



BIMM 143

Introduction to Bioinformatics

Barry Grant
UC San Diego

<http://thegrantlab.org/bimm143>

HELLO
my name is

BARRY

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HELLO
HER my name is

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Office Hours:
[SignUp](#)

Location:
Muir #3266

Introduce Yourself!

Your preferred name,
Place you identify with,
Major area of study/research,
Favorite joke (optional)!

Today's Menu

Course Logistics

Website, screencasts, survey, ethics, assessment and grading.

Learning Objectives

What you need to learn to succeed in this course.

Course Structure

Major lecture topics and specific learning goals.

Introduction to Bioinformatics

Introducing the *what, why and how* of bioinformatics?

Bioinformatics Database

Hands-on exploration of several major databases and their associated tools.

<http://thegrantlab.org/bimm143/>

The screenshot shows a web browser window with the URL http://bioboot.github.io/bimm143_W18/ in the address bar. The page content is as follows:

UC San Diego
BIMM 143
A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

Course Director
Prof. Barry J. Grant (Email: bjgrant@ucsd.edu)

Instructional Assistant
Alexander Sharp (Email: arsharp@ucsd.edu)

Course Syllabus
[Winter 2018 \(PDF\)](#)

Overview
Bioinformatics - the application of computational and analytical methods to biological problems - is a rapidly maturing field that is driving the collection, analysis, and interpretation of the avalanche of data in modern life sciences and medical research.
This upper division 4-unit course is designed for biology majors and provides an introduction to the principles and practical approaches of bioinformatics as applied to genes and proteins.
An integrated lecture/lab structure with hands-on exercises and small-scale projects emphasizes modern developments in genomics and proteomics. A detailed listing of

Twitter icon | GitHub icon | Email icon | RSS icon

<http://thegrantlab.org/bimm143/>

Screenshot of the BIMM 143 Winter 2018 website.

The page title is "Bioinformatics (BIMM 143, Winter 2018)".

The course director is Prof. Barry J. Grant (Email: bjgrant@ucsd.edu)

The instructional assistant is Alexander Sharp (Email: arsharp@ucsd.edu)

The course syllabus is available as a [Winter 2018 \(PDF\)](#).

Overview: Bioinformatics - the application of computational and analytical methods to biological problems - is a rapidly maturing field that is driving the collection, analysis, and interpretation of the avalanche of data in modern life sciences and medical research.

Learning Goals: This upper division 4-unit course is designed for biology majors and provides an introduction to the principles and practical approaches of bioinformatics as applied to genes and proteins.

Assignments & Grading: An integrated lecture/lab structure with hands-on exercises and small-scale projects emphasizes modern developments in genomics and proteomics. A detailed listing of assignments and grading criteria will be provided.

Ethics Code:

Navigation: The sidebar includes links to Home, Gmail, Google, Bitbucket, GitHub, News, Disqus, BGGN-213, BIMM-143, and Google Docs. Social media icons for Twitter, GitHub, LinkedIn, and RSS feed are also present.

What essential concepts and skills should YOU attain from this course?

The screenshot shows a web browser window with the URL `blobboot.github.io/bimm143_W18/goals/` in the address bar. The page content is as follows:

UCSanDiego

BIMM 143

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

[Overview](#)

[Lectures](#)

[Computer Setup](#)

[Learning Goals](#) (This link is highlighted with a red box)

[Assignments & Grading](#)

[Ethics Code](#)

Learning Goals

At the end of this course students will:

- Understand the increasing necessity for computation in modern life sciences research.
- Be able to use and evaluate online bioinformatics resources including major biomolecular and genomic databases, search and analysis tools, genome browsers, structure viewers, and select quality control and analysis tools to solve problems in the biological sciences.
- Be able to use the R environment to analyze bioinformatics data at scale.
- Understand the process by which genomes are currently sequenced and the bioinformatics processing and analysis required for their interpretation.
- Be familiar with the research objectives of the bioinformatics related sub-disciplines of Genomics, Transcriptomics and Structural bioinformatics.

In short, students will develop a solid foundational knowledge of bioinformatics and be able to evaluate new biomolecular and genomic information using existing bioinformatic tools and resources.

Specific Learning Goals

At the end of this course students will:

- Understand the increasing necessity for computation in modern life sciences research.
- Be able to use and evaluate online bioinformatics resources and analysis tools to solve problems in the biological sciences.
- Be able to use the R environment to analyze bioinformatics data at scale.
- Be familiar with the research objectives of the bioinformatics related sub-disciplines of Genome informatics, Transcriptomics and Structural informatics.

In short, you will develop a solid foundational knowledge of **bioinformatics** and be able to evaluate new biomolecular and genomic information using **existing bioinformatic tools and resources.**

Specific Learning Goals....

What I want you to know by course end!

The screenshot shows a web browser window with the URL bioboot.github.io/bimm143_W18/goals/. The page title is "Specific Learning Goals". The main content area contains a paragraph about teaching goals and a list of learning objectives with their corresponding lecture numbers. The "Learning Goals" link in the sidebar is highlighted with a red box.

Specific Learning Goals

Teaching toward the specific learning goals below is expected to occupy 60%-70% of class time. The remaining course content is at the discretion of the instructor with student body input. This includes student selected topics for peer presentation, as well as one student selected guest lecture from an industry based genomic scientist.

All students who receive a passing grade should be able to:

	Lecture(s):
1 Appreciate and describe in general terms the role of computation in hypothesis-driven discovery processes within the life sciences.	1, 2, 20
2 Be able to query, search, compare and contrast the data contained in major bioinformatics databases and describe how these databases intersect (GenBank, GENE, UniProt, PFAM, OMIM, PDB, UCSC, ENSEMBLE).	2, 12, 13
3 Describe how nucleotide and protein sequence and structure data are represented (FASTA, FASTQ, GenBank, UniProt, PDB).	3, 10
4 Be able to describe how dynamic programming works for pairwise sequence alignment and appreciate the differences between global and local alignment along with their major application areas.	4, 5
5 Calculate the alignment score between two nucleotide or protein sequences using a provided scoring matrix and be able to perform BLAST, PSI-BLAST, HMMER and protein structure based database	5, 10

BIMM 143

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

[Overview](#)

[Lectures](#)

[Computer Setup](#)

[Learning Goals](#)

[Assignments & Grading](#)

[Ethics Code](#)

Course Structure

Derived from specific learning goals

The screenshot shows a web browser window with the following details:

- Title Bar:** Shows the URL `bloboot.github.io/bimm143_W18/lectures/` and various browser icons.
- Header:** BIMM 143 Home Gmail Goal Bitbucket GitHub News Discus EGNN-213 BIMM-143 GDocs
- Left Sidebar (UCSD BIMM 143):**
 - UCSanDiego** logo
 - BIMM 143**
 - A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.
 - Navigation links: Overview, Lectures (highlighted with a red box), Computer Setup, Learning Goals, Assignments & Grading, Ethics Code.
- Main Content (Lectures):**

Lectures

All Lectures are Tu/Th 9:00-12:00 pm in Warren Lecture Hall 2015 (WLH 2015) ([Map](#)). Clicking on the class topics below will take you to corresponding lecture notes, homework assignments, pre-class video screen-casts and required reading material.

#	Date	Topics for Winter 2018
1	Tu, 01/09	Welcome to Bioinformatics Course introduction, Learning goals & expectations, Biology is an information science, History of Bioinformatics, Types of data, Application areas and introduction to upcoming course segments, Student computer setup
2	Th, 01/11	Bioinformatics databases and key online resources NCBI & EBI resources for the molecular domain of bioinformatics, Focus on GenBank, UniProt, Entrez and Gene Ontology. Hands on with BLAST, GenBank, OMIM, GENE, UniProt, Muscle, PFAM and PDB bioinformatics tools and databases
3	Tu,	Sequence alignment fundamentals, algorithms and applications Homology, Sequence similarity, Local and global alignment, classic

Course Structure

Derived from specific learning goals

The screenshot shows a web browser window with the URL blobboet.github.io/bimm143_W18/lectures/. The page title is "Lectures".
The sidebar on the left has links: UC San Diego, BIMM 143, Overview, Lectures (highlighted with a red box), Computer Setup, Learning Goals, Assignments & Grading, and Ethics Code.
The main content area displays a table of lectures:

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3	Tu,	Sequence alignment fundamentals, algorithms and applications Homology, Sequence similarity, Local and global alignment, classic

Class Details

Goals, Class material, Screencasts & Homework

The screenshot shows a web browser window with the URL blobstore.github.io/bimm143_W16/lectures/l1 in the address bar. The page content is as follows:

UCSanDiego

BIMM 143

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

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1: Welcome to Foundations of Bioinformatics

Topics:

Course introduction, Learning goals & expectations, Biology is an information science, History of Bioinformatics, Types of data, Application areas and introduction to upcoming course segments, Student 30-second introductions, Student computer setup.

Goals:

- Understand course scope, expectations, logistics and [ethics code](#).
- Understand the increasing necessity for computation in modern life sciences research.
- Get introduced to how bioinformatics is practiced.
- Complete the [pre-course questionnaire](#).
- Setup your [laptop computer](#) for this course.

Material:

- Pre class screen casts (also see below):
 - SC1: [Welcome to BIMM-143](#),
 - SC2: [What is Bioinformatics?](#) and
 - SC3: [How do we do Bioinformatics?](#).
- Lecture Slides: [Large PDF](#), [Small PDF](#)
- [Handout: Class Syllabus](#)

Homework

Goals, Class material, Screencasts & Homework

The screenshot shows a web browser window with the URL blobbo洽github.io/bimmm143_W16/lectures/M1. The page content includes:

- UC San Diego** logo
- BIMM 143** title
- A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.
- Overview**, **Lectures**, **Computer Setup**, **Learning Goals**, **Assignments & Grading**, and **Ethics Code** navigation links.
- Homework:**
 - [Questions](#)
 - Readings:**
 - [PDF1: What is bioinformatics? An introduction and overview](#)
 - [PDF2: Advancements and Challenges in Computational Biology](#)
 - [Other: For Big-Data Scientists, 'Janitor Work' Is Key Hurdle to Insights](#) New York Times, 2014.
- Screen Casts:**

Welcome to "Foundations of Bioinformatics" (BGGN-213)

The video player displays a thumbnail of a man speaking in front of a colorful molecular model. The video controls show a play button, volume, time (2:05 / 4:06), and other standard video controls. The URL <http://thegrantlab.org/bggn213> is visible at the bottom of the video frame.

1 Welcome to BIMM-143: Course introduction and logistics.

Homework

Goals, Class material, Screencasts & Homework

The screenshot shows a web browser window with the URL blobbo洽github.io/b-mm143_W16/lectures/M1. The page content includes:

- Homework:**
 - Questions
 - Readings:
 - PDF1: [What is bioinformatics? An introduction and overview](#)
 - PDF2: [Advancements and Challenges in Computational Biology](#)
 - Other: [For Big-Data Scientists, 'Janitor Work' Is Key Hurdle to Insights](#) New York Times, 2014.
- Screen Casts:**
 -

On the left side of the browser window, there is a sidebar for the course BIMM 143, UC San Diego, featuring:

- UCSanDiego logo
- BIMM 143
- A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD
- Overview
- Lectures
- Computer Setup
- Learning Goals
- Assignments & Grading
- Ethics Code

Homework

Goals, Class material, Screencasts & **Homework**

The screenshot shows a Google Forms survey titled "BIMM143 Lecture 1 Homework (W18)". The survey begins with a question asking students to answer the following questions. The first question is a required field for an email address. The second question asks which operating system is most frequently used for bioinformatics tool development, with options for Windows, iOS, Unix, and Perl. The third question asks which database contains primarily protein sequences, with an option for GenBank.

docs.google.com/forms/d/e/1FAIpQLSeqDGQCYYIWKcvPsc3Unk4SsgAEdTHRJp...

BIMM 143 Home Gmail Goal Bitbucket GitHub News Discus EGNN-213 BIMM-143 GDocs

BIMM143 Lecture 1 Homework (W18)

Please answer the following questions

* Required

Email address *

Your email

Which of the following operating systems is most frequently used for bioinformatics tool development 1 point

- Windows
- iOS
- Unix
- Perl

Which of the following databases contains primarily protein sequences 1 point

- GenBank

Homework

Goals, Class material, Screencasts & **Homework**

docs.google.com/forms/d/e/1FAIpQLSeqDGQCYYIWKcvPsc3Unk4SsgAEdTHRJp...

BIMM 143 Home Gmail Goal Bitbucket GitHub News Discus EGNN-213 BIMM-143 GDocs

BIMM143 Lecture 1 Homework (W19)

Please answer the following questions

* Required

Homework is due before the next weeks class!

Which of the following operating systems is most frequently used for bioinformatics tool development 1 point

Windows

iOS

Unix

Perl

Which of the following databases contains primarily protein sequences 1 point

GenBank

Side Note: **Why stick with this course?**

Provides a hands-on practical introduction to major bioinformatics concepts and resources.

Covers modern hot topics and the intimate coupling of informatics with biology - highlighting the impact of computing advances and 'big data' on biology!

Designed for biology majors with no programming experience or high level math skills.

Provides a hook for increasing computational and data science competencies in the biosciences - valuable high demand translational skills!

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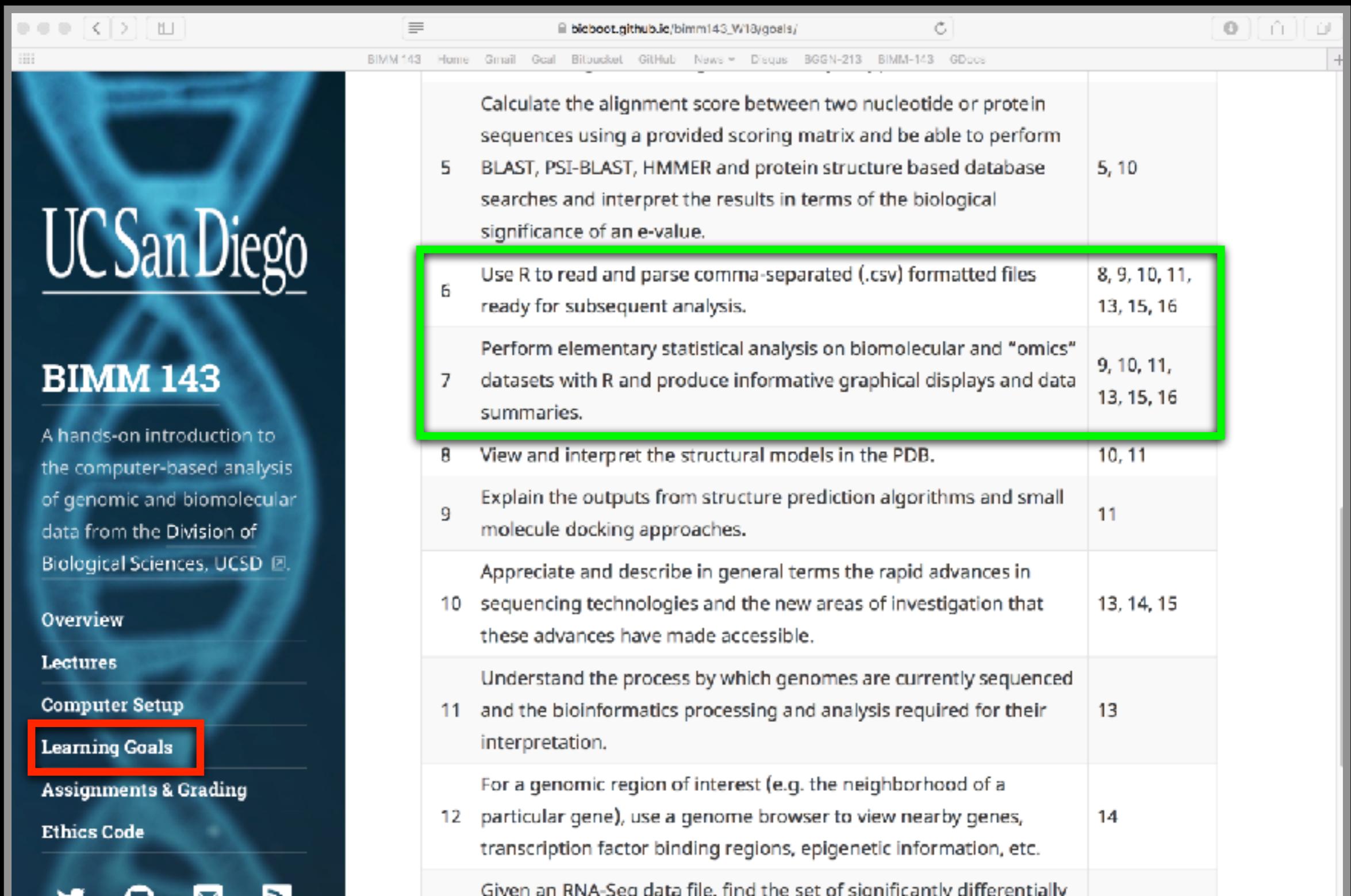
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BIMM-143 Learning Goals....

Data science R based learning goals



The screenshot shows a web browser displaying the BIMM-143 Learning Goals page. The page has a dark blue background with the UC San Diego logo and the course name 'BIMM 143' prominently displayed. On the left, a sidebar lists navigation links: Overview, Lectures, Computer Setup, Learning Goals (which is highlighted with a red box), Assignments & Grading, and Ethics Code. The main content area contains a table with 12 learning goals, each with a number, a description, and a list of associated numbers. Goals 6 and 7 are highlighted with a green box. A red arrow points downwards from the bottom right corner of the page.

5	Calculate the alignment score between two nucleotide or protein sequences using a provided scoring matrix and be able to perform BLAST, PSI-BLAST, HMMER and protein structure based database searches and interpret the results in terms of the biological significance of an e-value.	5, 10
6	Use R to read and parse comma-separated (.csv) formatted files ready for subsequent analysis.	8, 9, 10, 11, 13, 15, 16
7	Perform elementary statistical analysis on biomolecular and "omics" datasets with R and produce informative graphical displays and data summaries.	9, 10, 11, 13, 15, 16
8	View and interpret the structural models in the PDB.	10, 11
9	Explain the outputs from structure prediction algorithms and small molecule docking approaches.	11
10	Appreciate and describe in general terms the rapid advances in sequencing technologies and the new areas of investigation that these advances have made accessible.	13, 14, 15
11	Understand the process by which genomes are currently sequenced and the bioinformatics processing and analysis required for their interpretation.	13
12	For a genomic region of interest (e.g. the neighborhood of a particular gene), use a genome browser to view nearby genes, transcription factor binding regions, epigenetic information, etc.	14
	Given an RNA-Seq data file, find the set of significantly differentially expressed genes.	

BIMM-143 Learning Goals....

Delve deeper into “real-world” bioinformatics

UC San Diego

BIMM 143

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

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view and interpret the structural models in the PDB.		
9	Explain the outputs from structure prediction algorithms and small molecule docking approaches. Appreciate and describe in general terms the rapid advances in sequencing technologies and the new areas of investigation that these advances have made accessible. Understand the process by which genomes are currently sequenced and the bioinformatics processing and analysis required for their interpretation.	11 13, 14, 15 13
12	For a genomic region of interest (e.g. the neighborhood of a particular gene), use a genome browser to view nearby genes, transcription factor binding regions, epigenetic information, etc.	14
13	Given an RNA-Seq data file, find the set of significantly differentially expressed genes and use online tools to interpret gene lists and annotate potential gene functions.	15, 16
14	Perform a GO analysis to identify the pathways relevant to a set of genes (e.g. identified by transcriptomic study or a proteomic experiment).	16
15	Use the KEGG pathway database to look up interaction pathways.	17
16	Use graph theory to represent biological data networks.	17, 18
17	Understand the challenges in integrating and interpreting large heterogeneous high throughput data sets into their functional	19

These support a major learning objective

At the end of this course students will:

- Understand the increasing necessity for computation in modern life sciences research.
- Be able to use and evaluate online bioinformatics resources and analysis tools to solve problems in the biological sciences.
- Be able to use the R environment to analyze bioinformatics data at scale.
- Be familiar with the research objectives of the bioinformatics related sub-disciplines of Genome informatics, Transcriptomics and Structural informatics.

Why use R?

Productivity

Flexibility

Designed for data analysis

IEEE 2016 Top Programming Languages

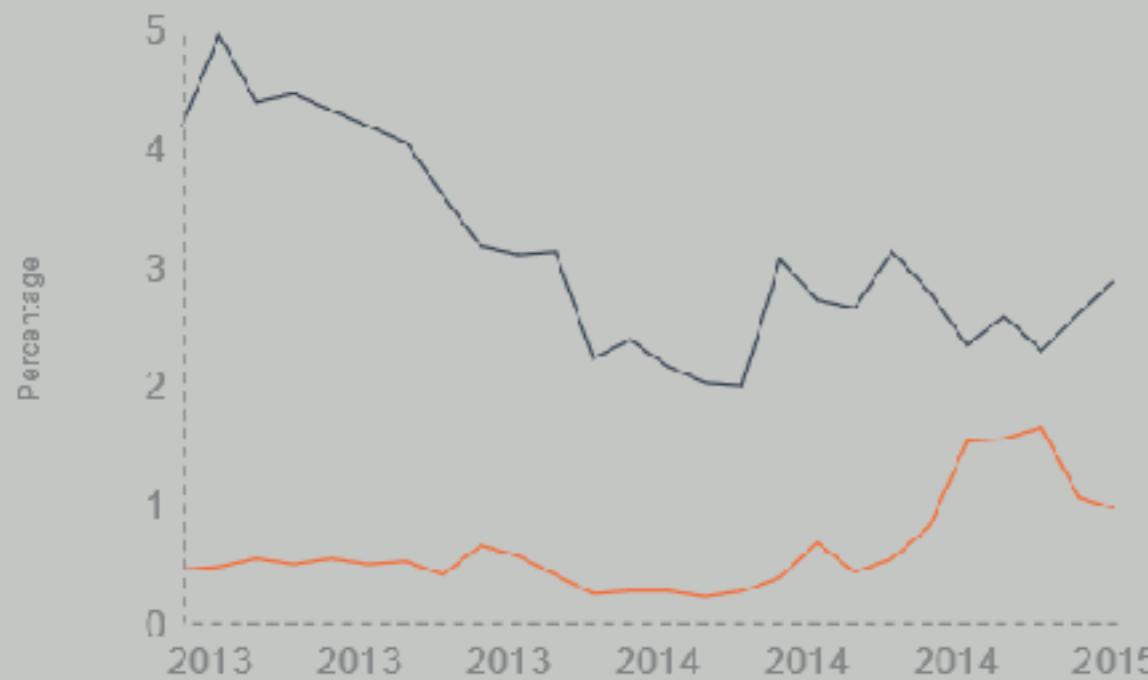
Language Rank	Types	Spectrum Ranking
1. C		100.0
2. Java		98.1
3. Python		98.0
4. C++		95.9
5. R		87.9
6. C#		86.7
7. PHP		82.8
8. JavaScript		82.2
9. Ruby		74.5
10. Go		71.9

<http://spectrum.ieee.org/computing/software/the-2016-top-programming-languages>

R and Python: The Numbers

Popularity Rankings

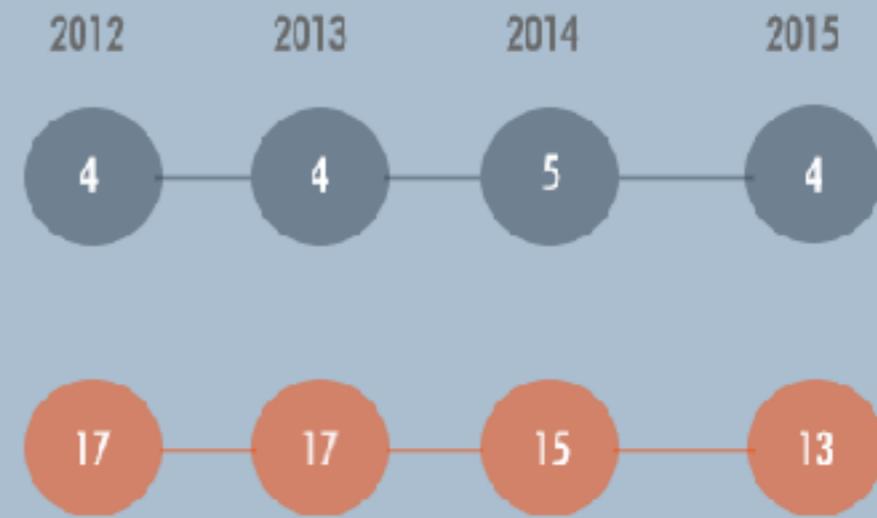
R and Python's popularity between 2013 and February 2015 (Tiobe Index)



Redmonk ranking, comparing the relative performance of programming languages on GitHub and Stack Overflow (September 2012 and January 2013, 2014, 2015)

Python

R



Jobs And Salary?

2014 Dice Tech Salary Survey:
Average Salary For High Paying Skills and Experience



\$ 115,531



\$ 94,139

[http://www.kdnuggets.com/2015/05/r-vs-python-data-science.html?
utm_medium=email&utm_source=flipboard](http://www.kdnuggets.com/2015/05/r-vs-python-data-science.html?utm_medium=email&utm_source=flipboard)

- R is the “lingua franca” of data science in industry and academia.
- Large user and developer community.
 - As of Jan 8th 2018 there are 12,039 add on **R packages** on [CRAN](#) and 1,473 on [Bioconductor](#) - more on these later!
- Virtually every statistical technique is either already built into R, or available as a free package.
- Unparalleled exploratory data analysis environment.

Today's Menu

Course Logistics

Website, screencasts, survey, ethics, assessment and grading.

Learning Objectives

What you need to learn to succeed in this course.

Course Structure

Major lecture topics and specific learning goals.

Introduction to Bioinformatics

Introducing the *what, why and how* of bioinformatics?

Computer Setup

Ensuring your laptop is all set for future sections of this course.

OUTLINE

Overview of bioinformatics

- The what, why and how of bioinformatics?
- Major bioinformatics research areas.
- Skepticism and common problems with bioinformatics.

Online databases and associated tools

- Primary, secondary and composite databases.
 - Nucleotide sequence databases (GenBank & RefSeq).
 - Protein sequence database (UniProt).
 - Composite databases (PFAM & OMIM).

Database usage vignette

- How-to productively navigate major databases.

Q. What is Bioinformatics?

“Bioinformatics is the application of computers to the collection, archiving, organization, and analysis of biological data.”

... Bioinformatics is a hybrid of biology and computer science

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- ... Bioinformatics is a hybrid of biology and computer science
- ... **Bioinformatics is computer aided biology!**

Q. What is Bioinformatics?

“Bioinformatics is the application of computers to the collection, archiving, organization, and analysis of biological data.”

- ... Bioinformatics is a hybrid of biology and computer science
- ... **Bioinformatics is computer aided biology!**

Computer based management and analysis of biological and biomedical data with useful applications in many disciplines, particularly genomics, proteomics, metabolomics, etc...

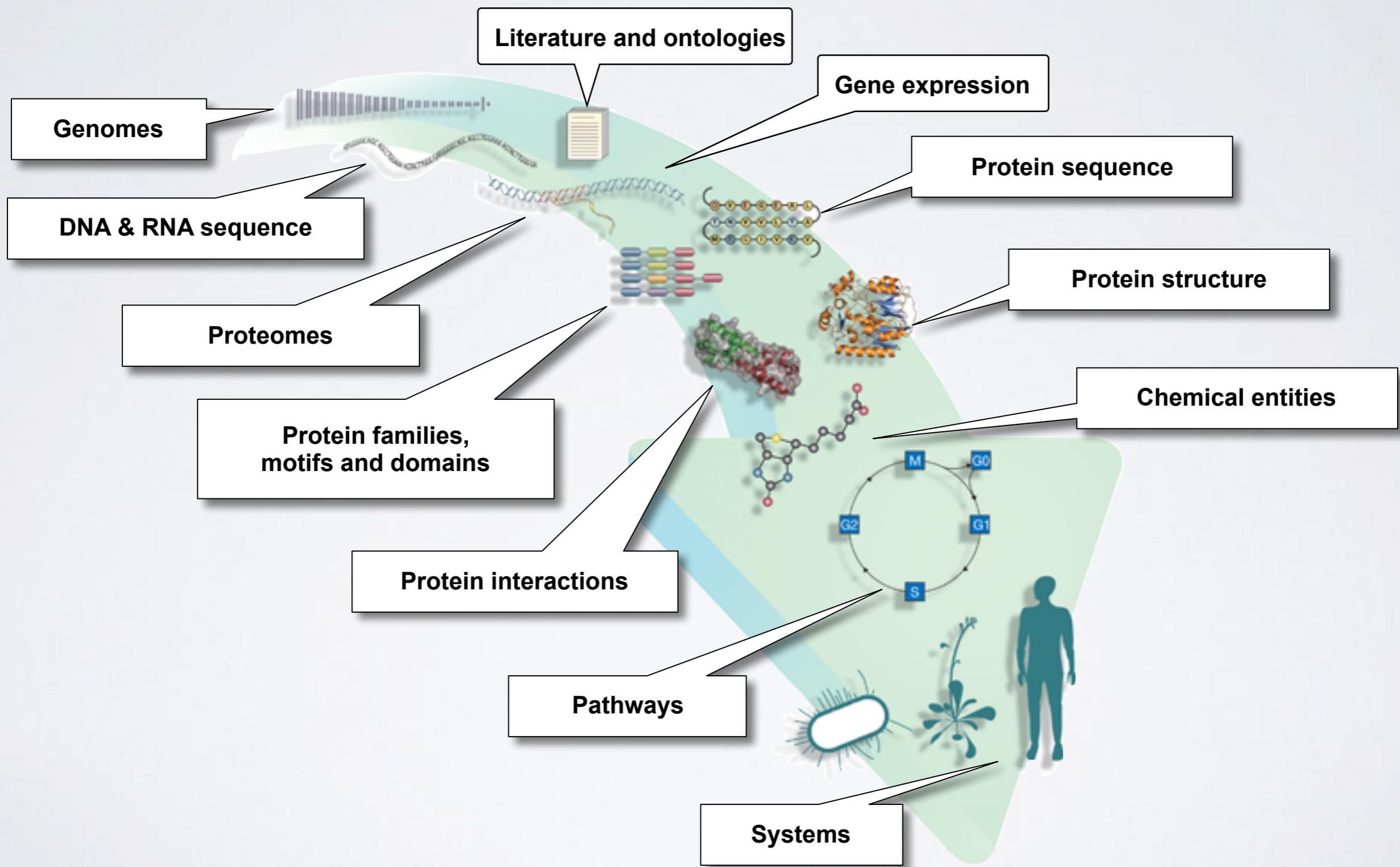
MORE DEFINITIONS

- ▶ “Bioinformatics is conceptualizing biology in terms of **macromolecules** and then applying “**informatics**” techniques (derived from disciplines such as applied maths, computer science, and statistics) to **understand** and **organize** the information associated with these molecules, on a **large-scale**.
Luscombe NM, et al. Methods Inf Med. 2001;40:346.
- ▶ “Bioinformatics is research, development, or application of **computational approaches** for expanding the use of **biological, medical, behavioral or health data**, including those to **acquire, store, organize and analyze** such data.”
National Institutes of Health (NIH) (<http://tinyurl.com/l3gxr6b>)

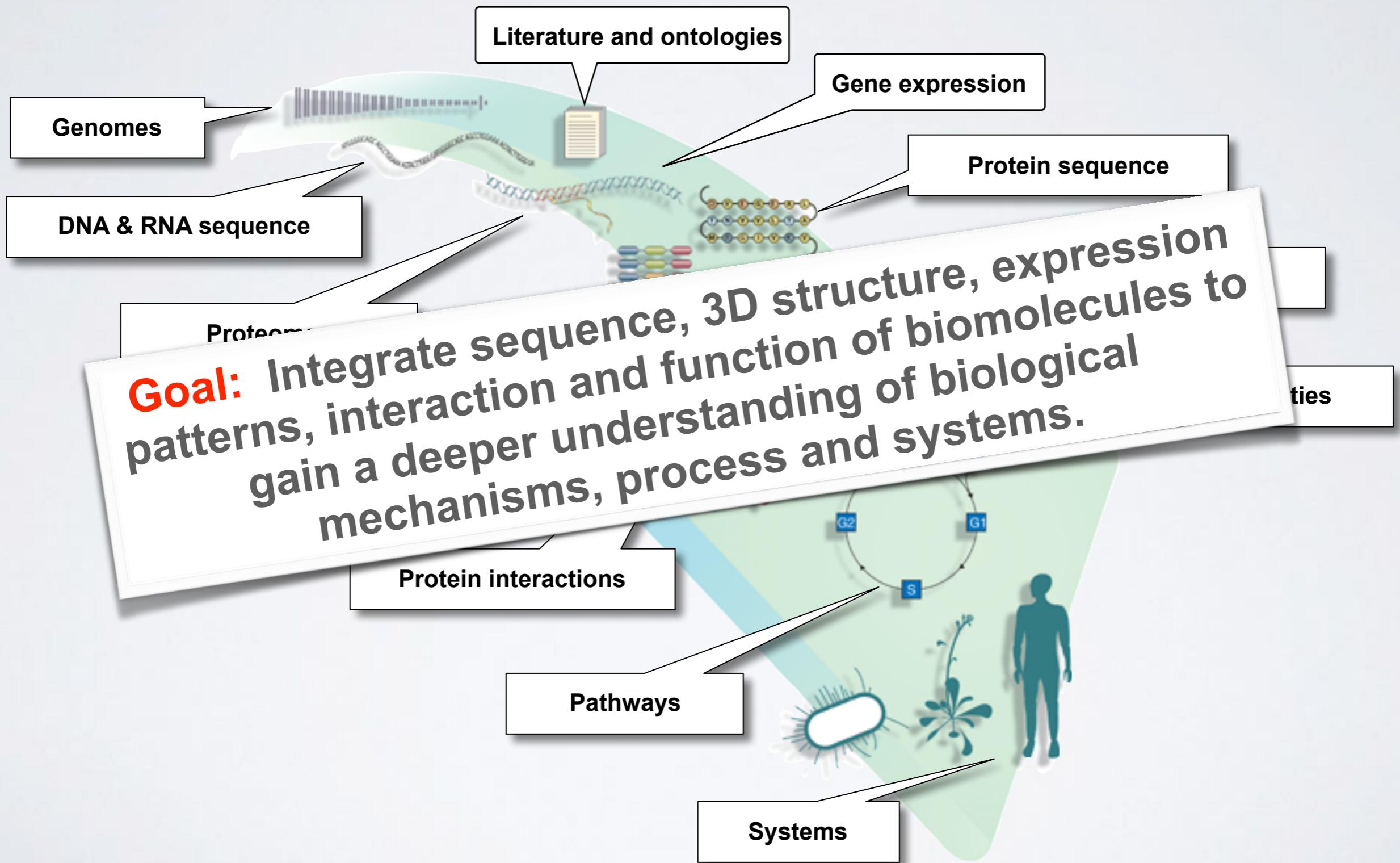
MORE DEFINITIONS

- ▶ “Bioinformatics is conceptualizing biology in terms of **macromolecules** and then applying “**informatics**” (derived from disciplines such as applied mathematics, science, and statistics) to **understand** and **analyze** the information associated with these molecules, on a **large-scale**.
Luscombe NM, et al. Methods 2001;40:346.
 - ▶ “Bioinformatics is the search, development, or application of computer approaches for expanding the use of biological, medical, behavioral or health data, including those to acquire, store, organize and analyze such data.”
National Institutes of Health (NIH) (<http://tinyurl.com/l3gxr6b>)
- Key Point:** Bioinformatics is Computer Aided Biology*

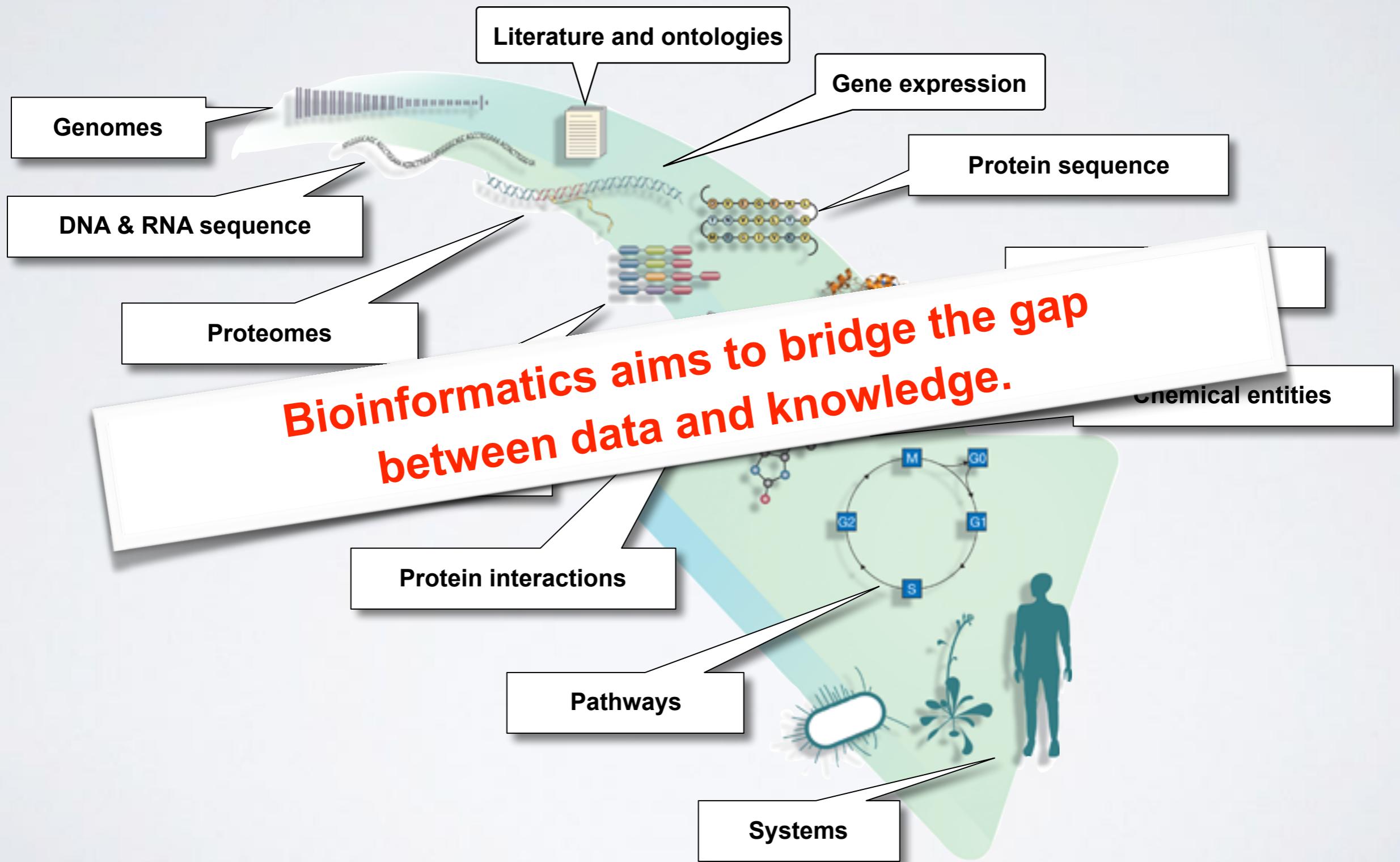
Major types of Bioinformatics Data



Major types of Bioinformatics Data



Major types of Bioinformatics Data



BIOINFORMATICS RESEARCH AREAS

Include but are not limited to:

- Organization, classification, dissemination and analysis of biological and biomedical data (particularly '-omics' data).
- Biological sequence analysis and phylogenetics.
- Genome organization and evolution.
- Regulation of gene expression and epigenetics.
- Biological pathways and networks in healthy & disease states.
- Protein structure prediction from sequence.
- Modeling and prediction of the biophysical properties of biomolecules for binding prediction and drug design.
- Design of biomolecular structure and function.

With applications to Biology, Medicine, Agriculture and Industry

Where did bioinformatics come from?

Bioinformatics arose as molecular biology began to be transformed by the emergence of molecular sequence and structural data

Recap: The key dogmas of molecular biology

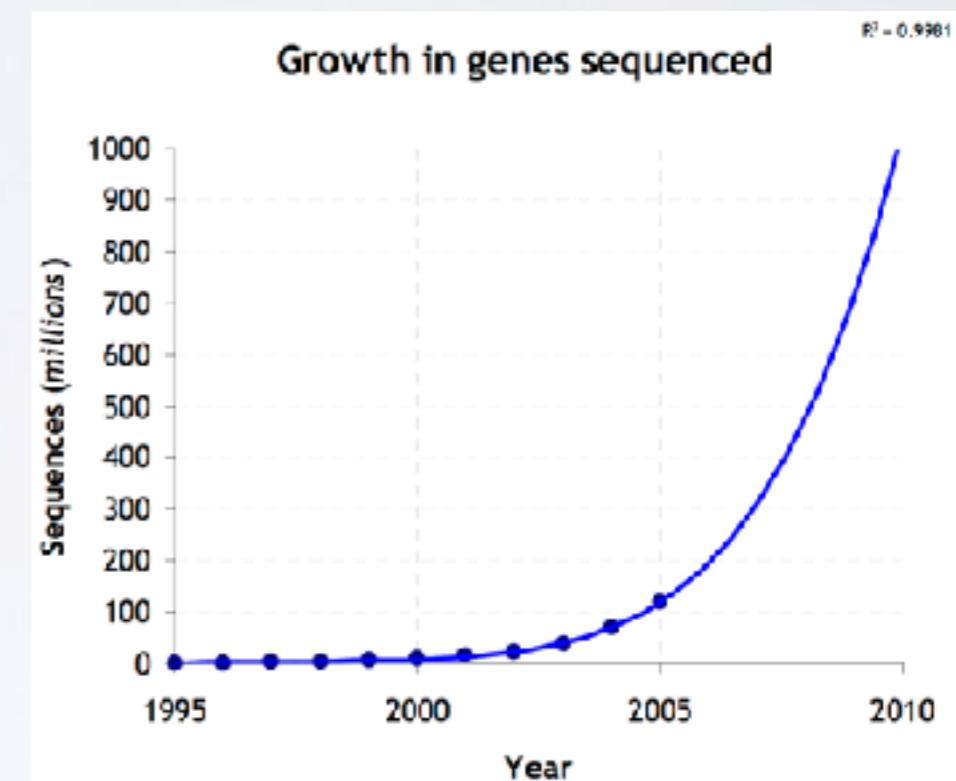
- *DNA sequence determines protein sequence.*
- *Protein sequence determines protein structure.*
- *Protein structure determines protein function.*
- *Regulatory mechanisms (e.g. gene expression) determine the amount of a particular function in space and time.*

Bioinformatics is now essential for the archiving, organization and analysis of data related to all these processes.

Why do we need Bioinformatics?

Bioinformatics is necessitated by the rapidly expanding quantities and complexity of biomolecular data

- Bioinformatics provides methods for the efficient:
 - ▶ **storage**
 - ▶ **annotation**
 - ▶ **search and retrieval**
 - ▶ **data integration**
 - ▶ **data mining and analysis**

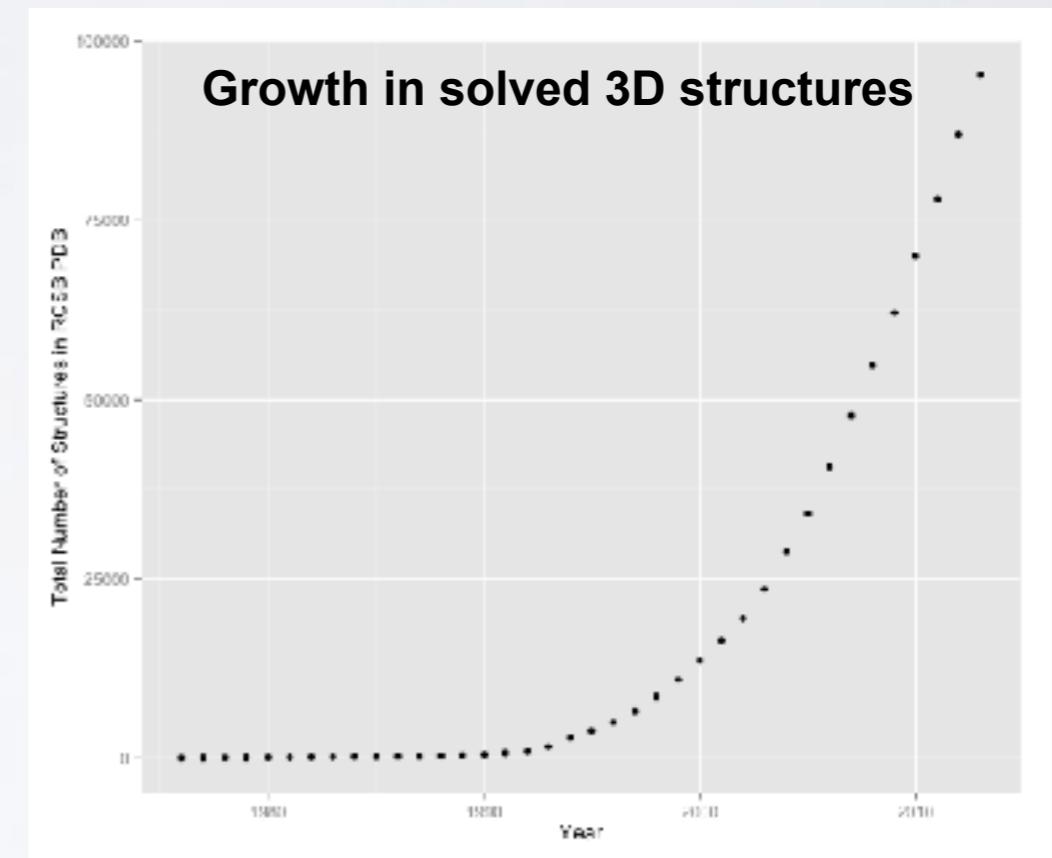


E.G. data from sequencing, structural genomics, proteomics, new high throughput assays, etc...

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E.G. data from sequencing, structural genomics, proteomics, new high throughput assays, etc...

How do we do Bioinformatics?

- A “*bioinformatics approach*” involves the application of **computer algorithms**, **computer models** and **computer databases** with the broad goal of understanding the action of both individual genes, transcripts, proteins and large collections of these entities.



How do we *actually* do Bioinformatics?

Pre-packaged tools and databases

- Many online
- Most are free to use
- Time consuming methods require downloading...

Advanced tool application & development

- Mostly on a UNIX environment
- Knowledge of programming languages frequently required
(e.g. R, Python, Perl, C, Java, Fortran)
- May require specialized high performance computing...

How do we *actually* do Bioinformatics?

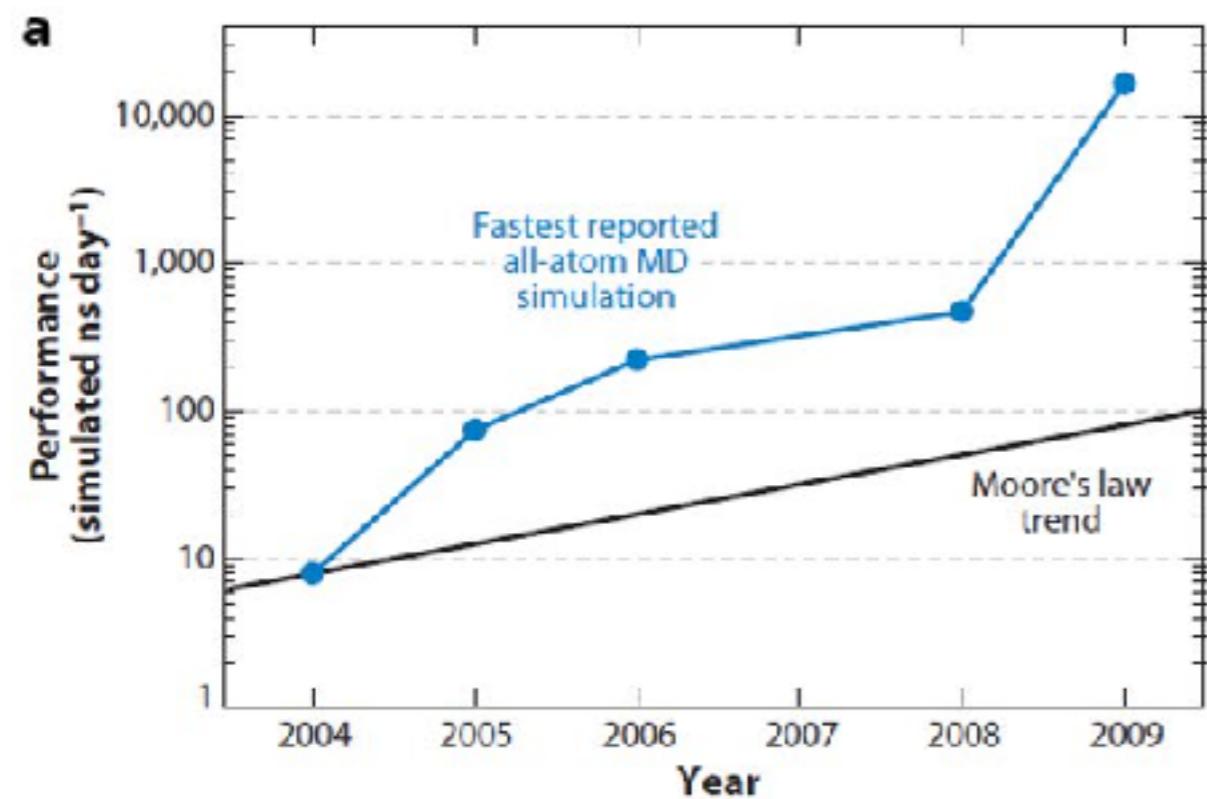
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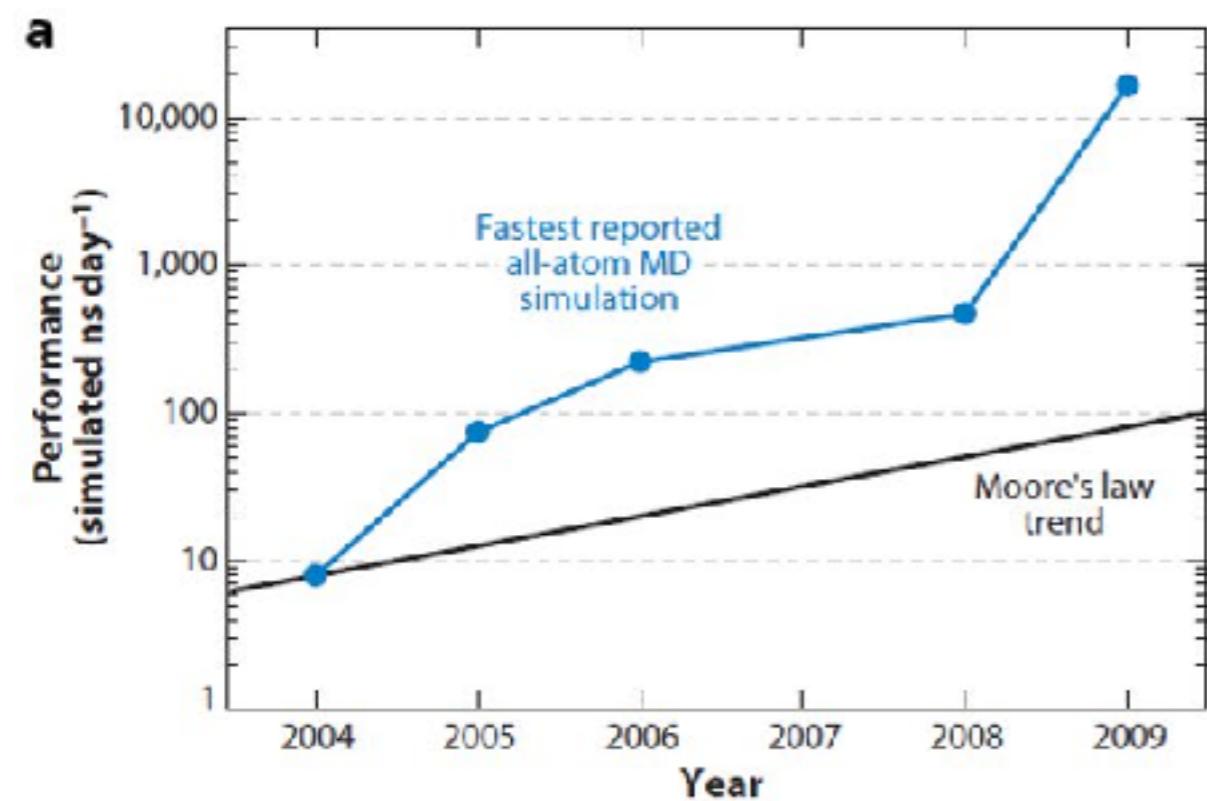
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- Mostly on a UNIX environment
- Knowledge of programming languages frequently required
(e.g. R, Python, Perl, C, Java, Fortran)
- May require specialized high performance computing...

SIDE-NOTE: SUPERCOMPUTERS ANDGPUS



SIDE-NOTE: SUPERCOMPUTERS AND GPUS



HOW COMPUTERS HAVE CHANGED

DATE	COST	SPEED	MEMORY	SIZE
1967	\$10M	0.1 MHz	1 MB	WALL
2013	\$14,000	1 GHz	10 GB	LAPTOP
CHANGE	10,000	10,000	10,000	10,000

If cars were like computers then a new Vehc
would cost \$3, would have a top speed of
1,000,000 Km/hr, would carry 50,000
adults and would park in a shadow.



Skepticism & Bioinformatics

We have to approach computational results the same way we do wet-lab results:

- Do they make sense?
- Is it what we expected?
- Do we have adequate controls, and how did they come out?
- Modeling is modeling, but biology is different...

What does this model actually contribute?

- Avoid the miss-use of ‘black boxes’

Skepticism & Bioinformatics

Gunnar von Heijne in his old but quite readable treatise, *Sequence Analysis in Molecular Biology; Treasure Trove or Trivial Pursuit*, provides a very appropriate conclusion:

- “Think about what you’re doing; use your knowledge of the molecular system involved to guide both your interpretation of results and your direction of inquiry; use as much information as possible; and do not blindly accept everything the computer offers you”.
- Key-Point: **Avoid the miss-use of ‘black boxes’!**

Common problems with Bioinformatics

Confusing multitude of tools available

- ▶ Each with many options and settable parameters

Most tools and databases are written by and for nerds

- ▶ Same is true of documentation - if any exists!

Most are developed independently

Notable exceptions are found at the:

- **EBI** (European Bioinformatics Institute) and
- **NCBI** (National Center for Biotechnology Information)

General Parameters

Max target sequences

Select the maximum number of aligned sequences to display

Short queries Automatically adjust parameters for short input sequences

Expect threshold

Word size

Max matches in a query range

Scoring Parameters

Matrix

Gap Costs Existence: 11 Extension: 1

Compositional adjustments Conditional compositional sco

Filters and Masking

Filter Low complexity regions

Mask Mask for lookup table only
 Mask lower case letters

PSI/PHI/DELTA BLAST

Upload PSSM Optional Choose File no file selected

PSI-BLAST Threshold

Pseudocount

Even Blast has many settable parameters

STEP 3 - Set your PROGRAM

FASTA

MATRIX	GAP OPEN	GAP EXTEND	KTUP	EXPECTATION UPPER VALUE	EXPECTATION LOWER VALUE
BLOSUM50	-10	-2	2	10	0 (default)

DNA STRAND	HISTOGRAM	FILTER	STATISTICAL ESTIMATES		
N/A	no	none	Regress		

SCORES	ALIGNMENTS	SEQUENCE RANGE	DATABASE RANGE	MULTI HSPs
50	50	START-END	START-END	no

SCORE FORMAT

Default

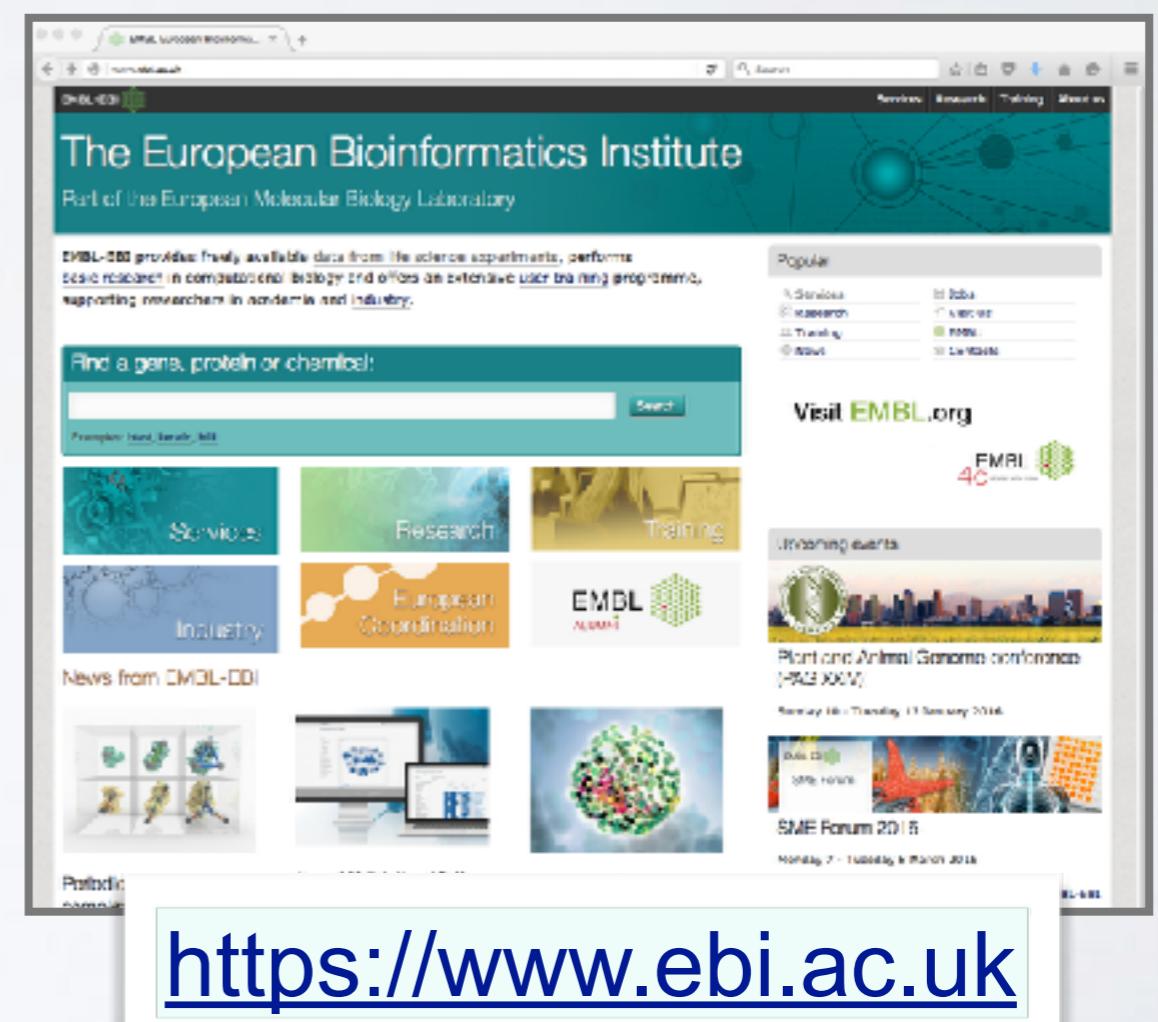
Related tools with different terminology

Key Online Bioinformatics Resources: NCBI & EBI

The NCBI and EBI are invaluable, publicly available resources for biomedical research



The screenshot shows the NCBI homepage with a blue header "National Center for Biotechnology Information". Below it is a navigation bar with links to "NCBI Resources", "How To", "Sign in to NCBI", "All Databases", and a search bar. The main content area includes a "Welcome to NCBI" section, a "Get Started" section with links to tools, downloads, how-to guides, and submissions, and a "3D Structures" section featuring a 3D molecular model. On the left is a sidebar with links to various NCBI databases like Resource List (A-Z), All Resources, Chemicals & Biosassays, Data & Software, DNA & RNA, Domains & Structures, Genes & Expression, Genetics & Medicine, Genomes & Maps, Homology, Literature, Proteins, Sequence Analysis, Taxonomy, Training & Tutorials, and Variation.



The screenshot shows the EMBL-EBI homepage with a green header "The European Bioinformatics Institute, Part of the European Molecular Biology Laboratory". Below it is a search bar and a "Find a gene, protein or chemical" input field. The main content area features sections for "Services", "Research", "Training", "Industry", "European Coordination", and "News from EMBL-EBI". There are also sections for "Upcoming events" (Plant and Animal Genome conference) and "Past Events" (SME Forum 2015). A sidebar on the right lists "Popular" links such as Advanced Research, Research, Training, News, and Contact. The footer includes the EMBL logo and a "4C" logo.

<http://www.ncbi.nlm.nih.gov>

<https://www.ebi.ac.uk>

National Center for Biotechnology Information (NCBI)

- Created in 1988 as a part of the National Library of Medicine (NLM) at the National Institutes of Health
- NCBI's mission includes:
 - ▶ Establish **public databases**
 - ▶ Develop **software tools**
 - ▶ **Education** on and dissemination of biomedical information
- We will cover a number of core NCBI databases and software tools in the lecture



<http://www.ncbi.nlm.nih.gov>

National Center for Biotechnology Information

NCBI Resources How To Sign in to NCBI

All Databases Search

NCBI Home Resource List (A-Z) All Resources Chemicals & Bioassays Data & Software DNA & RNA Domains & Structures Genes & Expression Genetics & Medicine Genomes & Maps Homology Literature Proteins Sequence Analysis Taxonomy Training & Tutorials Variation

Welcome to NCBI

The National Center for Biotechnology Information advances science and health by providing access to biomedical and genomic information.

[About the NCBI](#) | [Mission](#) | [Organization](#) | [Research](#) | [RSS Feeds](#)

Get Started

- [Tools](#): Analyze data using NCBI software
- [Downloads](#): Get NCBI data or software
- [How-To's](#): Learn how to accomplish specific tasks at NCBI
- [Submissions](#): Submit data to GenBank or other NCBI databases

3D Structures

Explore three-dimensional structures of proteins, DNA, and RNA molecules. Examine sequence-structure relationships, active sites, molecular interactions, biological activities of bound chemicals, and associated biosystems.

Popular Resources

PubMed Bookshelf PubMed Central PubMed Health BLAST Nucleotide Genome SNP Gene Protein PubChem

NCBI Announcements

New version of Genome Workbench available 06 Sep An integrated, downloadable applicati

<http://www.ncbi.nlm.nih.gov>

National Center for Biotechnology Information

NCBI Resources How To Sign in to NCBI

All Databases Search

NCBI Home Resource List (A-Z) All Resources Chemicals & Bioassays Data & Software DNA & RNA Domains & Structures Genes & Expression Genetics & Medicine Genomes & Maps Homology Literature Proteins Sequence Analysis Taxonomy Training & Tutorials Variation

Welcome to NCBI

The National Center for Biotechnology Information provides access to unique information, tools and resources in the fields of medicine, health and biology.

About the NCBI | Mission | Our History

Get Started

- Tools: Analyze data using NCBI's bioinformatics tools
- Downloads: Get NCBI data files and software
- How-To's: Learn how to access and use NCBI resources
- Submissions: Submit data to NCBI's databases

3D Structures

Explore three-dimensional structures of proteins, DNA, and RNA molecules. Examine sequence-structure relationships, active sites, molecular interactions, biological activities of bound chemicals and associated biosystems.

Popular Resources

PubMed Bookshelf PubMed Central PubMed Health BLAST Nucleotide Genome SNP Gene Protein PubChem

Resources

Central Health

Announcements

New version of Genome Workbench available 06 Sep An integrated, downloadable application

A screenshot of the NCBI homepage. The sidebar on the left lists various resources like NCBI Home, Resource List (A-Z), and 3D Structures. The main content area features a 'Welcome to NCBI' section and a 'Get Started' list. On the right, there's a 'Popular Resources' sidebar containing links to PubMed, Bookshelf, PubMed Central, PubMed Health, BLAST, Nucleotide, Genome, SNP, Gene, Protein, and PubChem. A red bracket on the right side of the sidebar groups the 'Gene', 'Protein', and 'PubChem' links, while three separate red arrows point to the 'PubMed', 'BLAST', and 'Gene' links respectively.

<http://www.ncbi.nlm.nih.gov>

National Center for Biotechnology Information

NCBI Resources How To Sign in to NCBI

All Databases Search

NCBI Home Resource List (A-Z)

Welcome to NCBI
The National Center for Biotechnology Information advances science

Popular Resources PubMed

Notable NCBI databases include:
GenBank, **RefSeq**, **PubMed**, **dbSNP**

and the search tools **ENTREZ** and **BLAST**

Homology Literature Proteins Sequence Analysis Taxonomy Training & Tutorials Variation

databases

3D Structures
Explore three-dimensional structures of proteins, DNA, and RNA molecules. Examine sequence-structure relationships, active sites, molecular interactions, biological activities of bound chemicals and associated biosystems

Protein PubChem

NCBI Announcements
New version of Genome Workbench available 06 Sep
An integrated, downloadable applicati

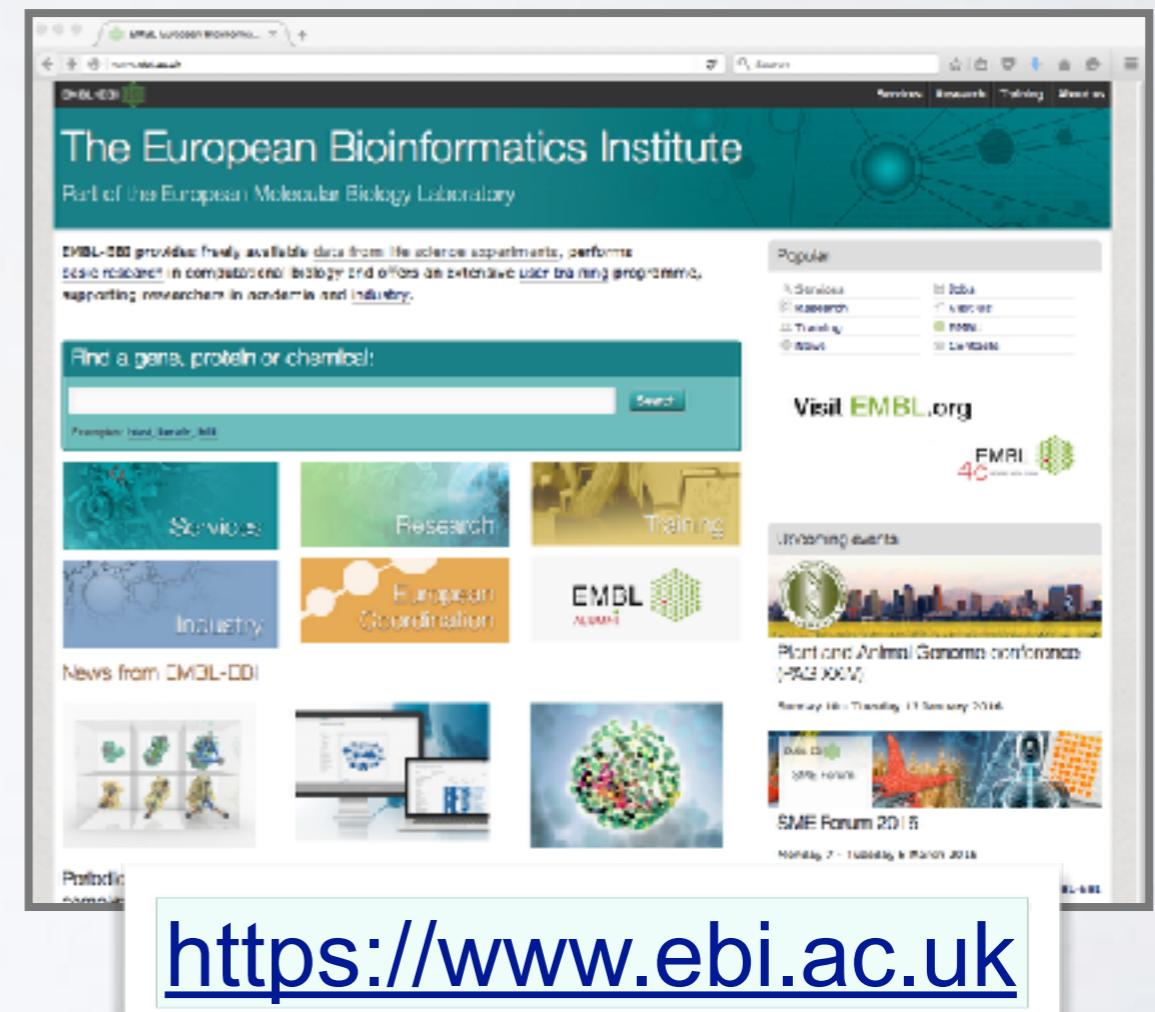
Key Online Bioinformatics Resources: NCBI & EBI

The NCBI and EBI are invaluable, publicly available resources for biomedical research



The screenshot shows the NCBI homepage with a blue header "National Center for Biotechnology Information". Below it is a navigation bar with links for "NCBI Resources", "How To", "Sign in to NCBI", "All Databases", and a search bar. The main content area includes sections for "Welcome to NCBI", "Get Started", "3D Structures", and "NCBI Announcements". The "Popular Resources" sidebar lists PubMed, Bookshelf, PubMed Central, PubMed Health, BLAST, NUCOTIDE, GenBank, SNP, Gene, Protein, and PubChem.

<http://www.ncbi.nlm.nih.gov>



The screenshot shows the EBI homepage with a green header "The European Bioinformatics Institute". Below it is a navigation bar with links for "Reviews", "Research", "Training", and "About us". The main content area includes a search bar for "Find a gene, protein or chemical", sections for "Services", "Research", "Training", "Industry", "European Coordination", and "News from EMBL-EBI". The right sidebar features a "Popular" section with links for "Datasets", "Search", "Training", and "News", and a "Visit EMBL.org" section with a link to "EMBL-EBI".

<https://www.ebi.ac.uk>

European Bioinformatics Institute (EBI)

- Created in 1997 as a part of the European Molecular Biology Laboratory (EMBL)
- EBI's mission includes:
 - ▶ providing freely available **data and bioinformatics services**
 - ▶ and providing advanced **bioinformatics training**
- We will briefly cover several EBI databases and tools that have advantages over those offered at NCBI



The EBI maintains a number of high quality curated **secondary databases** and associated tools

The screenshot shows the homepage of the EMBL European Bioinformatics Institute (EBI) at www.ebi.ac.uk. The page features a dark blue header with the EMBL-EBI logo, a search bar, and navigation links for Services, Research, Training, and About us. The main content area has a teal background with the text: "The European Bioinformatics Institute Part of the European Molecular Biology Laboratory". Below this, a paragraph describes the institute's mission: "EMBL-EBI provides freely available data from life science experiments, performs basic research in computational biology and offers an extensive user training programme, supporting researchers in academia and industry." A search bar allows users to "Find a gene, protein or chemical" with examples like "blast, keratin, bfl1...". To the right, a "Popular" sidebar lists links for Services, Research, Training, News, Jobs, Visit us, EMBL, and Contacts. A "Visit EMBL.org" section features the EMBL 40th anniversary logo. Another sidebar for "Upcoming events" promotes the "Plant and Animal Genome conference (PAG XXIV)".

EMBL European Bioinforma... [+/-](#)

www.ebi.ac.uk [Search](#) [Services](#) [Research](#) [Training](#) [About us](#)

The European Bioinformatics Institute

Part of the European Molecular Biology Laboratory

EMBL-EBI provides freely available data from life science experiments, performs basic research in computational biology and offers an extensive user training programme, supporting researchers in academia and industry.

Find a gene, protein or chemical:

Examples: blast, keratin, bfl1...

Search

Services

Research

Training

EMBL ALUMNI

Industry

European Coordination

News from EMBL-EBI

Popular

Services

Research

Training

News

Jobs

Visit us

EMBL

Contacts

Visit EMBL.org

EMBL 40 YEARS 1974-2014

Upcoming events

Plant and Animal Genome conference (PAG XXIV)

Sunday 10 - Tuesday 12 January 2016

The EBI maintains a number of high quality curated **secondary databases** and associated tools

The screenshot shows the EBI Services website (www.ebi.ac.uk/services) with a banner featuring a molecular structure. The top navigation bar includes links for Services, Research, Training, and About us.

Services

Overview A to Z Data submission Support

Bioinformatics services

We maintain the world's most comprehensive range of **freely available** and up-to-date **molecular databases**. Developed in collaboration with our colleagues worldwide, our services let you share data, perform complex queries and analyse the results in different ways. You can work locally by downloading our data and software, or use our **web services** to access our resources programmatically. You can read more about our services in the journal *Nucleic Acids Research*.

Popular

- Ensembl
- UniProt
- PDBc
- ArrayExpress
- ChEMBL
- BLAST
- Europe PMC
- Reactome
- Train online
- Support

Service news

Training

DNA & RNA
genes, genomes & variation

Gene expression
RNA, protein & metabolite expression

Proteins
sequences, families & motifs

Structures
Molecular & cellular structures

Systems
reactions, interactions & pathways

Chemical biology
chemogenomics & metabolomics

Ontologies
taxonomies & controlled vocabularies

Literature
Scientific publications & patents

Cross domain
cross-domain tools & resources

The EBI maintains a number of high quality curated **secondary databases** and associated tools

The screenshot shows the EBI Services website (www.ebi.ac.uk/services) with a banner for 'Bioinformatics services'. Below the banner, there are nine service categories arranged in a grid:

- DNA & RNA (genes, genomes & variation)
- Gene expression (RNA, protein & metabolite expression)
- Proteins (sequences, families & motifs) - This box is highlighted with a red border.
- Structures (Molecular & cellular structures)
- Systems (reactions, interactions & pathways)
- Chemical biology (chemogenomics & metabolomics)
- Ontologies (taxonomies & controlled vocabularies)
- Literature (Scientific publications & patents)
- Cross domain (cross-domain tools & resources)

To the right of the services grid is a 'Popular' sidebar containing links to Ensembl, UniProt, PDBe, ArrayExpress, and ChEMBL, each with its respective logo. A large image of a monarch butterfly is visible in the background of the sidebar area. At the bottom right, there is a 'Training' section with a blurred image of a person working at a computer.

<https://www.ebi.ac.uk>

The EBI makes available a wider variety of **online tools** than NCBI

Proteins

Popular services

 UniProt	UniProt: The Universal Protein Resource The gold-standard, comprehensive resource for protein sequence and functional annotation data.	Quick links <ul style="list-style-type: none">○ Popular services in this category○ All services in this category○ Project websites in this category
 InterPro	InterPro A database for the classification of proteins into families, domains and conserved sites.	
 PRIDE	PRIDE: The Proteomics Identifications Database An archive of protein expression data determined by mass spectrometry.	
 Pfam	Pfam A database of hidden Markov models and alignments to describe conserved protein families and domains.	
 Clustal Omega	Clustal Omega Multiple sequence alignment of DNA or protein sequences. Clustal Omega replaces the older ClustalW alignment tools.	
 HMMER	HMMER - protein homology search Fast sensitive protein homology searches using profile hidden Markov models (HMMs). Variety of different search methods for querying against both sequence and HMM target databases.	
 InterProScan 5	InterProScan 5 searches sequences against InterPro's predictive protein signatures. Please note that InterProScan 4.8 has been retired.	

The EBI also provides a growing selection of **online tutorials** on EBI databases and tools

The screenshot shows the homepage of the EMBL European Bioinformatics Institute (EBI) at www.ebi.ac.uk. The page features a dark blue header with the EMBL-EBI logo, a search bar, and navigation links for Services, Research, Training, and About us. Below the header is a teal banner with the text "The European Bioinformatics Institute" and "Part of the European Molecular Biology Laboratory". A large graphic of interconnected nodes is visible on the right side of the banner. The main content area includes a search bar for finding genes, proteins, or chemicals, and several colored boxes for Services, Research, Training, Industry, European Coordination, and EMBL ALUMNI. A red box highlights the "Training" section. To the right, there's a "Popular" sidebar with links to Services, Research, Training, News, Jobs, Visit us, EMBL, and Contacts. A "Visit EMBL.org" section features the EMBL 40th anniversary logo. Below it is an "Upcoming events" section for the Plant and Animal Genome conference (PAG XXIV), showing a city skyline and the conference logo.

EMBL European Bioinforma... [+](#)

www.ebi.ac.uk [Search](#)

EMBL-EBI

Services | Research | Training | About us

The European Bioinformatics Institute

Part of the European Molecular Biology Laboratory

EMBL-EBI provides freely available data from life science experiments, performs basic research in computational biology and offers an extensive user training programme, supporting researchers in academia and industry.

Find a gene, protein or chemical:

Search

Examples: blast, keratin, bfl1...

Services

Research

Training

Industry

European Coordination

EMBL ALUMNI

Popular

Services

Research

Training

News

Jobs

Visit us

EMBL

Contacts

Visit EMBL.org

EMBL 40 years 1974-2014

Upcoming events

Plant and Animal Genome conference (PAG XXIV)

Sunday 10 - Tuesday 12 January 2016

The EBI also provides a growing selection of **online tutorials** on EBI databases and tools

The screenshot shows a web browser displaying the EMBL-EBI Training online course page. The URL in the address bar is www.ebi.ac.uk/training/online/course/using-sequence-similarity-searching-tools-embl-ebi. The page title is "Using sequence similarity searching tools at EMBL-EBI: webinar". The main content area features a video player showing a thumbnail of the webinar presentation. The thumbnail has a blue header with the text "Using sequence similarity search tools at EMBL-EBI" and "Finding homologous sequences with BLAST, FASTA, PSI-Search etc.". Below the header is a photo of a man (Andrew Cowley) and his contact information: andrew.cowley@ebi.ac.uk and support@ebi.ac.uk. The video player shows a progress bar at 0:03 / 37:42. To the left of the video player is a sidebar titled "Course content" with links to "Using sequence similarity searching tools at EMBL-EBI: webinar" and "Contributors". Below this is a "Print Course" button. To the right of the video player is a "Popular" sidebar with links to "Train online", "Find us", and "Funding". Another sidebar titled "Find us at..." lists links to "Open days and career days", "Conference exhibitions", "EMBL courses and events", "Genome campus events", and "Science for schools". At the bottom of the page, a summary text states: "This webinar focuses on how to use tools like BLAST and PSI-Search to find homologous sequences in EMBL-EBI databases, including tips on which tool and database to use, input formats, how to change parameters and how to interpret the results pages."

Using sequence similarity e... X

www.ebi.ac.uk/training/online/course/using-sequence-similarity-searching-tools-embl-ebi

EMBL-EBI

Services Research Training About us

Train online

Training Train online Home Course list Glossary Support & Feedback Log in / Register

training • online • course-list • using-sequence-similarity-searching-tools-embl-ebi

Course content

Using sequence similarity searching tools at EMBL-EBI: webinar

Contributors

Print Course

Using sequence similarity searching tools at EMBL-EBI: webinar

Using sequence similarity search tools at EMBL-EBI

Finding homologous sequences with BLAST, FASTA, PSI-Search etc.

Andrew Cowley
andrew.cowley@ebi.ac.uk
support@ebi.ac.uk

0:03 / 37:42

Popular

Train online

Find us

Funding

Find us at...

Open days and career days

Conference exhibitions

EMBL courses and events

Genome campus events

Science for schools

This webinar focuses on how to use tools like BLAST and PSI-Search to find homologous sequences in EMBL-EBI databases, including tips on which tool and database to use, input formats, how to change parameters and how to interpret the results pages.

The EBI also provides a growing selection of **online tutorials** on EBI databases and tools

A screenshot of a web browser displaying the 'Train online | EBI Train online' website. The address bar shows the URL www.ebi.ac.uk/training/online/. The page header includes the EMBL-EBI logo and links for 'Find', 'Help', and 'Feedback'. A red 'Beta' badge is visible in the top right corner. The main navigation menu at the top includes 'Databases', 'Tools', 'Research', 'Training', 'Industry', 'About Us', and 'Help'. A secondary navigation bar on the left labeled 'Navigation' contains a link to 'Train online Home'. The central content area features a large heading 'Train online'.

Notable EBI databases include:
[ENA](#), [UniProt](#), [Ensembl](#)

and the tools [FASTA](#), [BLAST](#), [InterProScan](#),
[MUSCLE](#), [DALI](#), [HMMER](#)

Find a course

Browse by subject



[Genes and Genomes](#)



[Gene Expression](#)



[Interactions, Pathways, and Networks](#)

Next Class...

**MAJOR BIOINFORMATICS
DATABASES AND ASSOCIATED
ONLINE TOOLS**

Bioinformatics Databases

AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb, BBDB, BCGD, Beanref, BiolImage, BioMagResBank, BIOMDB, BLOCKS, BovGBASE, BOVMAP, BSORF, BTKbase, CANSITE, CarbBank, CARBHYD, CATH, CAZY, CCDC, CD4OLbase, CGAP, ChickGBASE, Colibri, COPE, CottonDB, CSNDB, CUTG, CyanoBase, dbCFC, dbEST, dbSTS, DDBJ, DGP, DictyDb, Picty_cDB, DIP, DOGS, DOMO, DPD, DPInteract, ECDC, ECGC, EC02DBASE, EcoCyc, EcoGene, EMBL, EMD db, ENZYME, EPD, EpoDB, ESTHER, FlyBase, FlyView, GCRDB, GDB, GENATLAS, Genbank, GeneCards, Genlilesne, GenLink, GENOTK, GenProtEC, GIFTS, GPCRDB, GRAP, GRBase, gRNAsdb, GRR, GSDB, HAEMB, HAMSTERS, HEART-2DPAGE, HEXAdb, HGMD, HIDB, HIDC, HIVdb, HotMolecBase, HOVERGEN, HPDB, HSC-2DPAGE, ICN, ICTVDB, IL2RGbase, IMGT, Kabat, KDNA, KEGG, KloTho, LGIC, MAD, MaizeDb, MDB, Medline, Mendel, MEROPS, MGDB, MGI, MHCPEP5 Micado, MitoDat, MITOMAP, MJDB, MmtDB, Mol-R-Us, MPDB, MRR, MutBase, MycDB, NDB, NRSub, O-lycBase, OMIA, OMIM, OPD, ORDB, OWL, PAHdb, PatBase, PDB, PDD, Pfam, PhosphoBase, PigBASE, PIR, PKR, PMD, PPDB, PRESAGE, PRINTS, ProDom, Prolysis, PROSITE, PROTOMAP, RatMAP, RDP, REBASE, RGP, SBASE, SCOP, SeqAnaiRef, SGD, SGP, SheepMap, Soybase, SPAD, SRNA db, SRPDB, STACK, StyGene, Sub2D, SubtiList, SWISS-2DPAGE, SWISS-3DIMAGE, SWISS-MODEL Repository, SWISS-PROT, TeIDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene, URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, etc ..!!!!

Bioinformatics Databases

AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb, BBDB, RCCP, Beanref, CANSITE, CarbBank, CARBHYD, CATH, CAZy, ChickGBASE, Colibri, COPE, CottonDB, dbSTS, DDBJ, DGP, DictyDb, ECGC, EC02DBASE, FlyBase, GDB, HEPDB, HumanProteome, KEGG, MHCDB, MycoDB, PDBe, PDB, Pfam, PhosphoBase, PigBASE, PIR, PKR, PMD, PPDB, PRESAGE, PRINTS, ProDom, Prolysis, PROSITE, PROTOMAP, RatMAP, RDP, REBASE, RGP, SBASE, SCOP, SeqAnaiRef, SGD, SGP, SheepMap, Soybase, SPAD, SRNA db, SRPDB, STACK, StyGene, Sub2D, SubtiList, SWISS-2DPAGE, SWISS-3DIMAGE, SWISS-MODEL Repository, SWISS-PROT, TelDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene, URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, etc ..!!!!

There are lots of Bioinformatics Databases

For a annotated listing of major bioinformatics databases please see the online handout

< Major Databases.pdf >

Side-note: Databases come in all shapes and sizes



Databases can be of variable quality and often there are multiple databases with overlapping content.

Primary, secondary & composite databases

Bioinformatics databases can be usefully classified into *primary*, *secondary* and *composite* according to their data source.

- **Primary databases** (or archival databases) consist of data derived experimentally.
 - **GenBank**: NCBI's primary nucleotide sequence database.
 - **PDB**: Protein X-ray crystal and NMR structures.
- **Secondary databases** (or derived databases) contain information derived from a primary database.
 - **RefSeq**: non redundant set of curated reference sequences primarily from GenBank
 - **PFAM**: protein sequence families primarily from UniProt and PDB
- **Composite databases** (or *metadatabases*) join a variety of different primary and secondary database sources.
 - **OMIM**: catalog of human genes, genetic disorders and related literature
 - **GENE**: molecular data and literature related to genes with extensive links to other databases.

Today's Menu

Course Logistics

Website, screencasts, survey, ethics, assessment and grading.

Learning Objectives

What you need to learn to succeed in this course.

Course Structure

Major lecture topics and specific learning goals.

Introduction to Bioinformatics

Introducing the *what, why and how* of bioinformatics?

Bioinformatics Database

Hands-on exploration of several major databases and their associated tools.

Your Turn!

https://bioboot.github.io/bimm143_S18/lectures/#1

The screenshot shows a web browser window displaying a course website for BIMM 143. The URL in the address bar is https://bioboot.github.io/bimm143_S18/lectures/#1. The main content area features a large title "1: Welcome to Foundations of Bioinformatics". Below it, sections for "Topics", "Goals", and "Material" are listed with bullet points. A sidebar on the left contains links for "Overview", "Lectures" (which is highlighted with a red box), "Computer Setup", "Learning Goals", "Assignments & Grading", and "Ethics Code".

Topics:

Course introduction, Learning goals & expectations, Biology is an information science, History of Bioinformatics, Types of data, Application areas and introduction to upcoming course segments, Student 30-second introductions, Student computer setup.

Goals:

- Understand course scope, expectations, logistics and [ethics code](#).
- Understand the increasing necessity for computation in modern life sciences research.
- Get introduced to how bioinformatics is practiced.
- Complete the [pre-course questionnaire](#).
- Setup your [laptop computer](#) for this course.

Material:

- Lecture Slides: [Large PDF](#), [Small PDF](#),
- Lab: [Hands-on section worksheet](#)
- Feedback: [Muddy Point Assessment](#).
- Handout: [Class Syllabus](#)
- Computer [Setup Instructions](#).

BIMM-143: INTRODUCTION TO BIOINFORMATICS (Lecture 1)

Bioinformatics Databases and Key Online Resources

https://bioboot.github.io/bimm143_W18/lectures/#1

Dr. Barry Grant

Jan 2018

Overview: The purpose of this lab session is to introduce a range of bioinformatics databases and associated services available on the Web whilst investigating the molecular basis of a common human disease.

Sections 1 and 2 deal with querying and searching GenBank, GENE and OMIM databases at NCBI. Sections 3 and 4 provide exposure to EBI resources for comparing proteins and visualizing protein structures. Finally, section 5 provides an opportunity to explore these and other databases further with additional examples.

Side-note: The Web is a dynamic environment, where information is constantly added and removed. Servers "go down", links change without warning, etc. This can lead to "broken" links and results not being returned from services. Don't give up - give it a second go and try a search engine using terms related to the page you are trying to access.

Section 1

The following transcript was found to be abundant in a human patient's blood sample.

```
>example1
ATGGTGCATCTGACTCCGTGGAGAAGTCTGCCGTTACTGCCCTGTGGGCAAGGTGAACGTGGATGAAG
TTGGTGGTGAGGCCCTGGCAGGCTGCTGGTGGTCTACCCCTGGACCCAGAGGTTCTTGAGTCCTTGG
GGATCTGTCCACTCCTGATGCAGTTATGGGCAACCCCTAACGGTGAAGGCTCATGGCAAGAAAGTGCTCGGT
GCCTTAGTGAATGGCCTGGCTCACCTGGACAACCTCAAGGGCACCTTGGCACACTGAGTGAGCTGCACT
GTGACAAGCTGCACGTGGATCCTGAGAACTTCAGGCTCCTGGCAACGTGCTGGTCTGTGTGCTGGCCA
TCACCTTGGCAAAGAATTCACCCCACCAAGTGCAGGCTGCCTATCAGAAAAGTGGTGGCTGGTGTGGCTAAT
GCCCTGGCCCACAAGTATCACTAAGCTCGCTTCTGCTGTCCAATTT
```

The only information you are given is the above sequence so you must begin your investigation with a sequence search - for this example we will use NCBI's **BLAST** service at: <http://blast.ncbi.nlm.nih.gov/>

Note that there are several different "basic BLAST" programs available at NCBI (including nucleotide BLAST, protein BLAST, and BLASTx).

YOUR TURN!

- There are five major hands-on sections including:

1. BLAST, GenBank and OMIM @ NCBI	[~35 mins]
2. GENE database @ NCBI	[~15 mins]
— BREAK —	
3. UniProt & Muscle @ EBI	[~25 mins]
4. PFAM, PDB & NGL	[~30 mins]
— BREAK —	
5. Extension exercises	[~30 mins]

- ▶ Please do answer the last review question (**Q19**).
- ▶ We encourage discussion and exploration!

YOUR TURN!

- There are five major hands-on sections including:

	End times:
1. BLAST, GenBank and OMIM @ NCBI	[10:45 am]
2. GENE database @ NCBI	[11:00 am]
— BREAK —	— 11:10 am —
3. UniProt & Muscle @ EBI	[11:35 am]
4. PFAM, PDB & NGL	[12:05 pm]
— BREAK —	— 12:15 am —
5. Extension exercises	[12:45 pm]

- ▶ Please do answer the last review question (**Q19**).
- ▶ We encourage discussion and exploration!

SUMMARY

- Bioinformatics is computer aided biology.
- Bioinformatics deals with the collection, archiving, organization, and interpretation of a wide range of biological data.
- There are a large number of primary, secondary and tertiary bioinformatics databases.
- The NCBI and EBI are major online bioinformatics service providers.
- Introduced Gene, UniProt, PDB databases as well as a number of ‘boutique’ databases including PFAM and OMIM.

HOMEWORK

https://bioboot.github.io/bimm143_S18/lectures/#1

- Complete the **initial course questionnaire**:
- Check out the “**Background Reading**” material online:
- Complete the **lecture 1 homework questions**:

THANK YOU