Matthew Ragoza

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Education

University of Pittsburgh, Pittsburgh, PA — Aug. 2021 - Present
Ph.D. student in Intelligent Systems Program
- Advised by Dr. Kayhan Batmanghelich, current GPA 4.00/4.00

University of Pittsburgh, Pittsburgh, PA — Aug. 2012 - Dec. 2016
B.S. in computer science and neuroscience, minor in chemistry
- Graduated *magna cum laude* with GPA 3.63/4.00

Research Experience

Tissue elasticity reconstruction with physics-informed neural networks — Aug. 2021 - Present
Department of Biomedical Informatics, University of Pittsburgh
Graduate Student Researcher, PI: Dr. Kayhan Batmanghelich
- Improved the robustness of elasticity reconstruction from displacement data in biological tissue by solving partial differential equations with deep learning
- Combined data-driven learning from MRI anatomical images with physical prior knowledge to further enhance elasticity reconstruction performance

Structure-based drug discovery with deep generative models — Jan. 2018 - Aug. 2021
Department of Computational and Systems Biology, University of Pittsburgh
Research Staff Member, PI: Dr. David Ryan Koes
- Trained conditional variational autoencoders to generate novel drug-like molecules within protein binding pockets by leveraging an atomic density grid representation
- Designed an algorithm for fitting valid molecular structures to 3D volumetric densities by iteratively detecting atoms and jointly optimizing their coordinates

Ligand pose optimization with convolutional neural networks — Jan. 2017 - Dec. 2017
Department of Computational and Systems Biology, University of Pittsburgh
Health Sciences Fellow, PI: Dr. David Ryan Koes
- Repurposed convolutional neural networks that were trained for protein-ligand scoring to be used for optimizing conformations of ligands within binding pockets
- Improved the robustness of convolutional neural networks for protein-ligand scoring by fine-tuning them with adversarially optimized molecular conformations

Protein-ligand scoring with convolutional neural networks — Sep. 2015 - Dec. 2016
Department of Computational and Systems Biology, University of Pittsburgh
Research Assistant, PI: Dr. David Ryan Koes
- Trained convolutional neural networks to predict binding of small molecules to target proteins and select binding conformations from sets of candidate poses

Optimization of sleep detection based on primate actigraphy data — Apr. 2014 - Dec. 2015
Department of Psychiatry, University of Pittsburgh
Research Assistant, PI: Dr. Judy Cameron and Dr. Neal Ryan
- Enhanced the classification of sleep-wake state based on non-human primate activity data by optimizing algorithm parameters using annotated videography

Peer-Reviewed Journal and Conference Papers

[1] **M. Ragoza** and K. Batmanghelich. "Physics-informed neural networks for tissue elasticity reconstruction in magnetic resonance elastography." In *26th International Conference on Medical Image Computing and Computer Assisted Intervention*, Oct. 2023. **(Early acceptance)**

[2] **M. Ragoza**, T. Masuda, and D. R. Koes. "Generating 3D molecules conditional on receptor binding sites with deep generative models." *Chemical Science*, vol. 13, pp. 2701-2713, Feb. 2022. DOI. (48 citations)

[3] A. T. McNutt, P. Francoeur, R. Aggarwal, T. Masuda, R. Meli, **M. Ragoza**, J. Sunseri, and D. R. Koes. "GNINA 1.0: molecular docking with deep learning." *Journal of Cheminformatics*, vol. 13, no. 43, Jun. 2021. DOI. (159 citations)

[4] J. Hochuli, A. Helbling, T. Skaist, **M. Ragoza**, and D. R. Koes. "Visualizing convolutional neural network protein-ligand scoring." *Journal of Molecular Graphics and Modelling*, vol. 84, pp. 96–108, Sep. 2018. DOI. (86 citations)

[5] **M. Ragoza**, J. Hochuli, E. Idrobo, J. Sunseri, and D. R. Koes. "Protein-ligand scoring with convolutional neural networks." *J Chem Inf Model*, vol. 57, no. 4, pp. 942–957, Apr. 2017. DOI. **(639 citations)**

[6] J. Sunseri, **M. Ragoza**, J. Collins, and D. R. Koes. "A D3R prospective evaluation of machine learning for protein-ligand scoring." *Journal of Computer-Aided Molecular Design*, vol. 30, no. 9, pp. 761–771, Sep. 2016. DOI. (20 citations)

Peer-Reviewed Workshop Papers

[1] **M. Ragoza**, T. Masuda, and D. R. Koes. "Learning a continuous representation of 3D molecular structures with deep generative models." In *Machine Learning for Structural Biology Workshop at NeurIPS 2020*, Vancouver, BC, Dec. 2020. arXiv. (25 citations)

[2] T. Masuda, **M. Ragoza**, and D. R. Koes. "Generating 3D molecular structures conditional on a receptor binding site with deep generative models." In *Machine Learning for Structural Biology Workshop at NeurIPS 2020*, Vancouver, BC, Dec. 2020. arXiv. (38 citations)

[3] **M. Ragoza**, L. Turner, and D. R. Koes. "Ligand pose optimization with atomic grid-based convolutional neural networks." In *Machine Learning for Molecules and Materials Workshop at NIPS 2017*, Long Beach, CA, Dec. 2017. arXiv. (25 citations)

Awards and Grants

- **2018 NCATS ASPIRE Design Challenge Winner** — Aug. 2019
  Recognized for creating predictive algorithms that help address the opioid crisis
- **XSEDE Allocation Request MCB190049** — Jun. 2019
  Granted 50,000 compute hours on Bridges GPU-AI cluster valued at $61,800
- **University of Pittsburgh Center for Research Computing Allocation** — Feb. 2019
  Granted 100,000 compute hours on H2P GPU cluster
- **Health Sciences Fellowship** — Jan. 2017
  Awarded a post-baccalaureate research fellowship at the University of Pittsburgh
- **NVIDIA GPU Award for Best GPU Poster** — Aug. 2016
  Awarded in computational division at 252nd ACS National Meeting & Exposition
- **Computer Science Day Best Poster Award** — Mar. 2016
  Selected by University of Pittsburgh Computer Science Department faculty

Oral Presentations

[1] **M. Ragoza** and K. Batmanghelich. "Physics-informed neural networks for tissue elasticity reconstruction in magnetic resonance elastography." Invited talk at *26th International Conference on Medical Image Computing and Computer Assisted Intervention*, Vancouver, BC, Oct. 2023.

[2] T. Masuda, **M. Ragoza**, and D. R. Koes. "Generating 3D molecular structures conditional on a receptor binding site with deep generative models." Spotlight talk presented at *Machine Learning for Structural Biology Workshop at NeurIPS 2020*, Vancouver, BC, Dec. 2020.

[3] **M. Ragoza**, L. Turner, and D. R. Koes. "Ligand pose optimization with atomic grid-based convolutional neural networks." Spotlight talk presented at *Machine Learning for Molecules and Materials Workshop at NIPS 2017*, Long Beach, CA, Dec. 2017.

Poster Presentations

[1] **M. Ragoza**, T. Masuda, and D. R. Koes. "Learning a continuous representation of 3D molecular structures with deep generative models." Poster presented at *Machine Learning for Structural Biology Workshop at NeurIPS 2020*, Vancouver, BC, Dec. 2020. Poster. Video.

[2] **M. Ragoza**, T. Masuda, and D. R. Koes. "Deep generative models for computational drug discovery." Poster presented at *CRC Advancing Research through Computing Symposium 2019*, Pittsburgh, PA, Mar. 2019. Poster.

[3] P. Francoeur, **M. Ragoza**, R. Rosenzweig, J. Sunseri, and D. R. Koes. "Gnina: deep learning for molecular docking." Poster presented at *256th ACS National Meeting & Exposition*, Boston, MA, Aug. 2018. Poster.

[4] J. Hochuli, **M. Ragoza**, and D. R. Koes. "Visualization of convolutional neural network scoring of protein-ligand binding." Poster presented at *253rd ACS National Meeting & Exposition*, San Francisco, CA, Apr. 2017. Poster.

[5] **M. Ragoza**, E. Idrobo, J. Hochuli, J. Sunseri, and D. R. Koes. "Convolutional neural networks for protein-ligand scoring." Poster presented at *252nd ACS National Meeting & Exposition*, Philadelphia, PA, Aug. 2016. Poster.

[6] **M. Ragoza**, J. Collins, N. Bastola, and D. R. Koes. "Convolutional neural networks for protein-ligand scoring." Poster presented at *Pitt CS Day 2016*, Pittsburgh, PA, Mar. 2016. Poster.

[7] J. Collins, **M. Ragoza**, J. Jensen, and D. R. Koes. "3Dmol.js: 3D structure visualization for the modern web." Poster presented at *251st ACS National Meeting & Exposition*, San Diego, CA, Feb. 2016. Poster.

[8] **M. Ragoza**, T. Liu, N. D. Ryan, and J. L. Cameron. "Optimization of an assessment strategy to accurately measure sleep in non-human primates from actigraphy data." Poster presented at *Western Psychiatric Institute and Clinic Research Day*, Pittsburgh, PA, Apr. 2015.

Technical Skills

Python, MATLAB, R, Bash/Linux, PyTorch, Git, Slurm, Jupyter Notebook, Latex GitHub

References

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