Bioinformatics
生物信息学

1. Introduction

Bioinformatics – Biological Big Data

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2015年9月14日

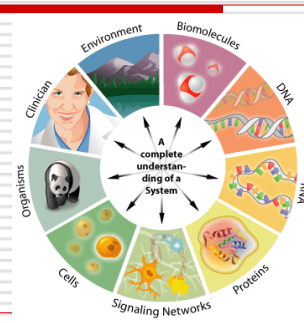
Question to you!

- What is Bioinformatics?
- How about bioinformatics research in ZJU, China and around the world?
- What are the current hot topics and future directions?
- How can you be a bioinformatian?

Puzzle for math & bio

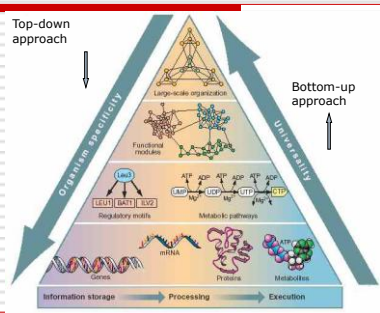
ScienceDaily (June 19, 2008)

The Wheel of Biological Understanding



http://www.cyberorissa.com/

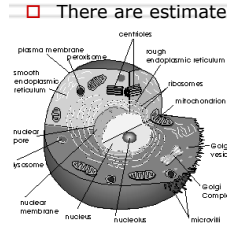
Two ways of looking a biological problem

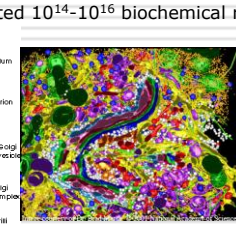


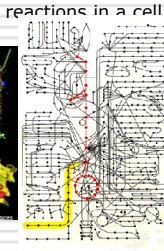
Life's Complexity Pyramid
(Oltvai-Barabasi, Science 10/25/

Biological Complexity

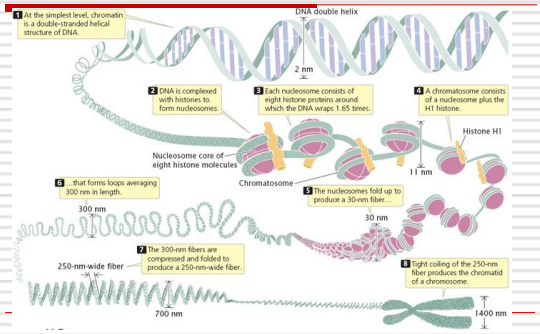
- In *Escherichia coli*, for instance, there are 225,000 proteins, 15,000 ribosomes, 170,000 tRNA-molecules, 15,000,000 small organic molecules and 25,000,000 ions inside the a few μm cell.
- There are estimated 10^{14}-10^{16} biochemical reactions in a cell





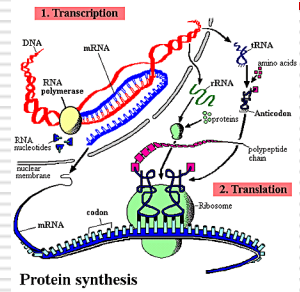


Eukaryotic Genome Complexity

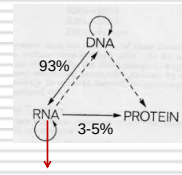


http://www.whfreeman.com/

中心法则



Francis Crick, 1958; *Nature* **227** , 1970

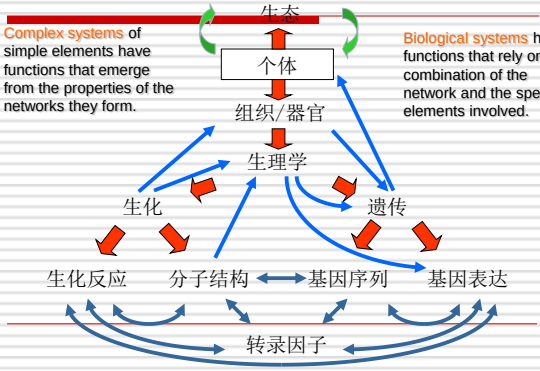


ncRNA (75% plants)

视频：life

Biological Systems

Complex systems of simple elements have functions that emerge from the properties of the networks they form.



Biological systems have functions that rely on a combination of the network and the specific elements involved.

Subdisciplines of biology

- *Biochemistry* 生物化学examines the rudimentary chemistry of life;
- *Molecular biology* 分子生物学studies the complex interactions of systems of biological molecules;
- *Cellular biology* 细胞生物学examines the basic building block of all life, the cell;
- *Physiology* 生理学examines the physical and chemical functions of the *tissues*, *organs*, and organ systems of an organism;
- and *Ecology* 生态学examines how various organisms interact and associate with their environment.

生物信息学大事记(一)

计算机科学	年份	生命科学
Blaise Pascal: mechanical calculators	1642	
Telegraph	1858	
	1859	Darwin's Origin of Species
	1865	Mendel's peas
	1869	DNA first isolated
Telephone	1876	
	1879	Mitosis observed
	1900	Rediscovery of Mendel's work
	1902	Orderly inheritance of disease observed Chromosome theory of heredity
	1909	The word gene coined
	1911	Fruit flies illuminate the chromosome theory
	1941	One gene, one enzyme
第一台电子管计算机ENIAC诞生	1943	x-ray diffraction of DNA
	1944	DNA is "transforming principle" Jumping genes
The first Computer Bug	1945	
Grace Murray Hopper: first compiler	1952	Genes are made of DNA
	1953	Francis Crick, James Watson和Maurice Wilkins发现DNA的双螺旋结构
	1955	第一个蛋白质序列(牛胰岛素)被测定
	1956	"生物学中的信息理论讨论会"于美国田纳西州的Gatlinburg召开

生物信息学大事记(二)

计算机科学	年份	生命科学
中国第一台电子管计算机研制成	1958	Edited by H. P. Yockey编辑的《生物学中的信息理论讨论会》出版
Telephone calls switched by computer, COBOL	1960	
Robert Berner: ASCII, computer mouse	1963	
Thomas Kurtz: BASIC	1964	
	1965	中国人工合成牛胰岛素结晶
	1968	First restriction enzymes described
Kenneth Thompson开发UNIX操作系统; Arpanet, Internet predecessor; the first computer hacker	1969	
Needleman-Wunsch序列比准算法	1970	
Ray Tomlinson wrote The first email program on Arpanet; the first personal computer	1971	
Dennis Ritchie发明C语言; NCSA developed Telnet	1972	First recombinant DNA
FTP	1973	First animal gene cloned
Bill Gates和Paul Allen成立微软; Bill Joy developed C shell (csh) and Vi text editor	1975	75-77:DNA sequencing
David Boggs invent Ethernet; Stephen Wozniak et al found Apple Computer.	1976	First genomic engineering company
Ward Christensen started The first computerized bulletin board system (CBBS). TCP split into TCP and IP	1978	
Usenet born; Brian Kernighan published C program language. Apple Computer introduced Apple II+	1979	
First computer virus. DNS is conceived by David Mills; Smith-Waterman序列比准算法; MS-DOS	1981	中国实现酵母丙氨酸转移核糖核酸的人工合成

生物信息学大事记(三)

计算机科学	年份	生命科学
Andreas von Bechtolsheim etal found Sun Microsystems; GNU by Richard Stallman; SMTP is published	1982	
Korn shell (ksh) relased by David Korn	1983	
The X window system is released by Robert W. Scheiffler; Apple introduce macintosh System 1.0	1984	
Bjarne Stroustrup创建C++语言; Apple introduce macintosh System 2.0 视窗微软问世 windows 1.0	1985	Kary Mullis创立PCR技术; 生物信息学专业期刊(CABIOS)创刊; 德国生物信息学会议(GCB)举行;
Apple introduce macintosh System 3.0	1986	日本核酸序列数据库DDBJ诞生; 蛋白质数据库SWISS-PROT建立; 中国开始实施高技术研究发展的"8.6.3计划"
Larry Wall推出Perl语言 Apple introduce macintosh System 4.0; Windows 2.0	1987	
Compact Disk Recordable (CD-R); Pearson实现FASTA程序 Apple introduce macintosh System 6.0	1988	美国国家生物技术信息中心（NCBI）成立;
MPEG audio Layer III (MP3) patent; the JPEG standard is adopted; Tim Berners-Lee, WWW protocol	1989	
Altschul实现BLAST程序; HTTP 1.0 标准发布; Arpanet ceases to exist (INTERNET). Archie by Alan Emtage created.	1990	国际人类基因组计划(HGP)启动; 第一届国际电脉、超级计算和人类基因组会议在美国佛罗里达州会议中心举行;
Gopher by Paul Lindner. Python by Guido van Rossum; Tim Berners-Lee announce the WWW project; Linus Torvalds releases Linux versions 0.01; Sun Microsystems release Solaris1.0 Apple introduce macintosh System 7.0	1991	
Mosaic web browser 1.0 released. CERN announced WWW would be free to anyone. Microsoft windows NT3.1;FreeBSD version 1.0 released	1993	欧洲生物信息学研究所（EBI）获准成立; 第一届ISMB国际会议美国国家医学图书馆(NLM)举行; HGP新5年计划;中国开始参与人类基因组计划

生物信息学大事记(四)

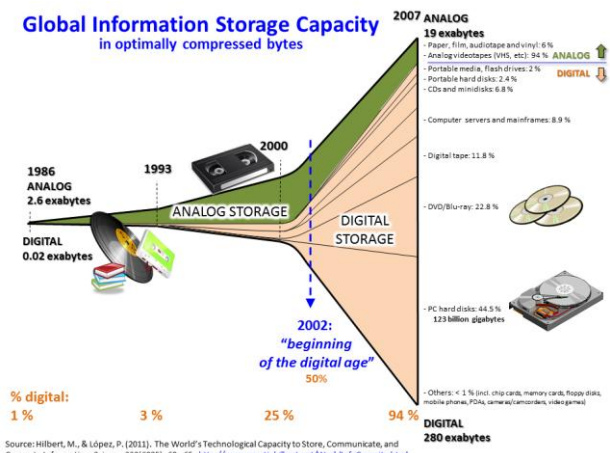
计算机科学	年份	生命科学
[illegible]	1994	Marc Wilkins提出蛋白质组(Proteome)的概念; 加拿大基因组计划
Opera web browser released. David Filo and Jerry Yang start their guide, later yahoo.com First spam messages is posted. Netscape web browser released. Linux kernel 1.0 The first alpha version of Ruby relased by Yukihiro Matsumoto		
Sun launches Java. Apache web server 0.6.2 released Jata Vlonen announces the SSH Internet explorer 1.0 released Microsoft rease Windows 95	1995	人类基因组物理图谱完成 日本信息生物学中心（CIB）成立
Larry Page and Sergey Brin, search engine BackRub, later Google. POP3 is published. W3C推出XML工作草案. Microsoft release windows NT4.0 Linux kernel 2.0; OpenBSD2.0	1996	Affymetrix生产商用DNA芯片 北京大学蛋白质工程和植物遗传学工程国家实验室加入欧洲分子生物学网络（EMBnet）
DVD format released Mac OS 8 released	1997	大肠杆菌基因组完成 北京大学生物信息学中心(CBI)成立; 中国科学院召开"DNA芯片的现状与未来"和"生物信息学"香山会议
CIH virus by Chen Ing-Hou, first known virus to target the flash BIOS Windows 98	1998	亚太生物信息学网络（APBioNet）成立; 瑞士生物信息学研究所（SIB）成立; 美国Celera遗传公司成立; 线虫基因组完成; CABIOS期刊更名为bioinformatics 中国人类基因组研究北方中心（北京）和南方中心（上海）成立 线虫基因组完成
Apple introduce Mac OS 9 and Mac OS X Server Linux kernel 2.2	1999	人类22号染色体序列完成 中国获准加入人类基因组计划，成为第六个国际人类基因组计划参与国

生物信息学大事记(五)

计算机科学	年份	生命科学
Windows 2000	2000	德、日等国科学家宣布基本完成人体第21对染色体的测序工作 果蝇基因组完成 中国科学院上海生命科学研究院生物信息中心(SIBI)成立
Windows XP Linux kernel 2.4	2001	美、日、德、法、英、中6国科学家和美国Celera公司联合公布人类基因组图谱及初步分析结果 首届全国生物信息学会议(CCB)举行; 中国完成籼稻基因组工作框架图
	2002	老鼠基因组完成
Windows Server 2003, Sony Blu-Ray DVD, DragonFly BSD project announced, Linux kernel 2.6	2003	HGP完成
IBM's Blue gene/L super computer, Internet speed record broken 7.57gb/s, Pioneer announce optical drives to store 500GB of data, Optical network speed record broken 101gb/s	2004	Proteomics: Decoding the Genome NGS
	2005	黑猩猩、狗基因组测序完成 中德计算生物所成立
	2006	Paleogenomics: digging out fossil DNA PiRNA
谷歌和IBM 合作推动云计算	2007	Human Genetic Variation
英特尔发布酷睿i7 处理器	2008	千人基因组测序计划启动; 拟南芥1001株系测序启动
我国"天河一号"超级计算机以每秒2.57.0万亿次	2010	外显子测序

作业1

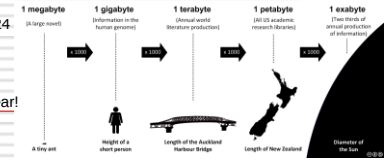
- Key development in the past 5 years
  - Biology
  - Computer science
  - Information technology

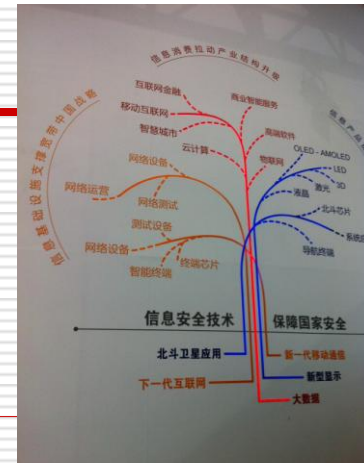


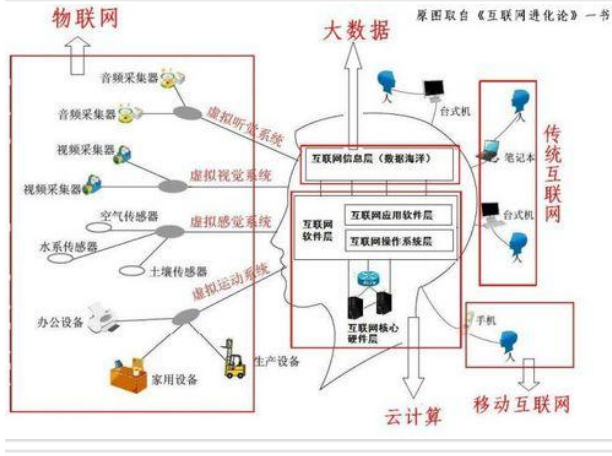
Source: Hilbert, M., & López, P. (2011). The World's Technological Capacity to Store, Communicate, and Compute Information. *Science*, 332(6025), 60 –65. http://www.martinhilbert.net/WorldInfoCapacity.html

- Byte字节数
- Kilobyte (KB) 10^3 =
- Megabyte (MB) 10^6
- Gigabyte (GB) 10^9 =
- Terabyte (TB) 10^{12} =
- Petabyte (PB) 10^{15} =
- Exabyte (EB) 10^{18} $=2^{60}$ 人类文明开始至2003年：5ET
- Zettabyte (ZB) 10^{21}
- Yottabyte (YB) 10^{24}

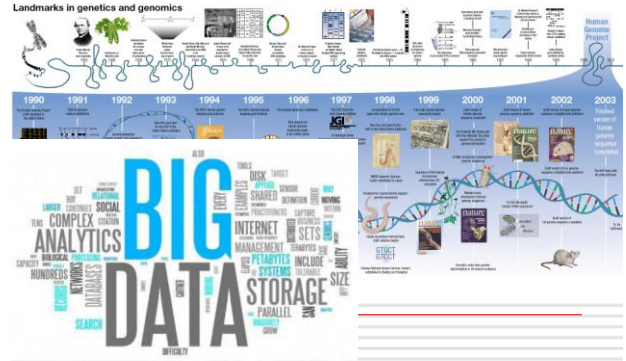
EBI stores 20 petabytes
CERN generates 15 PB every year!



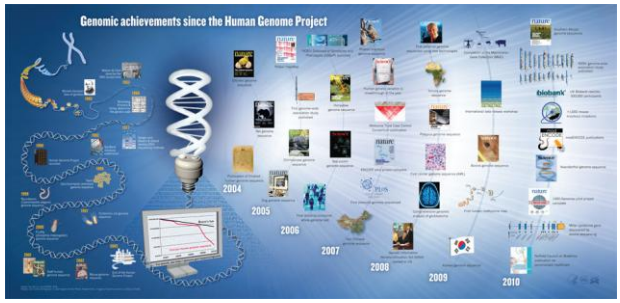




Genetics & Genomics

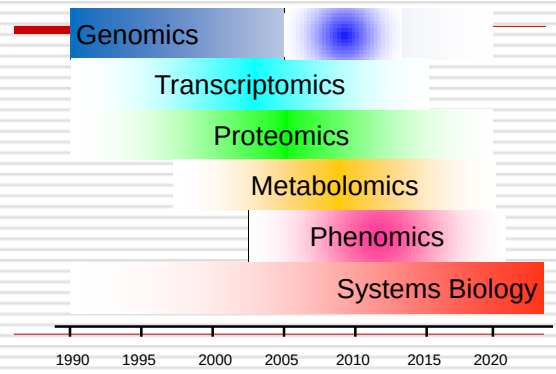


Genomic achievements since HGP



Nature 2011, 470: 204–213

Omics to Systems Biology



新一代基因测序仪和功能基因组学

Ion Proton　NextSeq 500　HiSeq 2500　MiSeq　Ion PGM

新一代测序平台的出现为**转录组**和**基因组**测序提供了非常好的机遇，不论是在测序价格上还是在精度上都具有很高的可选择性。

比如，通过对作物在冷驯化或干旱适应或盐胁迫等逆境条件下的不同阶段上进行转录组测序，从而更好全面的检测作物在转录组水平上是如何应对极端环境。

illumina®

HiSeq X Ten

- cost **$10 millions**
- 125 bp read length
- $1000 per genome

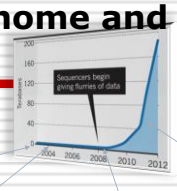
Oxford NANOPORE Technologies

MinION

- cost $900
- **80 kb** read length

Personal Genome and data

Every 10-12 month:
- **Data doubled**
- **Seq cost half**

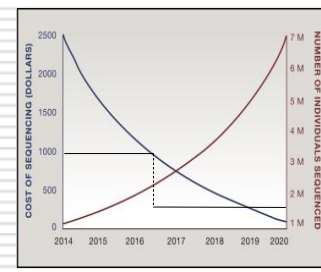


20 Billion $ (2001) 1 Billion $ /(2004) 1 Million $ (2008) 0.1 Million $ (2011

Mapping 24K genes (1990-2001)　Mapping 10-15M SNPs (2002-2008)　Sequencing the personal (2008)　Personal Genome Project (2011)

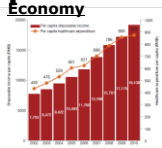
￥200/exome (2020)?

End of 2020, 90Million Chinese to be genome sequenced!

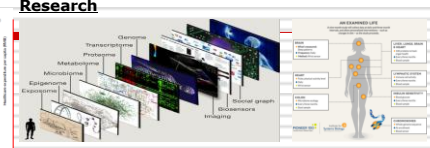


Biomedical big data for personalized medicine

Economy



Research



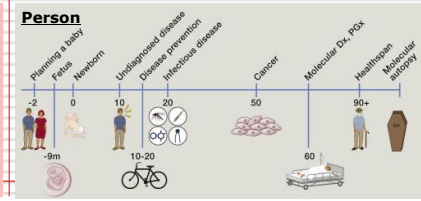
Year 2020

In China, Heathcare 2000yuan/person

Biomedical data ~EB（=1000PB）

Personal genomic sequencing

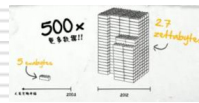
Person

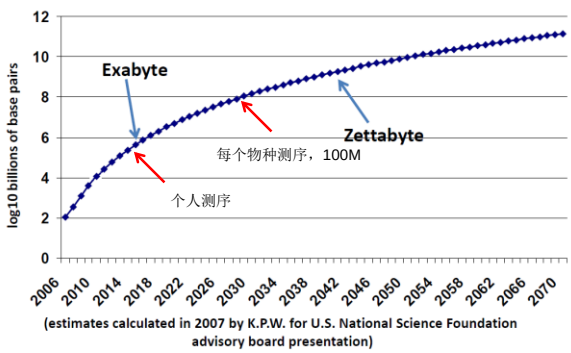


二代测序仪器的世界分布图

中国地区已经成为继北美和欧洲之后的**第3大**二代测序仪器设备拥有区，图中标注的数字为二代测序仪器数目，其中可以看出中国的二代测序仪器主要分布在深圳、北京和上海地区。

全球测序项目能力预测





基因组大数据商业化前景

解决基因组医学的商业应用瓶颈问题

传统医学：回顾式、经验性、封闭式、不确定性

The Problem of Big Data in Biology

A decade's progress

2003:
ABI 3730 Sequencer

Human Genome:
$2.7 Billion, 13 Years

2012:
Oxford Nanopore
MinION

Human Genome:
$900, 6 Hours

The Problem of Big Data in Biology

The New York Times **Business Day**

DNA Sequencing Caught in Deluge of Data

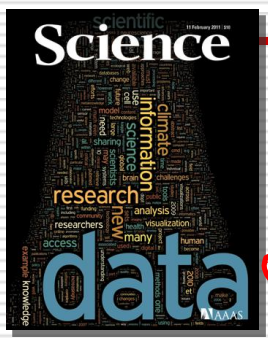
W. Richard McCombie, a professor of human genetics at the Cold Spring Harbor Laboratory, examining DNA samples.

By ANDREW POLLACK
Published: November 30, 2011

"BGI, based in China, is the world's largest genomics research institute, with 167 DNA sequencers producing the equivalent of 2,000 human genomes a day.

BGI churns out so much data that it often cannot transmit its results to clients or collaborators over the Internet or other communications lines because that would take weeks. Instead, it **sends computer disks** containing the data, via FedEx."

The Problem of Big Data in Biology



一个价值$1,000的基因组需要花费$100,000来解释？

生物学面临的大数据挑战

- 自人类基因组计划完成以来，以美国为代表，世界主要发达国家纷纷启动了生命科学基础研究计划，如国际千人基因组计划、DNA百科全书计划、英国十万人基因组计划等。这些计划引领生物数据呈爆炸式增长，目前每年全球产生的生物数据总量已达EB级，生命科学领域正在爆发一次数据革命，生命科学某种程度上已经成为大数据科学。

NIH Big Data to Knowledge (BD2K)

英国医学研究理事会（MRC）
“医学生物信息学计划”

生物信息学

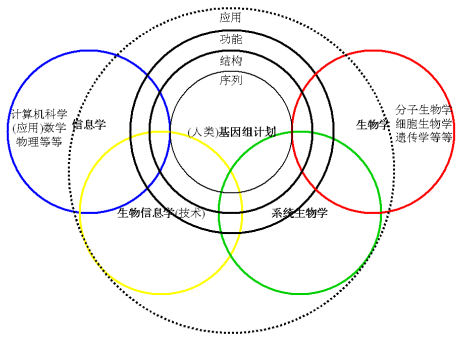
Biology + Informatics = Bioinformatics

But

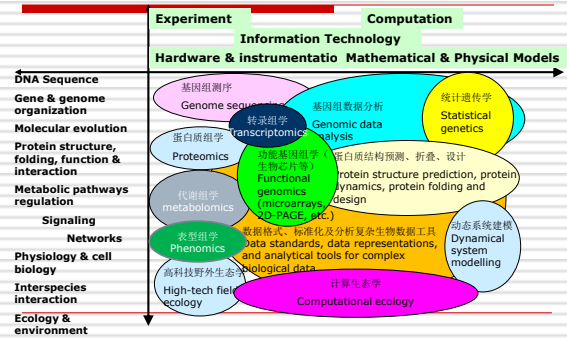
1 + 1 =/= 2

生物信息学是生物科学与信息科学的交叉学科，是利用计算机科学（信息学）的技术手段来研究生物学的数据，如对生物数据进行获取(retrival)，存储(storage)，传输(transfer)，计算(manuipulation)，分析(analysis)，模拟(simulation)，预测(prediction)等等的一门新兴学科，是21世纪科学发展的热点之一。

Biology, Bioinformatics, Systems Biology



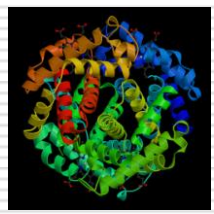
Bioinformatics

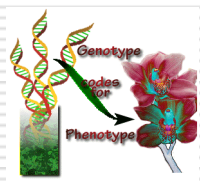


陈铭：整合生物信息学（2006）

Post-genomic era

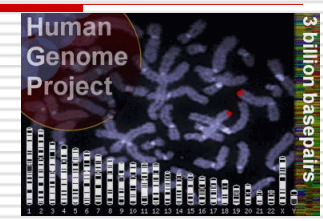
- Sequence → Structure → Function





研究对象

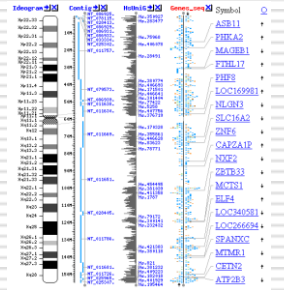
- *Molecular & Cellular Biology分子与细胞生物学*
- *BioPhysics生物物理学*
- *Brain&NeuroSci脑和神经科学*
- *Medicine&Pharmaceutics医药学*
- *Agriculture农牧渔林学*
- *Molecular&Ecological Evolution分子和生态进化*
- …



陈铭，后基因组时代的生物信息学，《*生物信息学*》，2004

研究内容

- Database数据库建设
- Data Mining & Integration数据库整合和数据挖掘
- Sequence Analysis序列分析
- Structural Analysis & Functional Prediction结构分析与功能预测
- Large Scale Expressional Profile Analysis大规模功能表达谱的分析
- Modeling and Simulation of BioPathways代谢网络建模分析
  - Reconstruction预测调控网络
  - Network Analysis网络普遍性分析
  - Modeling模型分析
- Program Development程序开发
- Commercialization商业化



陈铭，后基因组时代的生物信息学，《*生物信息学*》，2004

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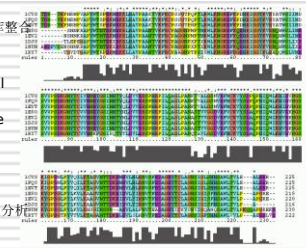

陈铭，后基因组时代的生物信息学，《*生物信息学*》，2004

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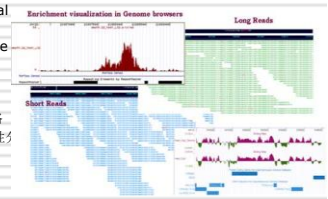

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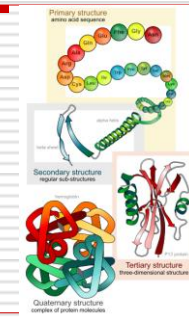

陈铭，后基因组时代的生物信息学，《*生物信息学*》，2004

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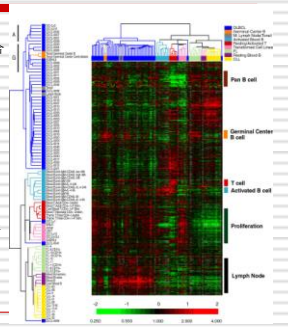

陈铭，后基因组时代的生物信息学，《*生物信息学*》，2004

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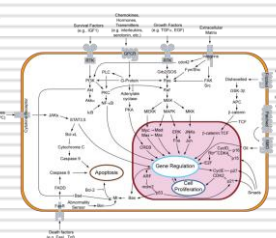
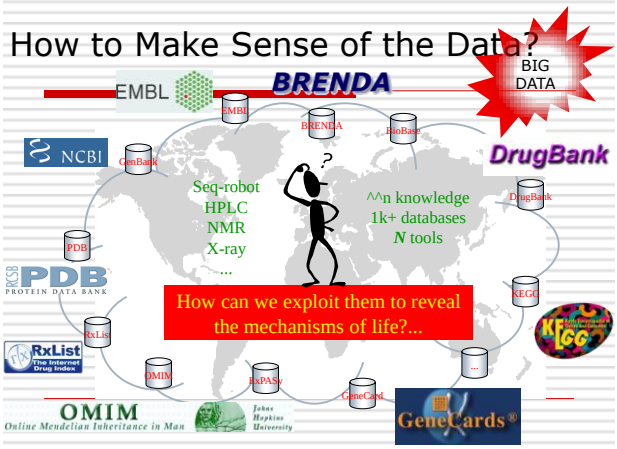
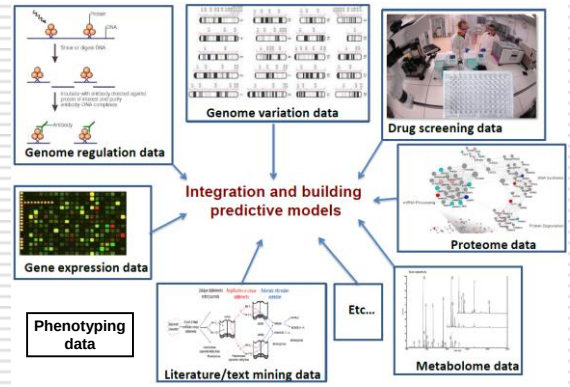


陈铭，后基因组时代的生物信息学，《*生物信息学*》，2004

How to Make Sense of the Data?



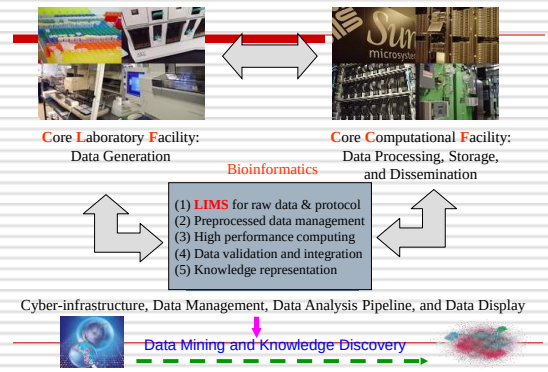
整合生物学



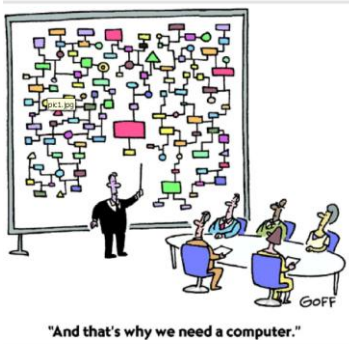
整合生物信息学

1. 整合生物信息学的研究领域
2. 生物数据挖掘与整合
3. 生命科学与生信技术的整合
4. 学科、人才的整合

陈铭，整合生物信息学，《*计算机教育*》，2006

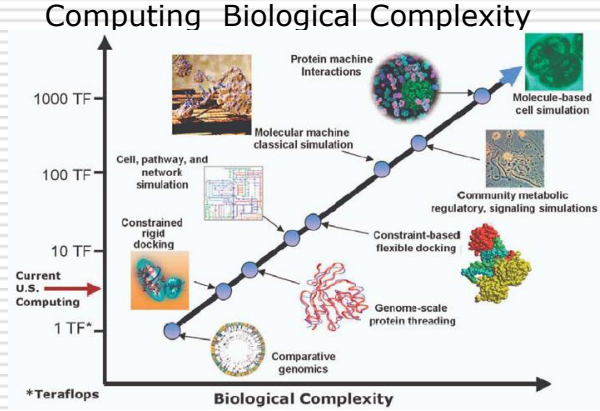


高通量数据分析对实验室的挑战

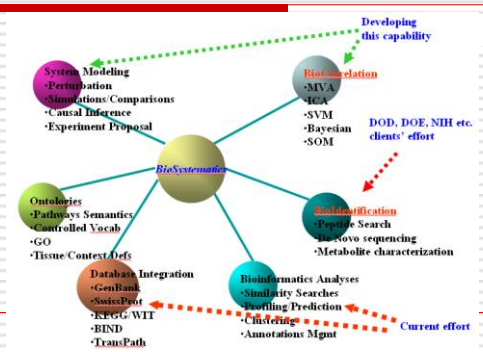


- 数据管理
- 数据解读
- 分析策略设计
- 分析方法选择
- 需要编程序？
- 键盘上的Linux

Computing Biological Complexity



Current Subfields in Computational Systems Biology



10 Useful Bioinformatics Skills to Have

- Bioinformatics is a highly specialized, technical field. You need a background in both biology and in information management, as well as specialized skills specific to the field of bioinformatics. Here are ten of those skills that it's good to have.

10 Useful Bioinformatics Skills to Have

1. Good communications skills. As a bioinformatics specialist, you will be communicating complex data to people with a variety of backgrounds. It's very much like being a translator. You have to know the languages involved, and you have to be an expert communicator in order to help people understand each other.

10 Useful Bioinformatics Skills to Have

2. Good teamwork skills. Bioinformatics is not for lone rangers. Researchers can sometimes work independently, but bioinformatics is about information and communication. You will be working on a team with people who have diverse backgrounds and differing areas of expertise. Good teamwork skills are essential.

10 Useful Bioinformatics Skills to Have

3. The ability to multitask. You will need to be able to handle several complex tasks at a time. This can be a high pressure job with deadlines that have to be met. The ability to multitask will help you manage your job with less stress.

10 Useful Bioinformatics Skills to Have

4. Flexibility. You may be moved from one project to another as your skills are needed. You may have to put aside a project you are working on to help someone with an urgent request. You may need to stop what you are doing and explain a computer model to a scientist. Flexibility is a key skill to have in bioinformatics.

10 Useful Bioinformatics Skills to Have

5. A working knowledge of biology and its applications. You don't have to be an expert in biology, but you do need to know what kind of information you are working with. It is especially useful to know about molecular biology and genetics and to understand recent genetic research.

10 Useful Bioinformatics Skills to Have

6. Proficiency in computer languages. You need to know basic programming languages like JAVA and HTML, SQL and PERL. Most bioinformatics programming utilizes PERL.

10 Useful Bioinformatics Skills to Have

7. Skill in data mining. Being able to extract data from multiple resources is invaluable.

10 Useful Bioinformatics Skills to Have

8. Good data visualization skills. You'll need to be able to take complex data and interpret it into models and other ways that make it understandable for biologists and other team members.

10 Useful Bioinformatics Skills to Have

9. Experience with bioinformatics tools, such as Blast, BLAT, sequence analysis algorithms and clustering tools.

10 Useful Bioinformatics Skills to Have

10. Experience in using bioinformatics resources, such as the UCSC genome browser and Entrez. You'll need to be familiar with the National Center for Bioinformatics (NCBI) and the database and analysis tools available on their website.

Bio-programming

- Computer
- Internet
- Web programing: HTML, XHTML, XML, SVG, XSL/XSLT, XQL, Java Script, CSS, Apache, IIS, CGI, asp, php, etc.
- Perl, Java, C++, Python, SQL, mySQL, etc.
- Open Source
- ~~Bioperl, Biojava, BioC++…~~

Keywords

- Database
- Web-based
- Parallel/grid/cloud computing
- Image analysis
- modeling
- Artificial intelligence
- Data mining
- ……

Data Mining

- 用得比较多的数据挖掘的技术方法：机器学习（归纳逻辑程序（Inductive Logic Programming），遗传算法（Genetic Algorithm），神经网络（Neural Network），统计方法（Statistical Methods），贝叶斯方法（Bayesian Methods），决策树（Decision Tree）和隐马尔可夫模型（Hidden Markov Model）等等 ），文本挖掘 ，网络挖掘

陈铭,生物信息学,2007

现状

- 美国
- 欧盟
  - 德国
  - 英国
  - 其他
- 日本
- 中国
- 俄罗斯等

- International Conference on Intelligent Systems for Molecular Biology (ISMB)
- European Conference on Computational Biology (ECCB)
- International Conference on Research in Computational Molecular Biology (RECOMB)
- Workshop on Algorithms in Bioinformatics (WABI)
- Pacific Symposium on Biocomputing (PSB)
- International Conference on Systems Biology (ICSB)
- Integrative Bioinformatics Workshop

现状?

- CBI:the Centre of BioInformatics at Peking University，罗静初
- BioSino:中国科学院上海生命科学研究院生物信息中心，陈诺南、李亦学
- BGI: 华大基因，杨焕明

生物信息学专业

- **浙江大学** 、北京大学、中国农业大学、南开大学、南京大学、中国科学技术大学、山东大学、中国科学院研究生院、清华大学、国防科学技术大学、上海交通大学、华中科技大学、南京林业大学、中南大学、中国药科大学

- 复旦大学、中山大学、云南大学、四川大学、东北大学、东南大学、暨南大学、重庆医科大学
- 北京师范大学、第三军医大学
- 吉林大学、上海大学、南京农业大学、西北农林科技大学、军事医学科学院

培养目标

- 本专业培养具有生物信息学基础理论、基本知识和科研技能，能在有关研究单位、高校或企事业单位从事生物信息学领域的科研、开发或教学工作的高级科学技术人才，并为生命科学、计算机科学等相关交叉学科输送研究生后备力量。

专业知识与能力

- 本专业（理学学士）学生的培养，重在双语教学，强化数学和计算机的基础，拓宽知识面，扎实现代生命科学基本知识的基础上，对学生进行生物信息学、生物学数据库技术、基因组学、蛋白质组学、分子遗传与进化、系统生物学和基因芯片数据分析等方面的基础理论、基础知识和基本科研技能的专业培养与训练。

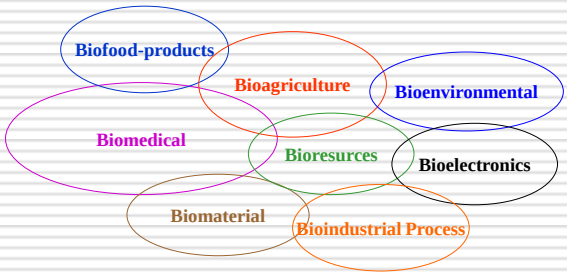
专业课程

- 生物化学、分子生物学、Linux应用技术基础、计算机网络应用技术、生物信息学、生物学数据库及实验、序列与基因组分析、蛋白质组学分析、系统生物学、生物芯片原理及数据分析等
- 分子遗传与分子进化、生物数据挖掘与知识发现、计算生物学导论、计算机辅助药物设计、生物代谢网络建模等

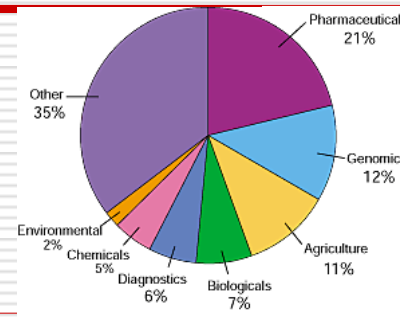
毕业情况

- 本专业具有良好的教学、科研与商业就业前景，80%以上的毕业生将继续读研或出国深造；
- 其余毕业生可在生物信息及其相关领域的科研机构和大专院校从事研究、开发、教学和管理工作。

Potential Biotech Industries

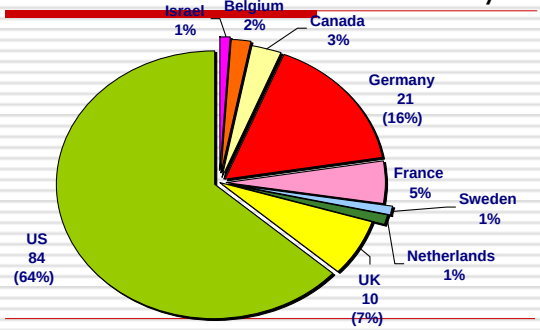


The changing marketplace of bioinformatics

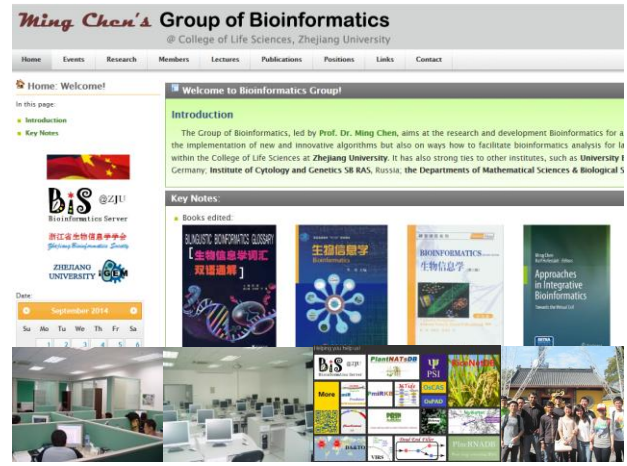


Nature Biotechnology 18, 1247 - 1249 (2000)

Global Bioinformatics Industry



Source: Genome Technology, 2001.02.01



Practice

- Quiz (10%)
- Exam (60%)
- Homepage (30%)
  - Apache httpd server
  - HTML
  - Sequence analysis