Harnessing Scientific AI for Knowledge Discovery in Virology

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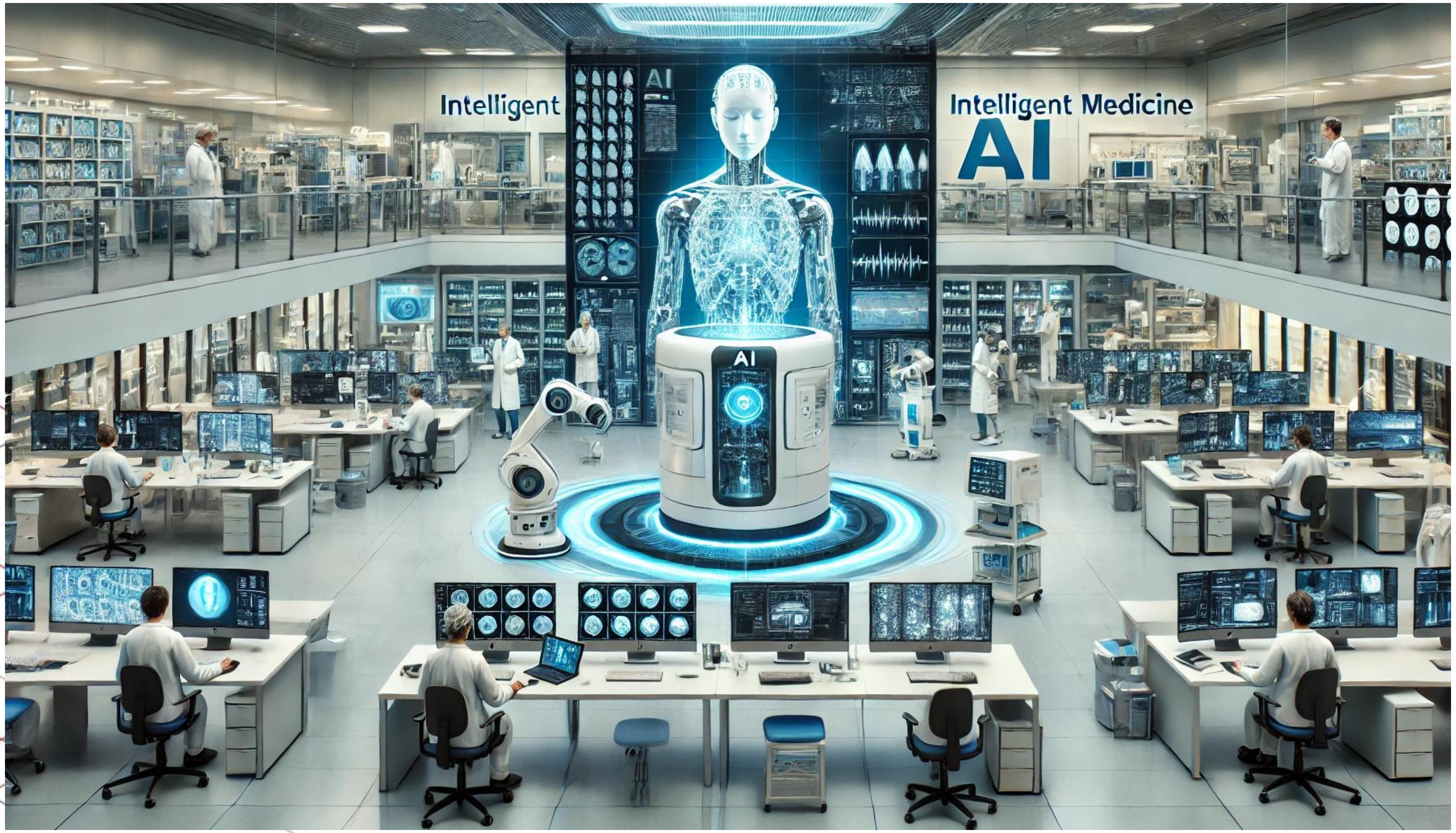
- In recent years, AI technology has achieved technological breakthroughs and is widely used in various fields of intelligent medicine, including: medical image inspection, disease-assisted diagnosis, surgery, hospital management, and medical big data integration.
- Moreover, AI is actively explored in emerging fields such as surgical robots, wearable devices, new drug discovery, precision medicine, epidemics prevention and control, and gene sequencing.
- In this talk, we focus on the applications of AI in domain of virological science.
  - Herein we will have the opportunity to look closely at some of the mentioned related fields.



Virological science and its subdomains

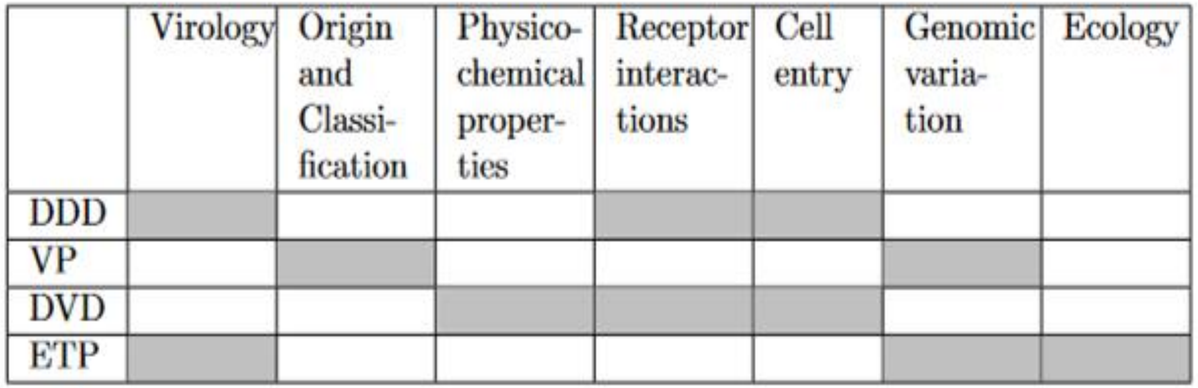
Virological science research is broadly categorized into the following seven subdomains:

1. **Virology:** Virology is the study of viruses — their structure, function, and genetics.
2. **Origin and Classification:** The origin and classification of a virus involve identifying its source (like which animal it came from) and its family or type.
3. **Physicochemical Properties:** This refers to the physical and chemical properties of the virus, such as stability at different temperatures or pH levels.
4. **Receptor Interactions:** What receptors on human cells do viruses use to gain entry? E.g., SARS-CoV-2 uses specific receptors (like ACE2) on human cells to gain entry.
5. **Cell Entry:** How the virus enters cells can affect how easily it spreads and how severe the infection can be.
6. **Genomic Variation:** Viruses like SARS-CoV-2 can mutate, leading to genomic variations that may affect their contagiousness and lethality.
7. **Ecology:** The ecological aspect studies the virus in relation to its environment, including how human interactions with wildlife might facilitate the emergence of new viruses.

AI Application Areas for Virology

1. **Disease Detection and Diagnosis**
2. **Virology and Pathogenesis**
3. **Drug and Vaccine Development**
4. **Epidemic and Transmission Prediction**

AI Application Areas in relation to Virological science



	Virology	Origin and Classification	Physico-chemical properties	Receptor interactions	Cell entry	Genomic variation	Ecology
DDD	▨			▨	▨		
VP		▨				▨	
DVD			▨	▨	▨		
ETP	▨					▨	▨

Table 1: Interactions between the domains of study in Virology (columns) and the AI methodology application areas (rows). The following acronyms are used in the first column. DDD: Disease Detection and Diagnosis, VP: Virology and Pathogenesis, DVD: Drug and Vaccine Development, ETP: Epidemic and Transmission Prediction

AI Application Areas for Virology

1. **Disease Detection and Diagnosis:** AI analyzes medical imaging and genetic data to quickly identify and classify viral infections.
2. **Virology and Pathogenesis**
3. **Drug and Vaccine Development**
4. **Epidemic and Transmission Prediction**

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Disease Detection and Diagnosis

- AI supports the diagnosis of infectious virological diseases through medical image inspections and provides non-invasive detection solutions to prevent medical personnel from contracting infections. Furthermore, the application of AI methods not only greatly shortens the imaging diagnosis time of radiologists but also improves the accuracy of the diagnosis.
- E.g., AI vision-based models were used in the detection of Covid-19 from chest X-ray and lung computed tomography (CT) imaging [1].
- The general application objectives are: image acquisition, organ recognition, infection region segmentation, and disease classification.

Reference

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Disease Detection and Diagnosis

- Lung CT Image Inspection
- Chest X-ray Image Inspection

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Lung CT Imaging

- What?
    - On a CT scan, COVID-19 usually shows up as cloudy spots called Ground Glass Opacity (GGO) around the edges or peripheral area of the lungs. Sometimes, these spots can be more solid. If the patient gets better, these cloudy spots will disappear and may leave behind some thin scar tissue.

Reference

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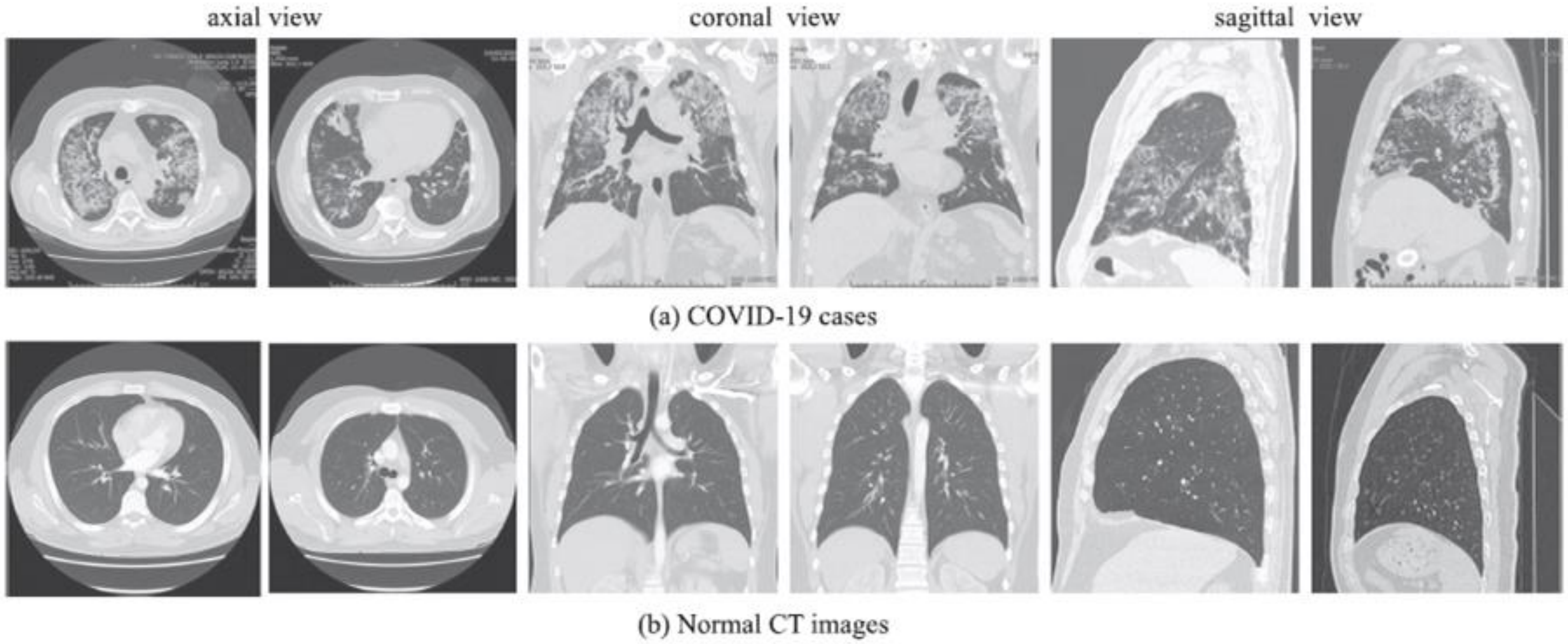
Lung CT Imaging



Examples of lung CT images of normal and COVID-19 cases

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

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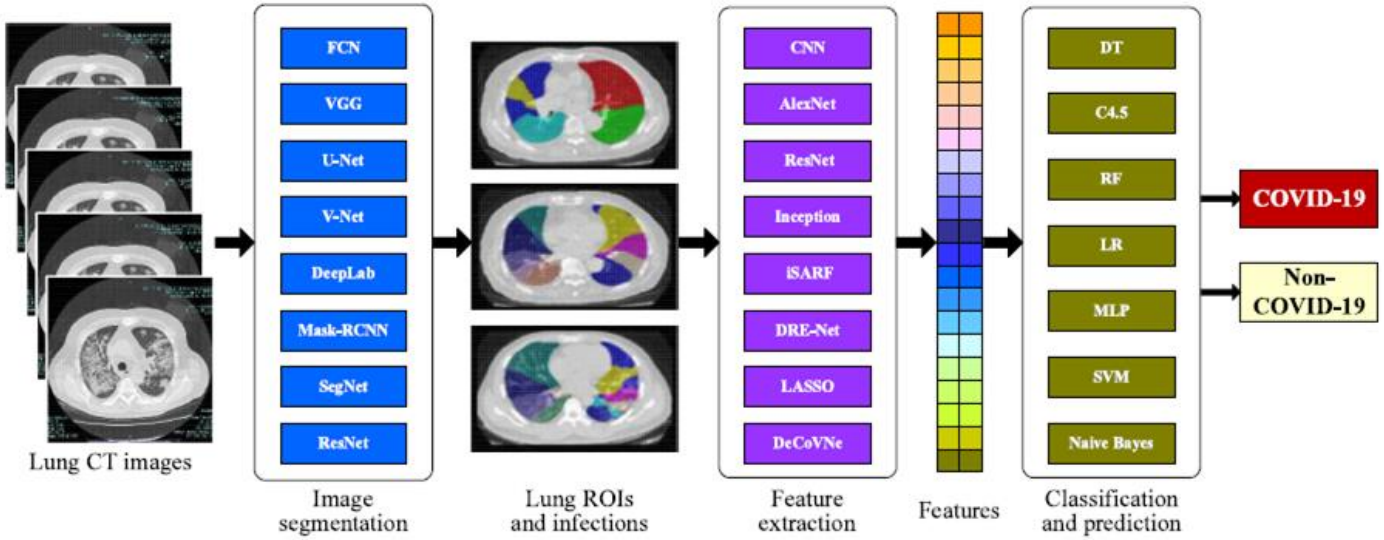

Representative AI architecture for CT image classification and Covid-19 inspection

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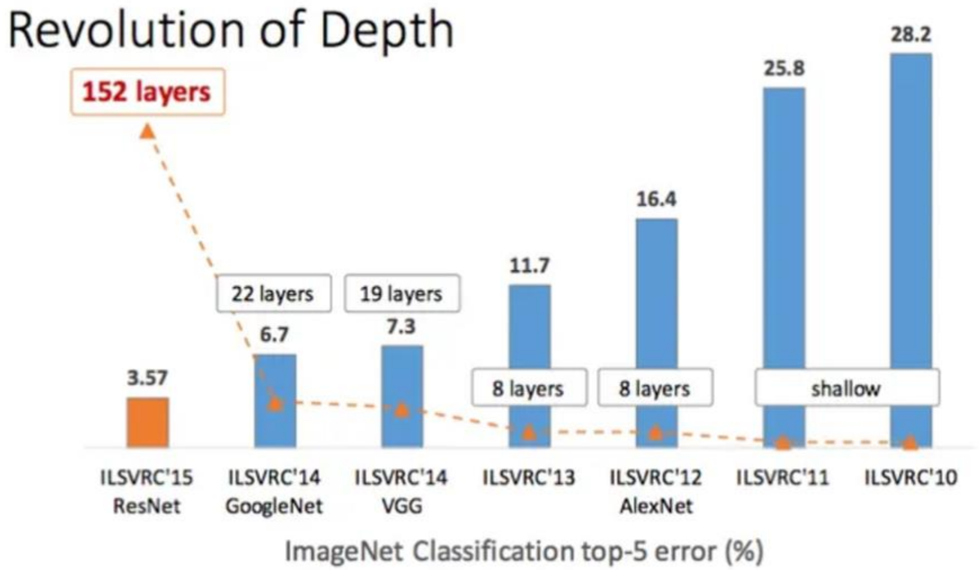
ResNet (Residual Networks)

- ResNet, short for Residual Networks is a classic neural network used as a backbone for many computer vision tasks.
- The fundamental breakthrough with ResNet was it allowed us to train extremely deep neural networks with 150+layers successfully. Prior to ResNet training very deep neural networks was difficult due to the problem of vanishing gradients.
    - This model was the winner of ImageNet challenge in 2015.



Reference

- He, K., Zhang, X., Ren, S., & Sun, J. (2016). Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp. 770-778).

ResNet (Residual Networks)

- ResNet first introduced the concept of skip connection. The figure below illustrates skip connection. The figure on the left is stacking convolution layers together one after the other. On the right is a representation of stacked convolution layers as before but now with also the original input added to the output of the convolution block. This is called skip connection.

Skip Connection Image from DeepLearning.AI

Reference

- He, K., Zhang, X., Ren, S., & Sun, J. (2016). Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp. 770-778).

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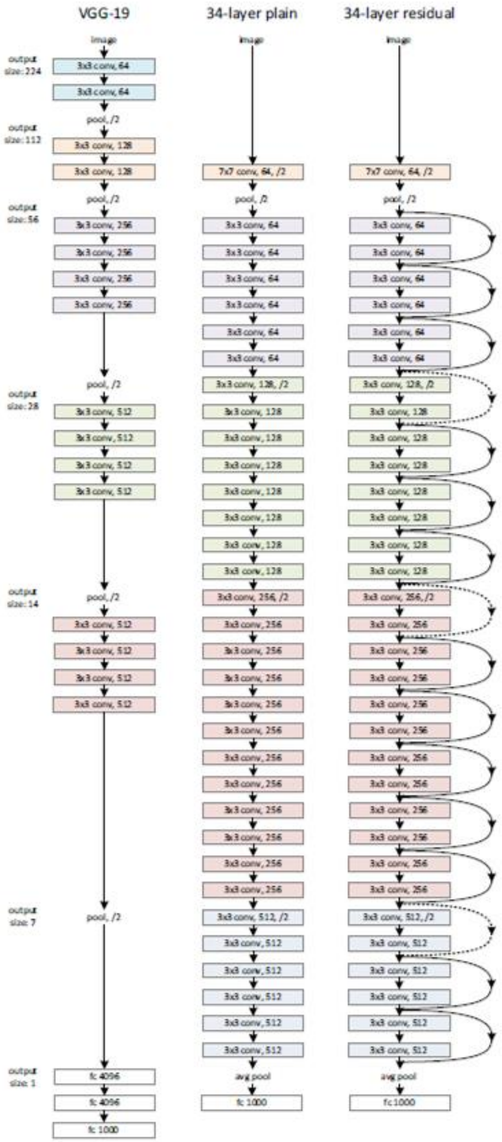
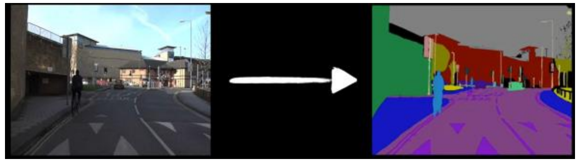


Reference

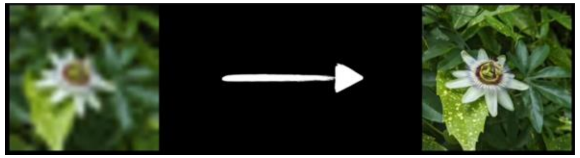
- He, K., Zhang, X., Ren, S., & Sun, J. (2016). Deep residual learning for image recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp. 770-778).

U-Net

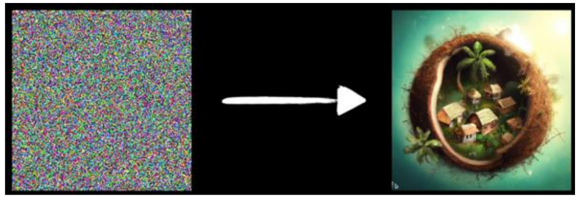
- U-Net was originally proposed for biomedical image segmentation tasks
    - However, due to its impressive performance, recently all of the cutting-edge generative models whether they be generative adversarial networks, or any of the diffusion model variants such as StableDiffusion, Imagen, or Dall-e 2 use the U-Net is one way or another.
- Applied in a wide spectrum of tasks:
    - image segmentation: mapping images to segmentation masks



    - super-resolution: upscaling low-resolution to high-resolution images



    - diffusion models: transform Gaussian noise to newly generated images

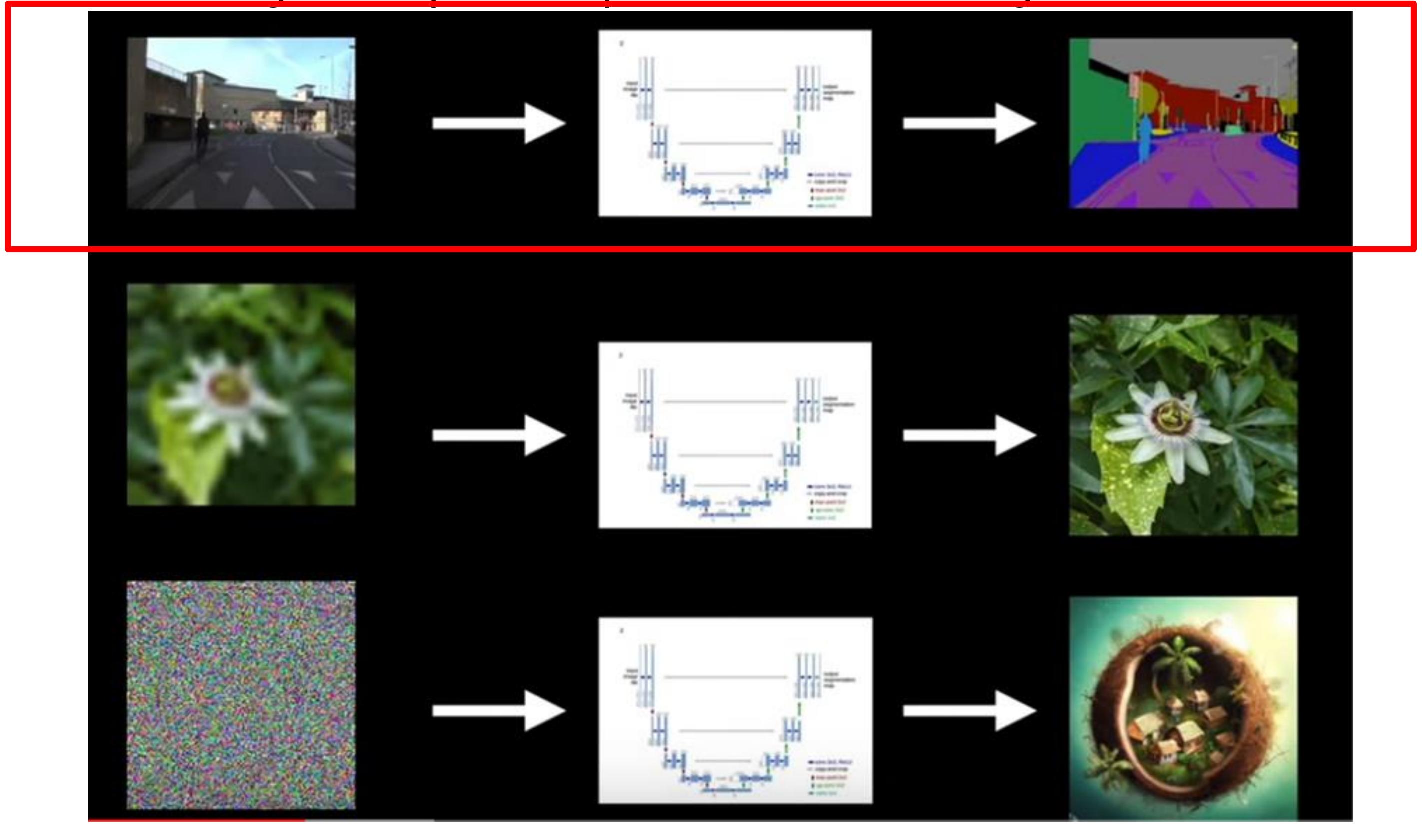


Reference

- Ronneberger, O., Fischer, P., & Brox, T. (2015). U-net: Convolutional networks for biomedical image segmentation. In *Medical image computing and computer-assisted intervention–MICCAI 2015: 18th international conference, Munich, Germany, October 5-9, 2015, proceedings, part III 18* (pp. 234-241). Springer International Publishing.

U-Net

- all of these tasks take an image as input and produce a new image



E.g., here we learn the mapping between the pixels of an image to the pixels of a segmentation mask

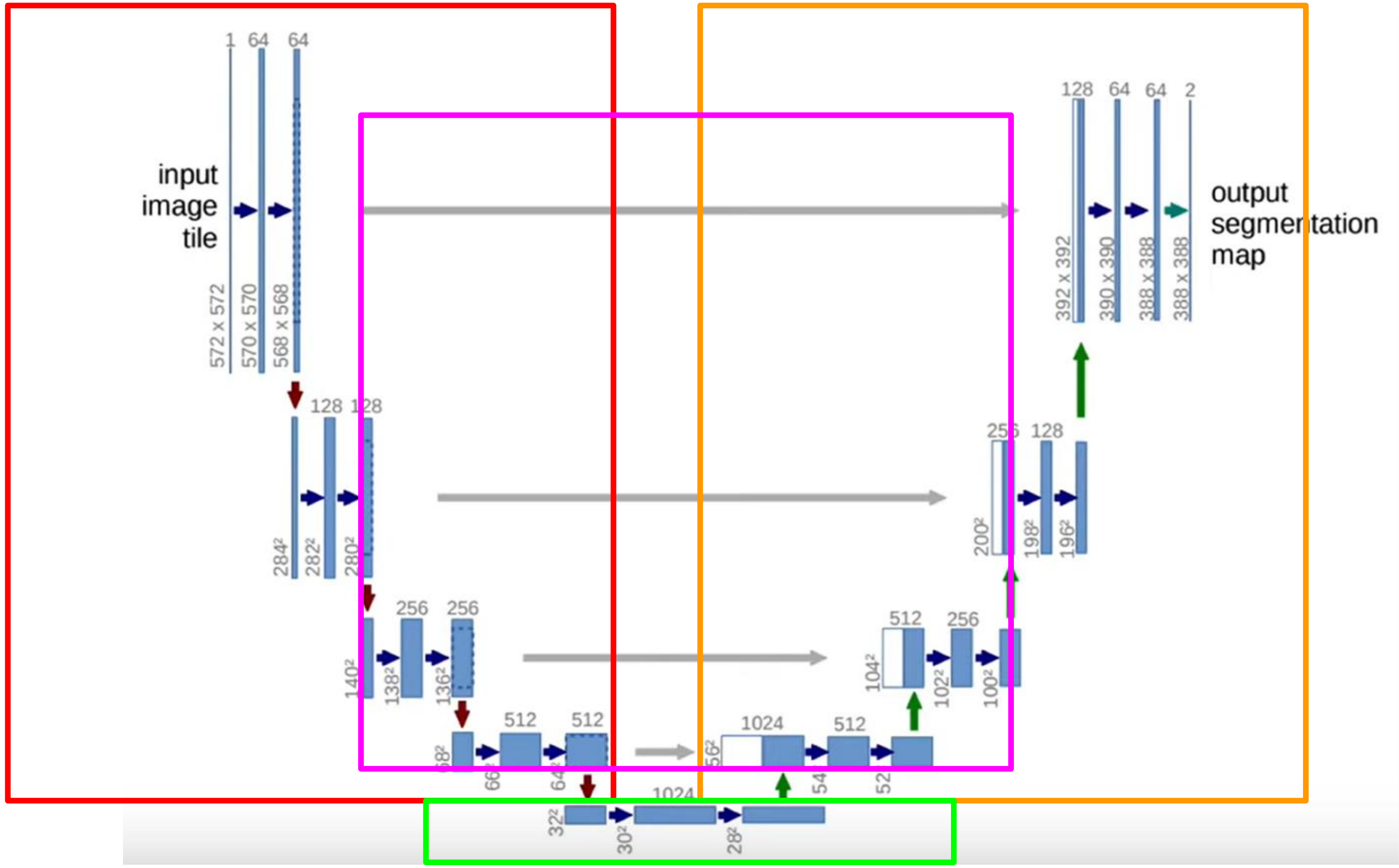
Reference

- Ronneberger, O., Fischer, P., & Brox, T. (2015). U-net: Convolutional networks for biomedical image segmentation. In *Medical image computing and computer-assisted intervention–MICCAI 2015: 18th international conference, Munich, Germany, October 5-9, 2015, proceedings, part III 18* (pp. 234-241). Springer International Publishing.

U-Net Architecture Overview

Skip connections

Encoder



Decoder

Bottleneck

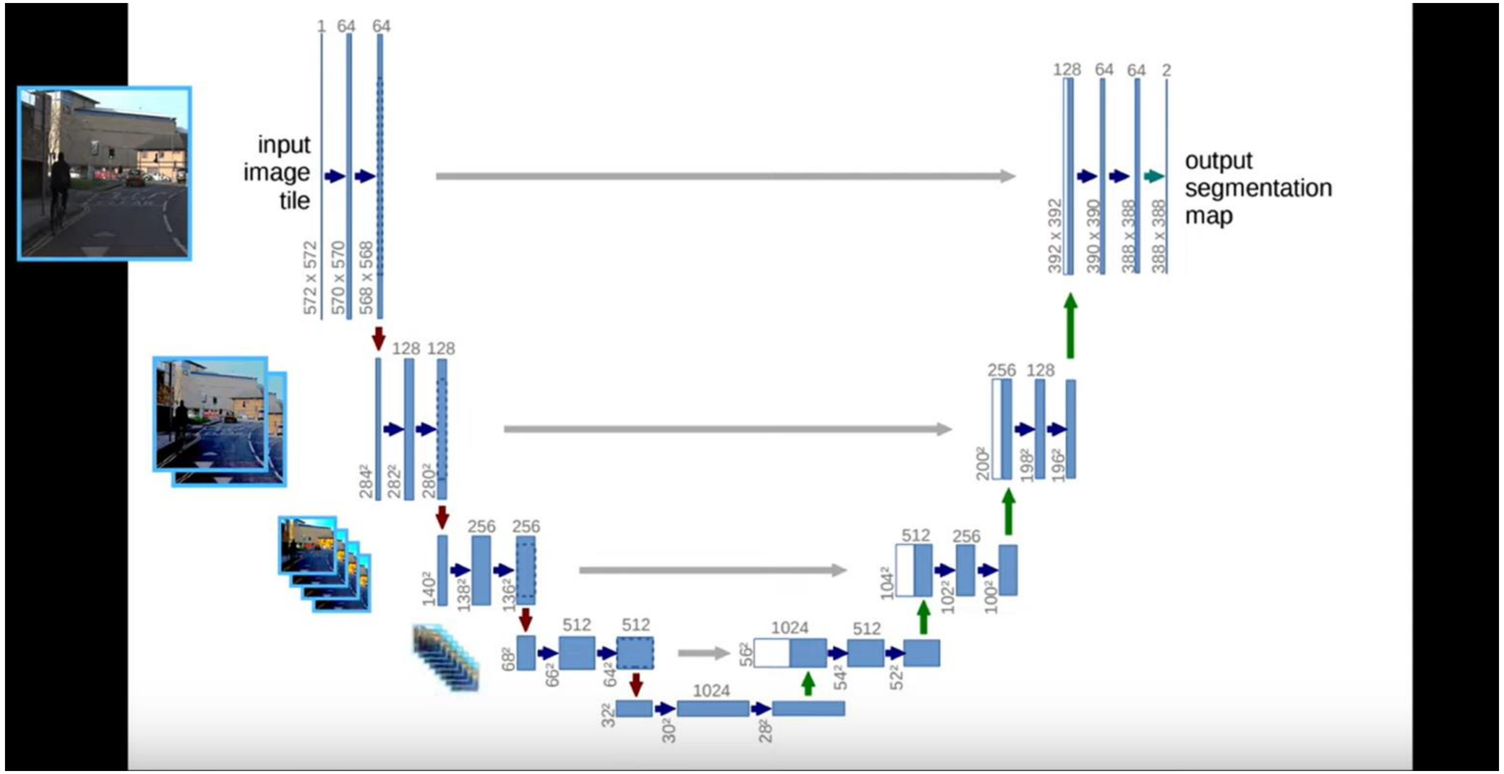
Reference

The U-Net (actually) explained in 10 minutes

https://youtu.be/NhdzGfB1q74?si=2U1h2eFqA9oSTE_6

U-Net: How does it work?

- An input image is first passed through the encoder, passing them through 3x3 convolutional layers and ReLU functions.
- At each stage, the image is downsampled with a 2x2 max pooling layer and the channels are doubled before passing them through the convolutional layers of the stage.
- This repeats all the way down to the bottleneck.



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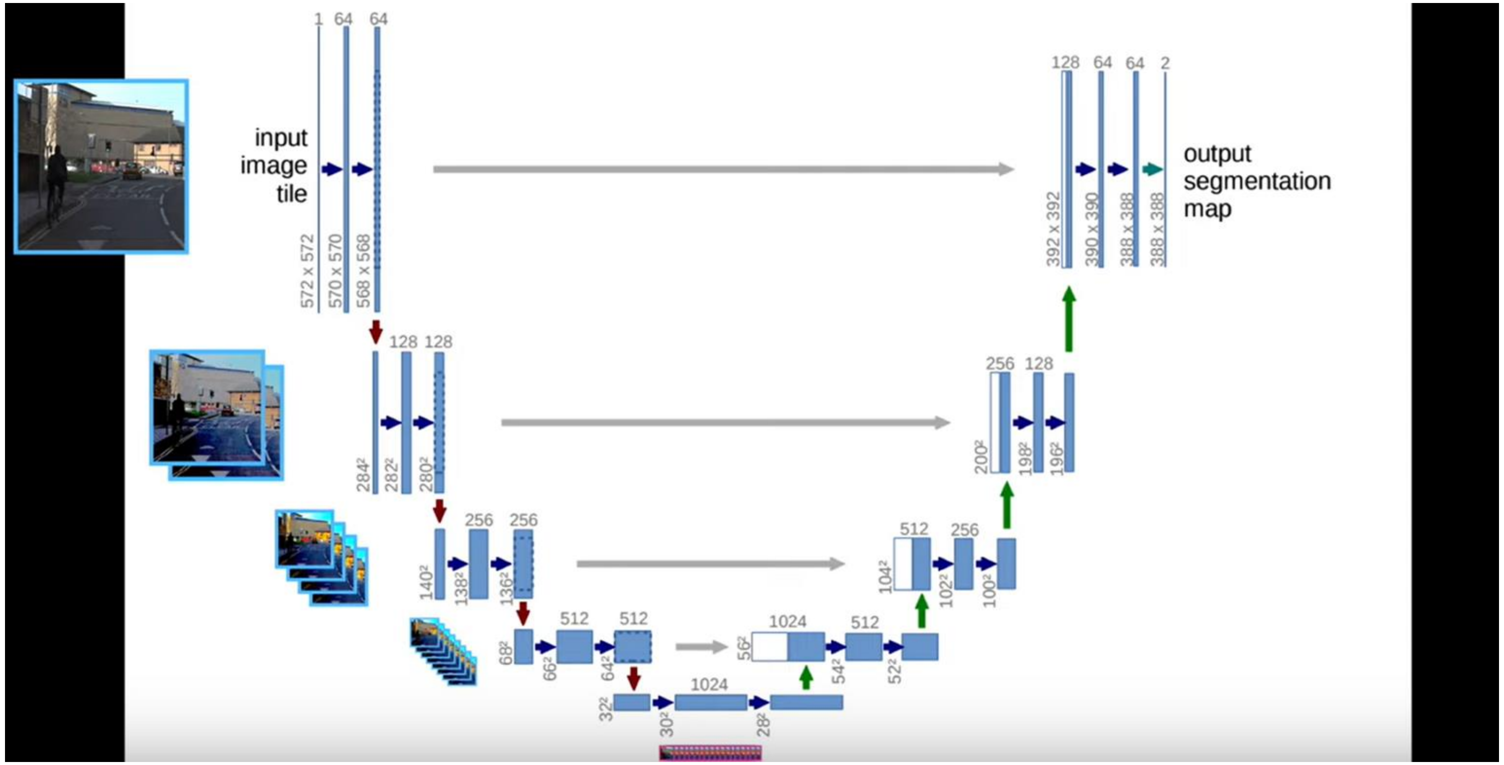

- At the bottleneck, the image is downsampled, features are passed through the convolutional layers, and then the features are upsampled to get back to the corresponding resolution before bottleneck.

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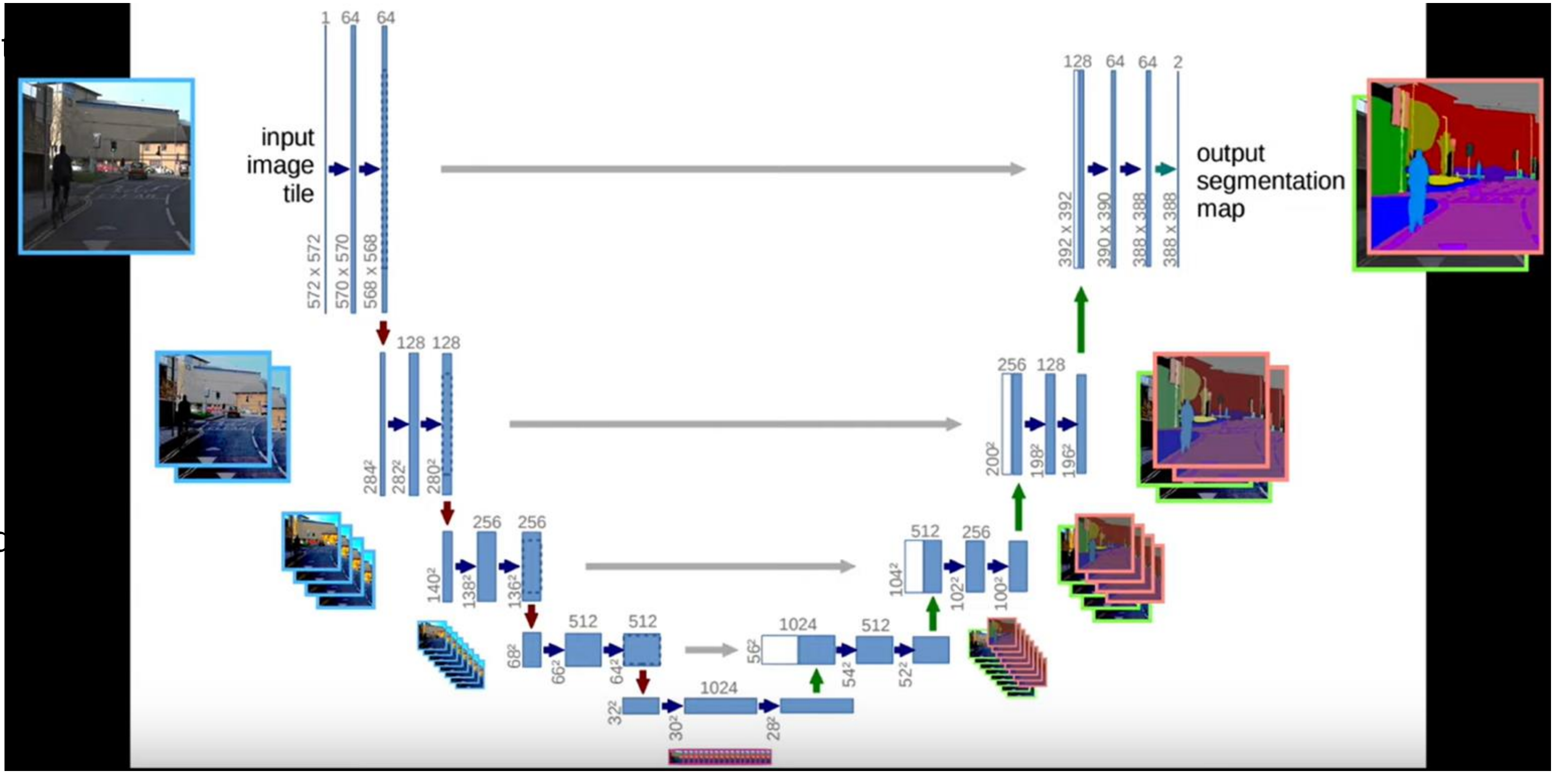
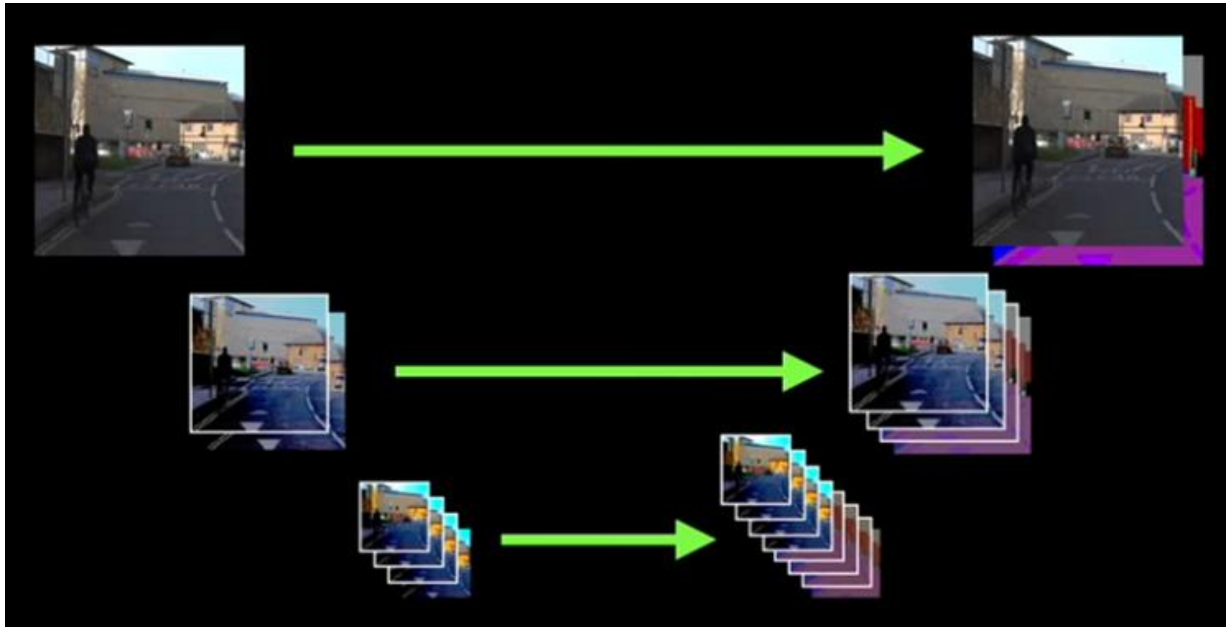


- At the bottleneck, the image is downsampled, features are passed through the convolutional layers, and then the features are upsampled to get back to the corresponding resolution before bottleneck.

- The features are now passed up the decoder where the features are upsampled stage-wise.
- At each stage the features are also concatenated with the encoder features by the skip connection paths.
- This pattern of upsampling, passing through convolutional layers, and concatenating the features repeats all the way to the final output layer.

U-Net

Since the connecting paths pass in copies of the input features, it makes it easier to gain pixel-perfect accuracy for tasks such as segmentation.



V-Net

A V-Net is similar to a U-Net, employing two symmetric contracting and expanding paths. However, in contrast with the U-Net, it exploits a fully-convolutional structure, with the presence of convolution operations exclusively and the absence of pooling layers.

- VNet employs residual connections and also uses strided convolutions for downsampling instead of max pooling

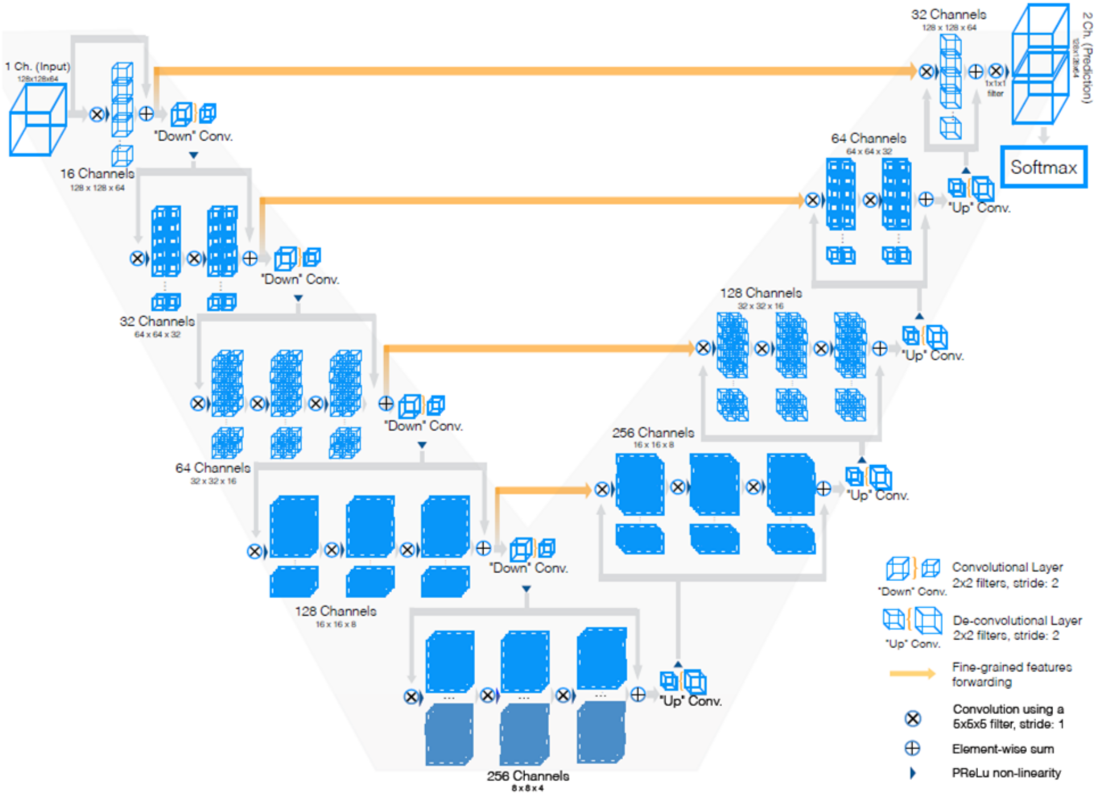


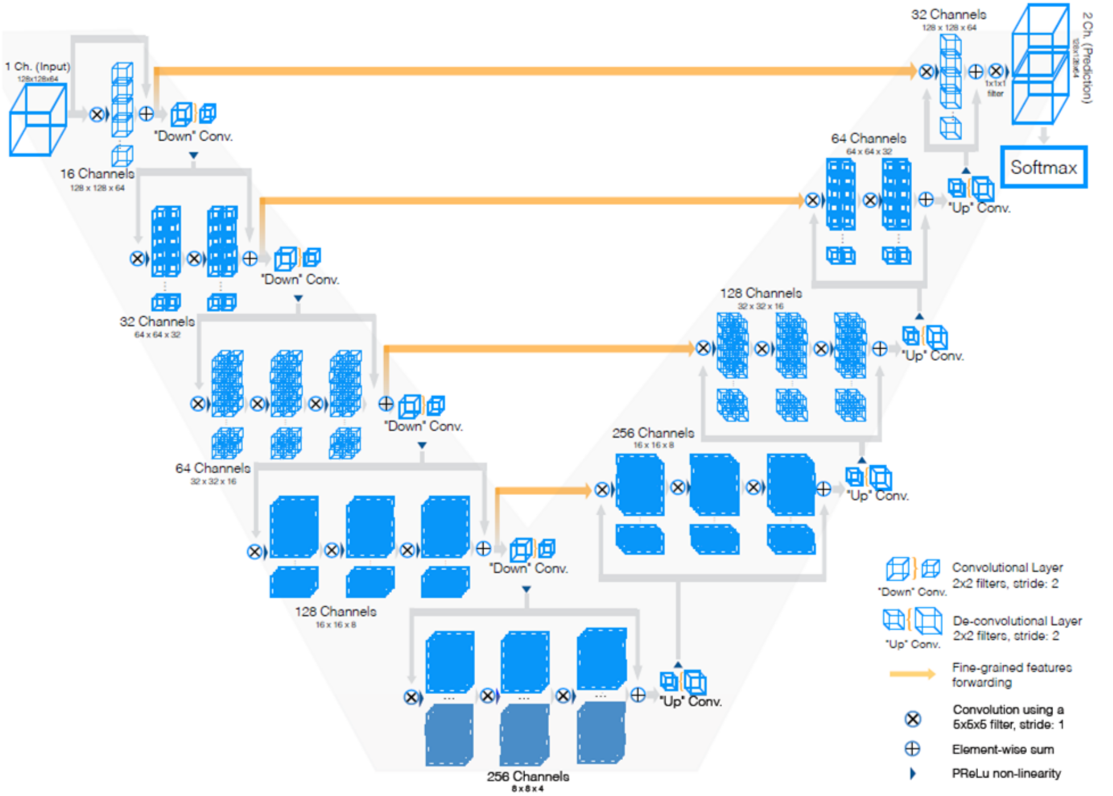
Fig. 2. Schematic representation of our network architecture. Our custom implementation of Caffe [5] processes 3D data by performing volumetric convolutions.

Reference

- Milletari, F., Navab, N., & Ahmadi, S. A. (2016, October). V-net: Fully convolutional neural networks for volumetric medical image segmentation. In *2016 fourth international conference on 3D vision (3DV)* (pp. 565-571). Ieee.

V-Net versus U-Net

- **U-Net:** Primarily designed for biomedical image segmentation. It's widely used for tasks like segmentation of cells, organs, or other structures in medical images.
- **V-Net:** Specifically designed for 3D medical image segmentation, such as MRI or CT scans, focusing on volumetric data.



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Lung CT Imaging

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    - Region Of Interest (ROI) segmentation,
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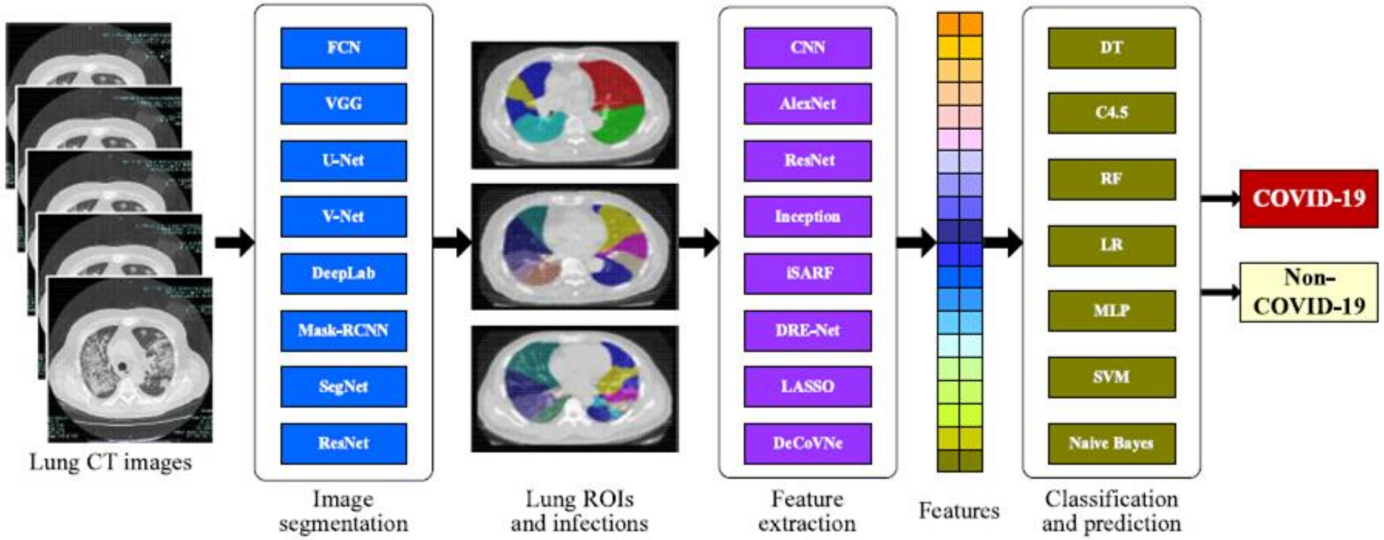

Representative AI architecture for CT image classification and Covid-19 inspection

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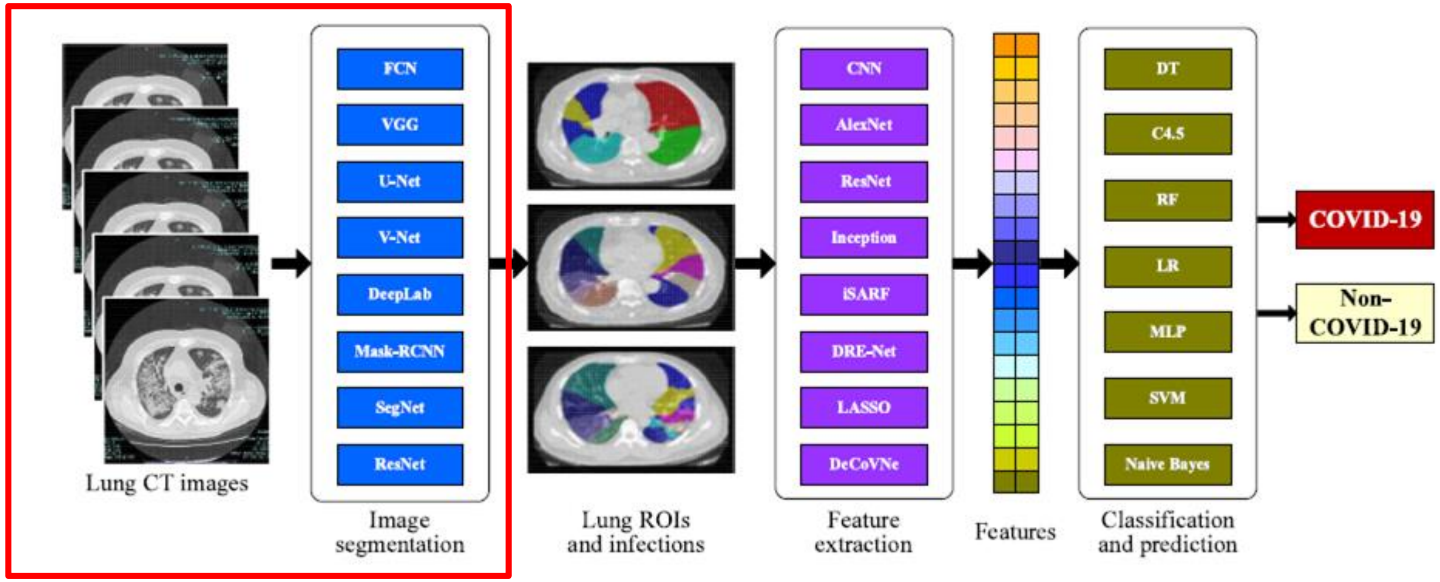

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Region of Interest (ROI) Segmentation

- Also known as the process of segmentation of lung organs in lung CT images such as lungs, lung lobes, bronchopulmonary segments, and infected regions or lesions.
    - Common methods: U-Net, V-Net, and VB-Net

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Lung CT Imaging - ROI Segmentation Approaches

- **Improved segmentation:**
  - Shan et al. (2021) collected 549 CT images from patients with confirmed COVID-19 and proposed an improved segmentation model (called VB-Net) based on the V-Net and ResNet models.
  - Chen et al. (2020) established a DL model based on the U-Net++ structure to extract the ROIs from each CT image and detect the training curve of suspicious lesions.
- **Classification:**
  - Xu et al. (2020) used a 3D DL model to segment the infection regions from lung CT images. Then, they built a classification model using ResNet and location-attention structures, and divided the segmented regional images into three categories, such as COVID-19, influenza-A viral pneumonia, and normal.
- **Lung organ detection:**
  - Li et al. (2020) used the U-Net segmentation model to extract lung organs as ROIs from each lung CT image.
  - Tang et al. (2021) used the VB-Net model to accurately segment 18 lung regions and infected regions from lung CT images, and further calculated 63 quantitative features.

Reference

- Shan, F., Gao, Y., Wang, J., Shi, W., Shi, N., Han, M., ... & Shi, Y. (2021). Abnormal lung quantification in chest CT images of COVID-19 patients with deep learning and its application to severity prediction. *Medical physics*, *48*(4), 1633-1645.
- Chen, J., Wu, L., Zhang, J., Zhang, L., Gong, D., Zhao, Y., ... & Yu, H. (2020). Deep learning-based model for detecting 2019 novel coronavirus pneumonia on high-resolution computed tomography. *Scientific reports*, *10*(1), 19196.
- Xu, X., Jiang, X., Ma, C., Du, P., Li, X., Lv, S., ... & Li, L. (2020). A deep learning system to screen novel coronavirus disease 2019 pneumonia. *Engineering*, *6*(10), 1122-1129.
- Li, L., Qin, L., Xu, Z., Yin, Y., Wang, X., Kong, B., ... & Xia, J. (2020). Artificial intelligence distinguishes COVID-19 from community acquired pneumonia on chest CT. *Radiology*.
- Tang, Z., Zhao, W., Xie, X., Zhong, Z., Shi, F., Ma, T., ... & Shen, D. (2021). Severity assessment of COVID-19 using CT image features and laboratory indices. *Physics in Medicine & Biology*, *66*(3), 035015.

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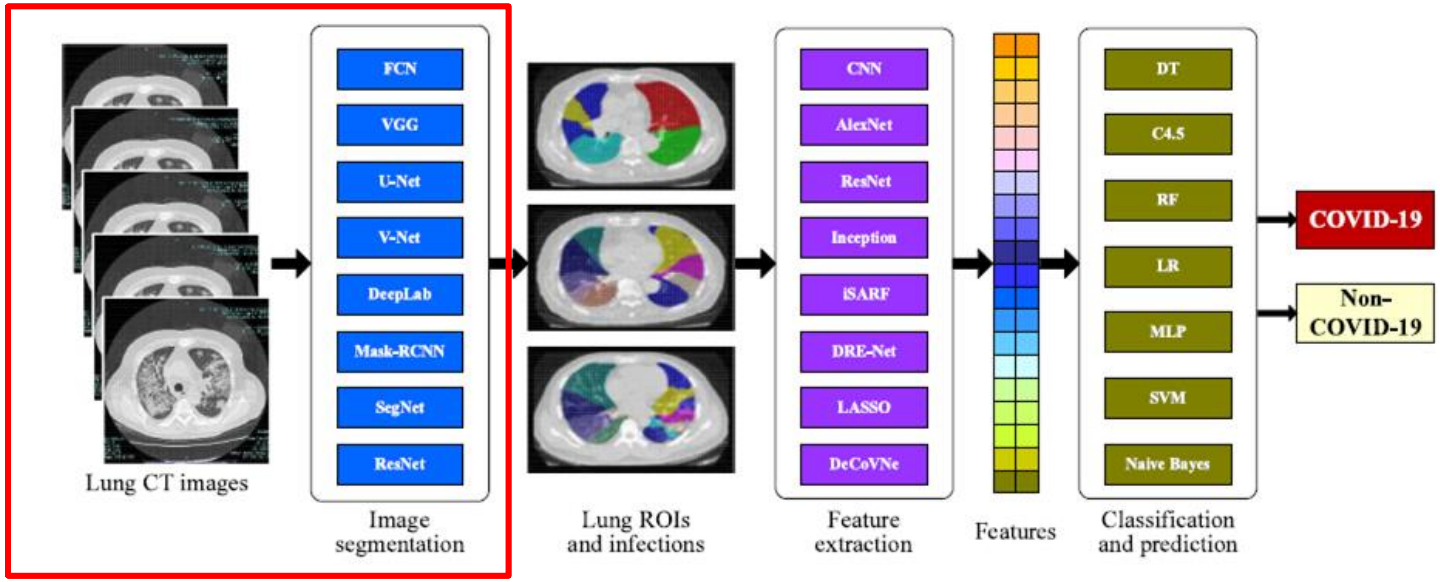

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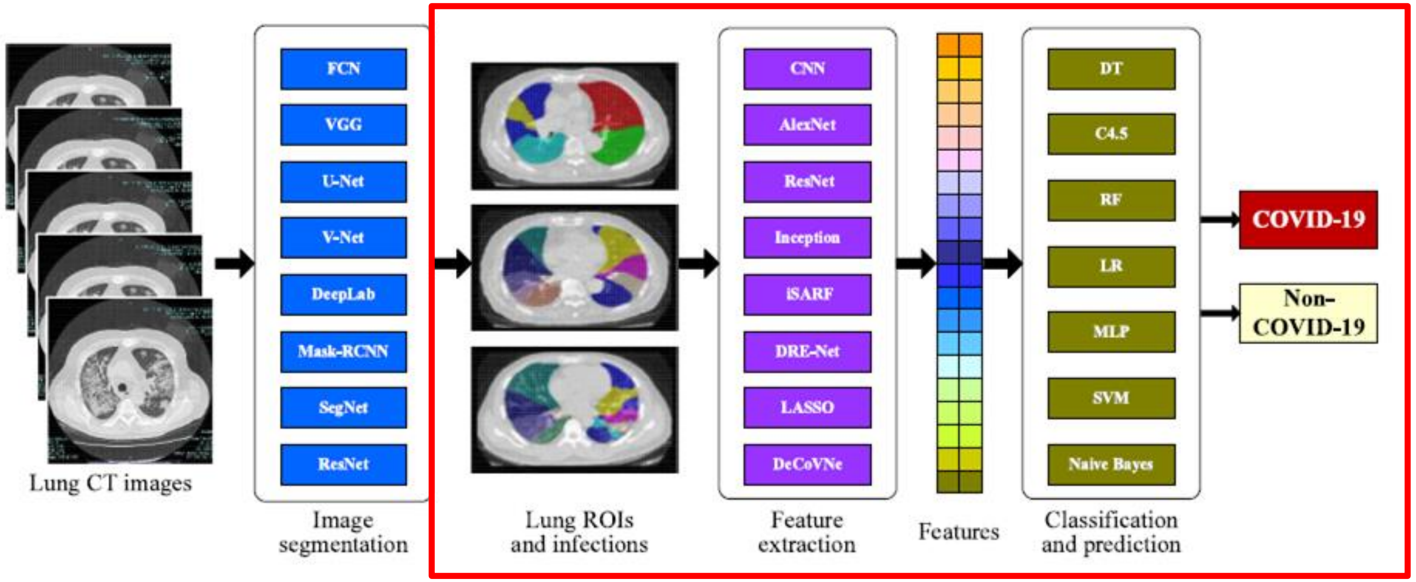

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Lung CT Imaging – Feature Extraction

Lung CT Imaging – Feature Extraction

Morphological Features Extracted from Lung CT Images:

- **Nodule Characteristics**: Size, shape, texture, and edges.
- **Texture Analysis**: Identifies patterns indicating pneumonia, fibrosis, or cancer.
- **Lung Volume and Shape**: Assessments for diseases like Chronic Obstructive Pulmonary Disease (COPD).
- **Wall Thickness**: Important for diagnosing bronchiectasis.
- **Airway Abnormalities**: Detection of deformities or blockages, relevant in asthma or bronchitis.
- **Vascular Structures**: Analysis of blood vessels for signs of pulmonary hypertension.
- **Cavitation**: Identification of cavities that suggest infections or necrotic tumors.

Lung CT Imaging - Covid-19 Classification Approaches

- Yue et al. (2020) collected 71 CT images from 52 patients with confirmed COVID-19 in 5 hospitals. They used radiobiological methods to extract 1,218 features from each CT image, and then performed LR and RF methods on these features to distinguish between short-term and long-term hospital stays.
- Shi et al. (2021) used the VB-Net model to segment lung and infection regions from CT images, and classified them based on 96 features (including 26 volume features, 31 digital features, 32 histogram features, and 7 surface features). Next, they proposed an iSARF method to classify features and predict COVID-19 disease. Comparative experiments show that the iSARF method is superior to LR, SVM, and NN methods

References

- Yue, H., Yu, Q., Liu, C., Huang, Y., Jiang, Z., Shao, C., ... & Qi, X. (2020). Machine learning-based CT radiomics method for predicting hospital stay in patients with pneumonia associated with SARS-CoV-2 infection: a multicenter study. *Annals of translational medicine*, *8*(14).
- Shi, F., Xia, L., Shan, F., Song, B., Wu, D., Wei, Y., ... & Shen, D. (2021). Large-scale screening to distinguish between COVID-19 and community-acquired pneumonia using infection size-aware classification. *Physics in medicine & Biology*, *66*(6), 065031

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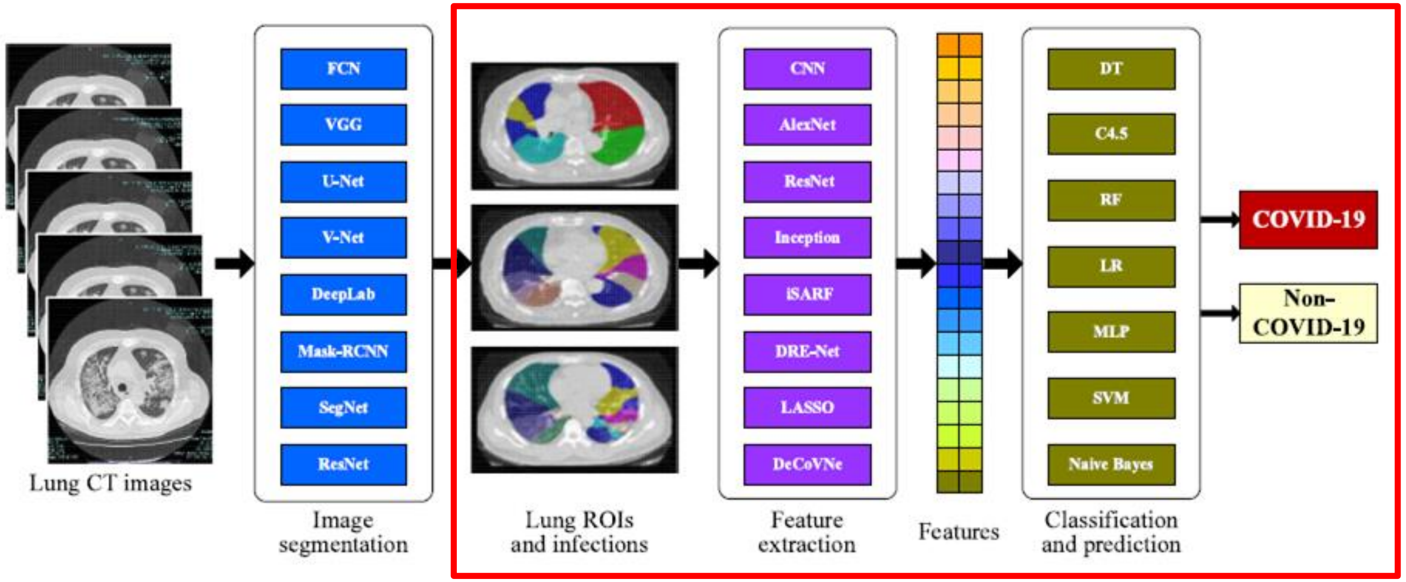

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Disease Detection and Diagnosis

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- Chest X-ray Image Inspection

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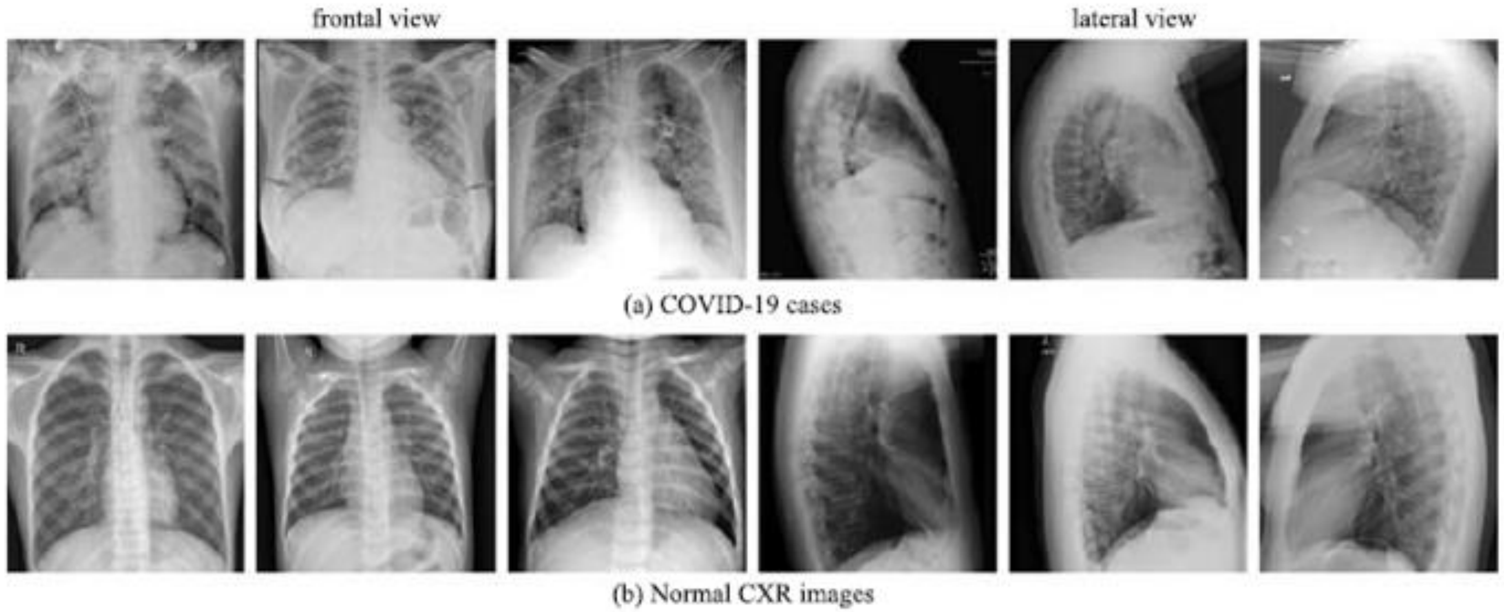
Chest X-ray Imaging

- What?
  - Compared with CT images, chest X-ray (CXR) images are easier to obtain in radiological inspections.
  - Although CXR imaging is a typical imaging method used for the diagnosis of COVID-19, it is generally considered to be less sensitive than CT imaging. Some CXR images of patients with early COVID-19 showed normal characteristics.
  - Radiological signs of COVID-19 CXR images include airspace opacity, Ground Glass Opacity (GGO), etc. In addition, the distribution of bilateral, peripheral, and lower regions is mainly observed.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Chest X-ray (CXR) Imaging



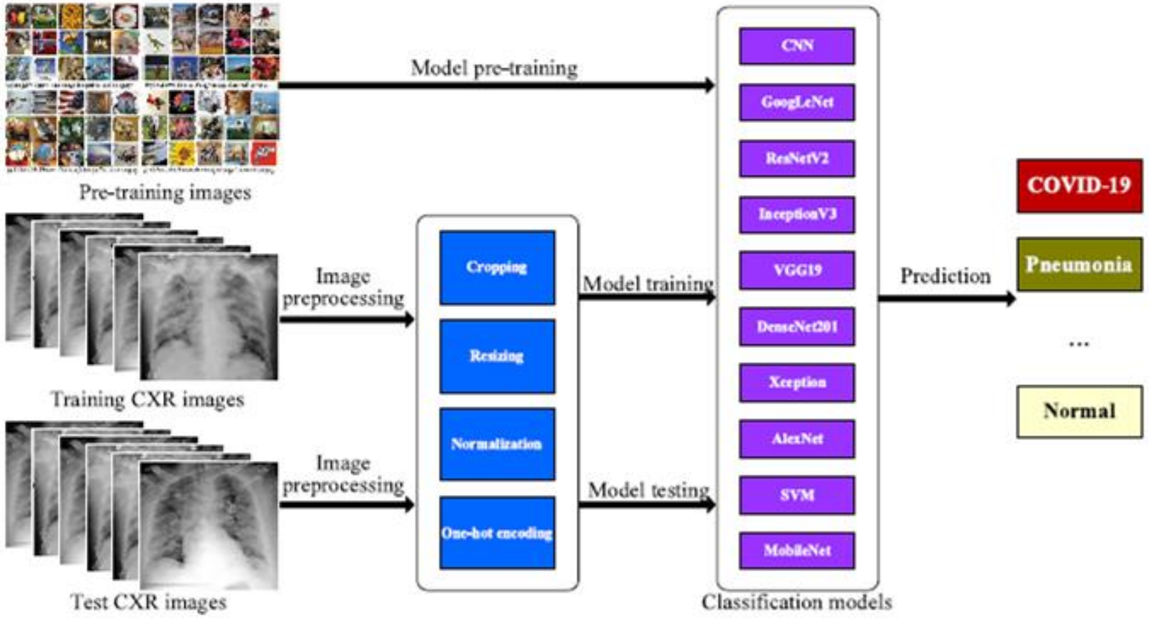
Examples of chest X-ray images of normal and COVID-19 cases.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Chest X-ray (CXR) Imaging

- The AI-based CXR image inspection for COVID-19 usually includes the following steps:
    - Data preprocessing,
    - DL model training, and
    - COVID-19 classification



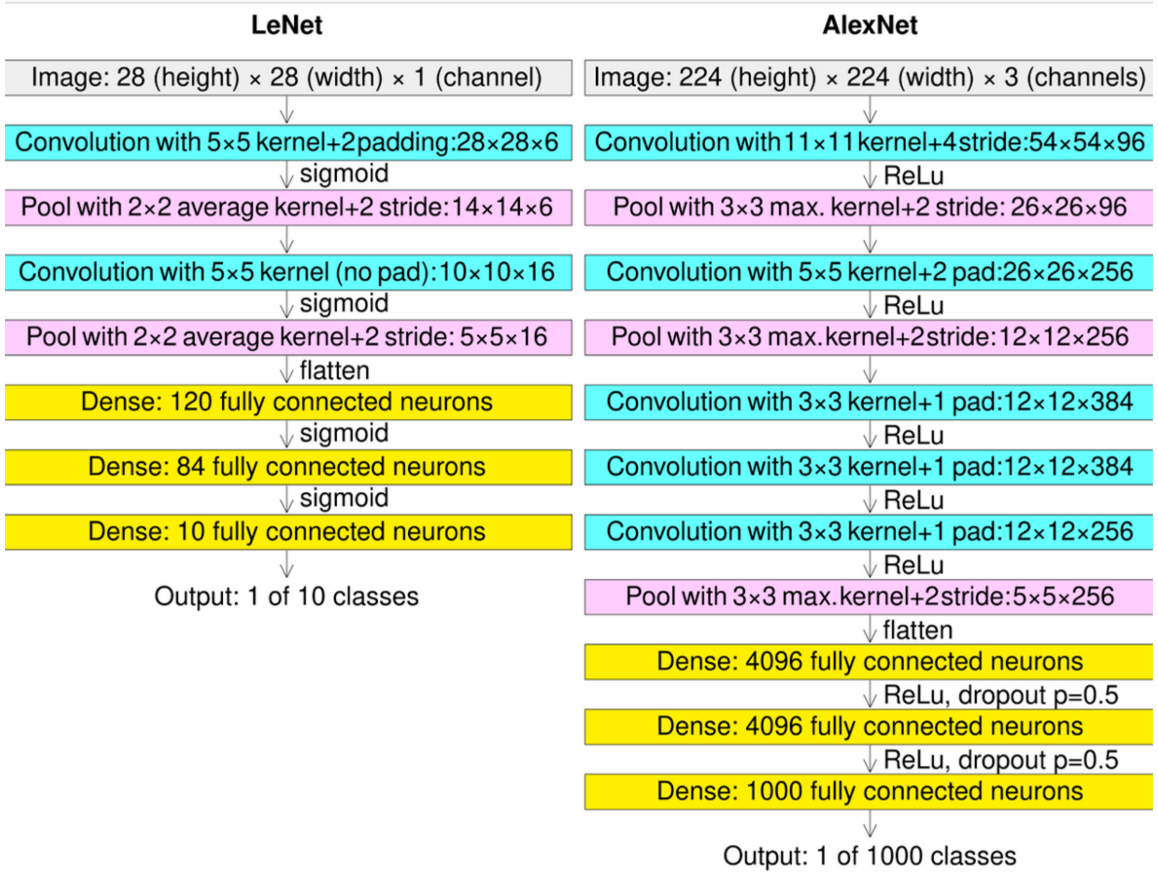
Representative AI architecture for CXR image classification and Covid-19 inspection

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

LeNet vs. AlexNet vs. VGG vs. Inception

- LeNet
    - 32x32 grayscale input image
    - 5-layer convolutional feature extractor
        - conv-pool-conv-pool-conv
    - 2-layer 10-way neural network classifier
- AlexNet
    - 11x11, 5x5, 3x3 convolutions, max pooling, dropout, ReLU activations, SGD with momentum
    - First deep convolutional neural net for ImageNet
        - Significantly reduced top 5 error from 26% to 15%
    - 60 million parameters
    - Trains on 2 GPUs for 6 days



LeNet

Image: 28 (height) × 28 (width) × 1 (channel)
Convolution with 5×5 kernel+2padding:28×28×6
sigmoid
Pool with 2×2 average kernel+2 stride:14×14×6
Convolution with 5×5 kernel (no pad):10×10×16
sigmoid
Pool with 2×2 average kernel+2 stride: 5×5×16
flatten
Dense: 120 fully connected neurons
sigmoid
Dense: 84 fully connected neurons
sigmoid
Dense: 10 fully connected neurons
Output: 1 of 10 classes

AlexNet

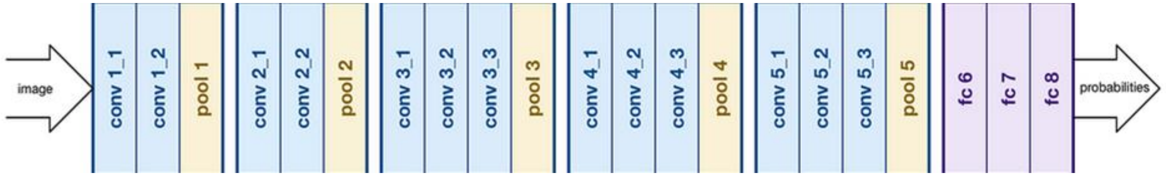
Image: 224 (height) × 224 (width) × 3 (channels)
Convolution with 11×11 kernel+4stride:54×54×96
ReLu
Pool with 3×3 max. kernel+2 stride: 26×26×96
Convolution with 5×5 kernel+2 pad:26×26×256
ReLu
Pool with 3×3 max.kernel+2stride:12×12×256
Convolution with 3×3 kernel+1 pad:12×12×384
ReLu
Convolution with 3×3 kernel+1 pad:12×12×384
ReLu
Convolution with 3×3 kernel+1 pad:12×12×256
ReLu
Pool with 3×3 max.kernel+2stride:5×5×256
flatten
Dense: 4096 fully connected neurons
ReLu, dropout p=0.5
Dense: 4096 fully connected neurons
ReLu, dropout p=0.5
Dense: 1000 fully connected neurons
Output: 1 of 1000 classes

References

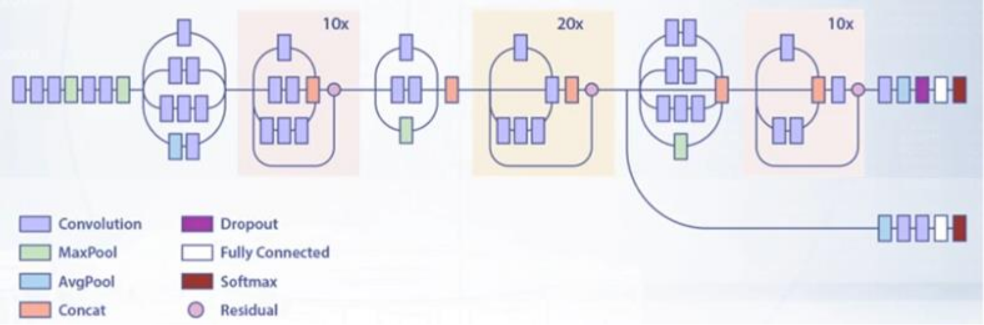
- LeCun, Y., Bottou, L., Bengio, Y., & Haffner, P. (1998). Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, *86*(11), 2278-2324.
- Krizhevsky, A., Sutskever, I., & Hinton, G. E. (2012). Imagenet classification with deep convolutional neural networks. *Advances in neural information processing systems*, *25*.

LeNet vs. AlexNet vs. VGG vs. Inception

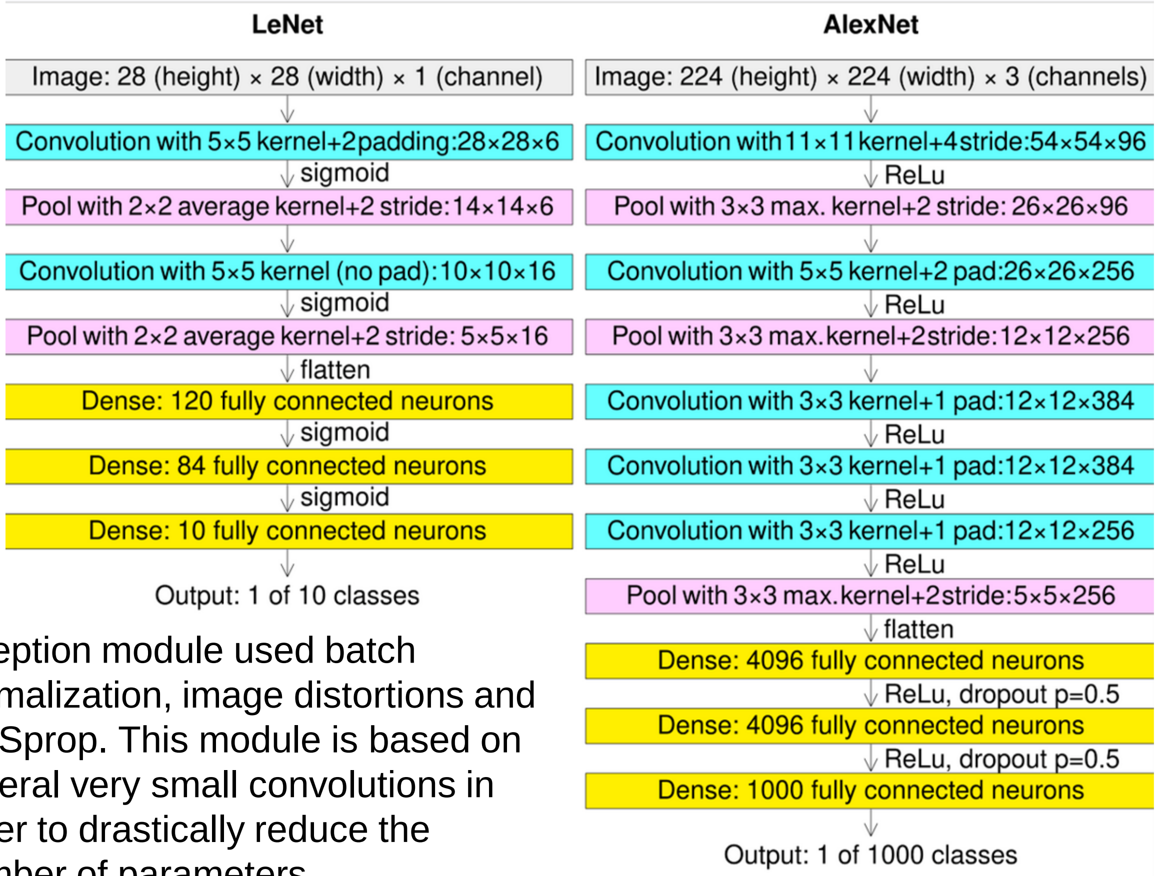
- VGG
  - Early variants in 16 or 19 convolution layers
  - Similar to AlexNet, only 3x3 convolutions
  - 138 million parameters
  - Trained on 4 GPUs for 2-3 weeks



- GoogleLeNet/Inception
  - Novel architecture with inception module* | 25M parameters | trains on 8 GPUs for 2 weeks



- Inception module used batch normalization, image distortions and RMSprop. This module is based on several very small convolutions in order to drastically reduce the number of parameters.
- Facilitates deep CNN - 22 layers with reduced parameters.



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sigmoid
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flatten
Dense: 120 fully connected neurons
sigmoid
Dense: 84 fully connected neurons
sigmoid
Dense: 10 fully connected neurons
Output: 1 of 10 classes

AlexNet

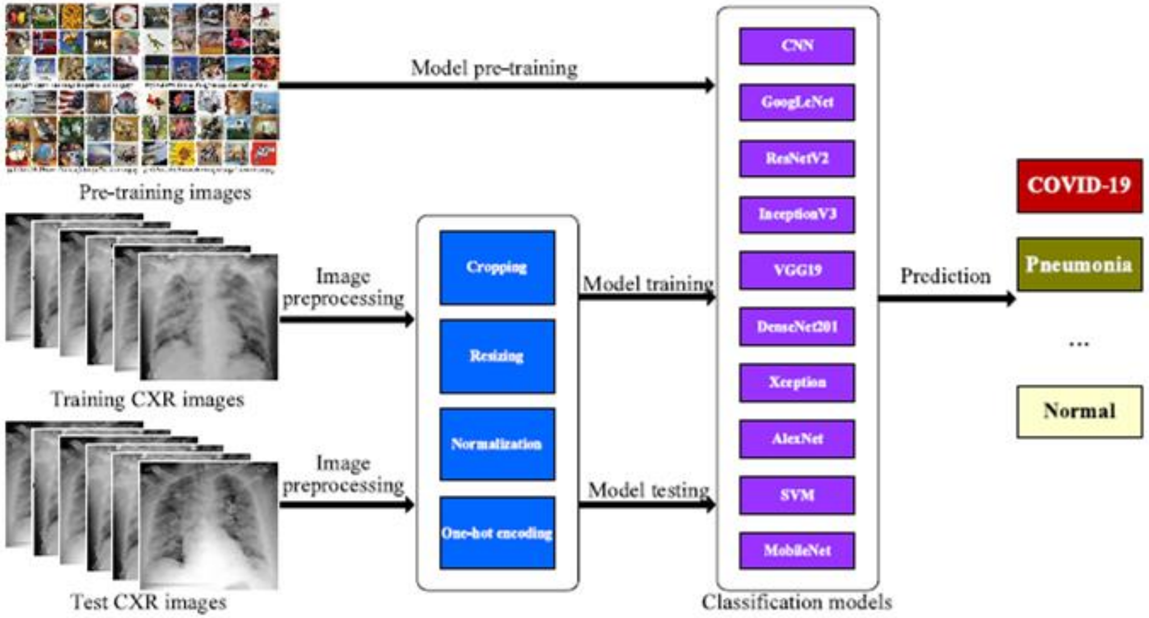
Image: 224 (height) × 224 (width) × 3 (channels)
Convolution with 11×11 kernel+4 stride:54×54×96
ReLu
Pool with 3×3 max. kernel+2 stride: 26×26×96
Convolution with 5×5 kernel+2 pad:26×26×256
ReLu
Pool with 3×3 max.kernel+2stride:12×12×256
Convolution with 3×3 kernel+1 pad:12×12×384
ReLu
Convolution with 3×3 kernel+1 pad:12×12×384
ReLu
Convolution with 3×3 kernel+1 pad:12×12×256
ReLu
Pool with 3×3 max.kernel+2stride:5×5×256
flatten
Dense: 4096 fully connected neurons
ReLu, dropout p=0.5
Dense: 4096 fully connected neurons
ReLu, dropout p=0.5
Dense: 1000 fully connected neurons
Output: 1 of 1000 classes

References

- Simonyan, K., & Zisserman, A. (2014). Very deep convolutional networks for large-scale image recognition. *arXiv preprint arXiv:1409.1556*.
- Szegedy, C., Liu, W., Jia, Y., Sermanet, P., Reed, S., Anguelov, D., ... & Rabinovich, A. (2015). Going deeper with convolutions. In *Proceedings of the IEEE conference on computer vision and pattern recognition* (pp. 1-9).

Chest X-ray (CXR) Imaging

- The AI-based CXR image inspection for COVID-19 usually includes the following steps:
    - Data preprocessing,
    - DL model training, and
    - COVID-19 classification



Representative AI architecture for CXR image classification and Covid-19 inspection

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

CXR Imaging - Covid-19 Classification Approaches

- **Nesting/Combining ML or DL models:**
    - Hemdan et al. (2020) proposed COVIDX-Net to help radiologists automatically diagnose COVID-19 based on CXR images. COVIDX-Net integrates 7 DCNN models, such as VGG19, DenseNet201, ResNetV2, InceptionV3, InceptionResNetV2, Xception, and MobileNetV2. Each model is separately trained on CXR images to classify the patient's status as COVID-19 positive or negative.
    - Sethy et al. (2020) used eleven DCNN models as CXR image feature extractors, including AlexNet, GoogLeNet, DenseNet, Inception, ResNet, VGG, XceptionNet, and InceptionResNet. Then, an SVM classifier classified the extracted image features to detect COVID-19.
    - Castiglioni et al. (2020) collected CXR data (610 images, including 324 COVID-19 cases) from Lombardy, Italy, and constructed a DCNN model to predict COVID-19. The DCNN model had 10 CNN models, with each of them using the ResNet-50 structure pre-trained on the ImageNet data set.
    - Ioannis et al. (2020) evaluated the performance of 5 DCNN models for medical image classification, including VGG19, MobileNetV2, Inception, Xception, and InceptionResNetV2. To address the shortcomings of the small-scale COVID-19 data set, each model is pre-trained on the ImageNet data set using the TL strategy.

Reference

- Hemdan, E. E. D., Shouman, M. A., & Karar, M. E. (2020). Covidx-net: A framework of deep learning classifiers to diagnose covid-19 in x-ray images. *arXiv preprint arXiv:2003.11055*.
- Sethy, P. K., & Behera, S. K. (2020). Detection of coronavirus disease (covid-19) based on deep features.
- Castiglioni, I., Ippolito, D., Interlenghi, M., Monti, C. B., Salvatore, C., Schiaffino, S., ... & Sardanelli, F. (2020). Artificial intelligence applied on chest X-ray can aid in the diagnosis of COVID-19 infection: a first experience from Lombardy, Italy. *MedRxiv*, 2020-04.
- Apostolopoulos, I. D., & Mpesiana, T. A. (2020). Covid-19: automatic detection from x-ray images utilizing transfer learning with convolutional neural networks. *Physical and engineering sciences in medicine*, *43*, 635-640.

CXR Imaging - Covid-19 Classification Approaches

- **Task-specific tailored networks:**
  - Zhang et al. (2020) proposed a new DL model, which consists of a backbone network, a classification module, and an anomaly detection module. The backbone network extracts the features of each input CXR image. The classification and anomaly detection modules respectively use the extracted features to generate classification scores and scalar anomaly scores.
  - Wang et al. (2020) introduced a COVID-Net DCNN model to identify COVID-19 cases based on CXR images. The COVID-Net model uses a large number of convolutional layers in a projection-expansion-projection design pattern. They collected 13,800 CXR images from 13,725 patients (including 183 COVID-19 patients) to establish a CXR database (called COVIDx) for training COVID-Net.

Reference

- Zhang, J., Xie, Y., Li, Y., Shen, C., & Xia, Y. (2020). Covid-19 screening on chest x-ray images using deep learning based anomaly detection. *arXiv preprint arXiv:2003.12338*, *27*(10.48550).
- Wang, L., Lin, Z. Q., & Wong, A. (2020). Covid-net: A tailored deep convolutional neural network design for detection of covid-19 cases from chest x-ray images. *Scientific reports*, *10*(1), 19549.

Disease Detection and Diagnosis

- Lung CT Image Inspection
- Chest X-ray Image Inspection

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Challenges: Lack of large-scale medical image datasets

- **Transfer learning:**
  - Maghdid et al. (2021) respectively used CNN and AlexNet models to train CXR and CT images and diagnose COVID-19 cases. Among them, the AlexNet model is pre-trained on the ImageNet data set to perform COVID-19 classification on the data sets in related work.
- **Tailored network models:**
  - **Innovative COVID-CAPS Model**: Developed by Afshar et al. (2020), this capsule network model (Hinton et al., 2018) is optimized for smaller chest X-ray datasets. It uniquely uses capsule-based layers to accurately identify and relate objects in images through spatial information, without relying on large-scale data sets.

Reference

- Maghdid, H. S., Asaad, A. T., Ghafoor, K. Z., Sadiq, A. S., Mirjalili, S., & Khan, M. K. (2021, April). Diagnosing COVID-19 pneumonia from X-ray and CT images using deep learning and transfer learning algorithms. In *Multimodal image exploitation and learning 2021* (Vol. 11734, pp. 99-110). SPIE.
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- Hinton, G. E., Sabour, S., & Frosst, N. (2018, February). Matrix capsules with EM routing. In *International conference on learning representations*.

Disease Detection and Diagnosis

- Image Inspection
    - Lung CT
    - Chest X-ray
- Other Detection Methods: Cough Sound Inspection

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Disease Detection and Diagnosis

- Image Inspection
    - Lung CT
    - Chest X-ray
- Other Detection Methods: Cough Sound Inspection

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Covid-19 Detection based on the Auditory/Sound Modality

- **Cough Sound Analysis:**
    - Schuller et al. (2021) discussed the potential application of computer audition (CA) and AI in analyzing the cough sounds of patients with COVID-19. They first analyzed the ability of CA to automatically recognize and monitor speech and cough under different semantics (such as breathing, dry and wet coughing or sneezing, speech during colds, eating behaviors, drowsiness, or pain). Then, they applied the CA technology to the diagnosis and treatment of patients with COVID-19. However, due to the lack of available data sets and annotation information, there are few studies on this technology in diagnosing COVID-19.
        - Orlandic et al. (2021) provided a COUGHVID cough dataset for COVID-19 diagnosis, which contains 20,000 crowdsourced cough records [146]. The cough records are labeled by experienced pulmonologists, and medical abnormalities are accurately diagnosed, thus providing a high-quality training dataset for MI/AI methods.
    - Wang et al. (2020) analyzed the respiratory patterns of patients with COVID-19 and other breathing patterns of patients with influenza and common cold. In addition, they proposed a respiratory simulation model (called BI-AT-GRU) for COVID-19 diagnosis. The BI-AT-GRU model includes a GRU neural network with a bidirectional and attention mechanism, and can classify 6 types of clinical respiratory patterns, such as Eupnea, Tachypnea, Bradypnea, Biots, Cheyne-Stokes, and Central-Apnea.

References

- Schuller, B. W., Schuller, D. M., Qian, K., Liu, J., Zheng, H., & Li, X. (2021). Covid-19 and computer audition: An overview on what speech & sound analysis could contribute in the sars-cov-2 corona crisis. *Frontiers in digital health*, *3*, 564906.
- Orlandic, L., Teijeiro, T., & Atienza, D. (2021). The COUGHVID crowdsourcing dataset, a corpus for the study of large-scale cough analysis algorithms. *Scientific Data*, *8*(1), 156.
- Wang, Y., Hu, M., Li, Q., Zhang, X. P., Zhai, G., & Yao, N. (2020). Abnormal respiratory patterns classifier may contribute to large-scale screening of people infected with COVID-19 in an accurate and unobtrusive manner. *arXiv preprint arXiv:2002.05534*.

AI Application Areas for Virology

1. **Disease Detection and Diagnosis:** AI analyzes medical imaging and genetic data to quickly identify and classify viral infections.
2. **Virology and Pathogenesis:** AI explores viral behaviors and mechanisms by analyzing genetic sequences and protein structures to understand how viruses originate, mutate, and cause disease.
3. **Drug and Vaccine Development**
4. **Epidemic and Transmission Prediction**

Virology and Pathogenesis

- The virology and pathogenesis of SARS-CoV-2 was another important scientific research area.
    - Virological studies included determining the origin and classification of SARS-CoV-2, physical and chemical properties, receptor interactions, cell entry, and the ecology and genomic variation of SARS-CoV-2.
    - Each of these phenomenon are determined by two kinds of biological molecules:
        - genes
        - proteins

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Virology and Pathogenesis

- The two main perspectives adopted for the virological/pathological research of SARS-CoV-2.
  - Proteomics - This involves studying all the proteins made by the virus, which helps understand what the virus does inside the body and how it causes illness.
  - Genomics - This is about examining the complete genetic material (DNA or RNA) of the virus. By looking at its genes, scientists can learn how the virus spreads, changes, and possibly find ways to stop it.

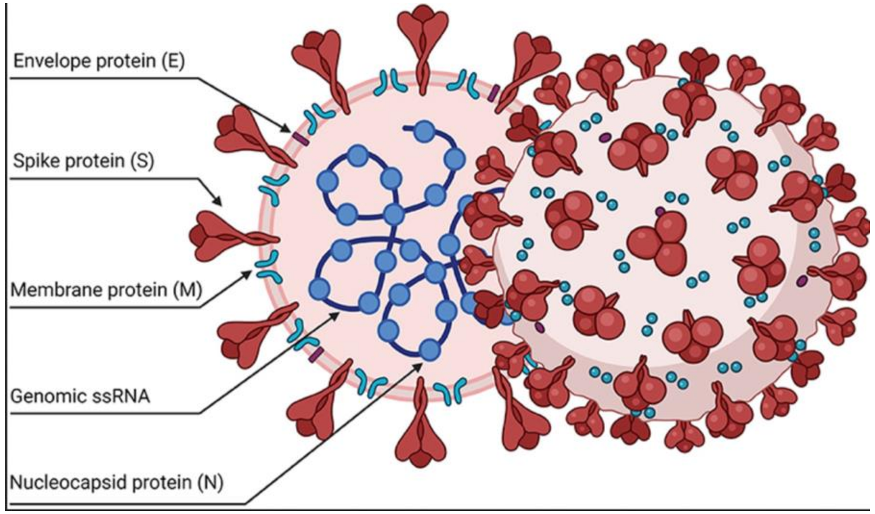
- In essence, the genes provide the instructions, and the proteins carry out the tasks.
  - Viruses are complex entities that consist of genetic material wrapped in a protein coat.
    - **Genetic Material**: This is the core of the virus, which can be either DNA or RNA. The genetic material contains the instructions for making more viruses, including the blueprints for viral proteins. It is the essential component that a virus injects into a host cell to hijack the cell's machinery and reproduce.
    - **Protein Coat (Capsid)**: This surrounds the genetic material. It protects the viral genes and helps deliver them into host cells. The protein coat is made up of smaller protein units called capsomeres, and it often determines the shape of the virus.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Virology and Pathogenesis

- In essence, the genes provide the instructions, and the proteins carry out the tasks.
  - Viruses are complex entities that consist of genetic material wrapped in a protein coat.
    - **Genetic Material**: This is the core of the virus, which can be either DNA or RNA. The genetic material contains the instructions for making more viruses, including the blueprints for viral proteins.
      - In case of SARS-COV-2, it is the genomic RNA
    - **Protein Coat (Capsid)**: This surrounds the genetic material. It protects the viral genes and helps deliver them into host cells. The protein coat is made up of smaller protein units called capsomeres, and it often determines the shape of the virus.
      - For SARS-COV-2, four types of structural proteins were confirmed, including nucleocapsid (N) proteins, envelope (E) proteins, membrane (M) proteins, and spike (S) proteins



Virology and Pathogenesis: **Proteomics**

Proteomic studies contribute to virology in the following ways:

- **Viral Protein Identification**: Identify all proteins produced by a virus, including structural and non-structural types.
- **Host-Virus Interactions**: Reveal interactions between viral proteins and host cell proteins, influencing infection outcomes.
- **Mechanisms of Pathogenesis**: Elucidate how viruses cause disease by studying protein expression and modifications.
- **Drug Targets and Antiviral Research**: Identify potential targets for antiviral drugs by focusing on critical viral or host proteins.
- **Vaccine Development**: Assist in vaccine creation by identifying immune system-recognizable viral surface proteins.
- **Monitoring Drug Resistance and Viral Evolution**: Detect protein changes that indicate drug resistance or provide insights into viral evolution.
- **Response to Treatment**: Monitor treatment efficacy by observing changes in the proteome of the host or virus.

Virology and Pathogenesis: **Proteomics**

- In this field, AI techniques are used to predict protein structures and analyze the interaction network between proteins and drugs.

References

- Ortega, J. T., Serrano, M. L., Pujol, F. H., & Rangel, H. R. (2020). Role of changes in SARS-CoV-2 spike protein in the interaction with the human ACE2 receptor: An in silico analysis. *EXCLI journal*, *19*, 410.
- Walls, A. C., Xiong, X., Park, Y. J., Tortorici, M. A., Snijder, J., Quispe, J., ... & Veesler, D. (2019). Unexpected receptor functional mimicry elucidates activation of coronavirus fusion. *Cell*, *176*(5), 1026-1039.
- Zhavoronkov, A., Aladinskiy, V., Zhebrak, A., Zagribelnyy, B., Terentiev, V., Bezrukov, D. S., ... & Ivanenkov, Y. (2020). Potential COVID-2019 3C-like protease inhibitors designed using generative deep learning approaches. ChemRxiv. *Preprint posted online on February*, *11*.

Virology and Pathogenesis: **Proteomics**

- Protein-folding problem
    - A protein is like a string of beads made of a sequence of different chemicals known as amino acids. These sequences are assembled according to the genetic instructions of an organism's DNA. Attraction and repulsion between the 20 different types of amino acids cause the string to fold in a feat of “spontaneous origami.” This forms the intricate curls, loops, and pleats of a protein’s 3D structure.
    - Predicting the protein-folding structure with AI was considered a “grand scientific challenge” known as the “protein-folding problem.”
        - CASP (Critical Assessment of Structure Prediction) was organized as a biannual contest by the Protein Structure Prediction Center to find the state of the art in modeling protein structure from amino acid sequence. Participants submitted models that attempted to predict a set of proteins for which the experimental structures were not yet public.
        - The breakthrough AlphaFold solution from the DeepMind team at Google research was determined at CASP.
            - At CASP14 in 2020, they presented AlphaFold 2– which demonstrated a level of accuracy so high that the community considered the protein–folding problem solved. This was even highly accurate when applied to predicting the protein folding structure of the SARS-COV-2 virus. (https://deepmind.google/technologies/alphafold/)

References

- Kryshtafovych, A., Schwede, T., Topf, M., Fidelis, K., & Moult, J. (2019). Critical assessment of methods of protein structure prediction (CASP)—Round XIII. *Proteins: Structure, Function, and Bioinformatics*, *87*(12), 1011-1020.
- Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., ... & Hassabis, D. (2021). Highly accurate protein structure prediction with AlphaFold. *nature*, *596*(7873), 583-589.

Virology and Pathogenesis: **Proteomics**

- Why is predicting protein-folding structure important in virology research?
    - **Improved Viral Mechanisms Understanding**: Predictive models clarify the structure and function of viral proteins, enhancing our understanding of viral lifecycle and mechanisms.
    - **Enhanced Drug Design**: Structure prediction enables precise targeting of viral proteins, facilitating the development of effective antiviral drugs.
    - **Vaccine Development**: Accurate protein structures help identify key immunogenic components, improving vaccine design and efficacy.
    - **Rapid Outbreak Response**: Quick structure prediction of novel viral proteins speeds up therapeutic and vaccine development during outbreaks.
    - **Understanding Antiviral Resistance**: Predictive modeling assesses how viral mutations may impact protein function and drug resistance, guiding the evolution of treatment strategies.

Virology and Pathogenesis: **Proteomics**

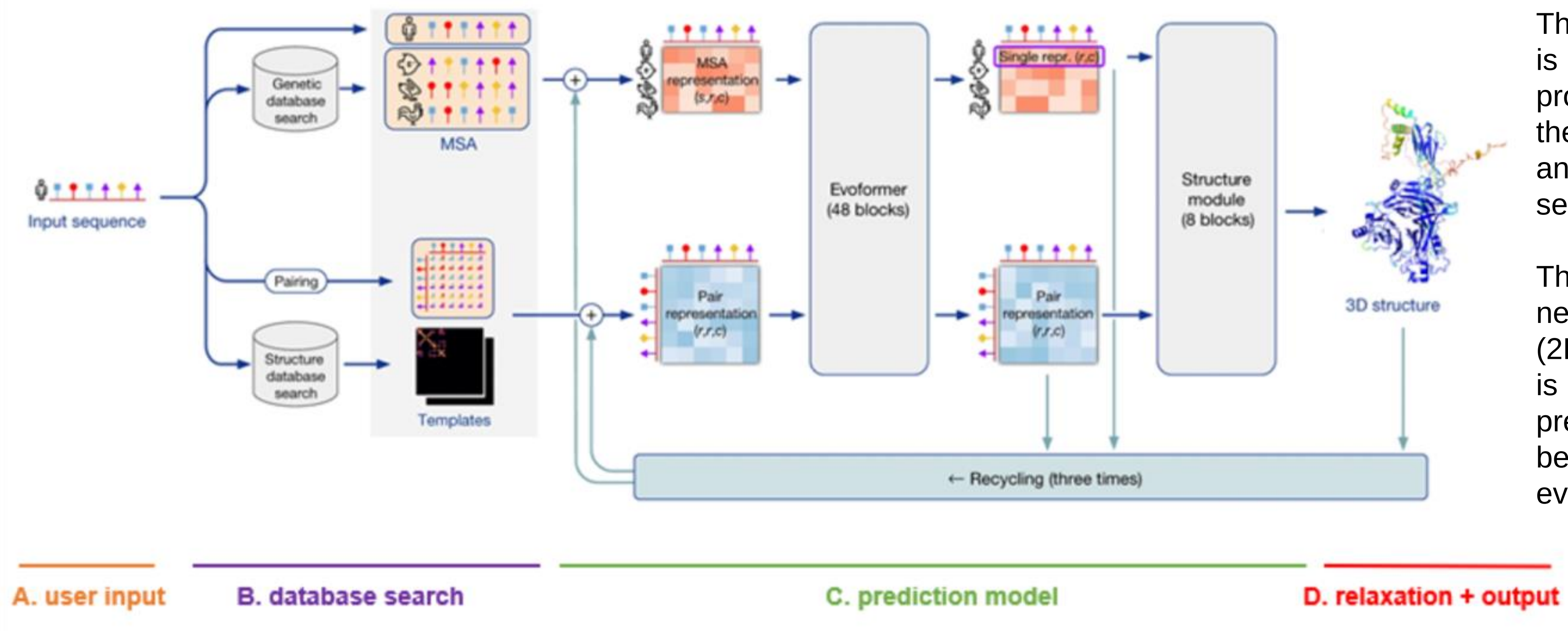
- Protein-folding problem: The AlphaFold Solution.
  - AlphaFold comprises the following modules:
    - **Core Architecture**: AlphaFold primarily uses transformer architectures, notably incorporating an attention mechanism that allows focusing on interactions crucial for protein folding.
      - Attention mechanisms have facilitated the breakthrough of large language models in the sphere of natural language technologies.
    - **Evoformer**: The innovative Evoformer module integrates evolutionary data and pairwise amino acid interactions, utilizing scaled dot-product attention to model protein sequence relationships.
    - **Integration of CNN Elements**: Incorporates elements inspired by convolutional neural networks, such as residual connections, which improve training stability and allow for deeper network architectures.
    - **Spatial Graph Convolutional Network**: Employs spatial graph convolutional networks to predict the distances and angles between amino acids, essential for constructing accurate 3D protein structures.
    - **Structure Module**: Converts relational and sequence data into precise 3D coordinates, refining the structure to ensure it’s chemically and physically plausible.
  - Thus, AlphaFold is a blend of technologies, combining transformers, graph neural networks, and CNN-inspired techniques to solve protein-folding prediction.

References

- Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A. N., ... & Polosukhin, I. (2017). Attention is all you need. *Advances in neural information processing systems*, *30*.
- Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., ... & Hassabis, D. (2021). Highly accurate protein structure prediction with AlphaFold. *nature*, *596*(7873), 583-589.

Virology and Pathogenesis: **Proteomics**

- **Protein Structure Prediction with AlphaFold**



The AlphaFold system consists of a feature extraction module and a distance prediction neural network.

The feature extraction module is responsible for searching for protein sequences similar to the input protein sequences and constructing multiple sequence alignments (MSA).

The distance prediction neural network is a two-dimensional (2D) ResNet structure, which is responsible for accurately predicting the distance between all residue pairs in every two protein sequences.

References

- Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., ... & Hassabis, D. (2021). Highly accurate protein structure prediction with AlphaFold. *nature*, *596*(7873), 583-589.

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Virology and Pathogenesis: **Genomics**

- Genomics was mainly used during Covid 19 to analyze the origin of SARS-CoV-2 and to inform vaccine development. AI algorithms were applied to compare the similarity of gene sequences, gene fragments, and miRNA predictions.

References

- Demirci, M. D. S., & Adan, A. (2020). Computational analysis of microRNA-mediated interactions in SARS-CoV-2 infection. *PeerJ*, *8*, e9369.
- Randhawa, G. S., Soltysiak, M. P., El Roz, H., de Souza, C. P., Hill, K. A., & Kari, L. (2020). Machine learning using intrinsic genomic signatures for rapid classification of novel pathogens: COVID-19 case study. *Plos one*, *15*(4), e0232391.

Virology and Pathogenesis: **Genomics**

- A research group used various machine learning (ML) techniques to study the genetic code of the COVID-19 virus. They aimed to figure out specific features of the virus's genetic material that would help them quickly categorize new viruses that are similar.
  - **Collecting Data:** They gathered the complete genetic blueprint of the COVID-19 virus from the NCBI database, related bat virus information from GISAID, and other virus sequences from the Virus-Host DB database.
  - **Analyzing the Genetic Code:** They used a method called chaotic game representation to convert the virus's genetic information into a format (a sequence of digital signals) that can be easily analyzed by computers.
  - **Further Analysis with Fourier Transform:** They transformed these digital sequences into a type of data called an amplitude spectrum using a mathematical technique known as the discrete Fourier transform. This helps to highlight different patterns in the data.
  - **Using Machine Learning:** They trained six different ML models (such as linear discriminant, linear SVM, quadratic SVM, fine KNN, subspace discriminant, and subspace KNN) to this data to see how well each model can classify and distinguish between different virus types based on the patterns they found.
  - **Testing the Models:** They then tested these models on 29 different COVID-19 virus sequences to see how accurately they can identify the COVID-19 virus.
  - **Results and Conclusion:** The results from their analysis supported the idea that the COVID-19 virus likely originated from bats and fits into a group of viruses known as beta-coronaviruses.

References

- Randhawa, G. S., Soltysiak, M. P., El Roz, H., de Souza, C. P., Hill, K. A., & Kari, L. (2020). Machine learning using intrinsic genomic signatures for rapid classification of novel pathogens: COVID-19 case study. *Plos one*, *15*(4), e0232391.

Virology and Pathogenesis: **Genomics**

- Another research group combined the latest in genetic science and AI to make better tests (e.g., improving RT-PCR) for detecting viruses, including COVID-19.
  - **Developing a CRISPR Tool**:
    - What is CRISPR? CRISPR-Cas is a revolutionary gene-editing technology that uses a specific enzyme (like Cas9) guided by RNA to precisely cut and modify DNA at targeted locations within an organism's genome. Two scientists were awarded the Chemistry Nobel Prize in 2020 for research on this technology.
      - CRISPR is like molecular scissors that can be programmed to target and cut specific sections of DNA
    - In this work, researchers adapted this tool not just to edit genes but to help in identifying viruses.
  - **Machine Learning**: They used different machine learning methods to understand and predict the variations in the genetic material of viruses. This helps in ensuring that the test remains effective even as the virus mutates or changes.
  - **Designing the Test**: Using the CRISPR technology, they designed an improved RT-PCR test. This new test can detect not just COVID-19 but 67 different respiratory viruses.

References

- Jinek, M., Chylinski, K., Fonfara, I., Hauer, M., Doudna, J. A., & Charpentier, E. (2012). A programmable dual-RNA–guided DNA endonuclease in adaptive bacterial immunity. *science*, *337*(6096), 816-821.
- Metsky, H. C., Freije, C. A., Kosoko-Thoroddsen, T. S. F., Sabeti, P. C., & Myhrvold, C. (2020). CRISPR-based surveillance for COVID-19 using genomically-comprehensive machine learning design. *BioRxiv*, 2020-02.

AI Application Areas for Virology

1. **Disease Detection and Diagnosis:** AI analyzes medical imaging and genetic data to quickly identify and classify viral infections.
2. **Virology and Pathogenesis:** AI explores viral behaviors and mechanisms by analyzing genetic sequences and protein structures to understand how viruses originate, mutate, and cause disease.
3. **Drug and Vaccine Development:** AI speeds up the design and testing of new drugs and vaccines by simulating molecular interactions and predicting immune responses.
4. **Epidemic and Transmission Prediction**

Drug and Vaccine Development

- Insights from proteomics and genomics research were critical in identifying targets for potential drugs and vaccines for SARS-CoV-2 and COVID-19.
    - Drug and vaccine proposals were made to interrupt virus replication and immune evasion.
- Role of Artificial Intelligence:
    - AI played a pivotal role in accelerating the development of drugs and vaccines.
    - Enabled rapid screening of vast chemical and biological data sets to identify viable candidates.
- Contribution to Smart Medicine:
    - AI applications in smart medicine significantly contributed to combating COVID-19.
    - Improved the speed and efficiency of research and development processes.
- Two areas:
    - Drug Development
    - Vaccine Development

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Drug and Vaccine Development

Drug and vaccine development are generally categorized into two main types:

1. **Small-Molecule Drug Discovery**: *This involves creating drugs that are made up of small, chemically manufactured molecules.* These are the typical kind of medicines you might find in pill form at the pharmacy, like aspirin or ibuprofen. They're usually designed to be easy to administer and can travel easily through the body to their target sites.
2. **Biological Product Development**: *This category includes drugs that are made from larger, more complex biological substances like proteins or antibodies, rather than simple chemicals.* These types of drugs often treat conditions that small molecules can't, and they might be used in treatments like vaccines, gene therapies, or treatments for diseases like cancer. Biological products are usually administered through injections or infusions because they are not as stable as small molecules when taken orally.

In simple terms, drug development can either focus on creating small chemical drugs that you swallow as pills or developing larger, biological treatments that are usually given through injections.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Drug Development: Small-molecule drug discovery

- A research work devised the MT-DTI (Molecule Transformer-Drug Target Interaction) model to predict binding interactions between existing drugs and proteins to identify potential drug candidates for COVID 19. In other words, to predict which existing drugs might effectively fight against COVID-19 by targeting a specific virus protein. This speeds up the process of finding treatments by narrowing down the list of potential drugs to those most likely to be effective.
    - **How it worked?** The MT-DTI model takes the detailed chemical structure of drugs (represented as SMILES strings) and the amino acid sequence information of proteins to predict the binding interactions between them, focusing on how the drug fits into the 3D structure of the protein. This helps researchers understand potential effectiveness and selectivity of drugs in targeting specific proteins.
    - **Data collection.** The team gathered data on the specific protein called 3C-like proteases, which the virus uses to reproduce, and related antiviral drugs and drug targets from databases like NCBI, Drug Target Common (DTC), and BindingDB.
    - **Results.** Their experiments suggested six drugs that might work against COVID-19, including well-known ones like Remdesivir and Ritonavir. Remdesivir, in particular, looked promising based on its performance in clinical trials, showing potential effectiveness in treating the virus.

Reference

- Beck, B. R., Shin, B., Choi, Y., Park, S., & Kang, K. (2020). Predicting commercially available antiviral drugs that may act on the novel coronavirus (SARS-CoV-2) through a drug-target interaction deep learning model. *Computational and structural biotechnology journal*, *18*, 784-790.

Drug Development: Small-molecule drug discovery

- Another line of research also contributed to the development of potential drug candidates targeting the SARS-CoV-2 3CLpro enzyme, critical for viral replication.
  - **Methodology**:
    - **AI Model**: Utilized a deep learning model combining reinforcement learning (RL) with recurrent neural networks (RNN) to analyze and classify protease inhibitors.
    - **Data Source**: Selected 2,515 protease inhibitor molecules from the ChEMBL database, represented in SMILES format.
  - **Outcome**:
    - **Selection and Ranking**: Ranked molecules based on their effectiveness in virtual screening, identifying top candidates for anti-SARS-CoV-2 activity.

Reference

- Bung, N., Krishnan, S. R., Bulusu, G., & Roy, A. (2020). De novo design of new chemical entities (NCEs) for SARS-CoV-2 using artificial intelligence.

Drug Development: Small-molecule drug discovery

- Another line of research leveraged the advanced deep Q learning network (called ADQN-FBDD) to generate potential compounds/molecules as anti-SARS-CoV-2 drugs.

Reference

- Tang, B., He, F., Liu, D., He, F., Wu, T., Fang, M., ... & Xu, D. (2022). AI-aided design of novel targeted covalent inhibitors against SARS-CoV-2. *Biomolecules*, *12*(6), 746.

Drug Development: Identification of protein targets

Hu et al. developed AI model to help find drugs that might work against various protein targets of the SARS-COV-2 virus.

- **Choosing Targets**: They started by selecting 8 proteins from the COVID-19 virus that the drugs could potentially target. These proteins are parts of the virus that are essential for it to survive and multiply.
- **Building the AI Model**: They used a specific type of deep learning (DL) model known as AtomNet. This model has special layers:
  - **Shared Layer**: This part learns common features that are useful across all the tasks the model performs.
  - **Task Processing Layer**: This part handles specific tasks, like predicting how well a drug might bind to each of the virus proteins.
- **Training the Model**: They improved the model by training it with data specific to coronaviruses. This training helps the model learn better how potential drugs might interact with the virus proteins.
- **Predicting Drug Binding**: After training, the model can predict which drugs are likely to bind effectively to the virus proteins. It gives each potential drug a score based on how well it's expected to bind.
- **Selecting Drugs**: They used the model to find the top 10 drugs that might be best at targeting three key proteins of the virus: RdRp, 3CLpro, and a papain-like protease, which previous studies identified as important for the virus.

Reference

- Hu, F., Jiang, J., & Yin, P. (2022). Prediction of potential commercially available inhibitors against sars-cov-2 by multi-task deep learning model. *Biomolecules*, *12*(8), 1156.

Drug Development: Identification of protein targets

Another team of researchers used advanced computing and AI techniques to quickly and efficiently find drugs that might be repurposed to treat COVID-19, focusing on those already approved for other infectious diseases.

- **Using Powerful Computers**: They used High-Performance Computing (HPC) to analyze large volumes of data, such as drug properties and their interactions with the virus.
- **Virtual Drug Screening**: To run a bunch of tests to quickly sift through thousands of chemicals to see which ones might effectively fight against COVID-19 as a way to narrow down potential drug candidates from a large pool without doing physical experiments in a lab initially.
- **Molecular Docking**: Used computer simulations to see how well each drug fits into the virus’s proteins, kind of like finding the right key for a lock. A good fit means the drug could potentially stop the virus from functioning properly.
- **Machine Learning Analysis**: They used two types of AI models — neural networks (NN) and Naive Bayes — to further evaluate which drugs are most likely to work against the virus. These models look at data from already known drugs and predict which could be good candidates for treating COVID-19.
- **Selecting Drug Candidates**: Based on their analyses, several drugs, previously approved for other diseases like hepatitis C, were selected as potential treatments for COVID-19. This is because their properties suggested they could also be effective against this virus.

Reference

- Kadioglu, O., Saeed, M., Greten, H. J., & Efferth, T. (2021). Identification of novel compounds against three targets of SARS CoV-2 coronavirus by combined virtual screening and supervised machine learning. *Computers in biology and medicine*, *133*, 104359.

Vaccine Development

Drug and vaccine development are generally categorized into two main types:

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Vaccine Development

- Three Types of COVID-19 Vaccines:
    - **Whole Virus Vaccines**: These vaccines use a form of the virus that has been killed or weakened so it can’t cause disease, but still triggers the immune system to respond and build immunity.
    - **Recombinant Protein Subunit Vaccines**: These include only specific pieces of the virus (often a protein) rather than the whole virus. These pieces are enough to train the immune system to recognize and fight the virus without risking a real infection.
    - **Nucleic Acid Vaccines (RNA and DNA vaccines)**: These vaccines use genetic material (either RNA or DNA) that provides cells in the body with instructions to produce a virus protein themselves. Once produced, this protein prompts an immune response.
- Role of AI in Vaccine Development:
    - AI technology helps in designing and developing these vaccines, but it does so in a less direct way compared to its applications in other fields.
    - Instead of being at the forefront, AI usually works behind the scenes in vaccine development. It might analyze data to predict how effective a vaccine could be or help understand which vaccine designs might be most successful.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Vaccine Development

- AI algorithms help vaccine developers understand exactly which parts of the COVID-19 virus should be targeted to provoke a strong and effective immune response, making the vaccines more effective. In general it includes three modules:
    - **AI Algorithms - netMHC and netMHCpan**: These are specific types of AI software designed to analyze immune system responses. They focus on understanding how our bodies recognize and fight off infections.
    - **Epitope Prediction**: An epitope is a small part of a virus (like COVID-19) that is recognized by the immune system. Predicting epitopes means identifying which parts of the virus are most likely to trigger an immune response. This is crucial for designing vaccines because it helps scientists know which pieces of the virus to include in the vaccine to best stimulate the immune system.
    - **Developing COVID-19 Vaccines**: Using the netMHC and netMHCpan algorithms, researchers can better design vaccines that effectively target the COVID-19 virus by focusing on the right epitopes.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Vaccine Development: Approaches

- Herst and the team used AI to find small parts of the COVID-19 virus protein that could be used to train the human immune system to recognize and fight the virus effectively in a vaccine. They carefully analyzed these parts using multiple AI methods to choose the best options for a potential vaccine.
    - **Obtaining Protein Sequences**: Herst et al. started their research by collecting the protein sequences of the SARS-CoV-2 virus from a database called GenBank.
    - **Trimming Protein Sequences**: They used an algorithm called MSA (Multiple Sequence Alignment) to break down the nucleocapsid phosphoprotein (a specific protein of the virus) into smaller pieces, called peptides. Peptides are short chains of amino acids that are part of the protein.
    - **Predicting Peptide Sequences**: The researchers then used two AI algorithms, netMHC and netMHCpan, to analyze these peptides. These algorithms help predict which peptides might be recognized by the human immune system.
        - **Enhanced Prediction with netMHCpan**: The netMHCpan version of the algorithm is particularly advanced because it incorporates data from 215 different human HLA types. HLAs (Human Leukocyte Antigens) are molecules on the surface of cells that help the immune system recognize which substances are foreign and should be attacked.
    - **Calculating Vaccine Candidates**: To find the best candidates for a COVID-19 vaccine, they averaged the predictions from four different methods: Artificial Neural Networks (ANN), Support Vector Machines (SVM), netMHC, and netMHCpan. This average helped them determine the most promising peptides to use in a vaccine.

Reference

- Herst, C. V., Burkholz, S., Sidney, J., Sette, A., Harris, P. E., Massey, S., ... & Rubsamen, R. (2020). An effective CTL peptide vaccine for Ebola Zaire Based on Survivors’ CD8+ targeting of a particular nucleocapsid protein epitope with potential implications for COVID-19 vaccine design. *Vaccine*, *38*(28), 4464-4475.

Vaccine Development: Approaches

- Ward et al. used a detailed and high-tech approach to identify specific parts of the COVID-19 virus that could be important for developing vaccines or treatments. They made their findings accessible through an online tool to help further research and response efforts against the virus.
  - **Downloading Sequences**: Ward et al. started their study by downloading the genetic sequences of the COVID-19 virus from two big databases, NCBI and GISAID. These databases contain detailed information about the virus's genetic material.
  - **Generating Consensus Sequences**: They created what are called "consensus sequences" for each of the virus's proteins. A consensus sequence is a standard or average sequence that represents the most common form of the genetic sequence across different samples of the virus. This serves as a reference for further analysis.
  - **Epitope Prediction and Mapping**:
    - **i. Epitope Prediction**: The team used various tools to predict B cell epitopes. B cell epitopes are parts of the virus that can trigger an immune response from B cells (a type of white blood cell).
    - **ii. Mapping to Amino Acid Sequences**: They linked these epitopes to specific locations on the amino acid sequences of the virus genes. Amino acids are the building blocks of proteins.

Reference

- Ward, D., Higgins, M., Phelan, J. E., Hibberd, M. L., Campino, S., & Clark, T. G. (2021). An integrated in silico immuno-genetic analytical platform provides insights into COVID-19 serological and vaccine targets. *Genome medicine*, *13*, 1-12.

Vaccine Development

- Ward et al. used a detailed and high-tech approach to identify specific parts of the COVID-19 virus that could be important for developing vaccines or treatments. They made their findings accessible through an online tool to help further research and response efforts against the virus.
    - **Using AI for Further Prediction**: They applied the AI-based netMHCpan algorithm to predict peptides that bind to HLA-1. HLA-1 molecules are proteins on the surfaces of cells that help the immune system recognize which cells are infected and need to be destroyed. They found many variations (2,915 alleles) across all peptide lengths.
    - **Mapping with BLASTp Tool**: They used the BLASTp tool, a bioinformatics software, to link the short amino acid sequences (epitopes) they identified to the standard or known sequences of the COVID-19 virus proteins.
    - **Online Tool Development**: Finally, they created an online tool that researchers and others can use to analyze the genetic variations of the COVID-19 virus, predict epitopes, study similarities with other coronaviruses, and analyze potential proteins for vaccine development.

Reference

- Ward, D., Higgins, M., Phelan, J. E., Hibberd, M. L., Campino, S., & Clark, T. G. (2021). An integrated in silico immuno-genetic analytical platform provides insights into COVID-19 serological and vaccine targets. *Genome medicine*, *13*, 1-12.

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4. **Epidemic and Transmission Prediction:** AI uses historical data and current trends to model and forecast the spread of viral diseases, aiding in proactive public health planning.

Epidemic and Transmission Prediction

- Numerous researchers have participated in the prediction, spread, and tracking of the COVID-19 outbreak based on a wealth of data as follows:
    - The number of suspected, confirmed, cured, and dead COVID-19 cases in each country/region that was announced in real-time
    - In addition, passenger travel trajectories among other data points.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Epidemic and Transmission Prediction

- Patient Mortality and Survival Rate Prediction
- Outbreak and Transmission Prediction
- Social Control

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Epidemic and Transmission Prediction

- **Patient Mortality and Survival Rate Prediction:** Researchers collected clinical COVID-19 case data and used different AI methods to extract important features and to predict the mortality and survival rate of patients with COVID-19.

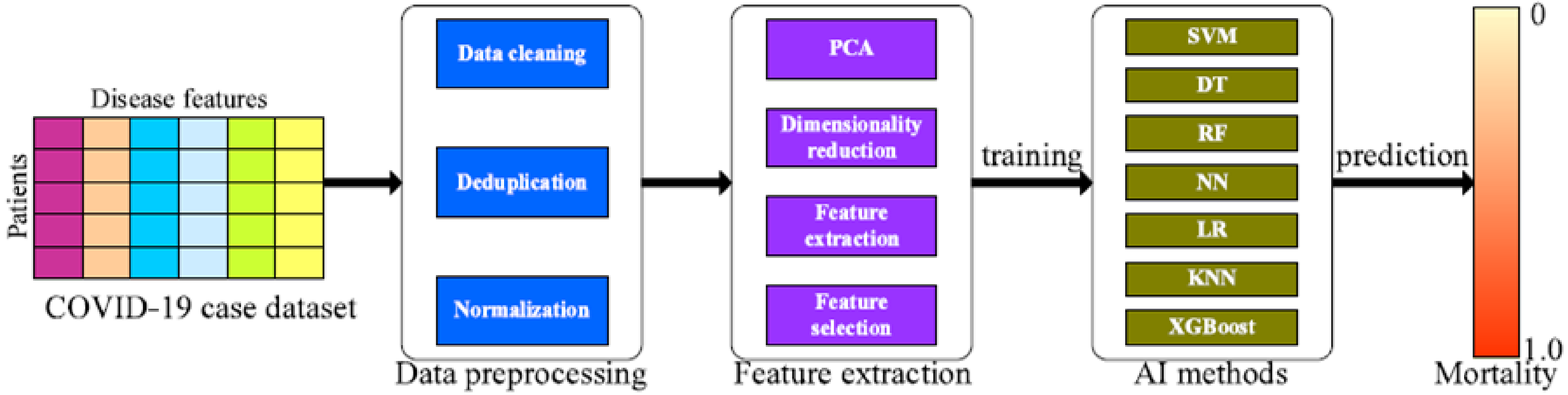

Figure. Representative AI architecture used for patient mortality and survival rate prediction

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Patient Mortality and Survival Rate Prediction: Approaches

- A research work used 6 AI methods to predict the mortality of patients with COVID-19.
  - **Base dataset:** They used public data of patients with COVID-19 from 76 countries/regions around the world
  - **Features:** 112 features, including 80 medical annotations and disease features and 32 features from the patients' demographic and physiological data. Based on the filtering method and wrapper method, 42 best features were extracted, such as demographic features, general medical information, and patient symptoms.
  - **Approach:** 6 AI methods (such as SVM, NN, RF, DT, LR, and KNN) are used to predict the mortality of patients with COVID-19.

Reference

- Mohammad, P., & Mahdi, S. (2020). Predicting Mortality Risk in Patients with COVID-19 Using Artificial Intelligence to help Medical Decision-Making. *Preprints arXiv*, *30*, v1.

Patient Mortality and Survival Rate Prediction: Approaches

- Sarkar et al. used the RF model to analyze the records of 433 patients with COVID-19 from Kaggle, and identified the important features and their impact on mortality. Experimental results show that patients over 62 years of age have a higher risk of death.

Reference

- Sarkar, J., & Chakrabarti, P. (2020). A machine learning model reveals older age and delayed hospitalization as predictors of mortality in patients with COVID-19. *MedRxiv*, 2020-03.

Patient Mortality and Survival Rate Prediction: Approaches

- Yan et al. analyzed a blood sample data set of 404 patients with COVID-19 in Wuhan, China, and used the XGBoost classification method to select three important biomarkers to predict the survival rate of individual patients. Experimental results with an accuracy of 90% indicate that higher LDH levels seem to play an important role in distinguishing the most critical COVID-19 cases.

Reference

- Yan, L., Zhang, H., Goncalves, J., Xiao, Y., Wang, M., Guo, Y., ... & Yuan, Y. (2020). A machine learning-based model for survival prediction in patients with severe COVID-19 infection.
- Yan, L., Zhang, H. T., Xiao, Y., Wang, M., Guo, Y., Sun, C., ... & Yuan, Y. (2020). Prediction of criticality in patients with severe Covid-19 infection using three clinical features: a machine learning-based prognostic model with clinical data in Wuhan. *MedRxiv*, 2020-02.

Epidemic and Transmission Prediction

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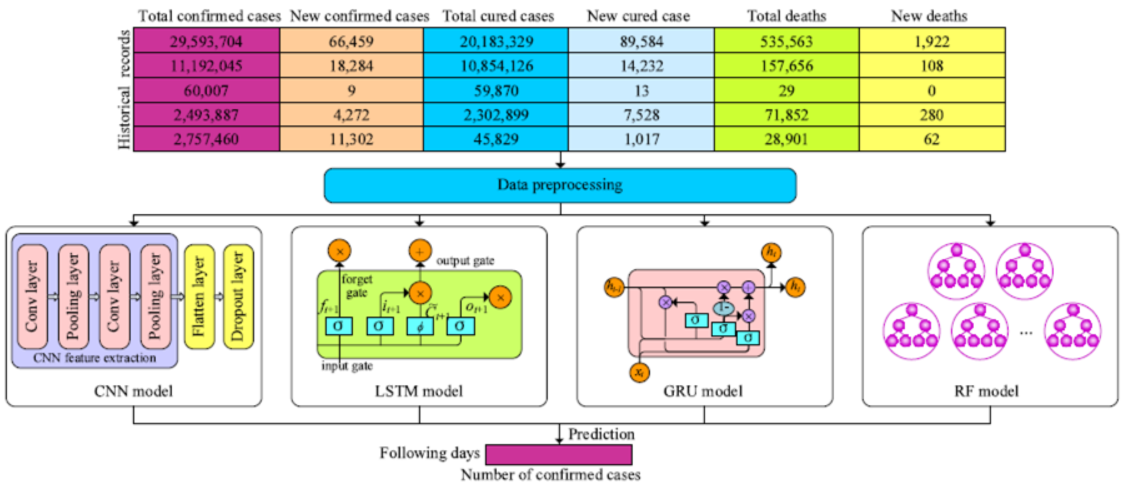
Epidemic and Transmission Prediction

- **Outbreak and Transmission Prediction:** Since the source of COVID-19 was found in Wuhan, China, hence, the outbreak and spread of COVID-19 in China received extensive attention.
    - Huang et al. used 4 DL models (such as CNN, LSTM, GRU, and MLP) to train and predict COVID-19 cases from 7 severely epidemic cities in China. The input of these DL models are the features of COVID-19 cases, including the number of confirmed cases, cured cases, and deaths. Based on the input of the previous 5 days, each model can predict the number of COVID-19 cases in the subsequent days.



Total confirmed cases	New confirmed cases	Total cured cases	New cured case	Total deaths	New deaths
29,593,704	66,459	20,183,329	89,584	535,563	1,922
11,192,045	18,284	10,854,126	14,232	157,656	108
60,007	9	59,870	13	29	0
2,493,887	4,272	2,302,899	7,528	71,852	280
2,757,460	11,302	45,829	1,017	28,901	62

Figure. Representative AI architecture for Covid 19 Outbreak Prediction

Reference

- Huang, C. J., Chen, Y. H., Ma, Y., & Kuo, P. H. (2020). Multiple-input deep convolutional neural network model for covid-19 forecasting in china. *MedRxiv*, 2020-03.

Outbreak and Transmission Prediction

- BlueDot, an AI company, was known to make accurate predictions for the COVID-19 outbreak.
  - They collected large-scale heterogeneous data from various sources, such as news reports, global ticketing data, animal diseases, global infectious disease alerts, and real-time climate conditions. Then, used filtering tools to narrow its focus; used various ML and NLP techniques to detect, mark, and display the potential risk frequency of COVID-19; and finally predicted the outbreak time of transmission.
  - It is worth mentioning that 9 days before the official announcement of the COVID-19 outbreak, BlueDot had accurately predicted the epidemic of COVID-19 and cities with a high risk of virus outbreaks.

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    - It is worth mentioning that 9 days before the official announcement of the COVID-19 outbreak, BlueDot has accurately predicted the epidemic of COVID-19 and cities with a high risk of virus outbreaks.

- In the same vein, Metabiota, another well-known AI company, collected large-scale data from social and nonsocial sources (such as biology, socioeconomic, political, and environmental data), and used technologies such as AI, ML, big data, and NLP to accurately predict the outbreak, spread, and intervention measures of COVID-19.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Outbreak and Transmission Prediction

- In addition to China, the outbreak and spread of COVID-19 in other countries including the United States, Italy, Spain, Iran, and Switzerland have also received widespread attention.
- A group of researchers proposed a system that connects fuzzy logic and neural networks, and uses an enhanced flower pollination algorithm for model parameter optimization and model training.
- Rizk et al. proposed an improved Multi-layer Feed-forward Neural Network (ISACL-MFNN) model, which uses an internal search algorithm (ISA) to optimize model parameters.
    - From the official COVID-19 data set reported by the WHO, data from January 22, 2020, to April 3, 2020, in the United States, Italy, and Spain were collected to train the ISACL-MFNN model and to predict the confirmed cases within the next 10 days.

Reference

- Al-Qaness, M. A., Ewees, A. A., Fan, H., & Abd El Aziz, M. (2020). Optimization method for forecasting confirmed cases of COVID-19 in China. *Journal of clinical medicine*, *9*(3), 674.
- Rizk-Allah, R. M., & Hassanien, A. E. (2022). COVID-19 forecasting based on an improved interior search algorithm and multilayer feed-forward neural network. *Medical Informatics and Bioimaging Using Artificial Intelligence: Challenges, Issues, Innovations and Recent Developments*, 129-152.

Outbreak and Transmission Prediction

- Marini et al. developed an agent-based AI platform, which accepts the entire Swiss population as input data to simulate and predict the spread of COVID-19 in Switzerland. It simulates people's daily trajectories by calibrating micro-census data, and effectively predicts individual contacts and possible transmission routes.

Reference

- Marini, M., Brunner, C., Chokani, N., & Abhari, R. S. (2020). Enhancing response preparedness to influenza epidemics: Agent-based study of 2050 influenza season in Switzerland. *Simulation Modelling Practice and Theory*, *103*, 102091.

Epidemic and Transmission Prediction

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- Social Control

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Epidemic and Transmission Prediction

- **Social Control:** When COVID-19 appeared, most countries in the world adopted different forms of social control, social alienation, school closures, and blockade measures to prevent the spread of the epidemic.

Reference

- Viner, R. M., Russell, S. J., Croker, H., Packer, J., Ward, J., Stansfield, C., ... & Booy, R. (2020). School closure and management practices during coronavirus outbreaks including COVID-19: a rapid systematic review. *The Lancet Child & Adolescent Health*, *4*(5), 397-404.

Social Control

- AI technologies have been widely used in epidemic control and social management, including individual temperature detection, video tracking, contact tracking, intelligent robots, etc.
- Many countries used smart devices equipped with AI to detect infected persons in public transportation places, such as airports and train stations.
  - For example, infrared cameras were used to scan high temperatures in a crowd, and different AI methods perform efficient analysis to detect whether an individual is wearing a mask in real time.
- DL-based video tracking technology was used to detect and track suspicious COVID-19 patients in public places.
- At the entrances and exits of cities, the identity information of each passing person was collected. Then, AI-based systems are used to efficiently query the travel history and trajectory of each passing individual to check whether they are from areas seriously affected by COVID-19.

Reference

- Chen, J., Li, K., Deng, Q., Li, K., & Philip, S. Y. (2019). Distributed deep learning model for intelligent video surveillance systems with edge computing. *IEEE Transactions on Industrial Informatics*.
- Chen, S., Yang, J., Yang, W., Wang, C., & Bärnighausen, T. (2020). COVID-19 control in China during mass population movements at New Year. *The Lancet*, *395*(10226), 764-766.

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Takeaways: Challenges

- Lack of available large-scale training data.
- Data imbalance between positive and negative samples.
- Massive noisy data and rumors.
- Limited knowledge in the intersection of computer science and medicine.
- Data privacy and human rights protection.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Takeaways: Directions for Future Work

- Few-shot learning and transfer learning.
- Improved video diagnosis methods.
- Patient prognosis management.
- Identification and filtering of fake news.
- Impact simulation and evaluation.
- Patient contact tracking.
- Intelligent robots.
- Intelligent Internet of Things.

Reference

- Chen, Jianguo, et al. "A survey on applications of artificial intelligence in fighting against COVID-19." *ACM Computing Surveys (CSUR)* 54.8 (2021): 1-32.

Thank you for your attention!

Questions/Discussion

Let’s connect via LinkedIn and continue this discussion together.

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