Pietro Bongini, Ph.D.

☑ pietro.bongini@gmail.com
ℝ ResearchGate D Orc:

ail.com in LinkedIn D OrcId GitHub





Current Position

- 2023 Present
- Research Associate through Research Grant in ING-INF/05 Information processing systems. University of Siena, Italy - Department of Information Engineering and Mathematics. Via Roma, 56, 53100 Siena SI. Project: Tuscany Health Ecosystem (PNRR)
 Spoke 9 Principal Investigator: Prof. Marco Maggini.

Research Interests

Machine Learning, Bioinformatics, Graph Neural Networks, Graph Generation, Drug Side-Effect Prediction, Graph Diffusion Models

Research Positions

2023 – Present	 Research Associate through Research Grant in ING-INF/05 - Information process- ing systems. University of Siena, Italy - Department of Information Engineering and Mathematics. Via Roma, 56, 53100 Siena SI. Project: Tuscany Health Ecosystem (PNRR) - Spoke 9 Principal Investigator: Prof. Marco Maggini.
2021 - 2023	Research Associate through Research Grant in INF/01 - Informatics. University of Pisa, Italy - Department of Computer Science. Largo Bruno Pontecorvo, 3, 56127 Pisa PI. Project: Artificial intelligence for pharmaceutical research, in collaboration with Chiesi Farmaceutici S.p.A. Principal Investigator: Prof. Corrado Priami.
2018 – 2022	Ph.D. Student in Smart Computing. University of Siena, Italy - Department of Information Engineering and Mathematics. Via Roma, 56, 53100 Siena SI. Thesis Title: "Graph Neural Networks for Molecular Data". Research Group: Siena Artificial Intelligence Laboratory. Advisors: Prof. Franco Scarselli, Prof. Monica Bianchini.

Education

- 2018 2022 Ph.D. in Smart Computing University of Florence, Italy Department of Information Engineering. Grade: Excellent with Honours. Thesis title: "Graph Neural Networks for Molecular Data". Advisors: Prof. Franco Scarselli and Prof. Monica Bianchini.
- 2015 2018 Master's Degree in Computer and Automation Engineering University of Siena, Italy
 Department of Information Engineering and Mathematics. Grade: 110 / 110 with Honours. Thesis title: "Glycine induced formation and druggability evaluation of protein surface pockets: A machine learning approach". Advisor: Prof. Monica Bianchini.
- 2011 2015 Bachelor's Degree in Information Engineering University of Siena, Italy Department of Information Engineering and Mathematics. Thesis title: "Classificazione di Proteine con Semantic Based Regularization" ("Protein Classification with Semantic Based Regularization"). Advisor: Prof. Michelangelo Diligenti.

Research Publications

Journal Articles



A. Visibelli, P. Bongini, A. Rossi, N. Niccolai, and M. Bianchini, "A deep attention network for predicting amino acid signals in the formation of α -helices," *Journal of Bioinformatics and Computational Biology*, vol. 18, no. 05, p. 2 050 028, 2020. *O* DOI: 10.1142/S0219720020500286.

P. Bongini, N. Niccolai, and M. Bianchini, "Glycine-induced formation and druggability score prediction of protein surface pockets," *Journal of Bioinformatics and Computational Biology*, vol. 17, no. 05, p. 1 950 026, 2019. *O* DOI: 10.1142/S0219720019500264.

Conference Proceedings

- M. Benini, P. Bongini, and E. Trentin, "A novel representation of graphical patterns for graph convolution networks," in *IAPR Workshop on Artificial Neural Networks in Pattern Recognition*, Springer, 2023, pp. 16–27. *O* DOI: 10.1007/978-3-031-20650-4_2.
- P. Bongini, "Graph neural networks for drug discovery: An integrated decision support pipeline," in IEEE MetroXraine 2023 Conference Proceedings, 2023.

M. Monaci, N. Pancino, P. Andreini, *et al.*, "Deep learning techniques for dragonfly action recognition.," in *Proceedings of the 9th International Conference on Pattern Recognition Applications and Methods -ICPRAM*, 2020, pp. 562–569.

N. Pancino, A. Rossi, G. Ciano, *et al.*, "Graph neural networks for the prediction of protein-protein interfaces.," in *ESANN - European Symposium on Artificial Neural Networks, Computational Intelligence and Machine Learning*, 2020.

S. Bonechi, M. Bianchini, P. Bongini, *et al.*, "Fusion of visual and anamnestic data for the classification of skin lesions with deep learning," in *International Conference on Image Analysis and Processing*, Springer, 2019, pp. 211–219. *O* DOI: 10.1007/978-3-030-30754-7_21.

Books and Chapters

5

2

P. Bongini, N. Pancino, F. Scarselli, and M. Bianchini, "Biognn: How graph neural networks can solve biological problems," in *Artificial Intelligence and Machine Learning for Healthcare*, Springer, 2023, pp. 211–231. *O* DOI: 10.1007/978-3-031-11154-9_11.

P. Bongini, A. Trezza, M. Bianchini, O. Spiga, and N. Niccolai, "Structural bioinformatics to unveil weaknesses of coronavirus spike glycoprotein stability," in *In Silico Modeling of Drugs Against Coronaviruses*, Springer, 2021, pp. 203–211. *9* DOI: 10.1007/7653_2020_59.

Ph.D. Thesis

P. Bongini, "Graph neural networks for molecular data," University of Florence - Ph.D. in Smart Computing, 2022.

Posters, Seminars, and Other Talks

- 2024 Pietro Bongini, "Graph Neural Networks for Molecular Data", Seminar held by Pietro Bongini at the AI4BA 2024 Summer School upon invitation, Siena, IT, June 28 2024.
 - Pietro Bongini, "Graph Neural Networks", Lecture held by Pietro Bongini at a UniSi-DIISM joint laboratory event, Siena, IT, June 13 2024.
- 2023 Pietro Bongini, Monica Bianchini, Franco Scarselli, "NextGeneration GNNs: Developing Universal Graph Handlers". Talk held by Pietro Bongini at AIxIA 2023 Machine Learning and Data Mining workshop, Rome, IT, November 9 2023.
 - Pietro Bongini, "Graph Neural Networks for Drug Discovery". Dissemination talk held by Pietro Bongini at AI4Girls, Siena, IT, July 19 2023.

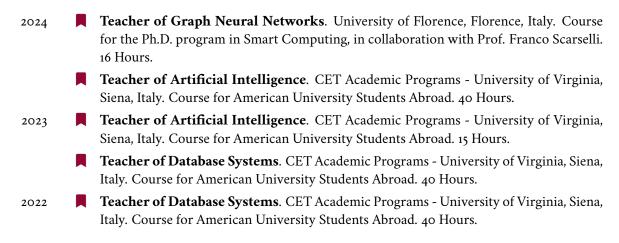
Posters, Seminars, and Other Talks (continued)

	Pietro Bongini, "L'AI per le relazioni tra entità e tra persone". Dissemination talk (in Italian) held by Pietro Bongini at Pint of Science 2023, Siena, IT, May 22 2023.
	Pietro Bongini, "Graph Neural Networks for Drug Discovery". Dissemination talk held by Pietro Bongini at SAIHub meetup @ Palazzo Sansedoni, Siena, IT, April 13 2023.
2022	Pietro Bongini, Monica Bianchini, Neri Niccolai, "Bioinformatic Survey of X/Gly genomic vari- ants". Talk held by Pietro Bongini at Bioinformatiha 9, Pisa, IT, September 16 2022.
	Elisa Messori, Monica Bianchini, Pietro Bongini, "Drug Side-Effect Prediction with Graph Neu- ral Networks". Talk held by Elisa Messori at BITS 2022, Verona, IT, June 29 2022.
	Pietro Bongini, "Graph Neural Networks for Molecualr Data". Seminar held by Pietro Bongini for Toscana Life Sciences upon invitation, Siena, IT, February 1 2022.
2021	Pietro Bongini, "Introduction to Artificial Intelligence, Machine Learning, and Deep Learning". Seminar held by Pietro Bongini for the UDIEMS student society upon invitation, Siena, IT, June 7 2021.
2020	Pietro Bongini, Monica Bianchini, Franco Scarselli, "Molecular Graph Generation with Graph Neural Networks". Talk held by Pietro Bongini at AIxIA 2020 - Machine Learning and Data Mining workshop, Online Event, November 26 2020.
	Pietro Bongini, Monica Bianchini, Neri Niccolai, "A possible strategy to fight Covid-19: interfer- ing with spike glycoprotein trimerization". Talk held by Pietro Bongini at Bright 2020 - La notte dei ricercatori, Online Event, November 27 2020.
2018	Pietro Bongini, Monica Bianchini, Neri Niccolai, "Engineering proteins with modulated activ- ities: a Structural Bioinformatics approach". Talk held by Pietro Bongini at Bioinformatiha 7, Siena, IT, October 26 2018.
2017	Simone Gardini, Guido Mangiavacchi, Pietro Bongini, Monica Bianchini, Neri Niccolai, "En- zyme Interface Composition Analysis". Poster presented at Bioinformatiha 6, Pisa, IT, October 20 2017.

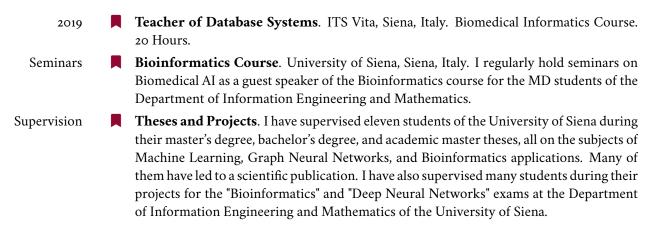
Organization of Events

- I participated in the organization of the Pint of Science festival in Siena, as a member of the team. Siena, IT, May 13-15 2024.
 - I took part in the organization of the first AI4BA (Artificial Intelligence for Biomedical Applications) Summer School. Siena, IT, June 24-28 2024.

Teaching Activities



Teaching Activities (continued)



Research Activities

Research Associate @ UniSi 📃 📕	Investigation of graph generators based on recurrent GNNs. Develop- ment of a generative autoencoder based on recurrent GNNs to generate different types of graphs with desired characteristics.
Ħ	Investigation of Graph Neural Network models and associated tech- niques to build a universal graph embedder. Development of graph au- toencoders based on recurrent GNNs for creating pre-trained GNN models that can be used on a whole graph domain (e.g. molecular graphs).
	Seminars on AI and its application to bioinformatics.
Research Associate @ UniPi 📃	Investigation of Machine Learning algorithms for the prediction of the efficacy of therapies for Chronic Obstructive Pulmonary Disease (COPD), in collaboration with Chiesi Farmaceutici S.p.A., with interpretable and fair predictors.
Ħ	Application of predictive techniques to the classification of patients in- volved in clinical studies on Pediatric Acute-onset Neuropsychiatric Syn- drome (PANS).
	Seminars on AI and its application to bioinformatics.
Ph.D. School 📃	Design, implementation, and experimentation of a molecular graph gen- eration method based on Graph Neural Networks.
	Programming a Tensorflow implementation of Composite Graph Neural Networks (CGNNs), a variant of GNNs which can handle graphs made of heterogeneous nodes and arcs; Experiments on Composite Graph Neural Networks.
	Design and implementation of DruGNN, a predictor of drug side–effects based on Composite Graph Neural Networks; This activity was carried out as a visiting researcher (though remotely due to the Covid–19 pan- demic) of the Computer Laboratory, University of Cambridge, under the supervision of Prof. Pietro Liò.
R	Maximum clique detection with Graph Neural Networks, for the identi- fication of binding sites in protein–protein interface graphs.
Ħ	Investigation of strategies based on Machine Learning aimed at acquiring and processing knowledge to counter the Covid-19 infection.
	Secondary structure prediction on aminoacid sequences using Long Short-Term Memories.

	Glycine mutation of protein structures and druggability evaluation of protein surface pockets for drug discovery.
	Speaker of seminars on Biomedical Applications of Graph Neural Net- works during lab meetings on a regular basis.
	Attendance to international conferences and summer schools, among which the ACDL 2019 summer school at Certosa di Pontignano, Siena (Italy), online attendance at NeurIPS 2020, and the presentation of a pa- per as a speaker at KES 2021 international conference held in Szczecin (Poland).
Master's Thesis	Programming and testing a software pipeline for the substitution of large aminoacids with glycine, with the aim of opening new protein surface pockets.
	Creating a dataset of pockets to train a druggability score regressor; Training a MLP regressor to assign druggability scores to new pockets,

on the basis of their chemical and structural features.

Authorship and Editorial Activities

Authorship	I have authored 27 scientific publications so far: 19 journal articles, 5 con- ference papers, 2 book chapters, and 1 Ph.D. Thesis. I am the first author of 15 of them (2 as unique author), among which important publications on "Neu- rocomputing" and the "IEEE/ACM Transactions on Computational Biology and Bioinformatics", and the last author (supervisor) of 2 of them.
Peer Review	I have peer-reviewed more than 65 submissions for many academic jour- nals and conferences. I peer–review for "Neurocomputing", "Neural Process- ing Letters", "Neural Networks", and the "International Joint Conference on Neural Networks" on a regular basis.
Editorial Appointments	In 2024, I have been appointed as a guest editor for the "Symmetry" jour- nal, on the special issue "Asymmetric and Symmetric Study on Biostatistics". In 2021/2022, I served as an associate editor for the "Mathematics" journal, working on the special issue "Mathematical Modelling and Machine Learning Methods for Bioinformatics and Data Science Applications II".

Professional Skills

Research Very good capacity of keeping up to date and individuating new research directions according to the relevant literature. Excellent knowledge of the literature on the topics of Graph Neural Networks, Graph Convolution Networks, Graph Generation, Drug Side–Effect Prediction (also Polypharmacy). Good knowledge of the literature on Machine Learning and Artificial Intelligence in general. Very good ability in developing and formalizing methods/algorithms and implementing them, also thanks to the programming skills. Excellent skill in writing/communicating the research methodology and its results, also assessing the usability of the findings and the future research directions left to explore.

Programming Excellent programming skills in Python; good programming skills in Java, C, C++, C#; very good experience with the TensorFlow, Keras, Pytorch, Scikit–learn, Numpy, Pandas, PyMol, Biopython, NetworkX, Matplotlib, and RdKit library packages; basic knowledge of many other libraries and packages in all the programming languages listed above.

Professional Skills (continued)

Platforms	Excellent knowledge of the Unity engine. Very good knowledge of Matlab and the PyMol molecular graphics platform. Excellent knowledge of LaTeX and Overleaf. Good knowledge of NetBeans, Visual Studio, the Anaconda virtual environment manager, and basic knowledge of Jupyter Notebooks. Very good skill in using Mi- crosoft Office (PowerPoint, Publisher, and Excel in particular) for postprocessing and presenting the results.
Communication	Very good communication skills developed during collaborative activities in the re- search environments; very good presentation skills acquired during the studies and the research work; excellent writing skills developed starting from the high–school period, through the university studies, and refined on more specific standards dur- ing the research work. Fluency in both written and spoken language in Italian and English.
Web	Good knowledge of HTML, CSS, and Javascript; basic knowledge of PHP and Word- press. Good level of experience in using the Leaflet Javascript library for creating interactive maps, together with OpenStreetMap data, and the Maperitive program for realizing custom map tiles for the web. These skills have been acquired during the studies, and then refined in personal projects unrelated to research.

Languages

Italian 📕 Native Speaker

English

Proficient(C2) Certificate of Proficiency in English (CPE), Cambridge ESOL (2017).

Short Description of Myself

I am a methodical, rational, yet very curious and passionate person. Even though I have a calm, patient, and reserved personality, I enjoy being involved in many social activities and projects. I really like collaborating with other people who put passion into their job, and I appreciate interdisciplinary projects very much. I have always been attracted by informatics and in particular by artificial intelligence, which I perceive as a new wonderful scientific field, but also as a valuable instrument to explore almost every field of science, from informatics to physics, from mathematics to biology and medicine. In particular, I have an interest for biomedical applications of artificial intelligence which dates back to the times of my Bachelor's degree, and which I have never stopped exploring and improving, as the subjects of my three theses testify. During the Bioinformatics course of my Master's degree, I discovered Graph Neural Networks. Since then, I have always been fascinated by the capabilities of this powerful and versatile type of neural network that can process structured data. This latter characteristic makes it the ideal model to process complex biomedical data, such as proteins, the human metabolism, and drug structures. I have devoted the main part of my Ph.D. research to the exploration of the capabilities of Graph Neural Networks in the biomedical field, and I wish to keep improving the existing methodologies in this direction. My interest in cross-discipline research stems from my curiosity for every aspect of life, and every field of knowledge, including history and sports. In my free time, I am a sports enthusiast and I regularly play tennis. Whenever I can, I go mountain-biking in the countryside. I also enjoy hiking in the mountains, especially in the Dolomites, and playing billiards, which has been the subject of one of my personal projects (unrelated to research activity). Moreover, I have a passion for cooking, mapping any kind of interesting stuff, reading various genres of books, and visiting interesting places.

Personal Projects

During my studies and in my free-time, I have carried out many interesting projects on different topics. This section is intended as a brief summary of the most interesting ones.

This project was carried out during my free-time, stemming from my interest in three topics: billiards, physics, and artificial intelligence. In 2016-2017, I developed a 2D simulator of various billiard games, including Italian billiards, English billiards, Snooker, and various pool games. The 2D simulator was programmed in Java. After acquiring knowledge with the Unity engine, the project was upgraded to 3D simulation, using Unity and C# scripts. Unfortunately, issues with real-time physics made the simulation not sufficiently realistic and the 3D project was eventually left unfinished. One of the goals of the project was to develop a Machine Learning agent that could learn to play billiards, but this goal was also abandoned after the issues with 3D simulation.

Architectural Rendering in Unity - I (2017)

For the "Design of Applications Systems and Services" exam of my Master's Degree, I created a set of "walkable" architectural renderings using the Unity engine. The rendered buildings were obtained from free web sources as 3D models, rendered (and texturized where needed) on Unity. I then developed a simple simulator, in which it was possible to walk inside the rendered building as in a first–person video–game, or to watch a pre–recorded tour. This was possible through a custom interface (a Windows executable) or through a browser Web–GL based interface. The project also included a small crowd evacuation simulation of a sports hall based on flock behavior modeling.

Architectural Rendering in Unity - II (2023-)

In my free-time, I am currently working on a Unity package for the Architectural Rendering of apartments. The package includes textures, materials, and objects for rendering structural components and furniture, as well as features for adapting new items that can be imported in .obj or .prefab formats. Components can be animated and made interactive with a bunch of C# scripts that allow to navigate the scene as in a first-person video-game, interacting with doors, windows, lights, shutters, roller shutters, drawers, house appliances, and other furniture items. Special items are also available to represent wiring, plumbing, and other systems in 3D.

Flaw Detector based on Convolutional Neural Networks (2016-2017)

For the "Advanced Digital Image Processing" exam of my Master's Degree, together with two fellow students, I built a flaw detector intended to improve a production line of plastic film. The plastic film could have as many as 20 different types of flaws, each of which represented a class (together with the "no-flaw" case) for our classifier based on CNNs. We trained and tested the model on a dataset of photos of flawed and pristine plastic films coming from a real production line, obtaining very good results.

AI-Powered Cannon Game (2016)

For the "Machine Learning" exam of my Master's Degree, together with two fellow students, I built a small 2D cannon shooting simulator controlled by a neural network. The objective was to train a neural network that could hit an opponent before being hit, in a variety of different positions and conditions. We programmed the environment with realistic physics (including wind effects) from scratch in Java, and trained a Multi–Layer Perceptron on it. A final test was carried out with 1-vs-1 matches against human opponents. The AI-controlled gun was able to deliver a successful hit on 70% of its shots, beating the human opponents in more than 90% of the matches.

Dichiarazioni relative al presente Curriculum Vitae

Il sottoscritto Pietro Bongini, nato a Siena (SI), il 05/03/1992, C.F. BNGPTR92C05I726B, residente in Siena (SI), via Dario Neri, 51, CAP 53100, dichiara che quanto riportato nel presente Curriculum Vitae corrisponde a verità, ai sensi delle norme in materia di dichiarazioni sostitutive di cui agli articoli 46 e 47 del D.P.R. 445/2000.