

Certificate Course

# Artificial Intelligence in Drug Development (AIDD)

October 2025 - May 2026

### **Key Highlights**

- Flipped-classroom approach
- 10-day virtual, expert led workshop
- End-to-end case studies
- Capstone Project

# Weekly Effort 4-6 Hours a Week



### **Learning Mode**

Online + 10-day virtual workshop





Students, Graduates and above



### Certification

Certificate of Completion/ Attendance

### **Learning Experience**

### Pre-recorded lectures, guided materials

Flexible learning that works with your schedule

### Mentors with global impact

Learn from the leading academic and industry experts

### 10 days immersive virtual workshop

Blend theory with hands-on, project based leaning experience

### **Licensed softwares & tools**

Complimentary to state of the art, industry standard softwares and tools

# **Structured Virtual Learning**

Oct 2025 - Feb 2026

- Self-Paced
- Access to lectures, materials & software
- · Assignments & exercises



# Project-Based Learning

Mar 2026 Mode: Online

Phase I

- Virtual workshop
- In-depth training
- Capstone project
- Case studies

### **Submission & Certification**

May 2026

- Project submission
- Final assessment
- Certification (Completion/attendance)



### **Frequently Asked Questions**

### Is there a qualifying mark to receive the final certification in this course?

Yes. To successfully complete the course and receive a digital certificate of completion, participants must achieve a minimum score of 70% in all required assignments. A certificate of attendance will be provided to the participants who complete phase one and attend the virtual workshop.

#### What if I miss an assignment deadline? Can I submit it later?

Assignments not submitted by the due date will be considered late. Late submissions are accepted until one week after the course end date. Please note that feedback will not be provided for late assignments.

### Will there be dedicated doubt-clearing sessions?

Yes. Weekly office hours will be conducted throughout the duration of the course to address participants' questions.

#### How long will I have access to the learning materials?

You will have access to the online platform, including videos and all course materials, for 12 months from the course start date. Access is limited to registered participants as per the terms of use.

#### What software tools will I learn?

Participants will receive hands-on training in Pumas and DeepPumas, advanced tools for pharmacometrics modeling and scientific machine learning.

#### How long will I have access to the licensed software?

Students: Free access (academic license).

Industry participants: A 6-month evaluation desktop license.

### What is the teaching methodology?

We follow a Flipped Classroom approach:

Phase 1: Self-paced learning of theoretical concepts.

Phase 2: Hands-on, collaborative virtual workshop to apply your knowledge.

#### Do I need prior experience in pharmacometrics or machine learning?

Prior exposure to basic machine learning is helpful but not required. The course is designed to build your knowledge from foundational concepts to advanced applications, making it accessible to participants without prior experience.

#### Can international participants apply?

Yes. International participants are welcome. Please note that the default country in the registration form is India—this can be updated during registration. For more information write to us at <a href="mailto:connect@sophas.net">connect@sophas.net</a>.

### Will I receive support after the course if I have further questions?

Yes. Participants will have access to discussion forums to engage with instructors and peers even after the course ends.

# **Course Highlights**



20+

Recorded video lectures and curated readings for foundational learning



10+

Hands-on assignments and exercises designed to reinforce key concepts in machine learning and SciML



Real-world case scenarios-SciML applications in drug development



10

Days of intensive virtual workshop with expert-led sessions



3

Phases: Virtual learning, virtual workshop, and project submission



1

Capstone project simulating advanced AI-driven analysis in drug development using real-world case data



Advanced software tools: Pumas & DeepPumas for Pharmacometrics & SciML



Led by global experts from Pumas-AI & AI/ML leader from A\*STAR



Training aligned with global regulatory expectations



Be part of a global learning community advancing Aldriven drug development in collaboration with PumasAl and SOPHAS



## Unit 1

# **Programme Modules**

### **Machine Learning Fundamentals**

Basic concepts

- Definition of "learning"
- · Continuous and discrete data
- Data imputation
- Model evaluation
- Cross-validation
- Hyper-parameters

Introduction to Supervised Learning

- Decision tree
- k-nearest neighbors (kNN)
- Ensembles
- Random forest
- Gradient boosting (XGBoost)

Introduction to Unsupervised Learning

- Principal component analysis
- k-means and k-medoids clustering

# Neural Networks and SciML (Scientific Machine Learning)

Neural Network (NN) Essentials

- Universal approximation theorem
- Perceptron
- Activation functions
- Multi-layer perceptron (MLP)
- NNs in supervised learning
- NNs in unsupervised learning

#### Regularization

- · Ridge regression
- LASSO (Least Absolute Shrinkage and Selection Operator)

Neural Networks in Low Data Regime

- Transfer learning
- Self-supervision
- Data augmentation

Time Series Modelling

- Discrete-time NNs (RNN, LSTM, GRU)
- Neural ordinary differential equations (NeuralODEs)
- Universal differential equations (UDEs)
- Scientific machine learning (SciML) for pharmacometrics

#### Explainability

- SHAPELY (SHapley Additive exPlanations)
- LIME (Local Interpretable Model-agnostic Explanations)

### **Generative Modeling**

Generative models

Unit 3

- Probabilistic principal component analysis
- Nonlinear mixed effects (NLME) models as generative models
- Variational autoencoder (VAE) as NLME + amortized learning
- Dimension reduction and clustering using generative models
- Normalizing flows

Conditional Generative Models

- Conditional VAE
- Scientific NLME models as conditional generative models
- Generative neural ODEs
- DeepNLME

Model Fitting and Evaluation

- Understanding the marginal likelihood
- Information criteria vs cross-validation

Generative adversarial networks (GANs)

- Adversarial learning and Jensen-Shannon divergence
- Optimal transport and Wasserstein GAN

### **Drug Development Case Studies**

Unit 4

### **Case Studies**



### Predicting drug response for a new patient

We will predict whether a new patient responds to a drug or not given their characteristics. This enables the identification of which variables are most associated with a drug response.



### **Predicting pharmacokinetic parameters**

We will predict the pharmacokinetic parameters of a patient given a number of baseline covariates. This allows for better baseline prediction of the drug exposure level over time.



### Modeling and predicting time-course of neutropenia

We will test and compare a machine learning (ML) model, the Friberg model, and a hybrid ML-Friberg model at modeling and predicting the time-course of neutropenia data.



### Tumor growth dynamics and overall survival

We will fit complex and diverse tumor size data and use it to predict overall survival in a population. This can be used to evaluate the efficacy of a new oncology treatment.



### **Clustering tumor responses**

We will cluster tumor size time-courses and other longitudinal data. This can be used to automatically identify sub-populations in the data.



### **Clustering and modeling biomarkers**

We will cluster a large list of biomarkers and identify which of them are most associated with a clinical endpoint.



### Better trial simulation using generative models

We will improve the quality of trial simulations from a model by enhancing it using generative machine learning.



### **Orientation Week**

The first week is an orientation to introduce you to fellow participants and familiarize with the learning platform and tools.

# Learning Journey



### Self-paced, Flexible **Online Learning**

Phase 1: Structured Virtual Learning, 5 months (1 Oct 2025 to 28 Feb 2026) Learn online through recorded lectures, guided materials, and licensed tools, with a flexible commitment of 4-6 hours/week.



### Office Hour Sessions

Attend weekly online sessions to clear doubts and review key concepts. Assignments will be graded by the grading team.



### **Weekly Goals**

As you begin the programme, focus on weekly goals like completing assignments before their deadlines.



### **Project-Based Workshop** (Virtual)

Phase 2: Project-Based Learning, 10 days (Mar 2026) Apply your knowledge through a hands-on capstone featuring real-world datasets, Pumas software, and expert sessions.



### **Final Submission & Certification**

Phase 3: Submission & Certification (May 2026)

Certificate of Attendance: For completing online sessions and virtual workshop Certificate of Completion: For successful project submission

### **Course Certificate**

Based on participation and performance, learners will be awarded one of the following:

- Certificate of Attendance: For those who complete the virtual learning and attend the online 10-day workshop.
- Certificate of Completion: For those who submit the capstone project and meet performance criteria.

These certificates formally acknowledge the participant's proficiency in leveraging artificial intelligence techniques to advance drug development processes and make data-driven decisions.





## Why This Programme?



Understand key machine learning concepts and their direct applications in pharmacometrics modeling and drug development workflows.

Work with advanced tools purpose-built for SciML & pharmacometrics modeling in realworld data environments.





Master AI techniques to identify prognostic factors, explore datasets, and make statistically sound decisions in clinical development.

Use tools like LIME and SHAP to interpret complex models and ensure transparency in drug development pipelines.





Align your AI-driven approaches with international regulatory standards relevant to model-informed drug development.

Dive into advanced modeling frameworks like DeepNLME and NeuralODEs that combine domain knowledge and deep learning.





Develop a robust approach to evaluating AI models and choosing between traditional, ML-based, or hybrid strategies.

Participate in a collaborative, interdisciplinary learning environment supported by SOPHAS and Pumas-AI thought leaders.



### **Course Instructors**



DR. MOHAMED TAREK
Senior Product Engineer
PumasAl

Dr. Tarek is a Senior Product Engineer at PumasAI and Research Affiliate at the University of Sydney. His expertise spans mathematical modeling, optimization, machine learning, and Bayesian inference. He holds a Ph.D. in Computer Science from UNSW, where he focused on accelerating topology optimization for automated structural design. He also maintains the open-source projects TopOpt.jl and Nonconvex.jl.



DR. VIJAY IVATURI
CEO
PumasAl

Dr. Ivaturi is a pharmacometrician, academic, and biotech leader advancing PK/PD modeling, precision dosing, and regulatory science. He is Co-Founder and CEO of PumasAI, President of ISoP, and Endowed Chair at the Center for Pharmacometrics, Manipal. He holds a B.Pharm from MAHE, an M.S. from St. John's University, and a Ph.D. from the University of Minnesota, followed by a postdoctoral fellowship at Uppsala University. His work drives innovation in model-informed drug development through science, education, and global collaboration.



**DR. JAMES LU**Senior PI, Bioinformatics Institute,
A\*STAR

Dr. Lu is Senior Principal Investigator at the A\*STAR Bioinformatics Institute, where he leads AI research in clinical data modeling and drug development. Formerly at Genentech, he pioneered the application of AI in drug R&D. He serves as Co-Chair of the IQ Consortium AI/ML Working Group and sits on the Editorial Board of CPT: Pharmacometrics & Systems Pharmacology.

### **Course Instructors**



MR. LUCAS PEREIRA
Product Engineer
PumasAl

Lucas holds a master's degree in mechanical engineering from Poli-USP, focusing on accelerating mechanical design through neural networks. During his research, he developed a profound interest in simulations, numerical analyses, AI and statistics. At PumasAI, he is a member of the product engineering team, driving advancements in AI and optimal design. This includes tutorials, features, maintenance, webinars, experiments and research.



**DR. ANTHONY BLAOM**Scientific Computing Consultant,
Co-Creator of MLJ

Dr. Blaom is a mathematical researcher who also works as a scientific computing consultant, with a special interest in Machine Learning. He is a co-creator and lead contributor to MLJ, the popular Julia machine learning platform launched by the Alan Turning Institute in 2019. Dr. Blaom has extensive experience teaching university mathematics and related subjects and has been a Mathematics Lecturer and a Computer Science Senior Research Fellow at the University of Auckland. He holds a Ph.D. degree in Mathematics (Caltech), an M.Sc. degree in Aeronautics (Caltech), and B.E. degree in Mechanical Engineering (Univ. of Melbourne). His current mathematical research is in the area of Differential Geometry.

# **Hands-on Learning with Pumas**

Pumas combines cutting-edge science, advanced artificial intelligence, and powerful computing to revolutionize and streamline the drug development process.



Designed to deliver precision, speed, and adaptability, Pumas is the fastest and most advanced tool for comprehensive drug development analysis. It integrates state-of-the-art algorithms and superior solver technology to handle complex pharmacokinetic and pharmacodynamic models, setting a new gold standard in the industry.

Pumas stands out with its unmatched technical capabilities and continuous innovation, driving the pace of innovation in pharmacometrics. Trusted by leading pharmaceutical companies and regulatory bodies worldwide, Pumas ensures that your drug development process is efficient, accurate, and regulatory-ready.





- Non-Compartmental Analysis
- Dose Proportionality & Bioequivalence
- Nonlinear Mixed-Effects Modeling
- Physiologically Based Pharmacokinetics
- Quantitative Systems Pharmacology
- Clinical Trial Simulations
- Bayesian Estimation





## Hands-on Learning with DeepPumas



DeepPumas<sup>™</sup> is a pioneering platform that unites scientific modeling with machine learning to drive business intelligence and healthcare insights. By combining domain expertise with advanced data-science techniques, it minimizes the need for massive datasets and accelerates decision-making.

Discover hidden connections across biomarkers, outcomes, QSP, QbB, genomic data, and more. Prevent overlooked trends, productivity losses, and the pitfalls of limited datasets. With DeepPumas<sup>TM</sup>, you can identify target patients, optimize manufacturing processes, and build more robust QSP models with greater confidence.

```
df = CSV.read("data.csv", DataFrame)
pop = read_pumas(
   df,
    observations=[:WBC];
    id=:ID,
    time=:TIME.
    rate=:RATE,
    covariates=[:x0],
    evid=: EVID,
    event_data=true,
# Define DeepNLME Model
deepnlme_model = @model begin
    @param begin
        tvKtr ∈ RealDomain(: lower = 0.01)
        tvSlope ∈ RealDomain(; lower = 0.01)
        tvB ∈ RealDomain(; lower = 0.01)
        tvB0 ∈ RealDomain(; lower = 0.01)
        \Omega \in PDiagDomain(; init = fill(0.1, 6))
        tvF_B ∈ MLPDomain(
```

## **Course Details**

Course Start Date: Ocotber 1, 2025

**Course Duration:** 8 months

**Couse Fee:** 

Category	INR (₹) Fee	USD (\$) Fee	EUR (€) Fee
Students	2,00,000	\$2,500	€2000
Academics	2,50,000	\$3,000	€2,500
Industry	4,00,000	\$4,500	€4000

Workshop Mode: Virtual



### **About Us**



PumasAI is a global healthcare intelligence company with a vision to accelerate precision healthcare for patients. Proprietary software developed by the company includes the Pumas suite of products, an integrated modeling and simulation platform designed to multiply productivity across the drug development lifecycle, and Lyv, a clinical decision support system that leverages patient history and targeted medical data for personalized healthcare delivery. Scientists at PumasAI provide consulting with leading pharmaceutical innovators in clinical pharmacology, model-informed drug development, pharmacometrics, front-end applications, and more.



Pumas



**Deep**Pumas



Pumas CP



**Ask**Pumas



Scientific & Strategic Consulting Services

### **Learn more**



### **About Us**



Society of Pharmacometrics & Health Analytics is a professional society dedicated specifically to quantitative sciences within clinical pharmacology and broadly in health data analysis

This society has its roots in the "Population Approach Group in India – PAGIN" started in the year 2008 and has successfully propagating pharmacometrics in India ever since. PAGIN is known around the world and recognized by other pharmacometric societies for its annual pharmacometric workshops. The SOPHAS society is working with an expanded mandate including health care data analytics along with our core focus on pharmacometrics in drug development and clinical applications.

### **Learn more**







# Register for the Artificial Intelligence in Drug Development course here

AIDD CERTIFICATE COURSE - REGISTER NOW

For bulk registrations, reach out to us at **connect@sophas.net** and unlock a smoother, faster onboarding experience.

### **Organized by**

PumasAI
Society of Pharmacometrics and Health Analytics (SOPHAS)