学习优化前沿与挑战

诺亚方舟实验室 Noah’s Ark Lab
李希君 Xijun Li

Security Level:

HUAWEI

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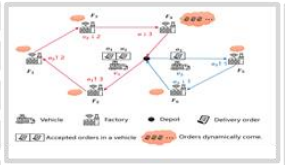
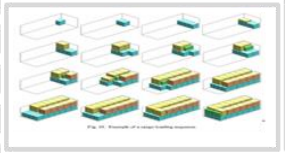
工业场景中的组合优化问题

场景

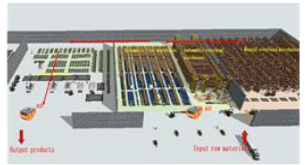
供应链



车队动态调度



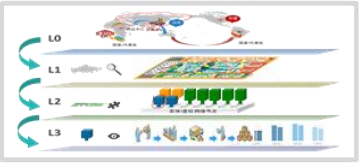
智能装箱



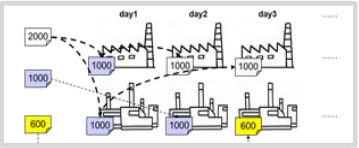
智能仓库调度

智能港口调度

物流调度



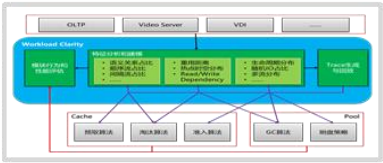
需求预测与网络规划



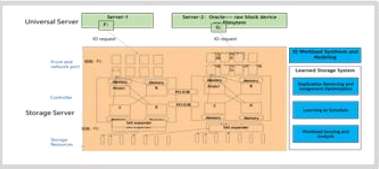
超大规模计划排产

计划排产

操作系统



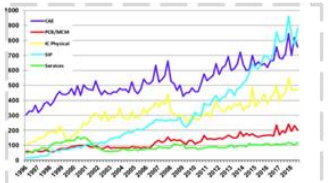
workload识别与预测

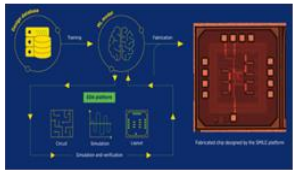


自动参数调优

计算机系统调优

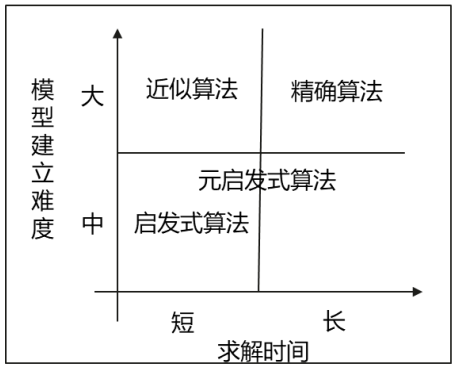
芯片EDA

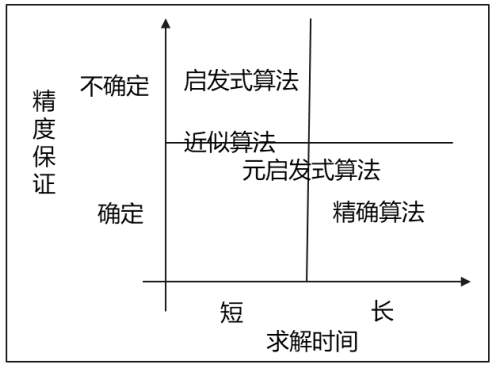


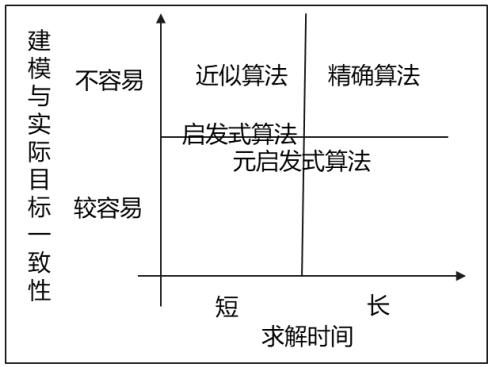


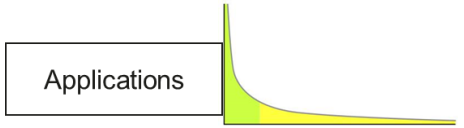
故障自动增量测试

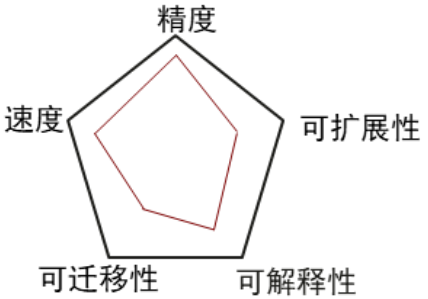
解决方案



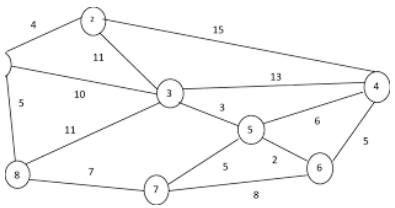


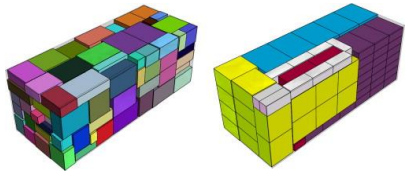


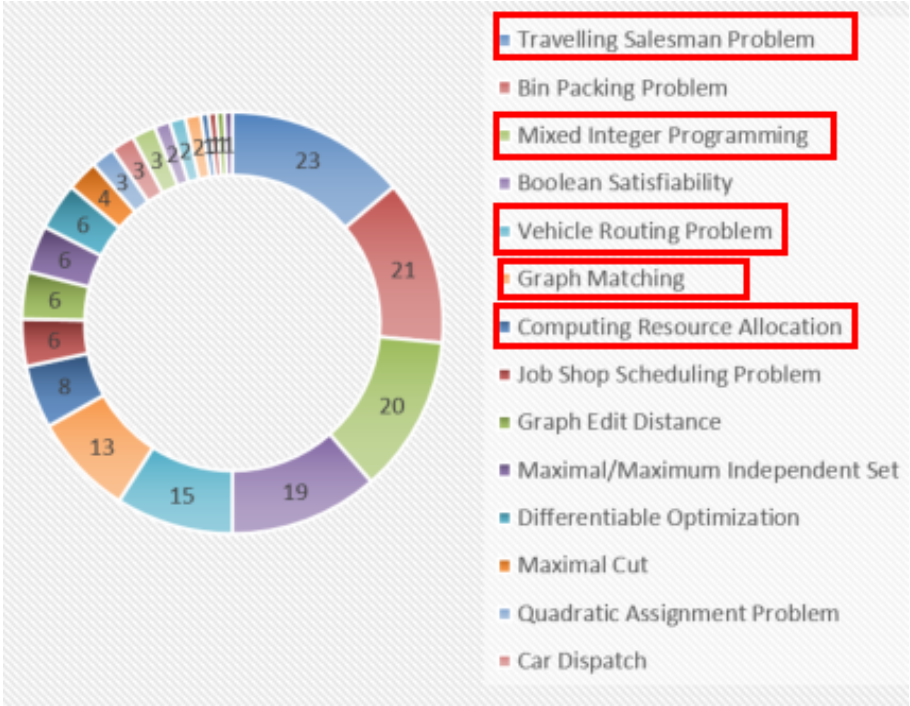




学习优化：将机器学习技术与优化技术“有机”结合，提升优化算法的速度/精度







近五年利用机器学习方法求解组合优化问题（L2O）的研究逐渐兴起

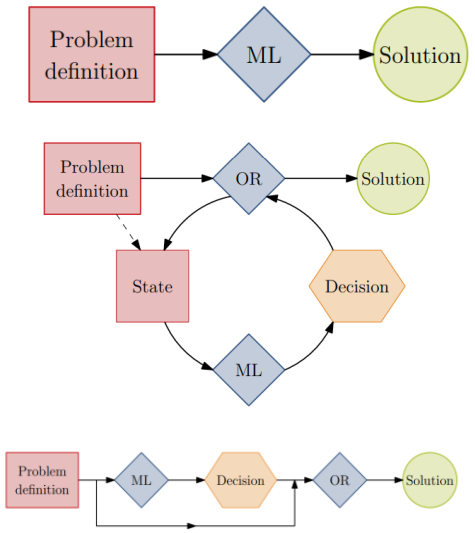
Machine Learning for Combinatorial Optimization: a Methodological Tour d'Horizon*

Yoshua Bengio[2,3], Andrea Lodi[1,3], and Antoine Prouvost[1,3]

yoshua.bengio@mila.quebec
{andrea.lodi, antoine.prouvost}@polymtl.ca

[1]Canada Excellence Research Chair in Data Science for Decision Making, École Polytechnique de Montréal
[2]Department of Computer Science and Operations Research, Université de Montréal
[3]Mila, Quebec Artificial Intelligence Institute

Bengio & Lodi等人发表题为Machine Learning for Combinatorial Optimization: a Methodological Tour d 'Horizon的论文。总结了利用机器学习技术求解组合优化问题的三种经典范式。



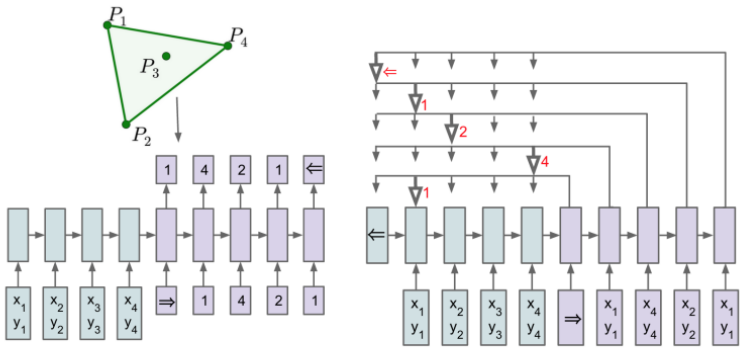
✓**范式1：** 端到端预测优化结果
✓**范式2：** 嵌入式评估函数（分支定界等算法）
✓**范式3：** AI调参（算法选择与参数配置）

✓**挑战1：** 高维空间，**可行域**的学习难题
✓**挑战2：** 序列决策，**最优路径**学习难题
✓**挑战3：** 不同组合优化问题的**分布泛化**

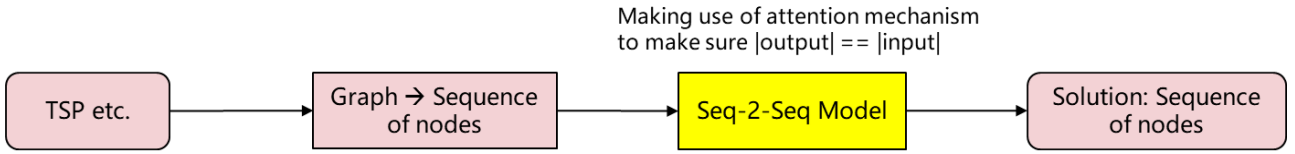
学习优化：端到端预测优化结果

Pointer Networks

Oriol Vinyals* Google Brain
Meire Fortunato* Department of Mathematics, UC Berkeley
Navdeep Jaitly Google Brain



(a) Sequence-to-Sequence (b) Ptr-Net



- ✓ **语音模型→组合优化:** 首次将语言模型中的**注意力机制(Attention Mechanism)**用于求解经典组合优化问题
- ✓ **核心idea：** 传统的seq2seq模型是无法解决输出序列的词汇表会随着输入序列长度的改变而改变的问题的。基于这种特点，作者考虑找到一种结构类似编程语言中的指针，每个指针对应输入序列的一个元素，从而可以直接操作输入序列而不需要特意设定输出词汇表，从而叫指针网络。
- ✓ **影响力：** 实验结果**没有超越启发式算法**的最优结果，但是由此开启了学习优化的热潮

General attention:

$$u_j^i = v^T \tanh(W_1 e_j + W_2 d_i) \quad j \in (1, \ldots, n)$$
$$a_j^i = \mathrm{softmax}(u_j^i) \quad j \in (1, \ldots, n)$$
$$d_i' = \sum_{j=1}^{n} a_j^i e_j$$

This paper:

$$u_j^i = v^T \tanh(W_1 e_j + W_2 d_i) \quad j \in (1, \ldots, n)$$
$$p(C_i | C_1, \ldots, C_{i-1}, \mathcal{P}) = \mathrm{softmax}(u^i)$$

Pointer networks

O Vinyals, M Fortunato, N Jaitly - Advances in neural …, 2015 - proceedings.neurips.cc

… • We propose a new architecture, that we call **Pointer** Net, which is simple and effective. It … softmax probability distribution as a "**pointer**". • We apply the **Pointer** Net model to three distinct …

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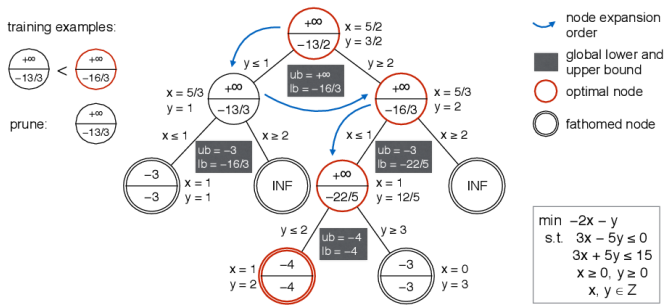
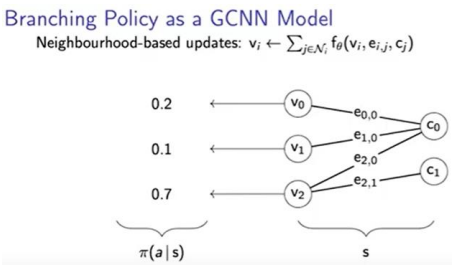
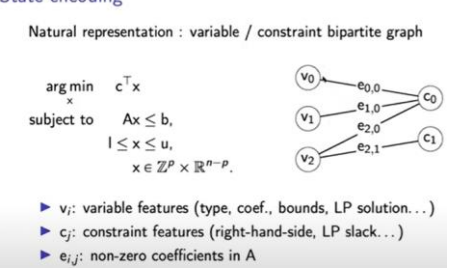
学习优化：嵌入式评估函数/AI调参

➢ Exact combinatorial optimization with graph convolutional neural networks, MILA, NeurIPS 2019



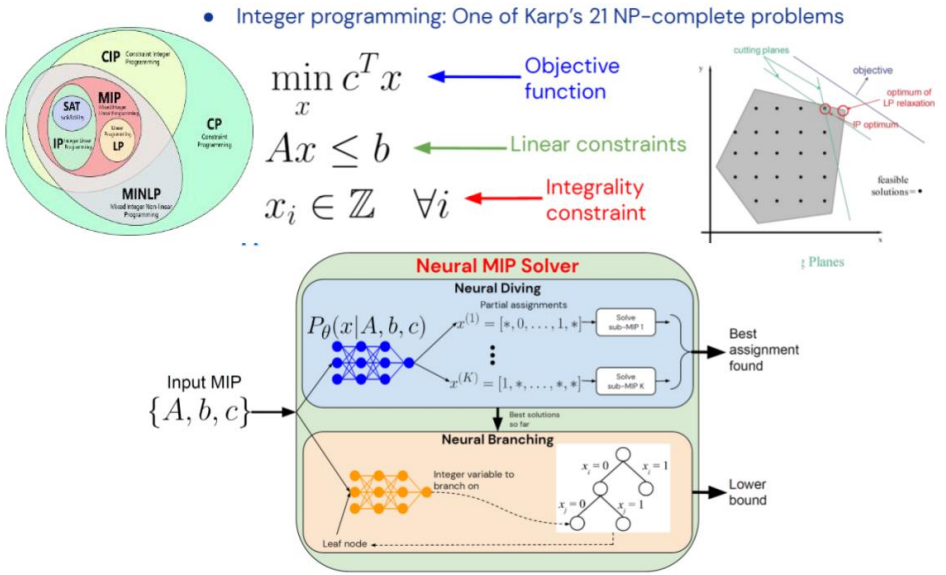
混合整数规划中的变量选择问题





- ✓ **数据表示：**数学规划矩阵→二部图表示→图卷积NN
- ✓ **模仿学习：**将变量选择策略表示为图卷积网络模型，并采用Imitation Learning拟合强分支策略(Strong Branching)
- ✓ **效果：**在同源数据集上显著超越求解器中经典变量选择算法
- ✓ **影响力：**成为NeurIPS 2021 ML4CO竞赛基线算法；MILA推出了一种学习优化框架Ecole

➢ Solving mixed integer programs using neural networks, DeepMind，arXiv 2020



混合整数规划中的变量选择与变量修整

- ✓ **生成模型+模仿学习：**采用生成模型进行变量修整的预测，利用模仿学习进行变量选择
- ✓ **效果：**在Google内部生产数据集上显著超越开源求解器SCIP的精度or效率
- ✓ **成本高昂：**该方法的训练开销巨大（百万美金GPU小时）

目录

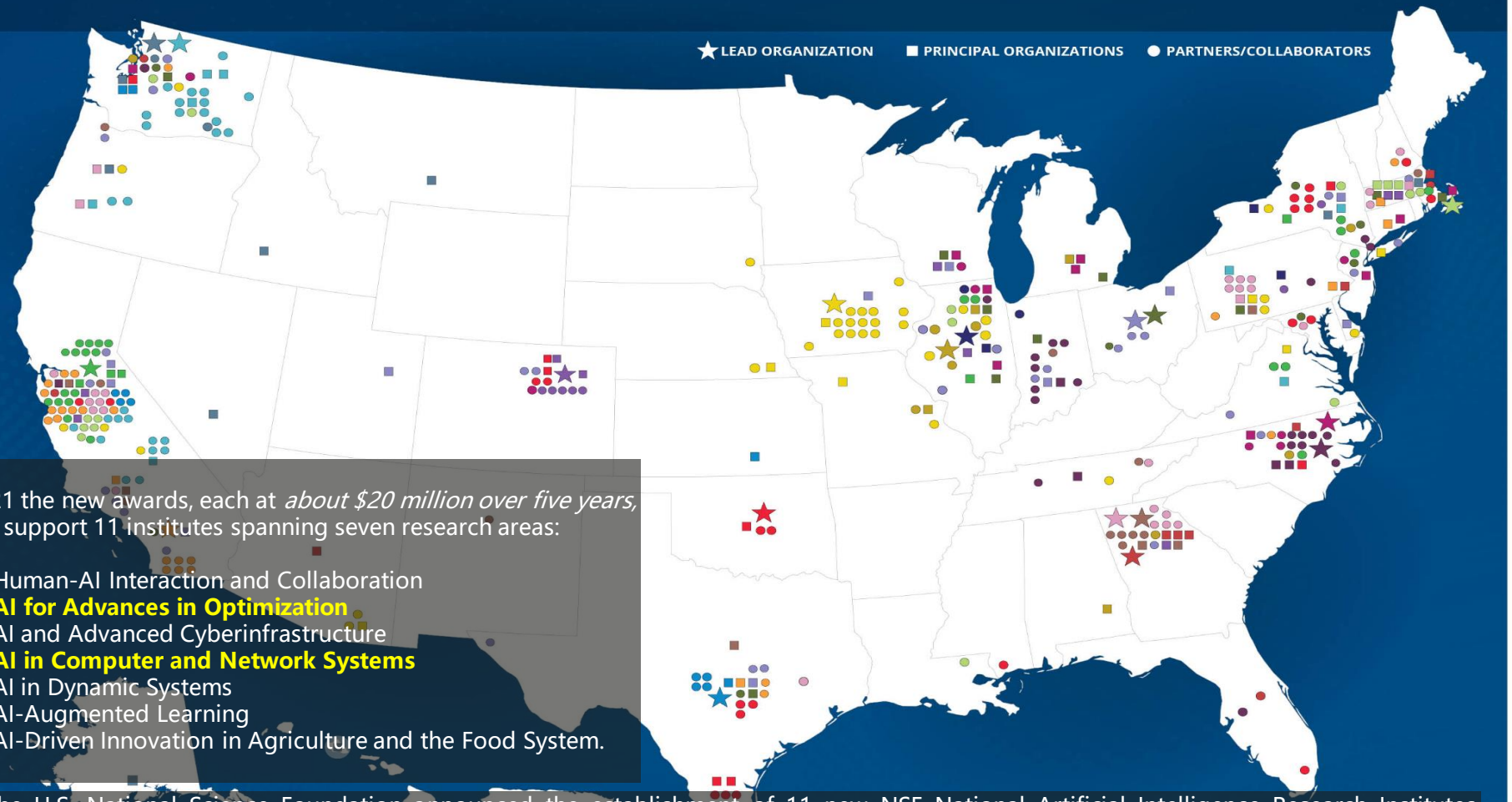
NSF2020/2021人工智能相关课题投资分布

NSF ARTIFICIAL INTELLIGENCE RESEARCH INSTITUTES

NSF-LED NATIONAL AI RESEARCH INSTITUTES

2020 *and* **2021** *awards*

*The U.S. National Science Foundation (NSF) announced a **$220** million investment in eleven new Artificial Intelligence (AI) Research Institutes, building on the first round of seven AI Institutes totaling **$140** million funded last year. **(The default map view below shows all awards combined).***



- NSF AI Institute for Research on Trustworthy AI in Weather, Climate, and Coastal Oceanography
- NSF AI Institute for Foundations of Machine Learning
- USDA-NIFA AI Institute for Next Generation Food Systems
- USDA-NIFA AI Institute for Future Agricultural Resilience, Management, and Sustainability (AIFARMS)
- NSF AI Institute for Student-AI Teaming
- Molecule Maker Lab Institute (MMLI): NSF AI Institute for Molecular Discovery, Synthetic, and Manufacturing
- NSF AI Institute for Artificial Intelligence and Fundamental Interactions
- NSF AI Institute for Collaborative Assistance and Responsive Interaction for Networked Groups (AI-CARING)
- NSF AI Institute for Learning-enabled Optimization at Scale (TILOS)
- NSF AI Institute for Optimization
- NSF AI Institute for Intelligent Cyberinfrastructure with Computational Learning in the Environment (ICICLE)
- NSF AI Institute for Future Edge Networks and Distributed Intelligence (AI-EDGE)
- NSF AI Institute for Edge Computing Leveraging Next Generation Networks (Athena)
- NSF AI Institute for Dynamic Systems
- NSF AI Institute for Engaged Learning
- NSF AI Institute for Adult Learning and Online Education (ALOE)
- USDA-NIFA AI Institute: Agricultural AI for Transforming Workforce and Decision Support (AgAID)
- USDA-NIFA AI Institute: AI Institute for Resilient Agriculture (AIIRA)

2021 the new awards, each at *about $20 million over five years,* will support 11 institutes spanning seven research areas:

- Human-AI Interaction and Collaboration
- **AI for Advances in Optimization**
- AI and Advanced Cyberinfrastructure
- **AI in Computer and Network Systems**
- AI in Dynamic Systems
- AI-Augmented Learning
- AI-Driven Innovation in Agriculture and the Food System.

"The U.S. National Science Foundation announced the establishment of 11 new NSF National Artificial Intelligence Research Institutes, building on the first round of seven institutes funded in 2020. **The combined investment of $220 million expands the reach of these institutes to include a total of 40 states and the District of Columbia."**

Information on approximate location of the Institutes' lead and principal organizations (staffing and/or activity), as well as their initial funded and unfunded partners. Collaborators related to an Institute may be represented with a single plot due to space limitations.

NSF2020/2021人工智能相关课题投资分布

NSF-LED NATIONAL AI RESEARCH INSTITUTES

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2020 Awards **2021** Awards

★ LEAD ORGANIZATION ■ PRINCIPAL ORGANIZATIONS ● PARTNERS/COLLABORATORS

This NSF **Artificial Intelligence (AI) Research Institute for Advances in Optimization** aims at delivering a paradigm shift in automated decision making at massive scales by fusing AI and Mathematical Optimization (MO), to achieve breakthroughs that neither field can achieve independently.

Led by the **Georgia Institute of Technology and partially funded by Intel**, this Institute will merge AI and mathematical optimization to create intelligent systems that can deliver decision-making at massive scales. Along with **supply chains, optimization** methods powered by AI will improve decision-making in **complex systems for energy, sustainability and circuit design**.

AWARDS

- NSF AI Institute for Research on Trustworthy AI in Weather, Climate, and Coastal Oceanography
- NSF AI Institute for Foundations of Machine Learning
- USDA-NIFA AI Institute for Next Generation Food Systems
- USDA-NIFA AI Institute for Future Agricultural Resilience, Management, and Sustainability (AIFARMS)
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- NSF AI Institute for Artificial Intelligence and Fundamental Interactions
- NSF AI Institute for Collaborative Assistance and Responsive Interaction for Networked Groups (AI-CARING)
- NSF AI Institute for Learning-enabled Optimization at Scale (TILOS)

NSF AI Institute for Optimization

LEAD:
Georgia Tech

PRINCIPAL ORGANIZATIONS:
- University of California – CA
- University of Southern California – CA
- Clark Atlanta University – GA
- University of Texas – TX
- Spelman College – GA

PARTNERS/COLLABORATORS:
- Georgia Center of Innovation for Logistics – GA
- Amazon Robotics – MA
- Georgia Dept of Economic Development – GA
- UPS – GA
- Girls Academic Leadership Academy – CA
- Gurobi Optimization – OR
- Ryder – GA
- Mosek ApS – Denmark
- Oak Ridge National Laboratory – TN
- Midcontinent Independent Systems Operator (MISO) – IN
- Los Alamos National Laboratory – NM
- Lawrence Livermore National Laboratory – CA
- Atlanta Public Schools – GA

- USDA-NIFA AI Institute: AI Institute for Resilient Agriculture (AIIRA)

The map reflects the approximate location of the Institutes' lead and principal organizations (staffing and/or activity), as well as their initial funded and unfunded partners.
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NSF2020/2021人工智能相关课题投资分布

NSF-LED NATIONAL AI RESEARCH INSTITUTES

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2020 *Awards* **2021** *Awards*

★ LEAD ORGANIZATION ■ PRINCIPAL ORGANIZATIONS ● PARTNERS/COLLABORATORS

TIIOS is a partnership of faculty from **University of California, San Diego, Massachusetts Institute of Technology, National University, University of Pennsylvania, University of Texas at Austin, and Yale University**. TILOS will pioneer learning-enabled optimizations that transform **chip design, robotics, communication networks**, and other use domains that are vital to our nation' s health, prosperity and welfare.

AWARDS

- NSF AI Institute for Research on Trustworthy AI in Weather, Climate, and Coastal Oceanography
- NSF AI Institute for Foundations of Machine Learning
- USDA-NIFA AI Institute for Next Generation Food Systems
- USDA-NIFA AI Institute for Future Agricultural Resilience, Management, and Sustainability (AIFARMS)
- NSF AI Institute for Student-AI Teaming
- Molecule Maker Lab Institute (MMLI): NSF AI Institute
- NSF AI Institute for Learning-enabled Optimization at Scale (TILOS)
- Transforming Workforce and Decision Support (AgAID)
- USDA-NIFA AI Institute: AI Institute for Resilient Agriculture (AIIRA)

NSF AI Institute for Learning-enabled Optimization at Scale (TILOS)

LEAD:
University of California - San Diego

PRINCIPAL ORGANIZATIONS:
- National University – CA
- University of Pennsylvania – PA
- MIT – MA
- Yale University – CT
- University of Texas – TX

PARTNERS/COLLABORATORS:
- Brain Corporation – CA
- Planck Aerosystem, Inc. – CA
- Allen Institute for Artificial Intelligence – WA
- Samsung Strategy and Innovation Center – CA
- Microsoft – CA
- TuSimple, Inc. – CA
- NVIDIA Corporation – CA
- Cadence Design Systems – CA
- Arm, Ltd. – CA
- Xilinx, Inc. – CA
- Synopsys, Inc. – NC
- Mentor Graphics (Siemens) – CA
- IBM – CA
- Samsung Austin R & D Center – TX
- Silicon Integration Initiative, Inc. – TX
- Ansys, Inc. – PA
- Western Digital CHIPS Alliance – CA
- Facebook – CA
- Sweetwater Union High School District – CA
- A Reason To Survive (ARTS) – CA
- SACNAS – CA
- Girl Scouts San Diego – CA
- FIRST – NH

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Artificial Intelligence Institute for Advances in Optimization (AI4OPT)

https://www.ai4opt.org/

It unifies the data-driven and model-driven approaches at the core of *AI and Operations Research (OR).* Its methodology thrusts include a new generation of *hybrid optimization solvers that learn to optimize, end-to-end learning and optimization to tightly integrate forecasting and decision making, and novel machine-learning methods based on combinatorial optimization.*

学术机构

Georgia Tech — Lead Organization

USC University of Southern California — Partner Organization

Berkeley UNIVERSITY OF CALIFORNIA — Partner Organization

UNIVERSITY OF TEXAS ARLINGTON — Partner Organization

业界投资

Argonne NATIONAL LABORATORY — Industrial Partner

Google — Industrial Partner

intel — Industrial Partner

ISO new england — Industrial Partner

kahua — Industrial Partner

KINAXIS — Industrial Partner

Los Alamos NATIONAL LABORATORY EST. 1943 — Industrial Partner

Ryder Ever better. — Industrial Partner

应用场景

- Logistics and Supply Chains
- Resilience and Sustainability
- Energy Systems
- Hardware Design and Control

基础研究

- Combinatorial Learning for Large Scale Datasets
- Optimization Solvers
- Reinforcement Learning
- Distributed Optimization
- End to End Optimization
- Decision Making under Uncertainty

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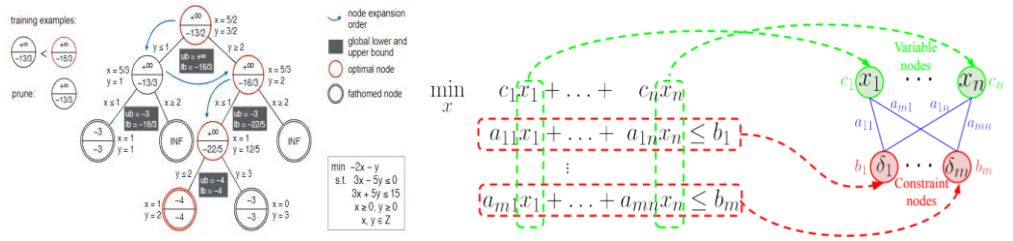
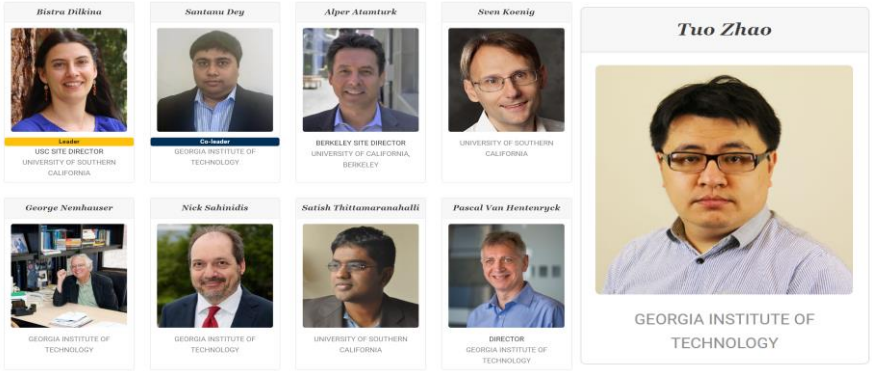
AI4OPT – 基础研究

Optimization Solver

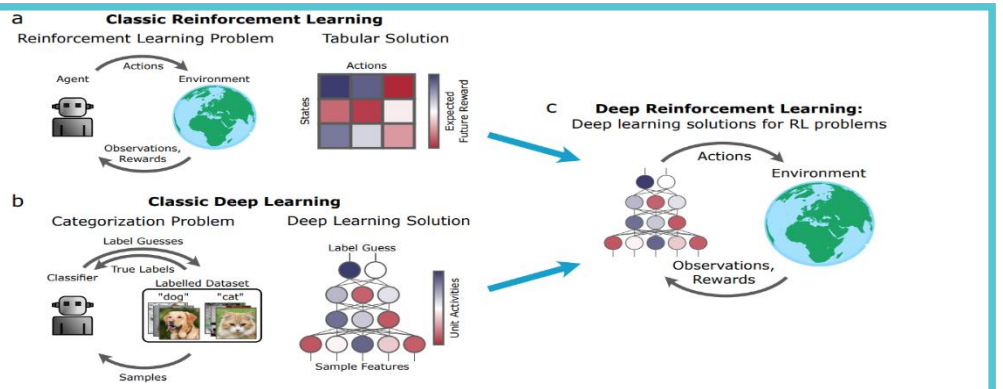


- ✓ **优秀实践：**传统优化求解器已经广泛应用于工业优化
- ✓ **新范式：**工业实际问题大量是同分布问题，过程数据同源，利用机器学习提升优化速度和精度
- ✓ 数据表示：数学规划问题转化为各种图数据、图网络
- ✓ 模块内替换：在传统求解器搜索框架（比如分支定界）替换核心模块
- ✓ 建模优化：利用强化学习等技术自动重优化数学模型

主要研究人员



Reinforcement Learning



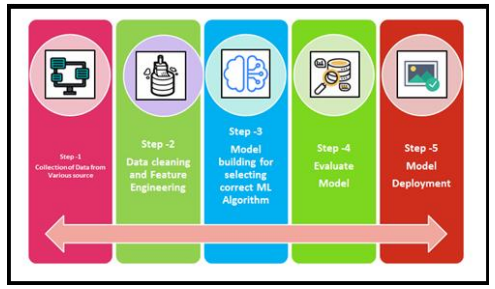
- ✓ 强化学习已在视频游戏、巡航、目的物操作等得到应用
- ✓ Value Function Approximation, Deep Q Learning, A2C
- ✓ **主攻方向：**Off-Policy RL, Safe RL, Representation Learning for RL

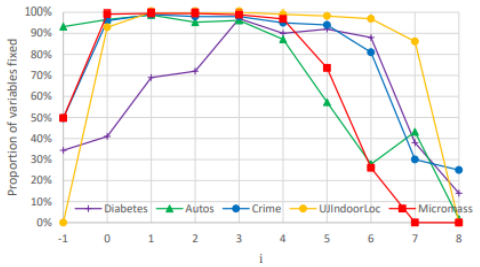
主要研究人员

[1] *Learning to run heuristics in tree search.* Elias B. Khalil, Bistra Dilkina, George L. Nemhauser, Shabbir Ahmed, and Yufen Shao. In IJCAI: International Joint Conferences on Artificial Intelligence Organization, pages 659–666, 2017.
[2] *Learning combinatorial optimization algorithms over graphs.* Hanjun Dai, Elias B Khalil*, Yuyu Zhang, *Bistra Dilkina, and Le Song.* In NeurIPS: Advances in neural information processing systems, 2017.
[3] *Learning to branch in mixed integer programming.* Elias Khalil, Pierre Le Bodic, Le Song, George Nemhauser, and Bistra Dilkina. In AAAI Conference on Artificial Intelligence, 2016.
[4] Yordle: An Efficient Imitation Learning for Branch and Bound. Qingyu Qu, Xijun Li, Yunfan Zhou. In NeurIPS 2022 ML4CO Competition

AI4OPT – 基础研究

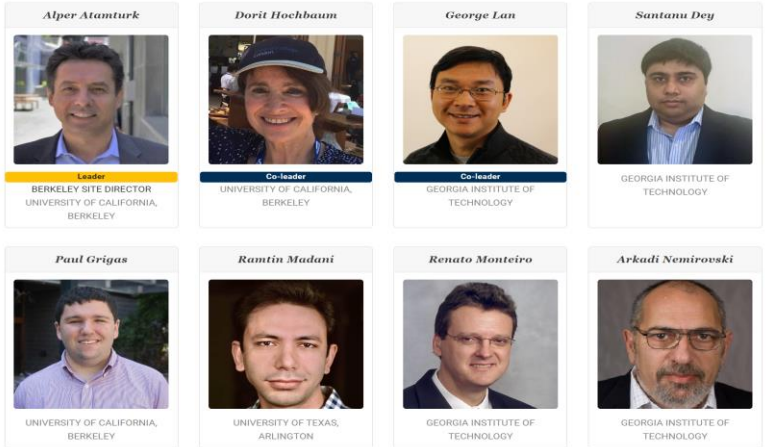
Combinatorial Learning for Large Scale Datasets



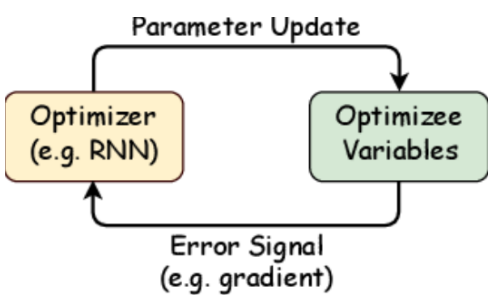


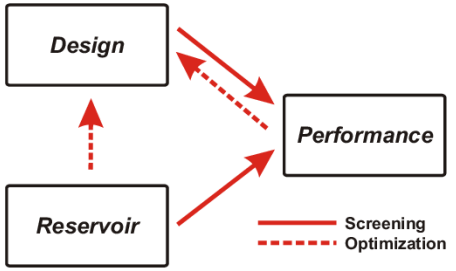
- ✓ 机器学习中的学习算法多维无约束凸优化，但优化过程中多发现是离散带约束问题
- ✓ Opt4AI: 利用传统离散组合优化技术（MIP等）提升AI学习算法效率和精度
- ✓ Meta Algorithms: 自动算法选择、自动模型选择等

主要研究人员



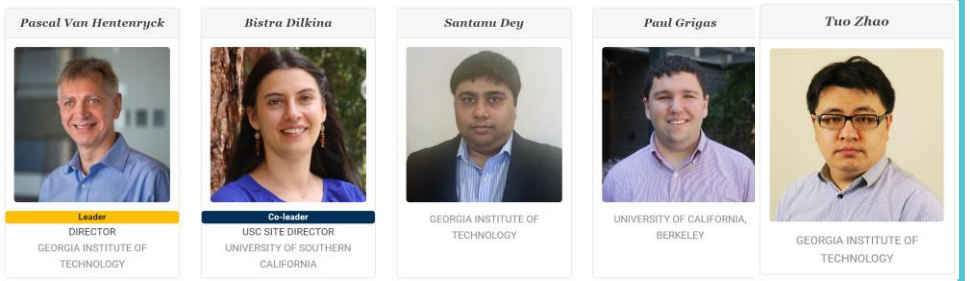
End to End Optimization





- ✓ Optimization Proxies: 利用机器学习逼近优化目标函数
- ✓ 端到端学习：Integrating optimization layers as parts of the deep-learning pipeline
- ✓ 学习优化：Replacing components of optimization models by machine-learning models

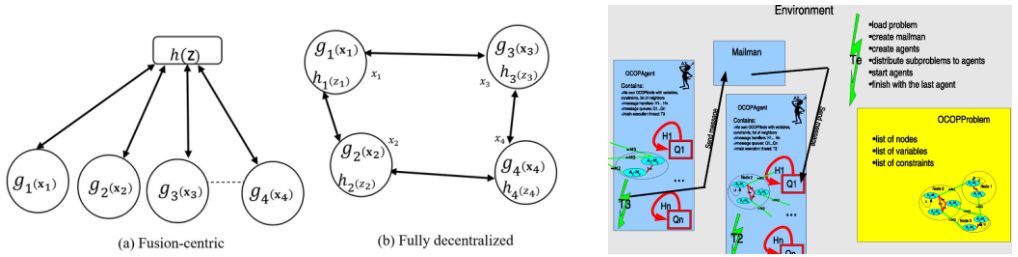
主要研究人员



[1] The max-cut decision tree: Improving on the accuracy and running time of decision trees. Jonathan Bodine and Dorit S Hochbaum. In Proceedings of the 12th International Joint Conference on Knowledge Discovery, Knowledge Engineering and Knowledge Management KDIR, volume , pages 59–70, 2020.
[2] Sparse and smooth signal estimation: Convexi- fication of l0 formulations. Alper Atamturk, Andres Gomez, and Shaoning Han. Journal of Machine Learning Research. (to appear).
[3] Safe screening rules for l0-regression from perspective relaxations. A. Atamturk and A. Gomes. Proceedings of the 37th International Conference on Machine Learning, pages 1–10, 2020.

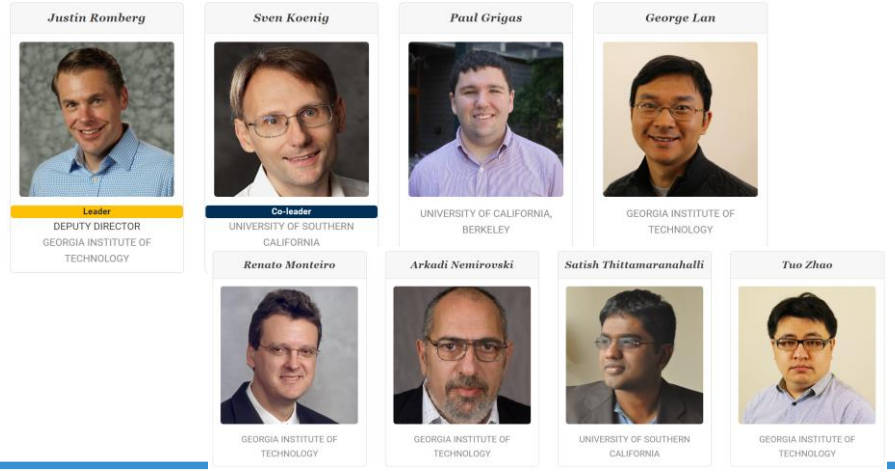
AI4OPT – 基础研究

Distributed Optimization

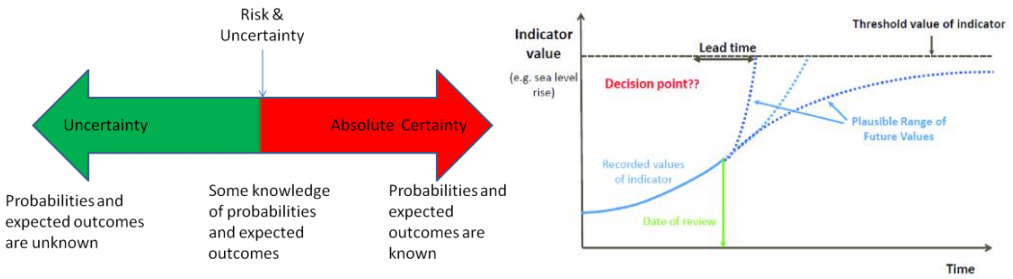


- ✓ 分布式通信和分布式计算的发展要求AI算法必须是实时的且去中心化的
- ✓ 研究方向：1）非凸连续优化的去中心化；2）分布式带约束优化问题；3）Multi-agent learning

主要研究人员

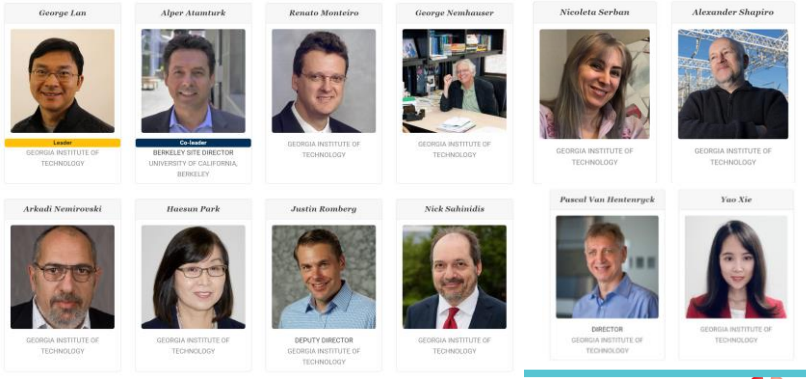


Decision Making Under Uncertainty



- ✓ 针对具有不确定性的大规模多阶段优化问题
- ✓ 研究兴趣: 1) 多阶段优化问题中的保真性、可追溯性、采样复杂度之间的tradeoff; 2) 系统复杂度分析和高效算法开发; 3）利用不确定性量化的结构信息求解多阶段不确定性优化问题

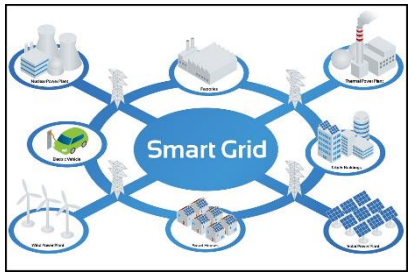
主要研究人员

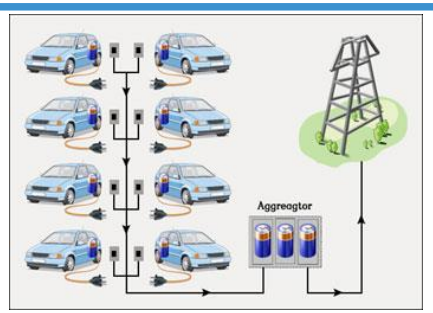


[1] Finite-time analysis of decentralized stochastic approximation with applications in multi-agent and multi-task learning. S. Zeng, T. Doan, and J. Romberg. arxiv:2010.15088, October 2020.
Lifelong multi-agent path finding in large-scale warehouses. J. Li, A. Tinka, S. Kiesel, J. Durham, S. Kumar, and S. Koenig. In Proceedings of the International Joint Conference on Autonomous Agents and Multiagent Systems (AAMAS), pages 1898–1900, 2020.
[2] Communication-efficient algorithms for decentralized and stochastic optimization. G. Lan, S. Lee, and Y. Zhou. Mathematical programming, 180(1):237–284, 2020.
[3] Task and path planning for multi-agent pickup and delivery. M. Liu, H. Ma, J. Li, and S. Koenig. In Proceedings of the International Joint Conference on Autonomous Agents and Multiagent Systems (AAMAS), pages 1152–1160, 2019.

AI4OPT – 应用场景

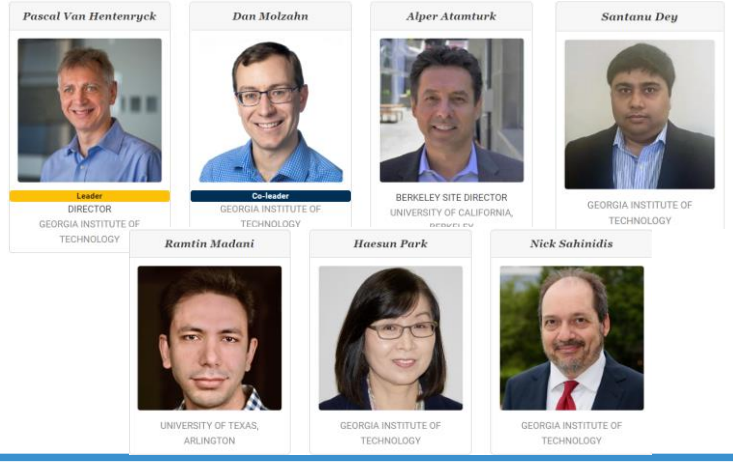
Energy Systems



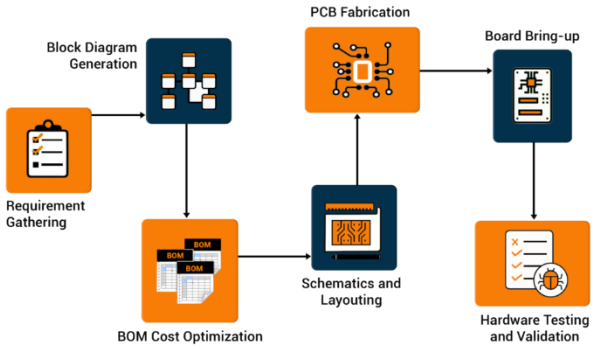


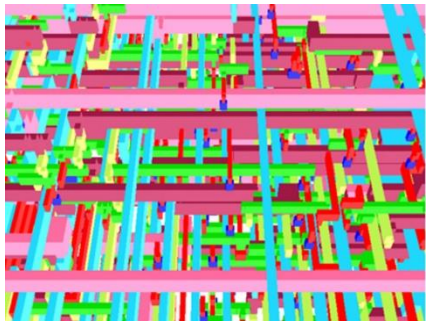
- ✓ 场景：1）太阳能、风能、混合能源的智能电网调度；2调度中的不确定性；3）新能源汽车普及使得电网调度问题更加复杂
- ✓ 技术路线：1）端到端学习优化；2）分布式优化；3）不确定性环境下的决策推理

主要研究人员



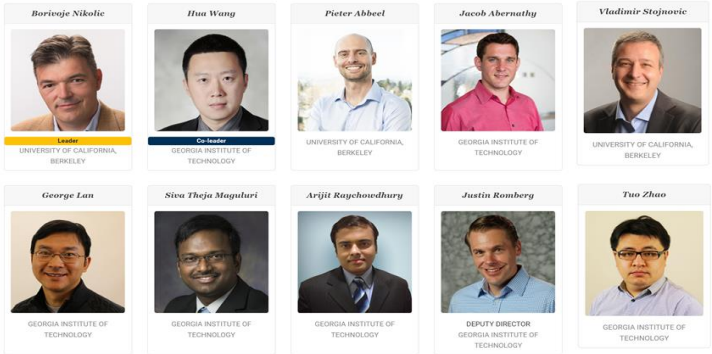
Hardware Design and Control





- ✓ 场景：1）数据驱动的逻辑综合；2）模拟混合信号 (AMS); 3) 毫米波电路；4）集成封装
- ✓ 技术路线：1）在线优化；2）强化学习；3）贝叶斯优化

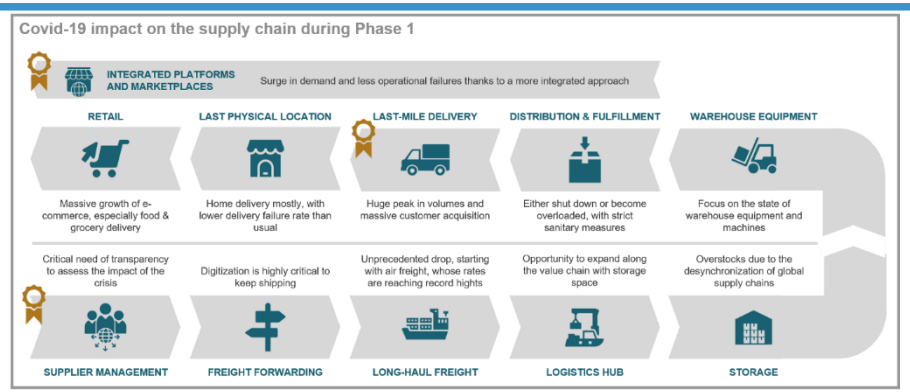
主要研究人员



[1] Learning Optimization Models for Large-Scale Security-Constrained Economic Dispatch. Wenbo Chen, Seonho Park, Mathieu Tanneau, and Pascal Van Hentenryck. In the Proceedings of the 22nd Power Systems Computation Conference (PSCC), June 27 – July 1, 2022 in Porto, Portugal.
[2] A Linear Outer Approximation of Line Losses for DC-based Optimal Power Flow Problems. Haoruo Zhao, Mathieu Tanneau, and Pascal Van Hentenryck. In the Proceedings of the 22nd Power Systems Computation Conference (PSCC), June 27 – July 1, 2022 in Porto, Portugal.
[3] Data-Driven Time Series Reconstruction for Modern Power Systems Research. Minas Chatzos, Mathieu Tanneau, and Pascal Van Hentenryck.Data-Driven Time Series Reconstruction for Modern Power Systems Research. In the Proceedings of the 22nd Power Systems Computation Conference (PSCC), June 27 - 2022 in Porto, Portugal.

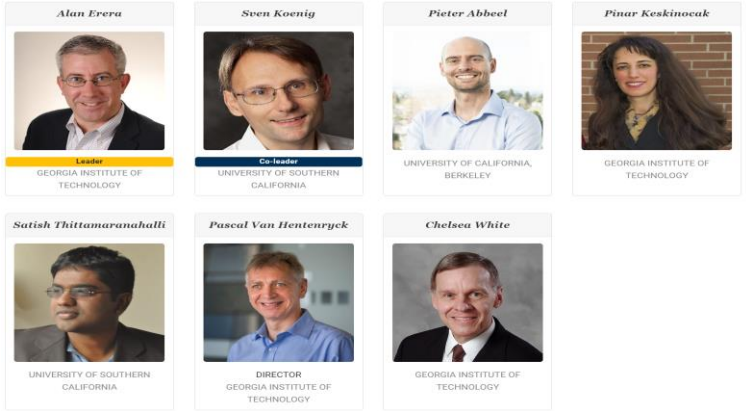
AI4OPT – 应用场景

Logistics and Supply Chain

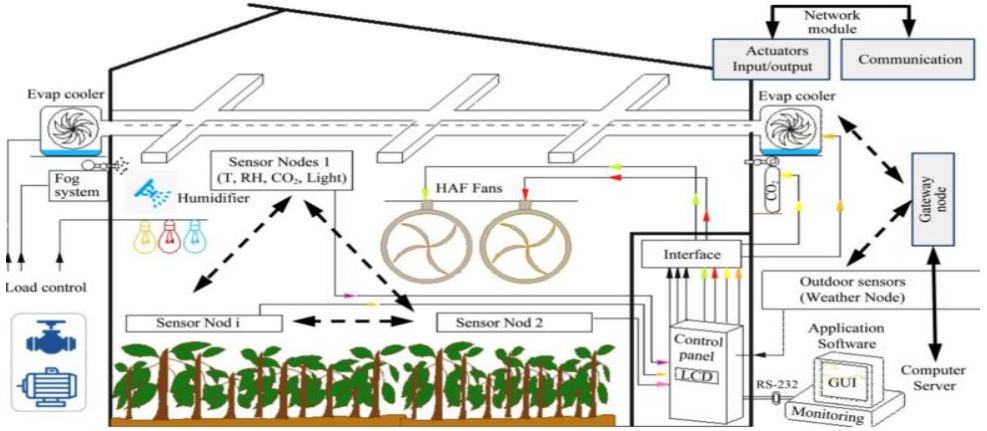


- ✓ 场景：1) Middle-mile networks; 2) 仓储优化； 3） 最后一公里配送系统；4）面向不确定性的集成调度 (Covid19)
- ✓ 技术路线：1）数据驱动的优化技术；2） 端到端优化；3）不确定性环境下的决策推理；4）强化学习

主要研究人员

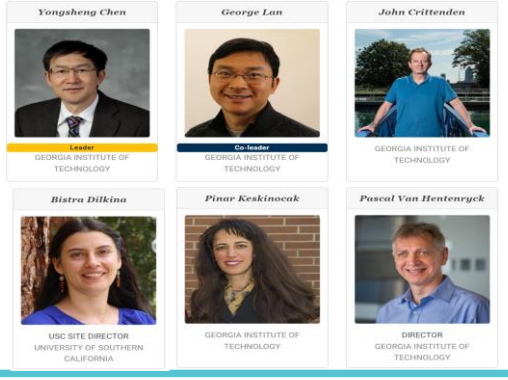


Resilience and Sustainability



- ✓ 场景：1）智慧农业（Controlled Environment Agriculture）；2）污水处理系统；3）食品质量检测系统
- ✓ 技术路线：1）在线优化；2）强化学习；3）数据驱动的优化技术

主要研究人员



[1] Constraint Programming for Scheduling, Pascal Van Hentenryck. Global Scheduling Seminar Series, April 2022.
[2] Fast Approximations for Job Shop Scheduling: A Lagrangian Dual Deep Learning Method. James Kotary, Ferdinando Fioretto, and Pascal Van Hentenryck. In the Thirty- Sixth AAAI Conference on Artificial Intelligence (AAAI-22), February 2022.

TILOS: The Institute for Learning-enabled Optimization At Scale

https://www.tilos.ai/

TIIOS is a partnership of faculty from *University of California, San Diego, Massachusetts Institute of Technology, National University, University of Pennsylvania, University of Texas at Austin, and Yale University*. TILOS will pioneer learning-enabled optimizations that transform *chip design, robotics, communication networks*, and other use domains that are vital to our nation' s health, prosperity and welfare.

学术机构

UC San Diego

MIT

Yale

TEXAS The University of Texas at Austin

Penn

业界投资

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Ai2 Ansys arm brainco corp cadence

CHIPS ALLIANCE facebook IBM Mentor A Siemens Business Microsoft

NVIDIA SAMSUNG Strategy & Innovation Center SAMSUNG AUSTIN SEMICONDUCTOR Si synopsys

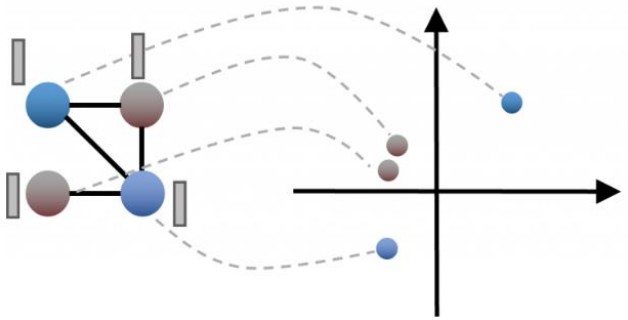
tusimple XILINX Western Digital

应用场景	**Chip Design**	**Networks**	**Robotics**
基础研究	Discrete and continuous optimization	Distributed, parallel, and federated optimization Dynamic decisions under uncertainty	Optimization on manifolds Nonconvex optimization in deep learning

HUAWEI

TILOS – 基础研究

Discrete and Continuous Optimization

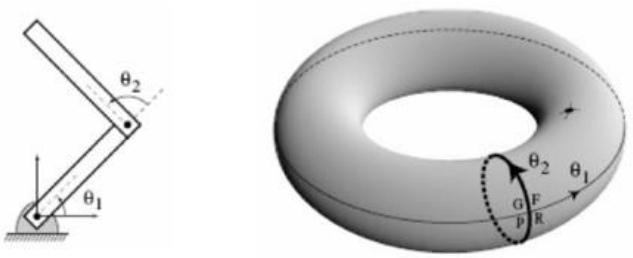


- ✓ 芯片设计中place-and-route等问题需要同时满足离散和连续约束
- ✓ 机器人控制问题中须同时考虑离散规划和分段连续最优控制
- ✓ 如何将机器学习技术嵌入上述混合优化问题；离散和连续优化问题是否可以互相促进；

Distributed and Parallel Optimization

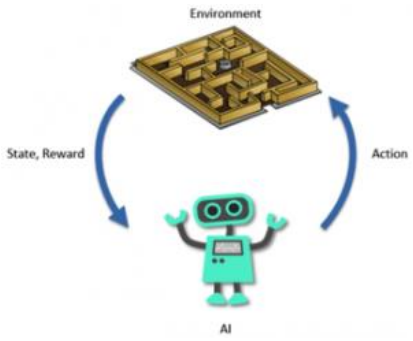
- ✓ 数据存储和训练成本远远超过单机的存储和计算能力上限
- ✓ 并行与分布式算法：关注通信开销，隐私，公平，安全性，分布式算法的收敛速率

Optimization and Sampling on Geometric Spaces



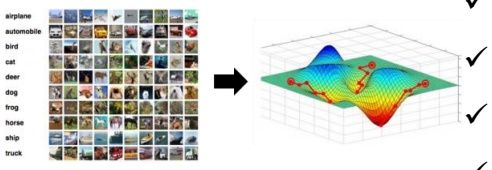
- ✓ 大量问题存在几何特征，该特征对算法设计的效率和精度极为重要
- ✓ 关注技术：李群，同空间，Grassmannians and Riemannian流形；利用流形对真实世界优化问题建模；并利用上述空间的几何特征设计高效优化和采样算法

Sequential Learning and Decision Making



- ✓ 序贯决策问题（机器人控制，自动网络调试）需要平衡探索和利用的关系
- ✓ Tradeoff between 精确度和计算开销
- ✓ 设计高效采样算法来有效解决数据利用问题
- ✓ 利用特殊的问题结构信息以加速数据利用

Nonconvex Optimization (and Beyond) in Deep Learning

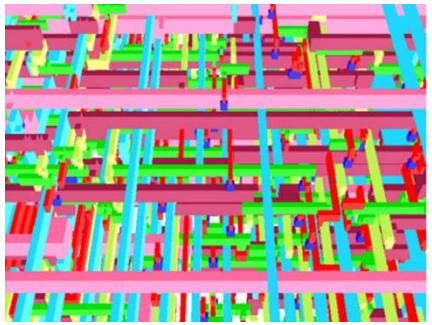


- ✓ 神经网络参数学习问题是非凸优化问题
- ✓ 非凸优化是computationally intractable
- ✓ 对基于梯度的非凸优化算法的理解
- ✓ 在随机和对抗的环境中做非凸优化

HUAWEI

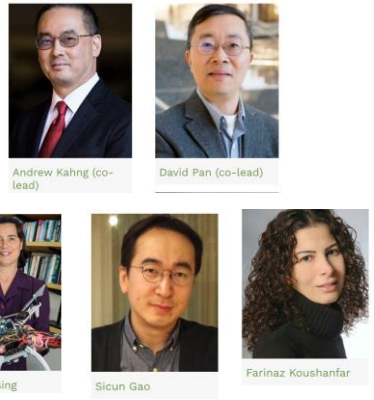
TILOS – 应用场景

Chip Design

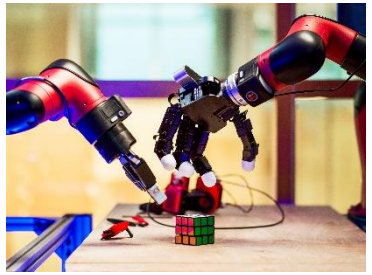


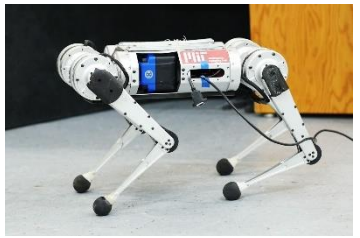
- ✓ 关注问题：1）从电路描述直接生成电路Layout；2）在验证环节探索下一代规模化突破；3）量化芯片设计中的隐私与安全成本
- ✓ 技术路线：1）利用cost landscape的结构信息；2）分布式采样和元启发搜索；3）设计高效元启发/启发式算子，构建算子数据库；4）将专家知识经验编码进优化和决策算法

主要研究人员



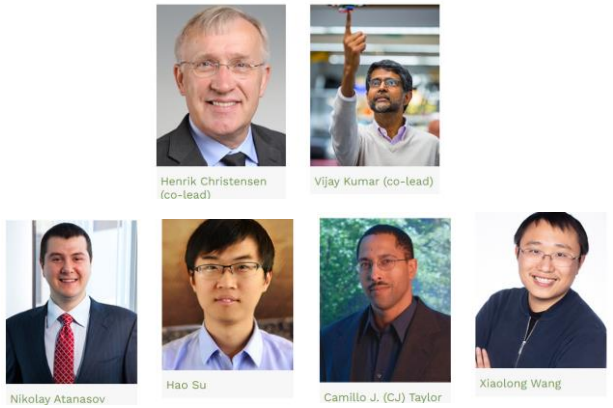
Robotics





- ✓ Graphical Models: 1）概率图模型；2）流形学习；3）大规模、在线学习
- ✓ Planning (Multi-agent)：在单和多agent系统下的kino动态规划问题
- ✓ 强化学习：1）离线的大规模多模态多目标的行为数据学习；2）在线实时优化
- ✓ Compositional Learning

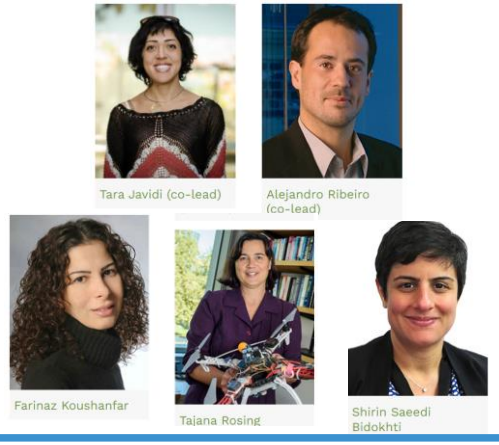
主要研究人员



Networks

- ✓ 多目标优化：面向混合离散连续优化问题的分布式随机优化算法；主动学习；联邦学习；
- ✓ 自治自愈网络：架构层面的超参数黑箱优化
- ✓ 专家和物理知识融入：利用机器学习技术表示专家知识和物理知识；Physic-based Neural Model in Signal Processing

主要研究人员



HUAWEI

目录

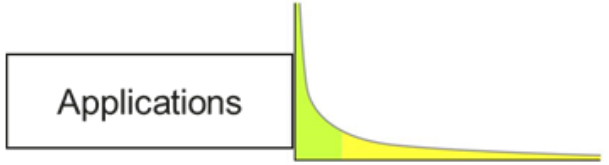
学习优化研究 – 求解器

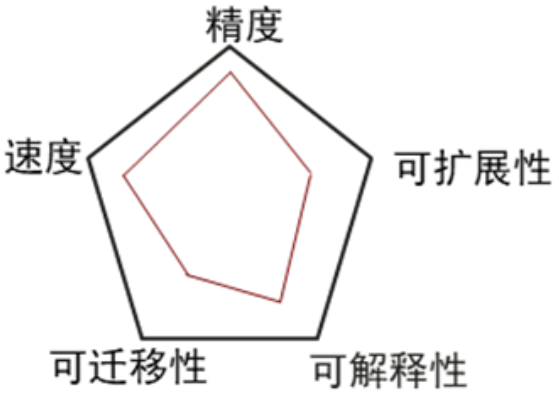
机器学习方法使能的MIP求解器方法 [1]

Method	Selection	Learning	Network	Representation	Remark
[Gasse *et al.*, 2019]	Variable	Reinforcement	GCN	Bipartite graph	Imitate strong branching
[Gupta *et al.*, 2020]	Variable	Supervised	GCN	Bipartite graph	Accelerate via dynamic embedding
[Sun *et al.*, 2020]	Variable	Reinforcement	PD policy	Subproblem set	Evolution strategy for training
[He *et al.*, 2014]	Node	Reinforcement	Standalone	Standalone	Imitate optimal oracle
[Yilmaz *et al.*, 2020]	Node	Supervised	MLP	Handcraft	Prune leaf
[Khalil *et al.*, 2016]	Variable	Supervised	SVM	Handcraft	Learning to rank
[Shen *et al.*, 2021]	Variable	Supervised	GCN	Bipartite graph	Combined with DFS
[Huang *et al.*, 2021b]	Cutting	Supervised	MLP	Handcraft	Large scale
[Zarpellon *et al.*, 2020]	Variable	Reinforcement	MLP	Handcraft	Imitate strong branching
[Tang *et al.*, 2020]	Cutting	Reinforcement	Attention & LSTM	Handcraft	Evolution strategy for training
[Nair *et al.*, 2021]	Variable	Reinforcement	GCN	Bipartite graph	Imitate strong branching
[Ding *et al.*, 2019]	Variable	Supervised	GCN	Tripartite graph	Extract connection information
[Alvarez *et al.*, 2014]	Variable	Supervised	ExtraTrees	Handcraft	Imitate strong branching

机器学习方法使能的SAT求解器方法 [2]

Methods	Networks	Learning	Solver Type	Instance Type
[Bünz and Lamm, 2017]	GNN	Supervised	Standalone	3-SAT
NeuroSAT [Selsam *et al.*, 2019]	GNN & LSTM	Supervised	Standalone	**SR**(n)
QuerySAT [Ozolins *et al.*, 2021]	GNN & Recurrent	Unsupervised	Standalone	k-SAT & Combinatorial
DG-DAGRNN [Amizadeh *et al.*, 2018]	DG-DAGRANN	Unsupervised	Standalone	k-SAT & Combinatorial
NeuroCore [Selsam and Bjørner, 2019]	GNN	Supervised	CDCL	SATCOMP
[Jaszczur *et al.*, 2020]	GNN & Attention	Supervised	DPLL & CDCL	**SR**(n)
Graph-Q-SAT [Kurin *et al.*, 2020]	GNN	Reinforcement	CDCL	3-SAT
NeuroGlue [Han, 2020a]	GNN	Supervised & Reinforcement	CDCL	SATCOMP
GVE [Zhang and Zhang, 2021]	GNN	Reinforcement	CDCL	SATCOMP
NeuroCuber [Han, 2020b]	GNN	Supervised	Cube-and-conquer	Combinatorial
NeuroComb [Wang *et al.*, 2021]	GNN	Supervised	CDCL	SATCOMP
[Yolcu and Póczos, 2019]	GNN	Reinforcement	SLS	3-SAT & Combinatorial
NLocalSAT [Zhang *et al.*, 2020]	GGCN	Supervised	SLS	Random





求解器特点：

✓可标准化

✓可验证，有保证

✓有可能被复制

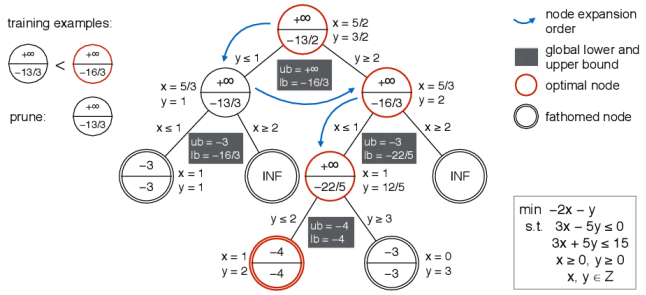
[1] Jiayi Zhang, Chang Liu, Junchi Yan, Xijun Li, Hui-Ling Zhen, Mingxuan Yuan: A Survey for Solving Mixed Integer Programming via Machine Learning. CoRR abs/2203.02878 (2022)

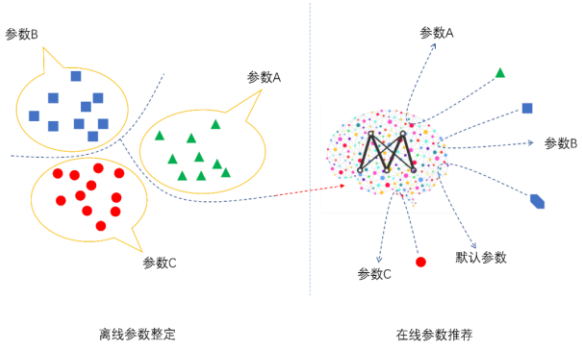
[2] Wenxuan Guo, Junchi Yan, Hui-Ling Zhen, Xijun Li, Mingxuan Yuan, Yaohui Jin: Machine Learning Methods in Solving the Boolean Satisfiability Problem. CoRR abs/2203.04755 (2022)

我们最近的一些尝试 – 学习优化求解器

与华为云联合参加AI顶会NeurIPS 2021 ML4CO求解器竞赛

Configuration task:





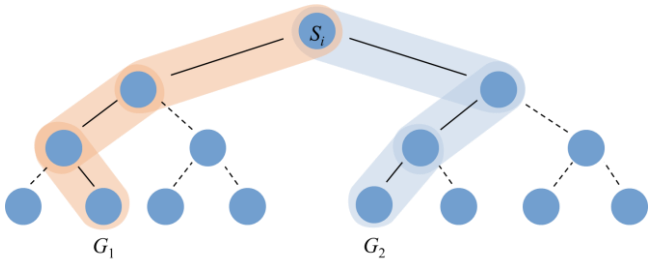
- ✓ 混合整数规划求解器(MIP Solver)是数学规划算法的集大成者。这些算法在MIP求解器内的实现涉及到大量超参数，如开源MIP求解器中**性能最为强劲的SCIP求解器提供了2617个超参数，其中超过2000个超参数与求解过程中的决策强相关。**
- ✓ **应用“离线参数整定”技术，实现综合BO调参：**求解器调参是一类“单次性能评估的时间、资源代价昂贵”的黑箱优化问题。针对这一类问题的常用技术方案是贝叶斯优化（Bayesian Optimization，BO）
- ✓ **基于“在线参数推荐”，完成从特征到类别的映射关系学习：**已知样本的精确类别划分与匹配是为未知样本推荐正确参数的先决条件。华为联合团队基于天筹AI求解器开发的技术积累，从MIP问题用例中抽取出上百个参数特征，并结合MIP问题三部图的图卷积特征，建立起MIP问题的精确画像。基于这些特征，应用无监督学习方法对匿名数据集实现类别划分。
- ✓ 获得该赛道的总榜第一

Dual task:

HEBO 河伯

Heteroscedastic Evolutionary Bayesian Optimisation

调参工具



Cumulative Reward

$$\min_{\phi} \sum_{i=1}^{m} [V_\phi(obs_i, set_i) - G_i]^2 + \lambda \|w\|^2 \quad s.t. \quad V_\phi(obs_i, set_i) \geq G_i, i = 1, ...m$$

$$L^K(\phi) = \sum_{i=1}^{m} (V_\phi(obs_i, set_i) - G_i)^2 \{\mathbf{1}_{(V_\phi \geq G_i)} + K \cdot \mathbf{1}_{(V_\phi < G_i)}\} + \lambda \|w\|^2$$

$$G_i > xV_\phi(obs_i, set_i)$$

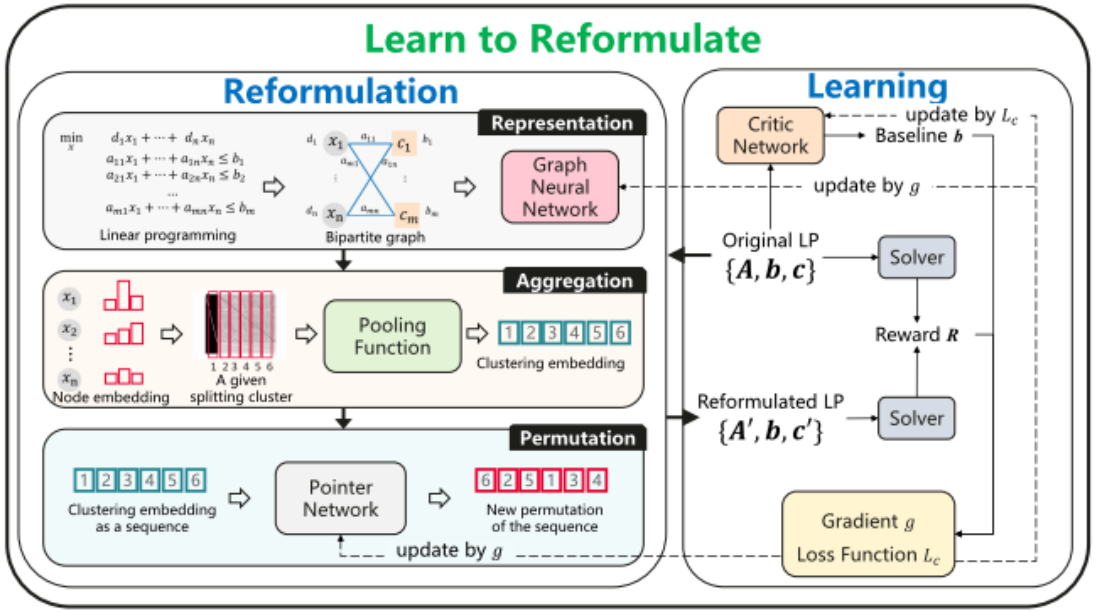
Best Action Imitation Learning (BAIL)

- ✓ A **hybrid sampling strategy** based on Pseudocost branching and active constraint methods to generate dataset.
- ✓ develop a **data selection method** based on BAIL algorithm to select the state-action pairs that possess higher cumulative reward.
- ✓ 利用更少的数据训练，性能大幅超越（40%+）基线算法(NeurIPS19)，获得该赛道总榜第二，学生榜单第一

[1] Li, Xijun, Qingyu Qu, Fangzhou Zhu, Jia Zeng, Mingxuan Yuan, Kun Mao, and Jie Wang. "Learning to Reformulate for Linear Programming." *arXiv e-prints* (2022): arXiv-2201.
[2] Qu, Qingyu, Xijun Li*, and Yunfan Zhou. "YORDLE: An Efficient Imitation Learning for Branch and Bound.“ NuerIPS 2021 ML4CO competition
[3] Gasse, Maxime, et al. "The Machine Learning for Combinatorial Optimization Competition (ML4CO): Results and Insights." arXiv preprint arXiv:2203.02433 (2022).

我们最近的一些尝试 – 学习优化求解器

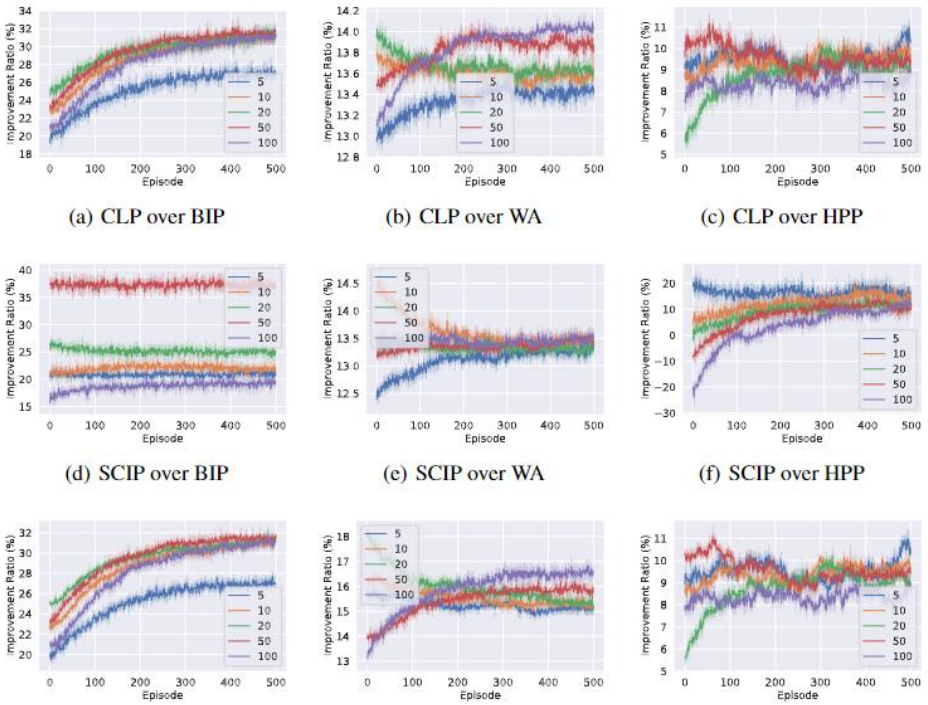
➢ **Learning to Reformulate for Linear Programming**



Reward $$R(\pi|l) = 1 - \frac{\mathcal{S}_{\mathcal{M}}(l|\pi)}{\mathcal{S}_{\mathcal{M}}(l)}$$

Distribution $$p(\pi|\{C_j\}_{j=1}^{M}) = \prod_{j=1}^{M} p(\pi(j)|\pi(<j), \{C_j\}_{j=1}^{M})$$

Loss $$\nabla_{\theta_G,\theta_P} J(\theta_G,\theta_P|l) = \mathbb{E}_{\pi\sim p_{\theta_G,\theta_P}(.|l)}[(R(\pi|l) - b(l)) \nabla_{\theta_G,\theta_P} \log p_{\theta_G,\theta_P}(\pi|l)]$$



(a) CLP over BIP (b) CLP over WA (c) CLP over HPP

(d) SCIP over BIP (e) SCIP over WA (f) SCIP over HPP

(g) Gurobi over BIP (h) Gurobi over WA (i) Gurobi over HPP

Figure 3: How different number of clustering block impacts the our method's performance

- ✓ **Formulation does matters!** (化简和初始解)
- ✓ 首次提出在建模端通过重排方式自动优化求解器效率
- ✓ 二部图+GCN提取数学规划规划问题结构信息
- ✓ 指针网络(Pointer Network)输出变量/约束重排序
- ✓ 强化学习方式训练上述网络

[1] Li, Xijun, Qingyu Qu, Fangzhou Zhu, Jia Zeng, Mingxuan Yuan, Kun Mao, and Jie Wang. "Learning to Reformulate for Linear Programming." *arXiv e-prints* (2022): arXiv-2201.

[2] Qu, Qingyu, Xijun Li*, and Yunfan Zhou. "YORDLE: An Efficient Imitation Learning for Branch and Bound." NuerIPS 2021 ML4CO competition

挑战与未来

1、**Learning from Data：数据 + 算力 + 算法。**

✓ OpenAI坚持AI第一定律（2018），2020年突围了大模型GPT-3/SaaS机会，孵化微软AI自动编程新业务Copilot。

✓ Google学习OpenAI，2021年思考搜索引擎转型对话系统，提出Pathways和SingleModel（多任务）战略。

2、**Heuristic Search + Data-driven：建模（NP难巨大搜索空间）+ 清晰目标函数 + 数据/仿真。**

✓ DeepMind坚持AI第二定律，突围AlphaFold2预测，2021年孵化新子公司Isomorphic Lab聚焦药物发现业务。

✓ DeepMind在控制领域探索，突破Data-driven可控核聚变、多任务控制器Gato。

✓ Tesla在神经网络进规控，加大探索力度。

3、**业务闭环，前途在应用（Heuristic Search + Learning Dynamic Data + Human Feedback）。**

✓ Tesla坚持AI第三定律，2021年突围“纯视觉”自动驾驶方案，从L2.9999进攻L4，带来新产业机会。

✓ Tesla的数据标注流水线，人工+自动。Scale AI自动驾驶数据标注初创公司，2021年估值73亿美金。

✓ Google超级APP闭环：2022 IO大会发布多个应用产品，NeRF技术地图商用仅仅两年，Multisearch学习OpenAI

Lookback for Learning to Branch

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Andrea Lodi, *CERC, Polytechnique Montréal, and Cornell Tech and Technion - IIT* — *andrea.lodi@cornell.edu*
M. Pawan Kumar, *University of Oxford* — *pawan@robots.ox.ac.uk*

- **学什么?** 经典优化算法已经比较完备，且在许多场景中得到应用，但是具体从完备的经典算法过程数据中学习什么是值得探索的。需要对经典算法的实现细节有充分的了解。
- **How to scale?** 学习优化求解器中采用图卷积神经网络提取数学规划特征，难以做大规模
- **如何稳定适用?** 实际场景中已经积累大量同分布的数学规划问题，亟待学习优化求解器在大规模场景中试炼

“未来的人工智能最重要的突破应该是与优化算法的紧密结合”
-- Michael I. Jordan

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Our group’s recent work

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Thank you.

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每个组织，构建万物互联的智能世界。

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