

# Konstantinos Pantazis

Data Scientist | Scientific AI | Industrial Process Optimisation | Digital Twins

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## PROFILE

Data scientist and applied mathematician with a Ph.D. in mathematics, building **scientific AI and machine-learning models for physical and industrial systems**. Experience spans **surrogate modelling, empirical/physics-informed feature engineering, optimisation, graph learning, uncertainty-aware evaluation, active learning, and production-oriented ML pipelines**. Current work focuses on a **digital food-extrusion intelligence platform** that combines recipe, process, lab-trial, and multiphysics descriptors to support virtual experimentation, calibrated prediction, and trust-aware recommendations. Strong interest in roles involving **complex systems, limited/noisy data, industrial decision support, and hybrid ML for real-world operational environments**.

## TECHNICAL SKILLS

**Scientific AI & Process Modelling:** surrogate modelling, model calibration, automated retraining, active learning, transfer learning, uncertainty quantification, statistical inference, process optimisation.

**Machine Learning & Analytics:** regression/classification, clustering, feature selection, feature engineering, model evaluation, graph ML, network alignment, graph matching, recommender systems

**Programming & Data Systems:** Python, SQL, R, MATLAB, VSCode, Power BI, REST APIs, scikit-learn, PyTorch, TensorFlow, Polars, NetworkX.

**LLMs & NLP:** HuggingFace, BioBERT, LangChain, RAG, RAGAS, TruLens, Pydantic, LLM APIs, graph-based retrieval.

## PROFESSIONAL EXPERIENCE

### Deus Ex Machina / PIPA AI

Sep. 2024 – Present

*Data Scientist*

Athens, Greece

- Own the ML/data-science intelligence layer for a **digital food-extrusion platform**, supporting virtual recipe screening, product-property prediction, process optimisation, and guided lab experimentation.
- Integrated recipe composition, controllable operating settings, historical lab trials, and multiphysics descriptors from mechanistic modelling into reproducible ML-ready pipelines, including target-specific feature-selection workflows.
- Developed staged predictive workflows combining extrusion-success classification, target-specific regression models for final product attributes, and optimisation routines for operator-controllable process settings.
- Implemented active-learning workflows to propose informative follow-up lab trials when model confidence is low, accelerating recipe onboarding and reducing unstructured trial-and-error experimentation.
- Built end-to-end ML pipelines for heterogeneous scientific and food datasets, including feature selection, automated retraining, BioBERT-based featurisation, hyperparameter tuning, and regression/classification models for sensory and molecular-property prediction.
- Engineered and evaluated LLM/RAG and graph-based RAG workflows for biomedical and scientific information extraction using frameworks such as RAGAS and TruLens, improving extraction accuracy from below 80% to 93% .
- Communicated clear, actionable insights through reports and presentations for both technical and non-technical stakeholders.

### Johns Hopkins University

Jun. 2022 – Jun. 2023

*Postdoctoral Fellow, Applied Mathematics & Statistics*

Baltimore, USA

- Developed statistical methods for network-valued and time-series-derived data, with applications to neuroscience, representation learning, dependence modelling, and downstream inference.
- Studied how network embeddings relate to classical statistical techniques such as PCA, focusing on model interpretation, dependence, effective sample size, clustering, and classification.
- Taught *Introduction to Optimization* and *Probability and Statistics for Biological Sciences and Engineering*, translating technical material for interdisciplinary audiences.

### Microsoft

May 2022 – Aug. 2022

*Joint E+D & MSR Research Intern*

Seattle, USA

- Modelled security incidents as graphs and implemented deep graph-similarity learning methods, including SimGNN, for relational incident analysis and risk exploration.

- Processed network-streaming security data and built interactive Power BI dashboards for large incident collections, supporting exploratory analysis and stakeholder-facing risk quantification.

### **DEVCOM Army Research Laboratory**

*Machine Learning Intern*

Jun. 2021 – Aug. 2021  
Washington, DC, USA

- Surveyed recommender-system methods and proposed collaborative filtering approaches for prioritising information objects in dynamic, high-volume decision environments.

## **SELECTED TECHNICAL WORK**

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### **Scientific AI for Food Extrusion Digital Twins**

Industry

- Built hybrid ML workflows for a real-world extrusion platform combining empirical lab data, controllable process settings, recipe information, and digital-twin descriptors to predict product properties and recommend feasible operating conditions.

### **Network Inference, Graph Matching & Relational ML**

Ph.D., postdoc, internships

- Developed graph-matching and joint-embedding methods for multiple networks, entity alignment, connectome analysis, social platforms, security incidents, and knowledge-graph signal recovery.

## **EDUCATION**

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### **University of Maryland, College Park**

*Ph.D. in Mathematics; dissertation: Statistical Inference across Multiple Graphs*

2019 – 2022  
USA

### **University of Massachusetts Amherst**

*Ph.D. Studies in Mathematics; transferred to UMD following advisor relocation*

2017 – 2019  
USA

### **National & Kapodistrian University of Athens**

*B.Sc. in Applied Mathematics*

2011 – 2016  
Greece

## **SELECTED PUBLICATIONS**

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- Hybrid multi-physics and machine-learning framework for prediction and optimization in twin-screw food extrusion. *Journal of Food Engineering*, under review, 2026.
- Optimizing the Induced Correlation in Omnibus Joint Graph Embeddings. *Journal of Computational and Graphical Statistics*, accepted, 2026.
- Clustered Graph Matching for Label Recovery and Graph Classification. *IEEE Transactions on Network Science and Engineering*, 2023.
- The Importance of Being Correlated. *Journal of Machine Learning Research*, 2022.
- Multiplex Graph Matching Matched Filters. *Applied Network Science*, 2022.