Systems eTraining in the Biosciences

Gerold Baier, UCL

SysMIC

INTERDISCIPLINARY SKILLS FOR BIOLOGICAL RESEARCH

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Systems eTraining in the Biosciences

Mathematics ✿ Informatics ✿ Computation

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Current problem in Bioscience Training

Biosciences advance
Training follows curricula
How can bioscientists stay up to date?

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Solution for Bioscience Training

Mathematics for precise, **quantitative** description
Computer programming for **digital** implementation
Engineering concepts for **rational** handling

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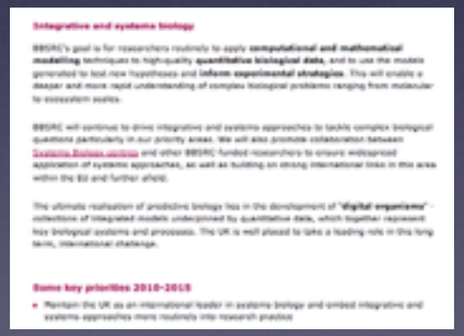
Systems eTraining in the Biosciences

BBSRC
bioscience for the future

Investing in world-class bioscience research and training on behalf of the UK public



Integrative and systems biology

BBSRC's goal is for researchers routinely to apply **computational and mathematical modelling** techniques to high-quality **quantitative biological data**, and to use the models generated to test new hypotheses and **inform experimental strategies**. This will enable a deeper and more rapid understanding of complex biological problems ranging from molecular to ecosystem scales.

BBSRC will continue to drive integrative and systems approaches to tackle complex biological questions particularly in our priority areas. We will also promote collaboration between Systems Biology centres and other BBSRC funded researchers to ensure widespread application of systems approaches, as well as building on strong international links in this area within the EU and further afield.

The ultimate realisation of predictive biology lies in the development of "**digital organisms**" - collections of integrated models underpinned by quantitative data, which together represent how biological systems and processes. The UK is well placed to take a leading role in this long term, international challenge.

Some key priorities 2010-2015

- Maintain the UK as an international leader in systems biology and embed integrative and systems approaches more routinely into research practice

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Integrative and systems biology

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Investing in world-class bioscience research and training on behalf of the UK public

2012-2016, £1m

1,250 places over 3 years

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SysMIC: the consortium

UCL, UL Birkbeck, U Edinburgh, OU

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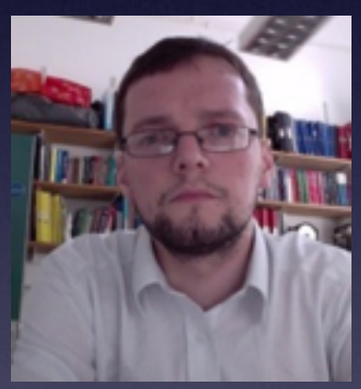
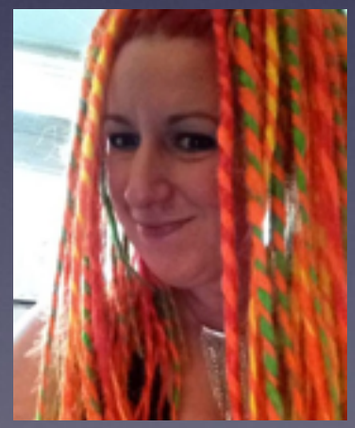
SysMIC: the UCL team

Geraint Thomas, Chris Barnes, Phil Lewis, Nadine Mogford, GB





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SysMIC Courses

Test:

September 2012 (20 London DTP students)

Currently:

about 400 trainees (different backgrounds)

[Reservation for April 2014: >200]

SysMIC Courses

BBSRC DTPs:

Oxford

Bristol / Bath / Exeter

Glasgow

Durham

Warwick

Manchester

Nottingham / Rothamstead

Reading

Cambridge

London (UCL, King's, RVC...)

Newcastle

Liverpool*

Edinburgh*

* from April 2014

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SysMIC Courses

Modular structure

3 modules – 6 months work – 5 hours / week

1: Basic skills

2: Advanced skills

3: Supervised projects

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SysMIC Online: Moodle

out

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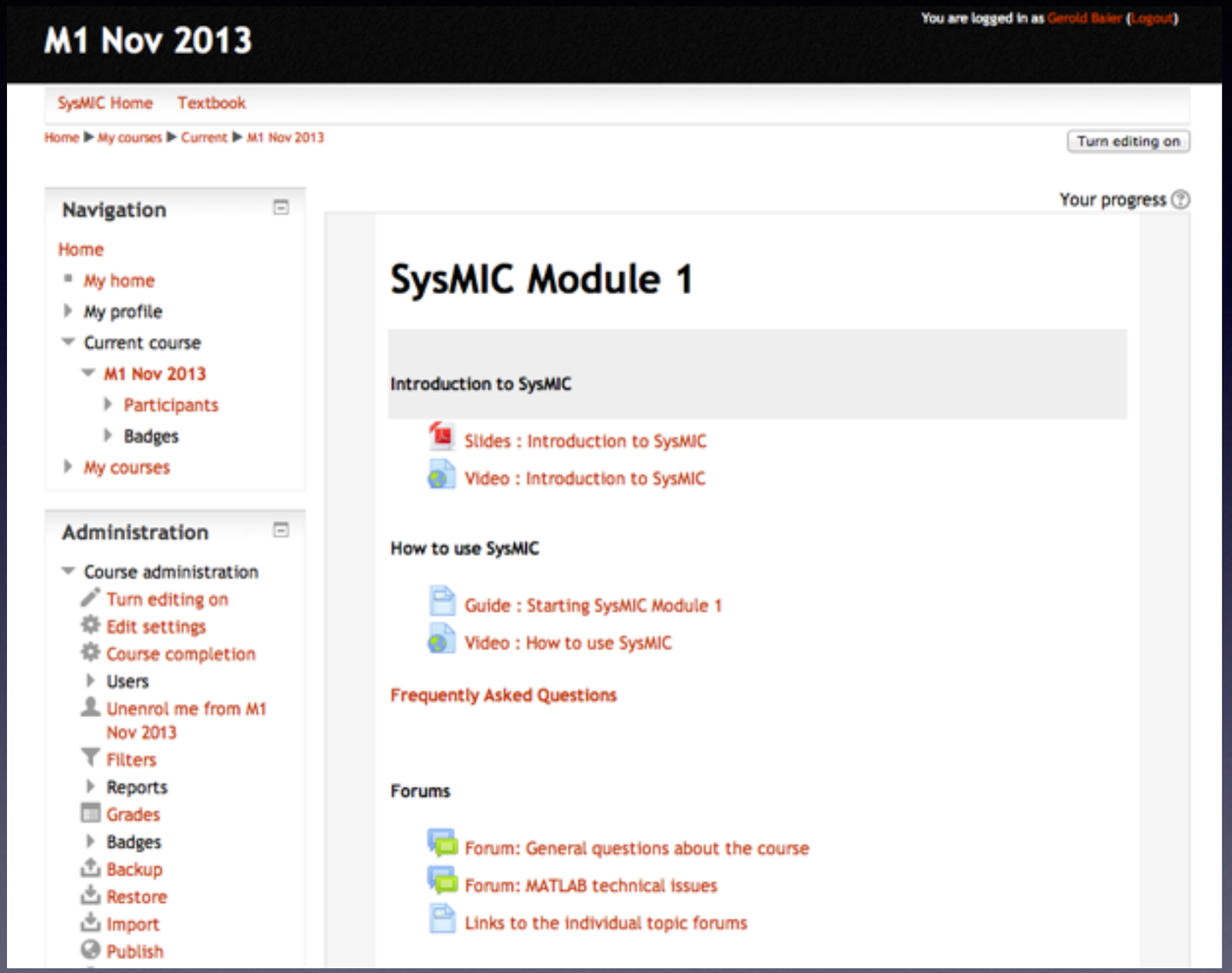

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SysMIC session

6

15th March - 28th March : 1.2 Functions and Calculus (session three)

Read the guide here for what to do in this session!

Forum: Functions and Calculus (session 3)
This is the place to ask questions if you don't understand something, or request help if you are having problems with this topic's assignment.

Materials
For this session read Biological Examples sections 1.8 and 1.9, and Mathematical Background section 2.4

- What to do in this session
- PDF : M1.2 Functions and Calculus materials (updated 15/3/13)
- Online interactive textbook: M1.2 Functions and Calculus materials

Assignment 6
From sections 1.8 and 1.9 complete and submit exercises 1.8.1 and 1.9.2. You will learn how to model two synthetic biological devices; the genetic toggle switch and the repressilator.

- Assignment 6 : Toggle switch and Repressilator
- Template for Assignment 6 (corrected for typo in Ex 1.8.1 equations)
- Repressilator you tube video

Quizzes
Read the materials in the Mathematical Background section 2.4, then attempt the quizzes:

- Quiz : Trigonometric functions (section 2.4.1) 20Qs
- Quiz : Calculus with trigonometric functions (section 2.4.1 and Appendix A) 15Qs
- Quiz : Complex numbers (section 2.4.2) 14Qs

Materials - Tasks - Tests

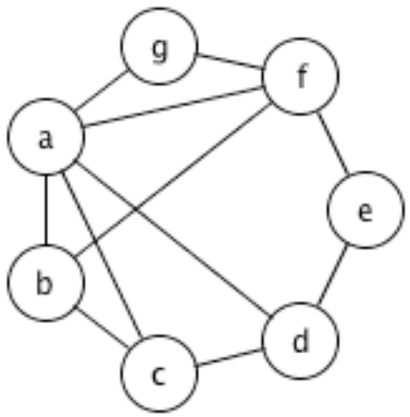
SysMIC quiz

Question 1

Complete

Marked out of 1.00

Look at this graph.



What is the clustering coefficent of node a?

Answer: 0.4

Node a has 5 neighbours, which are inter-connected by 4 edges (there are $\frac{5\times4}{2} = 10$ possibilities). Hence, the clustering coefficient of node a is $\frac{4}{10} = 0.4$.

Self-assessment

SysMIC forum

Topic 2 ▶ Forum: Networks (session 1)

Search forums

This is the place to ask questions if you don't understand something, or request help if you are having problems with this topic's assignment.

Add a new discussion topic

Discussion	Started by	Replies	Last post
Loop counts as two edges	Patrick Guest	1	Gordon Walsh Mon, 11 Feb 2013, 03:59 PM
Making changes to non-sequential nodes	Andrew Beggs	1	Gordon Walsh Wed, 30 Jan 2013, 02:28 PM
Nodes and Edges	Justin Slikas	5	Chris Barnes Mon, 28 Jan 2013, 09:47 AM
Problem with biolog function	Thomas Upton	3	Thomas Upton Tue, 22 Jan 2013, 04:36 PM

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SysMIC Interactive Applet

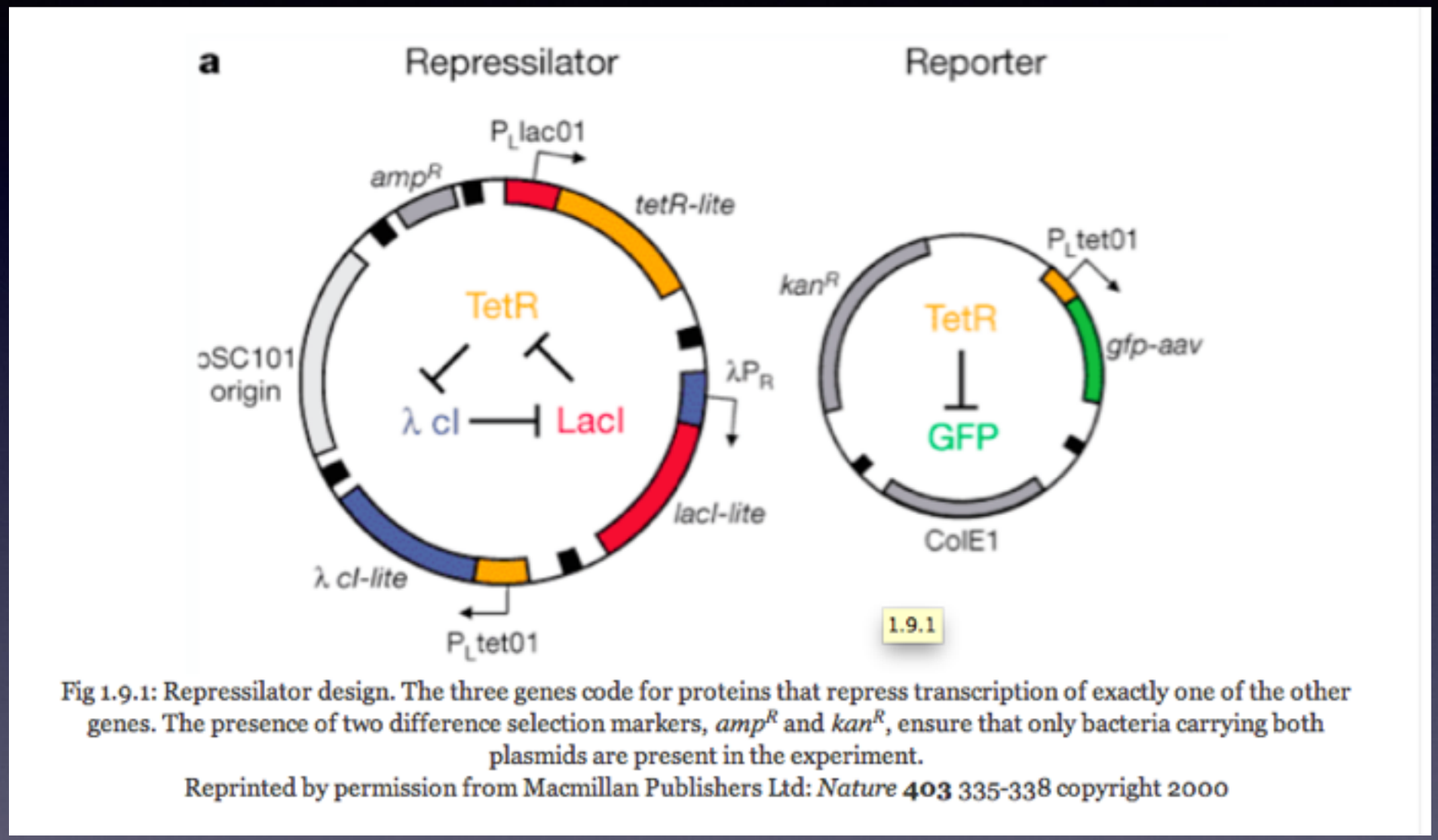

Fig 1.9.1: Repressilator design. The three genes code for proteins that repress transcription of exactly one of the other genes. The presence of two difference selection markers, amp^R and kan^R, ensure that only bacteria carrying both plasmids are present in the experiment.
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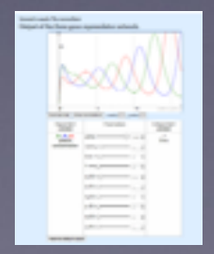
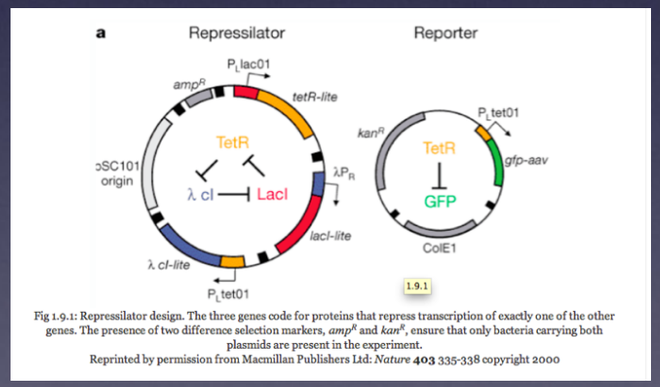
Repressilator

Elowitz, M B and Leibler, S, Nature 403 (6767), 335--338 (2000)



SysMIC Interactive Applet



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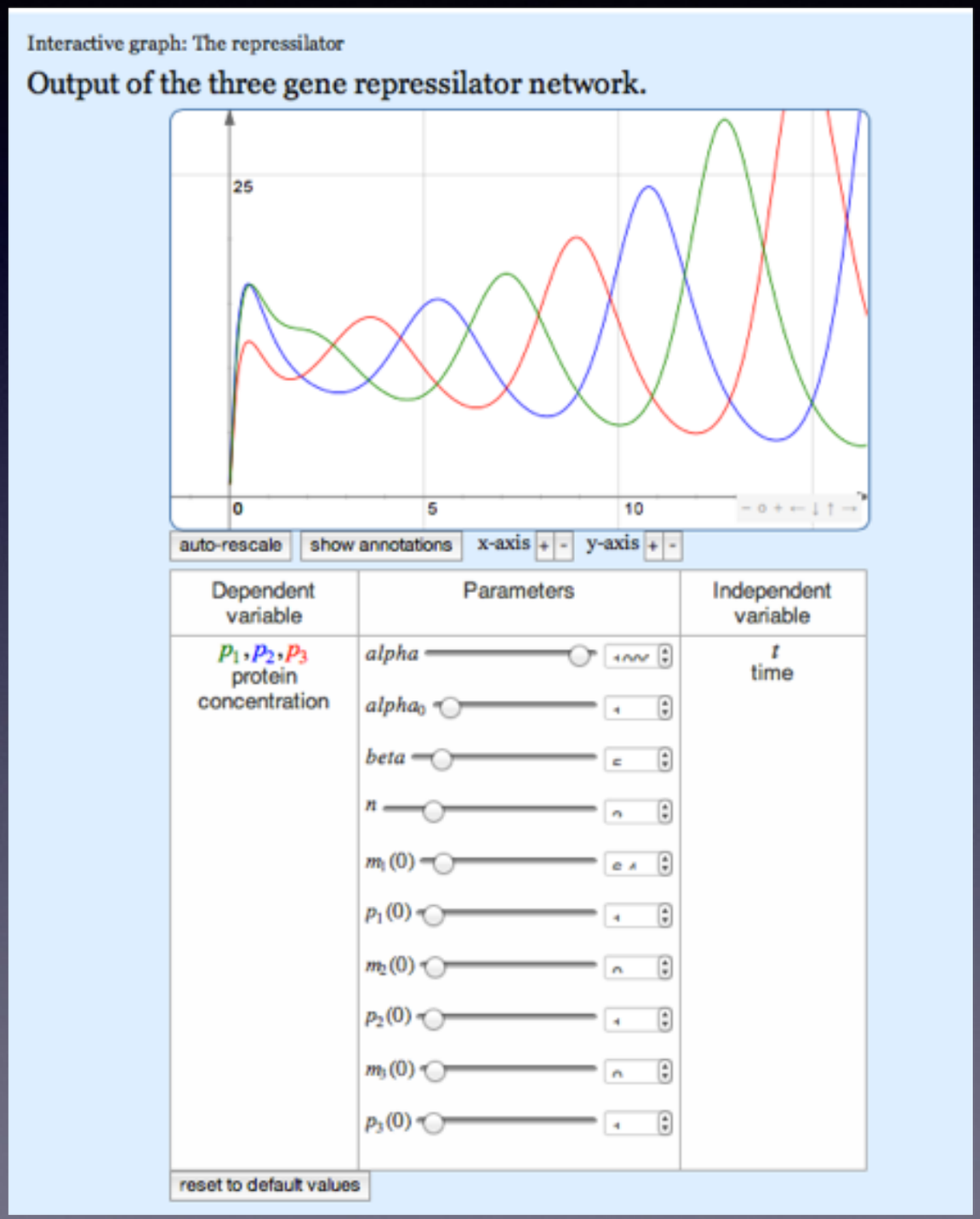

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SysMIC Exercises

Textbook PDF contains exercises but no solutions

Exercise 1.1.8

1. Verify Equation 1.1.8 separately for all three eigenvectors. Hint look at $\mathbf{L}\mathbf{v}_1 = \lambda_1\mathbf{v}_1$, $\mathbf{L}\mathbf{v}_2 = \lambda_2\mathbf{v}_2$ and $\mathbf{L}\mathbf{v}_3 = \lambda_3\mathbf{v}_3$

2. Show that multiplying an eigenvector by -1 does not alter your answer to part 1.

3. Which is the dominant eigenvalue-eigenvector pair?

SysMIC Exercises

Online version of textbook contains clickable solutions

Exercise 1.2.7

1. Calculate the covariance matrix from the ovarian cancer data. Plot the matrix using `imagesc`. Mark the healthy and patient groups.
   Solution:

```
load ovariancancer
covm = cov(obs');
imagesc(covm)
```

For output, see Figure 1.2.10

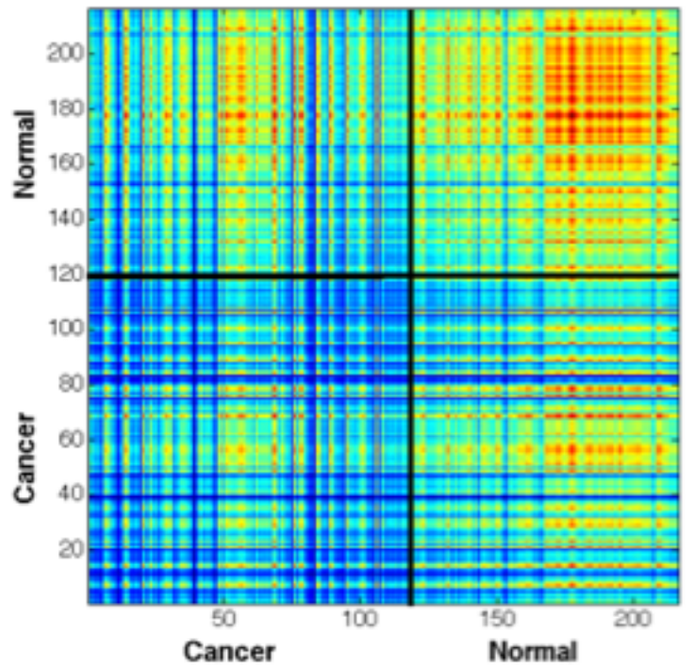

Figure 1.2.10: Covariance matrix of the ovarian cancer data. Anticorrelations are blue, correlations are red.

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Additional web materials

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Training Approach

Classical vs. Knowledge-based

SysMIC Training Approach

Classical

1. Applications of matrices

The solution of simultaneous linear equations is a task frequently occurring in engineering. In electrical engineering the analysis of circuits provides a ready example.
However the simultaneous equations arise, we need to study two things:

(a) how we can conveniently represent large systems of linear equations

(b) how we might find the solution of such equations.

We shall discover that knowledge of the theory of matrices is an essential mathematical tool in this area.

Representing simultaneous linear equations

Suppose that we wish to solve the following three equations in three unknowns x_1, x_2 and x_3:

$$\begin{aligned} 3x_1 + 2x_2 - x_3 &= 3 \\ x_1 - x_2 + x_3 &= 4 \\ 2x_1 + 3x_2 + 4x_3 &= 5 \end{aligned}$$

We can isolate three facets of this system: the **coefficients** of x_1, x_2, x_3; the **unknowns** x_1, x_2, x_3; and the **numbers** on the right-hand sides.
Notice that in the system

$$\begin{aligned} 3x + 2y - z &= 3 \\ x - y + z &= 4 \\ 2x + 3y + 4z &= 5 \end{aligned}$$

the only difference from the first system is the names given to the unknowns. It can be checked that the first system has the solution $x_1 = 2,\ x_2 = -1,\ x_3 = 1$. The second system therefore has the solution $x = 2, y = -1, z = 1$.
We can isolate the three facets of the first system by using **arrays** of numbers and of unknowns:

$$\begin{bmatrix} 3 & 2 & -1 \\ 1 & -1 & 1 \\ 2 & 3 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \\ 5 \end{bmatrix}$$

Even more conveniently we represent the arrays with letters (usually capital letters)

$$AX = B$$

Here, to be explicit, we write

$$A = \begin{bmatrix} 3 & 2 & -1 \\ 1 & -1 & 1 \\ 2 & 3 & 4 \end{bmatrix} \quad X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad B = \begin{bmatrix} 3 \\ 4 \\ 5 \end{bmatrix}$$

Here A is called the **matrix of coefficients**, X is called the **matrix of unknowns** and B is called the **matrix of constants**.

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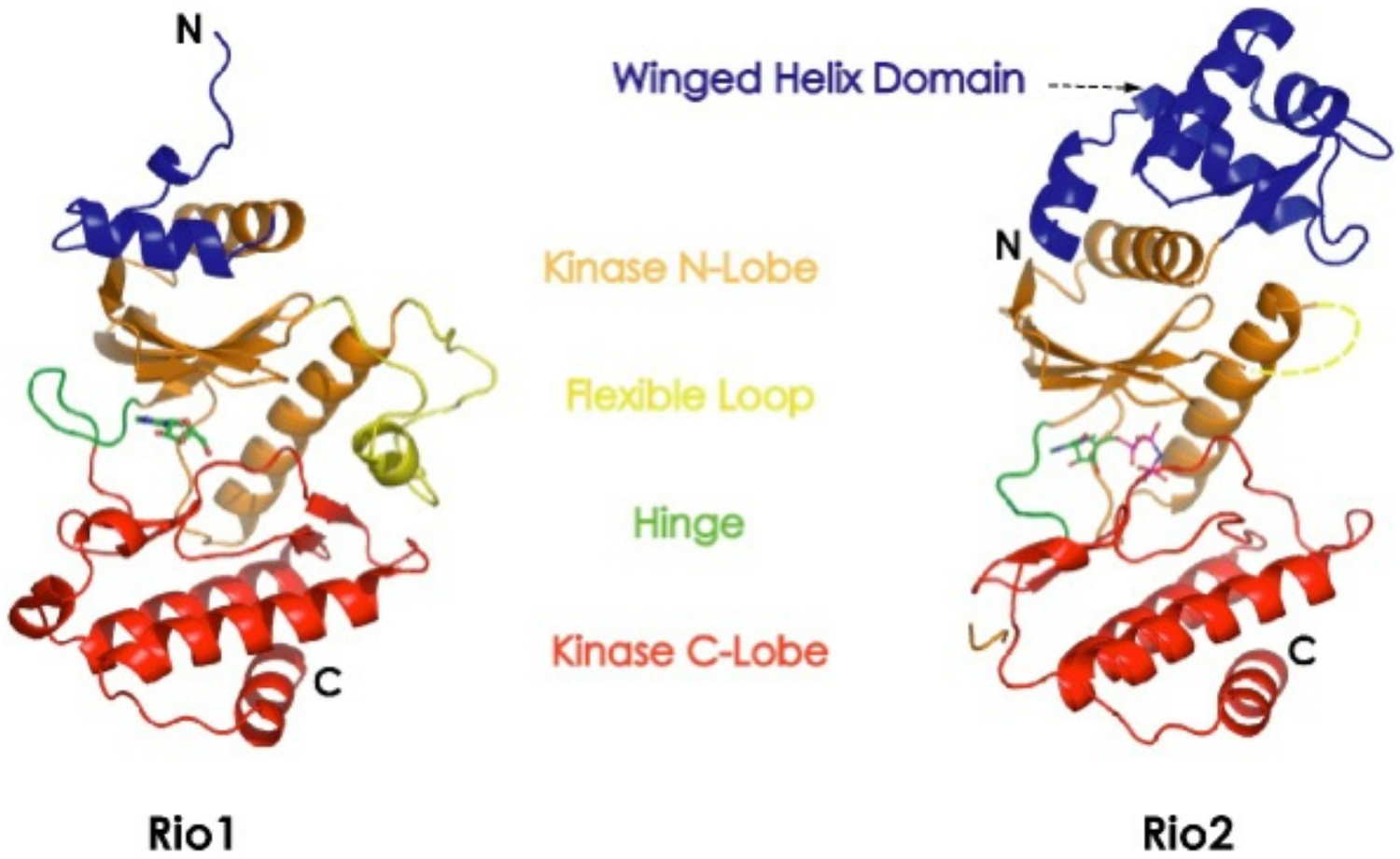
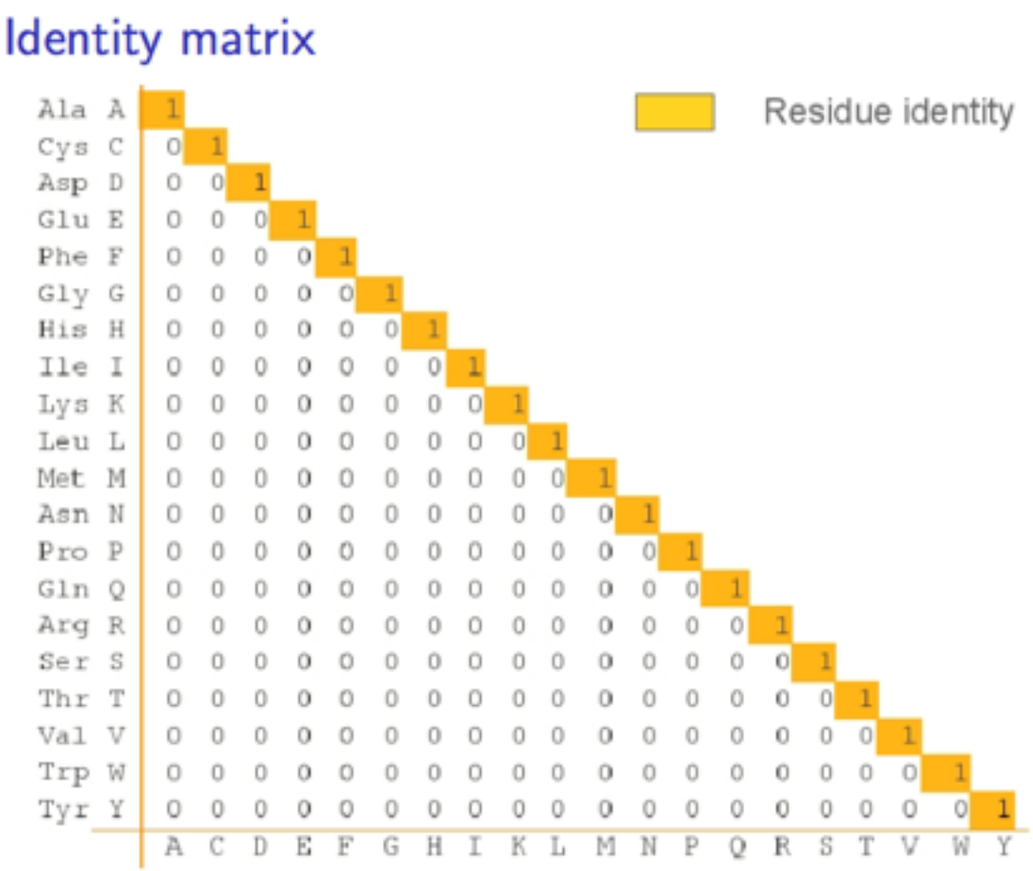
- Starting Point: Are two AA sequences similar? (Context: Find homologs of a new sequence)



SysMIC Training Approach

- Concept: Scoring matrix



BLOSUM-62

	C	S	T	P	A	G	N	D	E	Q	H	R	K	M	I	L	V	F	Y	W	
C	9																				C
S	-1	4																			S
T	-1	1	5																		T
P	-3	-1	-1	7																	P
A	0	1	0	-1	4																A
G	-3	0	-2	-2	0	6															G
N	-3	1	0	-2	-2	0	6														N
D	-3	0	-1	-1	-2	-1	1	6													D
E	-4	0	-1	-1	-1	-2	0	2	5												E
Q	-3	0	-1	-1	-1	-2	0	0	2	5											Q
H	-3	-1	-2	-2	-2	-2	1	-1	0	0	8										H
R	-3	-1	-1	-2	-1	-2	0	-2	0	1	0	5									R
K	-3	0	-1	-1	-1	-2	0	-1	1	1	-1	2	5								K
M	-1	-1	-1	-2	-1	-3	-2	-3	-2	0	-2	-1	-1	5							M
I	-1	-2	-1	-3	-1	-4	-3	-3	-3	-3	-3	-3	-3	1	4						I
L	-1	-2	-1	-3	-1	-4	-3	-4	-3	-2	-3	-2	-2	2	2	4					L
V	-1	-2	0	-2	0	-3	-3	-3	-2	-2	-3	-3	-2	1	3	1	4				V
F	-2	-2	-2	-4	-2	-3	-3	-3	-3	-3	-1	-3	-3	0	0	0	-1	6			F
Y	-2	-2	-2	-3	-2	-3	-2	-3	-2	-1	2	-2	-2	-1	-1	-1	-1	3	7		Y
W	-2	-3	-2	-4	-3	-2	-4	-4	-3	-2	-2	-3	-3	-1	-3	-2	-3	1	2	11	W

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Training Approach

- Task: create scoring matrix for two example sequences

Example

R	D	I	L	V	K	N	A	G	I

R	N	I	L	V	K	N	V	G	I

```
Identitäts-Matrix : 1 + 0 + 1 + 1 + 1 + 1 + 1 + 0 + 1 + 1 = 8
PAM250:             6 + 2 + 5 + 6 + 4 + 5 + 2 + 0 + 5 + 5 = 40
BLOSUM62:           5 + 1 + 4 + 4 + 4 + 5 + 6 + 0 + 6 + 4 = 39
```

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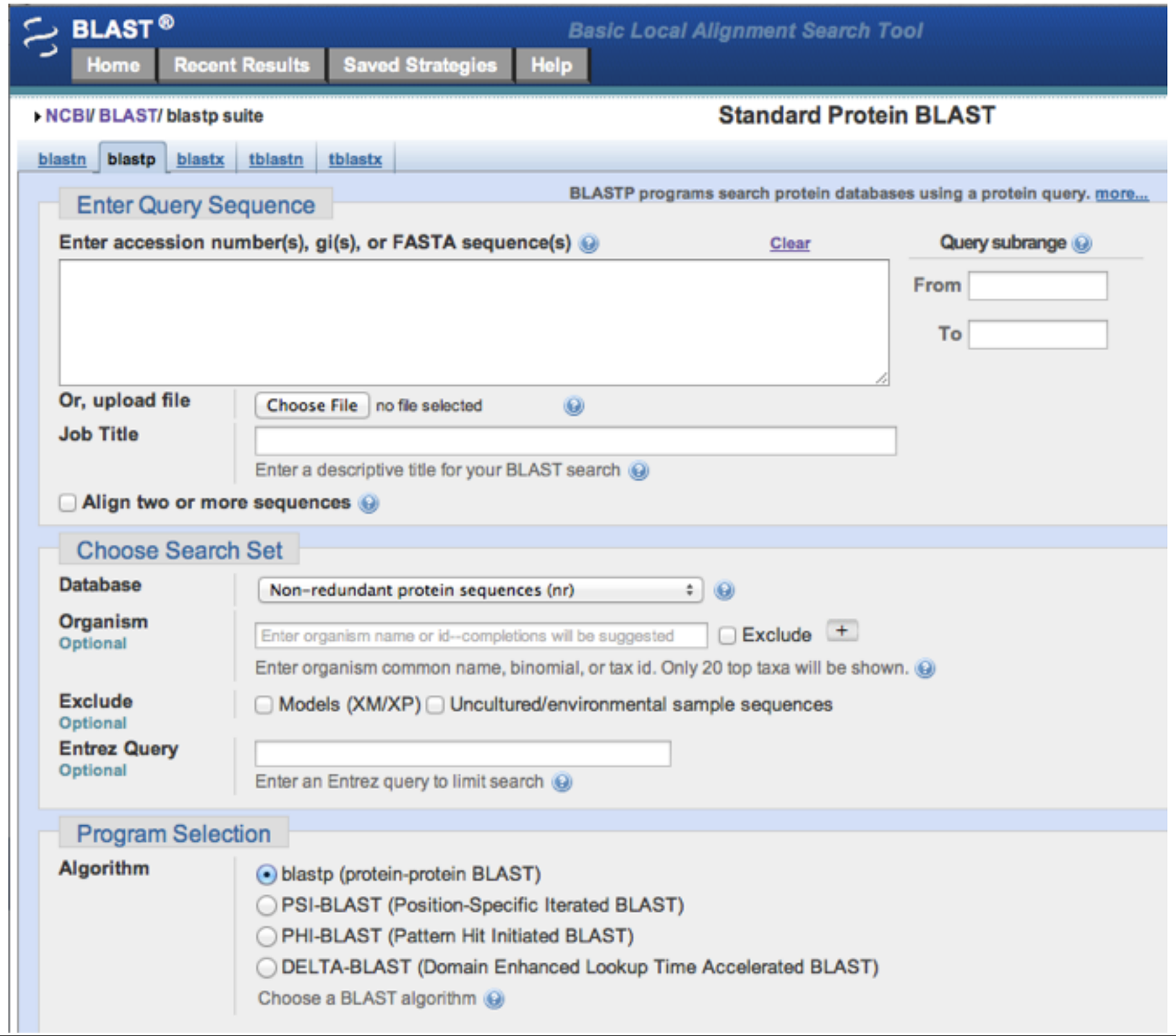
SysMIC Training Approach

NCBI Web Tool



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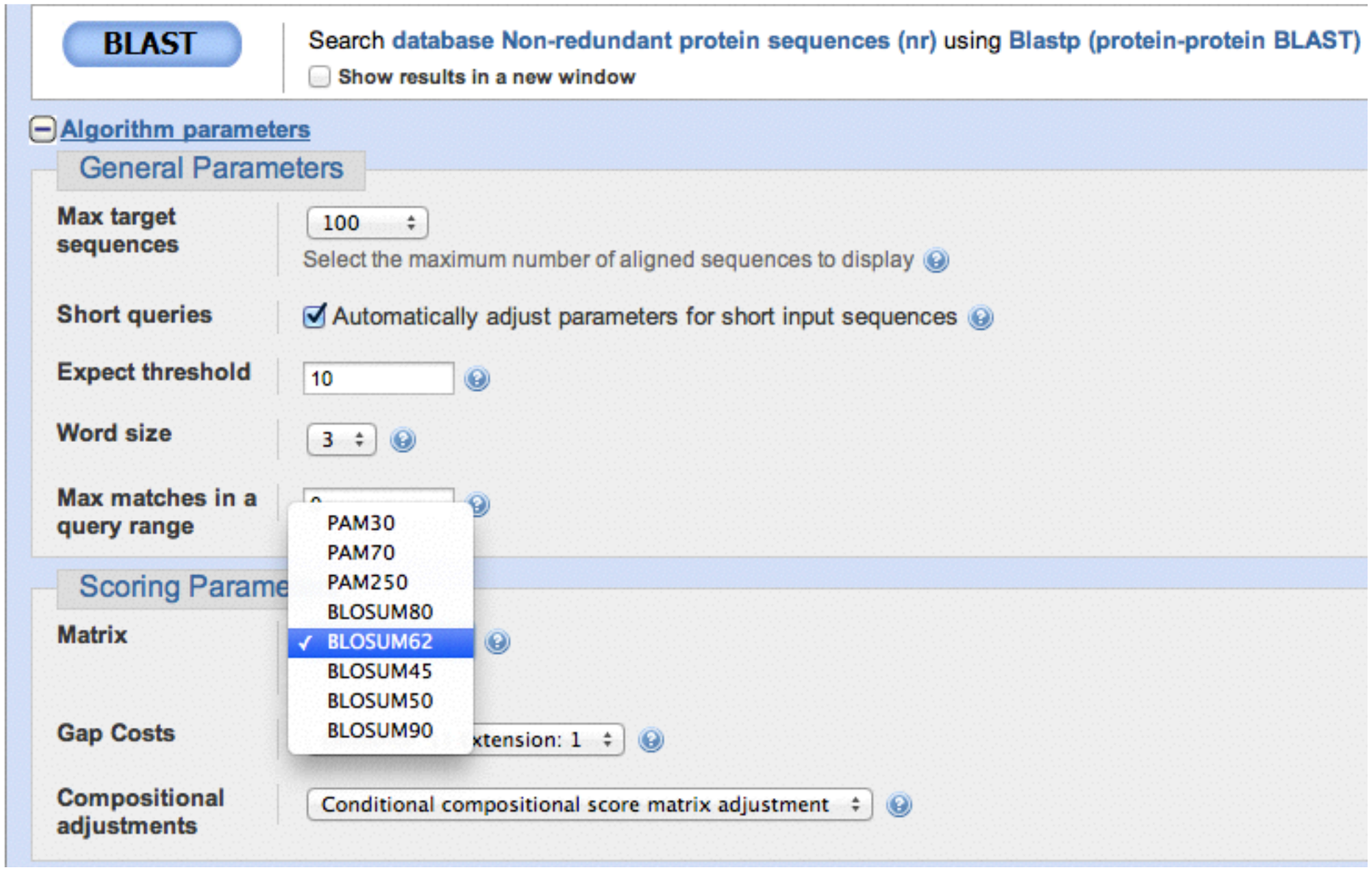
Use of Scoring Matrix



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Module 1 - Overview

- Basic MatLab
- Networks
- Modelling
- Statistics

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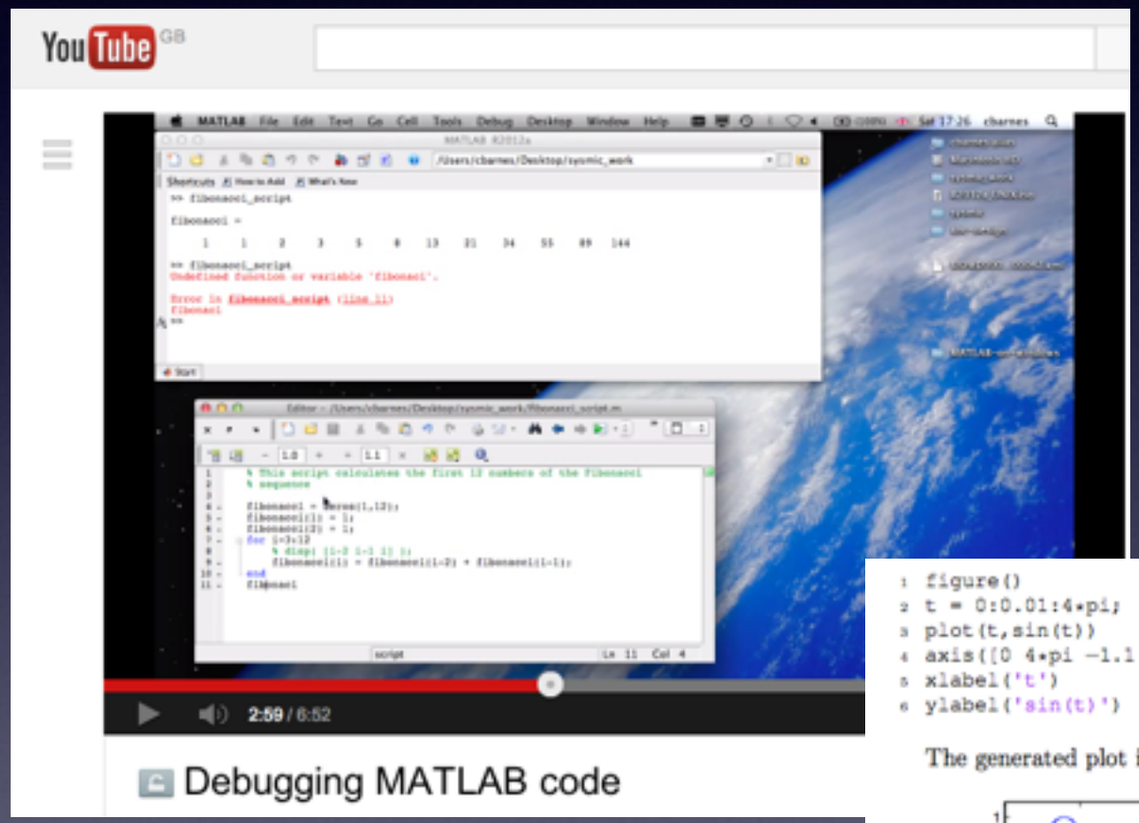
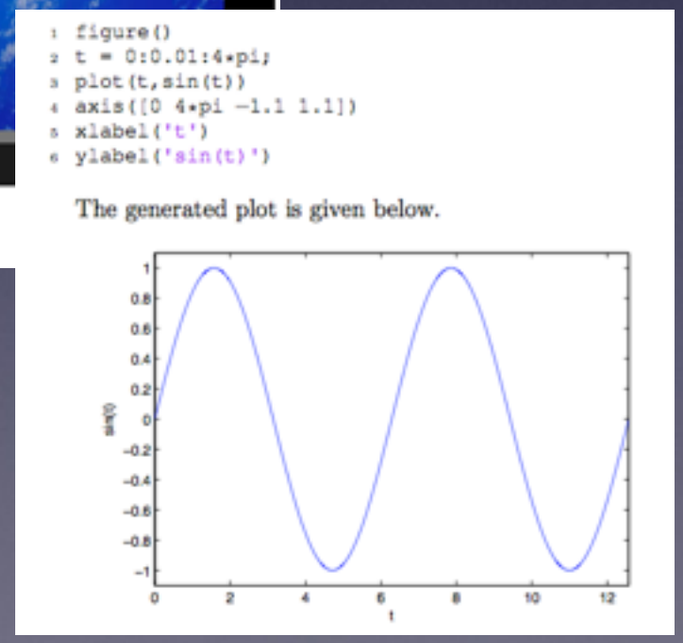




```
figure()
t = 0:0.01:4*pi;
plot(t,sin(t))
axis([0 4*pi -1.1 1.1])
xlabel('t')
ylabel('sin(t)')
```

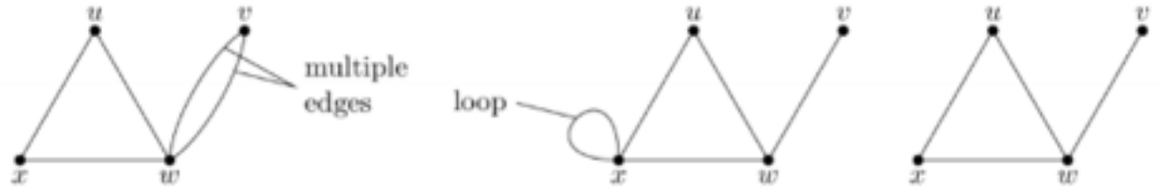
The generated plot is given below.

Module 1 - Overview

- Basic Matlab
- Networks
- Modelling
- Statistics

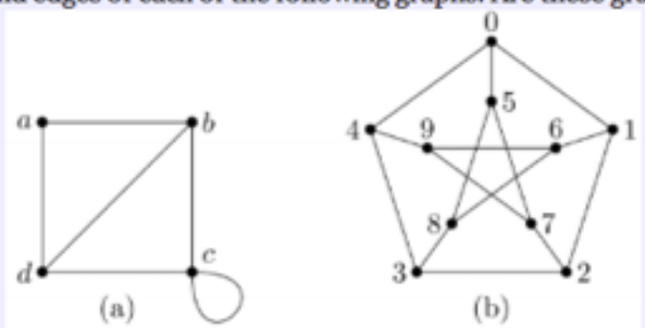
Definition
In a graph, two or more edges joning the same pair of vertices are **multiple edges**. An edge joining a vertex to itself is a **loop**.
A graph with no loops or multiple edges is a **simple graph**.

For example, graph (a) below has multiple edges and graph (b) has a loop, so neither is a simple graph. Graph (c) has no loops or multiple edges, and is therefore a simple graph.



Exercise 3.1.1

1. Write down the vertices and edges of each of the following graphs. Are these graphs simple graphs?



Solution

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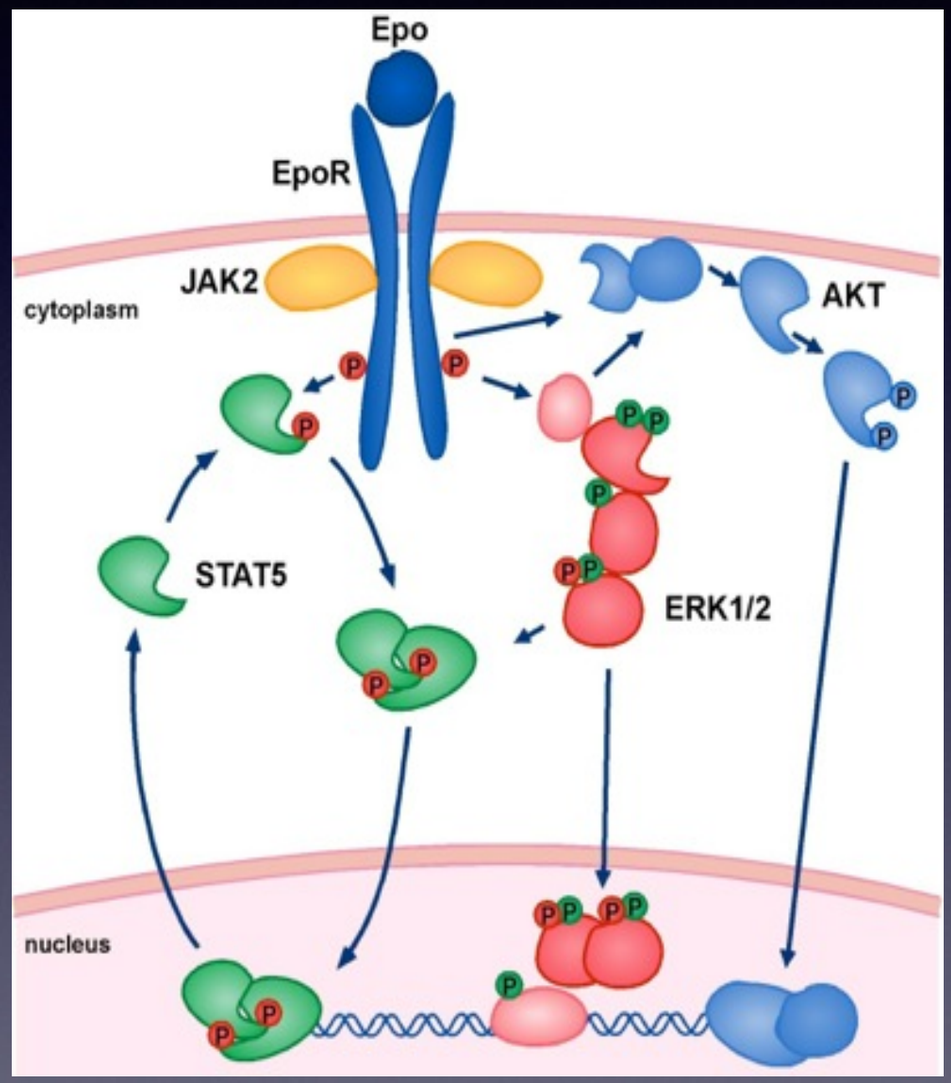
Module 1 - Overview

- Basic Matlab
- Networks
- Mechanistic Modelling
- Statistics



Epo Induced Signaling

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Module 1 - Overview

- Basic Matlab
- Networks
- Modelling
- Statistics

1 Introduction to R

1.1 Introduction and basics

1.1.1 What is R?

R is an open source programming language that is designed for data analysis and statistics. All information about R can be found here http://www.r-project.org/.

1.1.2 Getting, installing and starting R

R can be downloaded from the R project website which also contains links to installation instructions.

- Mac OS X : http://cran.r-project.org/bin/macosx/
- Windows : http://cran.r-project.org/bin/windows/base/
- Linux : http://cran.r-project.org/bin/linux/

Once installed R can be launched on Windows and Mac by running the R application. On Linux and Mac, R can also be run from a command window by typing `R` at the command prompt. To see which working directory R is running in you can do `getwd()` and also change working directories using the `setwd` function.

1.1.3 Four tips

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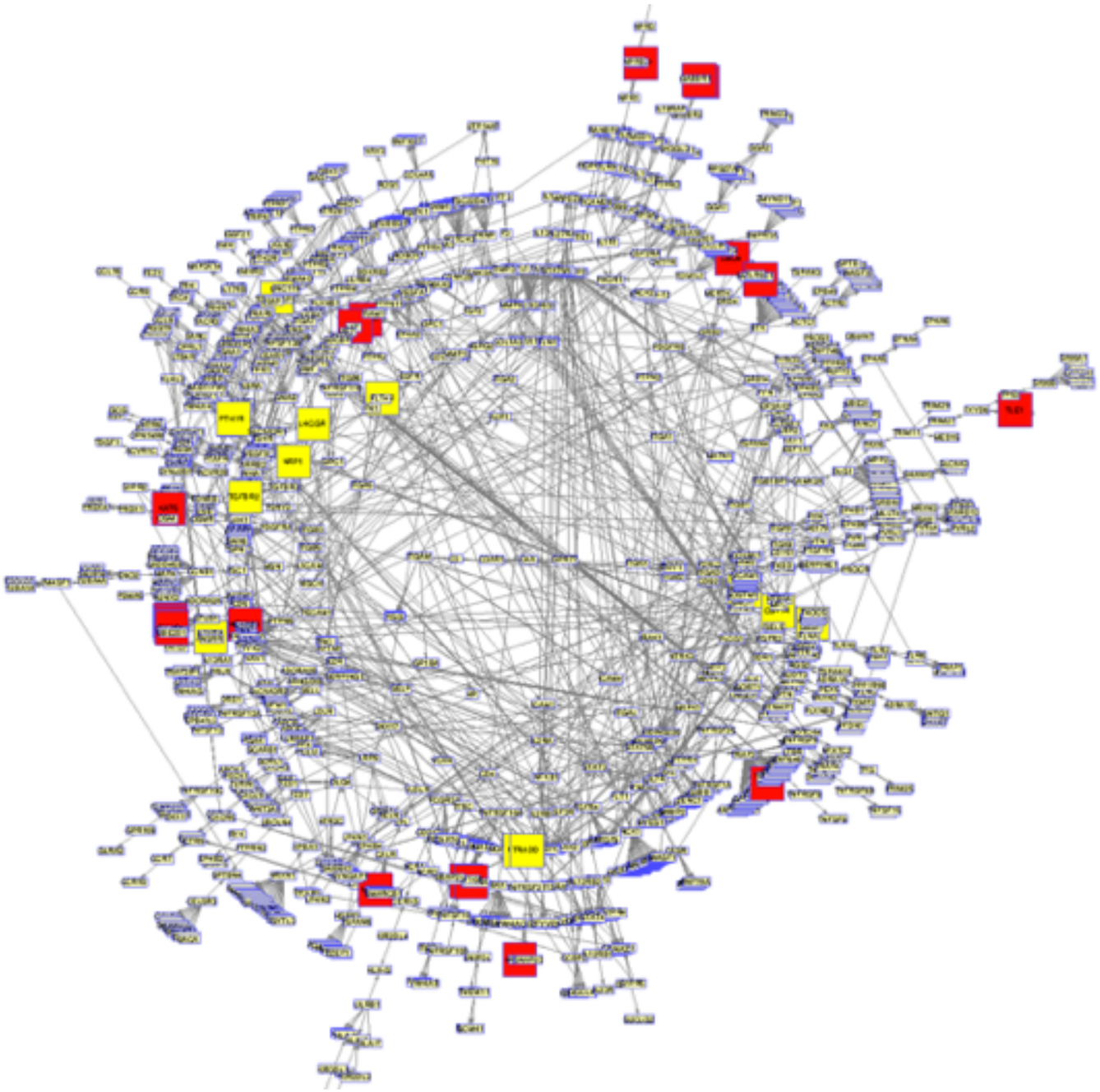
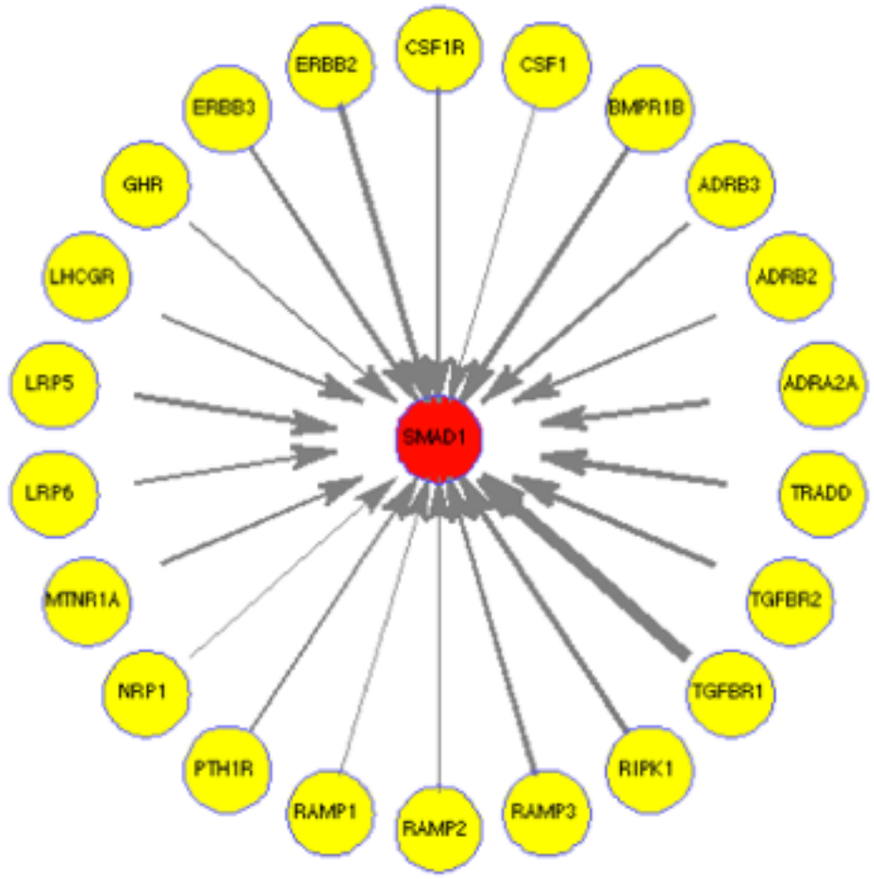
Training Outcomes





Network Analysis

Data:

A. Vinayagam, et al., A directed protein interaction network... Sci. Signal., 4(189):rs8, 2011.

Training Outcomes

Mini Projects

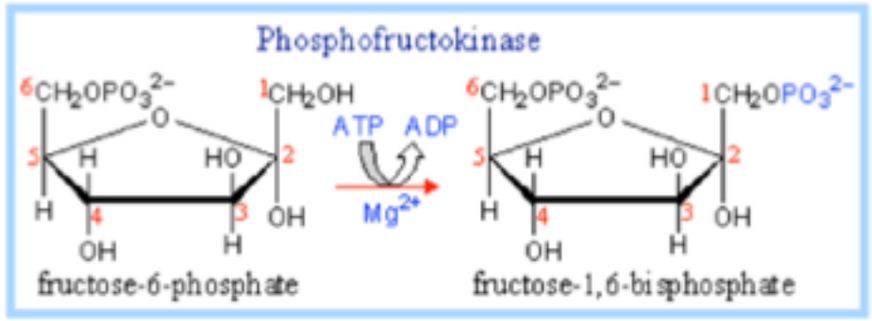


Figure 1.6.1: Reaction catalysed by mammalian PFK1.

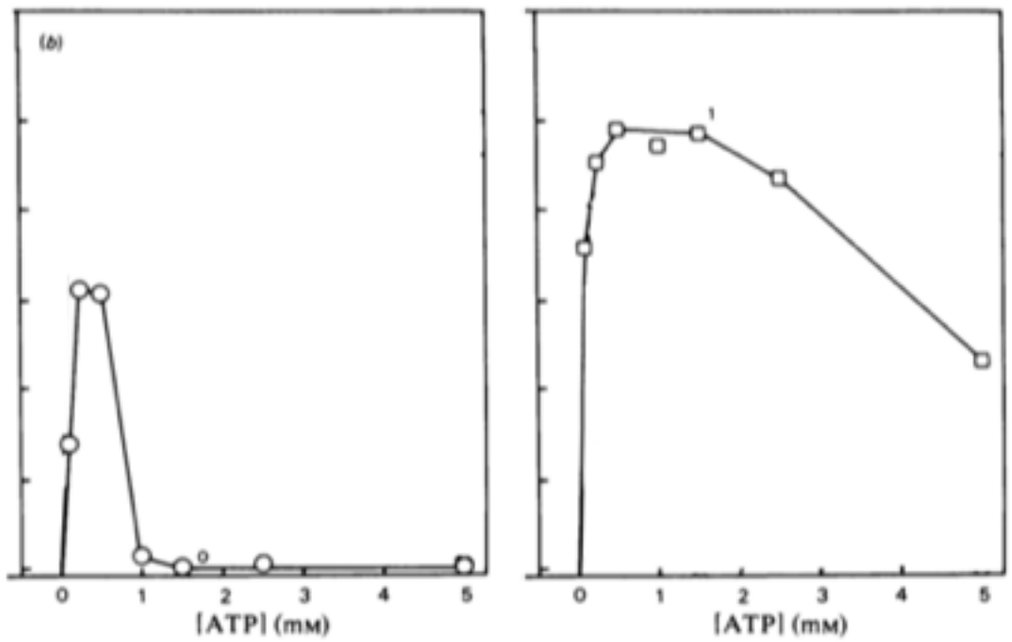
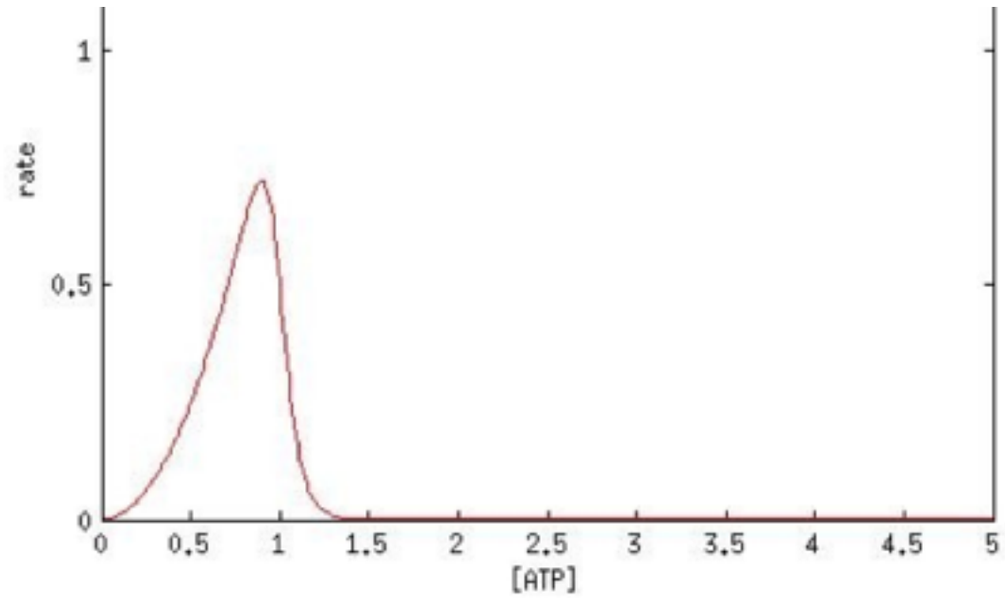


Figure 1.6.2: Rate of PFK as a function of [ATP] in the absence of F-2,6-BP.

Training Outcomes

Modelling

Simulation



MatLab Code

```
v = @(ATP,K,Vmax,n,m) Vmax*(ATP^n)/(K + ATP^m);
v1 = @(ATP) v(ATP,1,1,2.0,20.0);
limits = [5 0];
fplot(v1,limits,'r')
axis([0 5 0 1.5])
ylabel('rate')
xlabel('[ATP]')
```

Interpretation

Verbally describe two ways in which regulatory molecule F-2,6-BP could lead to the change in kinetics as depicted in Fig. 1.5.2 (right).

There are two Hill coefficients playing a role in this equation. “n” is related to ATP affinity in the reactive site of the enzyme. “m” is a value that characterizes the affinity of ATP for the inhibition site. PFK1 has some other binding sites for allosteric modulation, the most important one is the one for F-2,6-BP. As this molecule is not interacting with the catalytic site of the enzyme, it shouldn't be affecting the Vmax of the reaction. However, through conformational changes F-2,6-BP must be changing affinity rates. In order to increase the catalytic rate and avoid inhibition by ATP, F-2,6-BP can affect through two ways: decreasing km or/and the “m” coefficient. By reducing km the enzymatic affinity for F-6-P increases. On the other hand, the reduction of m equals to reduction of the ATP affinity for the inhibition site.

Training Assessment

Quizz

30 May 2013 10:36 AM	30 May 2013 10:37 AM	1 min 14 secs	0.00 ✗	16.67 ✓	0.00 ✗	0.00 ✗	16.67 ✓	16.67 ✓	50.00
30 May 2013 10:38 AM	30 May 2013 10:39 AM	43 secs	16.67 ✓	16.67 ✓	0.00 ✗	16.67 ✓	16.67 ✓	16.67 ✓	83.33
3 June 2013 10:37 AM	4 June 2013 10:43 AM	1 day	0.00 ✗	0.00 ✗	0.00 ✗	- ✗	0.00 ✗	0.00 ✗	0.00
4 June 2013 10:45 AM	4 June 2013 10:55 AM	10 mins 7 secs	16.67 ✓	16.67 ✓	16.67 ✓	16.67 ✓	16.67 ✓	16.67 ✓	100.00

SysMIC

Module 2 - Overview

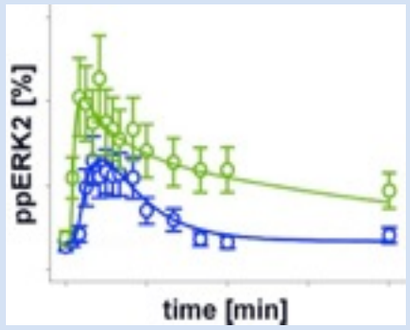
- Launch October 2013
- Six month duration, 5 hrs per week
- Apply tools from Module 1 to biological research
- Mathematical topics

✓ Functions of more than one variable
✓ More on linear systems
✓ Discrete systems
✓ Systems of ordinary differential equations
✓ Diffusion systems
✓ Stochastic systems
✓ Data handling
✓ Modelling challenges II

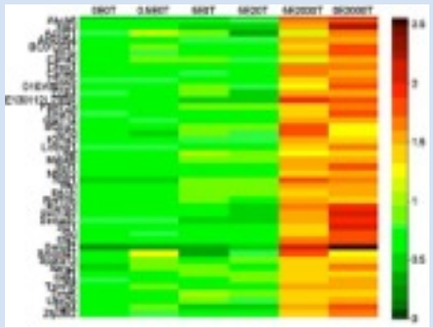
Systems Biology – Multiple Levels Perspective

Time-resolved quantitative data

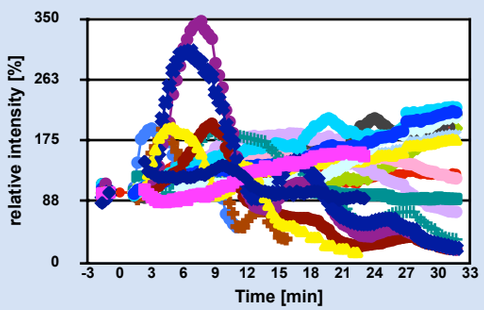
Mass spectrometry
Protein arrays
Immunoblotting
Luminex technology



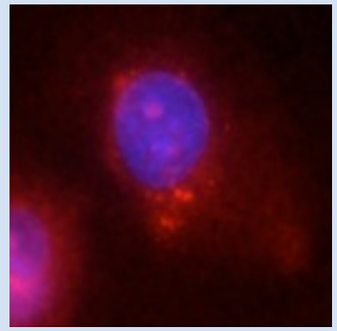
Next Generation
Sequencing
qRT-PCR



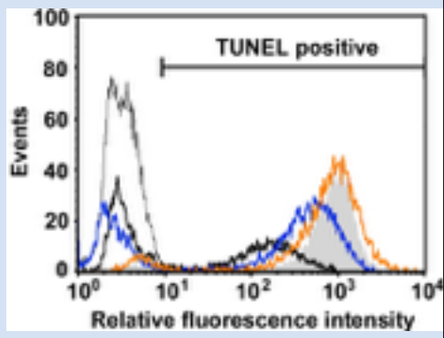
Live cell imaging
FRET, FCS



Immunofluorescence
Immunohistochemistry



TUNEL
Proliferation
Migration

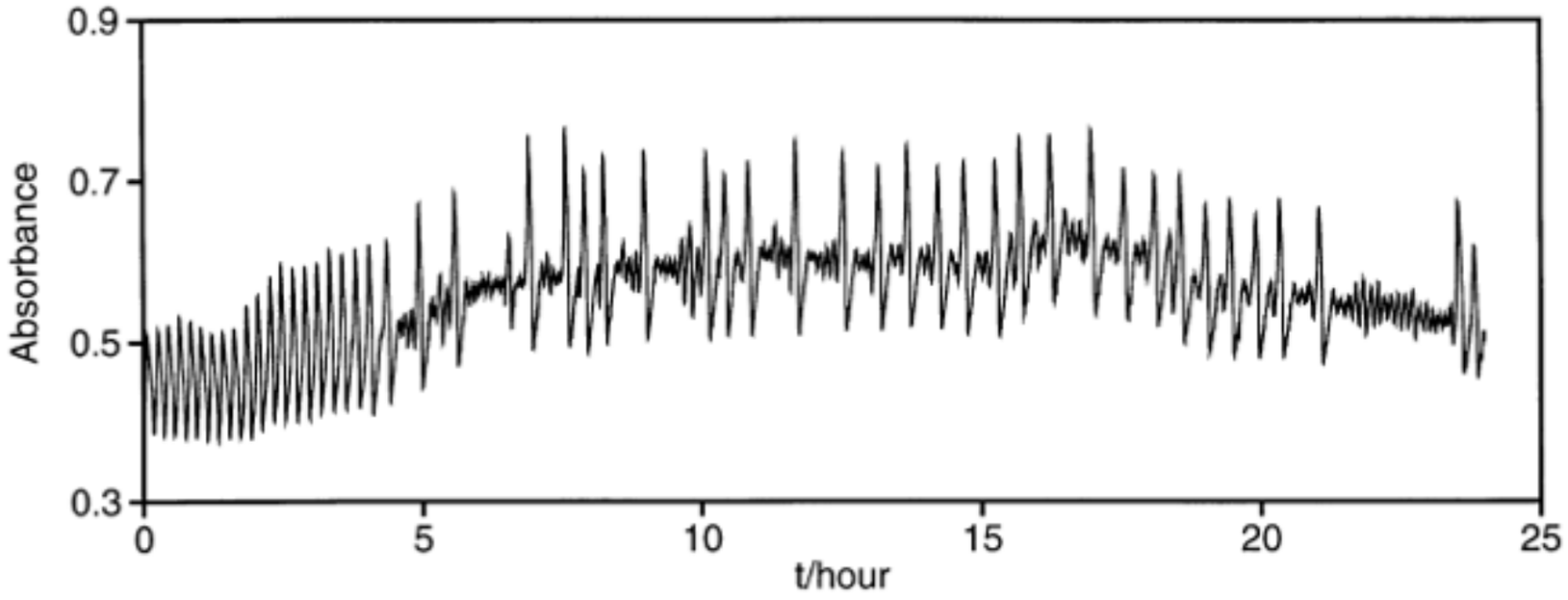


Protein | **mRNA, microRNA** | **Localization** | **Morphology** | **Process parameters**

Dynamic Pathway Model | **Network Model** | **Spatio-temporal Model** | **Multiscale Model**

Data-based Mathematical Models

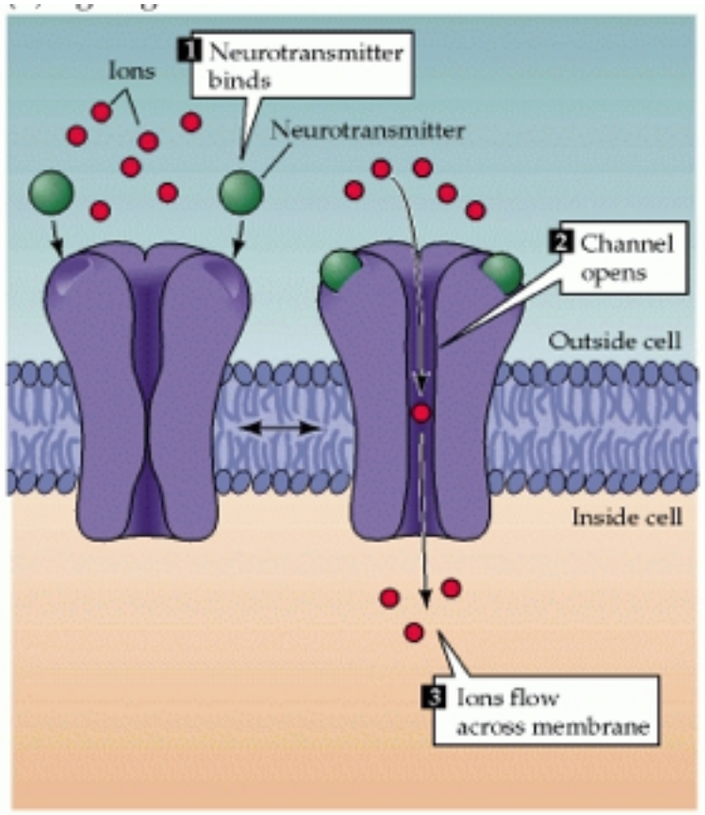
Reaction kinetics

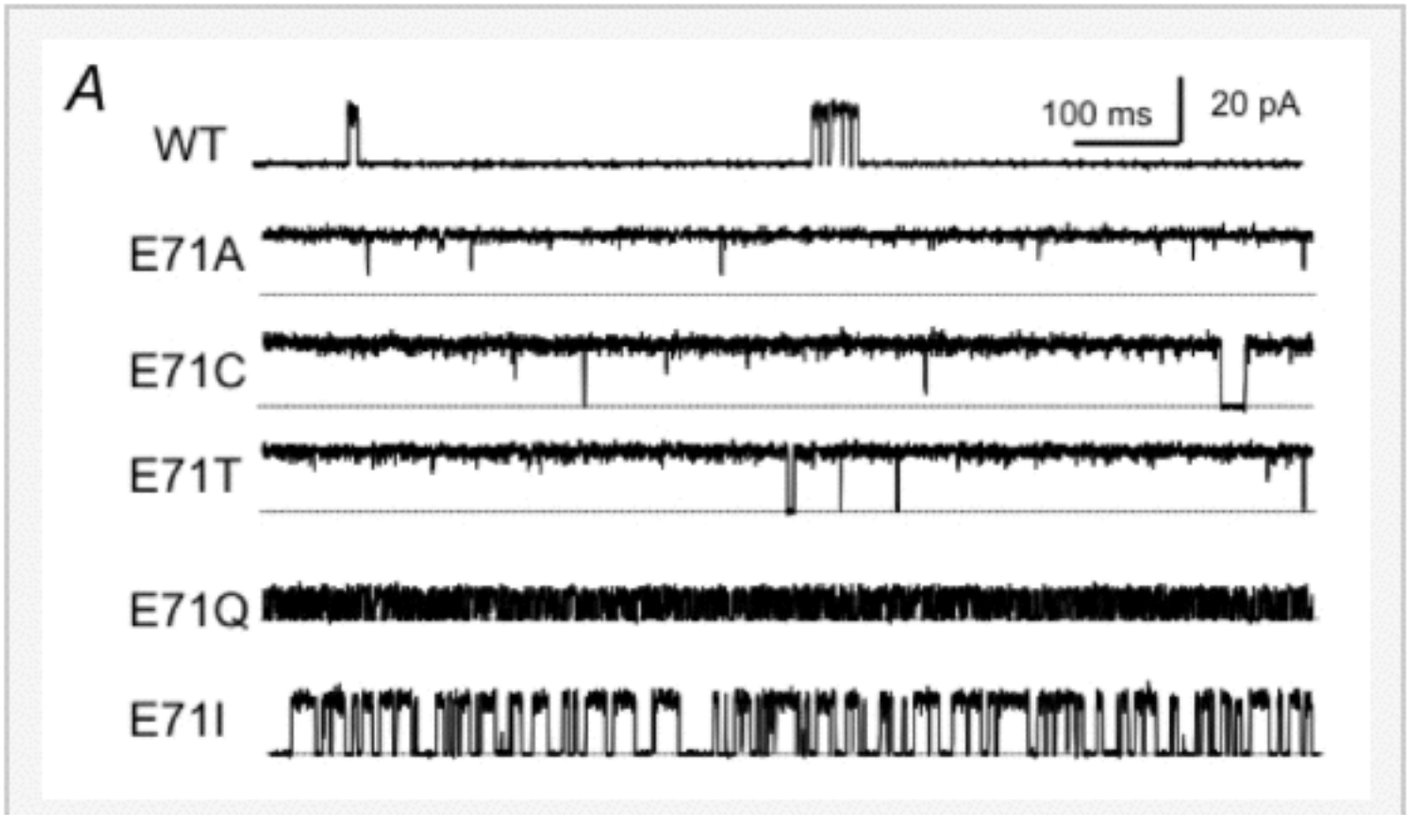


Glycolytic oscillations

Reaction	Rate expression
GLC + ATP → F6P + ADP	$\frac{V_1[ATP][GLC]}{(K_{1GLC}+[GLC])(K_{1ATP}+[ATP])}$
F6P + ATP → FBP + ADP	$\frac{V_2[F6P]^2[ATP]}{(K_2(1+k_2(\frac{[ATP]}{[AMP]})^2)+[F6P]^2)(K_{2ATP}+[ATP])}$

Ion channel gating

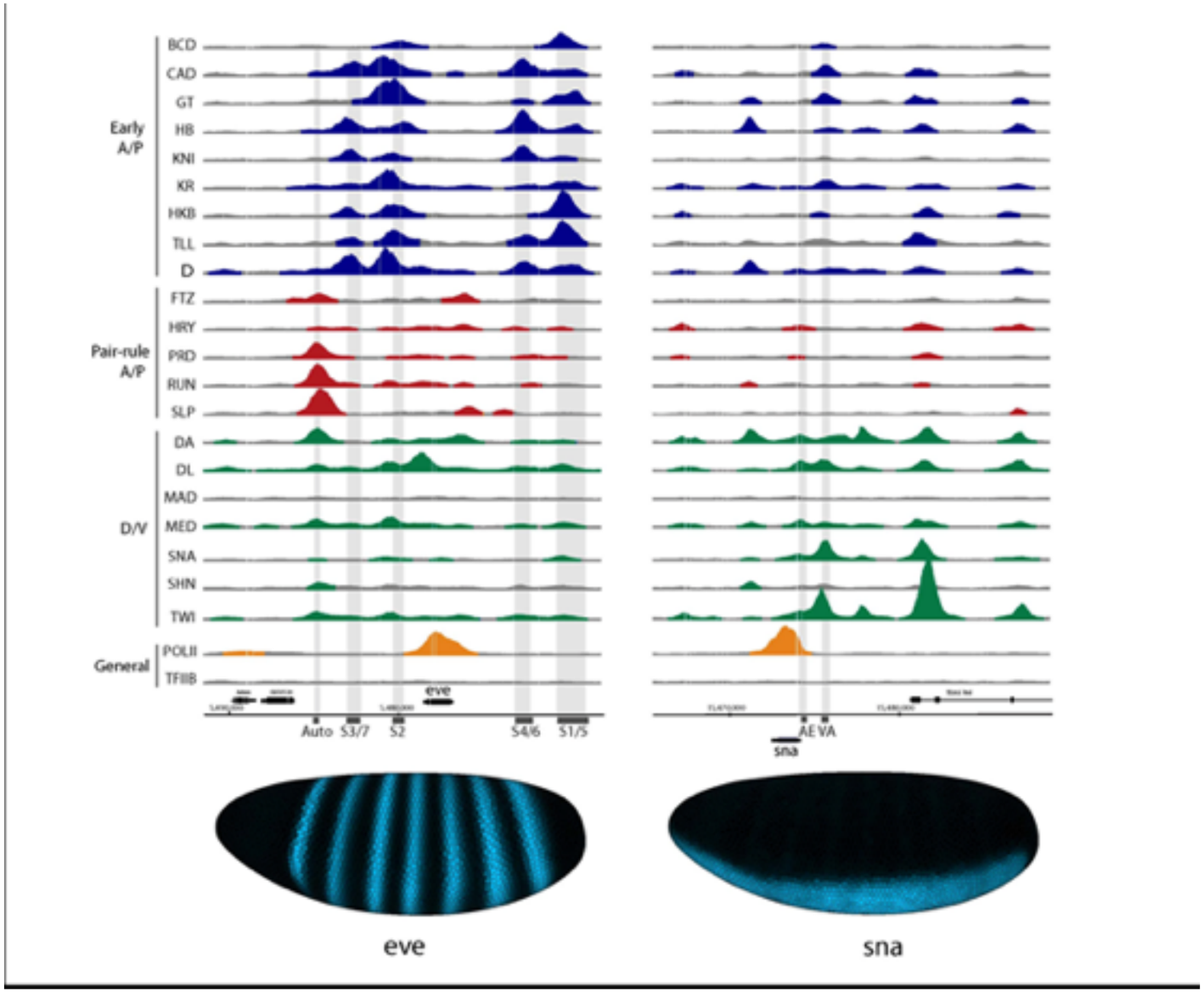




Transition matrix

$$\begin{pmatrix} P(X_{n-1}=0 \to X_n=0) & P(X_{n-1}=1 \to X_n=0) \\ P(X_{n-1}=0 \to X_n=1) & P(X_{n-1}=1 \to X_n=1) \end{pmatrix} = \begin{pmatrix} \gamma & 1-\delta \\ 1-\gamma & \delta \end{pmatrix}$$

Pattern formation



1.2.1 In one dimension - The Predator-Prey model

The model you will be presented with here is a discretised one dimensional reaction-diffusion system that represents two interacting (in our case, wholly dependent) populations, competing for existence.

Compared to Equation (1.2.5), our equations for the predator-prey model will be represented by

$$\frac{\partial u}{\partial t} = D_u \nabla^2 u + u(1 + u - \frac{\gamma u^2}{2} - \beta v), \tag{1.2.6}$$

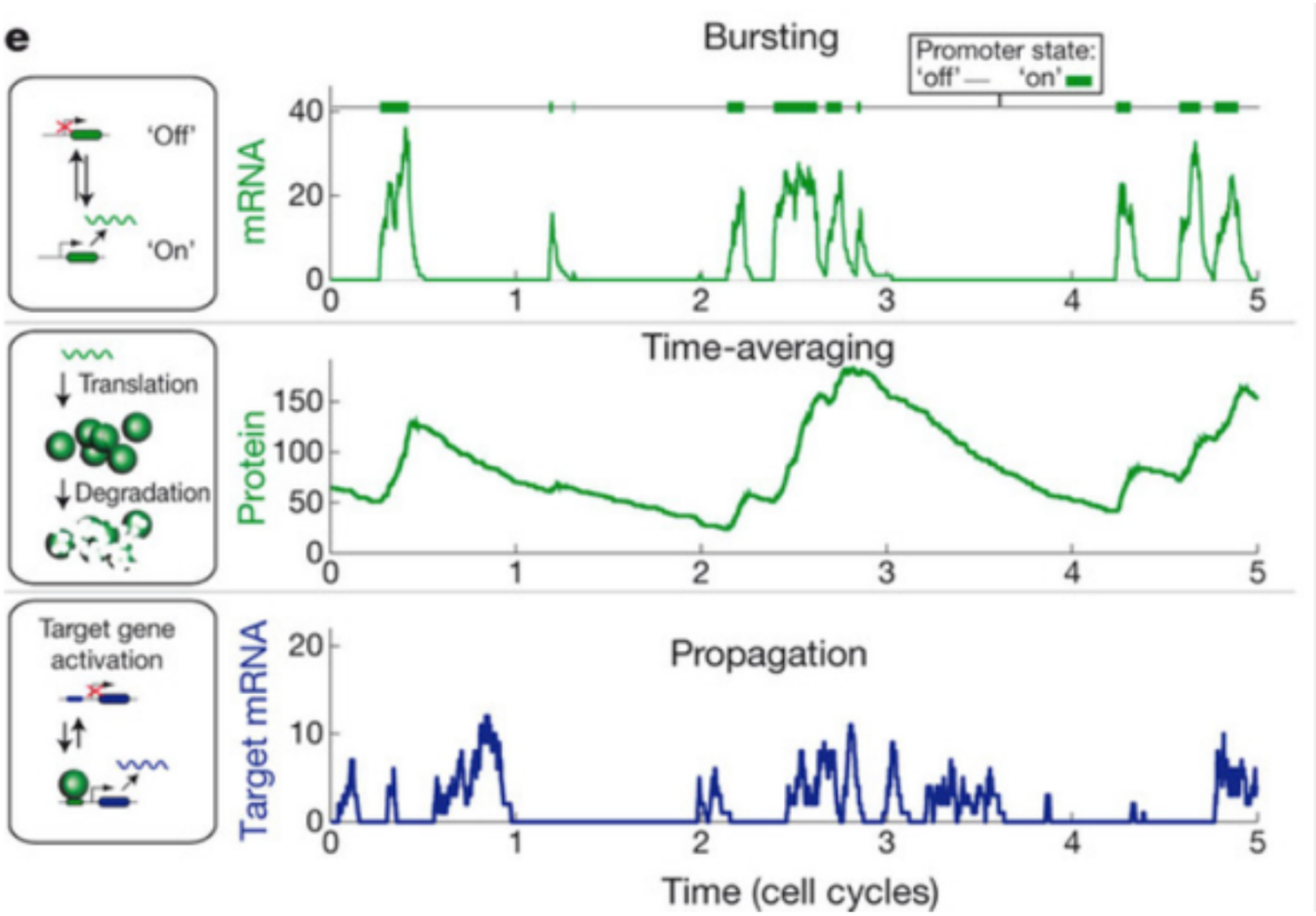
$$\frac{\partial v}{\partial t} = D_v \nabla^2 v + v(1 - v + \alpha u) \tag{1.2.7}$$

Reaction-diffusion models

Biological noise

Bistability is one of the origins of heterogeneity in biological system

- antibiotic resistance in bacteria
- this behaviour is exploited in many biological systems



Successful papers

Journal of Theoretical Biology 310 (2012) 143–159

Contents lists available at SciVerse ScienceDirect

Journal of Theoretical Biology

journal homepage: www.elsevier.com/locate/yjtbi

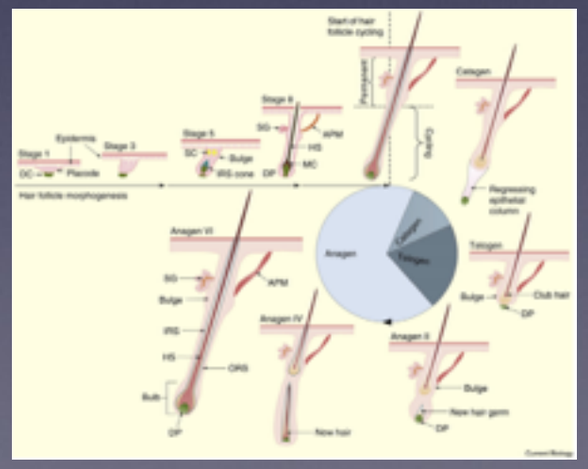
A prototypic mathematical model of the human hair cycle

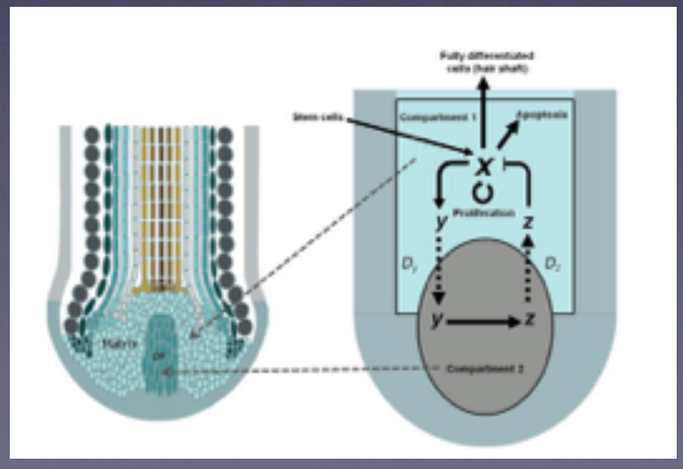
Yusur Al-Nuaimi [a,b,*,1], Marc Goodfellow [a,c,1], Ralf Paus [b,d], Gerold Baier [a]

[a] Doctoral Training Centre in Integrative Systems Biology, Manchester Interdisciplinary Biocentre, University of Manchester, UK
[b] Inflammation Sciences, School of Translational Medicine, Manchester Academic Health Sciences Centre, University of Manchester, UK
[c] Centre for Interdisciplinary Computational and Dynamical Analysis (CICADA), Alan Turing Building, University of Manchester, UK
[d] Department of Dermatology, University of Lübeck, Germany

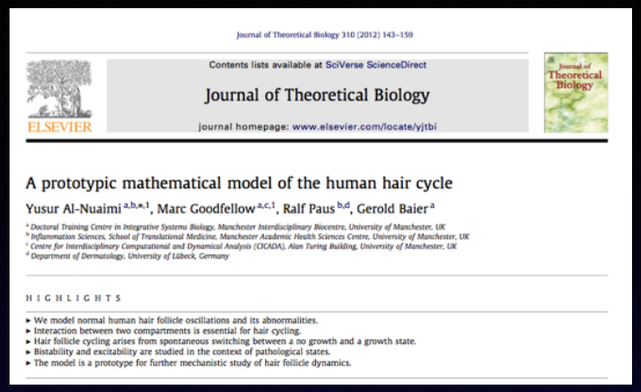
HIGHLIGHTS

- We model normal human hair follicle oscillations and its abnormalities.
- Interaction between two compartments is essential for hair cycling.
- Hair follicle cycling arises from spontaneous switching between a no growth and a growth state.
- Bistability and excitability are studied in the context of pathological states.
- The model is a prototype for further mechanistic study of hair follicle dynamics.





Successful papers



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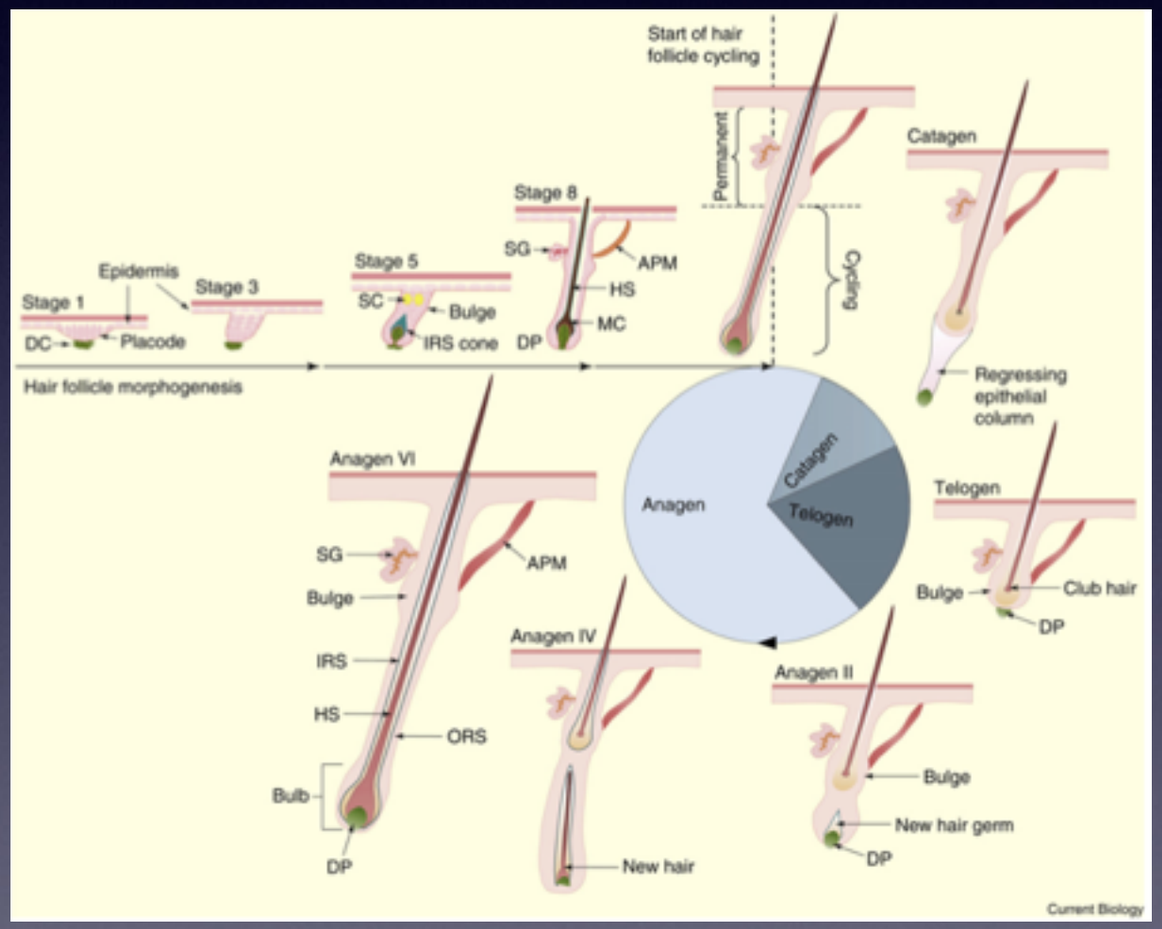
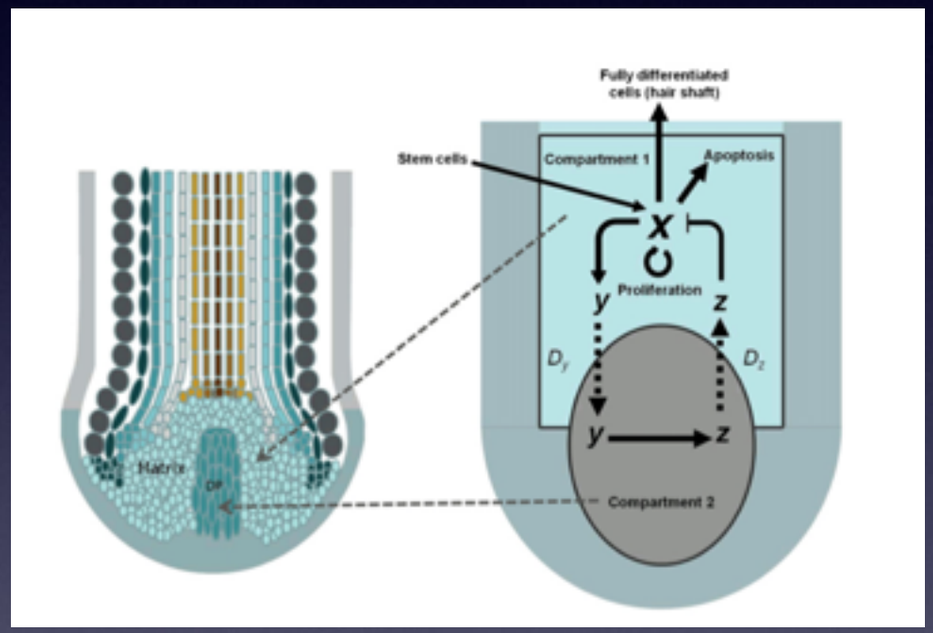
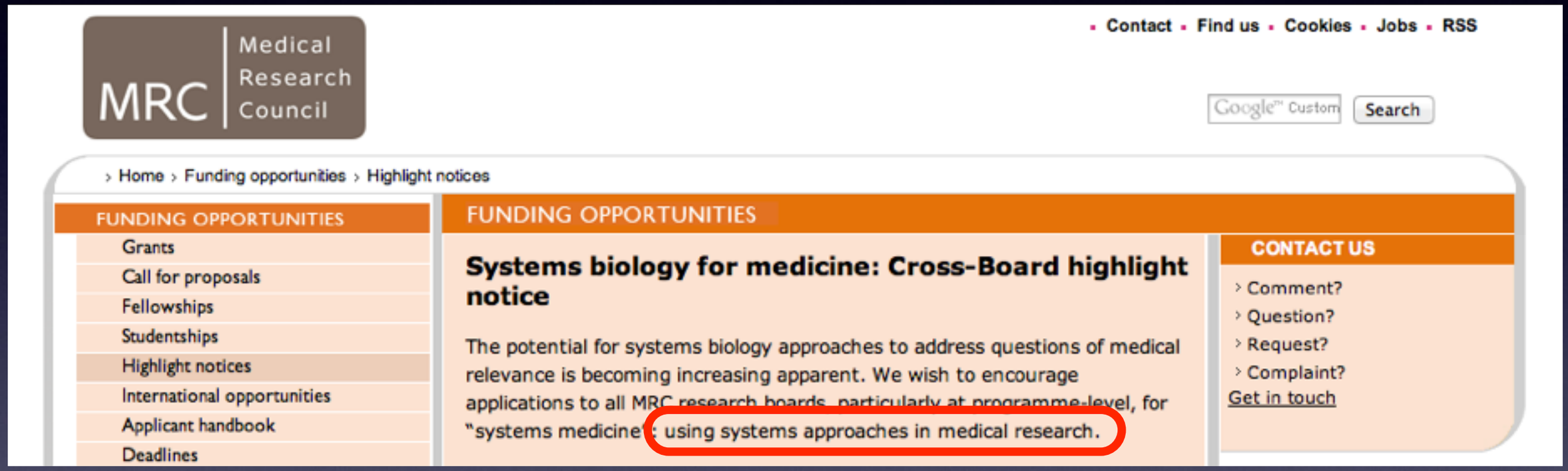




Grant Opportunities



Job Opportunities

Senior Scientist, **Quantitative Biology**
Flexus Biosciences - San Carlos, CA
Design and execution of sophisticated kinetic analyses of enzymes and receptors with novel inhibitors, antagonists etc. is a central component of this role....
Fitzii - 13 days ago - save job - block - email - more...

Quantitative Protein Biomarker LC-MS/MS Scientist
A10 - Andover, MA
Industry experience in biopharma preferred. Extensive expertise in the operation and maintenance of mass spectrometers....
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Head, Computational & Systems **Biology** Job
Johnson & Johnson ★★★★☆ 268 reviews - Spring House, PA
The role will be based in Spring House, PA. He/she will help select and retain highly qualified staff, develop capabilities of staff, and ensure that staff is...
Johnson & Johnson Family of Companies - 18 days ago - save job - block - email - more...

Scientist, **Quantitative Biology**
Flexus Biosciences - San Carlos, CA
He/She will be charged with delivering high quality potency, selectivity and characterization data to profile and evaluate compounds generated by our chemistry...
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Assistant Professor of **Biology** (Integrative Evolutionary Gen...
University of Alaska ★★★★★ 6 reviews - Fairbanks, AK
White Large Animal Research Station, Center for Alaska Native Health Research, Animal Quarters, Toolik Field Station, Spatial Ecology Laboratory, Alaska...
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Post Doctoral Associate- Computational **Biology**
Broad Institute ★★★★☆ 6 reviews - Cambridge, MA
□ Practical experience with analytical programming using R, MATLAB, or Python. □ Experience with computational analysis, algorithm development and statistics in...
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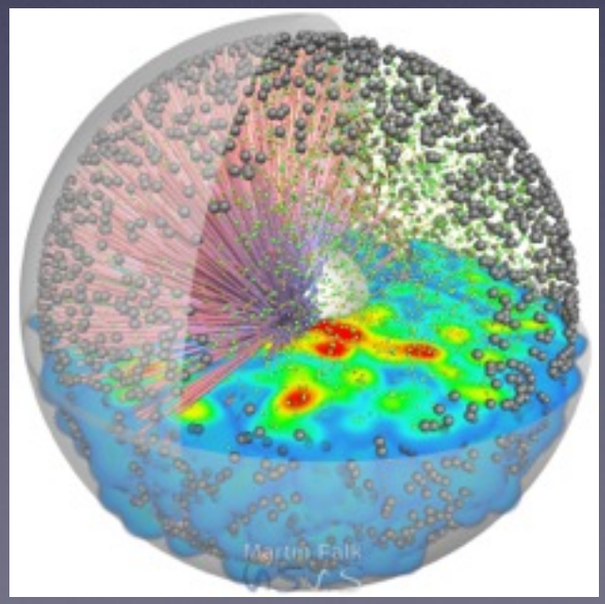
Senior Product Manager, Molecular **Biology**
MP Biomedicals - Solon, OH
MBA is strongly preferred. Formulate marketing plan to reach revenue plan for the molecular **biology** product, support growth of the product lines and increase...
MP Biomedicals LLC - 12 days ago - save job - block - email - more...

SysMIC Development

- Segment, annotate & hyperlink videos
- Live training sessions
- Virtual data environments (individual)



Systems eTraining in the Biosciences

Gerold Baier, UCL

SysMIC

INTERDISCIPLINARY SKILLS FOR BIOLOGICAL RESEARCH

University College London

Birkbeck College

The University of Edinburgh

The Open University