Bioinformatics and Data Science of Pandemics: Introduction

Alexander Schönhuth



Bielefeld University May 10, 2021

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Organization

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- Organization and introduction: *today*
- ► Full literature list available: *by May* 17
- ► How to present (brief): *May* 17
- ► How to write (brief): *shortly before presentations*
- **Presentations:** *from June 1:*
 - Each presentation 30-45 minutes (less in case of one presenter)
 - Up to two presentations per week, if that suits everyone's schedules
 - ▶ If desired/necessary, block seminar day possible as well
- **Technical Report:** *after presentation:*
 - Each report 8-15 pages
 - Optimally, report profits from feedback provided after presentation
 - Drafts can be submitted for discussion
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Motivation



MOTIVATION

- ► The Covid-19 crisis is a "bioinformatics" crisis
- ► Have a (truly) scientific look at topics of current interest
- The following is a list of suggested topics
- ▶ If you wish to discuss a different topic, please suggest
- ▶ In any case: scientific papers that deal with topic required



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Topics



PCR Test Design

- ► The Origin of SARS-CoV-2
- Virus Genome Assembly / Evolutionary Tracking
- Infection Wave Dynamics
- Drug Repurposing
- ► Any further? ...



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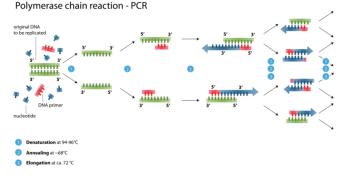


PCR Test Design



PCR TEST DESIGN

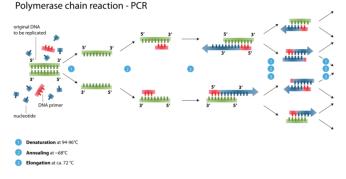
NIVERSITÄT



From: www.the-odin.com

- Primers need to anneal to target sequence
- Primers must not anneal against other sequences (related viruses)
- ► How to safely select such primers?

PCR TEST DESIGN



From: www.the-odin.com

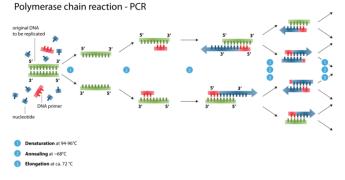
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- UNIVERSITÄT BIELEFELD

PCR TEST DESIGN: PAPERS

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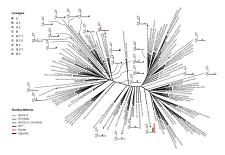
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The Origin of SARS-CoV-2



Origin

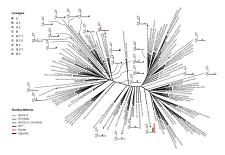


From: www.the-odin.com

- What are the viruses that are related with SARS-CoV-2 and how are they related?
- What are the driving evolutionary forces having shaped them (mutation, recombination)?
- How can we determine all of this and how certain can we be about our conclusions?



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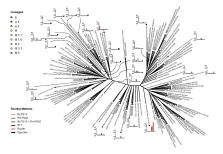


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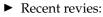
ORIGIN: PAPERS

Recent revies: https://doi.org/10.1007/s10311-020-01151-1

- Relation of virus lineage with other viruses: https://doi.org/10.1038/s41564-020-0771-4
- Uncertainty of origin (Nielsen): https://doi.org/10.1093/molbev/msaa316
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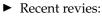


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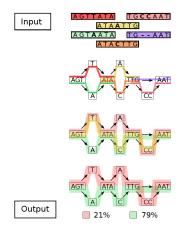


Virus Genome Assembly Evolutionary Tracking

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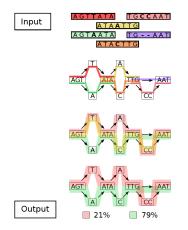
ASSEMBLY AND TRACKING



Constructing virus variation graph from input reads

- Viruses tend to infect hosts as ensemble of strains
- How to reconstruct all strains from an individual RNA/DNA sample?
- Once strains are reconstructed, how to put them into mutual context?
- Fast inspection of mutational status of infected people
- Overview of evolutionary status of pandemic
- Use graphs or trees

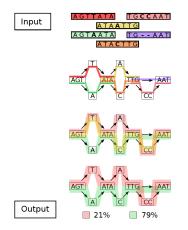
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Assembly and Tracking: Papers

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- Viral quasispecies assembly: https://genome.cshlp. org/content/27/5/835.full.html
- Full-length assembly using variation graphs: https: //doi.org/10.1093/bioinformatics/btz443

► Tracking:

- The Pantograph project (variation graphs): https://graphgenome.org/
- Phylogenetic trees ("nextstrain"): https: //doi.org/10.1093/bioinformatics/bty407



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Assembly and Tracking: Papers

► Assembly:

- Viral quasispecies assembly: https://genome.cshlp. org/content/27/5/835.full.html
- Full-length assembly using variation graphs: https: //doi.org/10.1093/bioinformatics/btz443
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Assembly and Tracking: Papers

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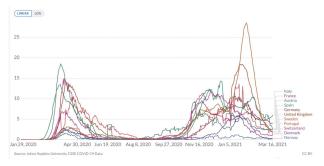
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Infection Wave Dynamics

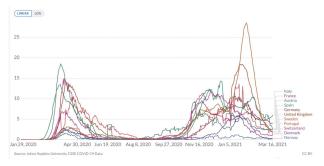
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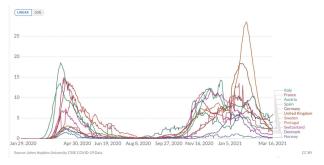
Covid-19 death count curves per countries in Europe

- Counts of infected/died people take particular shapes
- ▶ Why is that? Are there reliable models?
- How to estimate infection rate? (R-value)
- Do the curves behave in known / controllable ways?



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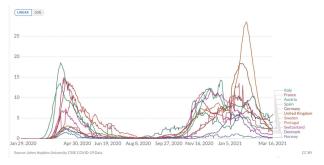
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► The R-Value:

- Popular overview: https://www.nature.com/ articles/d41586-020-02009-w
- Early dynamics of COVID-19: https: //doi.org/10.1016/S1473-3099(20)30144-4
- Stochastic non-linear dynamical systems: https: //doi.org/10.1093/biostatistics/kxs052
- Curve Fitting:
 - ► Gompertz curves:
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Infection Fatality Rate

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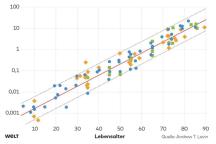
INFECTION FATALITY RATE

Infektionssterblichkeit nach Alter

(Regressionsanalyse)

- ······ Vorhersage-Intervall
- Studien mit repräsentativen Proben und Antikörperbestimmung
- Studien aus Ländern mit wenigen Fällen und umfassender Kontaktverfolgung
- Sonstige Studien

Sterberate in Prozent



Infection Fatality Rate (IFR) per age / study

When infected, how likely does one die?

- ▶ What role does age play?
- What are the techniques to provide reliable estimates?



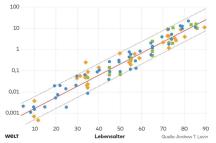
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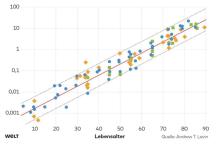
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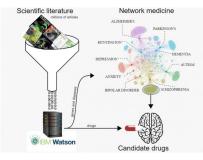


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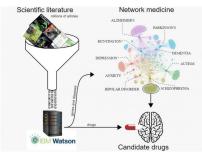




From: eurekalert.org

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- Different molecules may assume similar shapes
- Find such molecules in the context of particular disease

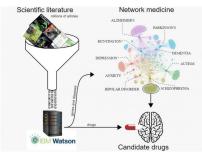




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DRUG REPURPOSING: PAPERS

Review: https://doi.org/10.1002/med.21728

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Thanks for your attention!

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