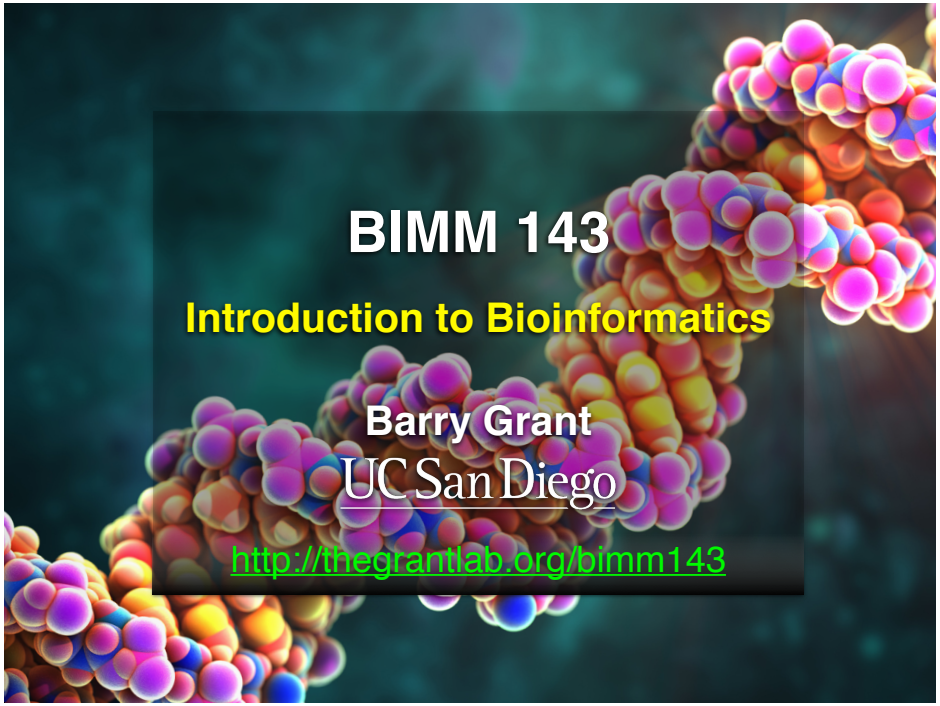


HELLO
my name is
BARRY
bjgrant@ucsd.edu

Office Hours:
SignUp

Location:
TATA, #2501

HELLO
HER ~~my~~ name is
ALENA
amartsul@ucsd.edu

HELLO
HER ~~my~~ name is
KELLY
kflander@ucsd.edu

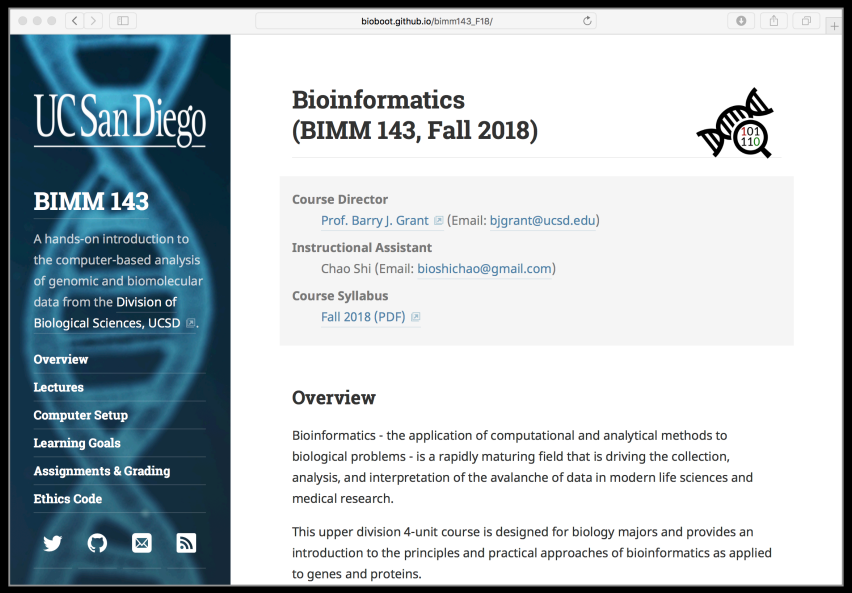
Introduce Yourself!

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

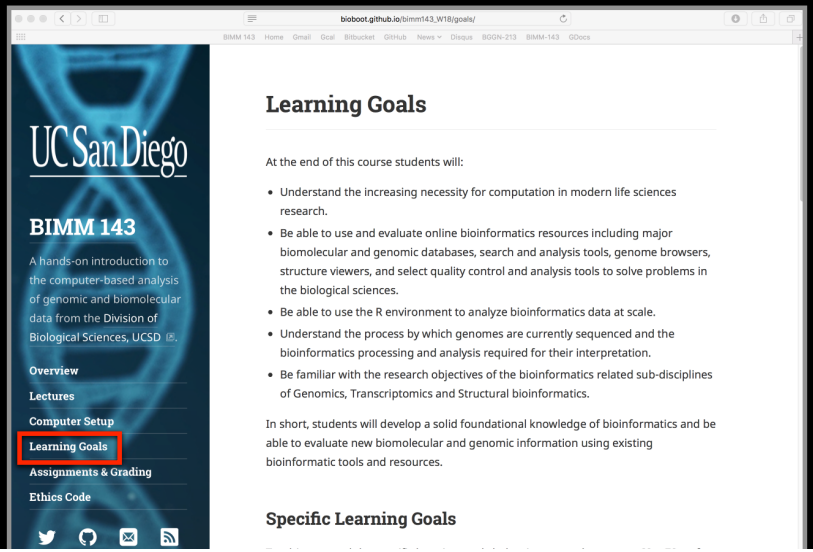
Today's Menu

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 leaning goals.
Introduction to Bioinformatis	**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/



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



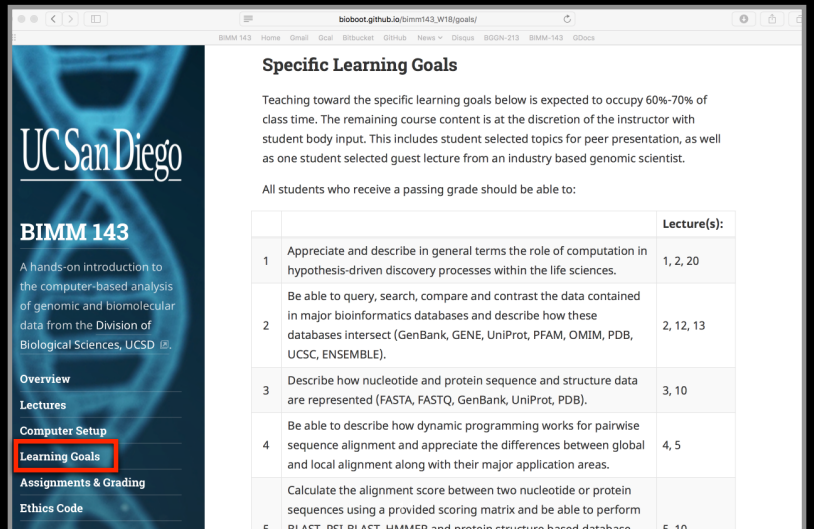
At the end of this course students will:

- 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**.

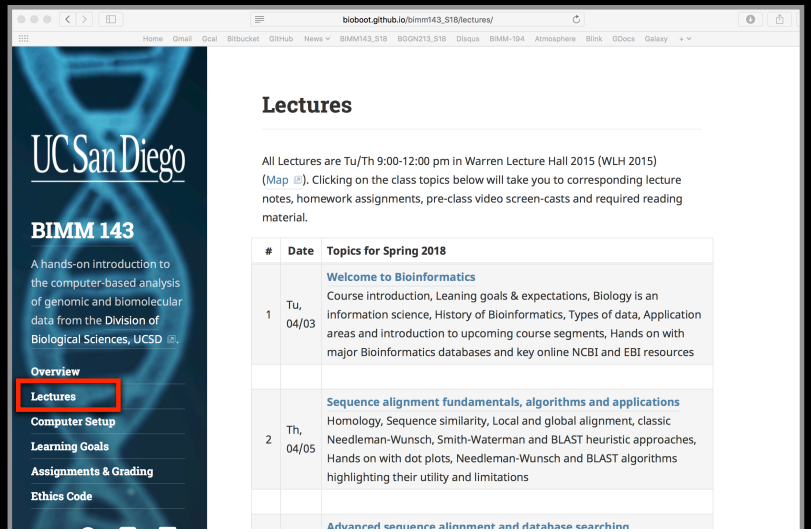
Specific Learning Goals....

What I want you to know by course end!



Course Structure

Derived from specific learning goals



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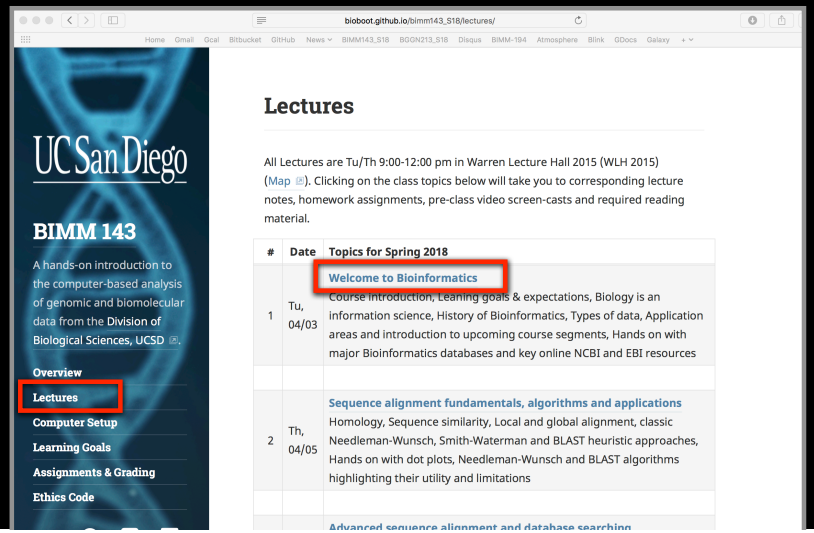
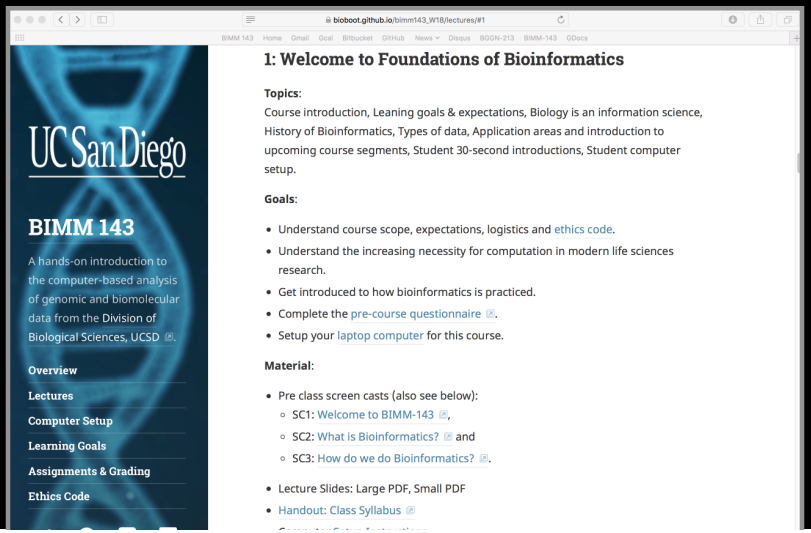


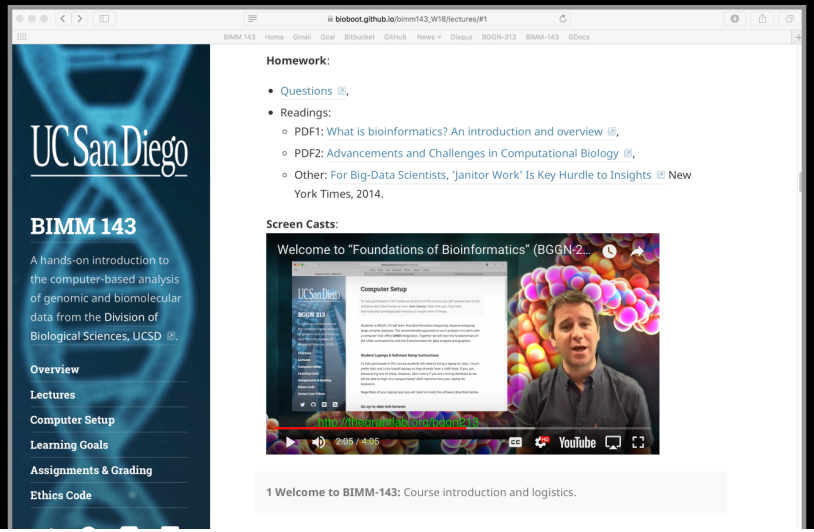
Class Details

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



Homework

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



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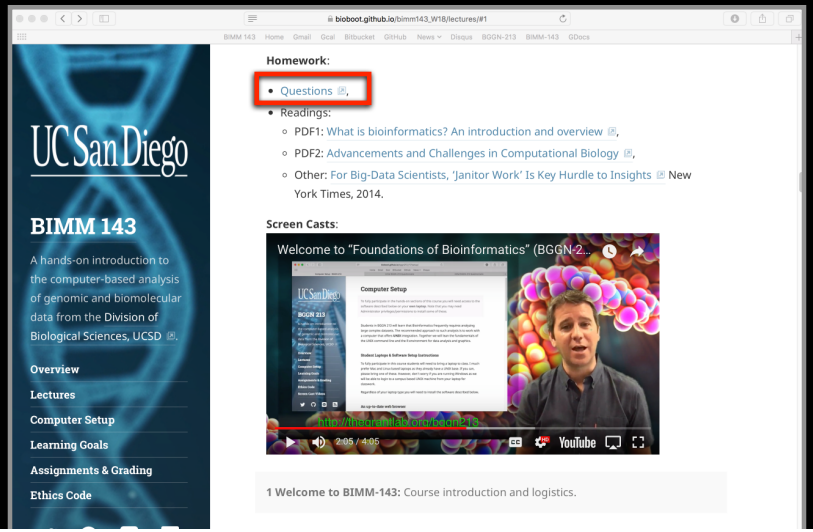

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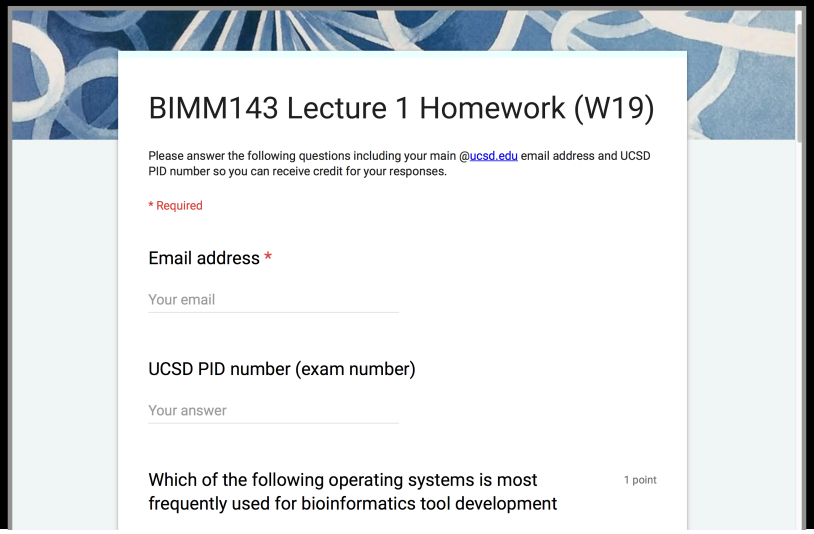

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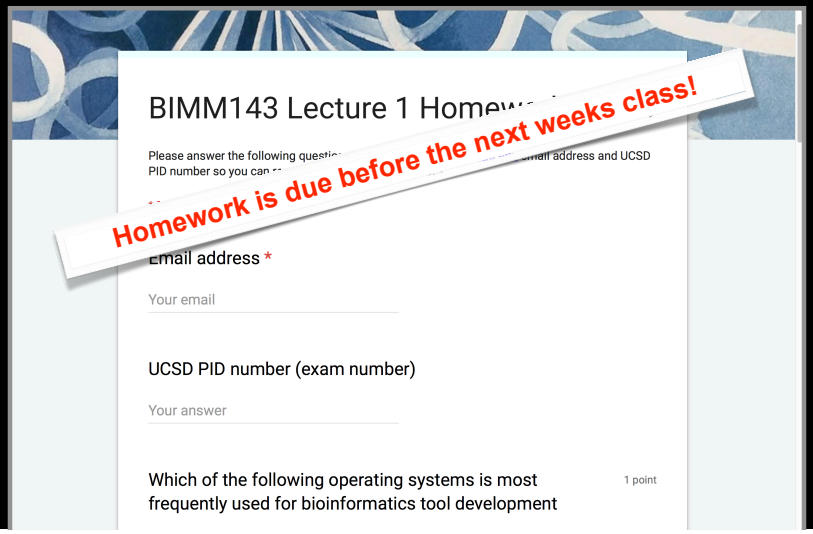

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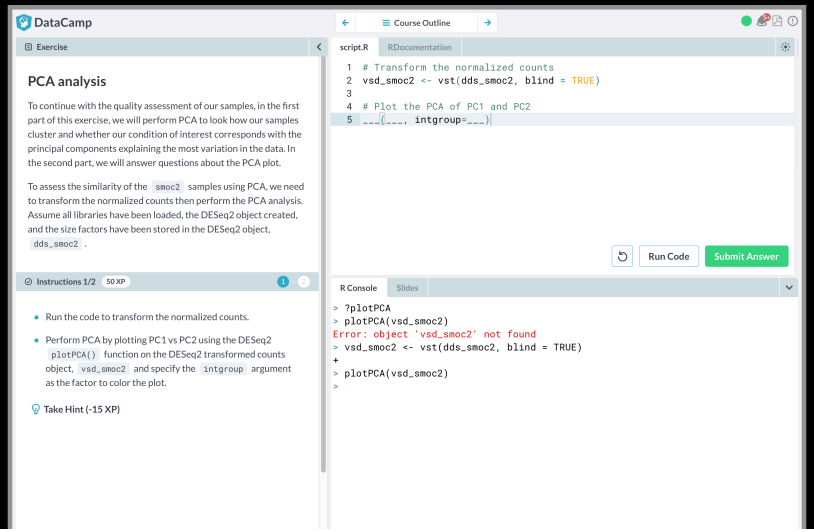
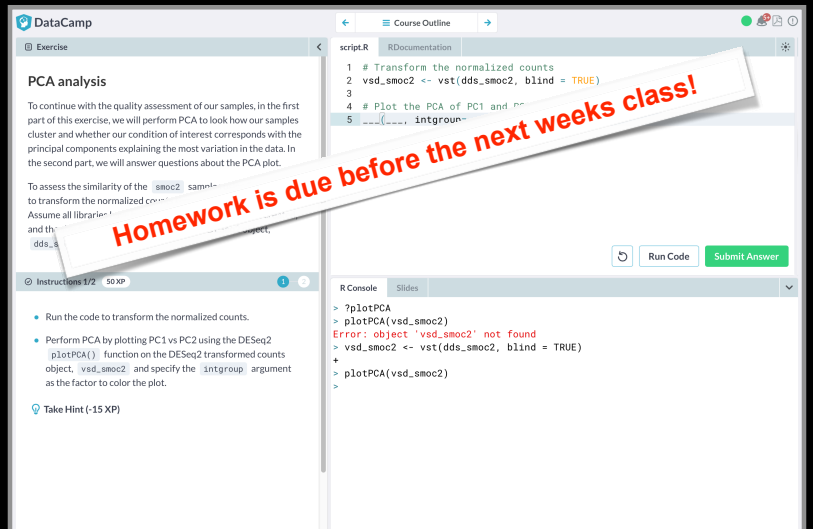


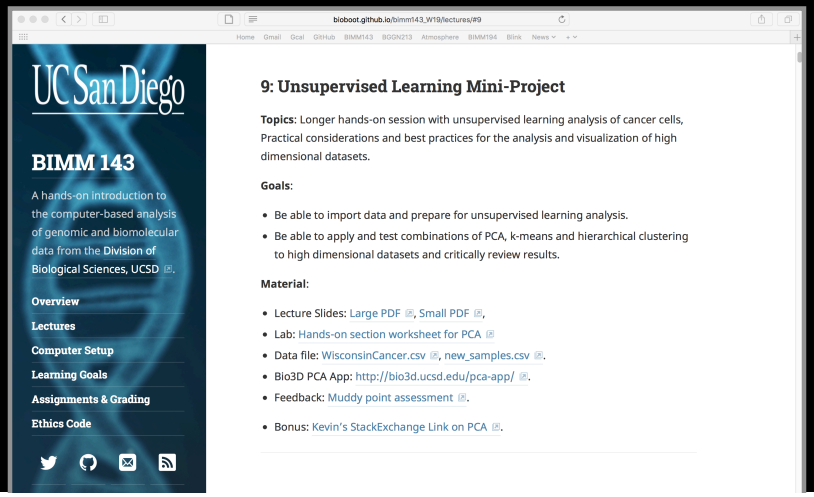
Homework (35% of course grade)

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



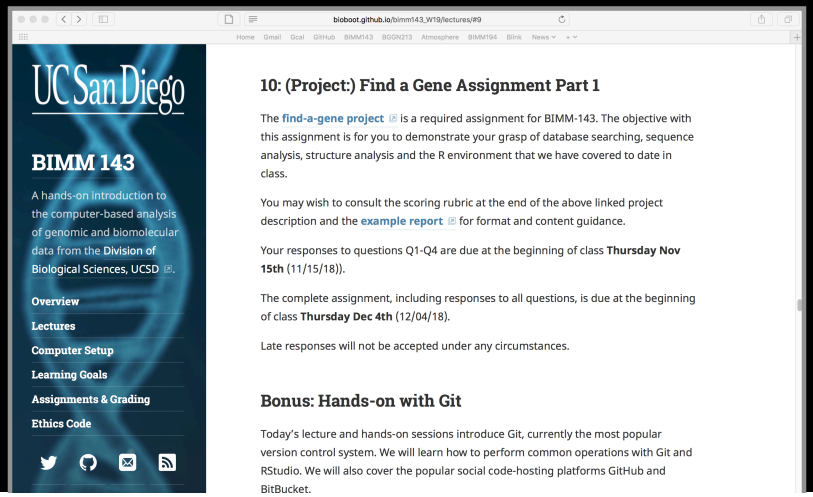
Projects

Week long **mini-projects** (x2),
and 1 five week main project



Projects (20% of course grade)

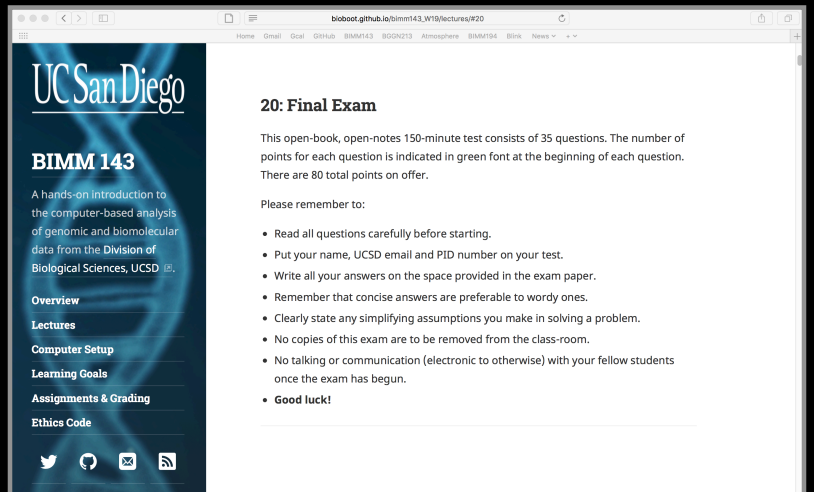
Week long mini-projects (x2),
and 1 five week **main project**



Final Exam

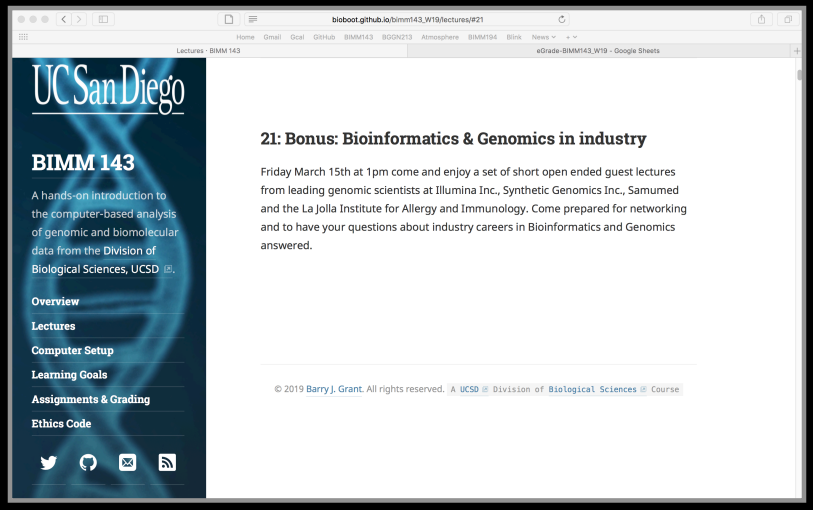
Open-book, open-notes 150-minute test

(45% of course grade)



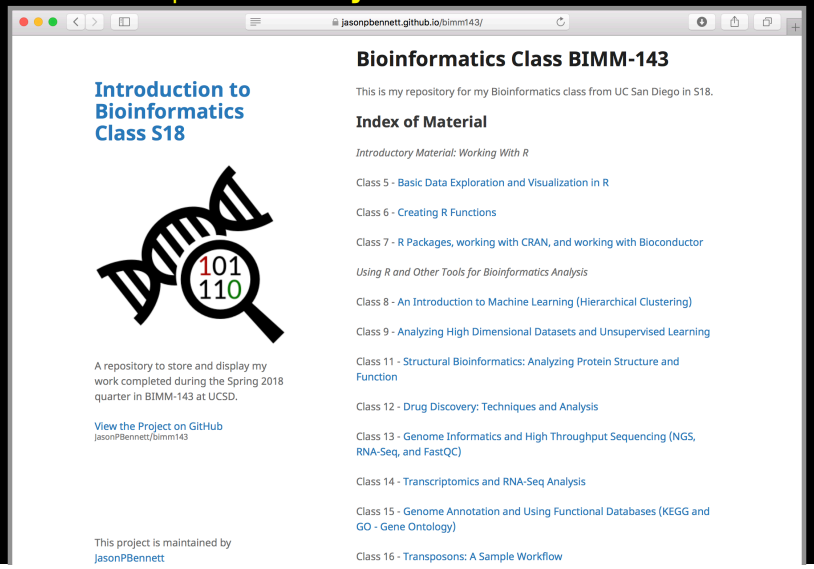
Bonus:

Bioinformatics & Genomics in industry



Bonus:

Online portfolio of **your** bioinformatics work!



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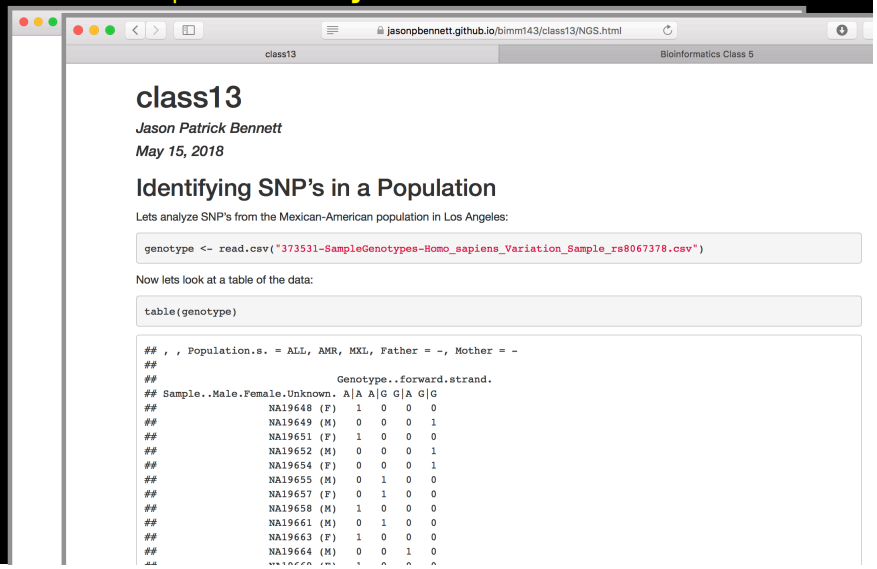

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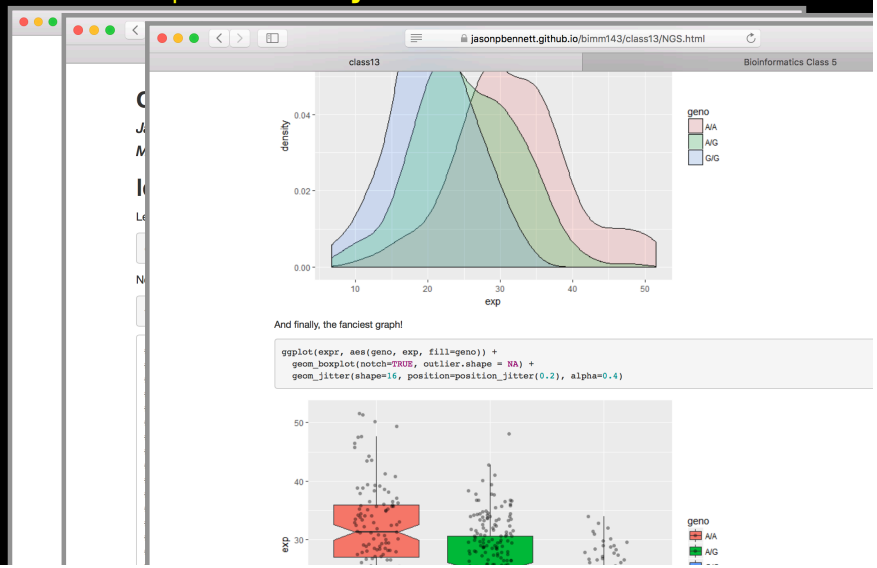

Side Note: Why stick with this course?

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 programing 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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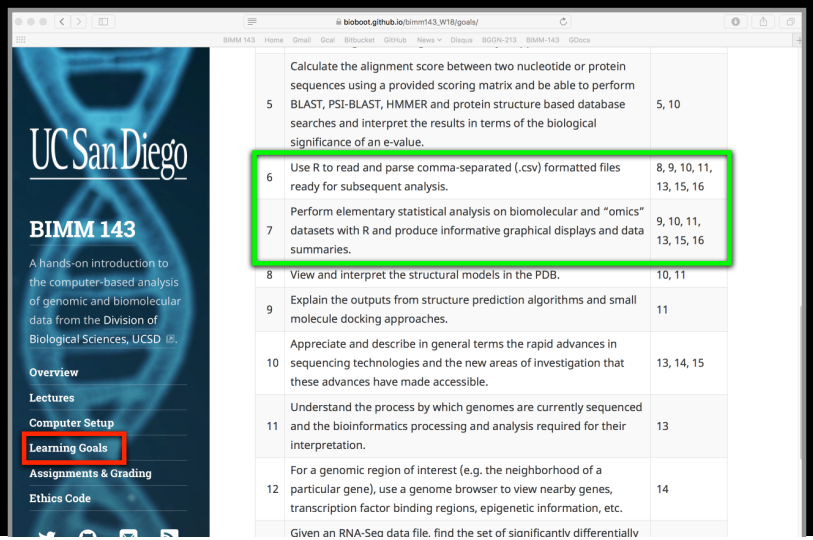
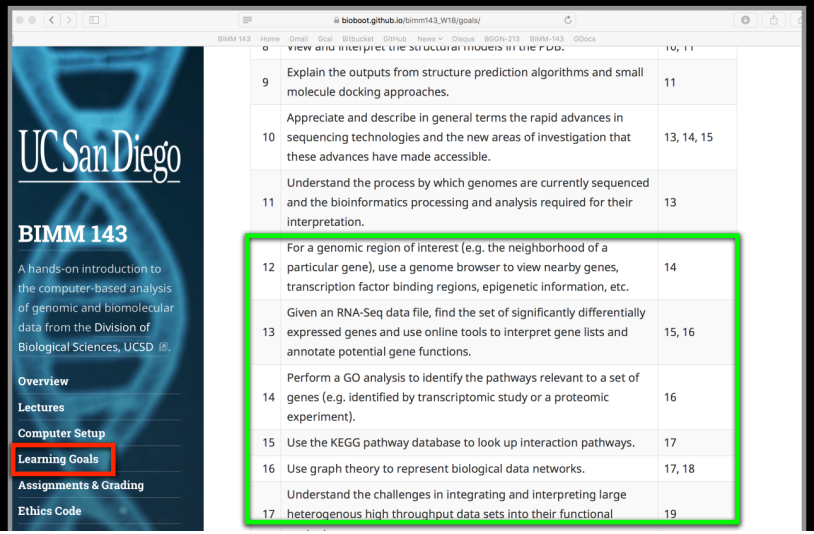
BIMM-143 Learning Goals....

Data science R based learning goals



BIMM-143 Learning Goals....

Delve deeper into "real-world" bioinformatics



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.

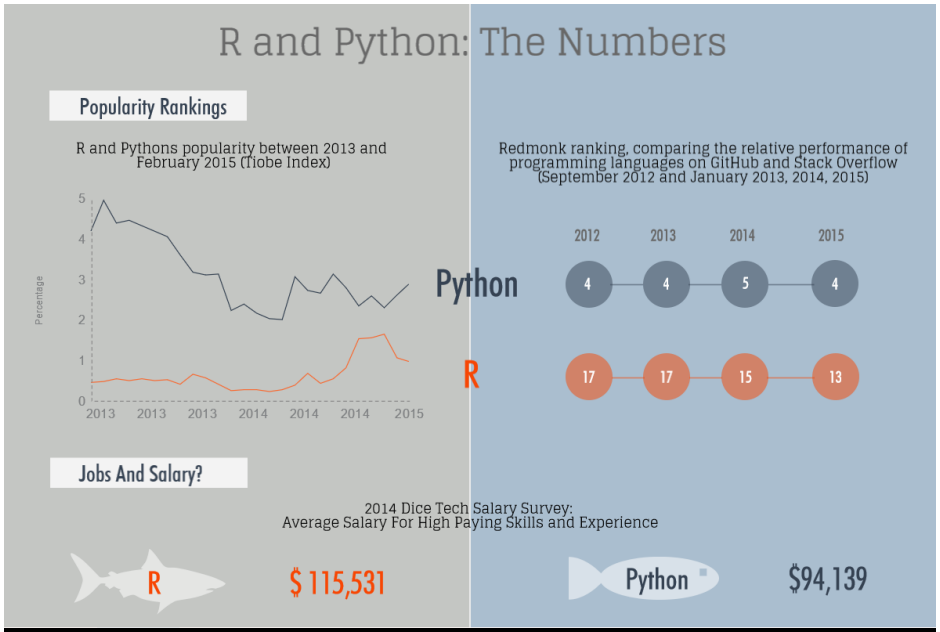
Why use R?

Productivity
Flexibility
Genomic 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

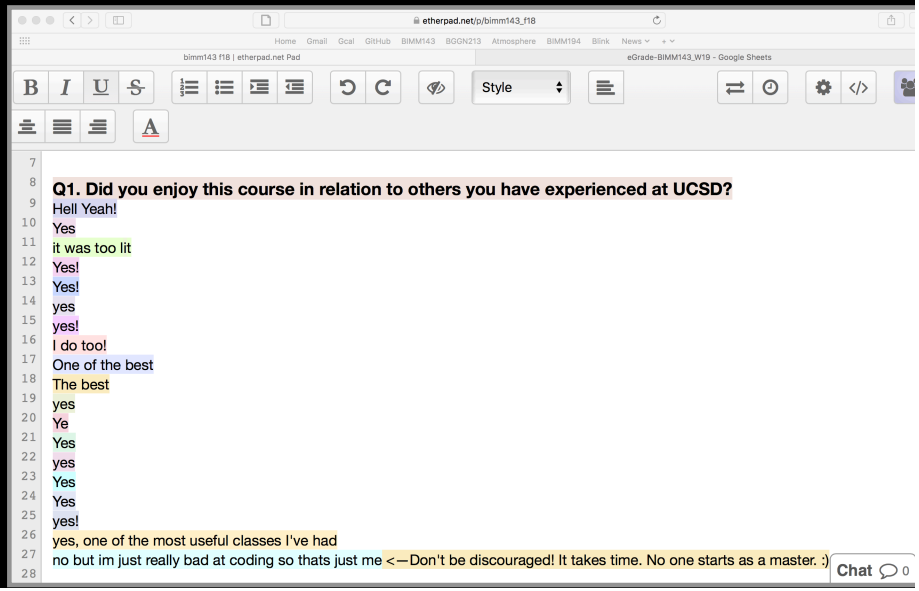
http://spectrum.ieee.org/computing/software/the-2016-top-programming-languages



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 and was designed specifically for data analysis.
- Large friendly user and developer community.
  - As of Jan 6th 2019 there are 13,645 add on **R packages** on **CRAN** and 1,649 on **Bioconductor** - more on these later!
- Virtually every statistical technique is either already built into R, or available as a free package.
- Unparalleled data analysis environment for **high-throughput genomic data**.

Past Student Opinions...



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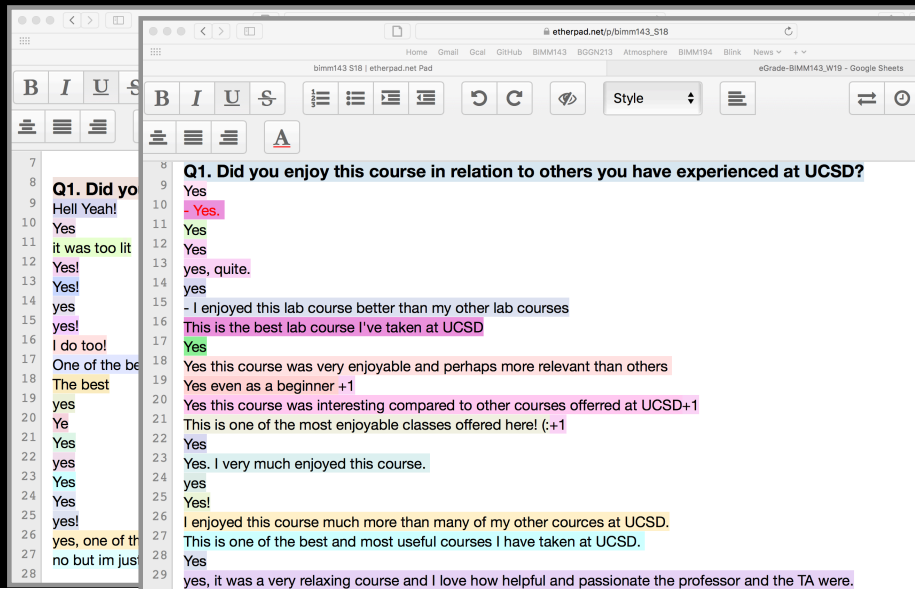

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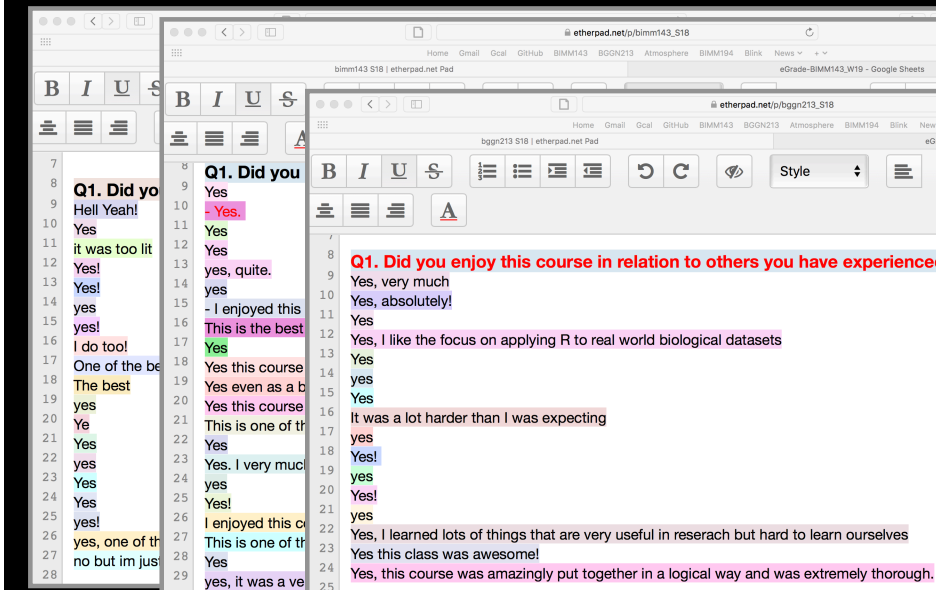

Q1. Did you enjoy this course in relation to others you have experience

Yes, very much
Yes, absolutely!
Yes
Yes, I like the focus on applying R to real world biological datasets
Yes
yes
Yes
It was a lot harder than I was expecting
yes
Yes!
yes
Yes!
yes
Yes, I learned lots of things that are very useful in reserach but hard to learn ourselves
Yes this class was awesome!
Yes, this course was amazingly put together in a logical way and was extremely thorough.

Instructor	Course	Term	Rcmnd Class	Rcmnd Instr	Study Hrs/wk	Avg Grade Expected	Avg Grade Received
Grant, Barry J	BIMM 143 - Bioinformatics Laboratory (A)	FA18	100.0 %	100.0 %	4.50	B+ (3.53)	N/A
Grant, Barry J	BIMM 143 - Bioinformatics Laboratory (A)	SP18	94.7 %	94.7 %	5.66	B+ (3.63)	B+ (3.35)
Grant, Barry J	BIMM 143 - Bioinformatics Laboratory (A)	WI18	100.0 %	100.0 %	5.64	B+ (3.64)	N/A
Grant, Barry J	BIMM 194 - Adv Topics-Molecular Bio (C)	WI18	92.9 %	100.0 %	1.30	A (4.00)	A (4.00)
Average for BIMM143:			98.2 %	98.2 %	5.27		

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Introduction to Bioinformatis	Introducing the *what*, *why* and *how* of bioinformatics?
Bioinformatics Database	Hands-on exploration of several major databases and their associated tools.

Q. What is Bioinformatics?

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… Bioinformatics is a hybrid of biology and computer science

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… **Bioinformatics is computer aided biology!**

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"*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)

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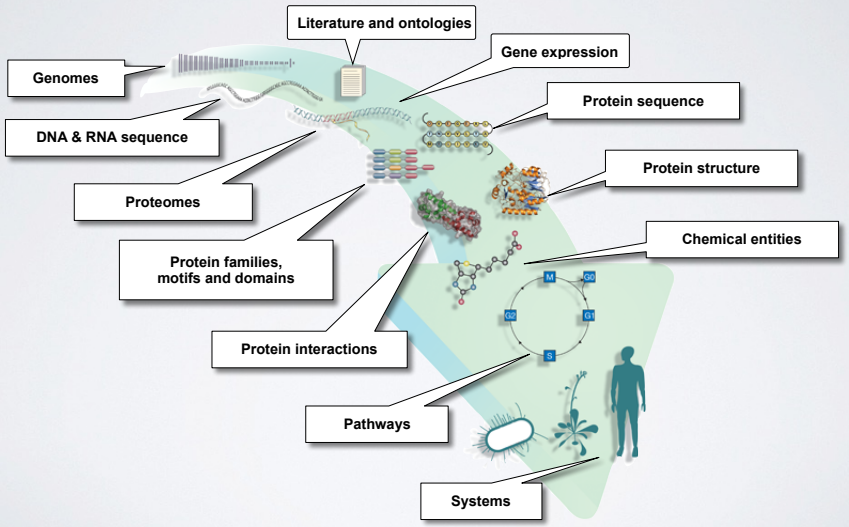
Key Point: Bioinformatics is Computer Aided Biology

Major types of Bioinformatics Data



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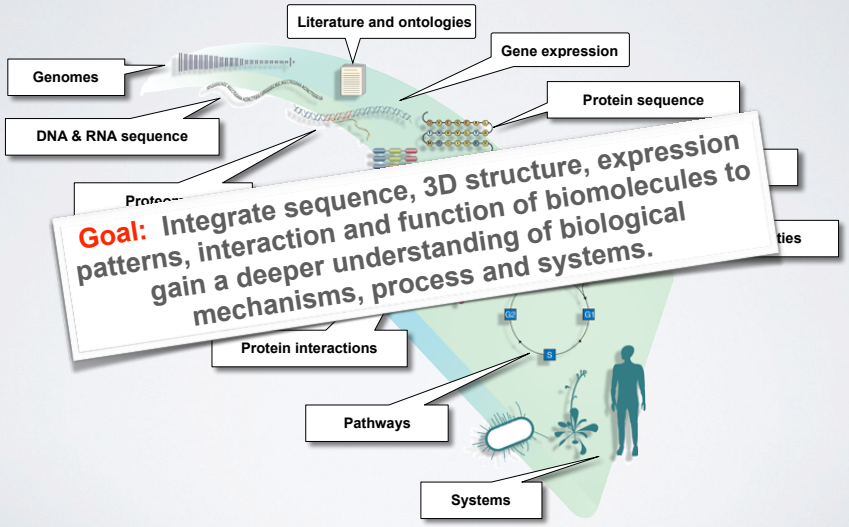
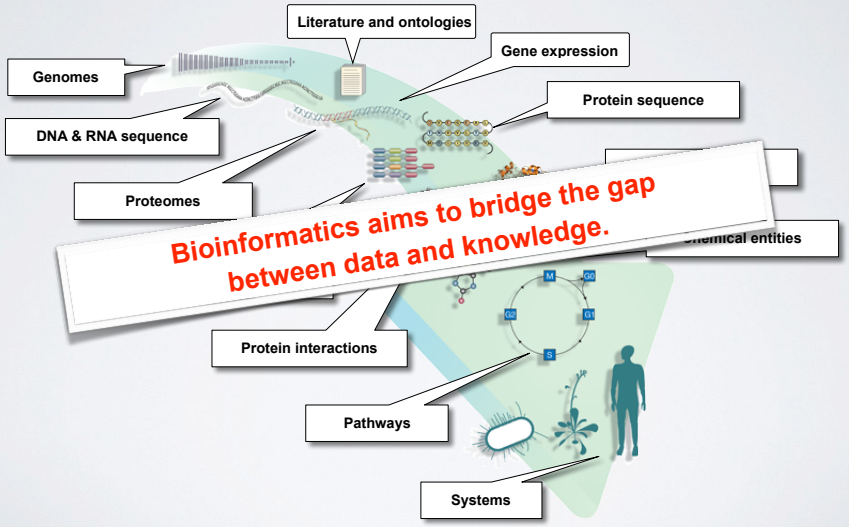


Goal: Integrate sequence, 3D structure, expression patterns, interaction and function of biomolecules to gain a deeper understanding of biological mechanisms, process and systems.

Major types of Bioinformatics Data



Bioinformatics aims to bridge the gap between data and knowledge.

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

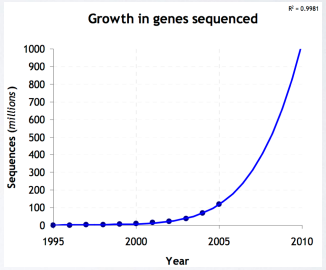
- *DNA sequence* determines *protein sequence*.
- *Protein sequence* determines *protein structure*.
- *Protein structure* determines *protein function*.
- *Regulatory mechanisms* (e.g. gene expression) determine the amount of a particular *function in space and time*.

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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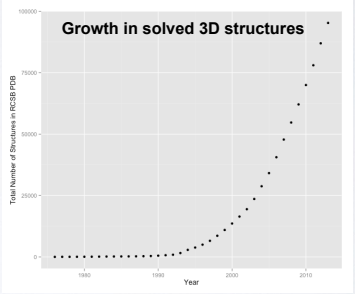

E.G. data from sequencing, structural genomics, proteomics, new high throughput assays, *etc*…

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.

DNA	→	RNA	→	Protein
Genome	→	**Transcriptome**	→	**Proteome**

x 1,000

x 100,000

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 programing languages frequently required (*e.g.* **R**, Python, Perl, C, Java, Fortran)
- May require specialized high performance computing…

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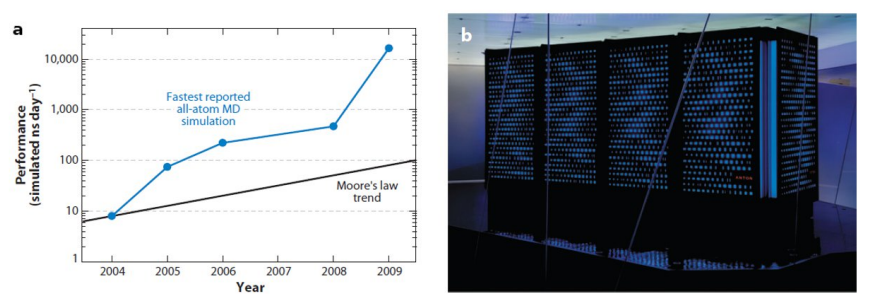
SIDE-NOTE: SUPERCOMPUTERS AND GPUS



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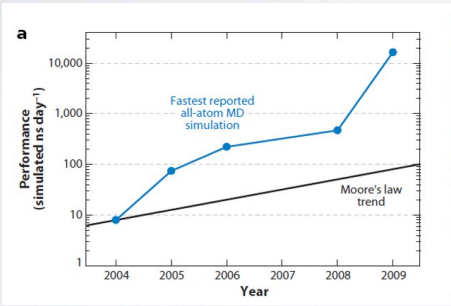
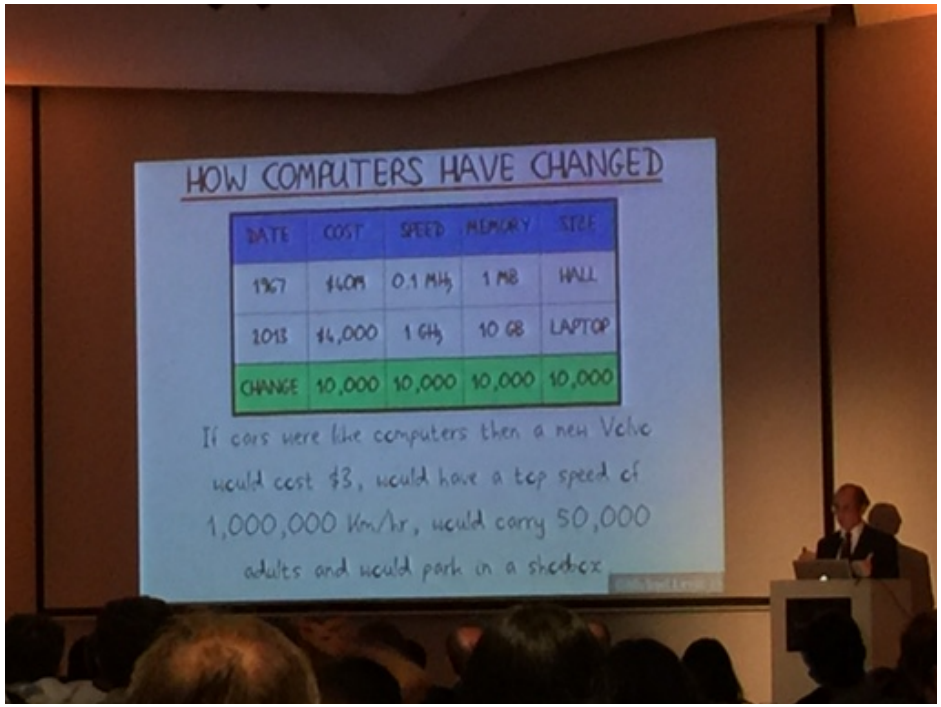




Skepticism & Bioinformatics

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 *"Sequence Analysis in Molecular Biology"* states:

➡"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'!**

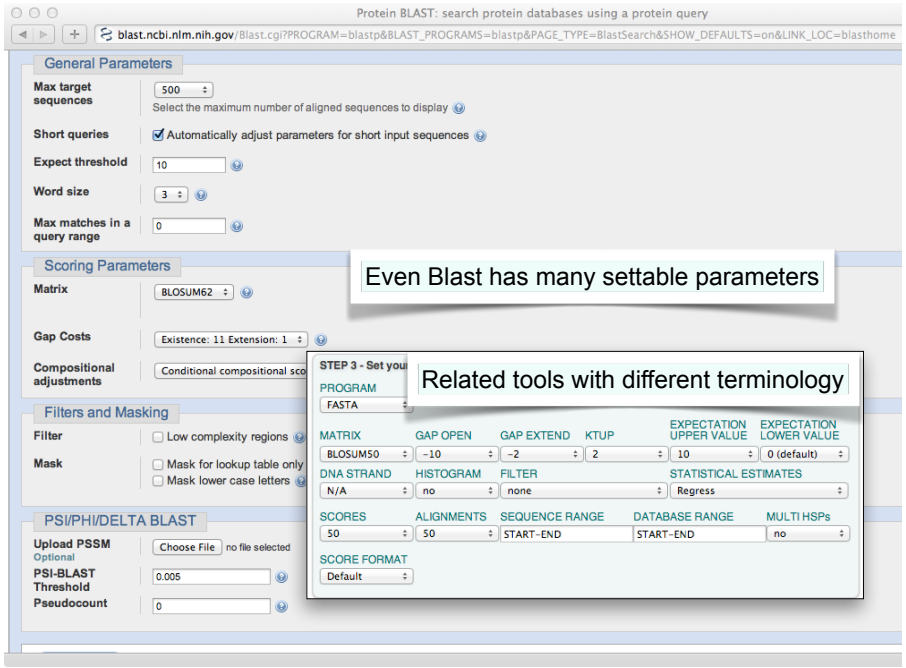
Common problems with Bioinformatics

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!

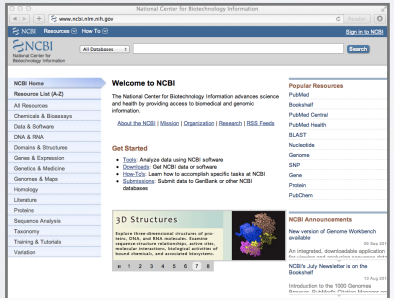
Most are developed independently

Notable exceptions are found at the:
- **EBI** (European Bioinformatics Institute) and
- **NCBI** (National Center for Biotechnology Information)

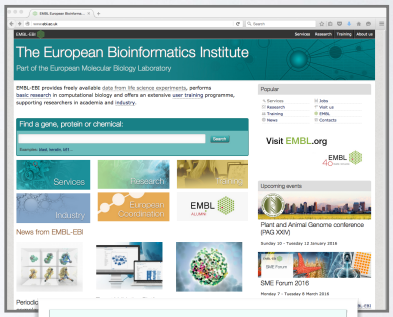


Key Online Bioinformatics Resources: NCBI & EBI

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



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



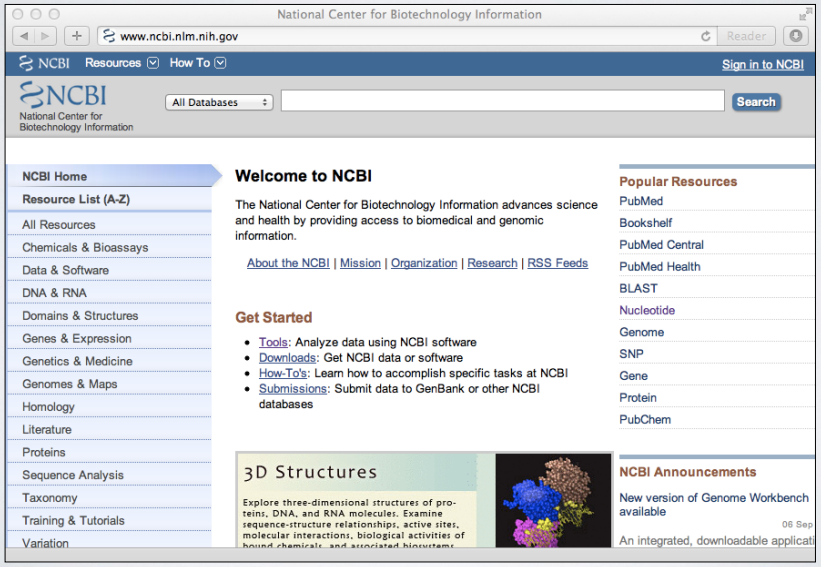
https://www.ebi.ac.uk

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



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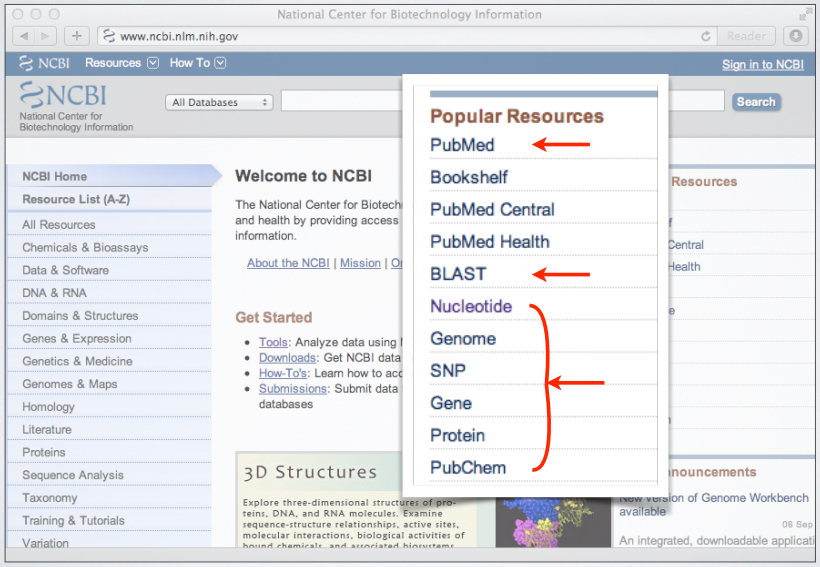

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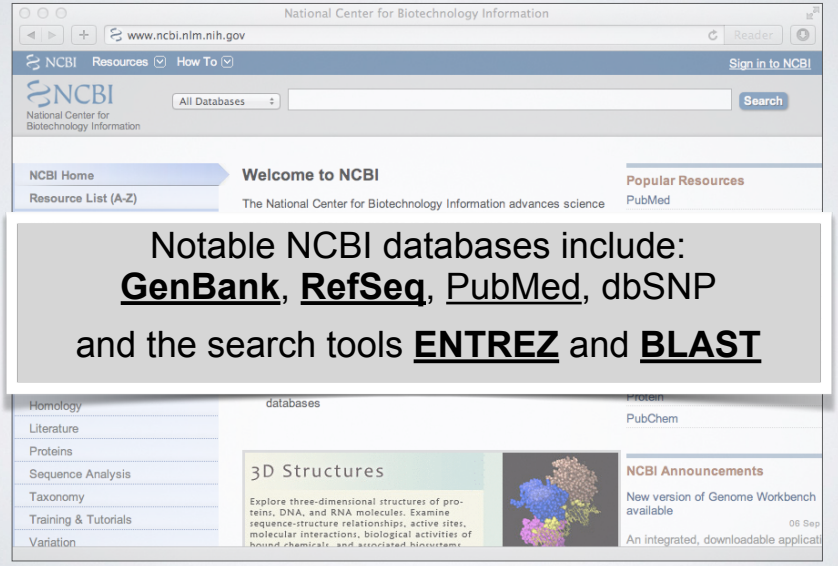
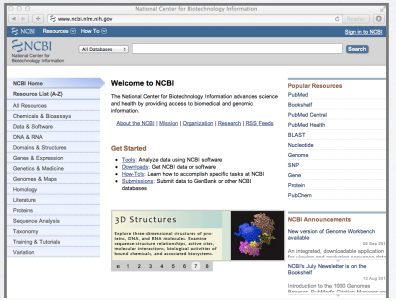


Notable NCBI databases include:
GenBank, **RefSeq**, PubMed, dbSNP

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

Key Online Bioinformatics Resources: NCBI & EBI

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



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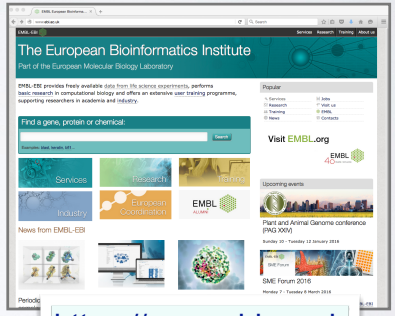


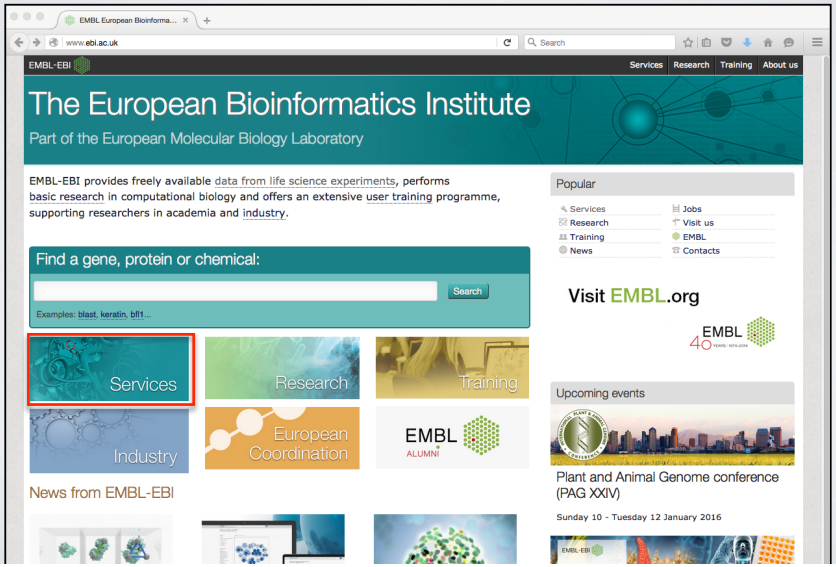
https://www.ebi.ac.uk

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



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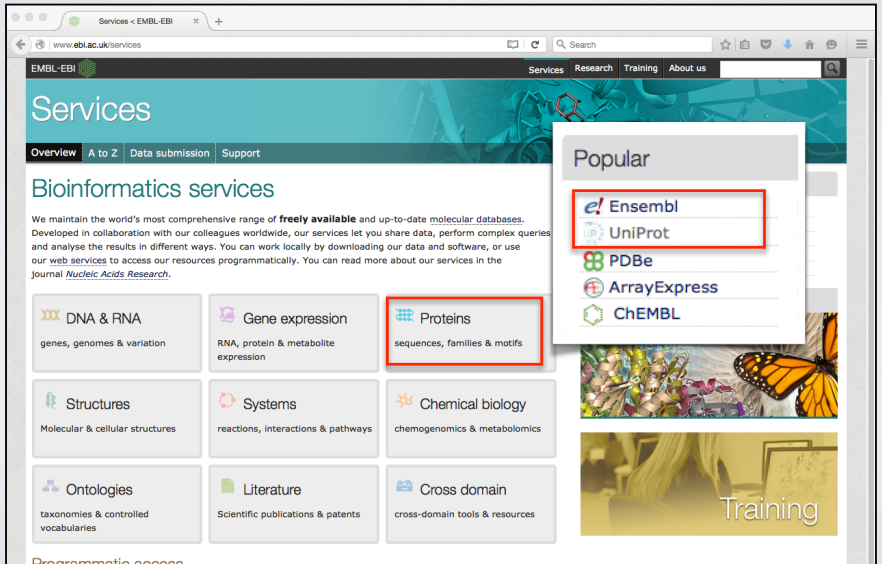
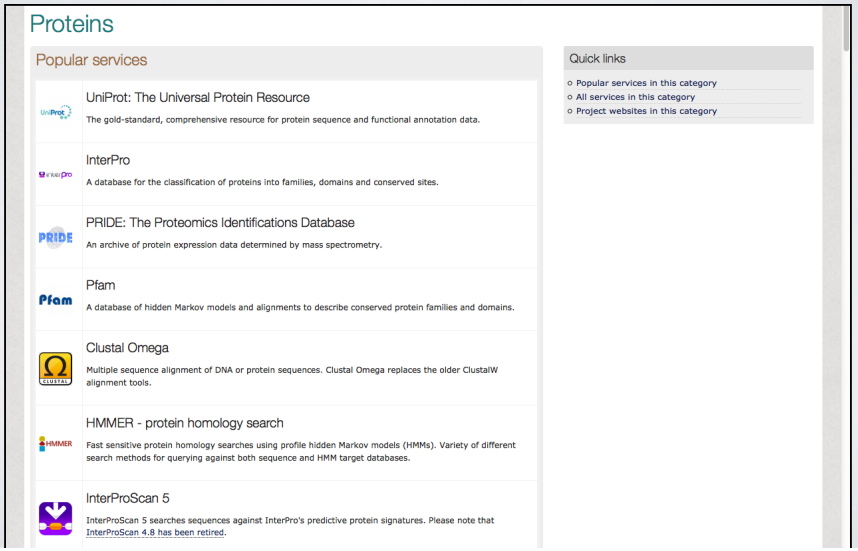
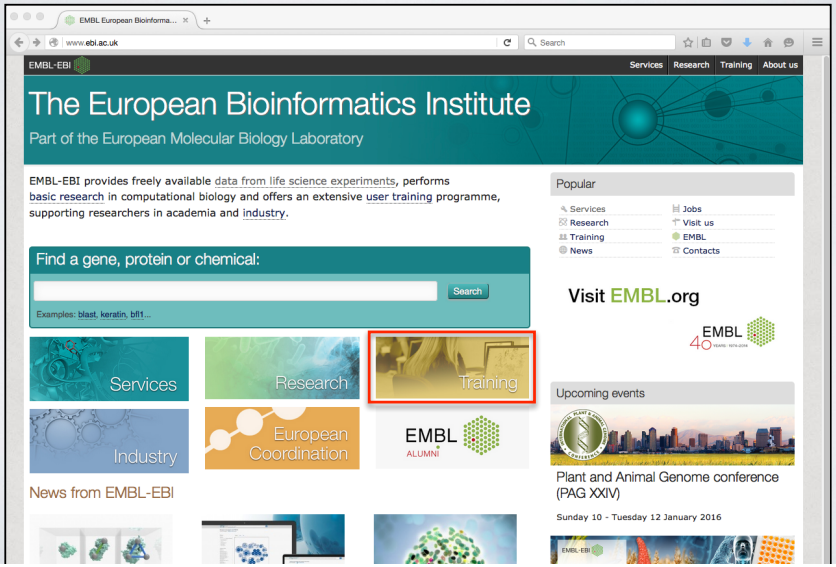


https://www.ebi.ac.uk

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



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



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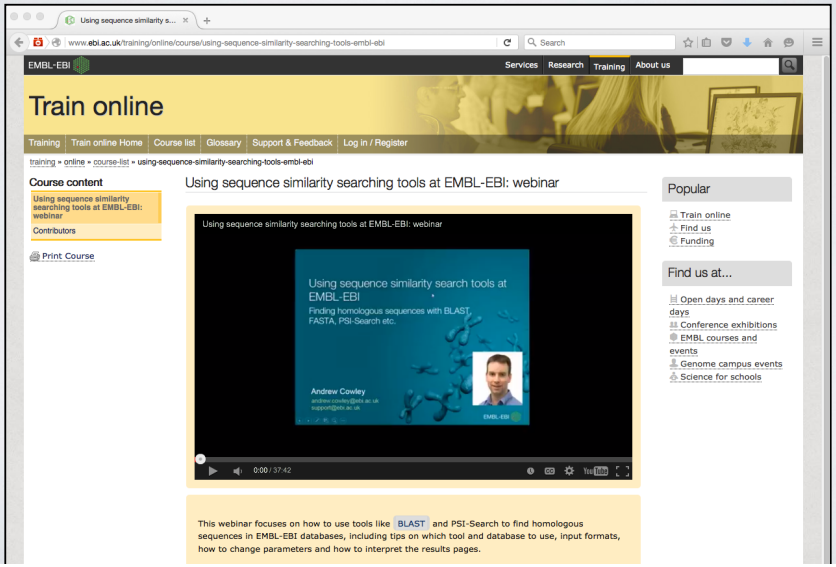

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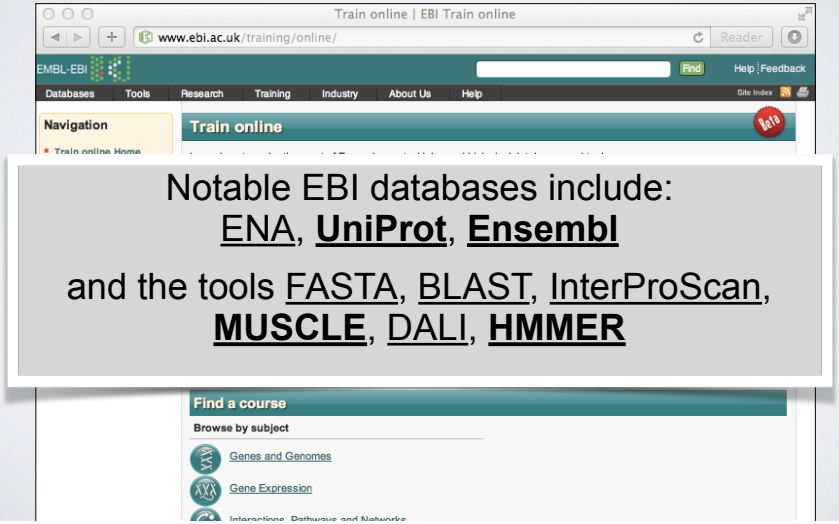


Notable EBI databases include:
ENA, **UniProt**, **Ensembl**

and the tools FASTA, BLAST, InterProScan, **MUSCLE**, DALI, **HMMER**

Bioinformatics Databases

AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb,BBDB, BCGD, Beanref, BioImage, 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, 0-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, TelDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene, URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, etc ..... !!!!

Bioinformatics Databases

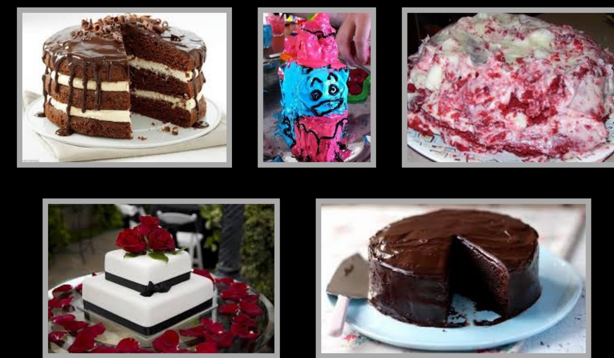
AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb, BBDB, BCGD, Beanref, BioImage, BioMagResBank, BIOMDB, BLOCKS, BovGBASE, BOVM... TKbase, CANSITE, CarbBank, CARBHYD, CATH, CAZY ... AP, ChickGBASE, Colibri, COPE, CottonDB ... bEST, dbSTS, DDBJ, DGP, DictyDb ... CDC, ECGC, EC02DBASE ... THER, FlyBase ... Link, G... DB, HAEMB, H... HotMolecBase, H... ZRGbase, IMGT, Kabat, KDNA, K... DB, Medline, Mendel, MEROPS, MGDB, MGI, MHC... OMAP, MJDB, MmtDB, Mol-R-Us, MPDB, MRR, MutBase, My... O-lycBase, OMIA, OMIM, OPD, ORDB, OWL, PAHdb, PatBase, PD... DB, 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



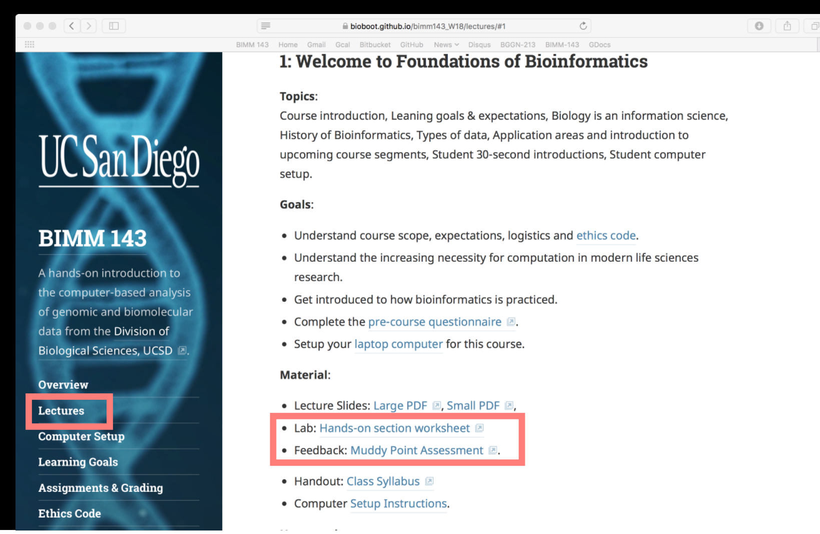
Databases can be of variable quality and often there are multiple databases with overlapping content.

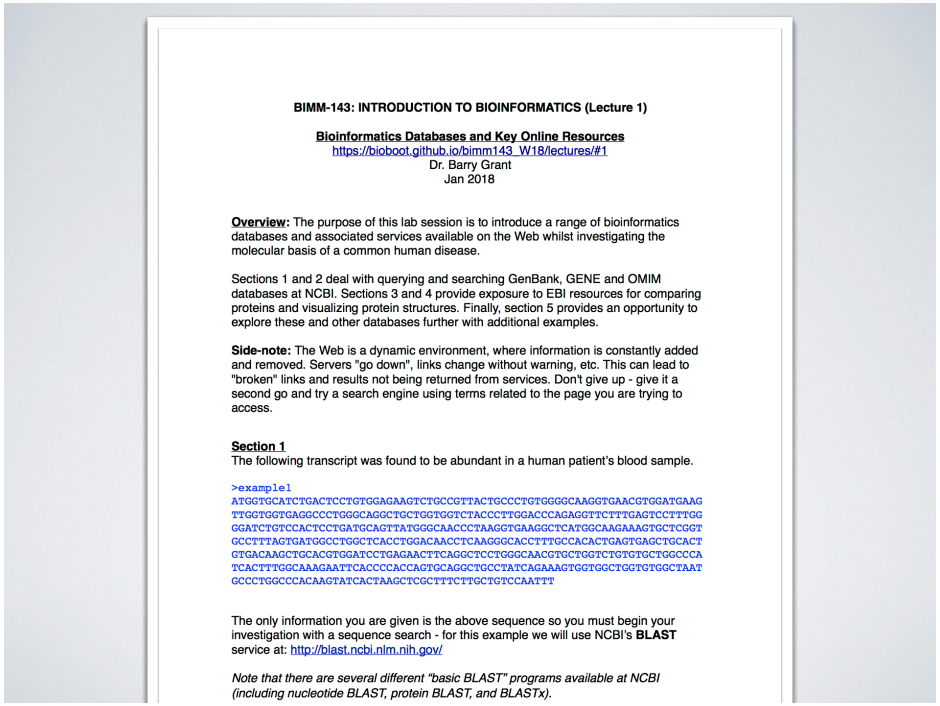
Today's Menu

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 leaning goals.
Introduction to Bioinformatis	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_W19/lectures/#1





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
ATGGTGCATCTGACTCCTGTGGAGAAGTCTGCCGTTACTGCCCTGTGGGGCAAGGTGAACGTGGATGAAG
TTGGTGGTGAGGCCCTGGGCAGGCTGCTGGTGGTCTACCCTTGGACCCAGAGGTTCTTTGAGTCCTTTGG
GGATCTGTCCACTCCTGATGCAGTTATGGGCAACCCTAAGGTGAAGGCTCATGGCAAGAAAGTGCTCGGT
GCCTTTAGTGATGGCCTGGCTCACCTGGACAACCTCAAGGGCACCTTTGCCACACTGAGTGAGCTGCACT
GTGACAAGCTGCACGTGGATCCTGAGAACTTCAGGCTCCTGGGCAACGTGCTGGTCTGTGTGCTGGCCCA
TCACTTTGGCAAAGAATTCACCCCACCAGTGCAGGCTGCCTATCAGAAAGTGGTGGCTGGTGTGGCTAAT
GCCCTGGCCCACAAGTATCACTAAGCTCGCTTTCTTGCTGTCCAATTT
```

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**	[10:35 am]
2. GENE database @ **NCBI**	[10:55 am]
— BREAK —	— 11:05 am —
3. UniProt & Muscle @ **EBI**	[11:30 am]
4. PFAM, PDB & NGL	[12:00 pm]
— BREAK —	— 12:10 am —
5. Extension exercises	[12:40 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.
- 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_W19/lectures/#1

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