero or the sum of all other regions)

1.7 Other

Multiple inputs:

- Multiple *outputs*: Joints are in the same place for each neuron
- Multiple *inputs*: Linear regions are convex polytopes in the multidimensional input space
- Shallow networks almost always have $D > D_{\text{in}}$ and create between $2^{D_{\text{in}}}$ and 2^D linear regions
- Deep networks with 1 input, 1 output and K layers of $D > 2$ hidden units can create a function with up to $(D + 1)^K$ linear regions

2 Training & Optimization

Given dataset $\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$, calculate mismatch using loss function:

$$L(\phi) = \frac{1}{N} \sum_{i=1}^N \ell(f_\phi(\mathbf{x}_i), \mathbf{y}_i)$$

We learn/fit the model by minimizing this loss:

$$\hat{\phi} = \arg \min_{\phi} L(\phi)$$

2.1 Loss Functions

Name	Formula	Type
Mean Squared Error (MSE)	$\frac{1}{N} \sum_{n=1}^N \ f_\phi(\mathbf{x}_n) - \mathbf{y}_n\ ^2$	Regression
Binary Cross-Entropy	$-\frac{1}{N} \sum_{n=1}^N [y_n \log \pi_n + (1 - y_n) \log(1 - \pi_n)]$	Binary Class.
Categorical Cross-Entropy	$-\frac{1}{N} \sum_{n=1}^N \sum_{d=1}^D y_{nd} \log \pi_{nd}$	Multi-Class
Negative Log-Likelihood (NLL)	$-\frac{1}{N} \sum_{n=1}^N \log p(\mathbf{y}_n f_\phi(\mathbf{x}_n))$	General

2.2 Maximum Likelihood Estimation (MLE)

Unless working with time series data, we assume that each data point is i.i.d:

$$p(\mathbf{y}_1, \dots, \mathbf{y}_N | \mathbf{x}_1, \dots, \mathbf{x}_N, \phi) = \prod_{i=1}^N p(\mathbf{y}_i | f_\phi(\mathbf{x}_i))$$

Maximising Likelihood is equivalent to minimising NLL, since log is monotonically increasing.
:

$$\hat{\phi} = \arg \max_{\phi} \prod_{i=1}^N p(\mathbf{y}_i | f_\phi(\mathbf{x}_i)) = -\arg \min_{\phi} \sum_{i=1}^N \log p(\mathbf{y}_i | f_\phi(\mathbf{x}_i))$$

Find parameters that maximise the probability of the data $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$ using loss:

$$L(\phi) = - \sum_{i=1}^N \log p(\mathbf{y}_i | f_\phi(\mathbf{x}_i))$$

Assuming that dimensions of each \mathbf{y}_i are independent the parameters:

$$p(\mathbf{y}_i | f_\phi(\mathbf{x}_i)) = \prod_{d=1}^D p(y_{id} | f_\phi(\mathbf{x}_i))$$

which yields the loss function

$$L(\phi) = - \sum_{i=1}^N \sum_{d=1}^D \log p(y_{id} | f_\phi(\mathbf{x}_i))$$

For multiclass classification, we had $p(\mathbf{y}_i | f_\phi(\mathbf{x}_i)) = \prod_{d=1}^D \pi_{id}^{y_{id}}$, so the **cross-entropy loss** is

$$L(\phi) = - \sum_{i=1}^N \sum_{d=1}^D y_{id} \log \pi_{id}$$

with class probabilities $\pi \in [0, 1]$, which sum to 1 ($\sum_d \pi_{id} = 1$):

$$\pi = \begin{bmatrix} \pi_1 \\ \vdots \\ \pi_K \end{bmatrix} = \begin{bmatrix} \text{softmax}(z_1) \\ \vdots \\ \text{softmax}(z_K) \end{bmatrix} = \begin{bmatrix} \frac{e^{z_1}}{\sum_d e^{z_d}} \\ \vdots \\ \frac{e^{z_K}}{\sum_d e^{z_d}} \end{bmatrix}$$

2.3 Gradient Descent

Minimize $L(\phi)$: initialise $\phi^{(0)}$ and update iteratively with **learning rate** η :

$$\phi^{(t+1)} = \phi^{(t)} - \eta \nabla_\phi L(\phi^{(t)}), \quad \nabla_\phi L(\phi) = \begin{bmatrix} \frac{\partial L(\phi)}{\partial \mathbf{W}^{(1)}} \\ \frac{\partial L(\phi)}{\partial \mathbf{b}^{(1)}} \\ \vdots \\ \frac{\partial L(\phi)}{\partial \mathbf{W}^{(L)}} \\ \frac{\partial L(\phi)}{\partial \mathbf{b}^{(L)}} \end{bmatrix} = \begin{bmatrix} \frac{\partial L(\phi)}{\partial \phi^{(1)}} \\ \frac{\partial L(\phi)}{\partial \phi^{(2)}} \\ \vdots \\ \frac{\partial L(\phi)}{\partial \phi^{(D)}} \end{bmatrix}$$

2.3.1 Stochastic Gradient Descent (SGD)

Draw minibatches $\mathcal{B}_t \subseteq \{1, \dots, N\}$ **without replacement**:

$$\phi^{(t+1)} = \phi^{(t)} - \sum_{i \in \mathcal{B}_t} \frac{\partial \ell_i(\phi^{(t)})}{\partial \phi}$$

where $\ell_i(\phi)$ is the loss of the i -th sample $(\mathbf{x}_i, \mathbf{y}_i)$ and $L(\phi) = \sum_{i=1}^N \ell_i(\phi)$. A full pass through the dataset is called an **epoch**.

2.3.2 Adam (Adaptive Moment Estimation)

Compute first and second moment of gradients:

$$\begin{aligned} \mathbf{m}^{(t+1)} &= \beta \mathbf{m}^{(t)} + (1 - \beta) \nabla_\phi \ell_i(\phi^{(t)}) \\ \mathbf{v}^{(t+1)} &= \gamma \mathbf{v}^{(t)} + (1 - \gamma) \nabla_\phi \ell_i(\phi^{(t)})^2 \end{aligned}$$

Compensate for initial values close to zero:

$$\tilde{\mathbf{m}}^{(t+1)} = \frac{\mathbf{m}^{(t+1)}}{1 - \beta^{t+1}}, \quad \tilde{\mathbf{v}}^{(t+1)} = \frac{\mathbf{v}^{(t+1)}}{1 - \gamma^{t+1}}$$

Update parameters after normalization by the second moment.

This way, we take the same step size in each direction (stable).

$$\phi^{(t+1)} = \phi^{(t)} - \eta \frac{\tilde{\mathbf{m}}^{(t+1)}}{\sqrt{\tilde{\mathbf{v}}^{(t+1)}} + \epsilon}$$

where η is the learning rate, and ϵ is a small constant to prevent division by zero.

2.4 Backpropagation

Used to calculate gradients $\nabla_\phi L(\phi)$.

3 Initialization & Regularization

3.1 Weight Initialization

Avoid vanishing/exploding gradients during backprop. Initialize $\phi_i \sim \mathcal{N}(0, \sigma^2)$. Below, $\alpha = 1$ for tanh and $\alpha = 2$ for ReLU.

3.1.1 He-Kaiming Initialization (ReLU)

$$\sigma^2 = \frac{2\alpha}{D_{\text{in}}} \iff \text{Var}[h_i^{(l)}] = \text{Var}[h_i^{(l-1)}]$$

3.1.2 Xavier-Glorot Initialization

$$\sigma^2 = \frac{2\alpha}{D_{\text{in}} + D_{\text{out}}}$$

3.2 Bias-Variance Tradeoff

Estimate the generalization error

$$E^{\text{gen}} = \mathbb{E}_{\mathbf{x}, \mathbf{y} \sim p_D(\mathbf{x}, \mathbf{y})} [L(f_\phi(\mathbf{x}), \mathbf{y})] = \int L(f_\phi(\mathbf{x}), \mathbf{y}) p_D(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$$

with a Monte-Carlo estimate:

$$E^{\text{gen}} \approx \frac{1}{N} \sum_{i=1}^N L(f_\phi(\mathbf{x}_i), \mathbf{y}_i)$$

where $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$ are sampled from $p_D(\mathbf{x}, \mathbf{y})$.

The expected generalization error if we train $f_{\phi(\mathcal{D})}$ on datasets $\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^N$ assuming a squared loss:

$$\begin{aligned} \mathbb{E}_{\mathcal{D}}[E^{\text{gen}}] &= \mathbb{E}_{\mathbf{x} \sim p_D(\mathbf{x})} \left[[\bar{\mathbf{y}}(\mathbf{x}) - \bar{f}_{\phi(\mathcal{D})}(\mathbf{x})]^2 + \text{Var}_{\mathcal{D}}[f_{\phi(\mathcal{D})}(\mathbf{x})] + \text{Var}[\mathbf{y}(\mathbf{x})] \right] \\ &= \text{Bias}^2 + \text{Variance} + \text{Irreducible Error} \end{aligned}$$

3.3 Regularization Techniques

3.3.1 Weight Decay

$$L'(\phi) = L(\phi) + g(\phi)$$

- ℓ^2 -regularization

- $g(\phi) = \frac{\lambda}{2} \|\phi\|_2^2 = \frac{\lambda}{2} \sum_{i=1}^D \phi_i^2$
- Gradient: $\frac{\partial g(\phi)}{\partial \phi_j} = \lambda \phi_j$

- ℓ^1 -regularization

- $g(\phi) = \lambda \|\phi\|_1 = \lambda \sum_{i=1}^D |\phi_i|$
- Gradient: $\frac{\partial g(\phi)}{\partial \phi_j} = \lambda \text{sign}(\phi_j)$

3.3.2 Other Regularization Techniques

- **Early stopping**
- **Data augmentation**
- **Injecting noise** to input data, activations, or weights
- **Ensemble methods:** bagging = bootstrap aggregating = resampling with replacement
- **Dropout:**
 - Randomly delete nodes with probability $\rho = 0.5$
 - At test time, multiply weights by ρ
 - Use as an ensemble of $2^{(\# \text{ of hidden nodes})}$ networks
- **Transfer learning**
- **Multi-task learning**
- **Self-supervised learning:** generative (with masks) or contrastive (with pairs)

4 Residual Neural Networks

Add an identity connection to prevent shattered (uncorrelated) gradients:

$$\mathbf{h}^{(l)} = \mathbf{h}^{(l-1)} + f_{\phi^{(l)}}(\mathbf{h}^{(l-1)})$$

Allows gradients to flow through:

$$\frac{\partial \mathbf{h}^{(l)}}{\partial \mathbf{h}^{(l-1)}} = I + \frac{\partial f_{\phi^{(l)}}(\mathbf{h}^{(l-1)})}{\partial \mathbf{h}^{(l-1)}}$$

5 Convolutional Neural Networks (CNNs)

Allow for **local connectivity** and **parameter sharing**.

Name	Symbol	Dimension	
Input Image	\mathbf{X}	$H \times W \times c_{\text{in}}$	
Kernel/Filter	\mathbf{W}	$w \times h \times c_{\text{in}} \times c_{\text{out}}$	
Bias	\mathbf{b}	$c_{\text{out}} \times 1$	TODO
Output Feature Map	\mathbf{Z}	$H' \times W' \times c_{\text{out}}$	
Stride	s	Scalar (or per dim)	
Padding	p	Scalar (or per dim)	

Important terms:

Kernel size, stride, padding, dilation rate (number of interspersed zero-values in kernel)

5.1 Invariance

FCN's have no notion of locality. We want layers to be **equivariant** to translations.

- **Equivariant:** $f(t(x)) = t(f(x))$
- **Invariant:** $f(t(x)) = f(x)$

The convolution operation is **equivariant** to translations.

5.2 Convolution Operation

Replace vectors with **tensors** indexed by (x, y, c) :

- Width: x
- Height: y
- **Channel:** c

Convolution weights are tensors $\mathbf{W} \in \mathbb{R}^{w \times h \times c_{\text{in}} \times c_{\text{out}}}$.

$$h_{x,y,c}^{(l)} = \sum_{c',m,n} h_{x+m,y+n,c'}^{(l-1)} W_{m,n,c',c} + b_c$$

Each convolution produces a new set of hidden variables = **feature map** or **channel**.

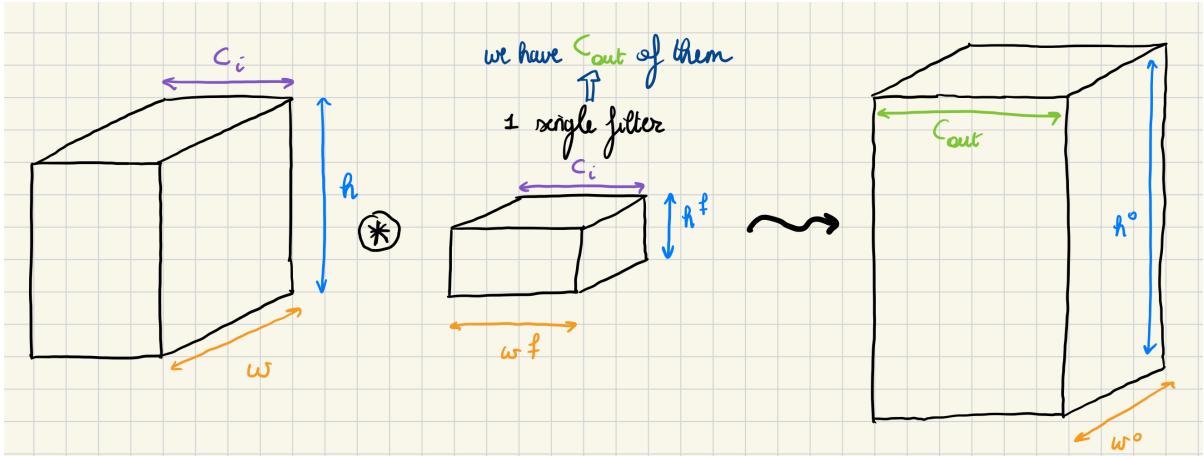
The **receptive field** of units in successive layers increases s.t. information from across the input is gradually aggregated.

5.3 Pooling

- **Increase channels in convolution layers**
- **Decrease resolution in pooling layers**

Variants of pooling:

- **Max Pooling**
- **Average Pooling**
- **Inverse Pooling:** Upsampling



5.4 Output dimensionality

Given:

- Input: $C_i \times w \times h$
- Filters: $C_i \times w_f \times h_f$
- Number of filters: C_o
- Stride: s
- Padding: p

Output:

- C_o channels
- Output width: $\left\lfloor \frac{w+2p-w_f}{s} + 1 \right\rfloor$
- Output height: $\left\lfloor \frac{h+2p-h_f}{s} + 1 \right\rfloor$

Each channel is a weighted sum of C_i input channels.

If we consider the kernel as a 4D tensor, the weights are shared across all output channels.
If we consider the kernel as a 3D tensor, each of the C_o kernels are different filters.

Each convolutional layer has $C_i \cdot C_o \cdot w_f \cdot h_f$ weights and C_o biases.

MaxPool halves the spatial dimensions: e.g. $13 \times 13 \times 256 \rightarrow 6 \times 6 \times 256$.

SoftMax layer has no parameters.

6 Recurrent Neural Networks (RNNs)

- Input of length T :

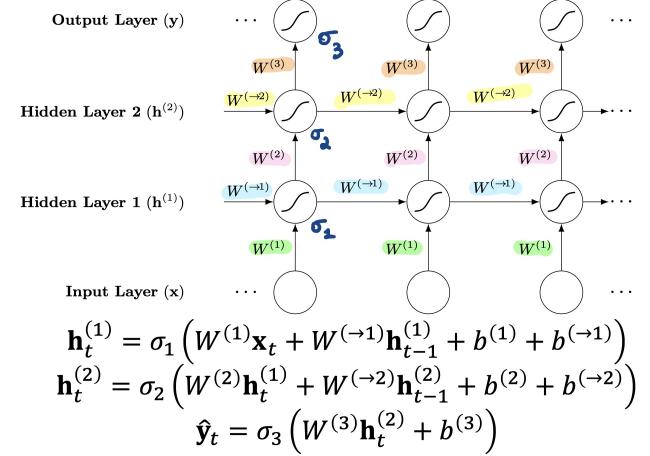
$$\mathbf{x} = \{\mathbf{x}_t\}_{t=1}^T, \quad \mathbf{x}_t \in \mathbb{R}^{D_x}$$

- Output of length S :

$$\mathbf{y} = \{\hat{\mathbf{y}}_t\}_{t=1}^S, \quad \hat{\mathbf{y}}_t \in \mathbb{R}^{D_y}$$

- The length T and S may vary between datapoints
- The length of the two sequences may differ: $T \neq S$

Name	Symbol	Dimension
Sequence length	T	Scalar
Input at Time t	\mathbf{x}_t	$D_x \times 1$
Hidden State at t	\mathbf{h}_t	$D_h \times 1$
Output at t	$\hat{\mathbf{y}}_t$	$D_y \times 1$
Input Weights	$\mathbf{W}^{(i)}$	$D_h \times D_x$
Recurrent Weights	$\mathbf{W}^{(-i)}$	$D_h \times D_h$
Output Weights	$\mathbf{W}^{(L)}$	$D_y \times D_h$
Biases	$\mathbf{b}^{(h)}, \mathbf{b}^{(y)}$	



6.1 MLE for RNNs

For an input-output pair

$$\begin{cases} \mathbf{x} = \mathbf{x}_1, \dots, \mathbf{x}_T \\ \mathbf{y} = \mathbf{y}_1, \dots, \mathbf{y}_S \end{cases}$$

we usually assume

$$p(\mathbf{y} | f_{\phi}(\mathbf{x})) = \prod_{t=1}^S p(\mathbf{y}_t | f_{\phi}(\mathbf{x}_t)) \quad (1)$$

$$= \prod_{t=1}^S p(\mathbf{y}_t | f_{\phi}(\mathbf{x}_{\leq t})) \quad (2)$$

6.2 Long Short-Term Memory (LSTM)

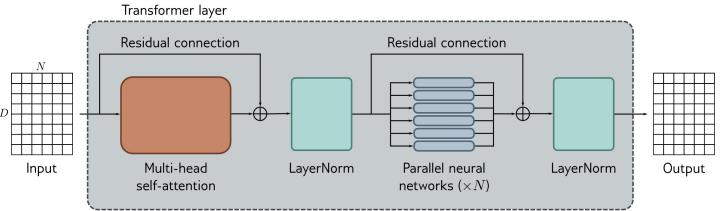
Gate/Component	Formula
Forget Gate	$f_t = \sigma(\mathbf{W}_f[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_f)$
Input Gate	$i_t = \sigma(\mathbf{W}_i[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_i)$
Cell Candidate	$\tilde{\mathbf{C}}_t = \tanh(\mathbf{W}_c[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_c)$
Cell State	$\mathbf{C}_t = f_t \odot \mathbf{C}_{t-1} + i_t \odot \tilde{\mathbf{C}}_t$
Output Gate	$\mathbf{o}_t = \sigma(\mathbf{W}_o[\mathbf{h}_{t-1}; \mathbf{x}_t] + \mathbf{b}_o)$
Hidden State	$\mathbf{h}_t = \mathbf{o}_t \odot \tanh(\mathbf{C}_t)$

7 Transformers & Attention

7.1 Notation and Dimensions

For sequences of length T' , embedding dim D' .

Name	Symbol	Dimension
Input Embeddings	\mathbf{X}	$T' \times D$
Queries	\mathbf{Q}	$T \times D$
Keys	\mathbf{K}	$T' \times D$
Values	\mathbf{V}	$T' \times D'$
Attention Weights	\mathbf{A}	$T \times T'$
Outputs	\mathbf{Y}	$T \times D'$
Number of Heads	h	-



7.2 Scaled Dot-Product Attention

$$\mathbf{A} = \text{softmax} \left(\frac{\mathbf{Q}\mathbf{K}^T}{\sqrt{D'}} \right)$$

where

$$\underbrace{\mathbf{Q}}_{T \times D} \cdot \underbrace{\mathbf{K}^T}_{D \times T'} \in \mathbb{R}^{T \times T'}$$

Compute attention (runtime $\mathcal{O}(n^2)!$) as weighted sum of values:

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \mathbf{AV}$$

In multiheaded attention (h heads):

- Reduce dimensions of \mathbf{Q} , \mathbf{K} , \mathbf{V} :

$$\begin{aligned} \mathbf{Q}_i &= \mathbf{Q}\mathbf{W}_i^Q \\ \mathbf{K}_i &= \mathbf{K}\mathbf{W}_i^K \\ \mathbf{V}_i &= \mathbf{V}\mathbf{W}_i^V \end{aligned}$$

- Compute attention for each head:

$$\begin{aligned} \mathbf{A}_i &= \text{softmax} \left(\frac{\mathbf{Q}_i \mathbf{K}_i^T}{\sqrt{D'}} \right) \\ \text{head}_i &= \mathbf{A}_i \mathbf{V}_i \end{aligned}$$

- Concatenate:

$$\text{MultiHead}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \text{Concat}(\text{head}_1, \dots, \text{head}_h)$$

- Project up to original dimension:

$$\text{MultiHead}(\mathbf{Q}, \mathbf{K}, \mathbf{V})\mathbf{W}_O$$

8 Unsupervised Deep Learning

8.1 Autoencoders (AE)

Encoder $f_\phi : \mathbf{x} \rightarrow \mathbf{z}$, Decoder $g_\theta : \mathbf{z} \rightarrow \hat{\mathbf{x}}$.

Name	Symbol	Dimension
Input	\mathbf{x}	$D_x \times 1$
Latent Code	\mathbf{z}	$D_z \times 1 (D_z < D_x)$
Reconstructed	$\hat{\mathbf{x}}$	$D_x \times 1$

- **Goal:** Learn compressed representation \mathbf{z} (bottleneck).
- **Loss:** Reconstruction loss (e.g., MSE).

$$L(\mathbf{x}, \hat{\mathbf{x}}) = \|\mathbf{x} - \hat{\mathbf{x}}\|^2 = \|\mathbf{x} - g_\theta(f_\phi(\mathbf{x}))\|^2$$

8.1.1 Limitation

We want to sample the latent space \mathbf{z} to generate new data. However, in standard AE, the latent space is not regularized, so sampling from it (e.g., $\mathbf{z} \sim \mathcal{N}(0, I)$) does not guarantee meaningful generations.

8.2 Variational Autoencoders (VAE)

Probabilistic generative model. We assume a generative process:

$$\mathbf{z} \sim p_\theta(\mathbf{z}), \quad \mathbf{x} \sim p_\theta(\mathbf{x}|\mathbf{z})$$

where $p_\theta(\mathbf{z})$ is the prior (usually $\mathcal{N}(0, I)$) and $p_\theta(\mathbf{x}|\mathbf{z})$ is the observation model.

8.2.1 Intractability

We want to maximize the marginal likelihood (evidence) $p_\theta(\mathbf{x})$:

$$p_\theta(\mathbf{x}) = \int p_\theta(\mathbf{x}, \mathbf{z}) d\mathbf{z} = \int p_\theta(\mathbf{x}|\mathbf{z}) p_\theta(\mathbf{z}) d\mathbf{z}$$

This integral is **intractable** because it requires integrating over all possible latent variables \mathbf{z} . Consequently, the true posterior $p_\theta(\mathbf{z}|\mathbf{x})$ is also intractable:

$$p_\theta(\mathbf{z}|\mathbf{x}) = \frac{p_\theta(\mathbf{x}, \mathbf{z})}{p_\theta(\mathbf{x})}$$

8.2.2 Amortized Variational Inference

To overcome this, we use **Variational Inference** with an approximate posterior $q_\phi(\mathbf{z}|\mathbf{x}) \approx p_\theta(\mathbf{z}|\mathbf{x})$. We use **Amortized Inference**, meaning the inference parameters ϕ (encoder weights) are shared across all data points, mapping \mathbf{x} to the parameters of $q_\phi(\mathbf{z}|\mathbf{x})$ (e.g., $\mu_\phi(\mathbf{x}), \sigma_\phi(\mathbf{x})$).

8.2.3 Objective: Evidence Lower Bound (ELBO)

We maximize the ELBO, which is a lower bound on the log-likelihood:

$$\begin{aligned} \log p_\theta(\mathbf{x}) \geq \text{ELBO} &= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|\mathbf{z})] - D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p_\theta(\mathbf{z})) \\ &= \text{Reconstruction Term} - \text{Regularization Term} \end{aligned}$$

8.2.4 Reparameterization Trick

To backpropagate through the sampling $\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}_\phi^2(\mathbf{x})\mathbf{I})$, we use:

$$\mathbf{z} = \boldsymbol{\mu}_\phi(\mathbf{x}) + \boldsymbol{\sigma}_\phi(\mathbf{x}) \odot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$$

This makes the sampling operation differentiable w.r.t. ϕ .

8.3 Semi-supervised Learning

Semi-supervised learning

- ≠ transfer learning!
- Little labeled data \mathbf{y}
- Lots of unlabeled data \mathbf{x}
- Auto-encode (unsupervised) to \mathbf{z}
- Train classifier on \mathbf{z} (supervised)