we all know about the current out break of coronavirus also known as covid 19 which

affected

more that 226 million like and taken 4 million of them .we have vaccines currently to build

immunity againsst these viruess

when we look into a case of epidemic ,even though we are advanced in technology than

ever before

why does the development of new drugs and vaccines take so long and how can we

improve the process?

Lets look into how much time it takes for a drug development process

to imrove this process of early stages there is branch called CADD whichuses existing chemical ,pharmacoogincatl and biological knowlege to do a virtual screening of possible molecules that can be used as drug .

What is a drug ..?drug is a checmical substance that affect the process of mind or body

used to treatment of any disease or abnormality

We have a receptor protein of interest like the green color thing here and a ligand ,which a molecule ,we use proceess called docking to find the binig affinity ..like the strength of interation between them.

receptor is the target to which a drug molecule binds itself

a key which fits in a lock

by binding to the receptor the drugs either enhance or inhibits is activity

conevtion tools sued for this process are autodock vina ,discovery studio.

Now we have a coronavirus protein and when we have a library of ligands . Instead of docking eacj ligand with and finding each and every binding affinity for scrrening them , our problem is to predict it biniding affinity from the ligand data.

Ligands are basically molecules that be represented as graphs.

Graphs consists of nodes and edges.The information of the graph can be represented as a adjacency matrix

conventional Machine Learning and Deep Learning tools are specialized in simple data types. Like images with the same structure and size.

unlike case of image data, we cannot resize or crop data like remove nodes in graphs.node so we need a representation of graph data and this can be done by using GNN models

for graphs we simply use the information in a nodes neighbourhood and combine it to a new embedding vector

one such message passing layer is graph convulution

in normal convvolution of images ,what happens is that the center node of that center pixel aggregates information from its neighbors, as well as from itself, to produce a new value.

Graph convolution uses average value of its neighbours.

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 simplified molecular-input line-entry system

The issue with this approach is that it depends on the arbitrary ordering of nodes that we

used in the adjacency matrix. In other words, such a model is not permutation invariant, and a

key desideratum for designing neural networks over graphs is that they should permutation

invariant (or equivariant).

what is drug designing ?

It is an inventive process of finding new medications based on th knowledge of a bilogical

target

it is complementary to the biomolecule target which they interact

lead finidings are using isolation og active subsance from the natural findings

modification of natural products ,broad screening of new snthetic substances

(the characters used to optimize a drug are

potentcy,selectivity,toxicity,metabolism,formulation)

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to reduce time cost and risk ,cadd is widely used for drug discovery process

create a new molecule &gt;doc molecule to the protein target -&gt; Analyze molecular

inerations -&gt;estimate binding strength -&gt; estimate drug like property

there are two main approaches to CADD , structure based ,ligand based