

# Bioinformatics and Computational Biology

(Opportunities & Challenges to solve complex problems)

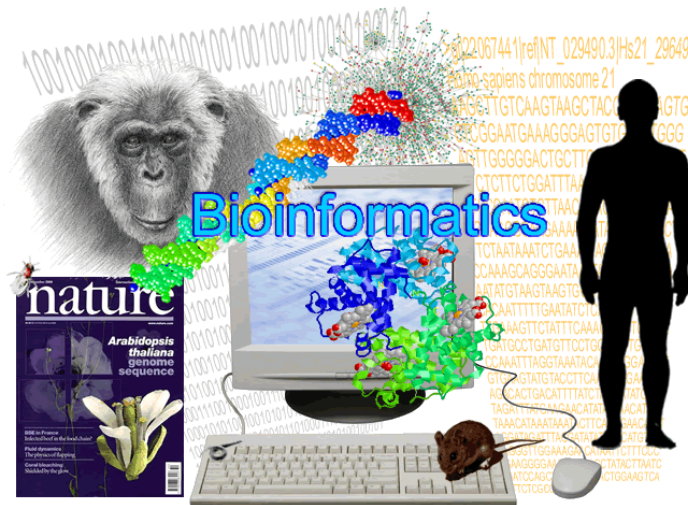


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# Bioinformatics

## Why it's useful...

- All of the information needed to build an organism is contained in its DNA. If we could understand it, we would **know how life works**.
  - Preventing and curing diseases like cancer (which is caused by mutations in DNA) and inherited diseases.
  - **Curing infectious diseases** (everything from AIDS and malaria to the common cold). If we understand how a microorganism works, we can figure out how to block it.
  - Understanding genetic and **evolutionary relationships** between species
  - Understanding **genetic relationships** between humans. Projects exist to understand human genetic diversity
  - Similarly, other Eukaryotes are being sequenced including plants, e.g. to understand **plant diseases**, their **tolerance under stress conditions** *etc.*
  - Prokaryotes, **Metagenome** sequencing.....



**Resistant**

**Susceptible**



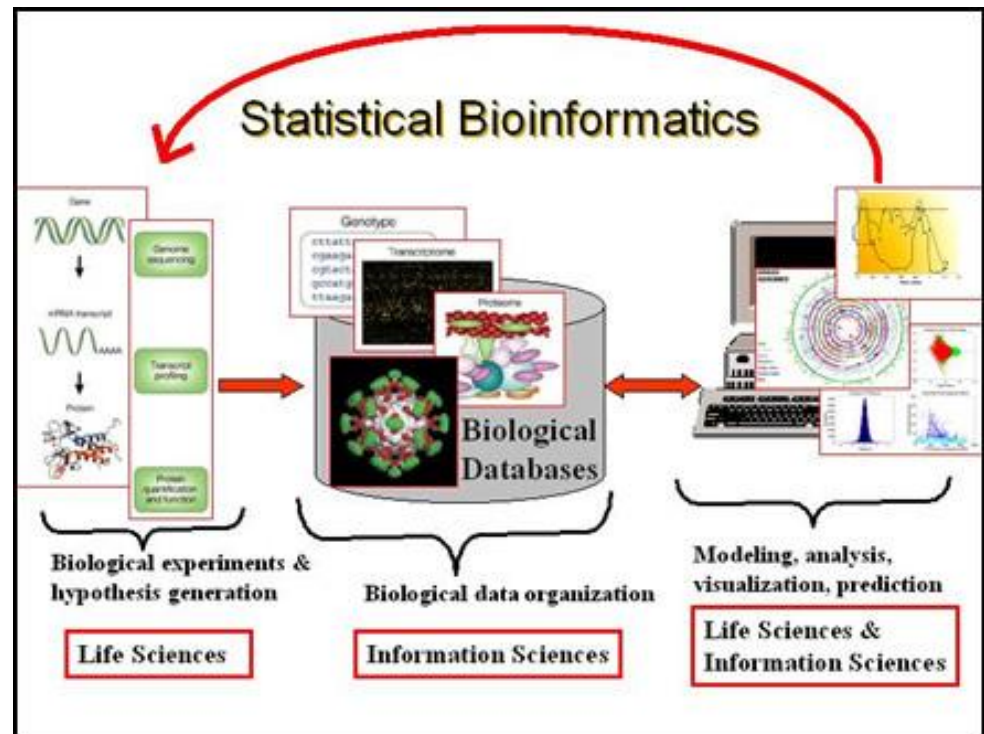
**Abiotic stress**

# Large-scale sequence analysis

## (Processing and Assembly)

Data Processing (e.g. EST to Unigene):

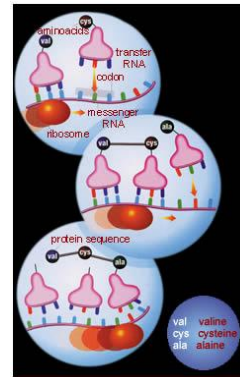
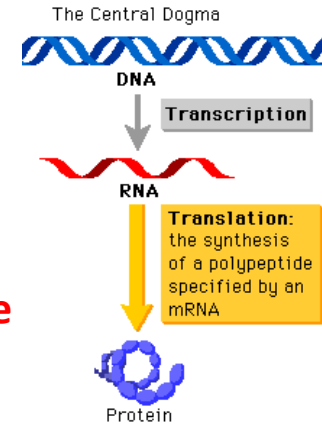
- EST cleaning (vector, adapter seqs etc.)
- Assembly (Tentative Consensus, Singletons)
- Unigenes
- Annotation



# Large-scale sequence analysis

(Annotation: adding biological information to sequence)

- **Annotation by homology (BLAST)**
  - requires a large, well annotated database of protein / nucleotide sequences
- **Annotation by sequence composition**
  - simple statistical/mathematical methods
- **Annotation by sequence features, profiles or motifs (InterProScan, PFAM)**
  - requires sophisticated sequence analysis tools
- **Annotation by Artificial Intelligence**
  - Identify 'known' from the 'unknowns' based on training the features from known samples
  - computational tools for prediction



What if there is **No** homology in the reference database or **NO HITS**?

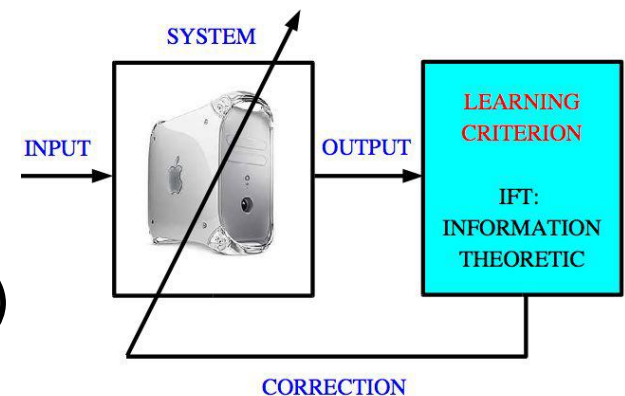
*(most of the time, this is the case.....)*

# Computational Intelligence

(offshoot of Artificial Intelligence)

- Machine Learning: an iterative *process* where a computer can **learn** from **experience E** with respect to some class of **tasks T** and **performance measure P**, if its performance at tasks T, as measured by P, improves with experience.

- Artificial Neural Networks (ANN)
  - Self-Organized Maps (SOMs)
- Bayesian statistics
- Decision tree learning
- Support Vector Machines (SVM)





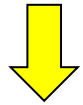
# Modeling of Biological Systems

## 'Omics' technologies

DNA



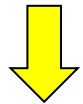
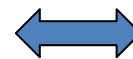
Gen*omics*



mRNA



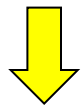
Transcript*omics*



Protein



Prote*omics*

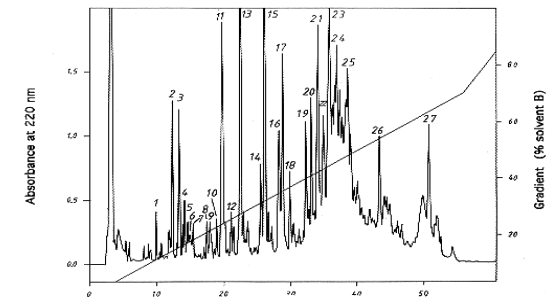
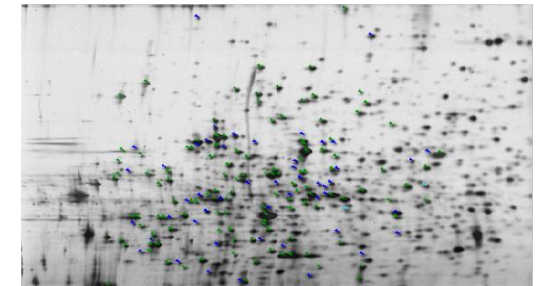
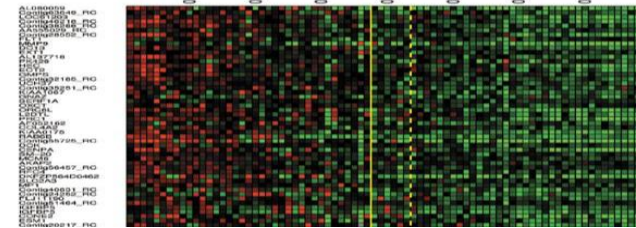


Metabolite

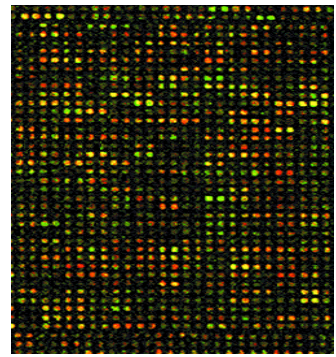


Metabol*omics*

```
Q 366 TAACCTTGAATAATCACCACAGCAAAAATATTTTACCATTAAAAAATCAGTCTTAGAAAT
T 29069186 TAACCTTGAATAATCACCACAGCAAAAATATTTTACCATTAAAAAATCAGTCTTAGAAAT
Q 426 GATTTATCTATTTTAAGATTTTAATCTAATTTAGTGAATCAAAAATTTTAAATCAGTGTG
T 29069246 GATTTATCTATTTTAAGATTTTAATCTAATTTAGTGAATCAAAAATTTTAAATCAGTGTG
Q 486 ATGGCAAATCTGCAAAAAGGTATTTGTACTTTTACATAAGGATCTTAGAAATATGGTATAA
T 29069306 ATGGCAAATCTGCAAAAAGGTATTTGTACTTTTACATAAGGATCTTAGAAATATGGTATAA
Q 546 AAACAATTTTGTGCTAGATGACAAGCAATTTTGAGCTTTTTTCTA
T 29069366 AAACAATTTTGTGCTAGATGACAAGCAATTTTGAGCTTTTTTCTA
```



# Artificial Intelligence in Bioinformatics



mRNA  
expression data

Subcellular  
Localization  
Prediction

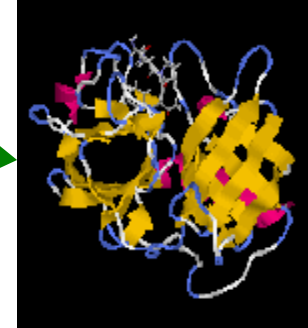
Metabolic Networks  
(identify pathways)



Metagenomics

Computational  
Epidemiology  
(Disease prediction)

Putative

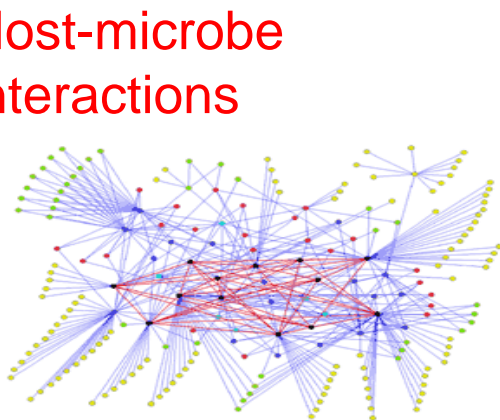


Function

Sequence signatures  
(gene, protein)

```
QFDACCFIDDVSKIYG-DYGP  
QFDACCFIDDVSKIYG-DHGP  
QFGACCFIDDVSKIFRLEDGPI  
QFDAC-FIDDVSKIFRLEDGPI  
RFDACCFIDDVSKIFRLEDGPI  
QFSVXCLIDDVSKIYR-HDGP  
QFPVCSIIDDLKMYR-HDSPV  
QFPVFCLIDDLSKIYR-DDGLI  
QFDARCFIDDLSKIYR-HDGQV  
QFDARCFIDDLSKIYR-HDGP  
RFDACCFIDDVSKICK-HDGPV  
QFDACCFIDDVSKICK-HDGPV
```

Gene Regulatory  
Networks



Host-microbe  
interactions

**Thank you for your kind attention!**

<http://bic.okstate.edu/> or <http://biochemistry.okstate.edu/>