**Math 496 T – Special Topic Undegrauate course. Spring of 2025.**

**Title:** Mathematics of Generative AI

**Instructor:** Michael Chertkov

**Course Prerequisites:** Successful completion (grade of A or B) in Linear Algebra (Math 215, or Math 310, or Math 313) and Calculus and Analysis (Math 223, or Math 254, or Math 355) is required.
**Programming** will be employed as a supportive tool for learning throughout the course. Students will be pointed to online resources to facilitate self-directed programming education, including guides on harnessing chat-based AI models to enhance the programming experience and associated learning tasks.
**Objectives:** Tailored for motivated juniors from mathematics, physics, astronomy, engineering, and other STEM disciplines, this course offers a deep dive into the synergy between classical and modern applied mathematics and contemporary Artificial Intelligence. Participants will:

- Explore the critical roles that differential equations and optimization play in AI's development.
- Develop proficiency in using linear algebra, differential analysis, and calculus for data-centric problem-solving.
- Learn to innovate with data and AI by applying sophisticated mathematical principles.
- Discover cutting-edge techniques and the latest research in applied mathematics, with a focus on machine learning, data science, and generative AI.
- Get primed for advanced studies in Applied Mathematics, paving the way for an accelerated Master's degree or professional path, grounded in a thorough comprehension of theory and its real-world applications.

**Texts and Additional Materials:** Essential reading for the course includes [1]:

- G. Strang, "Linear Algebra and Learning from Data" (2019) – A bridge between traditional linear algebra and the data-driven approach of modern AI.
- S.H. Strogatz, "Nonlinear Dynamics and Chaos" (2018) – An exploration into the complex world of dynamical systems and their chaotic behaviors.
- N. Gershenfeld, "The Nature of Mathematical Modeling" (1999) – techniques that are useful for modeling, both natural and otherwise.
- S.J.D. Prince, "Understanding Deep Learning" (2023) – Insights into the mechanisms and applications of deep learning technologies.
- S. Lynch, "Python for Scientific Computing and Artificial Intelligence" (2023) – A guide to leveraging Python in solving scientific computing challenges and AI development.
- S. H. Chan, "Tutorial on Diffusion Models for Imaging and Vision" `https://arxiv.org/abs/2403.18103`.

[1] We are dedicated to providing materials in a manner that does not impose additional financial burdens on students. Recognizing that not all required texts may be readily accessible online, we are exploring options to legally disseminate essential portions of the texts, such as individual chapters, to ensure all students have the necessary resources. Furthermore, we will investigate and offer alternative resources that are freely available to students to support their learning.

- W. Tang and A. Zhao, "Score-Based Diffusion Models via Stochastic Differential Equations – a Technical Tutorial", `https://arxiv.org/abs/2402.07487`
- M. Chen, S. Mei, J. Fan, M. Wang, "An Overview of Diffusion Models: Applications, Guided Generation, Statistical Rates and Optimization", `https://arxiv.org/abs/2404.07771`.

Additionally, comprehensive lecture notes will be made available.
**Tentative Course Schedule** (Total of 28 Lectures, Each 1.25 Hours):

- **Linear Algebra**: Topics include Linear Equations, Singular Value Decomposition, Compression, and Optimization. This section consists of 4 lectures, based on Strang's book, providing a mathematical foundation.
- **Differential Calculus**: Covers Automatic Differentiation, Differential Equations, Dynamical Systems, and Function Approximations via Neural Networks. This section includes 6 lectures, with materials from Strang, Gershenfeld, and Strogatz's books, preparing students for advanced topics.
- **Stochastic Calculus**: Introduces Basic Statistics and Probability Theory, Stochastic Processes, Statistical Inference, including Exact Inference, Markov Chain Monte Carlo and Variational methods. This section comprises 6 lectures, drawing from Strang and Prince's books, along with additional lecture notes.
- **Statistical Learning**: Observed and Hidden Data, Likelihood Optimization – Exact and Approximate, Sampling Methods, Boltzmann Machines, Bayesian Networks. This section consists of 6 lectures, using resources from Strang, Prince, and Lynch's books, supplemented with additional lecture notes.
- **Generative Models of AI**: Covers the Design and Understanding of Diffusion Models, their relationship and integration with other AI Tools and Techniques, and various Applications. This section includes 6 lectures, with content from lecture notes, enriched by Prince and Lynch's books, as well as recent reviews (by S. H. Chan, by W. Tang and A. Zhao and by M. Chen et al).

**Application Areas Targeted by the Course:** This course is designed to equip students with the mathematical foundations applicable across a broad spectrum of fields:
- **Physical Sciences:** Dive into areas like statistical mechanics, astrophysics, fluid mechanics, optics, quantum physics, accelerator physics, and materials science, showcasing the integral role of mathematics in understanding and advancing physical theories and technologies.
- **Engineering Sciences:** Explore applications in aerospace, mechanical engineering, robotics, transportation, energy systems, systems control, and optimization, highlighting mathematics as the backbone of engineering innovation and problem-solving.
- **Life Sciences:** Understand the mathematical underpinnings of genomics, molecular biology, neuroscience, biofluid dynamics, and epidemiology, illustrating how mathematics aids in deciphering complex biological phenomena.
- **Geosciences:** Examine the significance of mathematics in hydrology and atmospheric and ocean sciences, facilitating a deeper comprehension of Earth's systems.
- **Computer Sciences:** Delve into machine learning, data science, visualization, and natural language processing, areas where mathematics fuels the development of algorithms and tools for handling big data and artificial intelligence challenges.

This comprehensive curriculum aims to prepare students for a multitude of careers, fostering a seamless transition into specialized fields that rely on mathematical expertise for innovation and discovery empowered by AI.

**Contemporary Articles and Journal Club Presentations:**
To enrich the learning experience, students will have access to a curated list of cutting-edge research articles that delve into the practical applications of dynamical systems, stochastic calculus, and optimization within the realm of artificial intelligence. Key readings will include works by leading researchers in the field, such as [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12], offering students a broad perspective on contemporary advancements and methodologies:


[1] P. Vincent, "A Connection Between Score Matching and Denoising Autoencoders," *Neural Computation*, vol. 23, no. 7, pp. 1661–1674, Jul. 2011. [Online]. Available: https://direct.mit.edu/neco/article/23/7/1661-1674/7677

[2] J. Sohl-Dickstein, E. A. Weiss, N. Maheswaranathan, and S. Ganguli, "Deep Unsupervised Learning using Nonequilibrium Thermodynamics," Nov. 2015, arXiv:1503.03585 [cond-mat, q-bio, stat]. [Online]. Available: http://arxiv.org/abs/1503.03585

[3] J. Ho, A. Jain, and P. Abbeel, "Denoising Diffusion Probabilistic Models," Dec. 2020, arXiv:2006.11239 [cs, stat]. [Online]. Available: http://arxiv.org/abs/2006.11239

[4] Y. Song, J. Sohl-Dickstein, D. P. Kingma, A. Kumar, S. Ermon, and B. Poole, "Score-Based Generative Modeling through Stochastic Differential Equations," Feb. 2021, arXiv:2011.13456 [cs, stat]. [Online]. Available: http://arxiv.org/abs/2011.13456

[5] Q. Zhang and Y. Chen, "Diffusion Normalizing Flow," Oct. 2021, arXiv:2110.07579 [cs]. [Online]. Available: http://arxiv.org/abs/2110.07579

[6] T. Karras, M. Aittala, T. Aila, and S. Laine, "Elucidating the Design Space of Diffusion-Based Generative Models," Oct. 2022, arXiv:2206.00364 [cs, stat]. [Online]. Available: http://arxiv.org/abs/2206.00364

[7] L. Yang, Z. Zhang, Y. Song, S. Hong, R. Xu, Y. Zhao, Y. Shao, W. Zhang, B. Cui, and M.-H. Yang, "Diffusion Models: A Comprehensive Survey of Methods and Applications," Oct. 2022, arXiv:2209.00796 [cs]. [Online]. Available: http://arxiv.org/abs/2209.00796

[8] Q. Zhang and Y. Chen, "Path Integral Sampler: a stochastic control approach for sampling," Mar. 2022, arXiv:2111.15141 [cs]. [Online]. Available: http://arxiv.org/abs/2111.15141

[9] B. J. Holzschuh, S. Vegetti, and N. Thuerey, "Score Matching via Differentiable Physics," Jan. 2023, arXiv:2301.10250 [physics]. [Online]. Available: http://arxiv.org/abs/2301.10250

[10] M. Xu, L. Yu, Y. Song, C. Shi, S. Ermon, and J. Tang, "GeoDiff: a Geometric Diffusion Model for Molecular Conformation Generation," Mar. 2022, arXiv:2203.02923 [cs, q-bio]. [Online]. Available: http://arxiv.org/abs/2203.02923

[11] Y. Lipman, R. T. Q. Chen, H. Ben-Hamu, M. Nickel, and M. Le, "Flow Matching for Generative Modeling," Feb. 2023, arXiv:2210.02747 [cs, stat]. [Online]. Available: http://arxiv.org/abs/2210.02747

[12] T. Chen, G.-H. Liu, and E. A. Theodorou, "Likelihood Training of Schr\"odinger Bridge using Forward-Backward SDEs Theory," Apr. 2023, arXiv:2110.11291 [cs, math, stat]. [Online]. Available: http://arxiv.org/abs/2110.11291

This dynamic list will include the latest findings and insights. Students are encouraged to actively participate by contributing articles of interest, fostering a collaborative learning environment. Additionally, as part of the course's engagement activities, students will have the opportunity to present a 10-minute journal club presentation on selected articles or related topics. Although not mandatory, these presentations are incentivized with course credits, promoting active learning and critical thinking about current AI research trends.