

GUADALUPE GONZALEZ

PhD candidate in graph machine learning for therapeutics discovery

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I am a fourth-year PhD candidate in the Department of Computing at Imperial College London. I received my B.Sc. in Biomedical Engineering and M.Res. in Data Science before adventuring into the exciting field of deep learning on graphs advised by Prof. Michael Bronstein and Dr. Kirill Veselkov.

During the first part of my PhD I enjoyed developing graph machine learning methods leveraging genomic data to uncover molecules with disease-beating properties in foods within the [HyperFoods](#) project. Motivated by the drawbacks of modeling genetic perturbations using machine learning approaches alone, I currently work on developing causal graph machine learning algorithms to model genetic and chemical perturbations together with Dr. Marinka Zitnik at Harvard Medical School.

EDUCATION

Harvard University, US

*Visiting PhD, Supervised by Marinka Zitnik
Harvard Medical School*

Oct 2021 - Oct 2022 (in progress)

Imperial College London, UK

*PhD, Computing. Supervised by Michael Bronstein & Kirill Veselkov
Department of Computing, Faculty of Engineering*

2018 - 2023 (in progress)

Imperial College London, UK

*Master of Research, Biomedical Research - Data Science.
Department of Surgery and Cancer, Faculty of Medicine*

2017 - 2018

Distinction

Polytechnic University of Madrid, Spain

Bachelor of Science, Biomedical Engineering

2013 - 2017

Top of the class

RESEARCH EXPERIENCE

Harvard Medical School

Marinka Zitnik Lab - Visiting Graduate Student

Oct 2021 - Present

- **Modeling genetic perturbations with causal graph machine learning algorithms.** Motivated by the drawbacks of modeling genetic perturbations using machine learning approaches alone, I currently work on developing causal graph machine learning algorithms to model genetic and chemical perturbations for response prediction and perturbation discovery.

Imperial College London

Michael Bronstein Lab, Kirill Veselkov Lab - Graduate Student

Oct 2018 - Present

- **Graph neural model to predict combinatorial therapeutics against cancer.** Built novel graph neural architecture to leverage food molecule-drug pharmacodynamic interactions to modulate drug activity. Currently in wet-lab testing phase of predicted interacting food-drug combinations.
- **Meta-analysis of association of food items and risk of colorectal cancer.** Carried out meta-analysis of the association of several food items (garlic, nuts, tomatoes, cruciferous vegetables and citrus fruits) and the risk of colorectal cancer. [Publication](#)
- **Network ML maps phytochemically-rich Hyperfoods to fight COVID-19.** Using a network machine learning model to simulate effects of drugs, food molecules and COVID-19 on the genome, we predicted foods contributing to the prevention or recovery from COVID-19. [Publication](#)
- **Predicting anticancer hyperfoods with graph convolutional networks.** Building from our first study on hyperfoods, I introduced a graph neural model for anticancer hyperfoods prediction. [Publication 1](#)
[Publication 2](#)

- **HyperFoods: Machine intelligent mapping of cancer-beating molecules in foods.** Implemented and evaluated traditional neural models for anticancer molecule prediction within the [Hyperfoods](#) project. Carried out biological interpretability of model. Mined SQL database of food molecules to compile food items containing the predicted anticancer molecules.

Imperial College London

March 2018 - Oct 2018

Kirill Veselkov Lab - Master's Student Researcher

- Proposed and benchmarked machine learning algorithms for drug repositioning against cancer

Imperial College London

Oct 2017 - March 2018

Elsa Angelini Lab - Master's Student Researcher

- Proposed and benchmarked machine learning algorithms for the association of radiological and genomic features for glioblastoma patient stratification

PUBLICATIONS

1. Zhong, Z., **Gonzalez, G.**, Grattarola, D., Pang, J. (2022). Unsupervised Heterophilous Network Embedding via r-Ego Network Discrimination.
2. Borgas, P., **Gonzalez, G.**, Veselkov, K., Mirnezami, R. (2021). Phytochemically rich dietary components and the risk of colorectal cancer: A systematic review and meta-analysis of observational studies. *World Journal of Clinical Oncology*, 12(6), 482–499.
3. Laponogov, I.*, **Gonzalez, G.***, Shepherd, M., Qureshi, A., Veselkov, D., Charkoftaki, G., Vasiliou, V., Youssef, J., Bronstein, M., Veselkov, K. (2021). Network Machine Learning Maps 'Hyperfoods' to Fight COVID-19. *Human Genomics* 15(1): 1.* equal contribution.
4. **Gonzalez, G.**, Gong, S., Laponogov, I., Bronstein, M., Veselkov, K. (2021). Predicting anticancer hyperfoods with graph convolutional networks. *Human Genomics*, 15(1), 33.
5. **Gonzalez, G.**, Gong, S., Laponogov, I., Veselkov, K. and Bronstein, M. (2019). Graph Attentional Autoencoder for Anticancer Hyperfood Prediction. 2019 NeurIPS Graph Representation Learning Workshop.
6. Frasca, F*., Galeano, D.*, **Gonzalez, G.**, Laponogov, I., Veselkov, K., Paccanaro, A. and Bronstein, M. (2019). Learning interpretable disease self-representations for drug repositioning. 2019 NeurIPS Graph Representation Learning Workshop. * equal contribution.
7. Veselkov, K., **Gonzalez, G.**, Aljifri, S., Galea, D., Mirnezami, R., Youssef, J., Bronstein, M. and Laponogov, I. (2019). HyperFoods: Machine intelligent mapping of cancer-beating molecules in foods. *Scientific Reports*, 9(1).

AWARDS AND SCHOLARSHIPS

- 2019, IPAM (UCLA) Geometry and Learning from Data in 3D and Beyond Workshop IV travel grant.
- 2018, Dean's Prize. Faculty of Medicine, Imperial College London. Awarded to students achieving the highest overall Distinction grade on their master's course.
- 2017, Angel Barbero Martin de Vidales Foundation fellow. ETSIT, Polytechnic University of Madrid, Spain. Awarded to final-year students with outstanding academic records.
- 2016, 2015, 2014, Academic Excellence Scholarship. Community of Madrid, Spain. Awarded to undergraduate students with outstanding academic records.

VOLUNTEERING EXPERIENCE

Voluntary positions

- 2020 - 2021, [LOGML Summer School 2021](#) co-organizer. The London Geometry and Machine Learning summer school was a week-long event which took place in July 2021, in which early career researchers worked on practical projects under the guidance of experienced mentors. The summer school also featured prominent researchers in the fields of geometry and machine learning, as well as a company and networking night.

- 2019 - 2021, Co-president of [Women in Computing](#) (WiC) society at Imperial College London. Co-organized talks, workshops, and weekly activities for female and gender-minority PhD and staff members in the department of Computing. Led *WiC Entrepreneur* initiative to promote entrepreneurship among female students and staff members in the department of computing.
- 2019, Postgraduate Ambassador, Imperial College London.

Invited talks, panels, academic service

- 2022, Panelist at [LOGML Summer School 2022](#).
- 2021, Speaker, [So you have networks... now what?](#), Imperial Interdisciplinary Insights, Computational Biology Society, Imperial College London.
- 2021, Panelist, [GEMS Camp](#) College Panel.
- 2020, Speaker, [Applications of graph neural networks in computational biology](#), Geometry and Machine Learning Workshop for Medical Applications.
- 2020, Speaker, Informatics Meet-up, Department of Metabolism, Digestion and Reproduction, Imperial College London.
- Reviewer: TheWebConf (2022), HopperX1 (2019).

CO-SUPERVISIONS

Co-supervision of master's projects, Faculty of Medicine, Imperial College London

- 2021, The overlap score of genetic targets of food and drug molecules predicts their synergistic anticancer effect, Emma Zhang.
- 2021, Exploring dietary bioactive compounds on colorectal cancer radiation response using random walk with restarts, Yoyo Zhong.
- 2021, Drug combinations against colorectal cancer, Yuxi Wang.
- 2021, Combinatorial therapeutics against COVID-19, Jason Qiu.
- 2021, Drug combinations against lung cancer, Marco Gallotta.
- 2020, The COVID-19 pandemic and cancer – an opportunity for drug repurposing, Madelen Shepherd.
- 2020, COVID-19 and lung cancer: can we kill two birds with one stone?, Ahad Qureshi.

TEACHING EXPERIENCE

Imperial College London

- Graduate Teaching Assistant, Machine Learning, Faculty of Medicine, Fall 2021.
- Instructor, Workshop: *Big Data and the 'Dark Matter' of COVID*, Faculty of Medicine, Summer 2021.
- Graduate Teaching Assistant, Deep Learning, Faculty of Engineering, Summer 2020.
- Graduate Teaching Assistant, Big Data and Machine Learning, Faculty of Engineering, Summer 2019

Non-profit organizations

- In2Science instructor. Machine Learning sessions to encourage Year 12 students to progress into STEM research-intensive degrees, Summer 2020
- CodeFirstGirls instructor. Web programming in HTML, CSS, and JavaScript for girls with no experience in programming, to encourage them to pursue careers in STEM, Fall 2018

SKILLS

Programming languages Frameworks

Python, R, Matlab, Java, HTML, CSS, JavaScript, SQL
PyTorch, TensorFlow