#### Imperial Data Science and Al Winter School 2025

### Barin-Tumor

### Segmentation

Group 3
Li Xiangyu Su Yi Wu Kunzhen

# nnU-Net Introduction

#### nnU-Net



#### Detailed Configuration

Detailed configuration is more important than architectural design. nnU-Net uses a simple U-Net architecture, but transcends more complex parameters through good configuration.



#### Adaptable Configuration

Twenty-three publicly available biomedical image datasets were used in the development and evaluation of nnU-Net.

#### nnU-Net

a self-configuring method for deep learning-based biomedical image segmentation



#### Automated Configuration

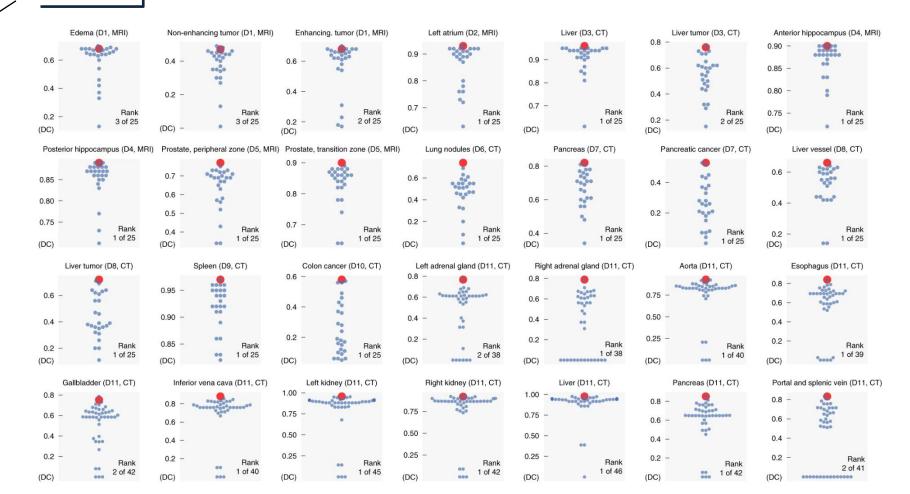
Systemize the complex manual method configuration process into fixed parameters, rule-based parameters and empirical parameters.



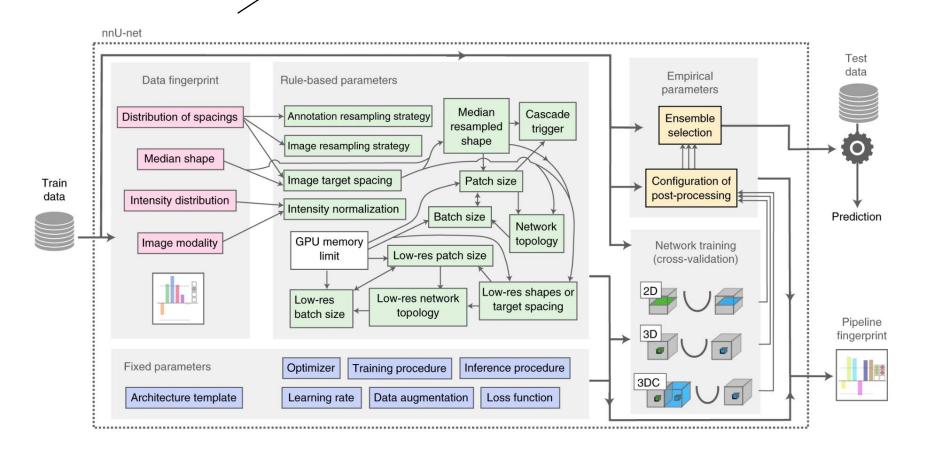
#### Easy Configuration

As an open source tool, nnU-Net can be used immediately by people who are not familiar with deep learning.

#### nnU-Net



#### nnU-Net: a self-configuring method for deep learning-based biomedical image segmentation



#### nnU-Net: a self-configuring method for deep learning-based biomedical image segmentation

|  | Design<br>choice                | Required input                         | Automated (fixed, rule-based or empirical) configuration derived by distilling expert knowledge (more details in online methods)                       |
|--|---------------------------------|--|--|
|  | Learning rate                   | -                                      | Poly learning rate schedule (initial, 0.01)  |
|  | Loss function                   | -                                      | Dice and cross-entropy   |
|  | Architecture template           | -                                      | Encoder–decoder with skip-connection ('U-Net-like') and instance normalization, leaky ReLU, deep supervision (topology-adapted in inferred parameters) |
|  | Optimizer                       | -                                      | SGD with Nesterov momentum ( $\mu = 0.99$ )  |
|  | Data<br>augmentation            | -                                      | Rotations, scaling, Gaussian noise, Gaussian blur, brightness, contrast, simulation of low resolution, gamma correction and mirroring                  |
|  | Training procedure              | -                                      | 1,000 epochs $\times$ 250 minibatches, foreground oversampling   |
|  | Inference<br>procedure          | _                                      | Sliding window with half-patch size overlap,<br>Gaussian patch center weighting  |
|  | Intensity<br>normalization      | Modality,<br>intensity<br>distribution | If CT, global dataset percentile clipping & z score with global foreground mean and s.d.  Otherwise, z score with per image mean and s.d.              |
|  | Image<br>resampling<br>strategy | Distribution of spacings               | If anisotropic, in-plane with third-order spline, out-<br>of-plane with nearest neighbor<br>Otherwise, third-order spline                              |
|  | Annotation resampling strategy  | Distribution of spacings               | Convert to one-hot encoding → If anisotropic, in-plane with linear interpolation, out-of-plane with nearest neighbor Otherwise, linear interpolation   |

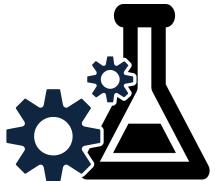
| Image target spacing                               | Distribution of spacings   | If anisotropic, lowest resolution axis tenth percentile, other axes median.  Otherwise, median spacing for each axis. (computed based on spacings found in training cases)   |
|--|--|--|
| Network<br>topology,<br>patch size,<br>batch size  | Median<br>resampled<br>shape, target<br>spacing, GPU<br>memory limit | Initialize the patch size to median image shape and iteratively reduce it while adapting the network topology accordingly until the network can be trained with a batch size of at least 2 given GPU memory constraints. for details see online methods. |
| Trigger of 3D<br>U-Net<br>cascade                  | Median<br>resampled<br>image size,<br>patch size                     | Yes, if patch size of the 3D full resolution U-Net covers less than 12.5% of the median resampled image shape  |
| Configuration<br>of low-<br>resolution 3D<br>U-Net | Low-res target<br>spacing or image<br>shapes, GPU<br>memory limit    | Iteratively increase target spacing while reconfiguring patch size, network topology and batch size (as described above) until the configured patch size covers 25% of the median image shape. For details, see online methods.                          |
| Configuration of post-processing                   | Full set of<br>training data<br>and<br>annotations                   | Treating all foreground classes as one; does all-but-largest-component-suppression increase cross-validation performance?  Yes, apply; reiterate for individual classes  No, do not apply; reiterate for individual foreground classes                   |
| Ensemble selection                                 | Full set of<br>training data<br>and<br>annotations                   | From 2D U-Net, 3D U-Net or 3D cascade, choose the best model (or combination of two) according to cross-validation performance   |

### nnU-Netv2 Implementation

### **Objective**

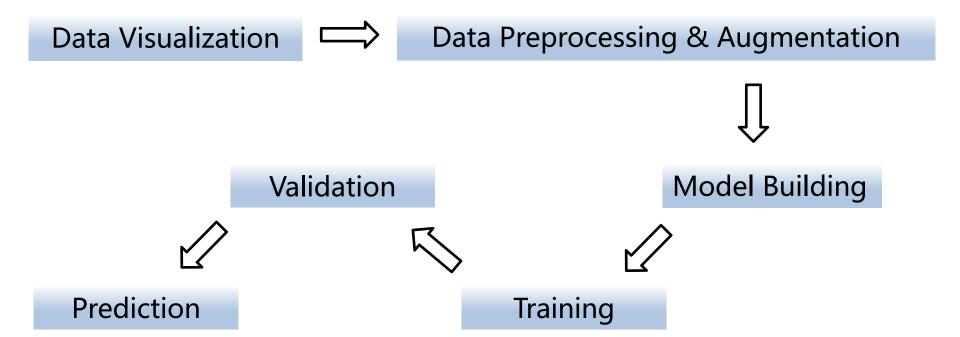


Medical image segmentation plays a crucial role in clinical diagnosis and treatment planning. Deep **learning-based segmentation** models, particularly the 3D U-Net architecture, have demonstrated remarkable performance in accurately delineating anatomical structures from MRI scans. This work presents a segmentation pipeline built upon nnUNetv2, incorporating advanced preprocessing, data augmentation, and a customized training framework to enhance model robustness and accuracy.



### **Brain-Tumor Segmentation Process**

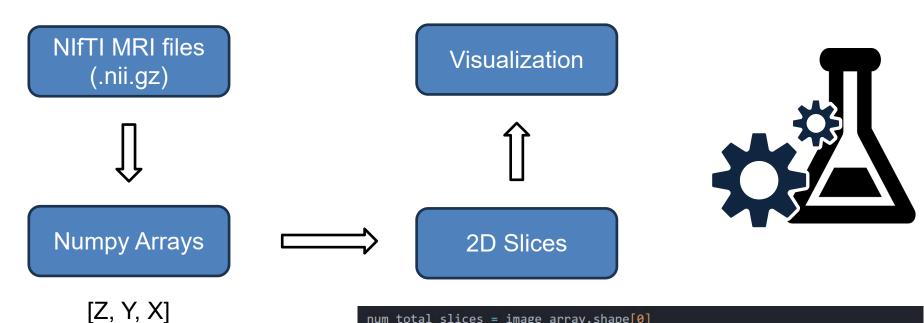




## MRI Volume Visualization

### **Data Visualization**





num\_total\_slices = image\_array.shape[0]
# Get `num\_slices` slices evenly distributed
slice\_indices = np.linspace(0, num\_total\_slices - 1, num\_slices, dtype=int)

Z: number of axial slices in the MRI scan

### **Prase the Data**





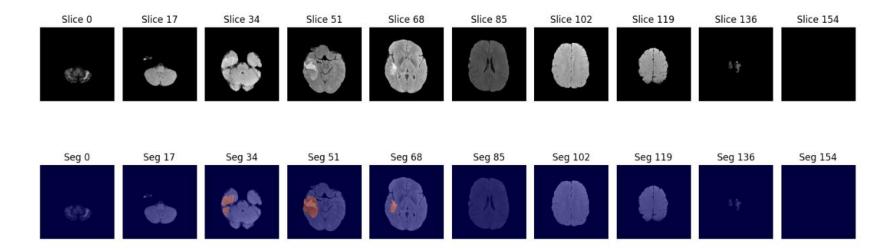


Figure 1: Example Visualization

### **Data Preprocessing**

### Track 2.1 Restructuring Dataset





dataset\_segmentation/train/xxx/xxx\_fld.nii



~/nnUNet\_raw/imagesTr/xxx/xxx\_fld.nii

dataset\_segmentation/train/xxx/xxx\_seg.nii



~/nnUNet\_raw/labelsTr/xxx/xxx\_seg.nii



### Track 2.2 Extracting Data Fingerprint



### Cropping Non-Zero Regions

Non-zero mask is created for each image and segmentation pair. This mask ensures that only the relevant part of the image is used for training.

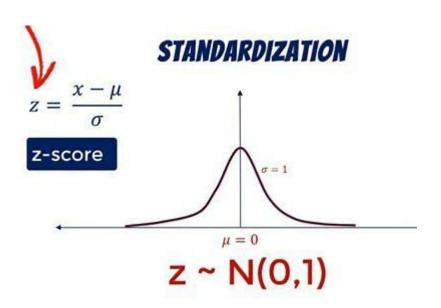
### Saving the Fingerprint

```
extract_fingerprints([task_id], check_dataset_integrity=True)
plans_identifier = plan_experiments([task_id])
num_processes = [4]
preprocess([task_id], plans_identifier, ['3d_fullres'], num_processes)
```

### Track 2.3 Preprocessing Individual Cases



#### Normalization



### Resampling

The original spacing (voxel size) of the images is adjusted to a targetspacing.

### **Data Augmentation**

### **Augmentation Techniques**

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**Patch Selection** 

**Spatial Transformations** 

Noise & Blur

**Brightness and Contrast** 

**Low Resolution & Gamma Transform** 

Mirroring and Masking

**Fixed-size patches** 

**Rotation, Scaling, Elastic Deformation** 

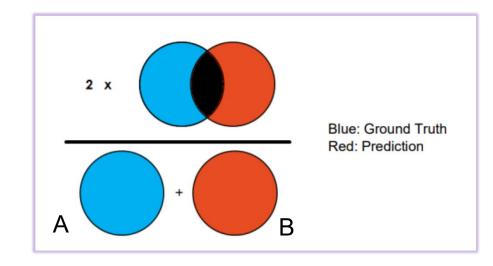
- Downsampling
- Adjust intensity distribution
- Applied specified axes
- Normalizes only within regions of interest

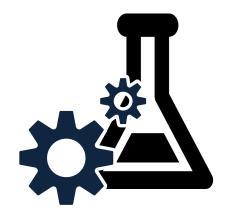
### Performance Metric

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### 4.1 Dice Similarity Coefficient

$$DSC = \frac{2 \cdot |A \cap B| + \text{smoothing}}{|A| + |B| + \text{smoothing}}$$





### 4.2 Cross-Entropy Loss





$$H(p,q) = -\sum_{x \in \mathcal{X}} p(x) \, \log q(x)$$
. (Eq.1)

Supports One-Hot Encoding

Works with one-hot encoded target labels

**Ensures Pixel Classification** 

Helps the model assign each pixel to the right class

### 4.3 Combined Loss Function

$$\mathcal{L} = w_{\text{dice}} \cdot \mathcal{L}_{\text{Dice}} + w_{\text{CE}} \cdot \mathcal{L}_{\text{CE}}$$

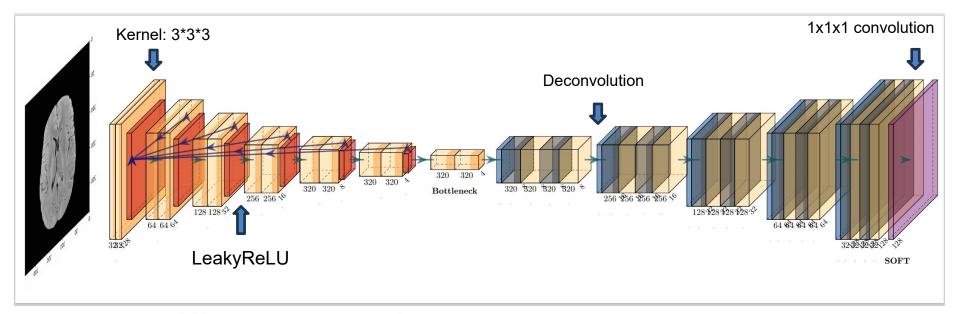


Ensures both accurate classification and well-defined segmentation boundaries.

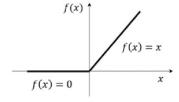
### Network Architecture

### **PlainConvUNet**

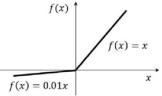








ReLU activation function



LeakyReLU activation function

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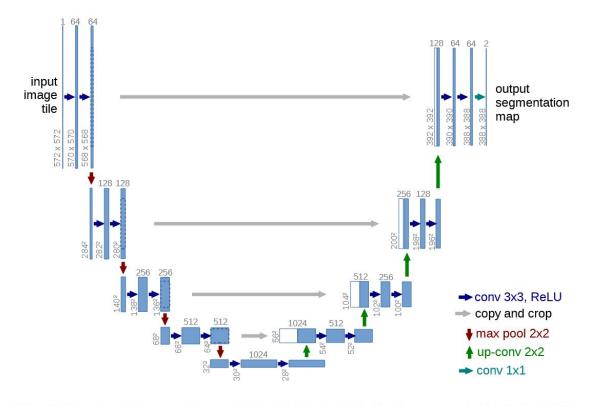
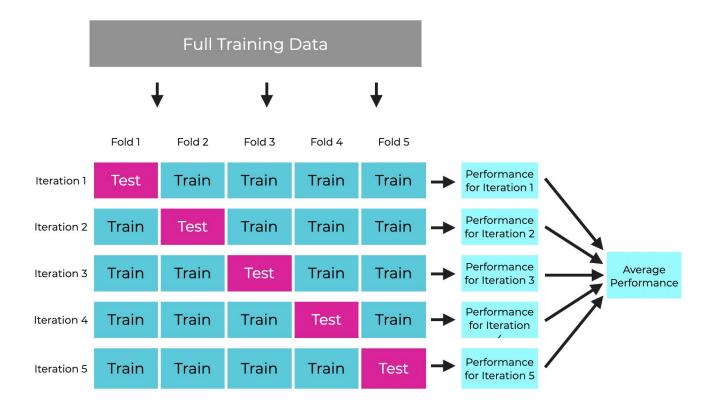


Fig. 1. U-net architecture (example for 32x32 pixels in the lowest resolution). Each blue box corresponds to a multi-channel feature map. The number of channels is denoted on top of the box. The x-y-size is provided at the lower left edge of the box. White boxes represent copied feature maps. The arrows denote the different operations.

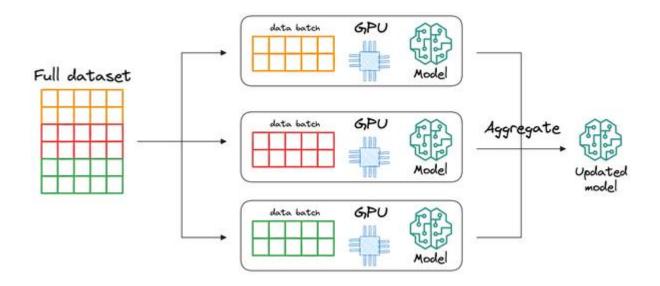


### **Trainer**

### **5-Fold Cross-Validation**



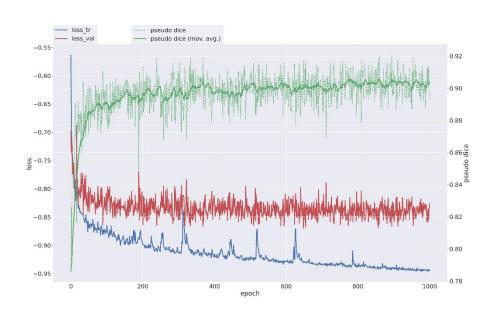
### **Multi-GPU Training**

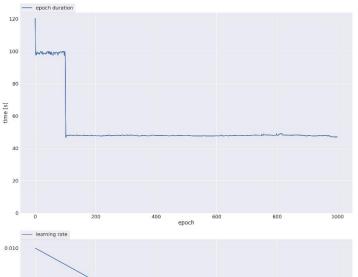


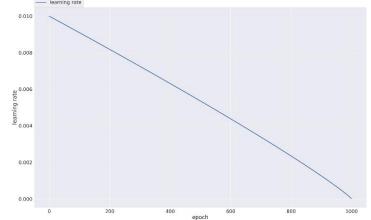
### Results

### **Training Process**

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### Validation Performance



- Fold 0: Mean Validation Dice: 0.9173
- Fold 1: Mean Validation Dice: 0.8910
- Fold 2: Mean Validation Dice: 0.8888
- Fold 3: Mean Validation Dice: 0.8911
- Fold 4: Mean Validation Dice: 0.9103
- Average Mean Dice Score: 0.8997

Hello,

Your model achieved a Dice score of 0.8875 and a 95 Hausdorff Distance of 11.5758 on our test set. Well done!

Best, Chengliang



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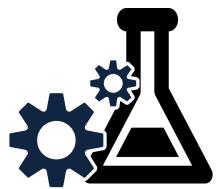
### Word Representation

### in **Biomedical Domain**

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Li Zhuoran Chen Xinjia Xu Zhesheng



The aim of this project is to analyze the text content and construct word representations suitable for the large scale document data in the biomedical field, and finally explore and analyze the application of word vectors.



### **Technological Process**



#### **Dataset**

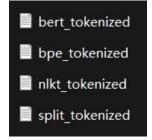


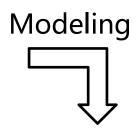
https://www.semanticscholar.org/cord19/

#### Core content



Tokenizer





```
Word: this, Vector: [ 0.23222321  0.12671019 -0.04556849 -0.06296597 -0.20533879]...

Word: be, Vector: [-0.11883736 -0.08993076 -0.18911168  0.00159133  0.03658859]...

Word: virus, Vector: [-0.00974345 -0.3625814  0.0456008 -0.5772487 -0.2413821 ]...

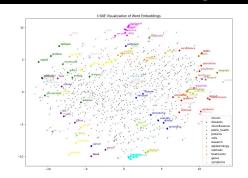
Word: coronavirus, Vector: [ 0.39919555 -0.37495816 -0.18429291 -0.10705779  0.3739001 ]...

Word: infection, Vector: [-0.34453392 -0.8504306  0.04829029  0.00951516 -0.33521503]...

Word: patients, Vector: [ 0.14964846 -0.24931104  0.19648291  0.3334433  0.10605083]...
```

### Representations

Visualisation & Application



### **Prase the Data**

### Prase the Data





#### **Overview of Dataset**

metadata.csv

--title

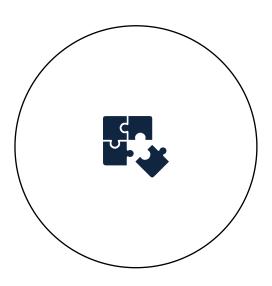
--abstract

|--authors

|--doi

. . . . . .

36.3G





#### **Selection of Content**

- Title
- Abstract

\*If missing, replaced with a 'Space'

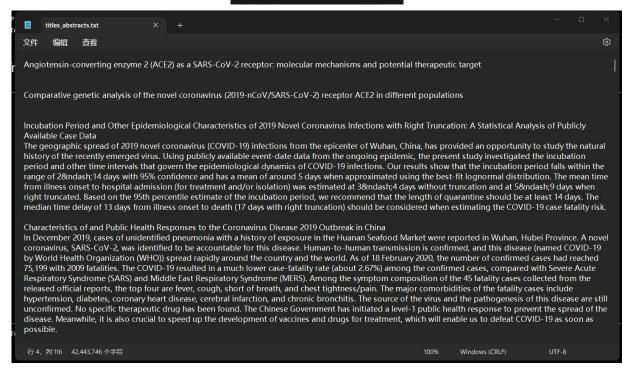
40.6M

#### Prase the Data



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titles\_abstracts.txt



#### PART 02

#### **Tokenization**

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#### Track 2.1 Use split() with regex



Input: content of file
Initialize empty list words
for each line in content do
 Split line using regex \W+
 Append tokens to words list
end for
Remove empty strings from words
Write result to file
Output: result of tokenization

Table 2.1: Weighted Random Sample of 20 Words

| source        | for         |
|---------------|-------------|
| acetate       | number      |
| rate          | enzymes     |
| peptide       | fruit       |
| MERS          | with        |
| in            | enzymes     |
| of            | respiratory |
| disease       | virus       |
| investigation | that        |
| activation    | the         |

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#### Track 2.2 Use NLTK tokenizer



Input: content of file Split content into sentences using sent\_tokenize() Initialize empty list words for each sentence in sentences do Tokenize sentence into words using word\_tokenize() Remove punctuations from sentence Convert all words to lowercase Append processed words to words end for Write result to file Output: result of tokenization

# Table 2.2: Top 20 Representative High-Frequency Words of Tokenized Result of NLTK

Tokenizer

| covid-19    | sars-cov-2   |
|-------------|--------------|
| 2019-n-ncov | infection    |
| pneumonia   | transmission |
| symptoms    | outbreak     |
| wuhan       | china        |
| case        | virus        |
| fever       | cough        |
| diagnosis   | treatment    |
| epidemic    | prevention   |
| control     | clinical     |

#### Track 2.3 Use Byte-Pair Encoding (BPE)



### from transformers import AutoTokenizer

Input: content of file Load pre-trained BERT tokenizer Set max\_length to 512 Initialize empty list result for each chunk of text with length max\_length do Tokenize chunk using BERT tokenizer Append tokenized chunk to result end for Write result to file Output: result of tokenization

#### **Table 2.3:**

Top 20
Representative High-Frequency
Words of
Tokenized
Result of
BERT
Tokenizer

| COVID-19  | SARS-CoV-2   |
|-----------|--------------|
| 2019-nCoV | virus        |
| infection | pneumonia    |
| symptoms  | transmission |
| patients  | diagnosis    |
| treatment | research     |
| outbreak  | cases        |
| china     | wuhan        |
| genome    | epidemiology |
| clinical  | prevention   |

#### Track 2.4 Build custom BPE



from tokenizers import
Tokenizer, models, trainers,
pre tokenizers

Input: content of file
Initialize BPE model
Set up the trainer for the model
Training BPE model with content
Save the trained BPE model
Tokenize content using trained
BPE model (as Track 2.3)
Write result to file
Output: result of tokenization

#### **Table 2.4:**

Top 20 Representative High-Frequency Words of **Tokenized** Result of Trained BPE Model Tokenizer

| corona       | virus        |
|--------------|--------------|
| infection    | COVID        |
| pneumonia    | epidemic     |
| transmission | cases        |
| patients     | symptoms     |
| treatment    | control      |
| quarantine   | diagnosis    |
| outbreak     | SARS         |
| MERS         | vaccine      |
| mortality    | epidemiology |

#### **Pros and Cons**



| Track                              | Efficiency | Accuracy  | Domain<br>Suitability | Ease of Use | Adaptability |
|------------------------------------|------------|-----------|-----------------------|-------------|--------------|
| Use split()<br>with regex          | High       | Low       | Low                   | Very High   | None         |
| Use NLTK<br>tokenizer              | Moderate   | Moderate  | Moderate              | Moderate    | Moderate     |
| Use Byte-Pair<br>Encoding<br>(BPE) | High       | Moderate  | Moderate              | Low         | Low          |
| Build new<br>Byte-Pair<br>Encoding | Moderate   | Very High | Very High             | Low         | Very High    |

#### PART 03

# **Build Word Representations**

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## Track 3.1 Use N-gram Language Modeling



N-gram language modeling represents words using **statistical** co-occurrence.

$$n=7$$

| 8 | the   | main           | symptoms       | of             | COVID-19       | are            | ?                       |
|---|---|----------------|----------------|----------------|----------------|----------------|-------------------------|
|   | $\omega_{t-6}$  | $\omega_{t-5}$ | $\omega_{t-4}$ | $\omega_{t-3}$ | $\omega_{t-2}$ | $\omega_{t-1}$ | $\boldsymbol{\omega_t}$ |
|   | $p(\omega_t   \omega_{t-n+1},, \omega_{t-1}) = \frac{C(\omega_{t-n+1},, \omega_{t-1}, \omega_t)}{C(\omega_{t-n+1},, \omega_{t-1})}$ |                |                |                |                |                |                         |

<sup>\*</sup>C counts the number of occurrences of the sequence

Embeddings are learned by constructing a co-occurrence matrix  $M_{ij} = p(\omega_j | \omega_i)$ . Embeddings are obtained by SVD decomposition of M:  $M = USV^T$ , where U is word embeddings and V is context embeddings.

## Track 3.1 Use N-gram Language Modeling



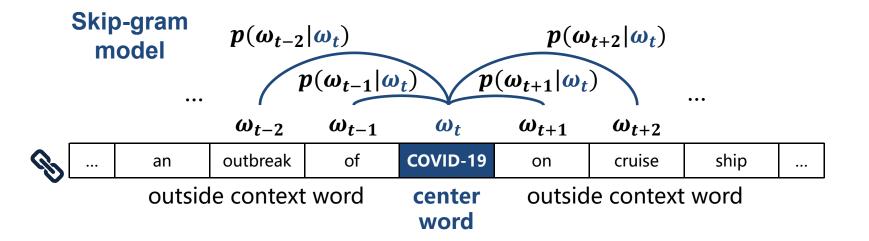
```
Word: based, Vector: [-0.00113634 0.00042914 0.00171392 -0.00094201 0.00194551]...
Word: simulate, Vector: [-0.00282291 0.00276994 0.0045483 0.00387259 -0.00197817]...
Word: exponential, Vector: [-0.00745408 -0.00210878 0.00366707 0.00557761 0.0008061]...
Word: synthesize, Vector: [-0.00195744 -0.00161151 0.00571776 -0.00158255 -0.00619846]...
Word: infected, Vector: [ 0.00098503 0.00135052 0.00025794 0.00151996 -0.00295611]...
Word: PCT, Vector: [-0.00361682 0.00107059 0.00450699 -0.00321555 -0.00355247]...
```

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## Track 3.2 Use Skip-gram with Negative Sampling



Skip-gram with Negative Sampling (SGNS) learns word embeddings by training a **neural network** to predict **context words** given a **target word**, while also distinguishing real context words from randomly sampled **negative words**.



## Track 3.2 Use Skip-gram with Negative Sampling

 $(1)_{+}$  1

 $(1)_{+}$  2

#### Nagetive sampling

window size=5

| _ |     |    | t-Z      | ·· t-1 | 337      | t+1 | 35 LTZ |      |     |
|---|-----|----|----------|--------|----------|-----|--------|------|-----|
| B | ••• | an | outbreak | of     | COVID-19 | on  | cruise | ship | ••• |
|   |     |    |          |        |          |     |        |      |     |

outside context **center** outside context word in window word word in window

(1)+

 $(1)_{+}$  1

(1)+12

- We use  $p(\omega_c|\omega_t) = \sigma(v_c^T v_t)$  to calculate  $p(\omega_c|\omega_t)$  with  $v_c$ (the vector of context word  $\omega_c$ ),  $v_t$ (the vector of target word  $\omega_t$ ) and function  $\sigma(x) = \frac{1}{1+e^{-x}}$
- Outside context words in window are selected as **positive samples**, while k **negative samples**  $\omega_n$  are drawn from a noise distribution.
- To maximize  $p(\omega_c|\omega_t)$  while minimize  $p(\omega_n|\omega_t)$ , the loss function simplifies to:  $L = -\log \sigma(v_c^T v_t) \sum_{n=1}^k \log \sigma(-v_n^T v_t)$

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#### Track 3.2

## **Use Skip-gram with Negative Sampling**

Model training

outside context center outside context word in window word word in window



For each context word, we update the vectors once. Then we move the window forward, traversing the entire content.

|     |    | 7        | window |          | •  |        |      |  |
|-----|----|----------|--------|----------|----|--------|------|--|
| ••• | an | outbreak | of     | COVID-19 | on | cruise | ship |  |
|     | an | outbreak | of     | COVID-19 | on | cruise | ship |  |
|     | an | outbreak | of     | COVID-19 | on | cruise | ship |  |

## Track 3.2 Use Skip-gram with Negative Sampling



```
Input: result of tokenization, window size, k
Initialize vectors randomly
for each sentence in result do
    for each target word in sentence do
        Set the window with the target word as the center
        for each context word in window do
            Randomly select k negative samples
            Caculate the loss function
            Update vectors based on gradient
Write model to file
Output: word representations
```

```
Word: be, Vector: [-0.04363129 -0.13416731 -0.04463265 0.42448187 0.1020665 ]...

Word: virus, Vector: [ 0.38384342 0.02390595 0.25144455 -0.32621083 0.22319743]...

Word: coronavirus, Vector: [ 0.34523997 -0.6191298 0.10023931 0.32888174 0.2146074 ]...

Word: infection, Vector: [-0.44734353 -0.3158639 -0.01379213 0.5342119 0.17223525]...

Word: patients, Vector: [ 0.3393421 -0.142002 0.5237385 0.3722622 0.3285995]...

Word: an, Vector: [ 0.15025043 -0.34280798 -0.30170983 0.20958054 -0.05775673]...
```

## Track 3.3 Use Contextualised Word Representation by MLM



Masked Language Model (MLM) is a technique used to learn contextualized word representations by training a model to predict randomly **masked words** in a sentence based on their **surrounding context**.

Given an input sequence  $\omega_1, \omega_2, ..., \omega_t$ , some tokens are randomly masked (e.g.  $\omega_m$ ), and the model learns to predict them:  $p(\omega_m | \omega_1, ..., \omega_{m-1}, [\text{MASK}], \omega_{m+1}, ..., \omega_t)$ 

Masked language model



surrounding context

masked word surrounding context

## Track 3.3 Use Contextualised Word Representation by MLM

• A transformer-based model (e.g. BERT) processes the full sequence bidirectionally, generating deep contextualized word embeddings. The loss function is typically the crossentropy loss over the masked tokens:

$$L = -\sum_{m} \log p(\boldsymbol{\omega}_{m} | \boldsymbol{h}_{m})$$

where  $h_m$  is the hidden representation of the masked token.

 This method enables embeddings to capture word sense variations and syntactic dependencies based on the given context.

## Track 3.3 Use Contextualised Word Representation by MLM

• In our implementation, we utilized BERT for embedding generation. Given the large number of parameters in BERT and the high computational cost of training, we employed **LoRA fine-tuning** to optimize the training process.

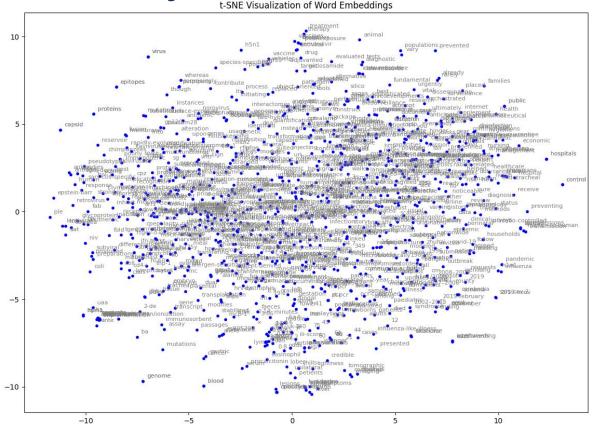
from transformers import BertTokenizer, BertForMaskedLM, Trainer, TrainingArguments from datasets import Dataset import torch from transformers import DataCollatorForLanguageModeling from peft import get\_peft\_model, LoraConfig, TaskType

#### PART 04

# **Explore the Word Representations**

## Track 4.1 Visualise the word representations by t-SNE

III • t-SNE is a dimensionality reduction algorithm that visualizes highdimensional data by mapping it into a lower-dimensional space (typically 2D or 3D) while preserving local structure and patterns.



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## Track 4.2 Visualise Biomedical Entities by t-SNE

• Biomedical Entities words are colored by category and highlighted in this section. In this graph, words marked with the same color tend

to cluster together, while words marked

with the different

from each other.

color tend to separate

epidemiology treatments -10

t-SNE Visualization of Word Embeddings

#### Track 4.3 Co-occurrence

 The words are selected in order from highest to lowest according to the statistical frequency of cooccurrence with the target word in the corpus.

- Cross-Domain Relevance
- Contextual Associations
- Broad Impact of COVID-19

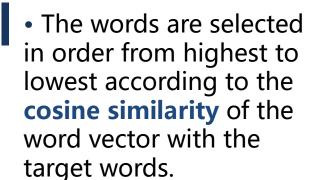
| <b>Co-occuring Word</b> | Frequency   |
|-------------------------|-------------|
| Covid                   | 0.009722719 |
| multiplicity            | 0.006220484 |
| flaviviral              | 0.005976294 |
| Lyme                    | 0.005395208 |
| productive              | 0.005248906 |
| obstructive             | 0.005074524 |
| mouth                   | 0.004548549 |
| persistent              | 0.004354533 |
| Alzheimer               | 0.004330223 |
| SFTSV                   | 0.004047467 |

#### Target word: 'coronavirus'

#### **Table 4.4:**

10 biomedical entities with the highest frequency of cooccurrence with coronavirus

#### Track 4.4 Semantic Similarity



$$Similarity = \frac{\boldsymbol{v_1} \cdot \boldsymbol{v_2}}{\|\boldsymbol{v_1}\| \cdot \|\boldsymbol{v_2}\|}$$

- Model Strengths
  - Error Handling
- Temporal and Specific References

| Semantic Similar<br>Word | Similarity  |
|--------------------------|-------------|
| novel                    | 0.632027924 |
| 2019-novel               | 0.618497908 |
| coronovirus              | 0.610034168 |
| abstract                 | 0.596071839 |
| provisionally            | 0.592935622 |
| 2019-ncov                | 0.58953917  |
| 2019                     | 0.587587357 |
| ncov-2019                | 0.576685071 |
| cov                      | 0.576638222 |
| 2019-novel               | 0.618497908 |

#### Target word: 'coronavirus'

#### **Table 4.3:**

10 biomedical entities with the highest semantic similarity with coronavirus

#### The end

## Thank you for your attention!

#### **Reference:**

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