RWTH AACHEN UNIVERSITY
Joint Research Center for Computational Biomedicine

UNIKLINIK RWTH AACHEN

Klinik für
Operative Intensivmedizin und
Intermediate Care

SMITH

Bericht zum DEA und VP

Use Case ASIC

28. Sept. 2022

Andreas Schuppert, Richard Polzin,
Konstantin Sharafutdinov, Chadi Barakat, Lars Küpfer

ASIC System – towards realizing the potential of clinical data

Smart Medical Information Technology for Healthcare

- DEA – Platform to enable Machine Learning for prognosis in ICU
- Virtual Patient – Extracting medical information from RWE data
- Exploring the (unexpected) value of multivariate data – is ARDS in Covid different?
- HPC – based model reduction – towards VP for clinical use

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Diagnostic Expert Advisor: Agenda

- Overview & Setup
- Application to Control Data
- Comparison to other models
- Stratification
- Individualization
- Outcome & Learnings

☆ Key Message marked on each slide

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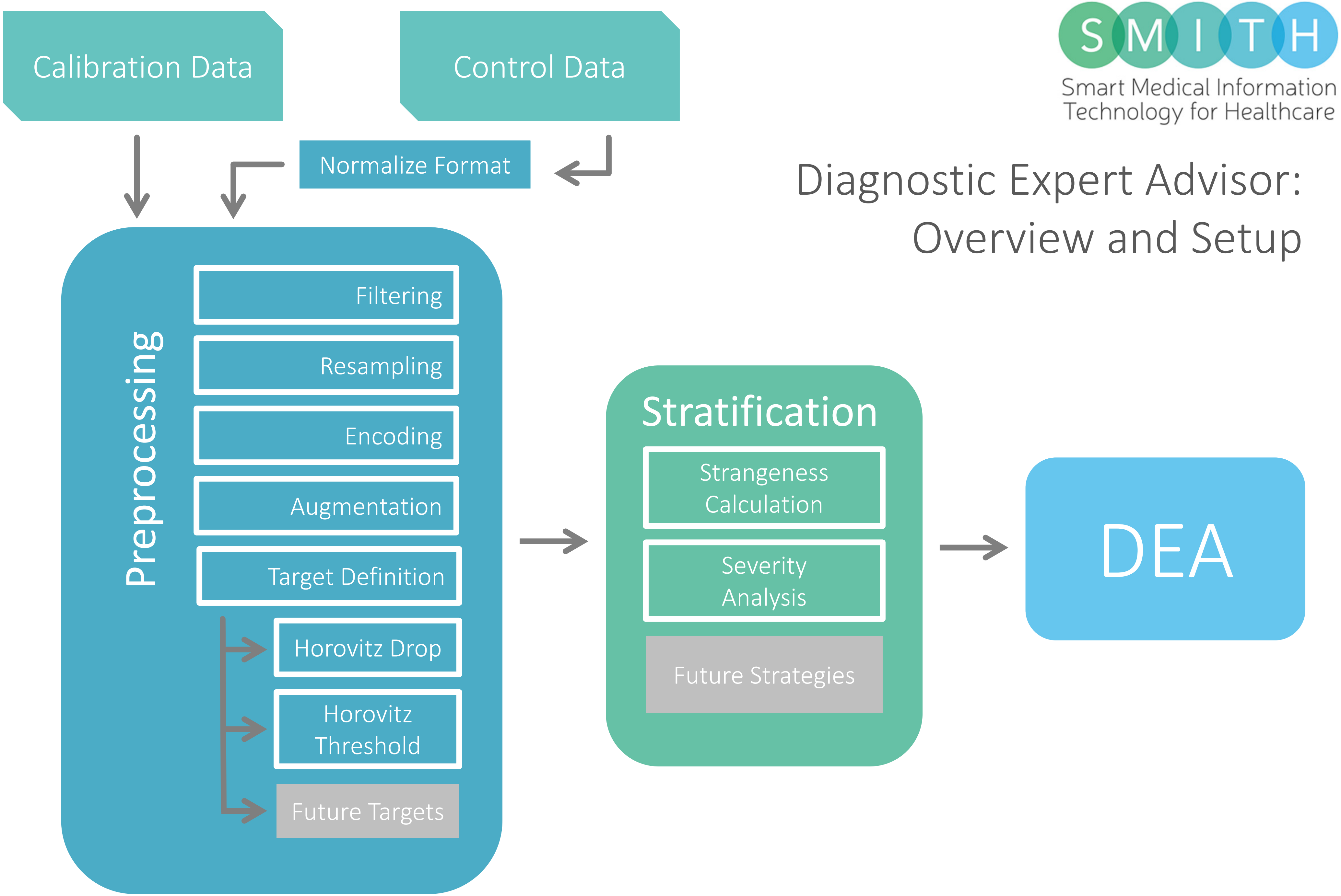
Diagnostic Expert Advisor: Overview and Setup



Titel: ASIC Workshop
Autor: Sharafutdinov
Schutzklasse: SMITH-intern
Folie:

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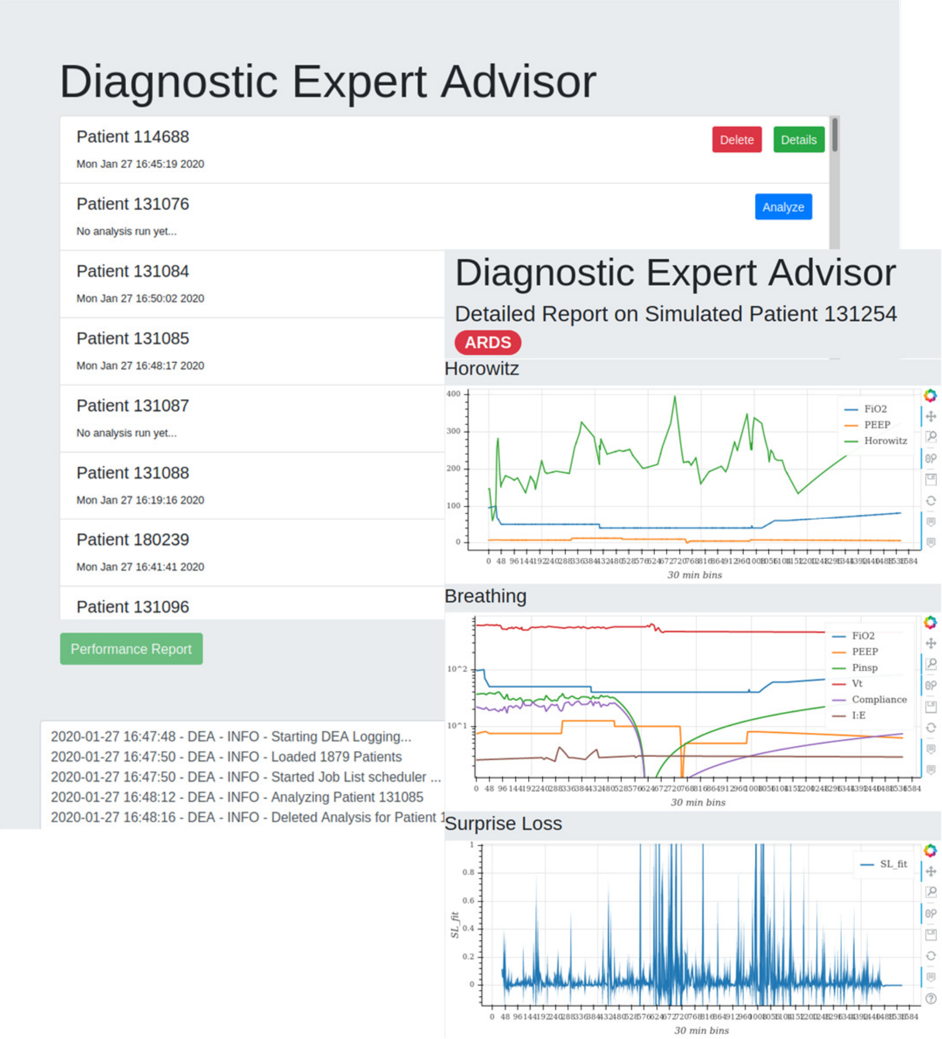
Diagnostic Expert Advisor: Overview and Setup

- Flexible Pipeline for DEA data preparation and training
  - Evaluated wide variety of models, preprocessing techniques and stratification approaches
  - Easily adaptable for new targtes, e.g.: stratification for covid, onset prediction for Sepsis, or other organ failures in conjunction with ARDS
- Interactive Web-UI for data exploration and application
  - Starting point for integration into hospitals



Diagnostic Expert Advisor

Patient 114688
Mon Jan 27 16:45:19 2020

Patient 131076
No analysis run yet...

Patient 131084
Mon Jan 27 16:50:02 2020

Patient 131085
Mon Jan 27 16:48:17 2020

Patient 131087
No analysis run yet...

Patient 131088
Mon Jan 27 16:19:16 2020

Patient 180239
Mon Jan 27 16:41:41 2020

Patient 131096

```
2020-01-27 16:47:48 - DEA - INFO - Starting DEA Logging...
2020-01-27 16:47:50 - DEA - INFO - Loaded 1879 Patients
2020-01-27 16:47:50 - DEA - INFO - Started Job List scheduler ...
2020-01-27 16:48:12 - DEA - INFO - Analyzing Patient 131085
2020-01-27 16:48:16 - DEA - INFO - Deleted Analysis for Patient 1
```

Diagnostic Expert Advisor

Detailed Report on Simulated Patient 131254

☆ Expandable Software Platform, applicable to more than ARDS

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Diagnostic Expert Advisor: Application to Control Data

- Control data for some hospitals available since 08/22

	Hospital 0	Hospital 2	Hospital 7	Hospital 8
Encounters	3,591	902	2,217	10,408
ROCAUC	0.88	0.83	0.86	0.82

- Large imbalance in distribution of cases
- Heterogenity in various aspects, e.g. strangeness → CH/VP
- Model generalizes well, achieving a mean ROCAUC of 0.83

☆ Different hospitals are handled well

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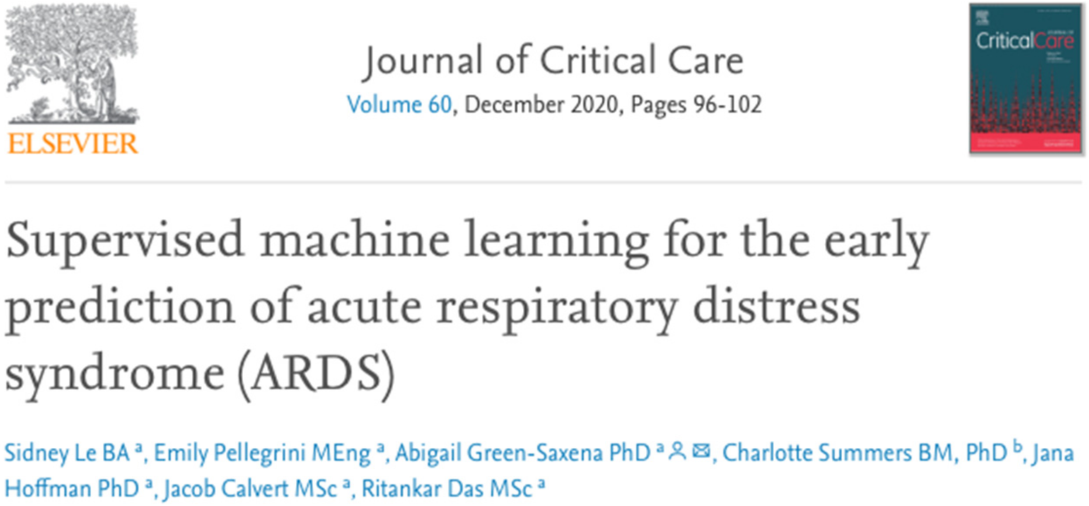
Diagnostic Expert Advisor: Comparison to other models

- There is no cohort like ours, thus comparison is complicated
- Prediction targets often differ as well
- E.g. Sidney et al.:
  - Prediction Target: *Horovitz < 300 and PEEP > 5*
  - Cohort: *Based on MIMIC III, excluding Tracheostomy in first 72 hours*
  - *Include Radiology Reports*
  - *Exclude Horovitz related information*



ELSEVIER

Journal of Critical Care
Volume 60, December 2020, Pages 96-102

Supervised machine learning for the early prediction of acute respiratory distress syndrome (ARDS)

Sidney Le BA [a], Emily Pellegrini MEng [a], Abigail Green-Saxena PhD [a], Charlotte Summers BM, PhD [b], Jana Hoffman PhD [a], Jacob Calvert MSc [a], Ritankar Das MSc [a]

☆ ASIC dataset is unique, our prediction target ambitious

Diagnostic Expert Advisor: Comparison to other models

- Many implementation details omitted in the paper
- No radiology reports available for DEA, only COI items

Prediction Horizon	At event	12h	24h	48h	96h
Sidney Et Al.	0.843	0.858	0.810	0.796	Not Tested
DEA	0.807	0.812	0.807	0.770	0.732

- -0.027 mean ROC AUC difference between Sidney Et Al. and DEA

☆ Performance at level of other published methods

Diagnostic Expert Advisor: Comparison to other models

- Sidney Et Al.: general population screening
- DEA focussed on ARDS/Horovitz prediction → Include Horovitz+

Prediction Horizon	At event	12h	24h	48h	96h
Sidney Et Al. *(Ohne Horovitz+)*	0.843	0.858	0.810	0.796	Not Tested
DEA *(Ohne Horovitz+)*	0.807	0.812	0.807	0.770	0.732
DEA *(Mit Horovitz+)*	0.965	0.975	0.960	0.897	0.840

- +0.123 ROC AUC difference between Sidney Et Al. and DEA+HV
- Prediction of Horovitz<300 and PEEP>5 of little clinical relevance

☆ Model performs very good at predicting “easier” ARDS targets

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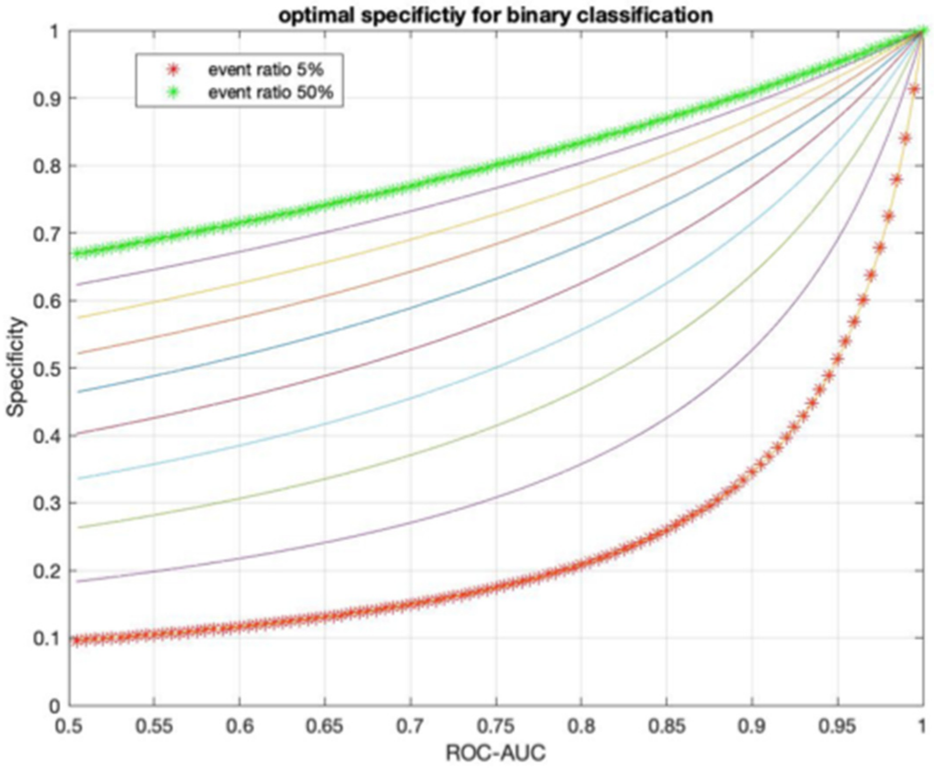
Diagnostic Expert Advisor: Stratification Strategy

- Even a high ROC AUC still leads to a large error rate, if the event is rare
- To be more applicable in the clinical context we need better results → Stratification
- Define risk classes based on
  - Acceptable error rates
  - Therapeutic options on true positives
  - Patient risk for false negatives



☆ Errors, Treatments on Alarm, Risk for patients: Need to finetune with the doctors

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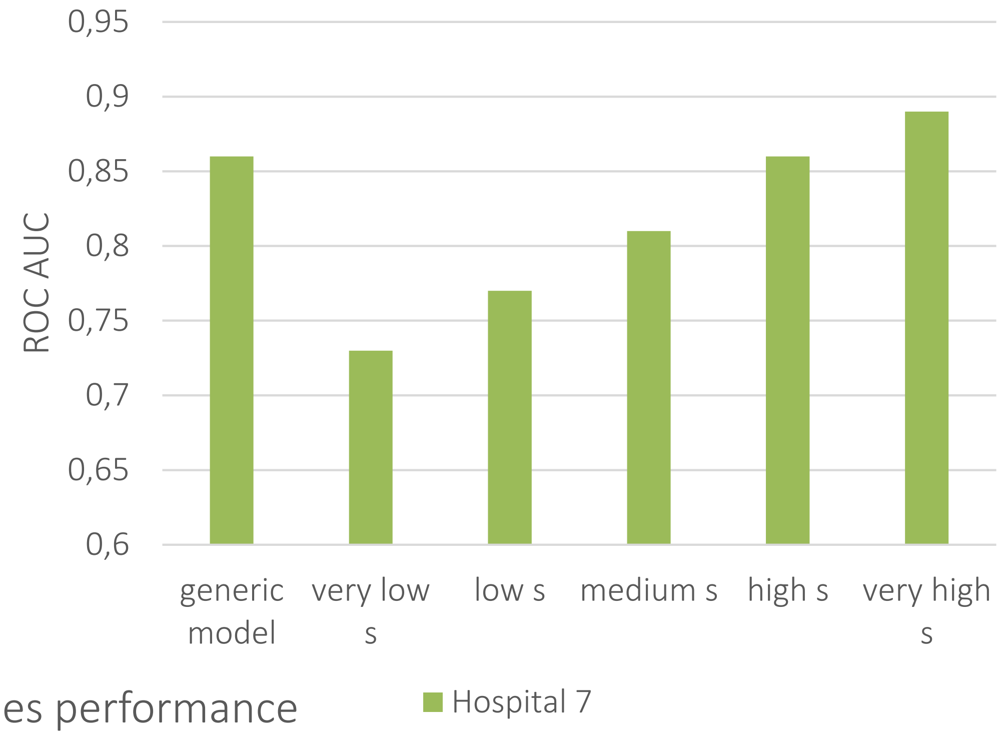
Diagnostic Expert Advisor: Stratification Strategy: Example

- Stratification based on “strangeness”: patients at high risk can often be found in sparsely populated data regions
- Develop dedicated models per strangeness group
- Especially for the very high strangeness cohort the prediction performance can be further increased



☆ Dedicated model for “strange” patients increases performance

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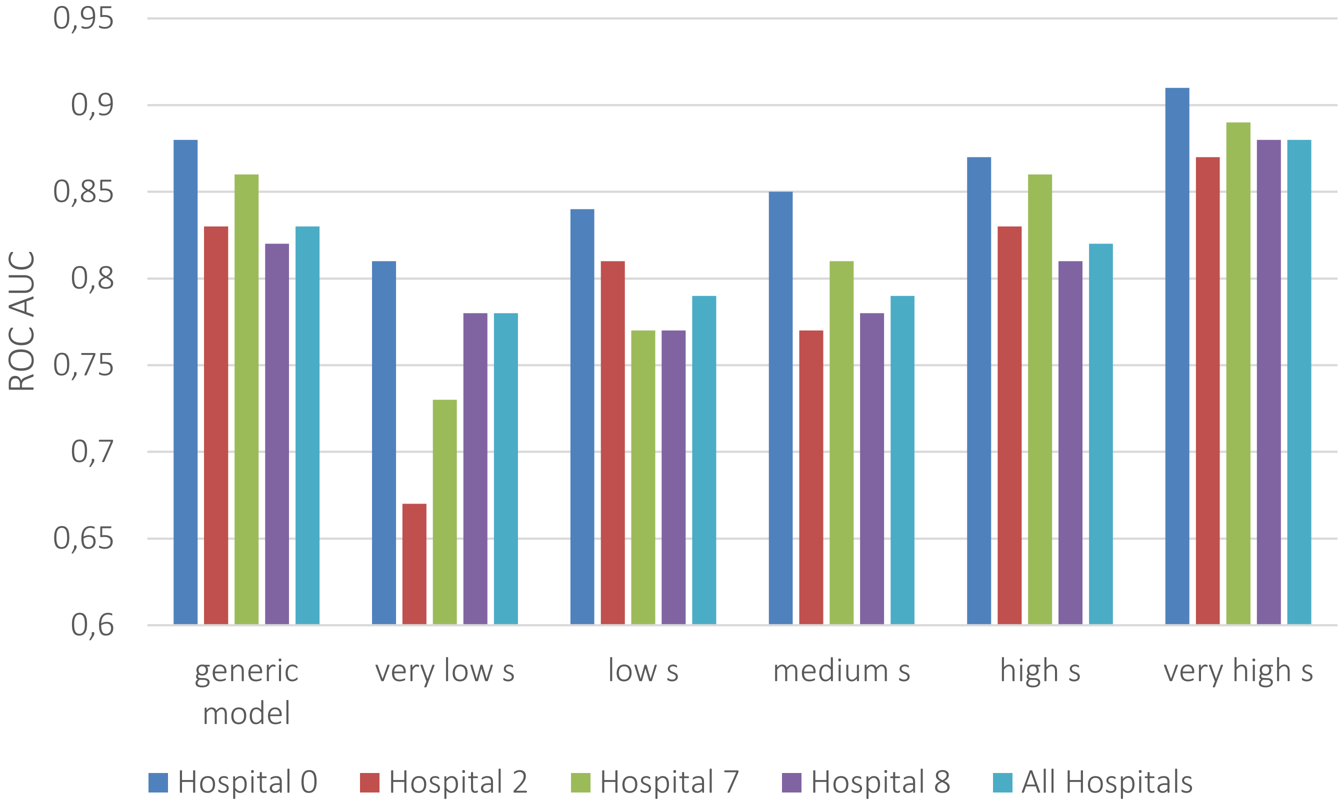
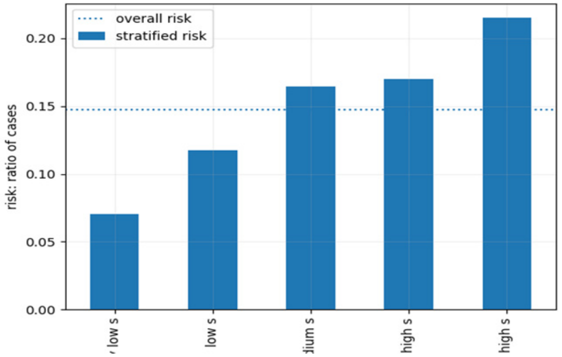
Diagnostic Expert Advisor: Stratification Strategy: Example

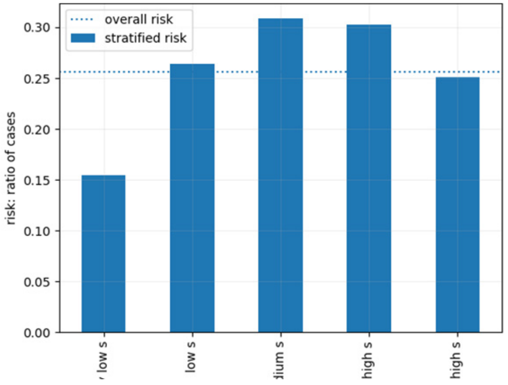
- Effect can be observed on all hospitals, even though the strangeness dynamics change significantly



Hospital 0



Hospital 8



☆ Stratification Concept works throughout all hospitals

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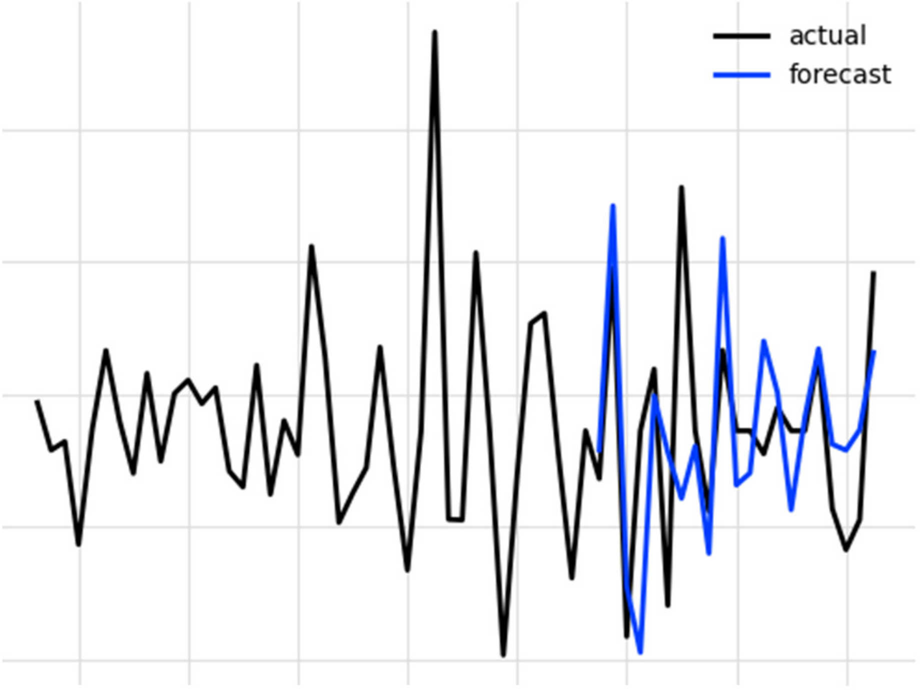
Diagnostic Expert Advisor: Individualization

- During the development of the DEA it could often be observed that for some patient a model would fit exceptionally well, though it would not generalize
- Testing the model fit on individual patients and deploying a good fitting model on a per-patient level could boost performance even further



Example: TFT Model predicting changes in Horovitz, good fit

- Potential to augment e.g. predicted Horovitz values, trend information or drop estimates to original model

☆ Individualization offers potential for even further performance increases

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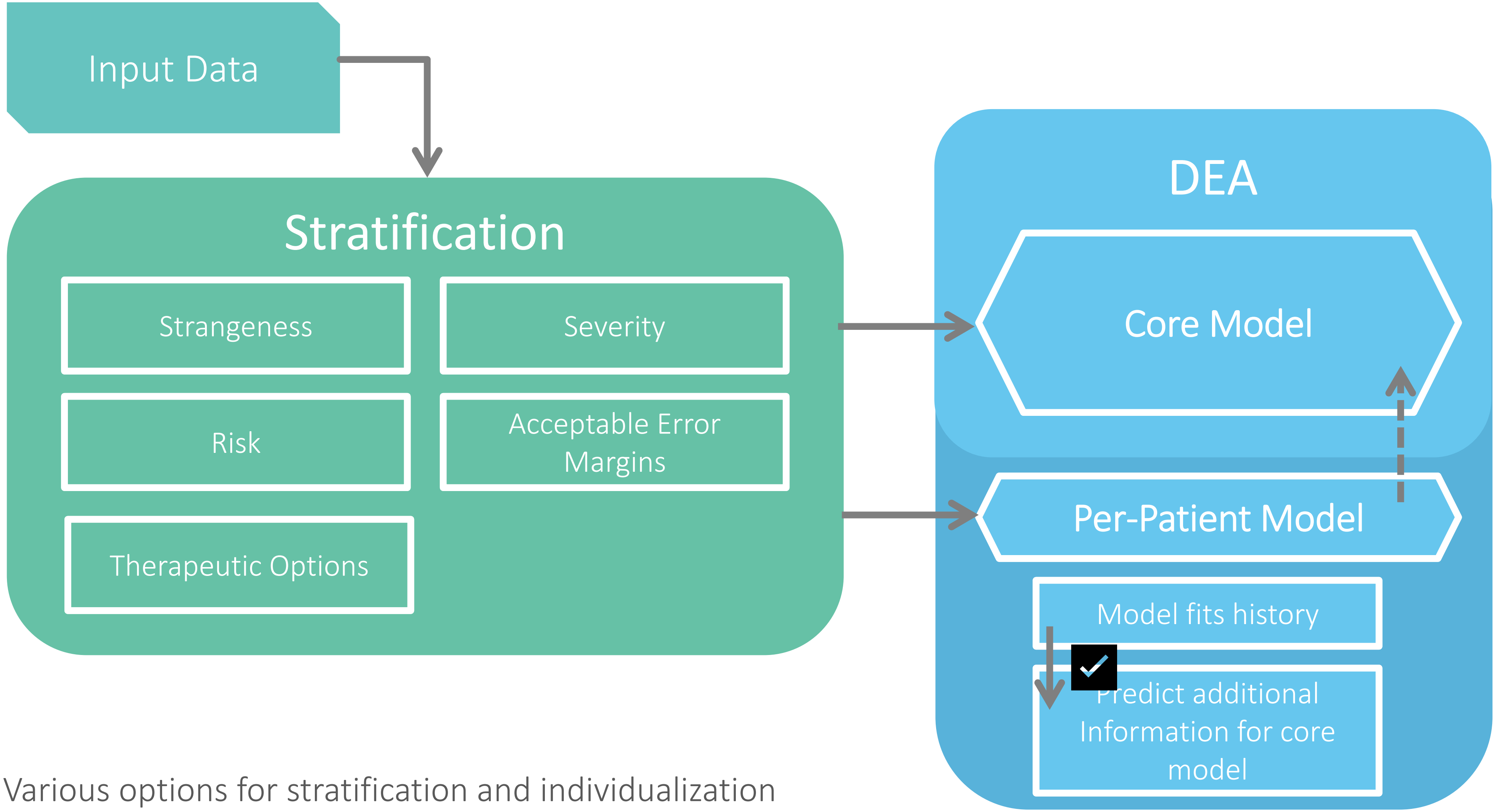
Diagnostic Expert Advisor: Individualization: Concept



☆ Various options for stratification and individualization

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Diagnostic Expert Advisor: Learnings

- Data Handling is a lot of work! (Control data only in July)
- Rare events require dedicated handling (high error rates)
- One-Model-Fits-All probably not fit for hospitals, especially as it neglects “high strangeness” patients
- Stratification based strategies required for smooth implementation (false alarms)
- Individualization (see VP as well) for the future

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Diagnostic Expert Advisor: Outcome

- Software Platform ready and expandable to future tasks
- Performance at, or above State of the Art
- Clinically relevant prediction target for lung damage
- Applicability across different hospitals, with fine-tuning possible
- Potential for future enhancements (further individualization)
- Potential for prediction of diverse outcomes (Multi-Organ failure, Sepsis)

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ASIC System – towards realizing the potential of clinical data

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Hybrid ICU data analysis framework

Problem:

- ICU datasets are different
- Once ICU data from different hospitals are pooled, strong selection bias is observed
- Outcomes of application of data based approaches are biased by the data origin

Solution:

1. **Generalization quality assessment framework:** estimates similarity between populations and pinpoints possible generalization issues

2. **Virtual patient modeling framework:** a filter to extract medically relevant information from noisy heterogeneous datasets and reduce selection bias

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Generalization quality assessment framework

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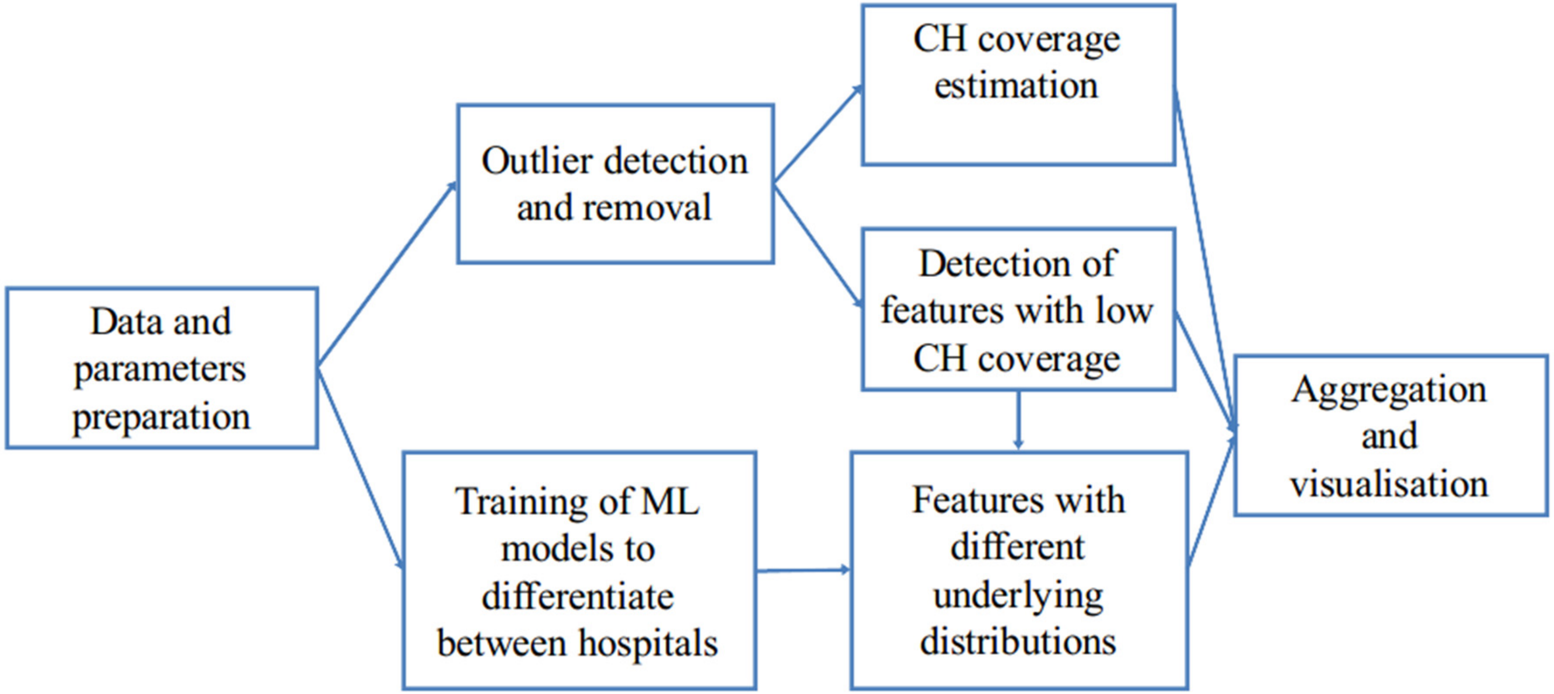
- Pipeline delivers
  1. estimate of **the similarity of different populations** in terms of the convex hull (CH) coverage and parameters with low CH coverage
  2. list of parameters with diverging underlying distributions

Pipeline consists of following steps:

1. Convex hull analysis for **a priori generalization assessment**
2. ML tool to find parameters with **differences in underlying distributions**


Data and parameters preparation
Outlier detection and removal
CH coverage estimation
Detection of features with low CH coverage
Training of ML models to differentiate between hospitals
Features with different underlying distributions
Aggregation and visualisation

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Generalization assessment: Results

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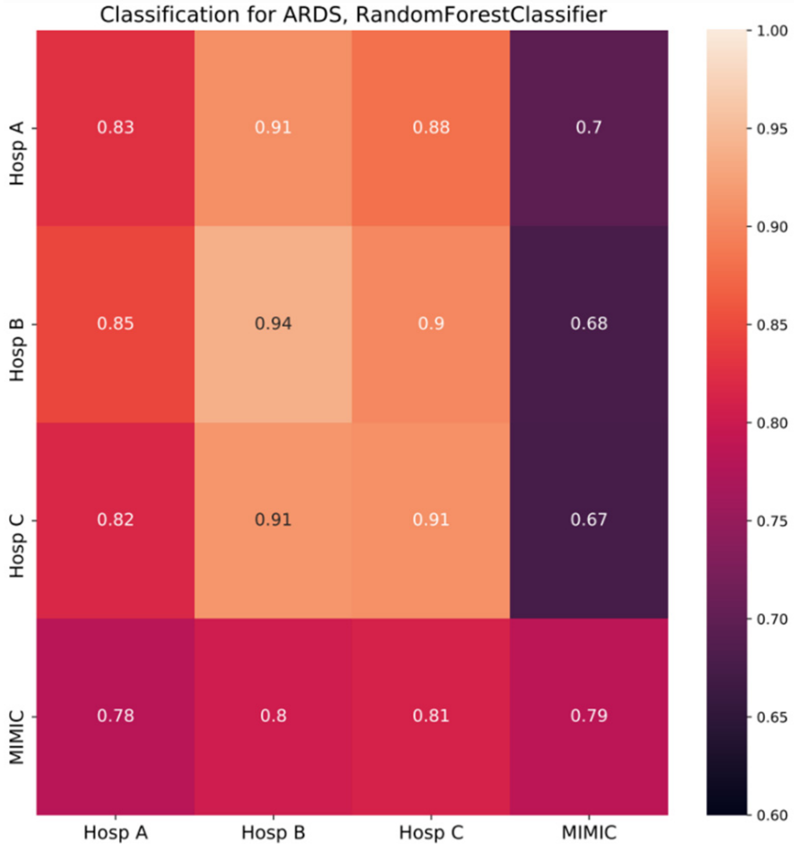

- Pipeline was applied on 3 German hospitals and MIMIC III dataset
- 2 clusters of datasets were observed – German hospitals and MIMIC
- Large performance drop for models for ARDS classification developed in German hospitals' once applied to MIMIC
- MIMIC models could not reach the same performance as specific German hospital models
- These results were supported by the CH analysis
- Features with low CH coverage and diverging distributions were found: PaO2, PEEP, FiO2 and tidal volume

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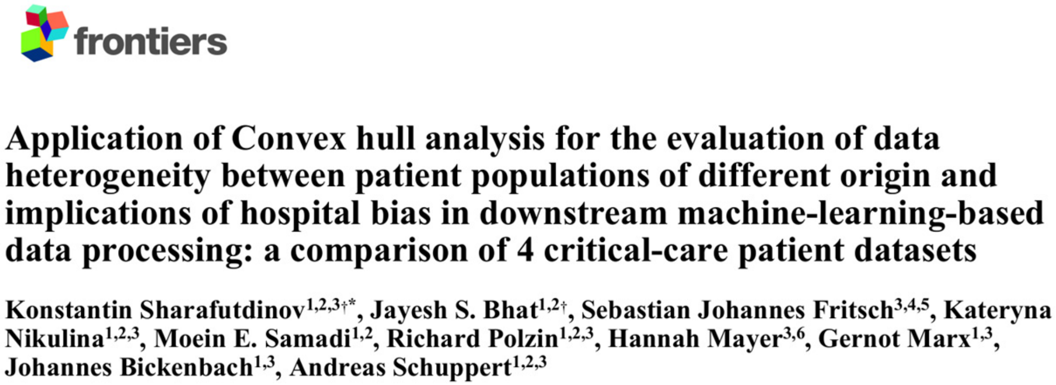
Generalization assessment: Conclusions

- Pipeline to assess generalization ability of ML models in different datasets (hospitals) has been developed
- Application of models developed on external datasets should be performed with care
- MIMIC data significantly differs from German hospitals
  - AI trained in Germany can have impaired performance by validation on MIMIC
  - Models trained in MIMIC do not reach specializaed performance of German models
  - Reasons for discrepancies: admission/treatment strategies, diverging ARDS labeling, timespans of data, etc.
- **Pooling of data as a possible solution**, but reduces performace in every single hospital

- Poor performance of validated models is a trend in healthcare
- This has to be considered by all AI/ML projects in intensive care
- “Gold Standard” databases are needed with harmonized data structures
- Novel methods for ML adaptation are needed

- Paper in review



frontiers

Application of Convex hull analysis for the evaluation of data heterogeneity between patient populations of different origin and implications of hospital bias in downstream machine-learning-based data processing: a comparison of 4 critical-care patient datasets

Konstantin Sharafutdinov[1,2,3†*], Jayesh S. Bhat[1,2†], Sebastian Johannes Fritsch[3,4,5], Kateryna Nikulina[1,2,3], Moein E. Samadi[1,2], Richard Polzin[1,2,3], Hannah Mayer[3,6], Gernot Marx[1,3], Johannes Bickenbach[1,3], Andreas Schuppert[1,2,3]

Virtual Patient Modeling Framework

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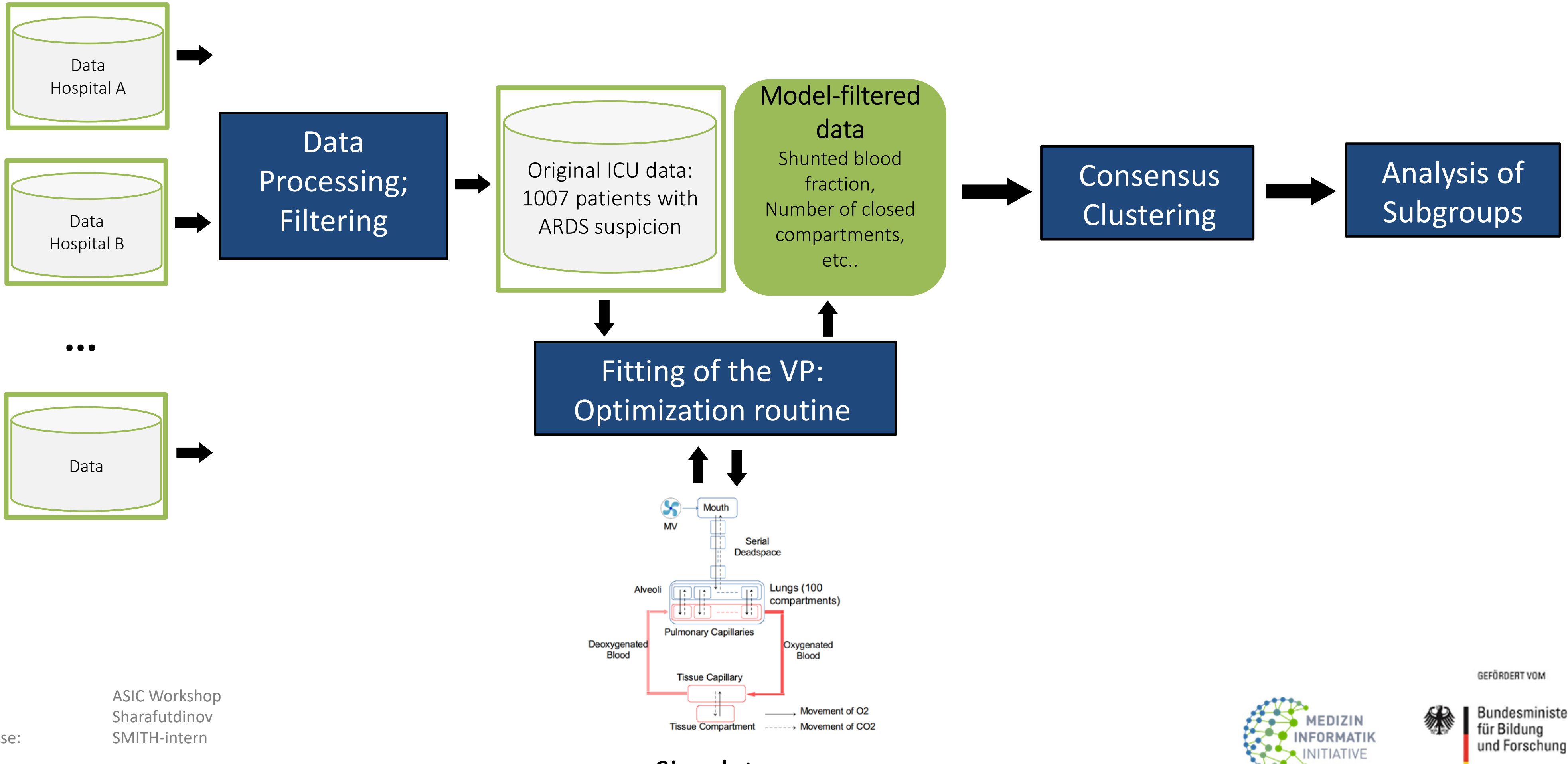
- **Problem**: pooling of datasets introduces selection bias
- **Solution**: VP modeling as a filter to extract medically relevant information from noisy heterogeneous datasets and reduce selection bias



Data Hospital A

Data Hospital B

...

Data

Data Processing; Filtering

Original ICU data: 1007 patients with ARDS suspicion

Model-filtered data
Shunted blood fraction, Number of closed compartments, etc..

Consensus Clustering

Analysis of Subgroups

Fitting of the VP: Optimization routine

Simulator

Titel:	ASIC Workshop
Autor:	Sharafutdinov
Schutzklasse:	SMITH-intern
Folie:	

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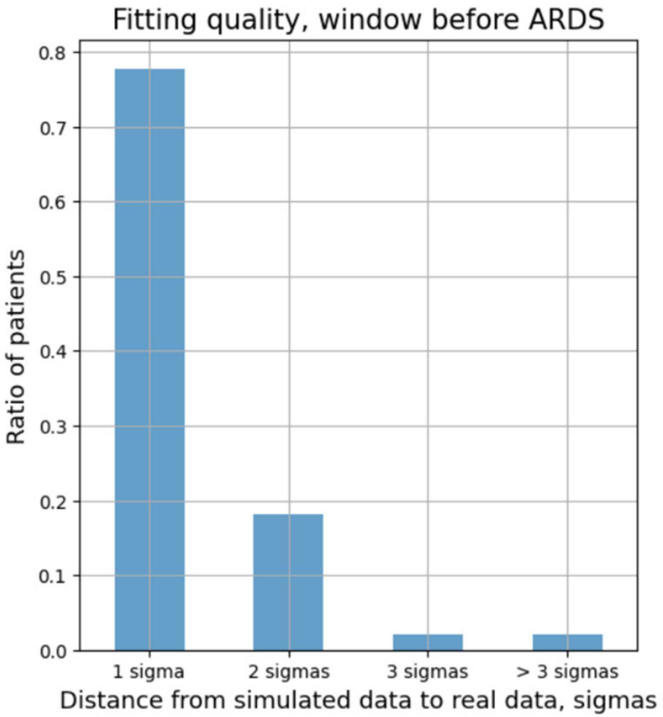
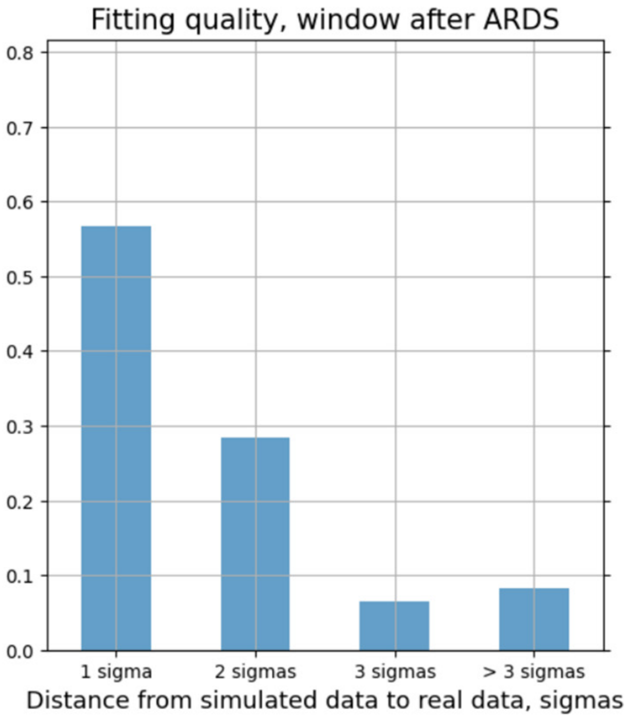
Virtual Patient: Goodness of fit

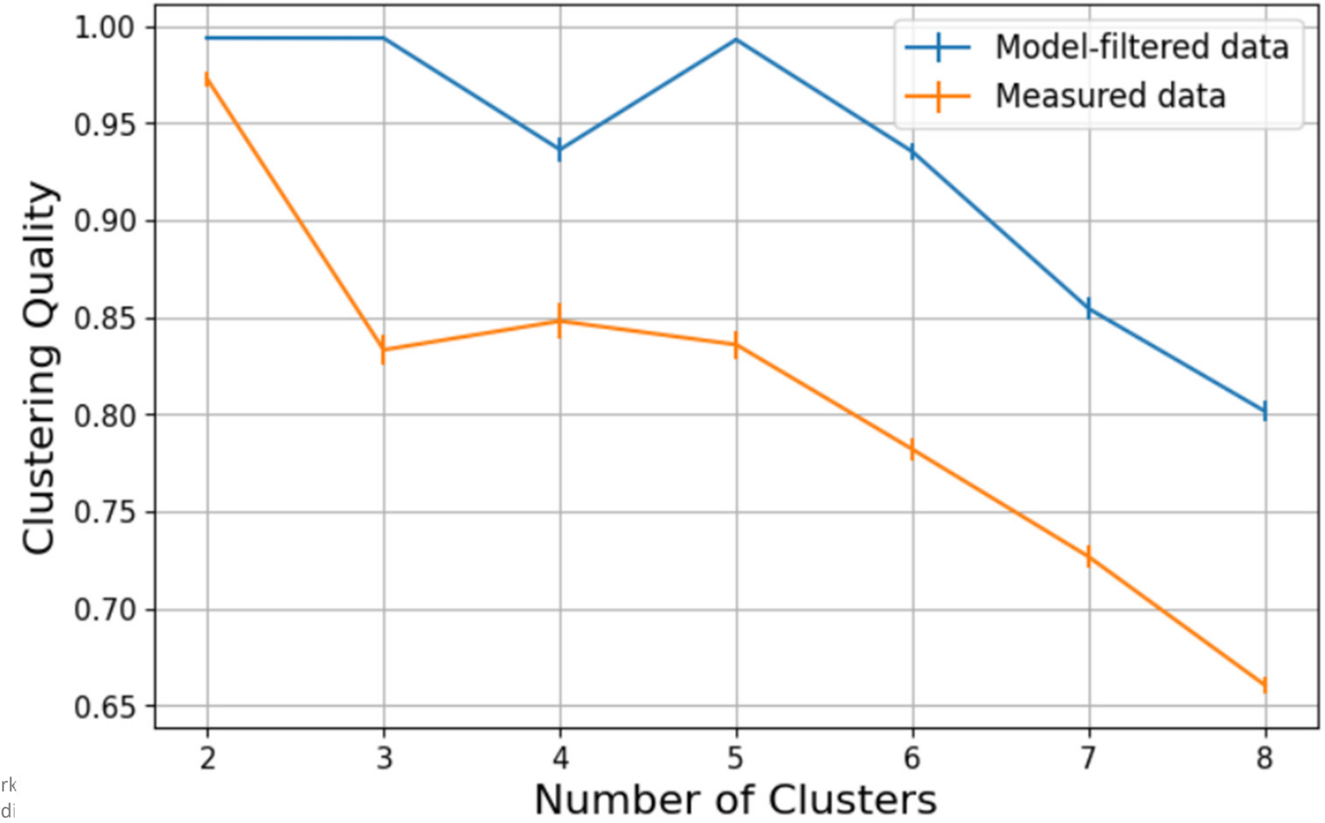




- Cohort of 1007 patients with ARDS suspicion (Horowitz < 300 for 24 hours)
- Before ARDS > 95% of patients can be fit well (2 σ) by the VP
- After ARDS > 84.5% of patients can be fit well
- Overall model shows good fit for 82% of patients (823 patients)
- **Model can fit data both before and after ARDS**

Virtual Patient as model filter

- Calculated list of parameters based on simulator outputs and VP parameters found in the optimization procedure
- Parameters include: number of closed compartments, ventilation, shunted blood fraction, etc. (overall 18 features)
- Performed consensus clustering on original measured data vs. model-based filtered data



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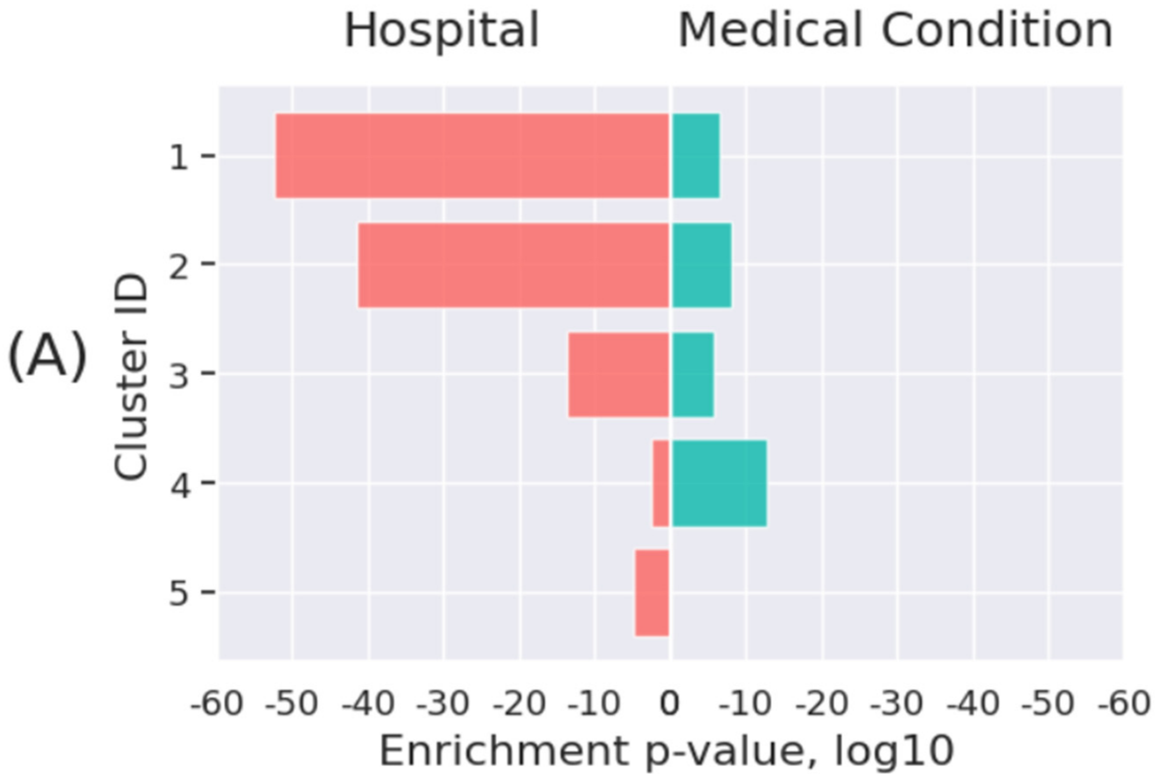
Virtual Patient as model filter

Clustering on **original data**:

- All clusters were found **to be driven by data from one or several hospitals** (enrichment with respect to the hospital)
- 4 out of 5 clusters were dominated by significant over-representation of underlying hospitals, i.e. the highest enrichment was observed with respect to the hospital and not to medical condition
- No ARDS cluster was observed



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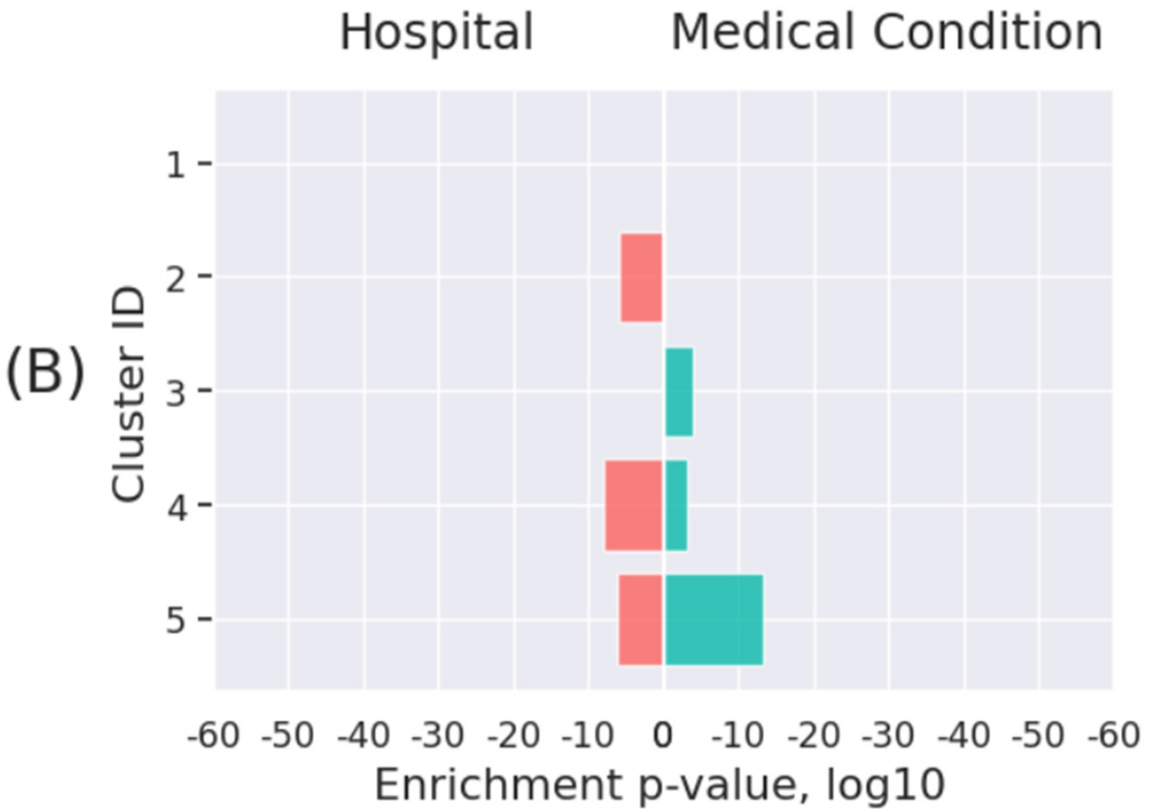
Virtual Patient as model filter

Clustering on **model-based filtered data**:

- **2 mixed clusters** were discovered (no enrichment with respect to a hospital)
- In other 3 clusters, where such over-representation was observed, it was lower, than in the clustering on measured original data
- **ARDS cluster was found**



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Virtual Patient: Results

- Applicability of modeling framework was tested on ARDS use case:
  - Relevant medical information of individual patients with suspicion for ARDS was extracted from observational data of mixed origin (data of 1000 ICU patients)

- Comparison of results of clustering on original measured data and on model-based filtered data revealed following observations:
  - More robust cluster configurations are observed in case of clustering on model-based filtered data
  - Filtered data allowed to reduce biases introduced by different hospitals
  - Filtered data allowed to discover clusters driven exclusively by medicine-related features
  - Filtered data allowed to discover an ARDS cluster.

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Virtual Patient: Conclusions

- A **virtual patient modeling framework** have been developed
  - VP model is adapted to single ICU patients, creating a cohort of digital twins of ICU patients
  - It can be used as a filter to extract medically relevant information from noisy heterogeneous datasets
  - Such modeling covers individuality of single patients and allows personalized modeling
  - It can be used to capture specific features of patient’s state and dynamics while reducing biases introduced by different datasets

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Hybrid ICU data analysis framework: Summary

- The issue of **poor generalization** of ML models and impaired performance in real-world setting becomes more important on the way to personalized medicine
- A strong need for generalization assessment methods
- One of the approaches to solve this issue is creation of gold standard datasets pooled from different hospitals
- Such pooling introduces **selection bias driven by data origin**

- A platform for heterogeneous ICU data integration and analytics has been developed including:
  - Generalization quality assessment framework for assessment of similarity between populations and discovery of possible generalization issues
  - Virtual patient modeling framework: a filter to extract medically relevant information from noisy heterogeneous datasets and reduce selection bias

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Multivariate Analytics: ARDS & Covid

- **Verwendbarer Datensatz aus ASIC – Studie:**

  ca. 4500 Patienten mit mechanischer Beatmung und ausreichender Annotation:

  - Snapshot – Datenstruktur: nur “schwerstmöglicher” Krankheitszustand erfasst
  - Keine Information zur Pathogenese bis zur ICU-Einweisung

  - 4139 Patienten ohne Covid
  - 495 Patienten mit Covid

- Features: Median von 38 routine ICU Parameter über Gesamtaufenthalt

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Globalanalyse mit tSNE

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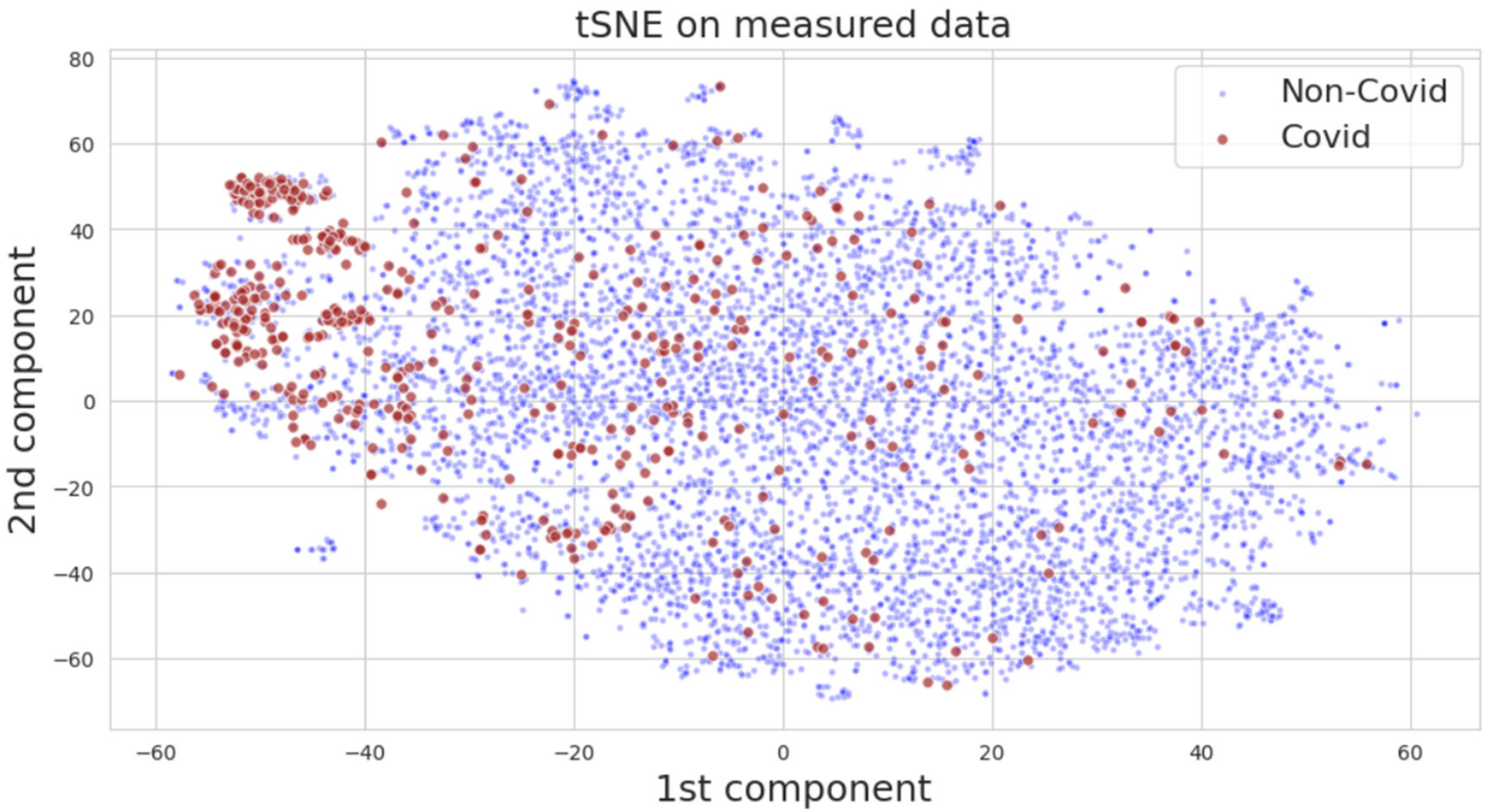

- Wenig markante Cluster
- 40% der Covid - Patienten zeigen Clusterstruktur
  - Häufung von ARDS und hoher Multimorbidität
  - Sehr hohe Mortalität (ca 90%)
- 60% der Covid – Patienten ähnlich zu nicht-Covid Patienten, niedrige Mortalität (20%)

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ARDS & Covid

Mortalität in Covid/severe ARDS Stratifizierung:

	no severe ARDS	severe ARDS
no Covid	0.3	0.54
Covid	0.27	0.6

- Ist die Mortalität ein ARDS-Problem?
- Ist ARDS in Covid lethaler als ohne Covid?

Caveat: Snapshot der Schwerstkranken Patienten: Multimorbidität

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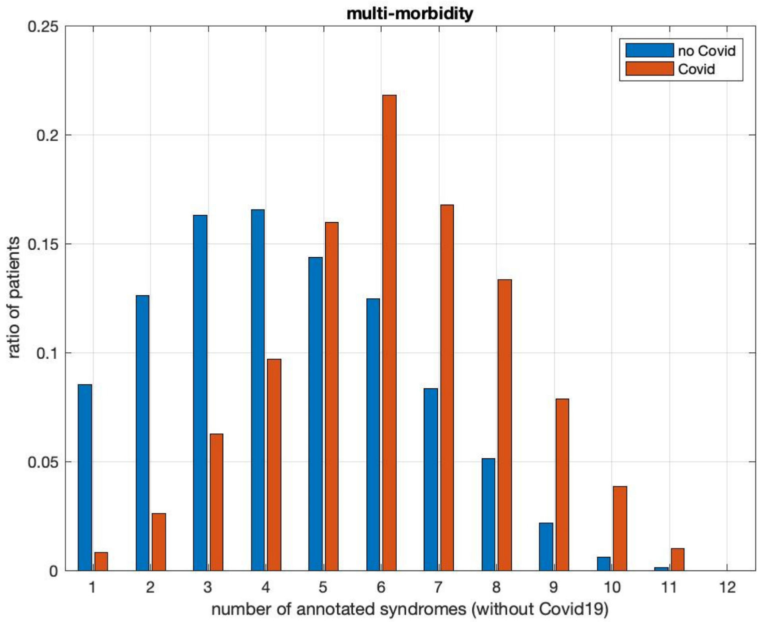
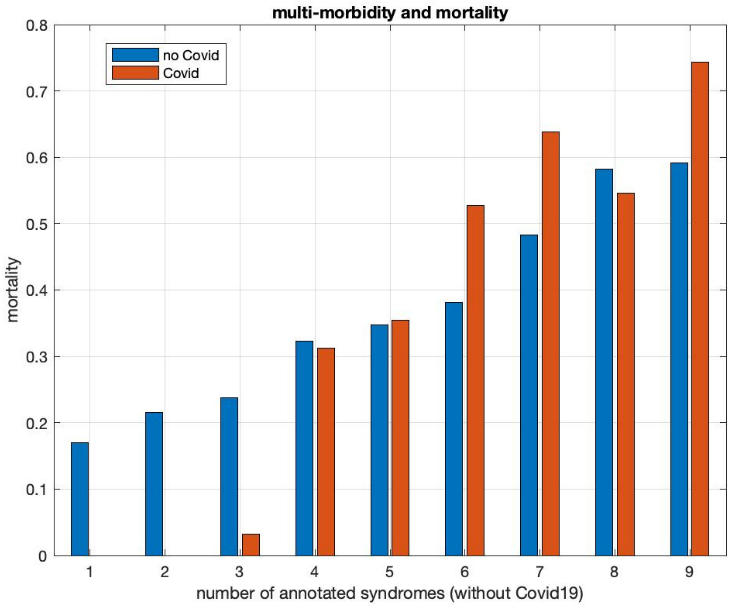
ARDS & Covid - Multimorbidität

- Covid-Patienten habe eine signifikant höhere Multimorbidität als nicht-Covid Patienten
  - 17 Risikofaktoren: Biometrie, Chronische Erkrankungen, Akutsyndrome
  - Mortalität ist **nur** eine Folge der Multimorbidität ?
  - Stratifizierung über **Multimorbiditätskontext** essentiell für belastbare Aussagen





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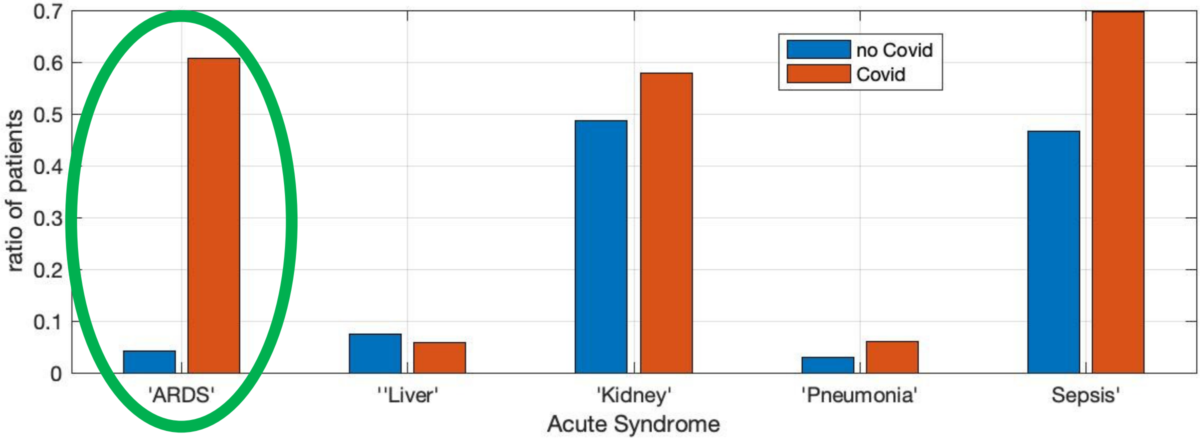
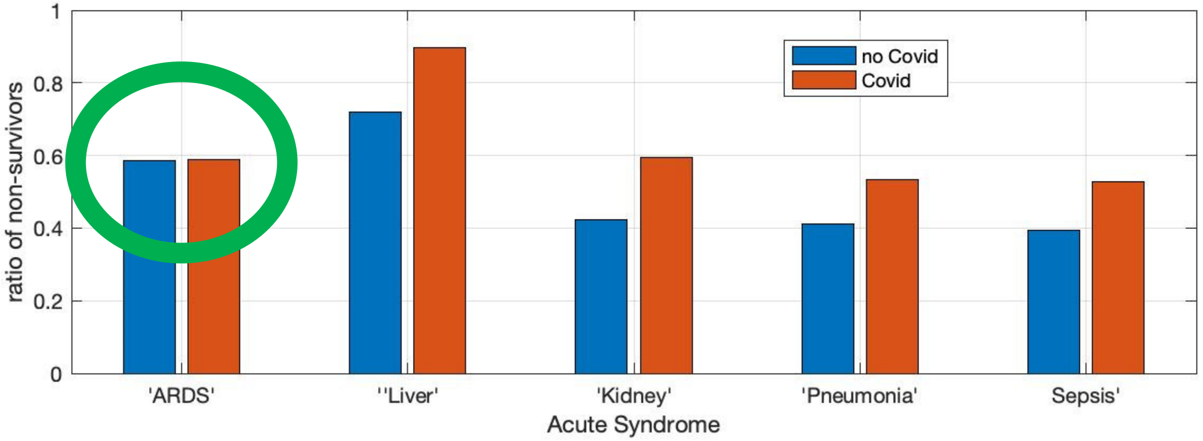
ARDS & Covid – Multi-Akutsyndrome

- Fokus auf ARDS / Leberversagen / Nierenversagen / Pneumonie / Sepsis
- Unifaktorielle Statistik zeigt hohe Prävalenz von (schwerem) ARDS in Covid
- Mortalität bei ARDS scheint nicht von Covid abzuhängen
- **Caveat!**

Prävalenz:



Mortalität:



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ARDS & Covid – Multi-Akutsyndrome

- **Multifaktorielle Stratifizierung nach Multi-Akutsyndromen**
  - Erfasst in Profilgruppen (>20 / >10 Patienten): 97% non-Covid, 92% Covid

ARDS	Liver Failure	Kidney Insuffizienz	Pneumonia	Sepsis	Sum of Syndromes	Prevalence non Covid	Prevalence Covid	Mortality non Covid	Mortality Covid
0	0	0	0	0	0	0.29331	0.086869	0.17298	0.16279
0	0	0	0	1	1	0.14593	0.076768	0.22682	0.13158
0	0	1	0	0	1	0.15753	0.034343	0.28988	0.29412
0	0	1	0	1	2	0.20826	0.11515	0.40023	0.36842
1	0	1	0	1	3	0.028026	0.27879	0.47414	0.68116
1	1	1	0	1	4	0.013288	0.058586	0.81818	0.89655
1	0	0	0	1	2	0.0079729	0.10707	0.30303	0.37736
1	0	1	1	1	4	0.0079729	0.060606	0.51515	0.53333
0	1	1	0	1	3	0.041556	0	0.73256	NaN
0	1	1	0	0	2	0.020295	0	0.63095	NaN
0	0	0	1	1	2	0.013047	0	0.24074	NaN
0	1	0	0	1	2	0.0079729	0	0.54545	NaN
0	0	1	1	1	3	0.016912	0	0.54286	NaN
0	1	0	0	0	1	0.0067649	0	0.25	NaN
0	0	0	1	0	1	0.0086978	0	0.13889	NaN
1	0	0	0	0	1	0	0.072727	NaN	0.36111
1	0	1	0	0	2	0	0.030303	NaN	0.53333

Mortalität Covid
<= Mortalität non-Covid

Mortalität Covid
> Mortalität non-Covid

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ARDS & Covid – Multi-Akutsyndrome

- **Multifaktorielle Stratifizierung nach Multi-Akutsyndromen**
  - In Risikoprofilgruppen **ohne** ARDS ist Mortalität Covid <= non Covid
  - In Risikoprofilgruppen **mit** ARDS ist Mortalität Covid > non Covid
  - Unterschied kann nicht durch chronische Erkrankungen / Biometrische Risikofaktoren erklärt werden.
- **Hypothese:** Covid-induziertes schweres ARDS unterscheidet sich von schwerem ARDS im “Normalfall”
- Deep Dive im Rahmen einer Masterarbeit (Start Sept. 22)

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ASIC System – towards realizing the potential of clinical data

Smart Medical Information Technology for Healthcare

- DEA – Platform to enable Machine Learning for prognosis in ICU
- Virtual Patient – Extracting medical information from RWE data
- Exploring the (unexpected) value of multivariate data – is ARDS in Covid different?
- HPC – based model reduction – towards VP for clinical use

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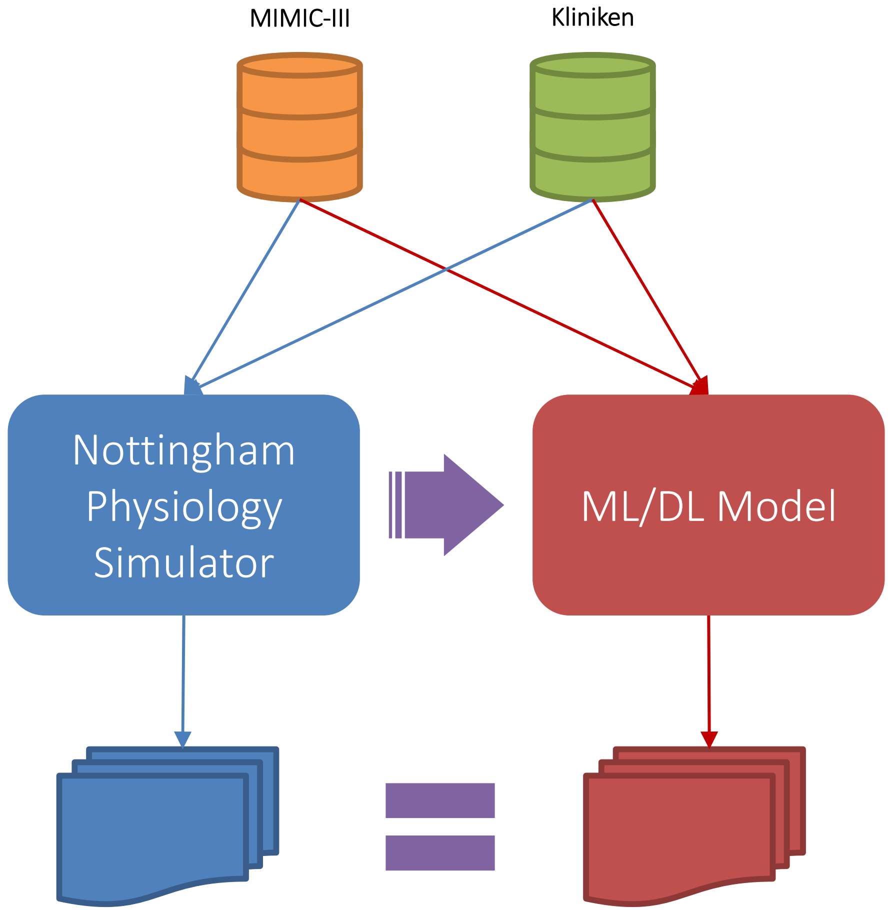
Virtual Patient Model Conversion - Foundations

- Nottingham Physiology Simulator (NPS)
  - Developed Hardman *et al.* and expanded by Das *et al.*
  - Mechanistic model to simulate the pulmonary and cardiovascular systems.
  - Built on Matlab and C.

- The objective is to migrate the model:
  - Same performance.
  - More portable.
  - More compatible.
  - Trainable to new data.



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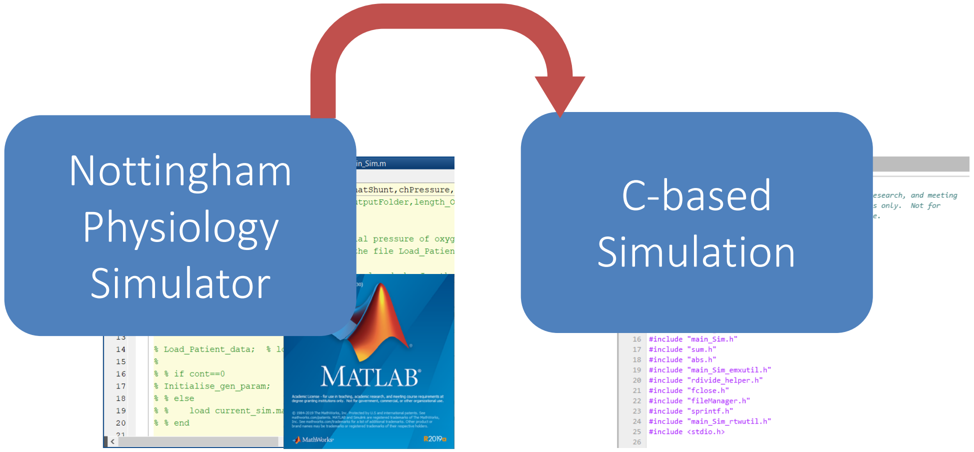
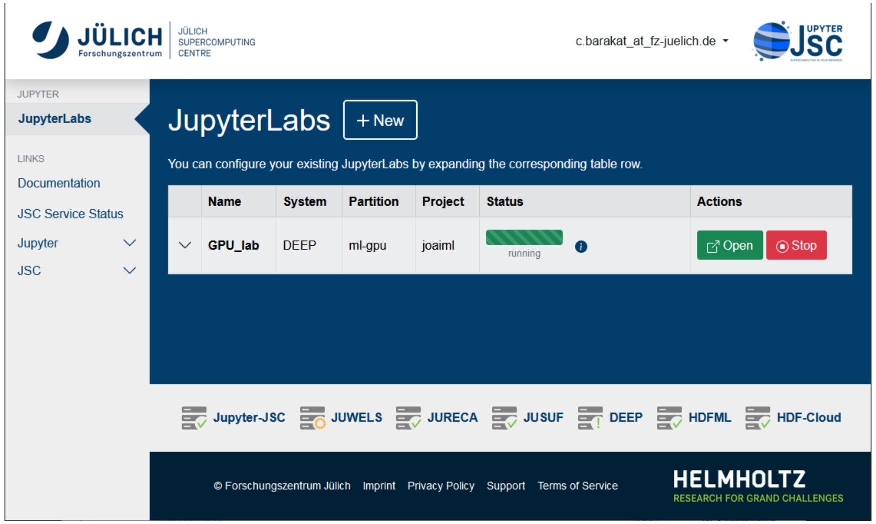
Virtual Patient Model – Preparing the Environment

- Convert the model completely to C.
- Set up a data storage and analysis environment on the DEEP Supercomputer.
- Use High-Performance Computing systems to run simulations in parallel in order to generate output data from the available patient data.
- Prepare an environment with the necessary modules and hardware to build and test the DL model.





JupyterLabs + New

You can configure your existing JupyterLabs by expanding the corresponding table row.

Name	System	Partition	Project	Status	Actions
GPU_lab	DEEP	ml-gpu	joaiml	running	Open Stop

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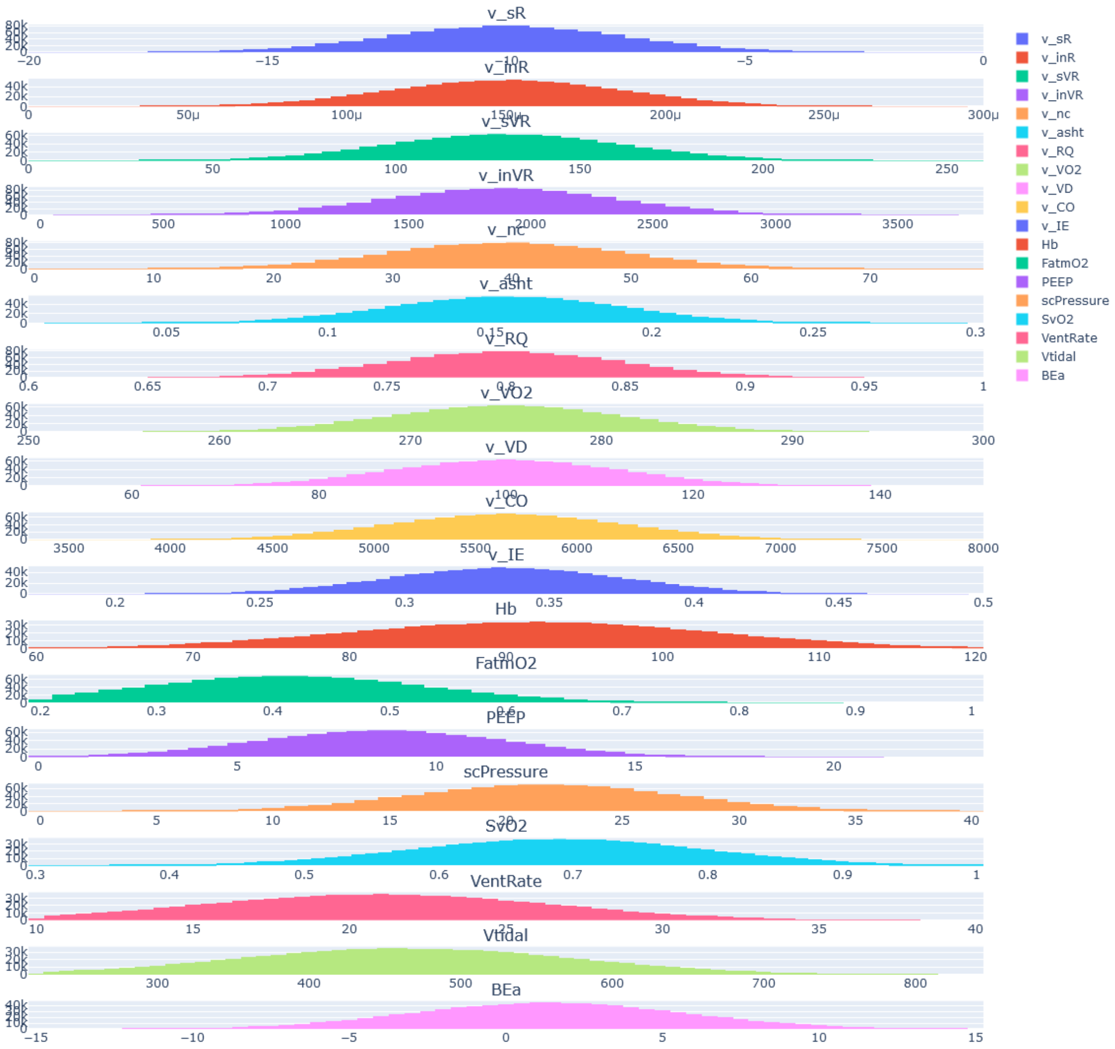
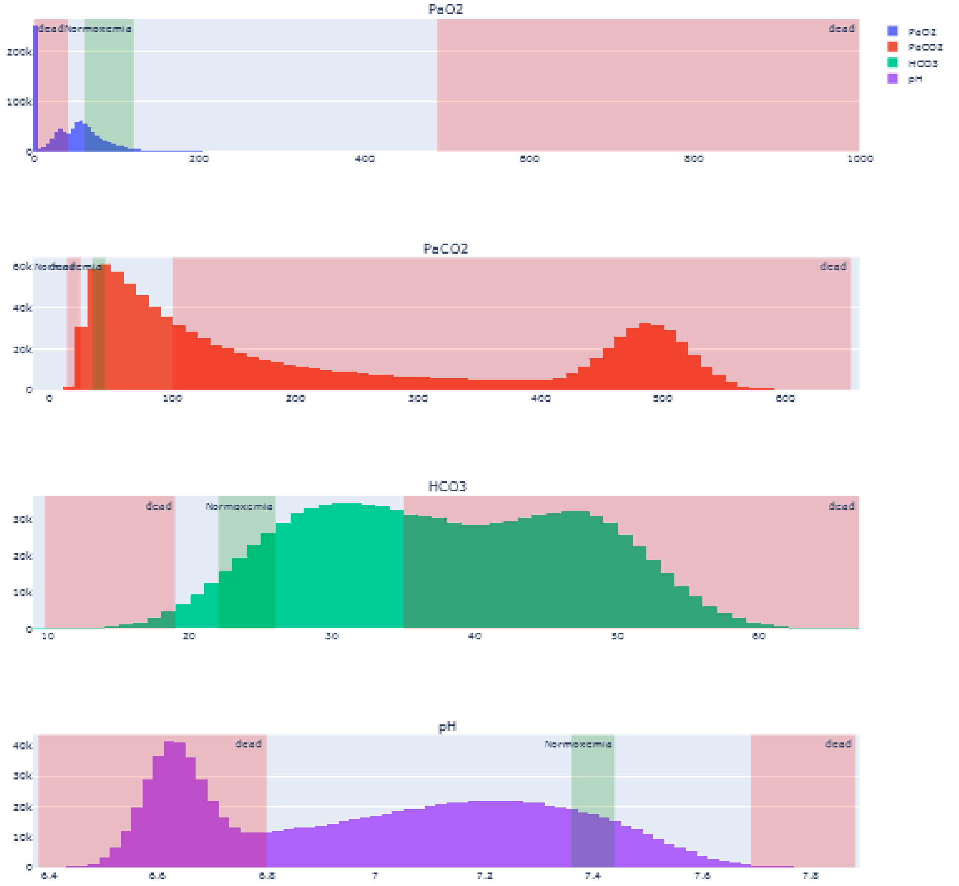
Data Visualisation on the Platform

SMITH
Smart Medical Information
Technology for Healthcare





Titel: ASIC Workshop
Autor: Sharafutdinov
Schutzklasse: SMITH-intern
Folie:

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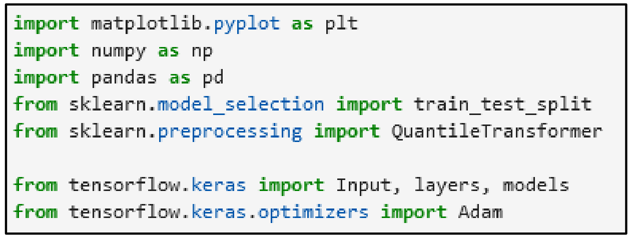
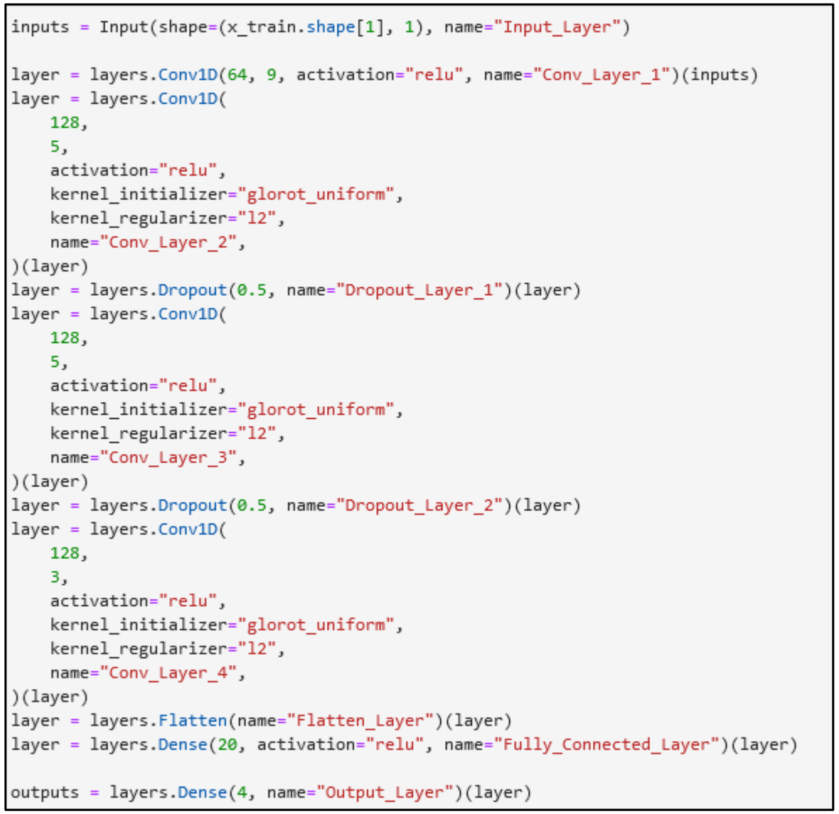
Model Training

- Several models built using Tensorflow and Keras.
- Tested deep fully-connected architectures and deep convolutional neural networks (CNNs) to determine the approaches with most potential for success.
- CNN performance was optimal in this case and a relatively simple model was built with room for tuning in the next step.
- Training process was greatly accelerated by having access to GPUs on the supercomputing nodes.



```python
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import QuantileTransformer

from tensorflow.keras import Input, layers, models
from tensorflow.keras.optimizers import Adam
```



```python
inputs = Input(shape=(x_train.shape[1], 1), name="Input_Layer")

layer = layers.Conv1D(64, 9, activation="relu", name="Conv_Layer_1")(inputs)
layer = layers.Conv1D(
    128,
    5,
    activation="relu",
    kernel_initializer="glorot_uniform",
    kernel_regularizer="l2",
    name="Conv_Layer_2",
)(layer)
layer = layers.Dropout(0.5, name="Dropout_Layer_1")(layer)
layer = layers.Conv1D(
    128,
    5,
    activation="relu",
    kernel_initializer="glorot_uniform",
    kernel_regularizer="l2",
    name="Conv_Layer_3",
)(layer)
layer = layers.Dropout(0.5, name="Dropout_Layer_2")(layer)
layer = layers.Conv1D(
    128,
    3,
    activation="relu",
    kernel_initializer="glorot_uniform",
    kernel_regularizer="l2",
    name="Conv_Layer_4",
)(layer)
layer = layers.Flatten(name="Flatten_Layer")(layer)
layer = layers.Dense(20, activation="relu", name="Fully_Connected_Layer")(layer)

outputs = layers.Dense(4, name="Output_Layer")(layer)
```

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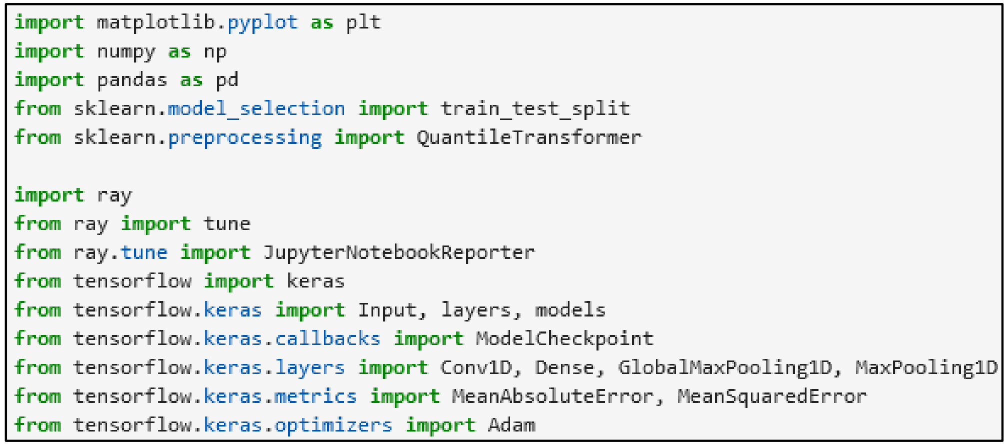
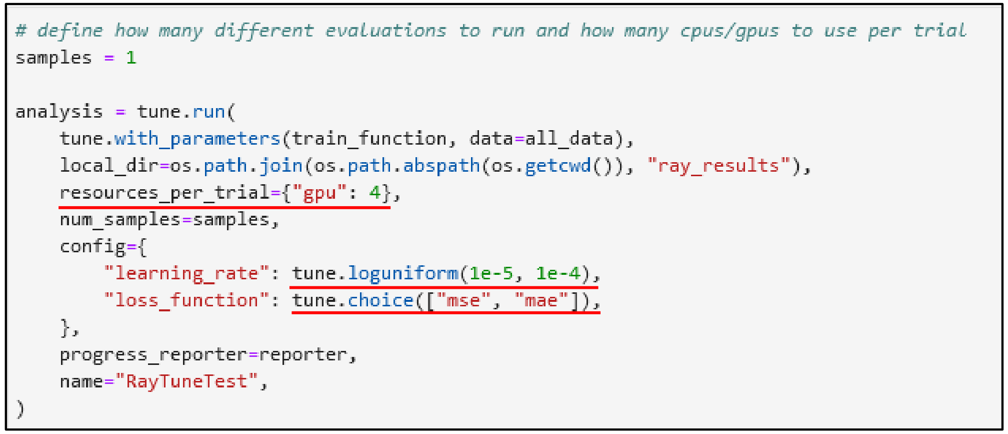
Hyperparameter Tuning

- Using Ray Tune we automated the hyperparameter tuning step.
- The module automatically produces the best performing combination of parameters.
- In this instance we configured the tuner to find the best values for only two parameters.
  - Can be expanded into the network structure.
  - Makes use of the available GPU resources.
  - Can be scaled up to a great extent across several nodes.



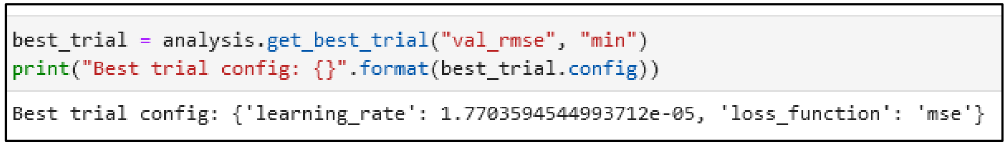
```python
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import QuantileTransformer

import ray
from ray import tune
from ray.tune import JupyterNotebookReporter
from tensorflow import keras
from tensorflow.keras import Input, layers, models
from tensorflow.keras.callbacks import ModelCheckpoint
from tensorflow.keras.layers import Conv1D, Dense, GlobalMaxPooling1D, MaxPooling1D
from tensorflow.keras.metrics import MeanAbsoluteError, MeanSquaredError
from tensorflow.keras.optimizers import Adam
```



```python
# define how many different evaluations to run and how many cpus/gpus to use per trial
samples = 1

analysis = tune.run(
    tune.with_parameters(train_function, data=all_data),
    local_dir=os.path.join(os.path.abspath(os.getcwd()), "ray_results"),
    resources_per_trial={"gpu": 4},
    num_samples=samples,
    config={
        "learning_rate": tune.loguniform(1e-5, 1e-4),
        "loss_function": tune.choice(["mse", "mae"]),
    },
    progress_reporter=reporter,
    name="RayTuneTest",
)
```



```python
best_trial = analysis.get_best_trial("val_rmse", "min")
print("Best trial config: {}".format(best_trial.config))
```

```
Best trial config: {'learning_rate': 1.7703594544993712e-05, 'loss_function': 'mse'}
```

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Results and Conclusions

- Building and training the model was greatly helped by the available hardware at JSC.
- The final model can be easily exported as a standalone model, and implemented in clinics:
  - Does not require special licenses or too much training to implement.
  - Runs offline and can be trained locally.

- The developed platform over which the work was done is of great use:
  - Can be accessed (with special permissions) on Jupyter@JSC
  - Can be implemented onto commercial Cloud Computing resources or University HPC resources.
  - Gives access to data processing and visualisation modules, as well as machine learning and hyperparameter tuning methods.

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Thank you for your attention!

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