華中科技大學数学中心

Center for Mathematical Sciences

中国 武汉

Wuhan China

Newsletter of the Center for Mathematical Sciences

2022 Winter

华中科技大学数学中心 简介

在建设世界一流大学的征程中，数学学科的作用异常重要。华中科技大学高瞻远瞩，于2013年成立数学中心。华中科技大学数学中心一方面倡导数学不同分支之间的相互交叉，激发新的合作研究，催生新的研究领域和研究群体。另一方面引领数学与工科、理科，医科及其它学科之间的合作研究，实现交叉创新、合作共赢。

作为我校国际交流与合作的平台，数学中心大力推动与发展“跨学科应用数学”合作研究。我们的跨学科合作研究领域包括数学与地球科学（物理海洋学和气候动力学）的交叉研究，以及数学与生命科学（计算和定量生物学）的交叉研究。

华中科技大学数学中心积极开展前瞻性研究，立足华中、辐射全国、影响海外。数学中心将国际先进的人才培养模式和研究机构运行机制有机融入到我国建设一流大学与一流学科的伟大事业之中，努力成为培养和聚集一流人才的平台，国际交流与合作的平台，科教运行机制以及人事体制改革试点的平台。

数学中心成员包括院士，国家特聘专家，外专千人计划专家，长江学者，青年学术英才，楚天学者，洪堡学者和华中学者。还有一批海内外知名访问学者，博士后，博士生，以及来自多个国家的留学生。数学中心设有李国平讲座教授，东湖讲座教授，东湖数学论坛，和郭友中数理科学讲座。

希望重要的数学发现萌芽于此，
希望新的研究领域和研究群体产生于此，
希望著名数学家和科学家在此留下足迹，
希望科技界更深刻地感受到数学的作用:
数学强，则科技强；科技强，则国家强！

数学中心官网

数学中心微信公众号

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華中科技大学数学中心

Center for Mathematical Sciences

Web:mathcenter. hust. edu. cn　　E-mail: mathcenter@hust.edu.cn

华中科技大学数学中心招收2023年免推硕士研究生

华中科技大学数学中心招收2023年秋季入学免推硕士研究生（面向有免推资格的本科生。本科专业不限）。

招生视频：http://x.eqxiu.com/s/3obeLrBg?eqrcode=1

华中科技大学数学中心网站：http://mathcenter.hust.edu.cn/

研究领域：包括随机动力系统，随机偏微分方程，随机分析，动力系统及其应用，几何与拓扑，偏微分方程，计算数学，应用数学，图像科学，数据科学与统计学，多尺度系统建模与计算模拟，数理地球科学和定量生物学。研究生指导团队实行双导师制，由本校专家和海外学者组成，包括院士，国家特聘专家，长江学者，青年学术英才，东湖讲座教授，楚天学者，优青，洪堡学者和华中学者。

数学中心已有来自世界各国的优秀学者，包括院士，教授，副教授/副研究员，助理教授，客座教授、访问学者，博士后以及博士研究生。他们从国内外（包括美国、英国、法国、德国、澳大利亚等国家）汇聚到美丽的江城武汉东湖之滨，共同致力于基础数学，计算与应用数学，概率与统计，数据科学，数学物理与交叉科学的发展。

欢迎有意愿的学生联系华中科技大学数学中心段金桥主任

（电邮：mathcenter@hust.edu.cn.）

欢迎加盟华中科技大学数学中心！

数学中心网址　　招生视频

華中科技大學数学中心

Center for Mathematical Sciences

Wuhan, China

Web：mathcenter. hust. edu. cn　　Email: mathcenter@hust.edu.cn

数学正在发生日新月异的变化。不仅数学内部各分支相互交融，共同推动数学向更高层次发展，而且科学与工程问题牵涉到越来越深的数学课题，对数学提出了重大挑战，激发了新的数学理论和方法的创立，从而推动数学本身的发展。数学也一直在背后推动着科学和工程技术的进步，为现代科学和高新技术的发展奠定坚实基础。世界强国必须是数学强国，数学弱国不可能是现代化强国，而现代高科技竞争同时包含数学研究的竞争。华中科技大学数学中心顺应科学发展趋势于2013年在武汉成立了。

数学中心宗旨

（1） 积极倡导数学不同分支之间的交叉研究；激发新的合作探索，催生新的研究领域和研究群体；
（2） 努力推动数学与科学，工程，医学之间的交叉研究；建立数学家和科学家之间的广泛联系，从而达到合作共赢；
（3） 聚集一流人才，培养优秀学生，做出一流学术研究，引领学科发展，服务国家和社会。

数学中心成员

数学中心已有来自世界各国的优秀学者，包括院士，教授，副教授/副研究员，助理教授，客座教授、访问学者，博士后以及博士研究生。他们从国内外（包括美国、英国、法国、德国、澳大利亚等国家）汇聚到美丽的江城武汉东湖之滨，共同致力于基础数学，计算与应用数学，概率与统计，数据科学，数学物理与交叉科学的发展。

数学中心诚聘海内外英才

无论您来自哪里，数学是我们的共同语言，欢迎您加入我们!

数学中心招聘网址:
https://www.mathjobs.org/jobs/list/16913

申请材料请寄段金桥老师:
mathcenter@hust.edu.cn

数学中心招聘二维码:

Open Positions in Wuhan Math Center

The Center for Mathematical Sciences, at Huazhong University of Science and Technology, Wuhan, China, is a mathematical research and education institution. Our mission is to promote interactions between mathematics and other disciplines, and to connect branches of mathematics. The Center's current research themes include stochastic mathematics, applied/computational mathematics, core mathematics, mathematical physics, and data science. Distinguished applicants in all areas of mathematical sciences will be considered.

Open Positions

• Assistant/Associate Professorships

Basic requirements:
A PhD degree in mathematical sciences or related fields, with distinguished research credentials.

• Postdoctoral fellows

Basic requirements:
New or recent PhD graduates in mathematical sciences or related fields, with distinguished research potential.

The compensation packages, including salary, start-up funds and housing allowance, are highly competitive, and are commensurate with qualification and experience.
The Center will also sponsor qualified candidates to compete for the National Junior Endowed Professorships.

How to Apply: Applicants should send these materials to mathcenter@hust.edu.cn:

1) A cover letter;
2) A curriculum vita with a list of 3 references;
3) A research statement.

Contact Us

Email Professor Jinqiao Duan: mathcenter@hust.edu.cn
Web Page: mathcenter.hust.edu.cn
Ads in MathJobs *https://www.mathjobs.org/jobs/list/16913*

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CONTENTS

目　录

News
新闻
东湖数学系列讲座 1
数学中心短课 6
2022 年 12 月召开华中科技大学数学中心学术年会 8
Academic Achievement
学术成果
2022 年已发表文章列表 9
Qualifying Exams
资格考试
Advanced Probability Theory Qualifying Exam 12
Functional Analysis Qualifying Exam 14
Popular Mathematics
数学热门话题
Take an online journey through the history of math
来一场在线的数学历史之旅吧 17
How a quantum technique highlights math's mysterious link to physics
量子技术如何凸显数学与物理学的神秘联系 20
A century ago, Alexander Friedmann envisioned the universe's expansion
一个世纪前，亚历山大·弗里德曼设想了宇宙的膨胀 24
Sensing the shape of functional proteins with topology
用拓扑学感知功能蛋白的形状 28

News
新闻

东湖数学系列讲座

华中科技大学数学中心于 2022 年 7 月-11 月顺利开展东湖数学系列讲座活动。讲座安排如下

报告题目：Some Recent Progress on Backward Stochastic Volterra Integral Equations
报告人：王寒霄（深圳大学）
时间：2022.07.08，周五，上午 10:00-11:00（北京时间）
腾讯会议 ID：543-460-996

报告摘要：

In this talk, we will briefly introduce some new results of backward stochastic Volterra integral equations (BSVIEs, for short). First, we will recall some classical results of BSDEs, type-I BSVIEs, and type-II BSVIEs. Some new estimates, features and applications of type-I BSVIEs will be also mentioned. For example, we will show that the generator of BSVIEs can be anticipating, but for BSDEs, the generator must be adapted. Next, we will introduce the type-III BSVIE and its connection with time-inconsistent optimal control problems. Indeed, type-III BSVIE has been a popular method for studying time-inconsistent control problems. Finally, we will introduce the path-dependent PDE approach to forward-backward SVIEs. A decoupling method of Volterra type stochastic Hamiltonian system will be also mentioned. The key technique is to establish a connection between linear type-II and type-III BSVIEs and to introduce the proper decoupling filed. This talk is based on some joint works with Yong (UCF), Zhang (USC), Zhou (NUS), and Sun (SUSTech).

报告人简介：

- 王寒霄，2014 年本科毕业于吉林大学，2020 年博士毕业于复旦大学，导师为国际数学家大会报告人雍炯敏教授。2017 年 10 月至 2019 年 5 月在美国中佛罗里达大学进行联合培养。2020 年 9 月至 2022 年 2 月在新加坡国立大学做博士后。2022 年 4 月至今任深圳大学数学与统计学院助理教授。主要从事随机控制和随机微分方程的研究。已在 Ann. I.H.P，ESAIM COCV，JDE，SICON 等期刊发表多篇学术论文。

报告题目：几类随机非线性系统的传播动力学
报告人：黄建华 教授（国防科技大学）
时间：2022.07.29，周五，上午 10:00-11:00（北京时间）
腾讯会议 ID：154-770-450

报告摘要：

在这个报告中，我们运用随机单调动力系统、遍历性、Feynman-Kac 公式和上下解等方法研究分布意义下，随机环境下种群之间相互作用分别为合作、竞争、竞争合作时，随机行波解的存在性和渐近传播速度的上、下届估计，分析噪声对传播速度的影响。最后用大偏差原理推导出广义 Feynman-Kac 公式，并由此给出纯跳噪声驱动的 KPP 方程的波速估计，该工作是与文豪、张亮和黎育红一起完成的。

报告人简介：

- 黄建华，国防科技大学数学教授，博士生导师，主要从事非线性系统的行波解及随机动力系统的动力学研究。先后完成 3 项国家自然科学基金面上项目和 2 项湖南省自然科学基金项目，参加 1 项国家自然科学基金重点项目研究。曾获得国家教学成果二等奖 1 次，湖南省自然科学二等奖和三等奖各 1 次。

报告题目：Explaining the reservoir computing phenomenon using randomized discrete-time signatures
报告人：Juan-Pablo Ortega Lahuerta (Nanyang Technological University)
时间：2022.08.05，周五，上午 10:00-11:00（北京时间）
Zoom ID：81880632959 Password：123456

报告摘要：

The possibility of uniformly approximating fading memory input/output systems using randomly generated state-space systems subjected to cheap training is a promising approach to the theory of recurrent neural networks that has been successfully implemented in many applications. In this talk we explain this surprising phenomenon by showing how the finite-dimensional random projections of certain universal infinite-dimensional approximants yield randomly generated state affine systems with linear readouts that exhibit excellent performance and, more importantly, provide a deep explanation of the reservoir computing phenomenon.

报告人简介：

- Juan-Pablo Ortega holds a first degree in Theoretical Physics from the Universidad de Zaragoza (Spain), a Masters and a PhD in Mathematics from the University of California, Santa Cruz, and a Habilitation degree from the Université de Nice (France). After a postdoc at the Ecole Polytechnique Fédérale de Lausanne (Switzerland) he became a researcher at the Centre Nationale de la Recherche Scientifique (CNRS, France). Before joining the Division of Mathematical Sciences of NTU, he taught mathematics at the Université Bourgogne Franche-Comté (France) and the University of St. Gallen (Switzerland). Prof. Ortega is a mathematician working on the learning and statistical modeling of dynamic processes like input/output systems, stochastic processes, dynamical and controlled systems, and time series. He is also interested in the applications of these topics to financial econometrics, mathematical finance, physiological signal treatment, and engineering. He has worked extensively in geometric mechanics, where he focuses on stability theory, symmetric systems, and their reduction.

报告题目：Well-posedness and wave-breaking for the stochastic rotation-two-component Camassa-Holm system

报告人：高洪俊 教授（东南大学）

时间：2022.08.26，周五，上午 10:00-11:00（北京时间）

腾讯会议 ID：315-679-496

报告摘要：

We study the global well-posedness and wave-breaking phenomenon for the stochastic rotation-two-component Camassa-Holm (R2CH) system. First, we find a Hamiltonian structure of the R2CH system and use the stochastic Hamiltonian to derive the stochastic R2CH system. Then, we establish the local well-posedness of the stochastic R2CH system by the dispersion-dissipation approximation system and the regularization method. We also show a precise blow-up criterion for the stochastic R2CH system. Moreover, we prove the global existence of the stochastic R2CH system occurs with high probability. At last, we consider transport noise case and establish the local well-posedness and another blow-up criterion.

报告人简介：

- 高洪俊，东南大学数学学院二级教授、博士生导师。担任 Stochastics and Dynamics 期刊编委。1994 年在北京应用物理与计算数学研究所获理学博士学位，目前主要研究兴趣为随机偏微分方程及其动力学。享受国务院政府特殊津贴，获得国防科工委科技进步奖一等奖和教育部自然科学二等奖等奖项，入选江苏省“青蓝工程”中青年学术带头人、江苏省“333”工程高层次人才、江苏省“青蓝工程”科技创新团队带头人。在包括 Adv. Math.、SIAM J. Math. Anal.、SIAM J. Appl. Dynamical Sys.、JLMS、IMRN、JDE 和中国科学在内的国内外重要期刊发表论文多篇。多次主持包括国家自然科学基金重点项目的基金项目多项，参与 973 项目，目前主持国家自然科学基金面上项目。

报告题目：Energy stable methods for phase-field surfactant model and simulation of droplet impact

报告人：Zhen Zhang (SUSTech)

时间：2022.11.11，周五，下午 3:00（北京时间）

腾讯会议 ID：809-897-479

报告摘要：

We develop energy stable and bound preserving schemes for phase-field surfactant model with moving contact lines. The desired properties of the schemes are rigorously proved. We numerically validate the accuracies of the schemes and apply them in simulating droplet impact problems. Qualitative agreements with experiments are obtained. Moreover, surfactants are observed to have effects on enhancing droplet deformation and reducing dissipations.

报告人简介：

- Zhen Zhang is an associate professor at the Department of Mathematics, Southern University of Science and Technology. He received his BA in mathematics from University of Science and Technology of China in 2007 and his PhD in applied mathematics from the Hong Kong University of Science and Technology in 2013. He worked as a postdoctoral fellow at Department of Mathematics in National University of Singapore from 2013 to 2015. His research interests include numerical analysis, multiphase moving contact line problems of complex fluids, multiscale modeling and simulation, phase-field modeling the modelling and its application in phase transition process, and sparse representation of data and feature selection in high dimensions.

报告题目：Simple implicit regularizations in deep learning
报告人：许志钦 教授（上海交通大学）
时间：2022.11.12，周六，上午 10:00-11:00（北京时间）
腾讯会议 ID：575-174-755

报告摘要：

Why do neural network models that look so complex usually generalize well? To understand this problem, we study deep learning training and find that some simple implicit regularization effects. The first is the frequency principle that neural networks learn from low frequency to high frequency. The second is the parameter condensation effect, which makes the number of neurons. We attempt to understand the mechanism of condensation from the embedding principle of loss landscape and gradient flow. We further derive the implicit regularization of Dropout and find that it can promote condensation formation and the flatness of the solution. These implicit regularizations all reflect the characteristic that neural networks tend to use simple functions to fit data in the training process, so as to achieve better generalization. Finally, I will discuss some important theoretical issues in neural networks.

报告人简介：

- Zhi-Qin John Xu is an associate professor at Shanghai Jiao Tong University (SJTU). Zhi-Qin obtain B.S. in Physics (2012) and a Ph.D. degree in Mathematics (2016) from SJTU. Before joining SJTU, Zhi-Qin worked as a postdoc at NYUAD and Courant Institute from 2016 to 2019. He published papers on Journal of Machine Learning Research, AAAI, NeurIPS, Communications in Computational Physics, SIMODS, European Journal of Neuroscience and Communications in Mathematical Science etc. He is a managing editor of Journal of Machine Learning.

数学中心短课

Mini-Course: Modern Quantum Mechanics and Its Application

Prof. Evgeniy Kiktenko, Prof. Aleksey K. Fedorov.

Zoom Meeting: 506 635 6571 Passcode: 202211

Schedule	Outline
Nov. 21, 2022 16:00-19:30 pm	Lecture 1a (AF) Lecture 2a (EK)
Nov. 23, 2022 16:00-19:30 pm	Lecture 2b (EK) Lecture 1b (AF)
Nov. 24, 2022 16:00-19:30 pm	Lecture 3a (EK) Lecture 4a (AF)
Nov. 25, 2022 16:00-19:30 pm	Lecture 3b (EK) Lecture 4b (AF)
Upcoming	Lecture 5-8

Lecture 1: Overview of quantum information technologies area

General overview of quantum information processing, history of quantum computing, basic principles and models of quantum computing.

Lecture 2: Basics of quantum mechanics formalism

Bra-, ket- notation, observables, von Neuman measurement and Born rule, tensor product and partial trace, Schrödinger, Heisenberg, and Dirac pictures of quantum dynamics, Schmidt decomposition, quantum entanglement and purification.

Lecture 3: Quantum and post-quantum cryptography

BB84 protocol, classical post-processing, concept of post-quantum cryptography.

Lecture 4: Quantum entanglement and its applications

Quantum entanglement and complexity of quantum states decription. Tesnor networks and matrix product states. Local hidden variables and Bell inequality. Quantum teleportaion and quantum superdense coding.

Lecture 5: Quantum computing in NISQ era

Physical platforms of quantum computing. Quantum machine learning. Quantum chemisty.

Lecture 6: Open quantum systems

Positive operator-valued measures (POVM), soft measurements, informationally complete POVM (IC-POVM), minimal IC-POVM (MIC-POVM), symmetric IC-POVM (SIC-POVM). Dynamics of open quantum systems, completely positive trace-preserving (CPTP) maps. Master equation.

Lecture 7: Quantum simulation for many-body systems

The use of quantum computers to simulate complex many-body quantum systems in analog and digital manners.

Lecture 8: Universal quantum computation

The concept of universal quantum computation. Universal set of gates and quantum error correction. Solovay-Kitaev theorem. “Quantum parallelism”. Quantum Fourier transform. Basic quantum algorithms: Bernstein-Vazirani, Saimon, Shor, Grover. Clifford gates and Gottesman-Knill theorem.

更多课程回放内容，关注哔哩哔哩官方账号：华中大数学中心

2022 年 12 月召开华中科技大学数学中心学术年会

时间：2022 年 12 月 8 日　　09:00-16:30

腾讯会议 ID：614 104 149（无密码）

年会安排：

序号	时间	汇报人	报告题目
1	9:00-9:30	付建勋	Three-nested folding models and its applications
2	9:30-10:00	高婷	基于随机动力系统的可解释性深度学习
3	10:00-10:30	郇真	Elliptic cohomology and 2-Vector Bundles
4	10:30-11:00	林聪萍	流动环境下的内质网几何动力学
5	11:00-11:30	刘超	On nonlinear Jeans instability
6	14:00-14:30	向茂松	微分分次几何中的同调类
7	14:30-15:00	徐海涛	格点系统中的边界态与谱带分析
8	15:00-15:30	殷钶	基于补偿凸变换的优化方法
9	15:30-16:00	张一威	动力系统中的热力学机制、大偏差与重分形分解的一点新进展
10	16:00-16:30	赵蒙	Electrically controlled self-similar evolution of viscous fingering patterns

Academic Achievement

学术成果

2022 年已发表文章列表

1. Lin L, Yang M, Duan J: Effective approximation for a nonlocal stochastic Schrödinger equation with oscillating potential. Zeitschrift für angewandte Mathematik und Physik, 2023, 74(1): 1-20.

2. Wang Z, Lv L, Duan J: Homogenization of Dissipative Hamiltonian Systems Under Lévy Fluctuations. Journal of Nonlinear Science, 2023, 33(1): 1-39.

3. Yang L, Gao T, Lu Y, Duan J, Liu T: Neural network stochastic differential equation models with applications to financial data forecasting. Applied Mathematical Modelling, 2023, 115: 279-299.

4. Zhang Y, Wang X, Wang Z, Duan J: Analysis of multiscale methods for stochastic dynamical systems driven by α-stable processes. Applied Mathematics Letters, 2023, 136: 108462.

5. Yuan S, Schilling R, Duan J: Large deviations for stochastic nonlinear systems of slow–fast diffusions with non-Gaussian Lévy noises. International Journal of Non-Linear Mechanics, 2023, 148: 104304.

6. Chen X, Duan J, Hu J, Li D: Data-driven method to learn the most probable transition pathway and stochastic differential equation. Physica D: Nonlinear Phenomena, 2023, 443: 133559.

7. Chen J, Hu J, Wei W, Duan J: A data-driven approach for discovering the most probable transition pathway for a stochastic carbon cycle system. Chaos: An Interdisciplinary Journal of Nonlinear Science, 2022, 32(11): 113140.

8. Chen S, Duan J: Instability of small-amplitude periodic waves from fold-Hopf bifurcation. Journal of Mathematical Physics, 2022, 63(11): 112702.

9. Lu Y, Li Y, Duan J: Extracting stochastic governing laws by non-local Kramers–Moyal formulae. Philosophical Transactions of the Royal Society A, 2022, 380(2229): 20210195.

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Qualifying Exams

资格考试

Advanced Probability Theory Qualifying Exam

Center for Mathematical Sciences Huazhong University of Science and Technology

December 2022

Note: This exam covers Le Gall: Measure Theory, Probability, and Stochastic Processes.

1. Let $(E,\mathcal{A})$ be a measure space, and let μ be a finite measure on E. If $(f_n)_{n\in\mathbb{N}}$ and f are real measurable functions on E, we say that f_n converges in μ-measure to f if, for every $\varepsilon>0$

$$\mu\left(\left\{x\in E:\left|f_n(x)-f(x)\right|>\varepsilon\right\}\right)\xrightarrow{n\to\infty}0$$

(1) Show that if $f_n(x)\to f(x),\mu(dx)$ a.e., then f_n converges in μ-measure to $f(x)$. Give an example (using Lebesgue measure) showing that the converse is not true in general.

(2) Show that, if the sequence f_n converges in μ-measure to f, we can find a subsequence $(f_{n_k})_{k\in N}$ such that $f_{n_k}(x)\to f(x)$ as $k\to\infty$, $\mu(dx)$ a.e.

(3) Show that (still under our assumption that μ is finite) the conclusion of the dominated convergence theorem remains valid if we replace the condition

$$f_n\xrightarrow{n\to\infty}f(x),\mu(dx)\ a.e.$$

by the weaker assumption f_n converges in μ-measure to f.

2. (1) Show that, if $\mu(E)<\infty$, one has $\|f\|_\infty=\lim\limits_{p\to\infty}\|f\|_p$ for any measurable function $f:E\to\mathbb{R}$.

(2) Show that the result of question (1) still holds when $\mu(E)=\infty$ if we assume that $\|f\|_p<\infty$ for some $p\in[1,\infty)$.

3. (20 points) Let $(X_n)_{n\in\mathbb{N}}$ be a sequence of independent and identically distributed random variables with values in $\mathbb{R}_+$. Show that, if $\mathbb{E}[X_1]<\infty$,

$$\limsup_{n\to\infty}\frac{X_n}{n}=0,\ a.s.,$$

whereas, if $\mathbb{E}[X_1]=\infty$,

$$\limsup_{n\to\infty}\frac{X_n}{n}=0,\ a.s.$$

4. Let $(X_n)_{n\in N}$ be a sequence of independent and identically distributed random variables in L^2, such that $\mathbb{E}[X_n]=0$ and $\upsilon ar(X_n)>0$. Set $S_n=X_1+\cdots+X_n$.

(1) Prove that

$$\limsup_{n\to\infty} \frac{S_n}{\sqrt{n}} = \infty,\ a.s.$$

(2) Prove that the sequence $S_n / \sqrt{n}$ does not converge in probability.

(3) Prove that the limit

$$\lim_{n\to\infty} \mathbb{P}(S_n > 0, S_{2n} < 0)$$

exists and compute this limit.

5. Let $(\mathcal{A}_n)_{n\in N}$ be a decreasing sequence of sub-σ-fields of $\mathcal{A}$, with $\mathcal{A}_1 = \mathcal{A}$, and let $X \in L^2(\Omega, \mathcal{A}, \mathbb{P})$.

(1) Prove that the random variables $\mathbb{E}\left[X \middle| \mathcal{A}_n\right] - \mathbb{E}\left[X \middle| \mathcal{A}_{n+1}\right]$, for $n \in \mathbb{N}$, are orthogonal in L^2, and that the series

$$\sum_{n\in\mathbb{N}} \left(\mathbb{E}\left[X \middle| \mathcal{A}_n\right] - \mathbb{E}\left[X \middle| \mathcal{A}_{n+1}\right]\right)$$

converges in L^2.

(2) Let $\mathcal{A}_\infty = \bigcap_{n\in\mathbb{N}} \mathcal{A}_n$. Prove that

$$\lim_{n\to\infty} \mathbb{E}\left[X \middle| \mathcal{A}_n\right] = \mathbb{E}\left[X \middle| \mathcal{A}_\infty\right], \text{ in } L^2.$$

Functional Analysis Qualifying Exam

Center for Mathematical Sciences Huazhong University of Science and Technology

Winter 2022

Reference:

Haim Brezis: Functional Analysis, Sobolev Spaces and Partial Differential Equations.

1. Let $E=\ell^1$, so that $E^*=\ell^\infty$. Consider $N=c_0$ as a closed subspace of E^*. Determine
$$N^\perp=\{x\in E;\langle f,x\rangle=0 \quad \forall f\in N\}$$
and
$$N^{\perp\perp}=\{f\in E^*;\langle f,x\rangle=0 \quad \forall x\in N^\perp\}$$
Check that $N^{\perp\perp}\neq N$.

2. Let E and F be two Banach spaces and let (T_n) be a sequence in $\mathcal{L}(E,F)$. Assume that for every $x\in E$, T_nx converges as $n\to\infty$ to a limit denoted by Tx. Show that if $x_n\to x$ in E, then $T_nx_n\to Tx$ in F.

3. Let E be a Banach space and let $K\subset E$ be a subset of E that is compact in the strong topology. Let (x_n) be a sequence in K such that $x_n\rightharpoonup x$ weakly $\sigma(E,E^*)$. Prove that $x_n\to x$ strongly.

4. Let $1\le p<\infty$ and $1\le q\le\infty$.
(a) Prove that $L^1(\Omega)\cap L^\infty(\Omega)$ is a dense subset of $L^p(\Omega)$.
(b) Prove that the set
$$\{f\in L^p(\Omega)\cap L^q(\Omega);\|f\|_q\le 1\}$$
is closed in $L^p(\Omega)$.
(c) Let (f_n) be a sequence in $L^p(\Omega)\cap L^q(\Omega)$ and let $f\in L^p(\Omega)$. Assume that
$$f_n\to f \text{ in } L^p(\Omega) \text{ and } \|f_n\|_q\le C.$$
Prove that $f\in L^r(\Omega)$ and that $f_n\to f$ in $L^r(\Omega)$ for every r between p and q, $r\neq q$.

5. Let $M\subset H$ be a closed linear subspace that is not reduced to $\{0\}$. Let $f\in H$, $f\notin M^\perp$.
(a) Prove that
$$m=\inf_{u\in M,|u|=1}(f,u)$$
is uniquely achieved.
(b) Let $\varphi_1,\varphi_2,\varphi_3\in H$ be given and let E denote the linear space spanned by

$\{\varphi_1, \varphi_2, \varphi_3\}$. Determine m in the following cases:

i. $M = E$,

ii. $M = E^{\perp}$.

(c) Examine the case in which $H = L^2(0,1)$, $\varphi_1(t) = t$, $\varphi_2(t) = t^2$, and $\varphi_3(t) = t^3$.

6. Let (λ_n) be a sequence of positive numbers such that $\lim_{n\to\infty} \lambda_n = +\infty$. Let V be the space of sequences $(u_n)_{n\geq 1}$ such that

$$\sum_{n=1}^{\infty} \lambda_n |u_n|^2 < \infty.$$

The space V is equipped with the scalar product

$$((u,\upsilon)) = \sum_{n=1}^{\infty} \lambda_n u_n \upsilon_n.$$

Prove that V is a Hilbert space and that $V \subset \ell^2$ with compact injection.

7. Let E be a Banach space and let $T \in \mathcal{L}(E)$.

(a) Assume that $T^2 = I$. Prove that $\sigma(T) \subset \{-1,+1\}$ and determine $(T - \lambda I)^{-1}$ for $\lambda \neq \pm 1$.

(b) More generally, assume that there is an integer $n \geq 2$ such that $T^n = I$. Prove that $\sigma(T) \subset \{-1,+1\}$ and determine $(T - \lambda I)^{-1}$ for $\lambda \neq \pm 1$.

(c) Assume that there is an integer $n \geq 2$ such that $T^n = 0$. Prove that $\sigma(T) = \{0\}$ and determine $(T - \lambda I)^{-1}$ for $\lambda \neq 0$.

(d) Assume that there is an integer $n \geq 2$ such that $\|T^n\| < 1$. Prove that $I - T$ is bijective and give an expression for $(I - T)^{-1}$ in terms of $(I - T^n)^{-1}$ and the iterates of T.

8. Fix a function $\varphi \in C_c^{\infty}(\mathbb{R})$, $\varphi \not\equiv 0$, and set $u_n(x) = \varphi(x+n)$. Let $1 \leq p \leq \infty$.

(a) Check that (u_n) is bounded in $W^{1,p}(\mathbb{R})$.

(b) Prove that there exists no subsequence (u_{n_k}) converging strongly in $L^q(\mathbb{R})$, for any $1 \leq q \leq \infty$.

(c) Show that $u_n \rightharpoonup 0$ weakly in $W^{1,p}(\mathbb{R})$ $\forall p \in (1,\infty)$.

9. Let $H = L^2(0,1)$ and consider the function $\varphi : H \to (-\infty, +\infty]$ defined by

$$\varphi(u) = \begin{cases} \dfrac{1}{2}\displaystyle\int_0^1 u'^2 & \text{if } u \in H^1(0,1), \\ +\infty & \text{if } u \in L^2(0,1) \text{ and } u \notin H^1(0,1). \end{cases}$$

(a) Check that φ is convex and lower semicontinuous.

(b) Compute $\varphi^*(f)$ for every $f \in H$.

10. Let $I = (0,1)$ and $1 \leq p \leq \infty$. Set

$$B_p = \left\{ u \in W^{1,p}(I);\ \|u\|_{L^p(I)} + \|u'\|_{L^p(I)} \le 1 \right\}.$$

(a) Prove that B_p is a closed subset of $L^p(I)$ when $1 < p \le \infty$; more precisely, B_p is compact in $L^p(I)$.

(b) Show that B_1 is not a closed subset of $L^1(I)$.

Popular Mathematics
数学热门话题

Take an online journey through the history of math
来一场在线的数学历史之旅吧

By Erin Wayman

数学的发展史大致可以分为四个时期。

第一时期是数学形成时期（远古——公元前六世纪），这是人类建立最基本的数学概念的时期。人类从数数开始逐渐建立了自然数的概念，简单的计算法，并认识了最基本、最简单的几何形式，算术与几何还没有分开。

第二时期是初等数学时期、常量数学时期（公元前六世纪——公元十七世纪初），这个时期的基本的、最简单的成果构成中学数学的主要内容，大约持续了两千年。这个时期逐渐形成了初等数学的主要分支：算数、几何、代数。

第三时期是变量数学时期（公元十七世纪初——十九世纪末），变量数学产生于 17 世纪，经历了两个决定性的重大步骤：第一步是解析几何的产生；第二步是微积分（Calculus）的创立。

第四时期是现代数学时期（十九世纪末开始），数学发展的现代阶段的开端，以其所有的基础——代数、几何、分析中的深刻变化为特征。

Around 1900 B.C., a student in the Sumerian city of Nippur, in what's now Iraq, copied a multiplication table onto a clay tablet. Some 4,000 years later, that schoolwork survives, as do the student's errors (10 times 45, for example, is definitely not 270). The work is a reminder that no matter how elegant or infallible mathematics may seem, it's still a human endeavor.

That's one lesson I took from "History of Mathematics," an online exhibit developed by the National Museum of Mathematics in New York City and Wolfram Research, a computational technology company. Bringing together the Sumerian tablet and more than 70 other artifacts, the exhibit demonstrates how math has been a universal language across cultures and throughout time.

Divided into nine "galleries," the exhibit sums up the development of key topics related to mathematics, including counting, arithmetic, algebra, geometry and prime numbers. Each

gallery has a short timeline and features a handful of artifacts that serve as entry points to explore some milestones in more depth.

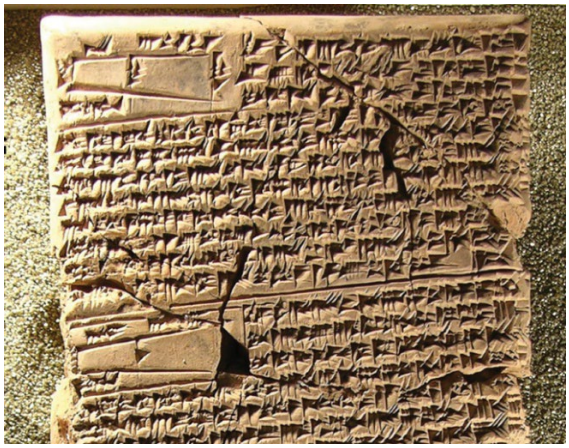
Among the highlights: The oldest known surviving calculating device, the Salamis Tablet, is a marble counting board from the Greek island of Salamis dating to 300 B.C. It's a precursor to the abacus. By moving pebbles across the board, a person could perform calculations. An early documented instance of using a symbol for "zero" as a placeholder (to, say, distinguish 1 from 10, 100 or 1,000) appears in the Bakhshali Manuscript, an Indian text dating to perhaps as early as A.D. 300. The manuscript's black dots eventually morphed into the open circles we know today as zeros. Also on display is *Al-Jabr*. Written in around 820 by Persian polymath Muḥammad ibn Mūsā al-Khwārizmī, the book established the field of algebra and gave the discipline its name. In 1557, the *Whetstone of Witte*, an English algebra text, introduced the modern equal symbol.

But the exhibit is more than just a collection of fun facts. As the galleries explain, humans' relationship with numbers goes back deep into prehistory. Modern math, however, stems from the rise of cities, with the need to keep track of people and supplies, and to undertake ever more complex construction projects.

Some mathematical principles must have been so vital to civilization's success that they appeared in many ancient cultures. Take the Pythagorean theorem. The Greek philosopher Pythagoras, who lived in the sixth century B.C., famously related the side lengths of a right triangle in the equation $a^2 + b^2 = c^2$. But a clay tablet reveals that people in Mesopotamia had worked out the relationship more than 1,000 years earlier. Ancient Chinese and Indian scholars were also familiar with the relationship.

Other math problems have had multiple solutions. The history of counting is littered with an array of methods for keeping track of numbers, from various forms of finger counting to the stringed recording devices called quipus, or khipus, used in the Inca Empire in the 1400s and 1500s. The placement and types of knots along a quipu's strings indicate different numerical values, though researchers today are still trying to understand exactly how to interpret the data recorded on these devices (*SN: 7/6/19 & 7/20/19, p. 12*).

This tablet, dated to as early as 2000 B.C., shows several math problems and drawings of trapezoids and triangles. The text suggests that people in Mesopotamia grasped the Pythagorean theorem long before the Greek philosopher Pythagoras, for whom the theorem is now named, lived.



Parts of the exhibit assume a high level of mathematical knowledge, such as some of the interactive features that give technical explanations behind some artifacts' mathematical principles. But a section of "learning journeys" aimed at "kids and others" provides materials that fill in some of the missing details from the main galleries and will appeal to adults whose memories of high school or college math are fuzzy.

"History of Mathematics" is a fascinating starting point for anyone interested in learning about the origins of the mathematical concepts that so many of us use every day but often take for granted.

How a quantum technique highlights math's mysterious link to physics

量子技术如何凸显数学与物理学的神秘联系

By Tom Siegfried

一项依赖于量子纠缠的技术扩展了数学问题的领域，其解决方案（理论上）可以得到验证。

It has long been a mystery why pure math can reveal so much about the nature of the physical world.

Antimatter was discovered in Paul Dirac's equations before being detected in cosmic rays. Quarks appeared in symbols sketched out on a napkin by Murray Gell-Mann several years before they were confirmed experimentally. Einstein's equations for gravity suggested the universe was expanding a decade before Edwin Hubble provided the proof. Einstein's math also predicted gravitational waves a full century before behemoth apparatuses detected those waves (which were produced by collisions of black holes — also first inferred from Einstein's math).

Nobel laureate physicist Eugene Wigner alluded to math's mysterious power as the "unreasonable effectiveness of mathematics in the natural sciences." Somehow, Wigner said,

math devised to explain known phenomena contains clues to phenomena not yet experienced — the math gives more out than was put in. “The enormous usefulness of mathematics in the natural sciences is something bordering on the mysterious and … there is no rational explanation for it,” Wigner wrote in 1960.

But maybe there’s a new clue to what that explanation might be. Perhaps math’s peculiar power to describe the physical world has something to do with the fact that the physical world also has something to say about mathematics.

At least that’s a conceivable implication of a new paper that has startled the interrelated worlds of math, computer science and quantum physics.

In an enormously complicated 165-page paper, computer scientist Zhengfeng Ji and colleagues present a result that penetrates to the heart of deep questions about math, computing and their connection to reality. It’s about a procedure for verifying the solutions to very complex mathematical propositions, even some that are believed to be impossible to solve. In essence, the new finding boils down to demonstrating a vast gulf between infinite and almost infinite, with huge implications for certain high-profile math problems. Seeing into that gulf, it turns out, requires the mysterious power of quantum physics.

Everybody involved has long known that some math problems are too hard to solve (at least without unlimited time), but a proposed solution could be rather easily verified. Suppose someone claims to have the answer to such a very hard problem. Their proof is much too long to check line by line. Can you verify the answer merely by asking that person (the “prover”) some questions? Sometimes, yes. But for very complicated proofs, probably not. If there are two provers, though, both in possession of the proof, asking each of them some questions might allow you to verify that the proof is correct (at least with very high probability). There’s a catch, though — the provers must be kept separate, so they can’t communicate and therefore collude on how to answer your questions. (This approach is called MIP, for multiprover interactive proof.)

Verifying a proof without actually seeing it is not that strange a concept. Many examples exist for how a prover can convince you that they know the answer to a problem without actually telling you the answer. A standard method for coding secret messages, for example, relies on

using a very large number (perhaps hundreds of digits long) to encode the message. It can be decoded only by someone who knows the prime factors that, when multiplied together, produce the very large number. It's impossible to figure out those prime numbers (within the lifetime of the universe) even with an army of supercomputers. So if someone can decode your message, they've proved to you that they know the primes, without needing to tell you what they are.

Someday, though, calculating those primes might be feasible, with a future-generation quantum computer. Today's quantum computers are relatively rudimentary, but in principle, an advanced model could crack codes by calculating the prime factors for enormously big numbers.

That power stems, at least in part, from the weird phenomenon known as quantum entanglement. And it turns out that, similarly, quantum entanglement boosts the power of MIP provers. By sharing an infinite amount of quantum entanglement, MIP provers can verify vastly more complicated proofs than nonquantum MIP provers.

It is obligatory to say that entanglement is what Einstein called "spooky action at a distance." But it's not action at a distance, and it just seems spooky. Quantum particles (say photons, particles of light) from a common origin (say, both spit out by a single atom) share a quantum connection that links the results of certain measurements made on the particles even if they are far apart. It may be mysterious, but it's not magic. It's physics.

Say two provers share a supply of entangled photon pairs. They can convince a verifier that they have a valid proof for some problems. But for a large category of extremely complicated problems, this method works only if the supply of such entangled particles is infinite. A large amount of entanglement is not enough. It has to be literally unlimited. A huge but finite amount of entanglement can't even approximate the power of an infinite amount of entanglement.

As Emily Conover explains in her report for *Science News*, this discovery proves false a couple of widely believed mathematical conjectures. One, known as Tsirelson's problem, specifically suggested that a sufficient amount of entanglement could approximate what you could do with an infinite amount. Tsirelson's problem was mathematically equivalent to

another open problem, known as Connes' embedding conjecture, which has to do with the algebra of operators, the kinds of mathematical expressions that are used in quantum mechanics to represent quantities that can be observed.

Refuting the Connes conjecture, and showing that MIP plus entanglement could be used to verify immensely complicated proofs, stunned many in the mathematical community. (One expert, upon hearing the news, compared his feces to bricks.) But the new work isn't likely to make any immediate impact in the everyday world. For one thing, all-knowing provers do not exist, and if they did they would probably have to be future super-AI quantum computers with unlimited computing capability (not to mention an unfathomable supply of energy). Nobody knows how to do that in even *Star Trek's* century.

Still, pursuit of this discovery quite possibly will turn up deeper implications for math, computer science and quantum physics.

It probably won't shed any light on controversies over the best way to interpret quantum mechanics, as computer science theorist Scott Aaronson notes in his blog about the new finding. But perhaps it could provide some sort of clues regarding the nature of infinity. That might be good for something, perhaps illuminating whether infinity plays a meaningful role in reality or is a mere mathematical idealization.

On another level, the new work raises an interesting point about the relationship between math and the physical world. The existence of quantum entanglement, a (surprising) physical phenomenon, somehow allows mathematicians to solve problems that seem to be strictly mathematical. Wondering why physics helps out math might be just as entertaining as contemplating math's unreasonable effectiveness in helping out physics. Maybe even one will someday explain the other.

A century ago, Alexander Friedmann envisioned the universe's expansion

一个世纪前，亚历山大·弗里德曼设想了宇宙的膨胀

By Tom Siegfried

1922 年，亚历山大·弗里德曼概述了宇宙的多种可能历史。宇宙膨胀是其中一种可能性。在宇宙膨胀的背景下，从宇宙大爆炸到现在的宇宙历史示意图。第一个弗里德曼方程描述了所有这些时期，从宇宙暴胀到大爆炸，再到现在和遥远的未来。即使在今天，该方程也非常准确。

For millennia, the universe did a pretty good job of keeping its secrets from science.

Ancient Greeks thought the universe was a sphere of fixed stars surrounding smaller spheres carrying planets around the central Earth. Even Copernicus, who in the 16th century correctly replaced the Earth with the sun, viewed the universe as a single solar system encased by the star-studded outer sphere.

But in the centuries that followed, the universe revealed some of its vastness. It contained countless stars agglomerated in huge clusters, now called galaxies.

Then, at the end of the 1920s, the cosmos disclosed its most closely held secret of all: It was

getting bigger. Rather than static and stable, an everlasting and ever-the-same entity encompassing all of reality, the universe continually expanded. Observations of distant galaxies showed them flying apart from each other, suggesting the current cosmos to be just the adult phase of a universe born long ago in the burst of a tiny blotch of energy.

It was a surprise that shook science at its foundations, undercutting philosophical preconceptions about existence and launching a new era in cosmology, the study of the universe. But even more surprising, in retrospect, is that such a deep secret had already been suspected by a mathematician whose specialty was predicting the weather.

A century ago this month (May 1922), Russian mathematician-meteorologist Alexander Friedmann composed a paper, based on Einstein's general theory of relativity, that outlined multiple possible histories of the universe. One such possibility described cosmic expansion, starting from a singular point. In essence, even without considering any astronomical evidence, Friedmann had anticipated the modern Big Bang theory of the birth and evolution of the universe.

"The new vision of the universe opened by Friedmann," writes Russian physicist Vladimir Soloviev in a recent paper, "has become a foundation of modern cosmology."

Friedmann was not well known at the time. He had graduated in 1910 from St. Petersburg University in Russia, having studied math along with some physics. In graduate school he investigated the use of math in meteorology and atmospheric dynamics. He applied that expertise in aiding the Russian air force during World War I, using math to predict the optimum release point for dropping bombs on enemy targets.

After the war, Friedmann learned of Einstein's general theory of relativity, which describes gravity as a manifestation of the geometry of space (or more accurately, spacetime). In Einstein's theory, mass distorts spacetime, producing spacetime "curvature," which makes masses appear to attract each other.

Friedmann was especially intrigued by Einstein's 1917 paper (and a similar paper by Willem de Sitter) applying general relativity to the universe as a whole. Einstein found that his original equations allowed the universe to grow or shrink. But he considered that unthinkable,

so he added a term representing a repulsive force that (he thought) would keep the size of the cosmos constant. Einstein concluded that space had a positive spatial curvature (like the surface of a ball), implying a "closed," or finite universe.

Friedmann accepted the new term, called the cosmological constant, but pointed out that for various values of that constant, along with other assumptions, the universe might exhibit very different behaviors. Einstein's static universe was a special case; the universe might also expand forever, or expand for a while, then contract to a point and then begin expanding again.

Friedmann's paper describing dynamic universes, titled "On the Curvature of Space," was accepted for publication in the prestigious *Zeitschrift für Physik* on June 29, 1922.

Einstein objected. He wrote a note to the journal contending that Friedmann had committed a mathematical error. But the error was Einstein's. He later acknowledged that Friedmann's math was correct, while still denying that it had any physical validity.

Friedmann insisted otherwise.

He was not just a pure mathematician, oblivious to the physical meanings of his symbols on paper. His in-depth appreciation of the relationship between equations and the atmosphere persuaded him that the math meant something physical. He even wrote a book (The World as Space and Time) delving deeply into the connection between the math of spatial geometry and the motion of physical bodies. Physical bodies "interpret" the "geometrical world," he declared, enabling scientists to test which of the various possible geometrical worlds humans actually inhabit. Because of the physics-math connection, he averred, "it becomes possible to determine the geometry of the geometrical world through experimental studies of the physical world."

So when Friedmann derived solutions to Einstein's equations, he translated them into the possible physical meanings for the universe. Depending on various factors, the universe could be expanding from a point, or from a finite but smaller initial state, for instance. In one case he envisioned, the universe began to expand at a decelerating rate, but then reached an inflection point, whereupon it began expanding at a faster and faster rate. At the end of the

20th century, astronomers measuring the brightness of distant supernovas concluded that the universe had taken just such a course, a shock almost as surprising as the expansion of the universe itself. But Friedmann's math had already forecast such a possibility.

No doubt Friedmann's deep appreciation for the synergy of abstract math and concrete physics prepared his mind to consider the notion that the universe could be expanding. But maybe he had some additional help. Although he was the first scientist to seriously propose an expanding universe, he wasn't the first person. Almost 75 years before Friedmann's paper, the poet Edgar Allan Poe had published an essay (or "prose poem") called Eureka. In that essay Poe described the history of the universe as expanding from the explosion of a "primordial particle." Poe even described the universe as growing and then contracting back to a point again, just as envisioned in one of Friedmann's scenarios.

Although Poe had studied math during his brief time as a student at West Point, he had used no equations in Eureka, and his essay was not recognized as a contribution to science. At least not directly. It turns out, though, that Friedmann was an avid reader, and among his favorite authors were Dostoevsky and Poe. So perhaps that's why Friedmann was more receptive to an expanding universe than other scientists of his day.

Today Friedmann's math remains at the core of modern cosmological theory. "The fundamental equations he derived still provide the basis for the current cosmological theories of the Big Bang and the accelerating universe," Israeli mathematician and historian Ari Belenkiy noted in a 2013 paper. "He introduced the fundamental idea of modern cosmology — that the universe is dynamic and may evolve in different manners."

Friedmann emphasized that astronomical knowledge in his day was insufficient to reveal which of the possible mathematical histories the universe has chosen. Now scientists have much more data, and have narrowed the possibilities in a way that confirms the prescience of Friedmann's math.

Friedmann did not live to see the triumphs of his insights, though, or even the early evidence that the universe really does expand. He died in 1925 from typhoid fever, at the age of 37. But he died knowing that he had deciphered a secret about the universe deeper than any suspected by any scientist before him. As his wife remembered, he liked to quote a passage from Dante: "The waters I am entering, no one yet has crossed."

Sensing the shape of functional proteins with topology

用拓扑学感知功能蛋白的形状

By Yunan Luo

蛋白质工程通过筛选巨大的突变空间来迭代优化蛋白质适应度，虽然受到实验能力的限制，但各种机器学习模型已经大大加快了蛋白质工程的速度。三维蛋白质结构具有进一步的优势，但其复杂的几何复杂性阻碍了其在深度突变筛选中的应用。持久同调是一种用于降低蛋白质结构复杂性的代数拓扑工具，在对给定数据的过滤过程中，它无法捕捉到同调形状的演变。引入一个拓扑提供的蛋白质适应度（TopFit）框架来补充蛋白质序列和结构嵌入。TopFit 采用集成回归策略，将持续谱理论（一种新的拓扑拉普拉斯算子）和两个辅助序列嵌入相结合，以捕获突变诱导的拓扑不变量、形状进化和序列差异。TopFit 的性能由包含 128,634 个变量的 34 个基准数据集进行评估，涉及各种蛋白质结构获取方式和训练集大小变化。

A topology-based approach is developed to better understand the relationship between protein structure and protein function.

Establishing connections between seemingly disparate fields of science may speed up the research process in one area by utilizing the techniques established in the other area as a jumping-off point. Writing for *Nature Computational Science*, Yuchi Qiu and Guo-Wei Wei[1] unveiled an algorithm that captures the structural features of functional proteins using methods in topology, a branch of mathematics that concerns the properties of shapes and spaces that are preserved under continuous deformations.

The scientific problem the authors studied is known as protein engineering, a biotechnology that involves the design and manipulation of protein sequences in order to create proteins with improved or new functions. A number of experimental techniques have been developed for engineering proteins, exemplified by directed evolution, a Nobel Prize-winning method that mimics the natural selection process to identify function-improved proteins through iterative rounds of variants screening and selection. Although well-established, directed evolution is still a costly and time-consuming process that requires screening an enormous number of protein variants in the mutational space to identify functional ones, and this is where machine learning (ML) may come in to assist[2].

The core computational problem in using ML for protein engineering is to map the protein sequence space to the protein fitness landscape. Due to the paucity of fitness data generated by experiments such as mutagenesis, recent studies have leveraged evolutionarily related sequence data to infer how likely a mutation is to affect function. This idea has led to two streams of approaches. One is to learn global evolutionary information from a large-scale corpus of protein sequences (for instance, UniProt) using protein language models[3–6], and the other is to learn local, more family-specific evolutionary information from the multiple sequence alignment of a target protein using ML algorithms such as Markov random fields or variational autoencoders[7,8]. Hybrid models that combine global and local information have also been developed to improve prediction performance[9,10].

Sequence data is not the only data we can use to infer protein fitness though. It is believed that protein structure data is also closely related to fitness, as the structure describes the biophysical properties of proteins and their functions more explicitly. The increasing availability of three-dimensional (3D) protein structures in the Protein Data Bank and the substantial coverage of high-quality predicted structures by AlphaFold[11] offer new opportunities to analyze protein fitness from a structure perspective. However, understanding the relationship between structure and function is a challenging task, in part due to the intricate complexity of structure data and the difficulty of developing ML models that can effectively capture structural features that are informative for fitness prediction.

Qiu and Wei demonstrated that the mathematical toolbox in topology can be adapted to address this challenge. They developed an ML algorithm called TopFit that can integrate structure data for navigating the protein fitness landscape. TopFit leverages persistent spectral theory (PST), a technique in topology that can be used to encode the topological and geometric features of a protein structure into a low-dimensional vector or embedding. PST can capture the structural features at various scales, from the locations of atoms to the interactions between residues and to the global shape of the whole 3D structure. Ultimately, this allows TopFit to sense the shape of functional proteins. To further improve the model's performance and robustness, PST embeddings were combined with protein language model embeddings and evolutionary scores, and an ensemble of predictors, including neural networks, kernel methods, and tree methods, was used to predict the fitness of a protein based on the combined embeddings. The authors conducted thorough evaluation experiments and

found that TopFit had good prediction accuracy for protein fitness prediction in protein engineering.

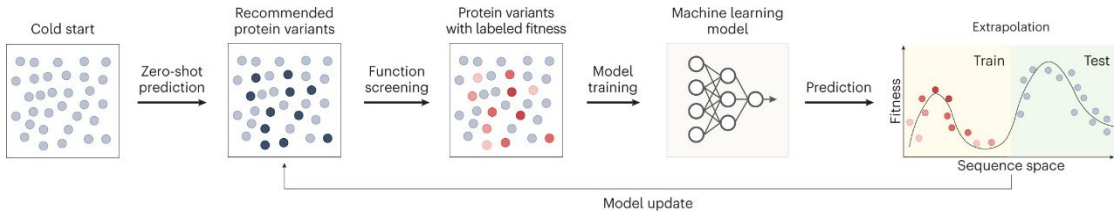


Fig. 1 | A schematic illustration of a machine learning workflow in protein engineering. When no fitness data is available for a target protein (cold start), zero-shot predictions are needed to recommend protein variants for experimental function screening. The obtained fitness data are then used to train a supervised machine learning model, which can be used to predict fitness for unseen protein variants (extrapolation) and identify promising variants to repeat the cycle.

The authors have made an important contribution to protein fitness prediction by incorporating protein structure data into ML models, also uncovering connections between two distinct areas — topology and protein engineering. Nevertheless, many interesting questions and challenges still remain (Fig. 1). One of the challenges is the 'cold start' problem, where no fitness data is available for a target protein to train the ML model. In this case, zero-shot predictions are often needed to recommend the protein variants for the first round of fitness screening. Unsupervised sequence-based ML models, such as pre-trained protein language models, have been shown to have good zero-shot prediction performance[10]. It would be interesting to investigate whether incorporating structure data into the pre-training process using methods such as PST can further improve the model's ability to make zero-shot predictions. Another important challenge is extrapolation, which aims to make predictions for unseen data, including novel protein sequences or sequences with fitness values outside the range of the training data. For example, it was noted by the authors that a simple ridge regression model outperformed more advanced, high-accuracy models, such as neural networks or boosting trees, for predicting fitness of multiple-mutation variants after being trained on single-mutation variants. Achieving both high-accuracy prediction and extrapolation is therefore a key challenge in developing ML models for protein engineering. Furthermore, exploring other paradigms or principles for modeling structure data is another interesting future direction. A notable trend in the ML community is the use of equivariant graph neural networks, which can learn effective representations that respect the physical symmetries of graph-like data, including molecular and protein structures[11].

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