

# Computational Molecular Biology and Bioinformatics

## Basics of Molecular Biology

Malay Bhattacharyya

Associate Professor

Machine Intelligence Unit  
Indian Statistical Institute, Kolkata

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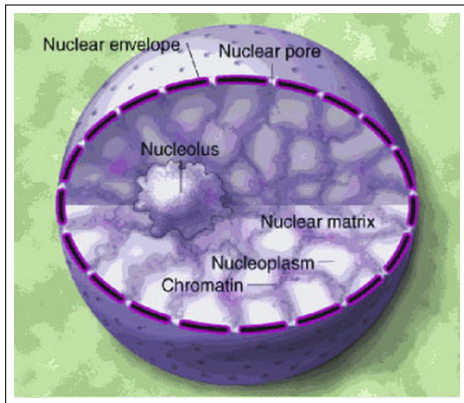


- 1 Molecular biology
  - Organism to cell
  - Cell to nucleus
  - Nucleus to chromosome
  - Chromosome to DNA
  - DNA to nucleotide
  - Transcription unit and promoter
  - DNA-RNA-mRNA
- 2 Central dogma of molecular biology
- 3 Scope of research
- 4 Suggested reading



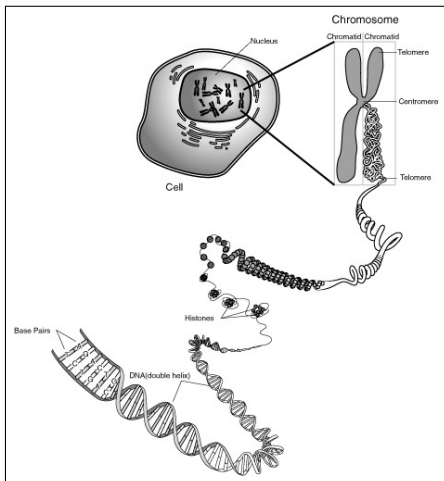


# Nucleus to chromosome



**Zooming from nucleus into the chromosome**

# Chromosome to DNA



**Zooming from chromosome into the DNA**

# DNA to nucleotide

```
... T T A C C G T C G G C A ...  
  | | | | | | | | | | | |  
... A A T G G C A G C C G T ...
```

**Note:** There are 3 billion base pairs in each cell to fit into a space of approximately  $6 \mu\text{m}$  across the human cells.

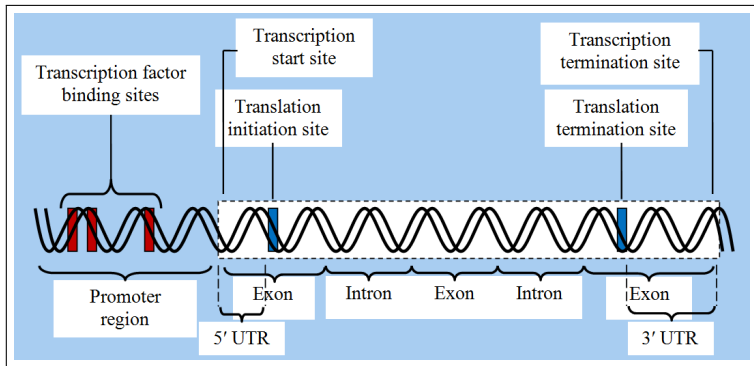
# This is your haystack!!!

... AATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
TTCGGTTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAAAAC  
AAATTGCCAATTTTGGCCAATTCGGAAAAATTTTCGGATTGCCAA  
TTCGGTTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAAAAC  
AAAAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
TTCGGCGGATTATTGCCAATTCCTCAAAGCCAATTCGGAAAAC  
CAAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
TTCGGTTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAAAAC  
TTCAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
GGGAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
ATCGGTTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAAAAC  
GAAAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
ATCGGTTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAA ...

# This is your haystack!!!

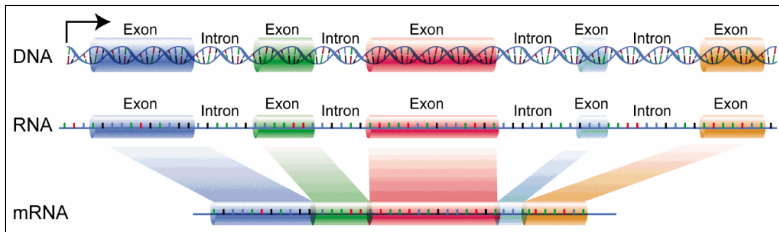
... AATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
 TTCGGTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAAAAC  
 AAATTGCCAATTTTGGCAATTCGGAAAAATTTTCGGATTGCCAA  
 TTCGGTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAAAAC  
 AAAAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
 TTCGGCGGATTATTGCCAATTCCTTCAAAGCCAATTCGGAAAAC  
 CAAAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
 TTCGGTTTC Blue eyes??? CGGAAAAGCCAATTCGGAAAAC  
 TTCAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
 GGGAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
 ATCGGTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAAAAC  
 GAAAATTTTCGGATTGCCAATTCGGAAAAATTTTCGGATTGCCAA  
 ATCGGTTTTCGGATTGCCAATTCGGAAAAGCCAATTCGGAA ...

# Transcription unit and promoter



**Organization of the transcription unit and promoter region**

# DNA-RNA-mRNA

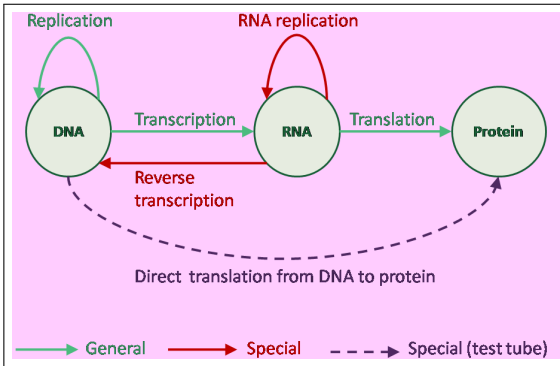


## The formation of DNA-RNA-mRNA

**Note:** The nucleotides A, T, C and G constitutes the DNA, whereas in RNA T is replaced by U.

# Central dogma of molecular biology

The central dogma of molecular biology comprises transcription followed by translation.



# Scope of research

“Biology is the only science in which multiplication is the same thing as division”

– Jupiter Scientific.

Molecular biology, which serves as a link between the genetics and biochemistry, covers the following areas:

- Sequence analysis
- Expression analysis
- Genetic analysis
- Epigenetic analysis
- System-level analysis
- Pathway analysis

# Resources

## Books:

- 1 C. Setubal and J. Meidanis: Introduction to Computational Molecular Biology, PWS Publishing Company, Boston, 1997.
- 2 P. A. Pevzner: Computational Molecular Biology – An Algorithmic Approach, MIT Press, 2000.
- 3 R. Durbin, S. R. Eddy, A. Krogh and G. Mitchison: Biological Sequence Analysis - Probabilistic Models of Proteins and Nucleic Acids, Cambridge University Press, 1998.
- 4 D. Gusfield: Algorithms on Strings, Trees, and Sequences, Cambridge University Press, USA, 1997.
- 5 H. Lodish, A. Berk, S. L. Zipursky, P. Matsudaira, D. Baltimore and J. Darnell: Molecular Cell Biology, W. H. Freeman, USA, 2000.
- 6 C.-I. Branden, J. Tooze: Introduction to Protein Structure, Garland Publishing, 1998.
- 7 A. Kowald, C. Christoph Wierling, E. Klipp, and W. Liebermeister: Systems Biology, Wiley-VCH, 2016.
- 8 B.O. Palsson: Systems Biology – Constraint based Reconstruction and Analysis, Cambridge University Press, 2015.

# Resources

## Journals:

- 1 WIREs Computational Molecular Science, Wiley.
- 2 Briefings in Bioinformatics, Oxford University Press.
- 3 Bioinformatics, Oxford University Press.
- 4 PLoS Computational Biology, PLoS.
- 5 IEEE/ACM Transactions on Computational Biology and Bioinformatics, IEEE-ACM.

## Conferences:

- 1 ISMB/ECCB
- 2 RECOMB

# Resources

## Other similar courses:

- 1 Serafim Batzoglou at Stanford – <https://web.stanford.edu/class/cs262>
- 2 Manolis Kellis at MIT – <https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-047-computational-biology-fall-2015>
- 3 Christopher Burge, David Gifford and Ernest Fraenkel at MIT – <https://ocw.mit.edu/courses/biology/7-91j-foundations-of-computational-and-systems-biology-spring-2014>
- 4 Curtis Huttenhower at Harvard – <https://canvas.harvard.edu/courses/71191>

# Evaluation criteria

## ① End-semester Evaluation:

- Written examination (50 marks)

## ② Internal Evaluation:

- Mid-semester examination (30 marks)
- Assignment submission (10 marks)
- Project work (10 marks)

**Web:** <https://www.isical.ac.in/malaybhattacharyya/Courses/CMBB/Fall2024>