CS4220: Knowledge Discovery Methods in Bioinformatics
Course Briefing

Wong Limsoon

Recommended "Pre-requisites"

- **Completed modules on**
  - Programming
  - Algorithms
  - Basic molecular biology
  - **ST2334 Probability & Statistics**
  - **CS2220 Introduction to Computational Biology**

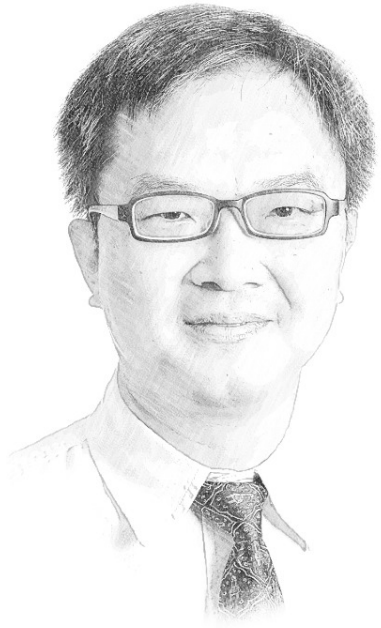
Objectives

- **Exposure to knowledge-discovery techniques**
- **Enhance flexible & logical problem-solving skill**
- **Understand bioinformatics problems and their solution in depth**
  - A modern network-based perspective

- **To achieve goals above, we expose students to case studies spanning gene expression and proteomic analysis, protein functional prediction, epistatic interaction analysis, etc.**

Professors

- **Wong Limsoon**



- **Anders Skanderup**

Contents of Course Overview

- Time Table
- Course Syllabus
- Course Homepage
- Teaching Style
- Project, Assignments, Exams
- Readings
- Assessment

- Quick Overview of Themes and Applications of Bioinformatics

Time Table

- **Lecture**
  - Tuesday 12nn-3pm at COM1-204
- **"Tutorial" (it is integrated into lecture)**

- **Emails**
  - wongls@comp.nus.edu.sg
  - skanderupamj@gis.a-star.edu.sg

- **Consultation**
  - Any time; just make appt

Course Syllabus

- **Essence of Biostatistics**
  - Statistical estimation
  - Hypothesis testing
  - Principle component analysis
- **Essence of Data Mining**
  - Clustering
  - Association rules
  - Classification
  - Class-imbalance learning
- **Gene Expression Analysis**
  - Basic gene expression analysis
  - Improving reproducibility
  - Dealing with small sample
- **Proteomic Profile Analysis**
  - Basic proteomic profile analysis
  - Improving consistency
  - Improving coverage
- **Batch effects**
  - Visualization
  - Normalization
  - PC1 removal
  - Batch effect-resistant feature selection
  - Batch effect-resistant classifiers
- **Network Perturbations in Disease Context**
- **Other classic or hot topics to be determined**

Teaching Style

- **Bioinformatics is a broad area**
- **Need to learn a lot of material by yourself**
  - Reading papers
  - Try the exercises
  - Practise on the w

And do this before each lecture

- **Don't expect to be told everything**

Assignments, Project, & Exam

- **Assignments (30-40% of marks)**
  - 3 to 4 assignments
  - Some are simple programming assignments
- **Project (20-30% of marks)**
  - Based on a case study in the class
  - 8-10 pages of report / ppt slides expected
- **Exam (40% of marks)**
  - 1 final open-book exam

Be Honest

- **Exam**
  - Absence w/o good cause results in ZERO mark
  - Cheating results in ZERO mark
- **Discussion on assignments & project is allowed**
- **Blatant plagiarism is not allowed**
  - Offender gets ZERO mark for assignment or exam
  - Penalty applies to those who copied AND those who allowed their assignments to be copied

Background Readings

- **Every lecture will be accompanied by a small set of "must-read" and "good-to-read" articles**

- **The "must-read" articles are considered lecture notes and are examinable**

Related Courses

- **CS2220 Introduction to Computational Biology**
  - Understand bioinformatics problems; interpretational skills
- **CS4330 Combinatorial Methods in Bioinformatics**
- **CS4220 Knowledge Discovery Methods in Bioinformatics**
  - Gene expression, proteomic profiling, protein interaction, transcription factor interaction, pathway perturbation
- **CS5238 Advanced Combinatorial Methods in Bioinformatics**
  - Seq alignment, whole-genome alignment, suffix tree, seq indexing, motif finding, RNA sec struct prediction, phylogeny reconstruction
- **CS6222 Computational frontier in precision medicine**
- **Etc …**

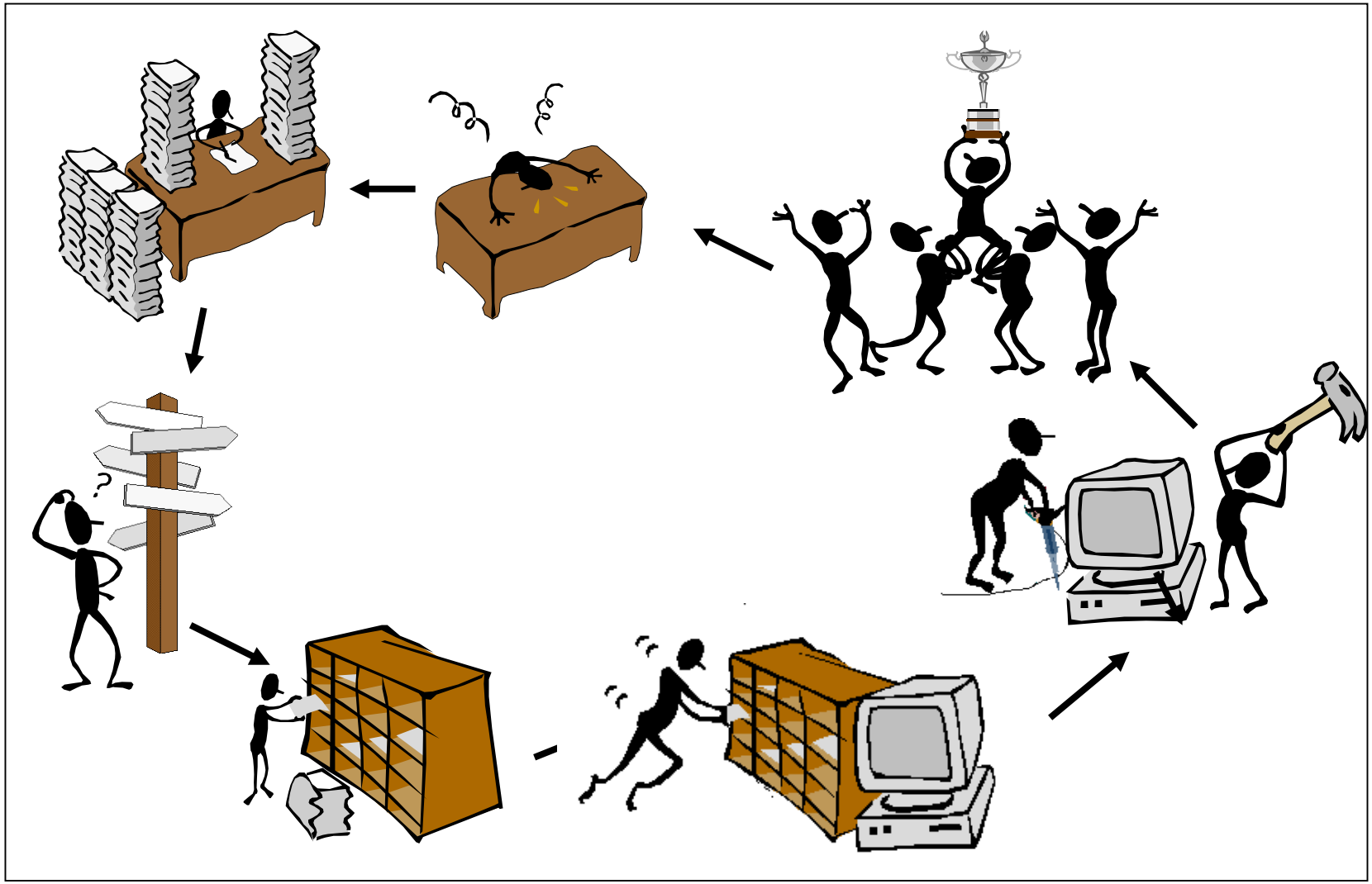
Any questions?

I hope you will enjoy this class ☺

Themes and Applications of Bioinformatics

These slides are for those who have not taken CS2220 to read at your own leisure

What is Bioinformatics?



Themes of Bioinformatics
Themes of This Course

Bioinformatics involves

Data Mgmt +
Knowledge Discovery +
Sequence Analysis +
Physical Modeling + ...

Knowledge Discovery =

Statistics + Algorithms + Databases

The Promises of Bioinformatics

To the patient:

Better drug, better treatment

To the pharma:

Save time, save cost, make more $

To the scientist:

Better science

Fulfilling the Promise via Drugs

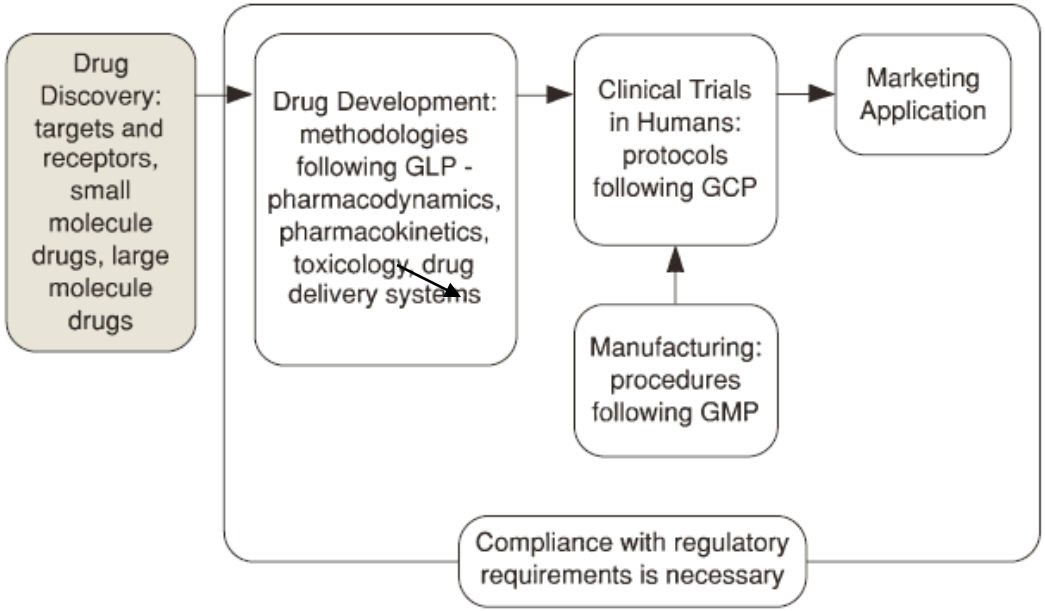


Figure from Rick Ng, *Drugs: From Discovery to Approval*

- **Bioinformatics is applicable to drug development**
- **Drug discovery: Design small molecules that bind target proteins**
  - Which proteins?
  - What should binding accomplish?
- **Biomarkers**

Pervasiveness of Bioinformatics

- **Bioinformatics is mandatory for large-scale biology**
  - e.g., High-throughput, massively-parallel measurements, or “lab on a chip” miniaturization
- **Computational data analysis is mandatory for indirect experimental methods**
  - e.g., reconstruction based on phase contrast or wave diffraction.
- **What about the rest of biology (and medicine) ?**
- **Limitless opportunities!**

Some Bioinformatics Problems

NUS National University of Singapore

- Biological Data Searching
- Biological Data Integration
- Gene/Promoter finding
- Cis-regulatory DNA
- Gene/Protein Network
- Protein/RNA Structure Prediction
- Evolutionary Tree reconstruction
- Infer Protein Function
- Disease Diagnosis
- Disease Prognosis
- Disease Treatment Optimization, ...

Commonly Used Data Sources

These slides are for those who have not taken CS2220 to read at your own leisure

Introductory References

- **S.K. Ng, "Molecular Biology for the Practical Bioinformatician", *The Practical Bioinformati*cian, Chapter 1, pages 1-30, WSPC, 2004**

- **Lots of useful videos,**
  http://www.as.wvu.edu/~dray/Bio_219.html

- **Materials from CS2220,**
  http://www.comp.nus.edu.sg/~wongls/courses/cs2220/2019