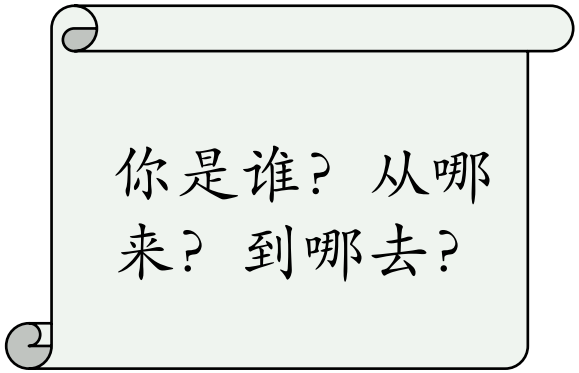
第一讲 绪论

高级机器学习

提纲

尝试回答如下问题:

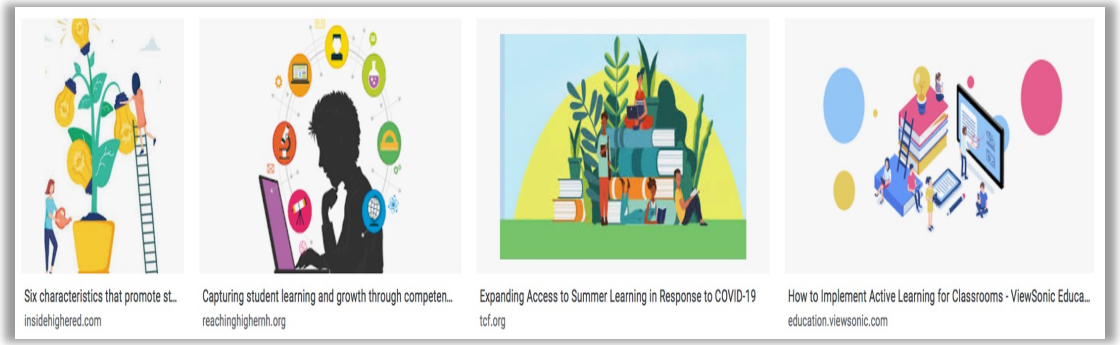
- 机器学习是什么?
- 机器学习从哪儿来?
- 机器学习能做什么?
- 机器学习到哪儿去?
- 机器学习与其它领域的关系?
- 机器学习前沿进展到哪儿找?
- …



机器学习

机器

学习



机器学习？

机器学习（Machine Learning）

1）人类学习利用**经验**不断提高性能

2）机器善于处理**数据**不断提高性能

能否把“经验”变成数据，让机器可以“模仿”人类进行学习

机器学习：机器利用数据学习人类经验，不断提高性能的过程

机器学习（Machine Learning）

机器学习是人工智能的核心领域之一，是实现智能化的关键

经典定义：利用经验改善系统自身的性能

经验 → 数据

随着该领域的发展，目前主要研究智能数据分析的理论和算法，并已成为智能数据分析技术的源泉之一

图灵奖连续授予在该方面取得突出成就的学者

Leslie Valiant
(1949 -)
(Harvard Univ.)

2010 年度

“计算学习理论”奠基人

Judea Pearl
(1936 -)
(UCLA)

2011 年度

“图模型学习方法”先驱

机器学习（Machine Learning）

机器学习是人工智能的核心领域之一，是实现智能化的关键

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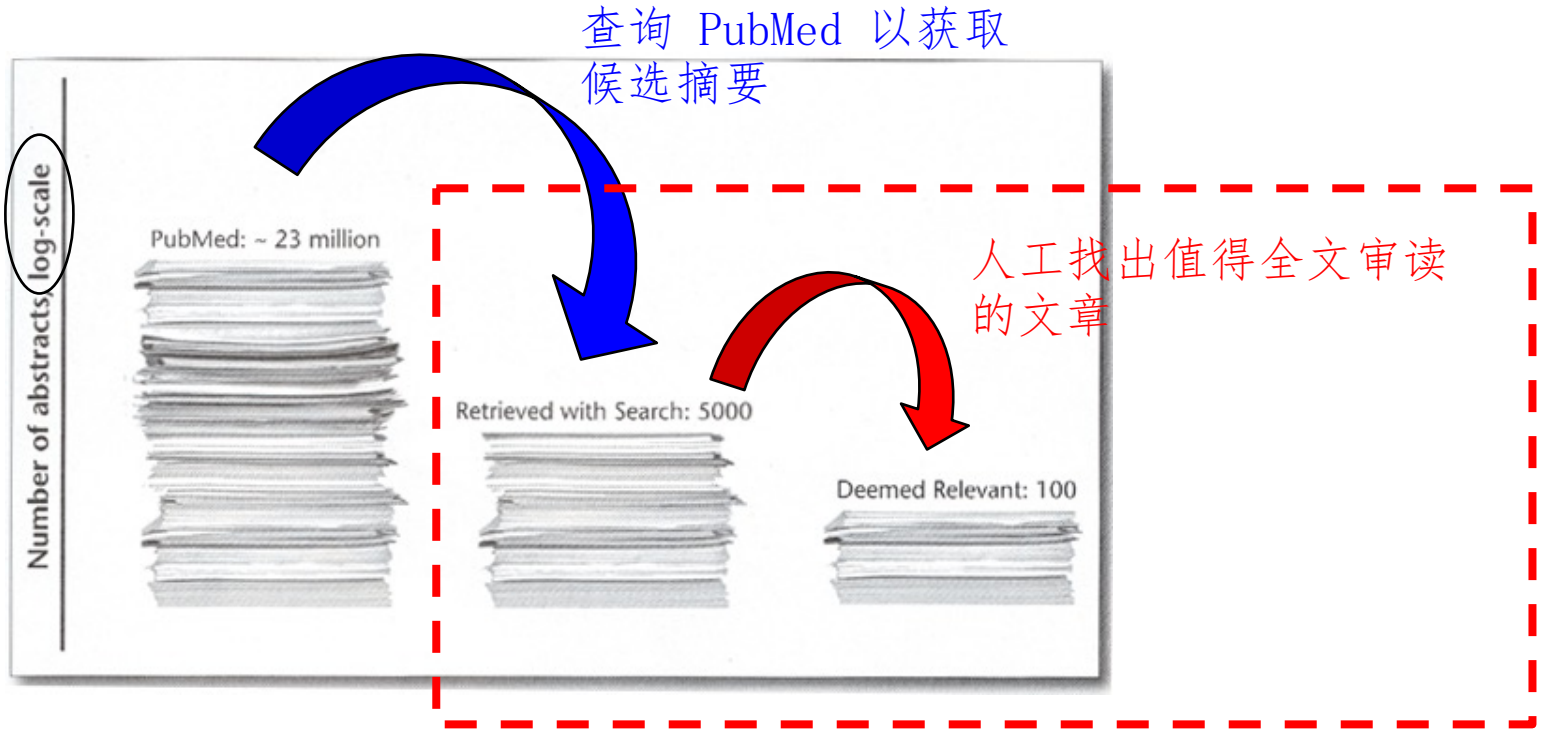
“深度学习三驾马车”
获2018年度图灵奖

一个例子：“文献筛选”

在“循证医学”（evidence-based medicine）中，针对特定的临床问题，先要对相关研究报告进行详尽评估



出自 [C. Brodley et al., AI Magazine 2012]

“文献筛选”

在一项关于婴儿和儿童残疾的研究中，美国Tufts医学中心筛选了约 33,000 篇摘要

尽管Tufts医学中心的专家效率很高，每篇摘要筛选时间只需 30 秒钟，但该工作仍花费了 250 小时

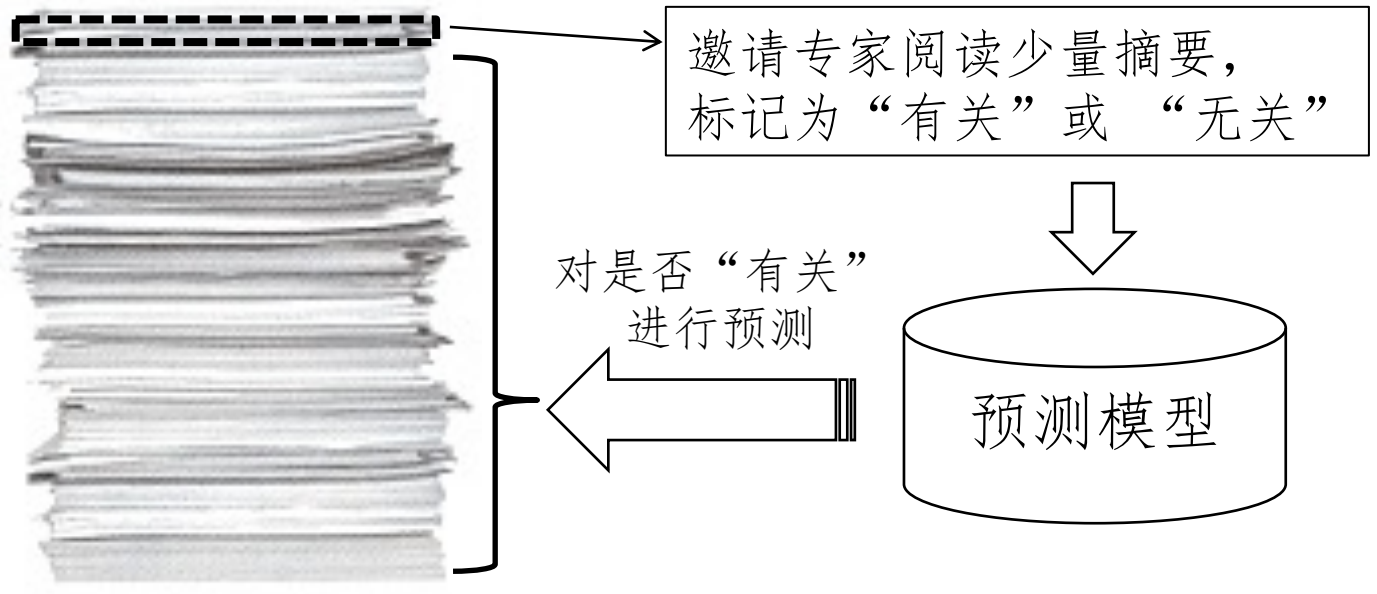
A portion of the 33,000 abstracts

每项新的研究都要重复这个麻烦的过程！

需筛选的文章数在不断显著增长！

“文献筛选”

为了降低昂贵的成本，Tufts医学中心引入了**机器学习**技术



- 人类专家只需阅读 50 篇摘要，系统的自动筛选精度就达到 93%
- 人类专家阅读 1,000 篇摘要，则系统的自动筛选敏感度达到 95%

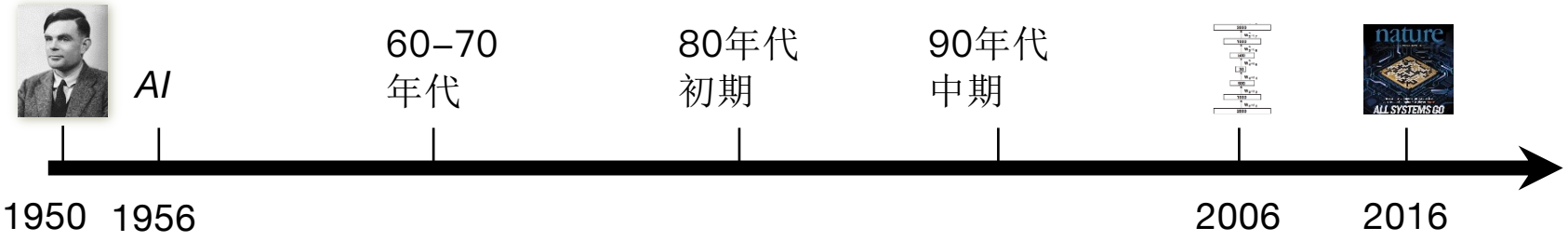
人类专家以前需阅读 33,000 篇摘要才能获得此效果

机器学习从何而来？

源自于人工智能的发展历史阶段

人工智能

推理期　知识期　学习期



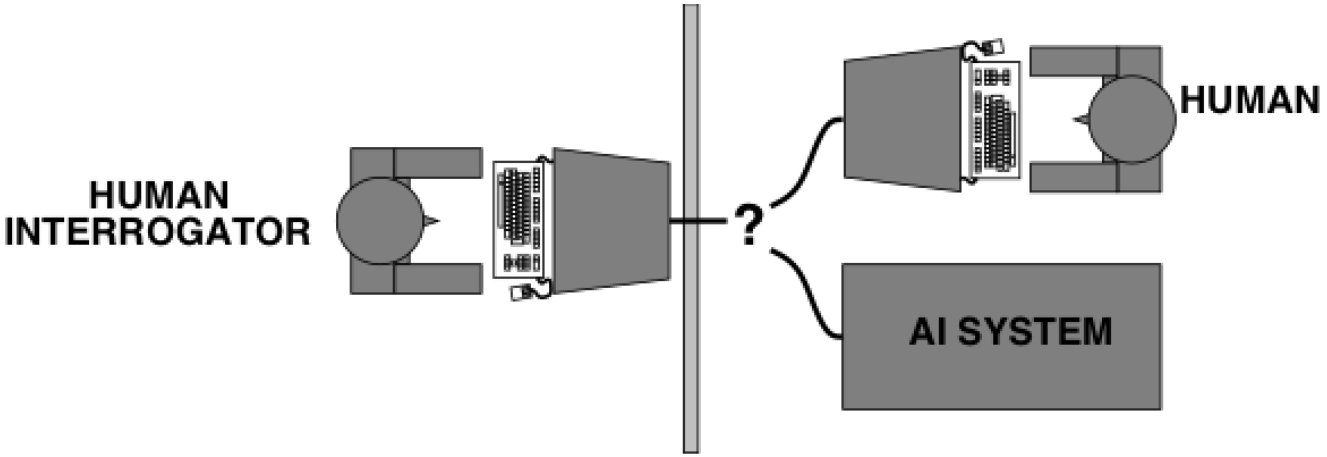
人工智能

1950

[Computing machinery and intelligence. Mind 49: 433-460, 1950.]

Alan Turing
1912-1954

Section 1: Imitation game (模仿游戏)



人工智能

AI

1950 1956

1956 Dartmouth 会议，命名 “Artificial Intelligence”

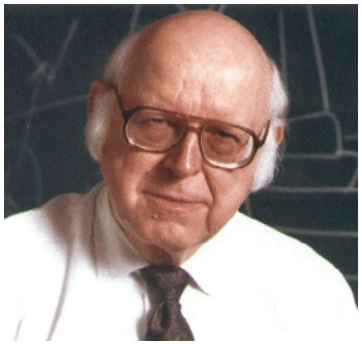
人工智能

AI

60–70
年代

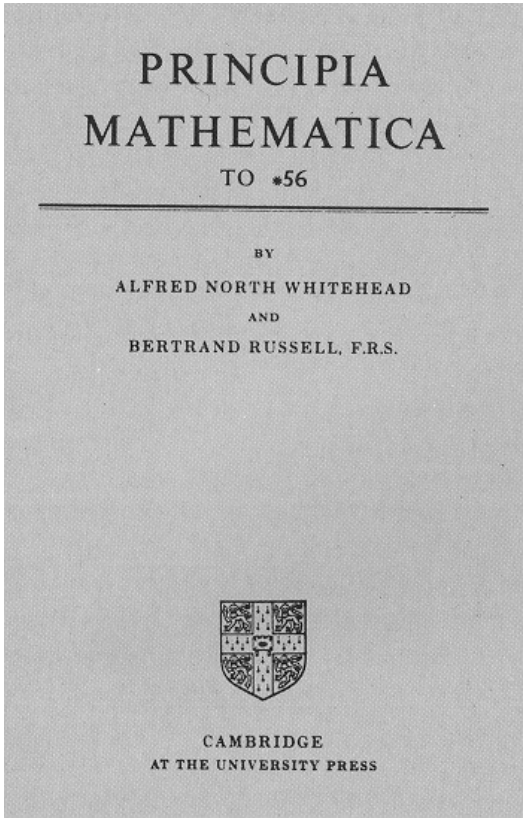
1950 1956

逻辑学家



Allen Newell

Herbert Simon



“逻辑理论家”程序在1952 年证明了著名数学家罗素和怀特海的名著《数学原理》中的38 条定理；在1963 年证明了全部52条定理，特别值得一提的是，定理2.85 甚至比罗素和怀特海证明得更巧妙.

人工智能

AI

60–70
年代

80年代
初期

1950 1956

专家系统

Edward Albert Feigenbaum

要使机器具有智能，就必须设法使机器拥有知识

人工智能

知识总结成计算机程序很困难；通过数据自动地让机器利用“知识”更为便利，那就是机器学习的优势

AI

60–70年代

80年代初期

90年代中期

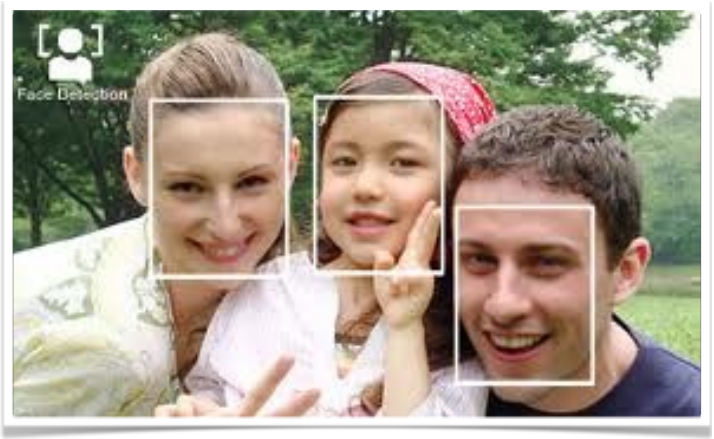
1950 1956

2006

机器学习

垃圾邮件过滤

人类识别系统



商品推荐系统

人工智能

AI

60–70
年代

80年代
初期

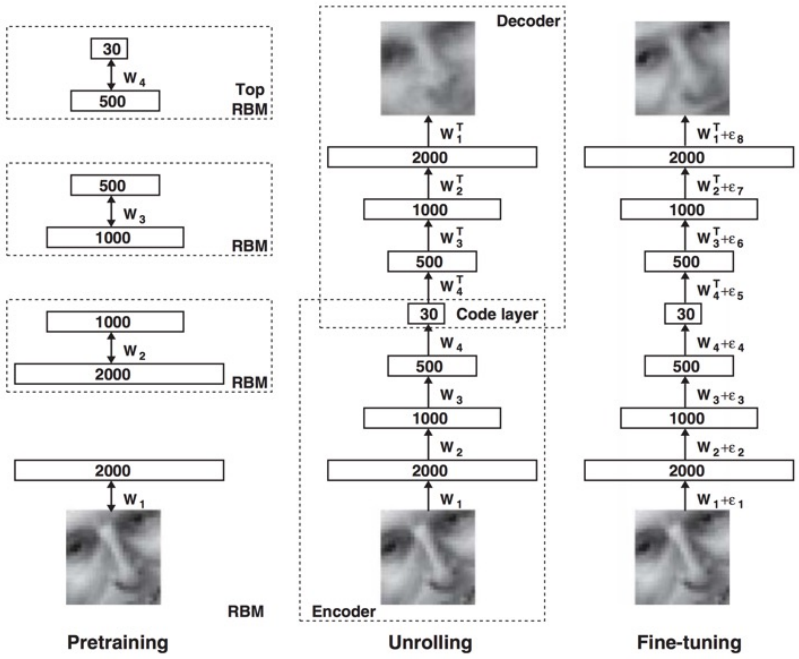
90年代
中期

1950 1956 2006 2016

机器学习 ⟶ 深度学习

Geoff Hinton

深度学习显著降低了机器学习应用者的门槛，
为机器学习技术走向工程实践带来了便利



2015年至今

《Nature》2015年2月统计学习先驱B. Schölkopf发文评论了基于学习的人工智能

《Nature》2015年5月发表7篇文章的专栏聚焦机器智能
深度学习、强化学习、概率机器学习、小型自主无人机

《Science》2015年7月发表人工智能专辑
机器学习、自然语言处理、计算理性、数据隐私

互联网巨头纷纷开源机器学习/深度学习系统
FBCUNN、TensorFlow、PaddlePaddle、Pytorch、SystemML、VELES

NVIDIA

专用于机器学习等计算任务的通用GPU

2015年至今

香港科技大学计算机系主任杨强教授（AAAI Fellow、IEEE Fellow、AAAS Fellow）：“现在我国人工智能的水平和国际几乎没有差距”

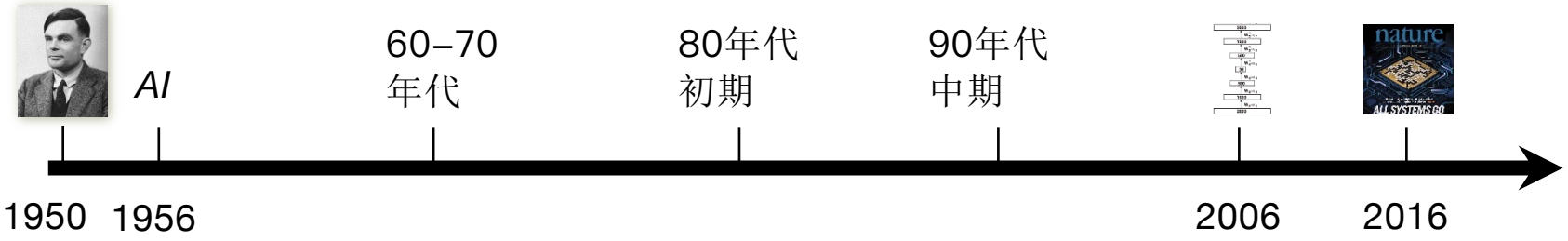
2015年国际人工智能联合大会（IJCAI 2015），中国投稿和录用论文数首次超过美国：欧盟、中国、美国

2020年即使受疫情影响，MLA线上人数超过45000人

微软亚洲研究院2015年11月开源了“分布式机器学习工具箱”
百度硅谷研究院也开源了其大规模深度学习系统

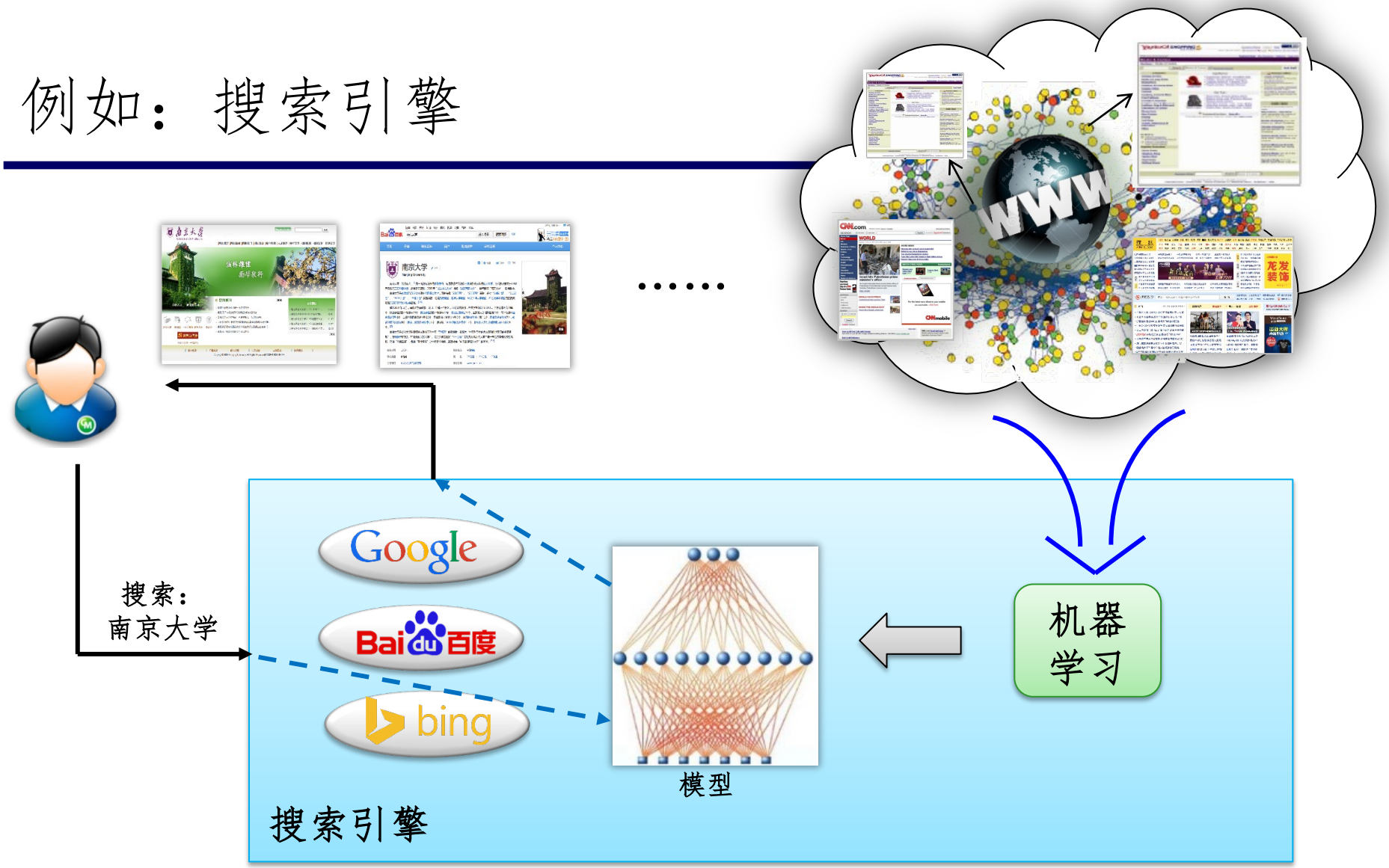
人工智能

推理期　知识期　学习期



机器学习有哪些应用？

例如：搜索引擎



机器学习技术正在支撑着各种搜索引擎

例如：自动汽车驾驶

车载摄像头

车载雷达

机器学习

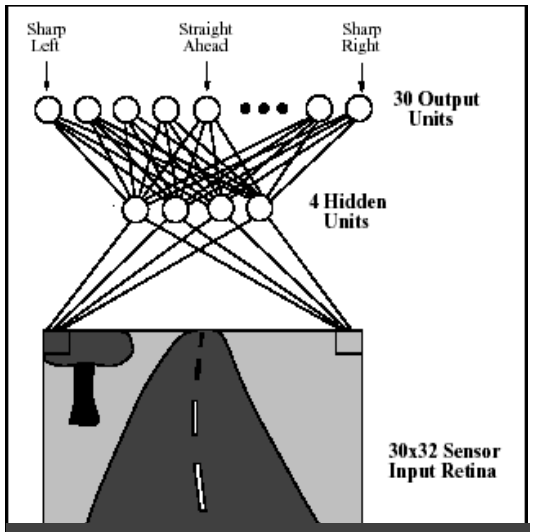
模型

方向盘旋转幅度

油门幅度

刹车幅度

控制汽车



美国在20世纪80年代就开始研究基于机器学习的汽车自动驾驶技术

DARPA Grand Challenge - 2004

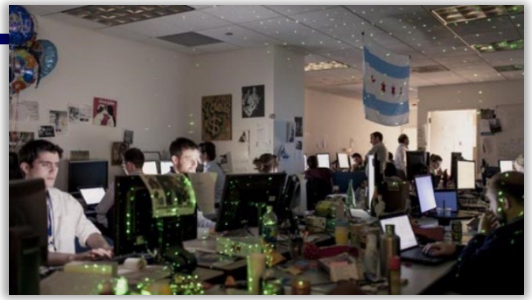
荒野中的无人车竞赛

Google 无人驾驶汽车 - 2016

新加坡无人驾驶出租车 - 2016

例如：帮助奥巴马胜选

《时代》周刊



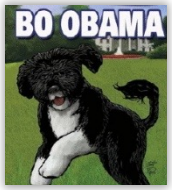
这个团队行动保密，定期向奥巴马报送结果；被奥巴马公开称为总统竞选的“核武器按钮”（“They are our nuclear codes”）

通过机器学习模型

◆ 个性化宣传

喜欢宠物？

奥巴马也有宠物！



喜欢篮球？

奥巴马也是篮球迷！

◆ 广告购买

精准定位不同选民群体，建议购买冷门广告时段，广告资金效率比2008年提高14%

◆ 筹款

和乔治克鲁尼/奥巴马共进晚餐对于年龄在40-49岁的美西地区女性颇具吸引力…… 乔治克鲁尼为奥巴马举办的竞选筹资晚宴成功募集到1500万美元

例如：AlphaGO

计算/预测出较高胜率的走法？

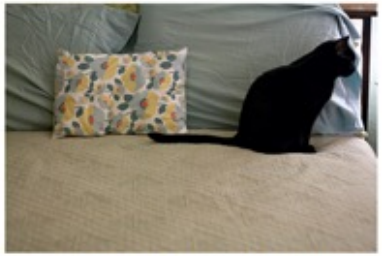
大量棋谱如何生成/利用

公开的计算难题，意义重大

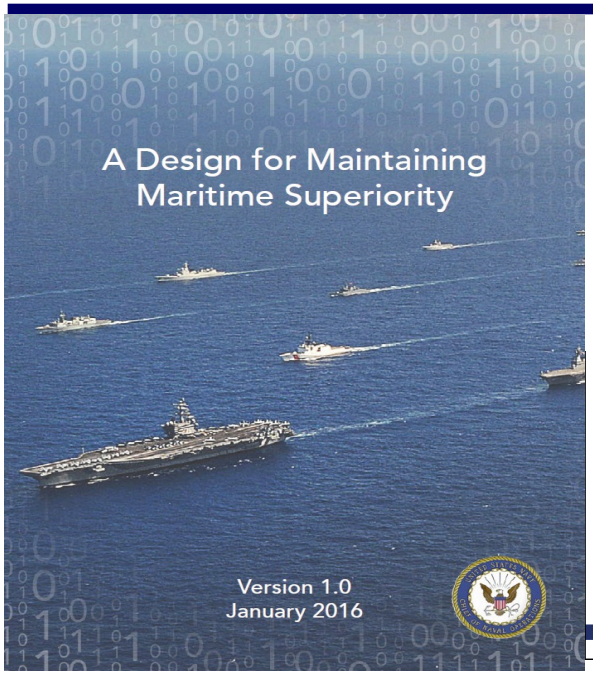
熟知的日常游戏，影响深远

例如：视频理解

计算机已可初步理解视频

Describes without errors	Describes with minor errors	Somewhat related to the image	Unrelated to the image
 A person riding a motorcycle on a dirt road.	 Two dogs play in the grass.	 A skateboarder does a trick on a ramp.	 A dog is jumping to catch a frisbee.
 A group of young people playing a game of frisbee.	 Two hockey players are fighting over the puck.	 A little girl in a pink hat is blowing bubbles.	 A refrigerator filled with lots of food and drinks.
 A herd of elephants walking across a dry grass field.	 A close up of a cat laying on a couch.	 A red motorcycle parked on the side of the road.	 A yellow school bus parked in a parking lot.

例如：美军海权纲领性文件



Conclusion

We will remain the world's finest Navy **only** if we all fight each an
better. Our competitors are focused on taking the lead – we mu
deny them. The margins of victory are razor thin – but decisive!
integrity, accountability, initiative, and toughness to execute the
in this Design, execute our mission, and achieve our end state. I
to lead you.

JOHN M. RICHARDSON

8

The third interrelated force is the increasing rate of technological creation and adoption. This is not just in information technologies, where Gordon Moore's projections of exponential advances in processing, storage, and switches continue to be realized. Scientists are also unlocking new properties of commonplace materials and creating new materials altogether at astonishing speeds. Novel uses for increasingly sophisticated robotics, energy storage, 3-D printing, and networks of low-cost sensors, to name just a few examples, are changing almost every facet of how we work and live. Genetic science is just beginning to demonstrate its power. Artificial intelligence is just getting started and could fundamentally reshape the environment. And as technology is introduced at an accelerating rate, it is being adopted by society just as fast – people are using these new tools as quickly as they are introduced, and in new and novel ways.

These thre
informati
interplay
must do
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And the
United St
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specifically on our vulnerabilities and are increasingly designed from the ground up to leverage the maritime, technological and information systems. They continue to develop and field information-enabled weapons, both kinetic and non-kinetic, with increasing range, precision and destructive capacity. Both China and Russia are also engaging in coercion and competition below the traditional thresholds of high-end conflict, but nonetheless exploit the weakness of accepted norms in space, cyber and the electromagnetic spectrum. The Russian Navy is operating with a frequency and in areas not seen for almost two decades, and the Chinese PLA(N) is extending its reach around the world.

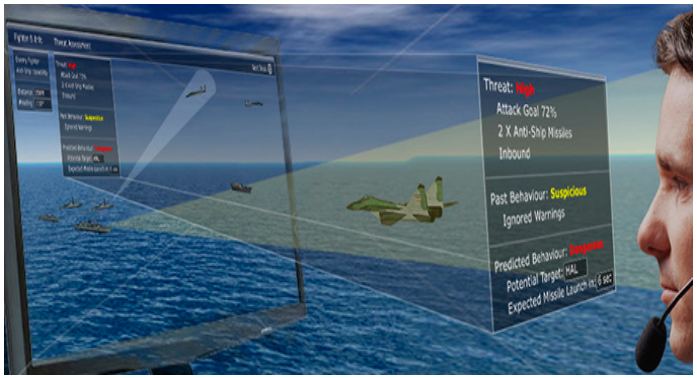
Russia and China are not the only actors seeking to gain advantages in the emerging security environment in ways that threaten U.S. and global interests. Others are now pursuing advanced technology, including military technologies that were once the exclusive province of great powers – this trend will only continue. Coupled with a continued dedication to furthering its nuclear weapons and missile programs, North Korea's provocative actions continue to threaten security in North Asia and beyond. And while the recent international agreement with Iran is intended to curb its nuclear ambitions, Tehran's advanced missiles, proxy forces and other conventional capabilities continue to pose threats to which the Navy must remain prepared to respond. Finally, international terrorist groups have proven their resilience and adaptability and now pose a long-term threat to stability and security around the world. All of these actors seek to exploit all three forces described above – the speed, precision and reach that

3

“人工智能开始并可以从根本上重塑（战场）环境…”

美海军作战部长John Richardson 2016年初签署的《保障制海权规划中明确指出人工智能的重要

例如：战场战术层面 （美）



眼镜蛇系统：

Coastal Battlefield Reconnaissance and Analysis (COBRA)

用于频海战斗舰，执行无人空中战术侦察。在两栖攻击之前，于海浪区和海滩区探测和定位雷区和障碍物

http://www.navy.mil/navydata/fact_display.asp?cid=2100&tid=1237&ct=2

http://www.navysbir.com/n15_1/N151-049.htm

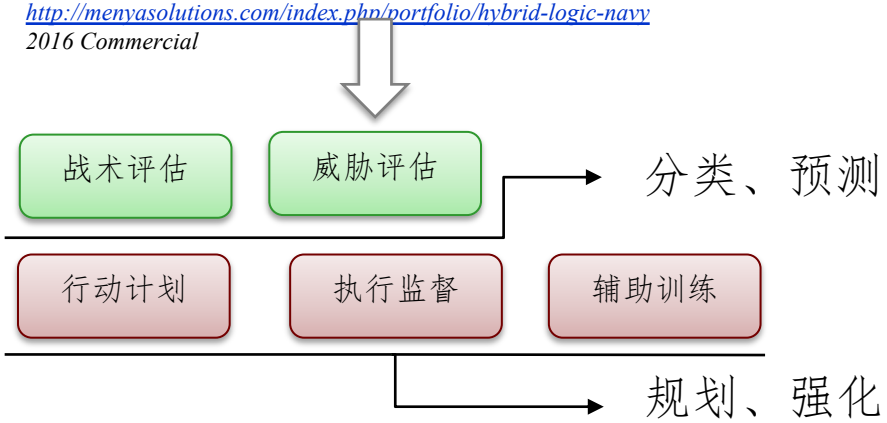
2015 US Navy Official

HybridLogic Navy:

一套自动的基于机器学习的代理，帮助人类和无人机理解战术状况，及时做出最佳决策，以对付海军作战中的威胁

http://menyasolutions.com/index.php/portfolio/hybrid-logic-navy

2016 Commercial



United States Navy

Fact File

AN/DVS-1 COASTAL BATTLEFIELD RECONNAISSANCE AND ANALYSIS - (COBRA)

The mission of the AN/DVS-1 Coastal Battlefield Reconnaissance and Analysis (COBRA) system is to conduct unmanned aerial tactical reconnaissance in the littoral battlespace for detection and localization of minefields and obstacles in the surf zone and beach zone prior to an amphibious assault. The COBRA airborne payload will be carried on the MQ-8 Fire Scout unmanned air system. This allows operators and other personnel to remain at a safe distance from the mine and obstacle belts and enemy direct and indirect fire. COBRA will be embarked in the Littoral Combat Ship (LCS) as part of the Mine Countermeasures (MCM) Mission Package (MP).

DESCRIPTION: The Coastal Battlefield and Reconnaissance (COBRA) program (Ref 1) is interested in technologies that facilitate automated target recognition (ATR) capabilities in aerial multi-spectral images for previously unseen environments and target types. Targets of interest include minefields and obstacles in various land and marine environments. Typically, ATR algorithms are developed offline (post-mission) using previously acquired test data sets. These algorithms are based on supervised learning methods (Ref 2) that incorporate data from a limited set of test fields. When data is acquired in new environments, the algorithms often must be re-optimized to have good performance in that environment, as well as maintain performance in previously seen environments. The process for performing this offline re-optimization is often costly since it requires the efforts of expert analysts to assimilate data sets, determine target truth, analyze target features, train the ATR classifiers and evaluate performance.

There is a need for innovative methods that can 1) incorporate information from new data sets into the ATR system as they are acquired, and 2) re-optimize ATR algorithms quickly across all known environments, including those of newly acquired data. Online Machine Learning (OML) algorithms (Ref 3-5) can potentially be used to "learn" in the field based on operator-provided results without affecting prior performance. The information collected online can be used to refine the prediction hypothesis (classifier) used in the ATR algorithms. In addition, the information may provide input for automated methods of optimizing ATR performance across all known data sets.

The proposed effort will develop innovative OML algorithms for ATR that can incorporate human operator decisions to optimize probability of detection and probability of false alarm performance in new environments and for new target types. These algorithms will be integrated into mission and post-mission analysis systems in which operators review acquired images. The algorithms will be implemented as object-oriented C++ code for insertion into the operator systems. Development of the online learning algorithms must be combined with identification of how the operator will interact with them to provide updated decision information. Robust optimization of the ATR algorithms may be performed post-mission, which will require the development of separate software tools for processing historical data sets. The OML algorithms and optimization tools developed in this effort will reduce program costs by minimizing the time required for optimizing ATR algorithms to perform well in unseen operational environments.

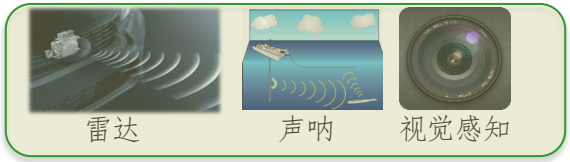
自动目标识别、监督学习以及在线学习技术被作为核心技术并多次提及

例如：战场战术层面 （英）

无人侦察快艇:

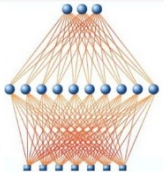
无人控制的情况下以50公里时速追踪快速目标并自动避障，进行跟踪、监视和间谍活动，或者用于海岸巡逻

http://www.telegraph.co.uk/news/2016/09/05/navy-unveils-robot-spy-speedboat/ *2016 Royal Navy Official /Commercial*



多源感知

机器学习



模型

控制模块

无人自动驾驶

船舶能源评估-条件优化和路由增强系统

Software to transform ship maintenance

September 21, 2016

SEA-CORES. Credit: University of Southampton

Researchers from the University of Southampton are to develop software that can monitor the equipment, fuel and energy performance of a ship at sea.

The University is part of the Ship Energy Assessment – Condition Optimisation & Routing Enhancement System (SEA-CORES) consortium, which provides a live model of ship performance on global operations. The development of the software is led by BAE Systems and is sponsored by Innovate UK.

SEA-CORES is able to correlate variables that could affect a ship's performance, such as energy consumption and different weather conditions. Using genetic algorithms to track and capture the live data, SEA-CORES provides those on board with a greater understanding of the vessel's capabilities across a wide range of operations.

Researchers from Electronics and Computer Science at the University of Southampton will work on monitoring loads on the ship and applying novel machine learning techniques to a domain that has largely been data poor.

Dr Sarvapali Ramchurn, who is leading the Southampton research group, said: "Unleashing such technologies on the marine sector is likely to have a huge impact. The work we are doing at Southampton in terms of autonomous systems and machine learning will help improve the efficiency of ships and detect potential issues before they cause major damage."

BAE Systems is developing and testing SEA-CORES on a commercial tanker provided by James Fisher Marine Services. The trial will analyse the vibration and trim performance of the vessel, its hull state and monitor the integrity of the ship's superstructure.

Chris Courtaux, Head of Engineering and Energy Services at BAE Systems, said: "SEA-CORES is able to consider all of the important components which affect the performance of a vessel during deployment.

"For instance, reducing speed may save fuel but increase the wear to the engine if below its optimum performance. This could in turn increase the maintenance requirements for these vessels and reduce their availability. It is crucial that we continue to analyse what more can be done to maintain these vessels in an efficient manner and increase the number of ships available for the Royal Navy fleet."

The software connects technologies in delivering fuel and engine optimisation through the use of the BAE Systems' Ship Energy Assessment System (SEAS), together with big data analysis by using System Information Exploitation (SIE) technology.

SEA-CORES has been developed in response to the increasing complexities of modern warships and the amount of data their systems produce. The technology could transform how the Royal Navy and BAE Systems maintain and support warships in the future by using the genetic algorithms to identify the relationships between a ship's systems, calculate their different permutations and ultimately recommend a strategy to optimise the vessel's performance.

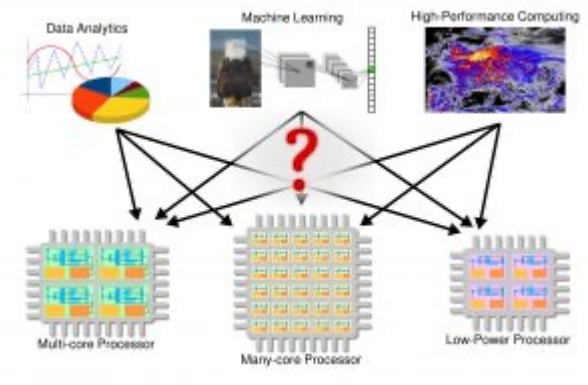
应对现代军舰日益复杂系统结构、针对其系统产生的海量数据而开发，能够有机组织军舰各个子系统，最终优化全舰效能

https://phys.org/news/2016-09-software-ship-maintenance.html

2016 Royal Navy Official / Commercial

遗传算法以及其他一些机器学习方法用于获取追踪数据和确定舰船子系统关联的任务中

例如：中长期战略层面 — 基础/技术研发

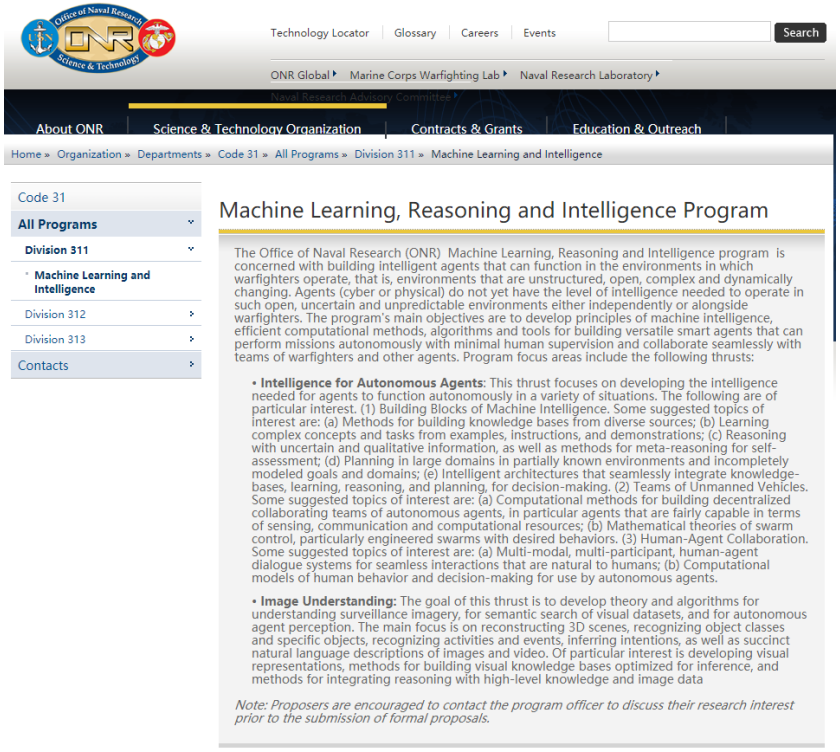


军用下一代机器学习处理器：

依托学习技术消除了海军开发人员选择架构的问题，由程序直接分析出最适合的处理器平台，最大化指令执行效率

http://futureforce.navylive.dodlive.mil/2017/07/popcorn-linux-software-for-a-diverse-world/

2017 US DOD Official



美海军研究院：

针对机器学习，特别对自主代理、图像理解展开全面研究

https://www.onr.navy.mil/en/Science-Technology/Departments/Code-31/All-Programs/311-Mathematics-Computers-Research/Machine-Learning-Reasoning-Intelligence

2017 US Navy Official / US Naval Research Division 311.

机器学习预往何处?

只是畅想一种可能的未来

华为-讲座

Deepseek

人工智能寒冬

1）低估智能的复杂性

2）脱离现实问题

90年代初，第二次人工智能寒冬

- AI硬件市场需求下跌
- 专家系统维护成本高昂
- 日本五代机失败
- DARPA大幅缩减AI项目资助

稳健性是硬伤

John Langford

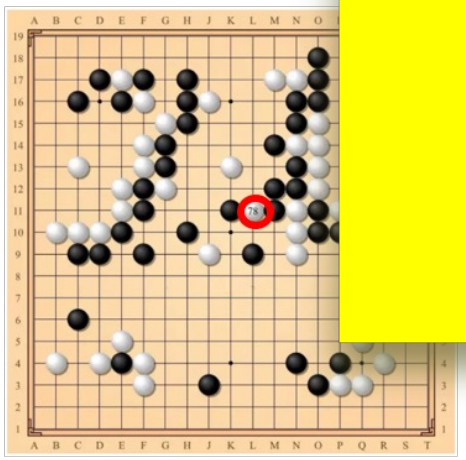
国际机器学习大会
ICML'12的程序主席

人类犯错：水平从九段降到八段

机器犯错：水平从九段降到业余

离“超越人类棋手”还远

“鲁棒性”是关键 ！



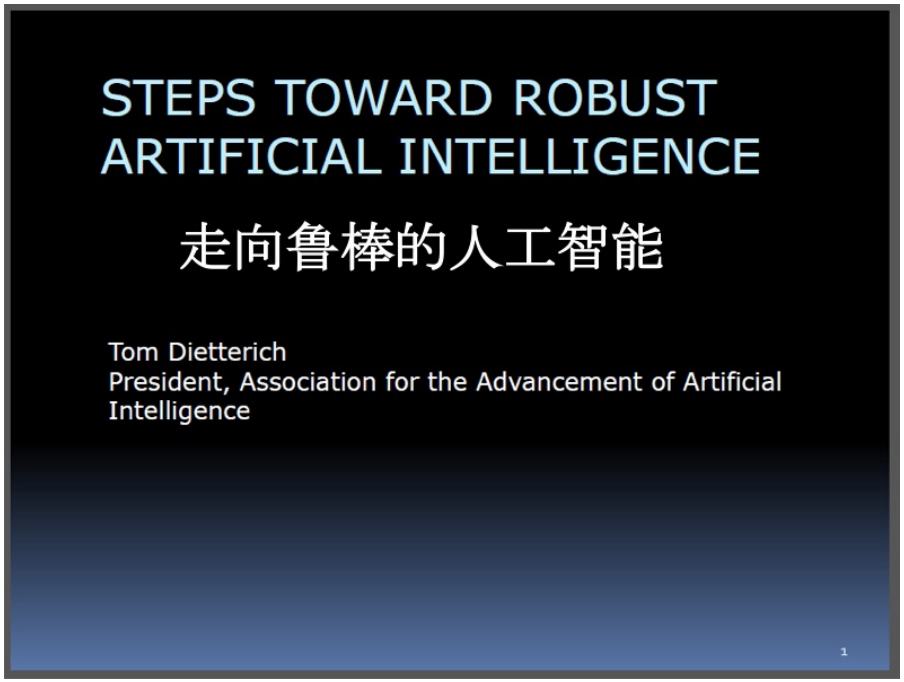
3月13日李世石九段的“神之一手”

phaGo以为自做得很好，但第87手迷惑了。们有麻烦了

错误出现在第79手犯了错误，但AlphaGo在第87手才发现

国际上对AI发展的探讨

AAAI “主席报告”
(“Presidential Address”)



Tom Dietterich

AAAI/AAAS/ACM Fellow
AAAI 现任主席
国际机器学习学会创始主席 （2001-2008）

国际上对AI发展的探讨

T. Dietterich强调：随着人工智能技术的发展，越来越多地面临“高风险应用”

因此，必须要有“鲁棒的**AI**”

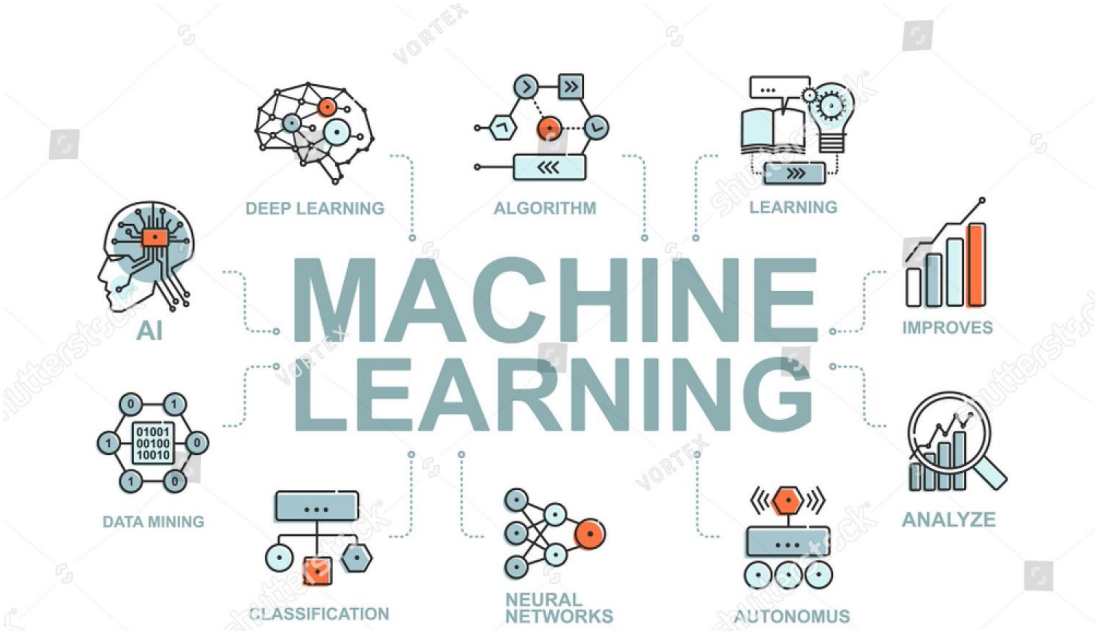
- 对人类用户错误鲁棒
- 对网络攻击鲁棒
- 对错误目标鲁棒
- 对不正确模型鲁棒
- 对未建模现象鲁棒

机器学习跟其它领域的关系

机器学习

机器学习：以数据为经验的载体，利用经验数据不断提高性能的计算机系统/程序/算法

广袤的交叉学科　　内容非常丰富



机器学习与其它领域的关系

- 机器学习与数据挖掘
  - 机器学习和数据挖掘都涉及数据分析
  - 机器学习、数据库、统计学是数据挖掘的关键支撑技术
  - 机器学习更偏技术方法，数据挖掘更偏应用些

- 机器学习与数据科学
  - 机器学习是数据科学实现智能化的关键步骤——数据智能分析
  - 数据科学还包括很多内容，例如收集、存储、传输、管理大数据
  - 大数据研究目的是为了利用大数据，没有机器学习提供数据分析技术，大数据利用无从谈起

机器学习与其它领域的关系

- 机器学习和计算机视觉
  - 机器学习是计算机视觉的核心技术
  - 计算机视觉是机器学习的重要应用
- 机器学习和自然语言处理、模式识别
  - 参考计算机视觉
- 机器学习和统计学
  - 统计学是机器学习的重要理论基础
- 机器学习和神经科学
  - 机器学习发展过程中，经常受到神经科学思想的启发
  - 神经科学发展比较缓慢，不够成熟，机器学习通常借鉴其思想，不会借鉴它的技术基础（例如，借鉴鸟儿造飞机，但是飞机的原理技术跟鸟没关系，主要靠物理、机械、材料等科学）

机器学习主要学术进展从哪得到

学术期刊

- AIJ 《Artificial Intelligence》
- JMLR 《Journal of Machine Learning Research》
- TPAMI《IEEE Trans. on Pattern Analysis and Machine Intelligence》
- TKDE《IEEE Trans. on Knowledge and Data Engineering》
- MLJ 《Machine Learning》
- TNNLS 《IEEE Trans. on Neural Network and Learning Systems》
- 国内：《中国科学 信息科学》
- …

学术会议

- ICML (International Conference on Machine Learning)
- NeurIPS (Neural Information Processing Systems)
- KDD (ACM SIGKDD Conf. on Knowledge Discovery and Data Mining)
- AAAI (AAAI conference on Artificial Intelligence)
- IJCAI (International Joint Conference on Artificial Intelligence)
- ICLR (International Conference on Learning Representation)
- 国内：MLA
- …

China Symposium on Machine Learning and Applications

中国机器学习及其应用研讨会

为了促进智能信息处理领域同行间的交流，陆汝钤院士发起组织了"智能信息处理系列研讨会"。“机器学习及其应用”研讨会自2002年开始，先后在上海、南京、北京、西安等地举行。该研讨会每年邀请海内外从事机器学习及相关领域研究的专家与会进行学术交流。研讨会不征文，不收取注册费，欢迎机器学习及相关领域的学者、研究生前来旁听特邀报告并参加讨论。为了促进机器学习及相关领域的研究生之间以及研究生与资深学者之间的交流，2006-2010年在机器学习及其应用研讨会（MLA）期间，同时举行了机器学习及其应用学生研讨会（SSMLA），此后该研讨会融入MLA的Poster session.

以下是各年会议的信息：

MLA'20		2020年11月，南京大学
MLA'19		2019年11月，天津大学
MLA'18		2018年11月，南京大学
MLA'17		2017年11月，北京交通大学
MLA'16		2016年11月，南京大学
MLA'15		2015年11月，南京大学
MLA'14		2014年11月，西安电子科技大学
MLA'13		2013年11月，复旦大学
MLA'12		2012年11月，清华大学
MLA'11		2011年11月，清华大学
MLA'10	SSMLA'10	2010年11月，南京大学
MLA'09	SSMLA'09	2009年11月，南京大学
MLA'08	SSMLA'08	2008年11月，南京大学
MLA'07	SSMLA'07	2007年11月，南京大学、南京师范大
MLA'06	SSMLA'06	2006年11月，南京大学、南京航空航

MLA'18 - The 16th China Symposium on Machine Learning and Applications

第十六届中国机器学习及其应用研讨会

2018年11月2-4日，南京大学，南京

会议首页
组织机构
特邀专家
会议日程
顶会论文交流
食宿安排
赞助支持
会议地点
会议文集
以往会议
会议照片

会议照片

所有照片均已缩小，若要查看原图，请点击图片

开幕式：

Michael K. Ng教授做大会报告：

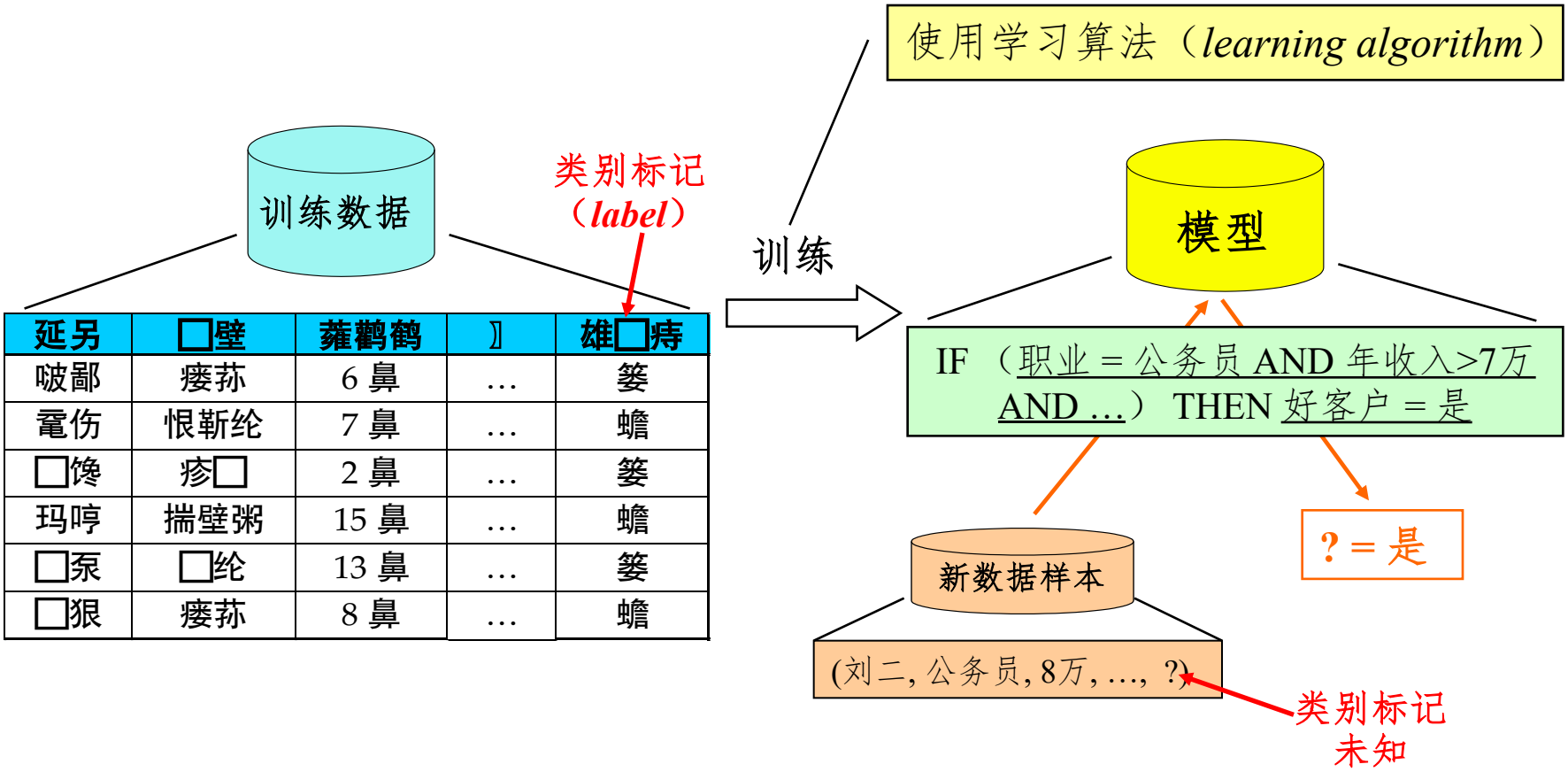
提纲

- 机器学习是什么?
  - 关键词：经验、数据、性能
  - 机器学习的经典过程
- 机器学习的历史和可能的未来?
  - 推理期、知识期、学习期
  - 可信稳健协同机器学习
- 机器学习是什么？能做什么?
  - 关键词：举1-2个例子说明
- 机器学习与其它领域的关系
  - 说出跟数据挖掘，大数据，计算机视觉，自然语言处理的关系?
- 机器学习前沿进展到哪儿找?
  - 能说出几个重要期刊和会议

机器学习

术语介绍

典型的机器学习过程



延另	□壁	薅鹳鹤	⟧	雄□痔
啵鄙	瘘荪	6 鼻	…	篓
鼋伤	恨靳纶	7 鼻	…	蟾
□馋	疹□	2 鼻	…	篓
玛哼	揣壁粥	15 鼻	…	蟾
□泵	□纶	13 鼻	…	篓
□狠	瘘荪	8 鼻	…	蟾

潜在意义

横：输入（数据） =》输出（标记）

纵：
历史（数据）
=》
未来（数据）

特征　　标记

编号	色泽	根蒂	敲声	好瓜
1	青绿	蜷缩	浊响	是
2	乌黑	蜷缩	沉闷	是
3	青绿	硬挺	清脆	否
4	乌黑	稍蜷	沉闷	否
1	青绿	蜷缩	沉闷	?

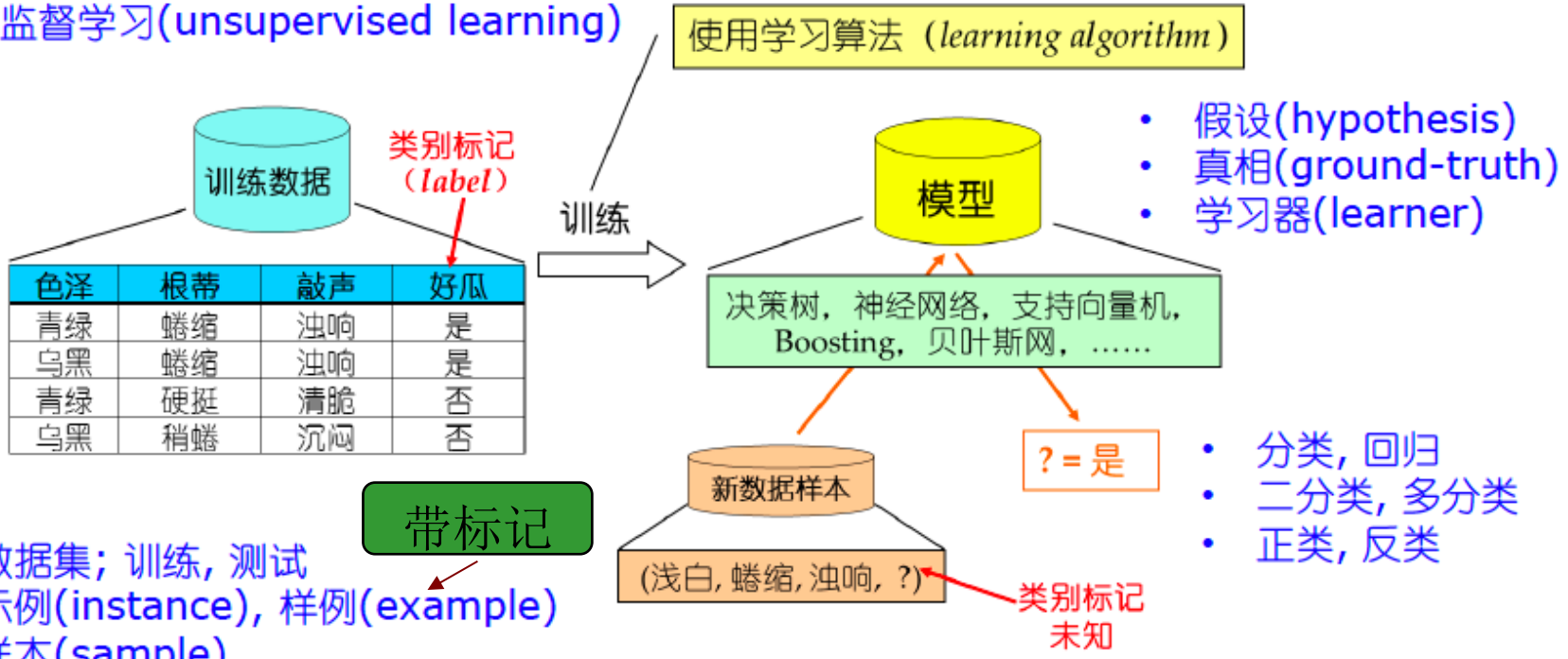
训练集

测试集

机器学习：面向未来的技术

基本术语

- 监督学习(supervised learning)
- 无监督学习(unsupervised learning)



- 假设(hypothesis)
- 真相(ground-truth)
- 学习器(learner)

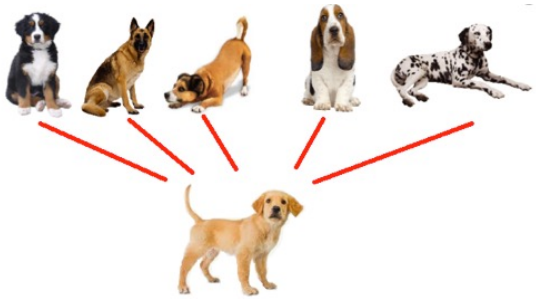
- 分类，回归
- 二分类，多分类
- 正类，反类

- 数据集；训练，测试
- 示例(instance)，样例(example)
- 样本(sample)
- 属性(attribute)，特征(feature)；属性值
- 属性空间，样本空间，输入空间
- 特征向量(feature vector)
- 标记空间，输出空间

- 未见样本(unseen instance)
- 未知“分布”
- 独立同分布(i.i.d.)
- 泛化**(generalization)**

学习的目标

机器学习技术的根本目标就是



模型具有泛化能力！

“简单理解”：应对未见样本的预测能力

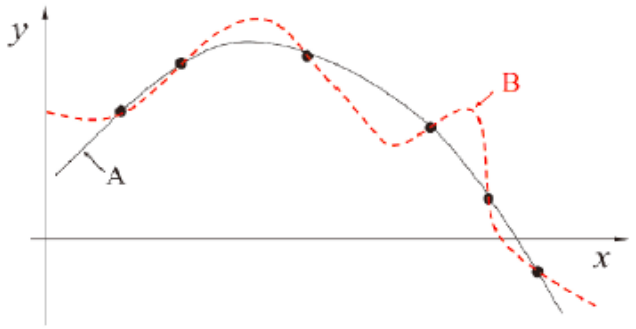
未来不可知，依靠“合理假设”，利用历史数据估计模型泛化能力

如：历史和未来数据来自于相同的分布
（I.I.D. 假设）

概念：归纳偏好（Inductive Bias）

“合理假设”不唯一，产生了模型的归纳偏好

机器学习算法在学习过程中对某种类型假设的偏好



A更好？
B更好？

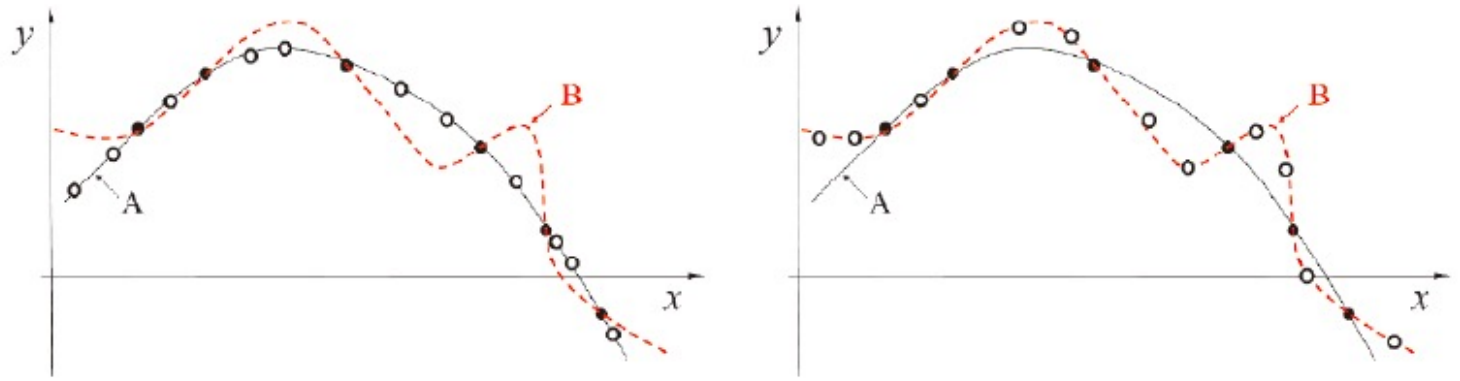
一般原则：
奥卡姆剃刀
(Ocam’s razor)

任何一个有效的机器学习算法必有其偏好

学习算法的归纳偏好是否与问题本身匹配，
大多数时候直接决定了算法能否取得好的性能！

“假设”好坏：No Free Lunch

没有免费的午餐！



(a) A 优于 B　　(b) B 优于 A

图 1.4　没有免费的午餐. (黑点: 训练样本; 白点: 测试样本)

NFL定理：一个算法 $\mathfrak{L}_a$ 若在某些问题上比另一个算法 $\mathfrak{L}_b$ 好，必存在另一些问题，$\mathfrak{L}_b$ 比 $\mathfrak{L}_a$ 好。

“假设”好坏：No Free Lunch

考虑二分类问题，且真实目标函数可以是任何函数 $\mathcal{X} \mapsto \{0,1\}$，函数空间为 $\{0,1\}^{|\mathcal{X}|}$. 对所有可能的 f 按均匀分布对误差求和，有

$$
\begin{aligned}
\sum_f E_{ote}(\mathfrak{L}_a|X,f) &= \sum_f \sum_h \sum_{\boldsymbol{x}\in\mathcal{X}-X} P(\boldsymbol{x})\ \mathbb{I}(h(\boldsymbol{x}) \neq f(\boldsymbol{x}))\ P(h \mid X, \mathfrak{L}_a) \\
&= \sum_{\boldsymbol{x}\in\mathcal{X}-X} P(\boldsymbol{x}) \sum_h P(h \mid X, \mathfrak{L}_a) \sum_f \mathbb{I}(h(\boldsymbol{x}) \neq f(\boldsymbol{x})) \\
&= \sum_{\boldsymbol{x}\in\mathcal{X}-X} P(\boldsymbol{x}) \sum_h P(h \mid X, \mathfrak{L}_a) \frac{1}{2} 2^{|\mathcal{X}|} \\
&= \frac{1}{2} 2^{|\mathcal{X}|} \sum_{\boldsymbol{x}\in\mathcal{X}-X} P(\boldsymbol{x}) \sum_h P(h \mid X, \mathfrak{L}_a) \\
&= 2^{|\mathcal{X}|-1} \sum_{\boldsymbol{x}\in\mathcal{X}-X} P(\boldsymbol{x}) \cdot 1\ .
\end{aligned}
$$

所有问题上的总误差与学习算法无关！

NFL定理的启示

NFL定理的重要前提：

所有“问题”出现的机会相同、或所有问题同等重要

实际情形并非如此；我们通常只关注自己正在试图解决的问题

脱离具体问题，空泛地谈论“什么学习算法更好”
毫无意义！

具体问题，具体分析！

另一种误区，在现实机器学习应用中…

把机器学习的“十八般兵器”都弄熟，
逐个试一遍，是不是就OK了？

NO！

“知己（算法）知彼（问题）”

1）熟悉各类算法的优势和局限

2）抓住问题的本质，主次轻重

3）适当变通，拿来就能用的情况不多