

Possibilities of applying AI in a pandemic

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Domain problem: [AI for social good \(AI4SG\)](#) - AI for Healthcare - infectious Diseases

New achievements and results enable the rapid and efficient application of AI methods and technology using infrastructure to produce results quickly and efficiently.

Addressing issues of dealing with infectious disease outbreaks with AI based solutions can be observed from two perspectives:

(1) Individual human-level:

- concerns on clinical health aspects:
 - **disease diagnosis:**
 - reliable detection vs. large-scale screening
 - from: biochemistry data, medical imaging/radiomics data (X-Ray, CT, MR), ...
 - examples:
 - Wang, S., Kang, B., Ma, J., Zeng, X., Xiao, M., Guo, J., ... & Xu, B. (2020). [A deep learning algorithm using CT images to screen for Corona Virus Disease \(COVID-19\)](#). *medRxiv*.
 - **clinical treatment/prevention:**
 - drugs discovery approaches (vaccine, antibody and small molecule development) / drug repurposing, predicting vaccine immunogenicity,
 - virtual screening tools (pyRX, AutoDock Vina) and databases (<https://zinc.docking.org/>), sequenced virus genome data, ...
 - examples:
 - Coronavirus puts drug repurposing on the fast track, <https://www.nature.com/articles/d41587-020-00003-1>
 - Coronavirus Deep Learning Competition, <https://www.youtube.com/watch?v=1LJgkovowgA>
 - Tomic, Adriana, et al. "[SIMON, an automated machine learning system, reveals immune signatures of influenza vaccine responses](#)." *The Journal of Immunology* 203.3 (2019): 749-759.
 - Lavecchia, Antonio. "[Deep learning in drug discovery: opportunities, challenges and future prospects](#)." *Drug discovery today* (2019).
- **clinical prediction:**

We suggest using the Vini in silico model of cancer [1] for VDS (virtual drug screening) against COVID-19 virus. Since there is no KEGG pathway for COVID-19 yet, VDS should be performed on ACE2 receptor of coronavirus [2], and the VINI model used in ultra-docking mode [3]. We believe this research should be conducted in three phases:

Phase A: The Vini model will perform VDS with existing antiviral drugs and their combinations. The maximum number of drugs in these combinations should not go beyond five, as with the more drugs chances for D2D (drug to drug) interactions rise exponentially. The list of current antiviral drugs is at <https://www.genome.jp/kegg/drug/br08350.html#2>

Phase B: In this phase, the Vini model will perform VDS in virtual chemical space [4], in order to find the novel drugs against the COVID-19 virus. The number of virtual chemical compounds will depend on the computing resources available, but at least several million compounds should be screened (to check if UNIRI is willing to join and borrow Bura resources for this search at no cost). The list of the most effective chemicals will be harmonized to exclude those with an unacceptable level of toxicity, and dose for which their chemical synthesis is too expensive or not possible. Free energy of binding between the hundred most effective (against ACE2 receptor) drug candidates and ACE2 will be recalculated with more precise MD tools like Gromacs or NAMD. Then, ten of the chemical compounds found as the most effective will be synthesized and tested in vitro.

Phase C: To check with the Lund University and RBI resources if they are willing to support this research. In that case, the Vini model can be additionally fed with transcriptomic (RNA-Seq) and quantitative proteomic (nLC-MS/MS) assay data. That would increase the efficacy of the Vini model in finding new drugs and allow personalized therapies against COVID-19 virus.

(2) Social system-level:

- concerns on predicting public reaction towards disease outbreaks:
- **public health aspects:**
 - epidemics monitoring,
 - tracking spread of coronavirus
 - Available dataset - 2019 Coronavirus dataset (January - February 2020):
 - <https://www.kaggle.com/brendaso/2019-coronavirus-dataset-01212020-01262020/activity>
 - detect signs of potential disease outbreaks from the collected (human behavioural) information
 - tracking s
 - epidemics forecasting
 - AI + complex network epidemiology models (<http://www.gleamviz.org/>, [Vespignani](#))
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 - epidemics control
 - methodology: AI (deep RL), complex networks (settings of disease maximization/minimization problem, network dismantling)
 - examples:
 - Probert, William JM, et al. "[Context matters: using reinforcement learning to develop human-readable, state-dependent outbreak response policies.](#)" *Philosophical Transactions of the Royal Society B* 374.1776 (2019): 20180277.
 - Bryan Wilder, Sze-Chuan Suen, and Milind Tambe. [Preventing infectious disease in dynamic populations under uncertainty.](#) In Thirty-Second AAAI Conference on Artificial Intelligence, 2018.
 - Ren, Xiao-Long, et al. "[Generalized network dismantling.](#)" *Proceedings of the National Academy of Sciences* 116.14 (2019): 6554-6559.

- COVID-19 and artificial intelligence: protecting health-care workers and curbing the spread, [https://www.thelancet.com/journals/landig/article/PIIS2589-7500\(20\)30054-6/fulltext](https://www.thelancet.com/journals/landig/article/PIIS2589-7500(20)30054-6/fulltext)
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- [artificial] complex systems (indirectly) affected with the outbreak:
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 - socio-economical, financial systems
 - political systems
 - [impacts of outbreaks on political stability](#)
 - Morens, David M., Gregory K. Folkers, and Anthony S. Fauci. "The challenge of emerging and re-emerging infectious diseases." *Nature* 430.6996 (2004): 242-249.
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We can also reason about the issues, from the point of view of two conceptual framework frameworks used in AISG survey: AEC (agent – environment – community) and DPP (descriptive – predictive – prescriptive) framework.

FRAMEWORK	DESCRIPTIVE	PREDICTIVE	PRESCRIPTIVE
AGENT	Disease diagnosis	Disease development predictions	Treatment recommendation
ENVIRONMENT	Drug discovery/development	Epidemic prediction	Preventing spread of illness
COMMUNITY	(subtyping)	(predictive phenotyping)	

AI SERVICE AND RESOURCES FROM SCIENCE

- Epidemic Intelligence Information System (EPIS)

Web based communication platform that allows nominated public health experts to exchange technical information to assess whether current and emerging public health threats have a potential impact in the EU.

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AI SERVICES FROM INDUSTRY

HealthMap, <https://en.wikipedia.org/wiki/HealthMap>

BlueDot - Automated infectious disease surveillance, <https://bluedot.global/>

- AI based early-warning system (NLP, ML) to track over 100 infectious diseases by analyzing about 100,000 articles in 65 languages every day
- Additional other data: traveler itinerary information and flight paths, information about an area's climate, temperature, or even local livestock

Metabiota - <http://metabiota.com/>

- data source: social media
- estimate the risk of a disease's spread causing social and political disruption, based on information like an illness's symptoms, mortality rate, and the availability of treatment.

DATA SOURCES AND RELEVANT AI GRAPH AND DATABASES

- Public Health Databases
- Online Medical Databases
- Social media sources
- EU level health databases
- National digital health databases
- Scientific research databases
- [European Centre for Disease Prevention and Control](#)

ADDITIONAL SCIENTIFIC LITERATURE

Wong, Zoie SY, Jiaqi Zhou, and Qingpeng Zhang. "[Artificial intelligence for infectious disease big data analytics.](#)" *Infection, disease & health* 24.1 (2019): 44-48.

- This paper provides discussion and visionary perspective on data usage and management for infectious diseases.
- It highlights the opportunity to make use of Artificial Intelligence (AI) methods to enable reliable and data-oriented disease monitoring and projection under this information age.
- It is foreseeable that together with reliable data management platforms AI methods will enable effective analysis of massive infectious disease and surveillance data to support risk and resource analysis for government agencies, healthcare service providers, and medical professionals in the future.

Ganasegeran, Kurubaran, and Surajudeen Abiola Abdulrahman. "[Artificial Intelligence Applications in Tracking Health Behaviors During Disease Epidemics.](#)" *Human Behaviour Analysis Using Intelligent Systems*. Springer, Cham, 2020. 141-155.

Aleksa Zlojutro, David Rey & Lauren Gardner. "[A decision-support framework to optimize border control for global outbreak mitigation](#)". (2019) 9:2216

- modeling framework that integrates both outbreak dynamics and outbreak control into a decision support tool for mitigating infectious disease pandemics that spread through passenger air travel.
- proposed border control strategies that exploit properties of the air traffic network structure and expected outbreak behavior

References

- [1] Tomic D, Skala K, Kranjcevic L, Pirkic B, Stifter S, and Smit I, Evaluation of the Efficacy of Cancer Drugs by Using the Second Largest Eigenvalue of Metabolic Cancer Pathways, *J Comput Sci Syst Biol*. 2018 July 11: 240-248.
- [2] Wan Y, Shang J, Rachel Graham R, Baric RS, Li F, Receptor recognition by novel coronavirus from Wuhan: An analysis based on decade-long structural studies of SARS, *Journal of Virology* Jan 2020, JVI.00127-20; DOI: 10.1128/JVI.00127-20
- [3] Tomic D, Davidovic D, Jangel V, Mesaric J, Skala K, Lipic T, Assessing the effectiveness of Autodock Vina in a large and unstructured environments for virtual drug screening, to be published in *Proc. of the 43rd Int. Mipro Convention*, 25-29.May, 2020, Opatija.
- [4] Lyu, J., Wang, S., Balias, T.E. et al. Ultra-large library docking for discovering new chemotypes. *Nature* 566, 224–229 (2019). <https://doi.org/10.1038/s41586-019-0917-9>
- [5] [16] Tomic D, Skala K, Pirkic B, Kranjcevic L, Predicting the effectiveness of combinatorial cancer therapies, In *Proc. of 42 Int. Convention Mipro*, 394-399, 2019, Opatija, Croatia, doi:10.23919/mipro.2019.8757131.