Artificial Intelligence in Drug Discovery
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Challenges and Future Role of Artificial Intelligence and Machine Learning in Pharmacovigilance

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26th DGRA Annual Congress
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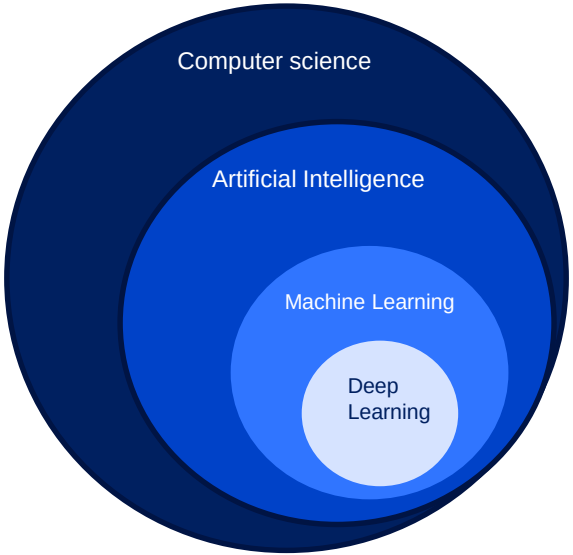


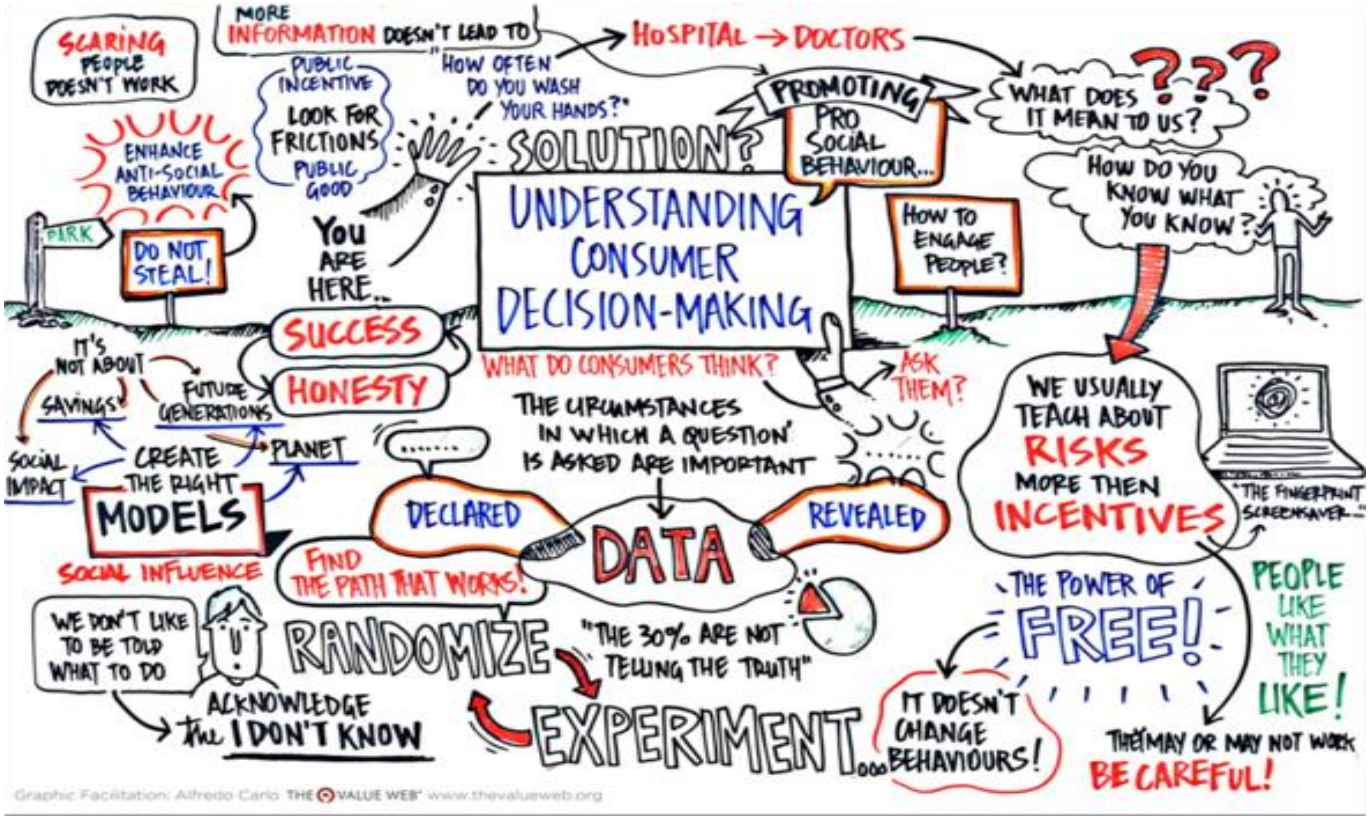
Definition Artificial Intelligence:

- Subfield of Computer Science
- Definition by European Commission‘s AI Communication *(2018)*
  - *"Artificial intelligence (AI) refers to systems that **display intelligent behaviour** by analysing their environment and taking actions – with **some degree of autonomy** – to **achieve specific goals**.*
  - *AI-based systems can be **purely software-based,** acting in the virtual world (e.g. voice assistants, image analysis software, search engines, speech and face recognition systems) or AI can be embedded in **hardware devices** (e.g. advanced robots, autonomous cars, drones or Internet of Things applications).”*

J.K. Aronso (Drug Safety (2022)45:407)

artificial intelligence *n.* a branch of computer science that involves the ability of a machine, typically a computer, to emulate specific aspects of human behaviour and to deal with tasks that are normally regarded as primarily proceeding from human cerebral activity. [Latin: *artificialis*, from *ars*, *artis*, art, and *facere* to make; *intelligens*, prp of *intellegere*, to understand, from *inter*, between, and *legere*, to choose]

AI in drug discovery - Challenges and future role of AI and ML in Pharmacovigilance



Real World Data (RWD): Information from observations of routine clinical practice (prospective and retrospective) Reference to the health status or healthcare of a defined population, i.e. data collection that routinely comes from a variety of different sources following authorization.

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KIMERBA Project at Paul-Ehrlich-Institut overview:

- Project duration: **March 2022 – December 2024**
- Funding: German Ministry of Health (Bundesministerium für Gesundheit, **BMG**)
- Project goal:

„Regulatory use of **Artificial Intelligence (AI)-assisted methods** for efficient **evaluation and regulation** **of vaccines and biomedical drugs**.“

  - **Digitization** of regulatory processes
  - **Facilitation** of improved and standardized regulatory processes **with AI**
    - Regulatory memory
    - Natural language processing (NLP) system
  - **AI use** for improved and standardized **pre- and post-approval** assessment

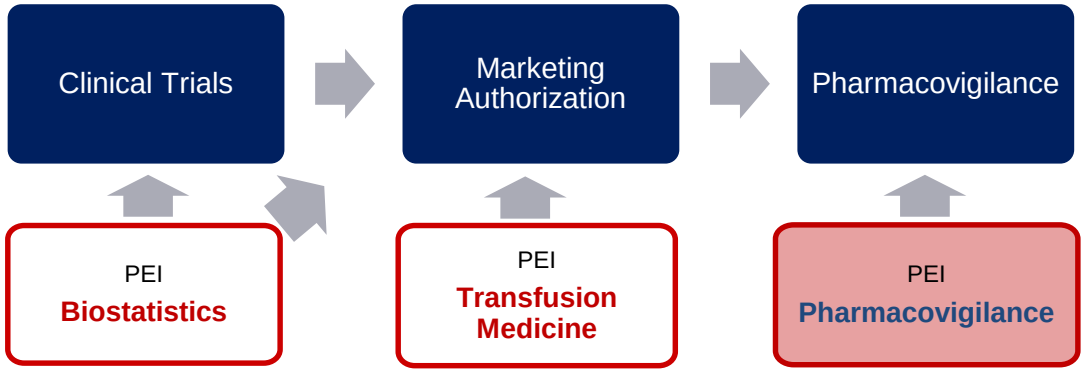
- Tools:
  - **Machine Learning (ML) / Natural Language Processing (NLP)**

KIMERBA – Research project at Paul-Ehrlich-Institut sponsored by BMG

„Regulatory use of **Artificial Intelligence (AI)-assisted methods** for efficient **evaluation and regulation** of vaccines and biomedical drugs.“

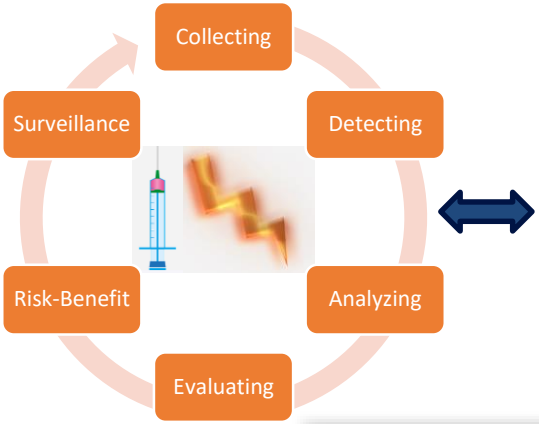
- **AI use** for improved and standardized **pre- and post-approval** assessment:

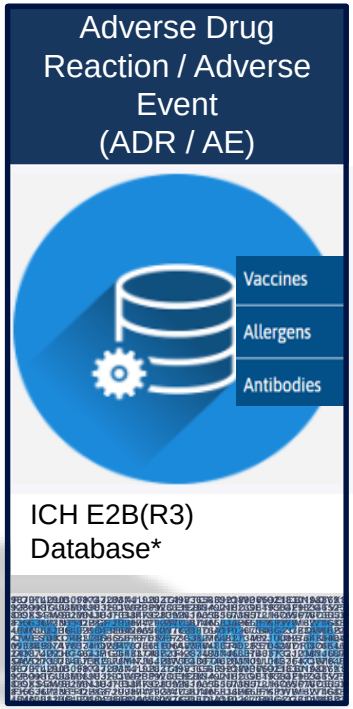
3 Focus Areas



Bundesministerium für Gesundheit

KIMERBA: Focus Area Pharmacovigilance





* ICH E2B(R3) = format of Individual Case Safety Reporting

Project objectives:

„Establishing ADR/AE Reporting via Mobile App to improve Vaccine Surveillance"

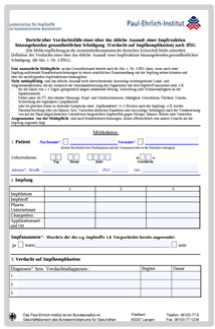
"Explore AI / ML-usage in Data Analysis of ADR Data"

"Digitization & Usage of AI in regulatory processes e.g. ADR Reporting"

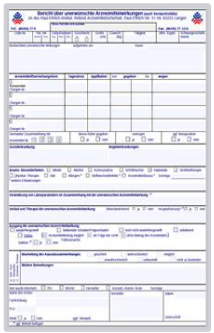
KIMERBA: Focus Area Pharmacovigilance

Scanned document images:

Form 1



Form 2



Doctor's Letter

Goals: extract main entities

- Patient and reporter information
- Suspected drugs
- Adverse reactions
- Relation extraction between Drugs and Reactions

Data Base

Approximately 7,603 PDF documents

- ~ 23,007 scanned pages
- ~ 2,955 structured reporting forms

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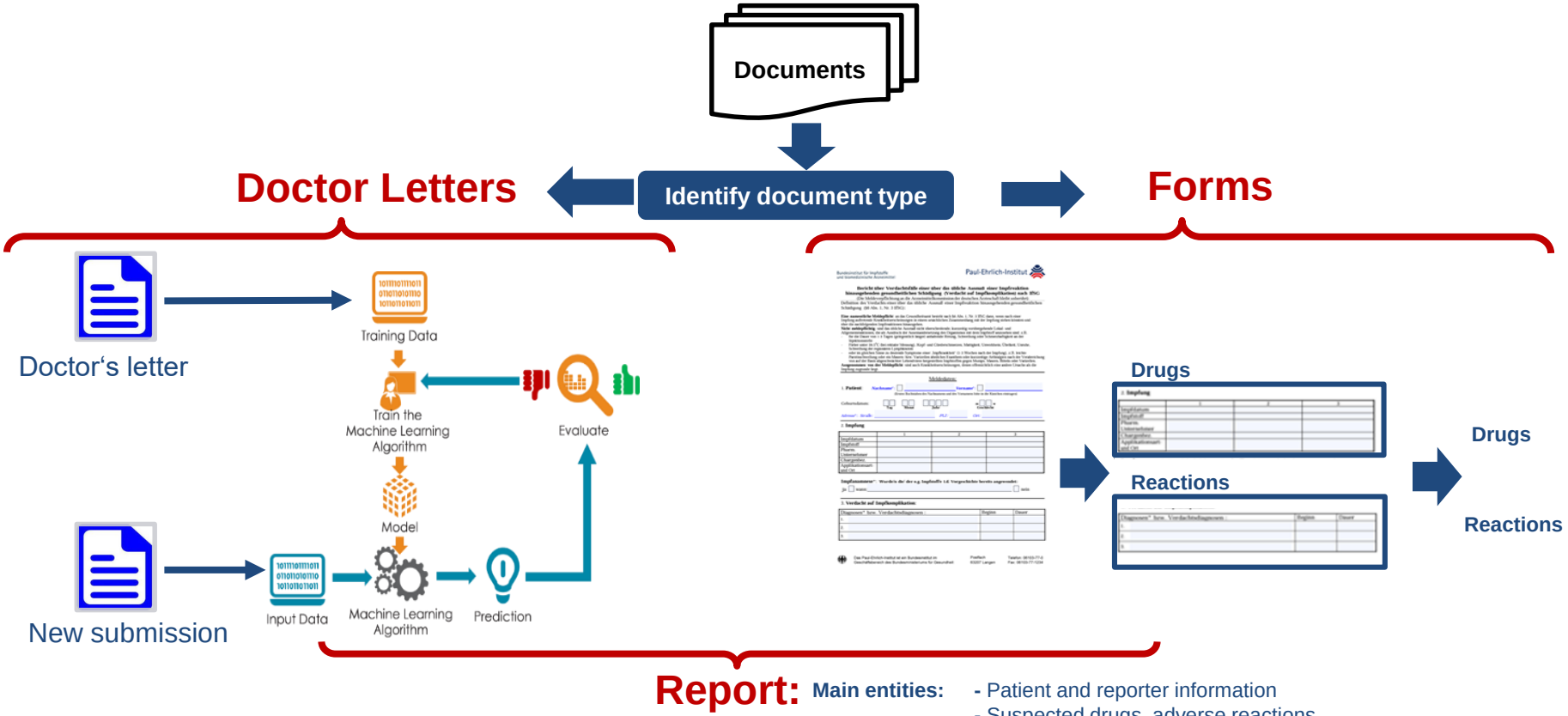


Report: **Main entities:**

- Patient and reporter information
- Suspected drugs, adverse reactions
- Relation extraction between Drugs and Reactions

AI-assisted Adverse Drug Reaction (ADR)
Data Analysis & Data Visualisation:

Available data: 2 datasets

- Dataset A ~ 350.000 patients: (app. 1 Mio data packages)
  - **Unsolicited** ADR reports on COVID-19 vaccines from inhouse **Vigilance One Ultimate database**

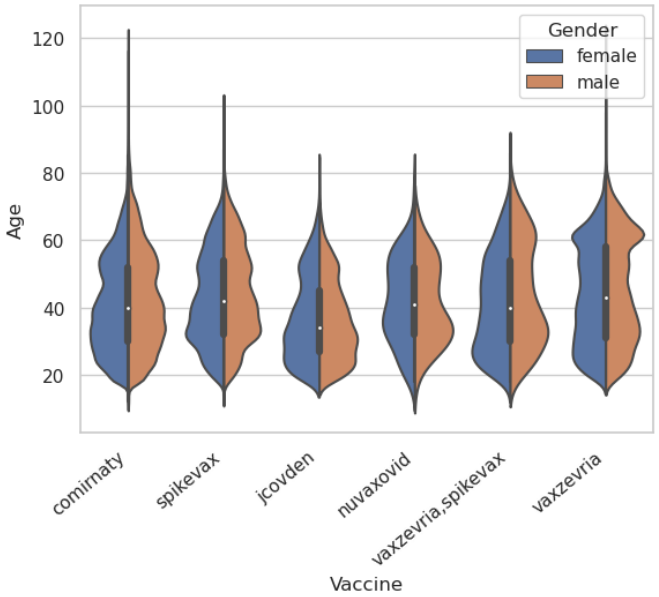
- Dataset B ~ 750.000 patients (app. 10 Mio data packages)
  - **Prospective questionnaire on tolerability of** COVID-19 vaccines reported during observational study SafeVac 2.0 (**ADR reporting via mobile-application**)

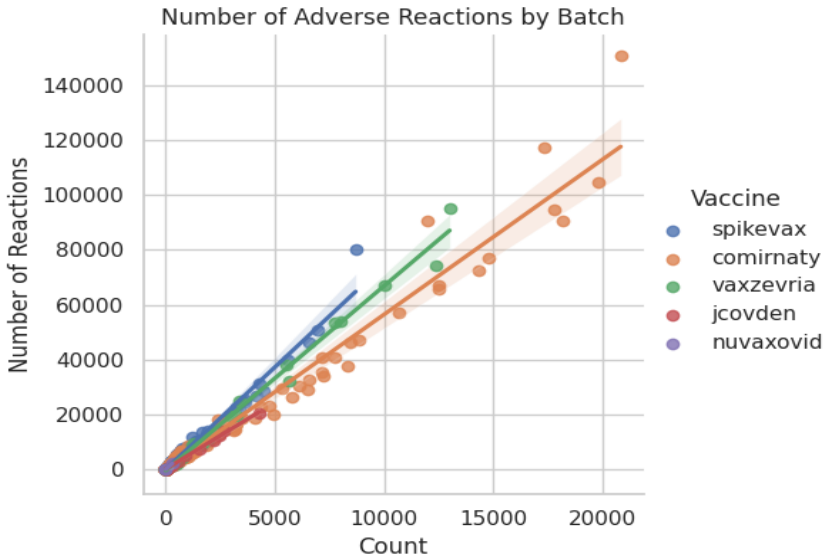
AI-assisted Adverse Drug Reaction (ADR) Data Analysis & Data Visualisation:

Goal: Use of AI / ML-techniques for…

- Data analysis
  - Descriptive analysis
  - Advanced analysis
    - » Identify hidden patterns (e.g. Cluster of Reports, Cluster of Drug-ADR-associations)
- Data visualisation
  - Enable visual discovery and communication of data characteristics, data insights, …

AI-assisted Adverse Drug Reaction (ADR) Data Analysis & Data Visualisation:





Résumé 2024

- Increased capacity is needed both for development of AI-based tools to increase efficiency in routine and standardised tasks in regulatory assessment.
- In routine and standardise procedures AI and ML based tools are likely to reduce errors linked to repetitive tasks.
- Hence, in the majority of processes in regulatory procedures AI an ML will have impacted on increasing data quality
- Finally, this investment could help to free up time from existing experts to focus specific tasks outside standardised pathways in regulatory processes.
- However, (nothing is for free) mind change is needed to accept, that investment infrastructure and AI and ML tools is warranted.

AI in drug discovery - Challenges and future role of AI and ML in Pharmacovigilance

Lead Research Group
- Dr. Renate König, (Head of FoG3)
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Acknowledgment to the KIMERBA- PhV Team at PEI

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