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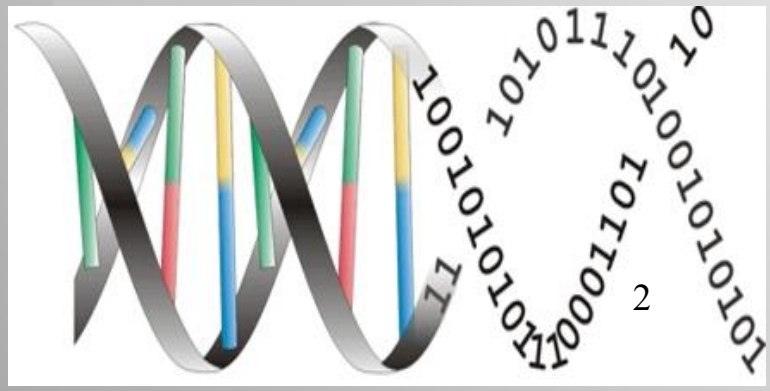
Programming for Computational & Systems Biology

Instructor: Paul Xie

Tue. & Thr. 9:35~10:50



Overview of Course

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- Introduction to programming skills in computational and systems biology. Topics include real world examples, such as processing genome or proteome data, and analyzing large-scale data. The idea of “big data” will be emphasized to help students with their coding skills to discovering new knowledge in biomedical sciences and solving biomedical problems.

Course Format

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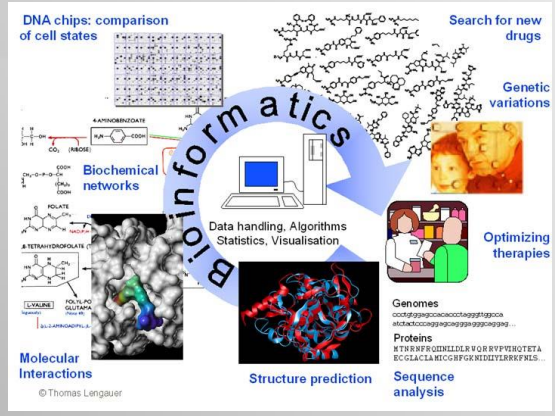
- Computer labs + lectures (3 hours/week)
- Coding concepts (some knowledge about biological data)
- 6-8 assignments, published on eLC, (30-40%)
  - Please upload them by the due days
- Paper review (10-20%)
- 1 term paper (50-60%)

Topics

- -Omics data, e.g. Genomics, Proteomics…
- Basic Programming, e.g. I/O, variables, string, loop, regular express, array…etc.
- Data retrieval & processing
- Data analysis
- Model & building model
- Clustering and Classification
- Prediction



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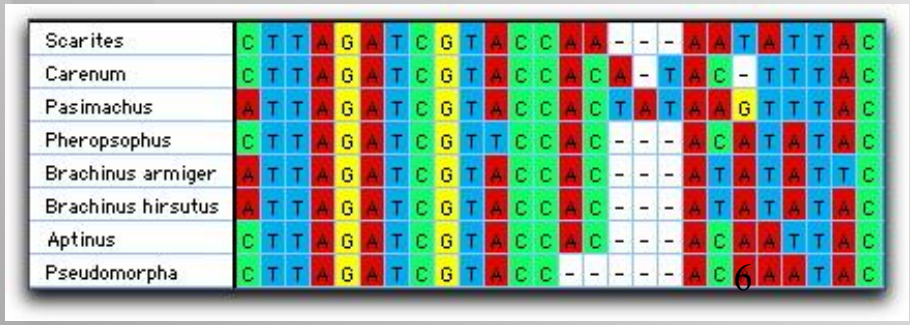
Data Array: List & Dictionary Transcription & Translation

Instructor: Paul Xie (4)



This Week

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- Random number
- Data array
  - List
  - Dictionary
- Average & Std. Dev.

Group Discussion

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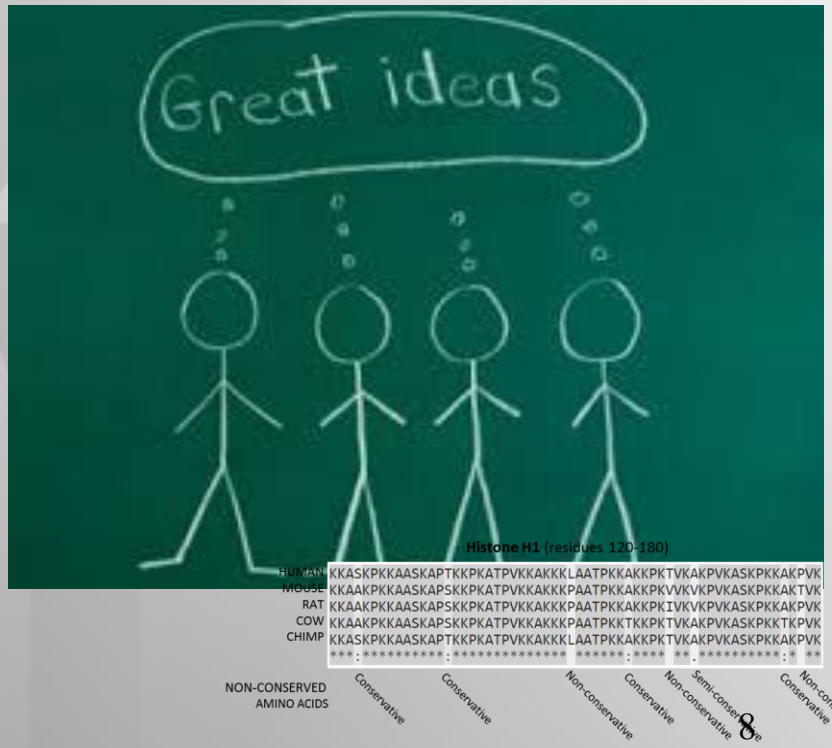

Python Time

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Open PyCharm

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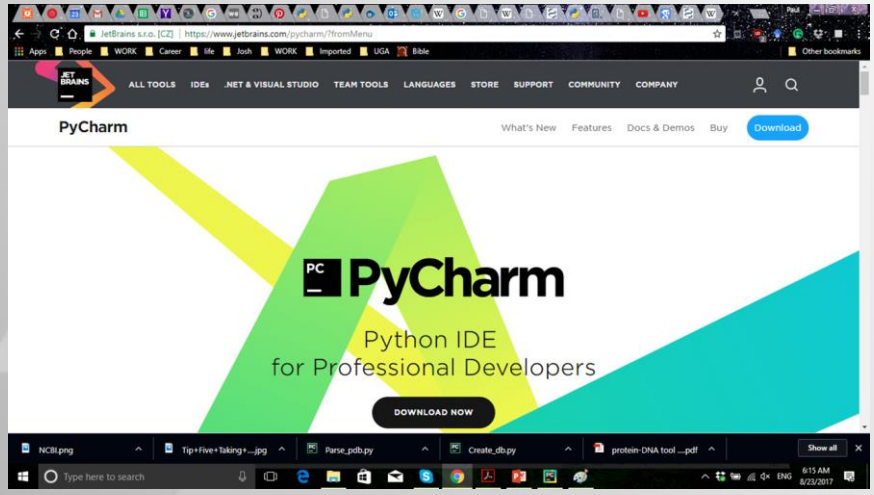
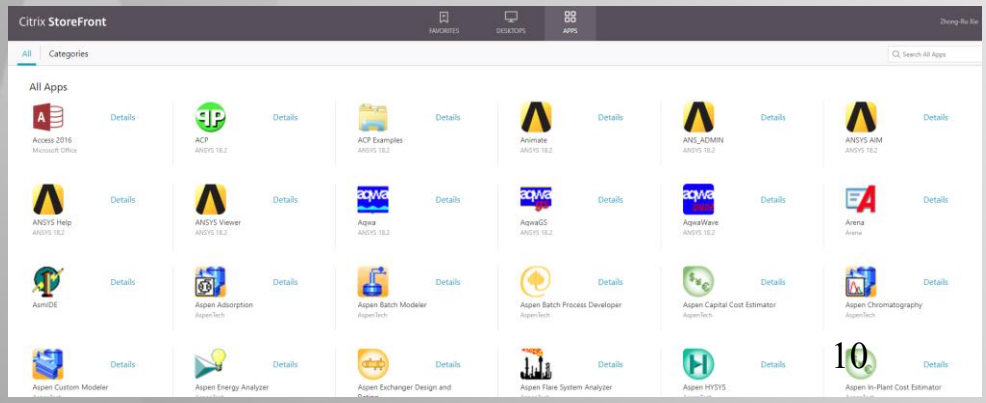
- Go to UGA CENGR Mylab
  - mylab.engr.uga.edu
- Login Citrix
  - Apps
  - PyCharm
  - New project





Syntax

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- Array
  - **List** is a collection which is ordered and changeable. Allows duplicate members. []
  - **Tuple** is a collection which is ordered and unchangeable. Allows duplicate members. ()
  - **Set** is a collection which is unordered and unindexed (unchageable). No duplicate members.{}
  - **Dictionary** is a collection which is unordered, changeable and indexed. No duplicate members. {key:200}

Code

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```
#array
def main():
    cars = ["Ford","Volvo","BMW"]
    for i in cars:
        print(i)

main()
```

Code

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```
#array
def show_array(cars):
    print(len(cars),'cars.\nThey are:')
    for i in cars:
        print(i)
    for i in range(10):
        print('-',end='')
    print()
……..
```

Code

```
……..
def main():
    cars = ["Ford","Volvo","BMW"]
    show_array(cars)
    cars.append("Honda")  #
    show_array(cars)
    cars.pop(2)
    show_array(cars)
    cars.insert(1,"Toyota")
    show_array(cars)
    print(cars.index("Honda"))
    cars.remove("Volvo")
    show_array(cars)
    cars.sort()
    show_array(cars)
    cars.reverse()
    show_array(cars)
main()
```

Exercise

- Random number ➔ array
- Calculate max, min, mean (average)
- Check redundant
  - Double loop
- Sort
  - Bubble sort

Water Level Marker

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- An array a[ ]
- A variable x to record highest (lowest) value
- (For loop)
  - Compare a[i] and x
  - Record the highest value

Average

- An array a[n]
- A variable s to record summary
- (For loop)
  - s += a[i];
- s /=n;

Practice

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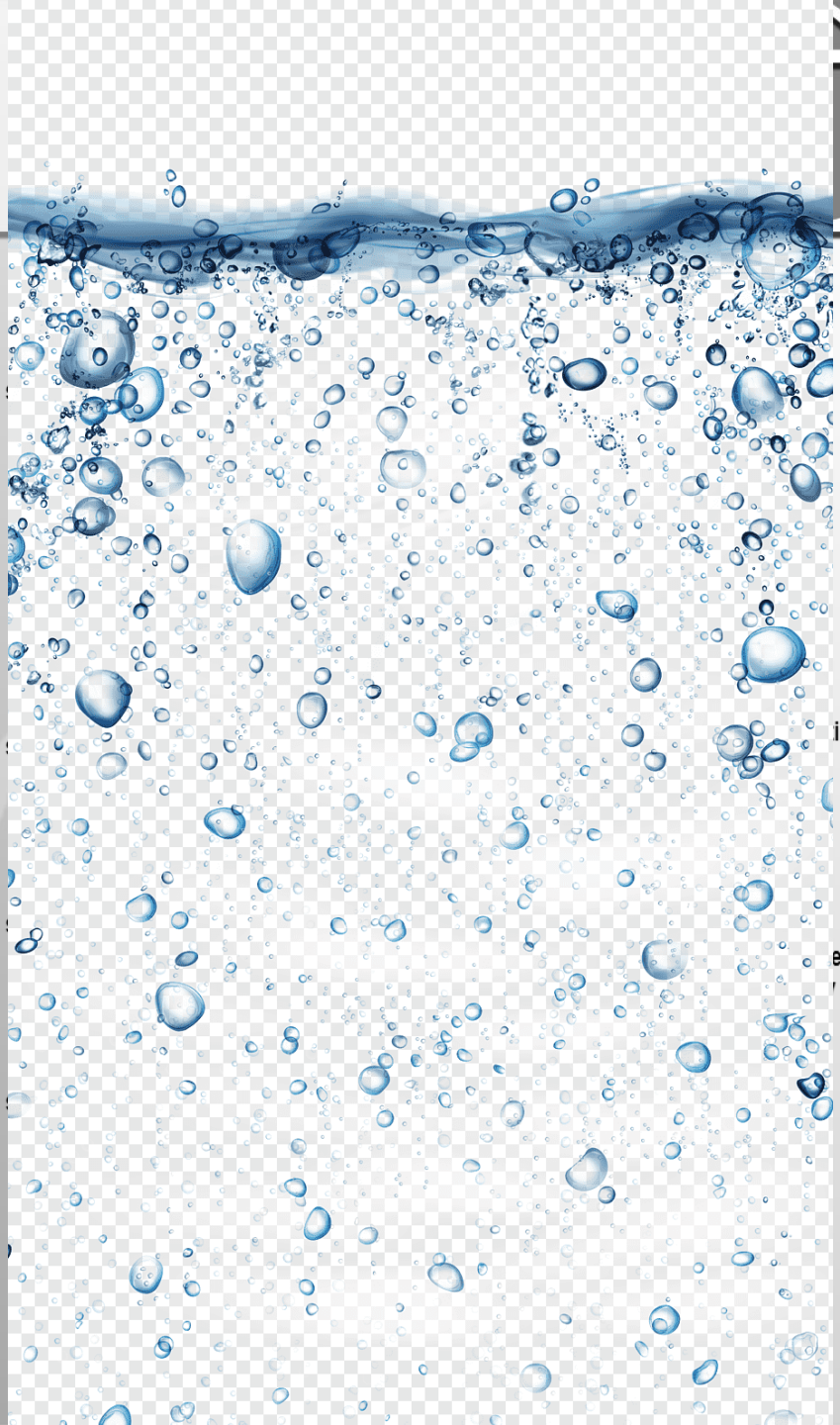
- Average and Standard deviation

$$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i-\overline{x})^2}=\sqrt{\frac{1}{N}\left(\sum_{i=1}^{N}x_i^2\right)-(\overline{x})^2}=\sqrt{\left(\frac{1}{N}\sum_{i=1}^{N}x_i^2\right)-\left(\frac{1}{N}\sum_{i=1}^{N}x_i\right)^2}.$$

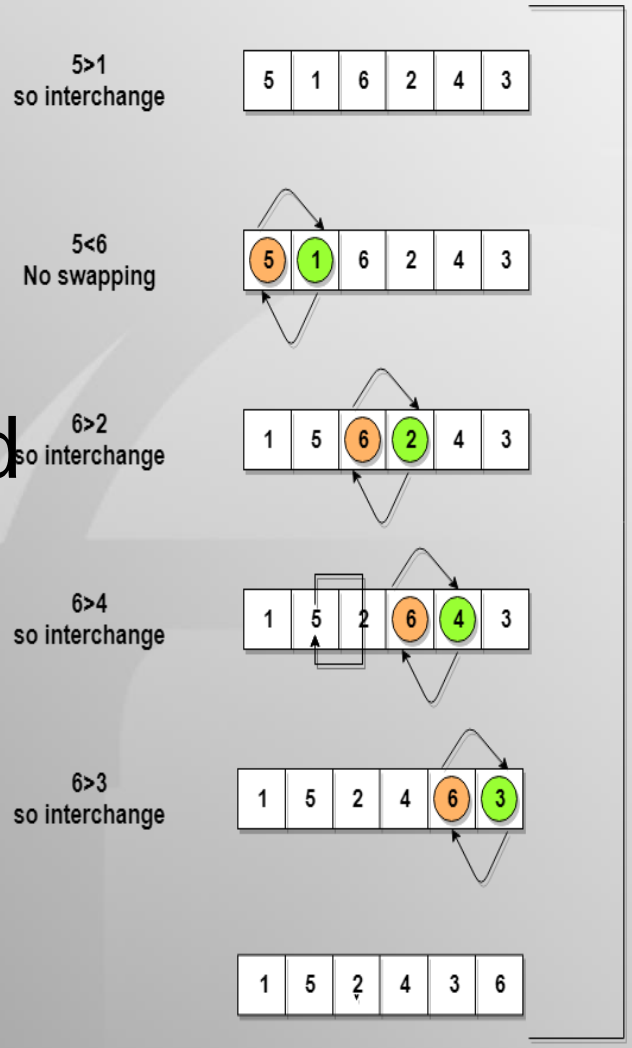
Bubble Sort

- An array a[n] contains n numbers
- How to sort them?
- Big bubbles is lighter (go up)



Bubble Sort

- An array a[ ]
- Double loops (loop #1 and #2)
- Compare numbers and switch



Non-redundant

- Lottery
- 5 or 6 non-redundant balls (numbers)
- For loop
  - Generate ball[i]
  - Compare balls

Taiwan Lottery

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- Prize
  - 1st (6 matches) : 82%
  - 2nd (5+special): 7%
  - 3rd (5 matches): 6.5%
  - 4th (4+special): 4.5%
  - 5th (4 matches): $80
  - 6th (3+special): $40
  - 7th (2+1 or 3 matches): $8
- ~56% of incomes

Exercises

- sort: from big to small
- List all Prime from 1 to 100
  - For loop
  - If /else
  - Array
  - Size unknown
- Store factorial in an array, e.g. 1! ~ 10!
  - Do we need to calculate 1!, 2!, 3!, … separately?

Multiplication Table

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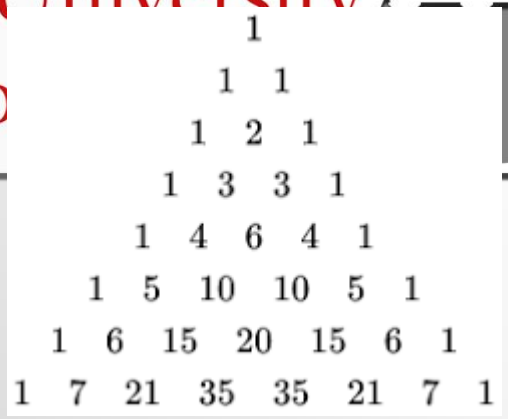
- Double Loop
- A loop inside another

```
a = []; b = []; c = []
for i in range(10):
    k = []; l = [];  m = []
    for j in range(10):
        k.append(i+1)
        l.append(j+1)
        m.append((i+1)*(j+1))
    a.append(k)
    b.append(l)
    c.append(m)
```

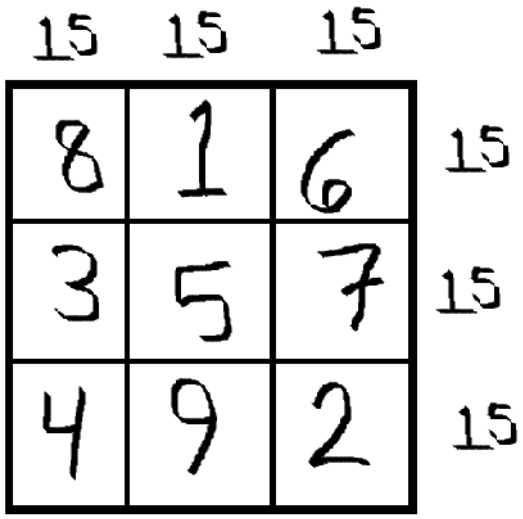
2D Array

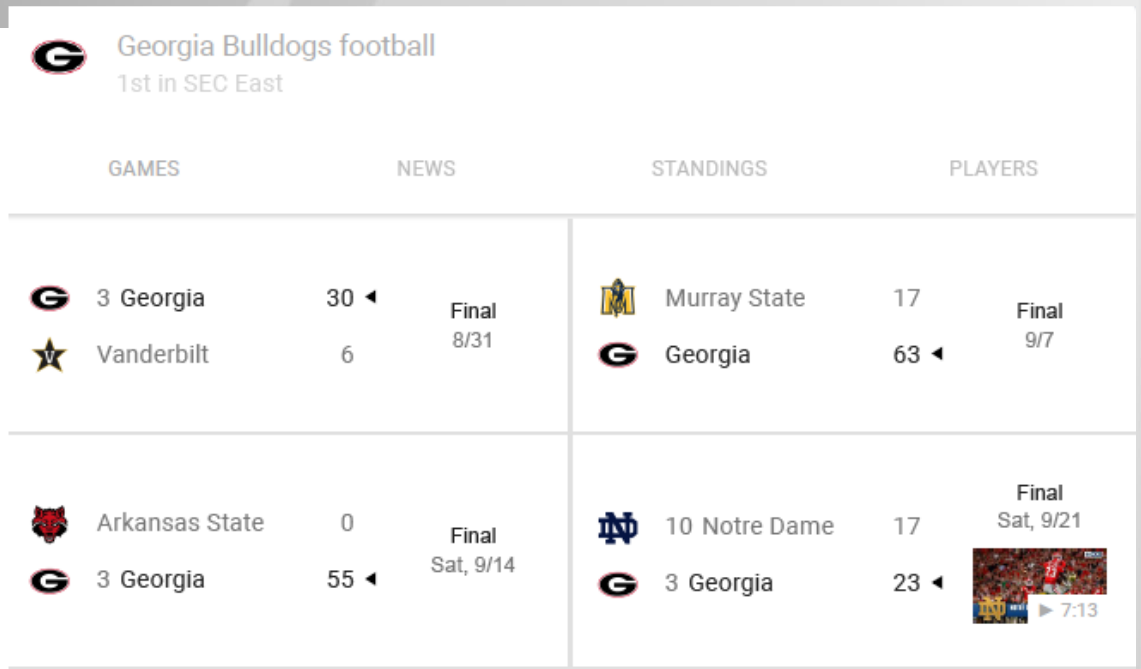
- a = [[0]*m for i in range(m)]
- Or, b = [1,2,3,4,5], c = [2,4,6,8,10],…
- a.append(b)
- a.append(c)
- …
- matrix

Exercise



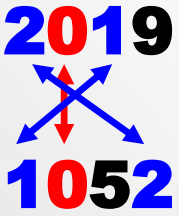
- Create a 2D array (list)
- 2d array for Dawgs score
- 2d array for your assignment scores
- Pascal triangle and Magic square





Exercise Quiz

- Please design a number guessing game called 1A2B



- Please randomly generate a 4-digit number with 4 different number (for example 2019)
- A player make a first guess, say 1024, compare two number2, 1 correct digit (0) has correct position ➔ 1A; and 2 correct digits has incorrect positions ➔ 2B
- Based on previous hints, keep guess until get it right

Open a File

- Syntax
- File_id = open(file_name, operation)
- ‘r’,’w’,’a’
- File_id.read()
- File_id.readline()
- File_id.readlines()

Syntax

- Array
- Dictionary
  - Key-value

Code


```
#dictionary
def main():
    cars =  {
        "brand": "Toyota",
        "model": "Corolla",
        "year": 2003
    }
    print(cars)
    cars["year"] = 2018
    cars["color"] = "red"
    cars["owner"] = "paul"
    cars["seller"] = "Toyota Athens"
    cars["plate"] = "Georgia"
    -------------------------
```

Code

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```
print(len(cars))
    for i in cars:
        print(i)
    for i in cars.keys():
        print(i)
    for i in cars.values():
        print(i)
    for x,y in cars.items():
        print(x,y)
    cars.popitem()
    cars.pop("seller")
    del cars[]
    print(cars)
```

Exercise

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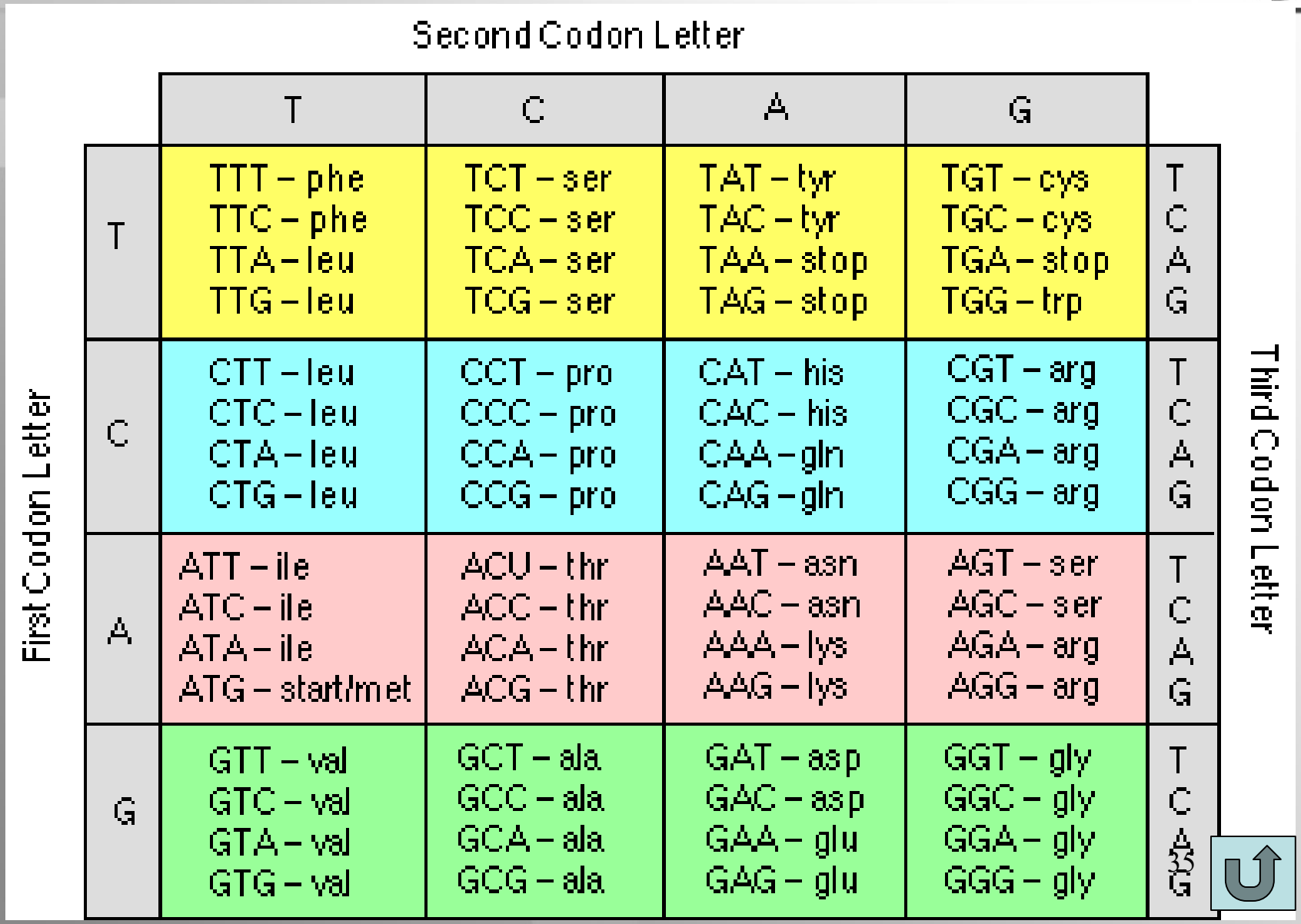
- Calculate the occurrence & frequency of amino acids (or nucleotides)
  - Open file(s)
  - Dictionaries
  - Loops
  - Counting
  - presentation

DNA → AA



First Codon Letter	Second Codon Letter: T	Second Codon Letter: C	Second Codon Letter: A	Second Codon Letter: G	Third Codon Letter
T	TTT – phe TTC – phe TTA – leu TTG – leu	TCT – ser TCC – ser TCA – ser TCG – ser	TAT – tyr TAC – tyr TAA – stop TAG – stop	TGT – cys TGC – cys TGA – stop TGG – trp	T C A G
C	CTT – leu CTC – leu CTA – leu CTG – leu	CCT – pro CCC – pro CCA – pro CCG – pro	CAT – his CAC – his CAA – gln CAG – gln	CGT – arg CGC – arg CGA – arg CGG – arg	T C A G
A	ATT – ile ATC – ile ATA – ile ATG – start/met	ACU – thr ACC – thr ACA – thr ACG – thr	AAT – asn AAC – asn AAA – lys AAG – lys	AGT – ser AGC – ser AGA – arg AGG – arg	T C A G
G	GTT – val GTC – val GTA – val GTG – val	GCT – ala GCC – ala GCA – ala GCG – ala	GAT – asp GAC – asp GAA – glu GAG – glu	GGT – gly GGC – gly GGA – gly GGG – gly	T C A G

Central Dogma

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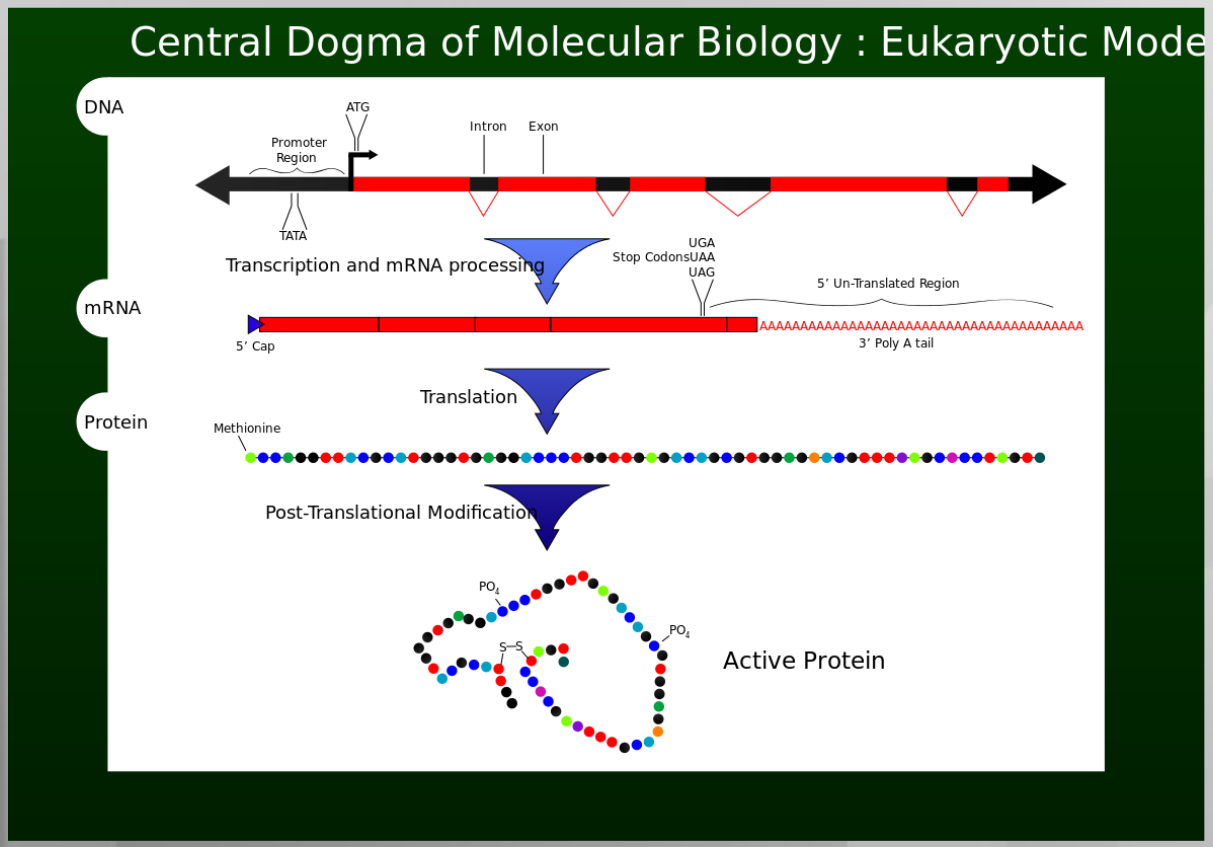
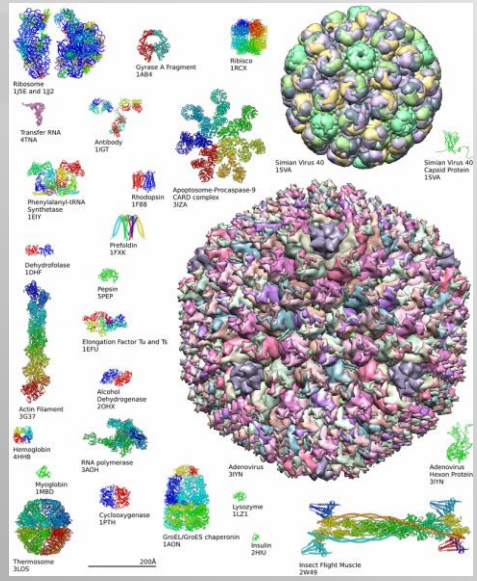
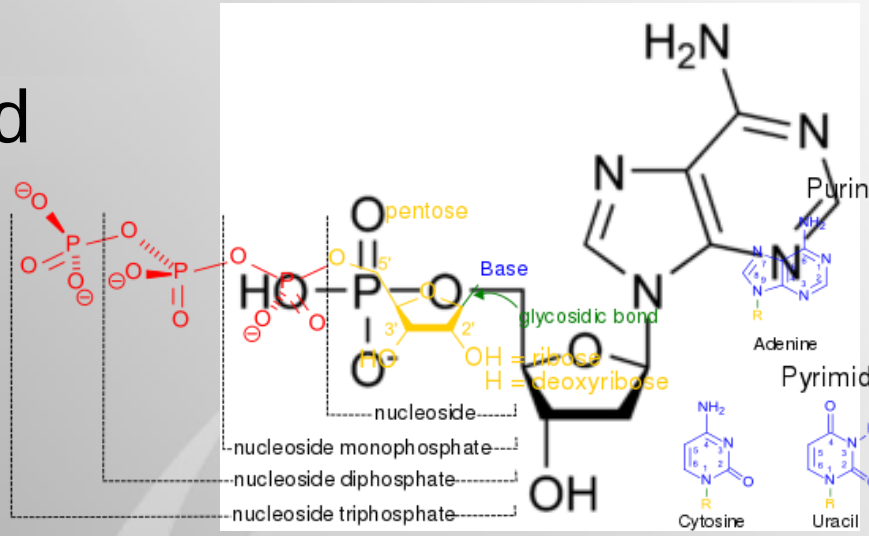


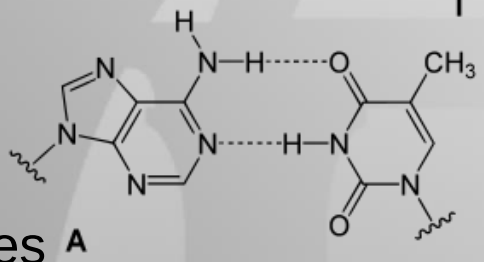
- DNA→RNA→ Protein
- Transcription & Translation (&Replication)

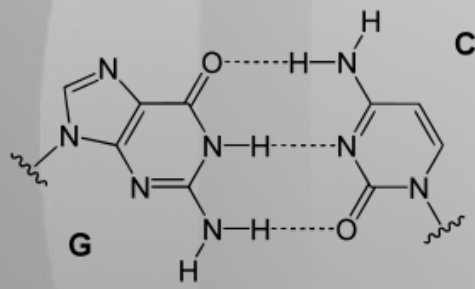


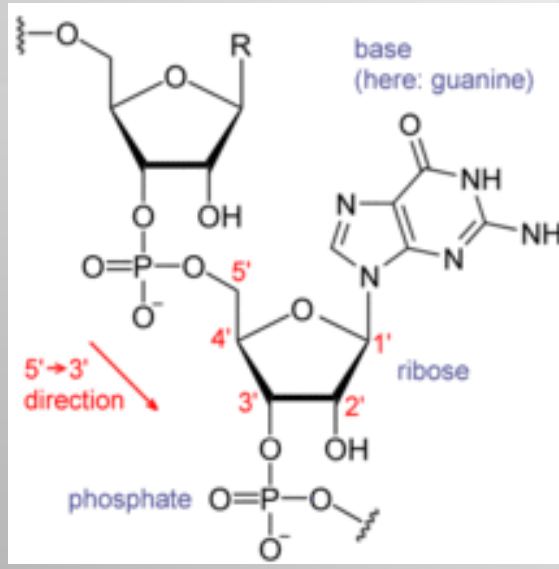
DNA & RNA

- Deoxyribonucleic acid
- Ribonucleic acid
  - Base: A, T/U, C, G
    - Adenine
    - Thymine
    - Uracil
    - Guanine
    - Cytosine
    - Purines & Pyrimidines
  - Ribose
  - Phosphate









Double Helix!

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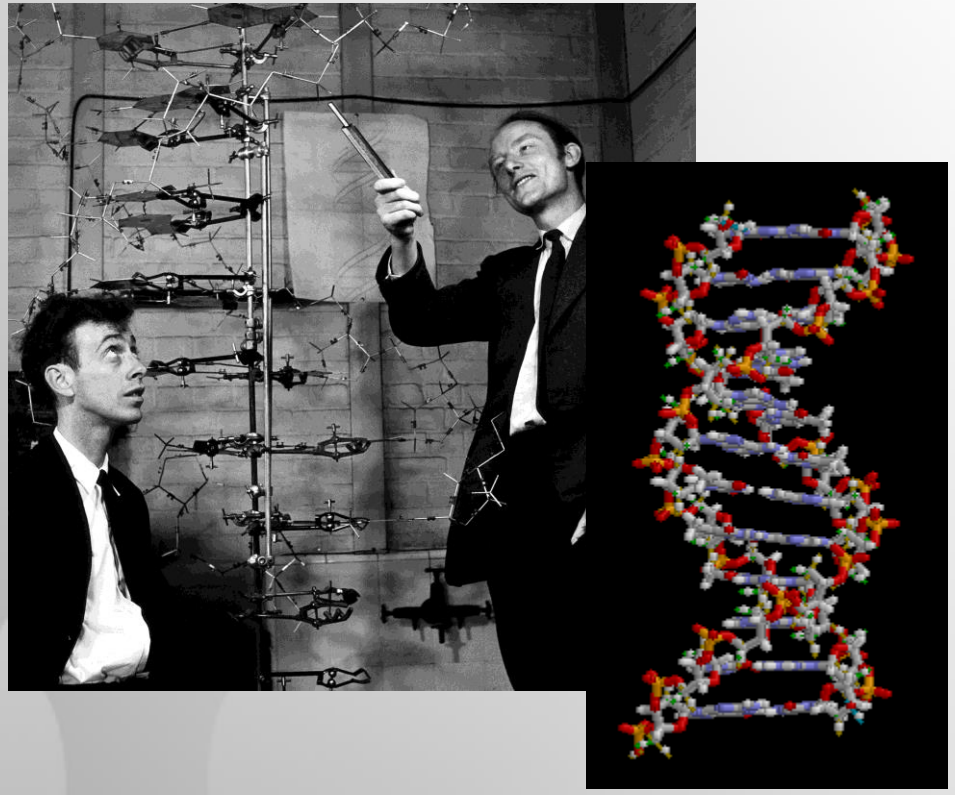
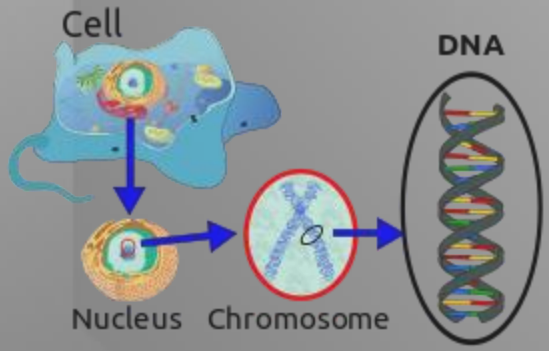
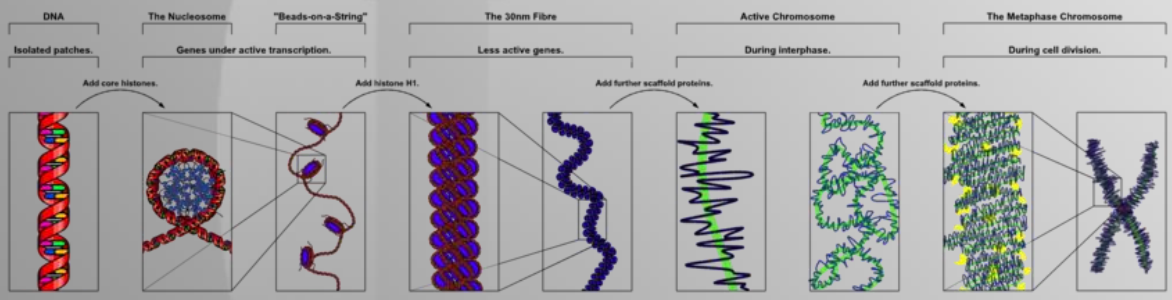
- Double helix
  - Chromosomes
- Replication
  - DNA-polymerase
- Transcription
- Translation

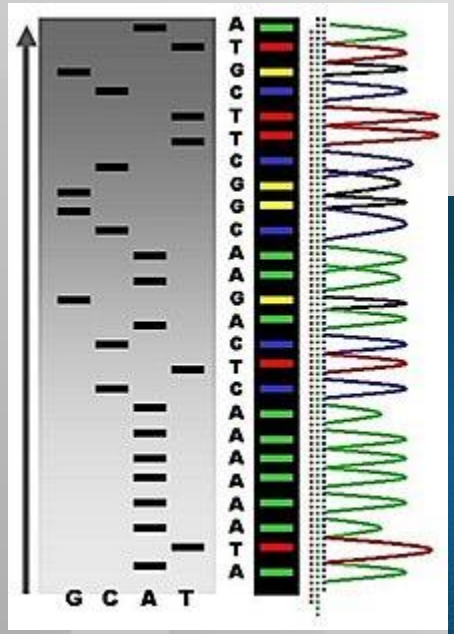


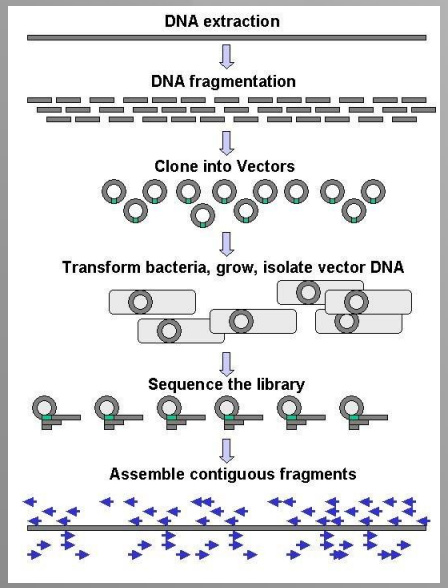


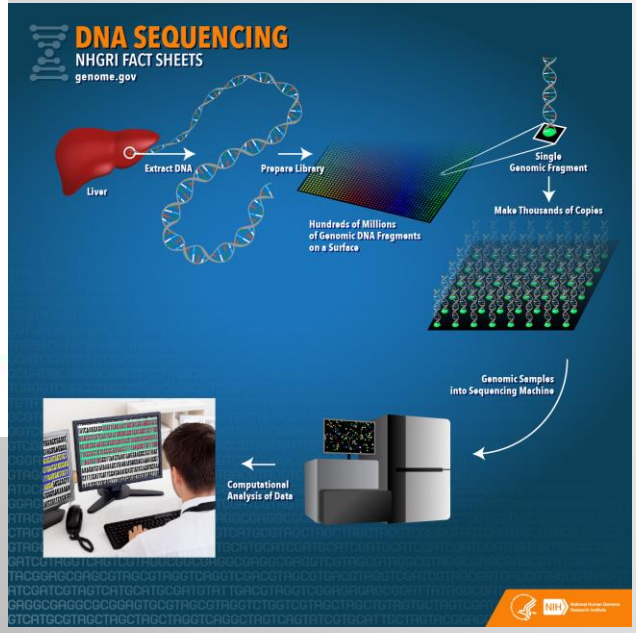


Sequencing

- Restriction Enzyme
- Gel & Electrophoresis

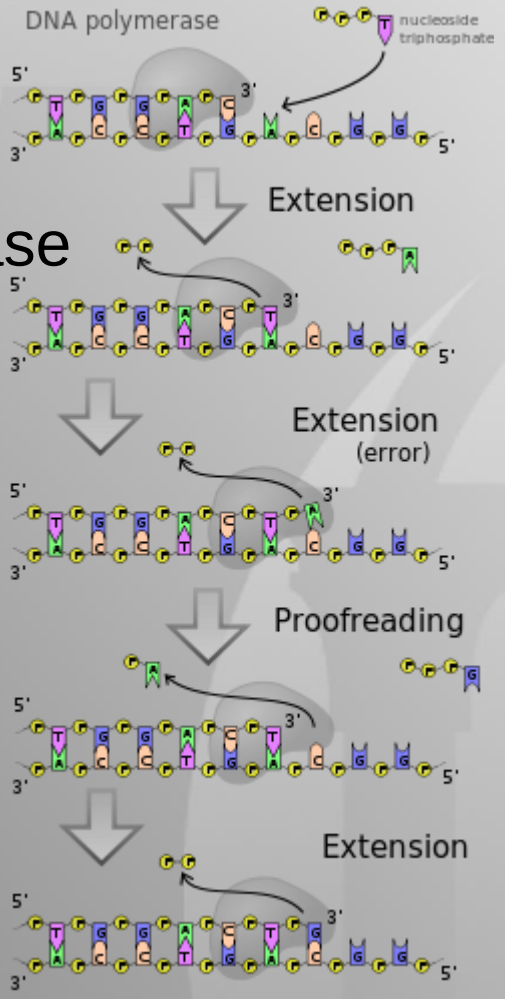


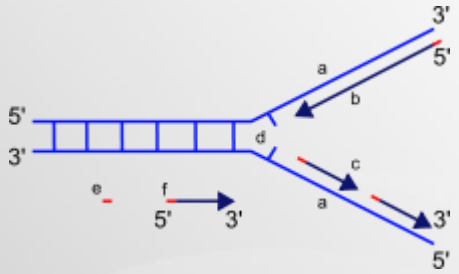


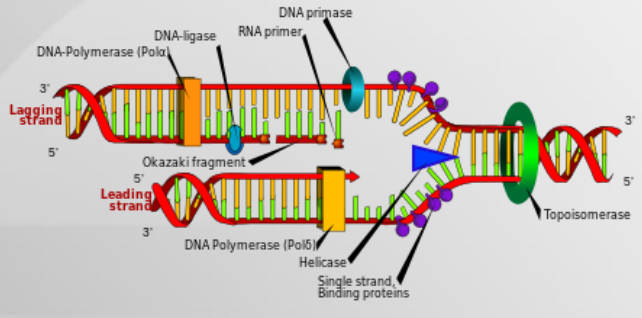


Replication

- Double helix
- Replication
  - DNA-polymerase
- Transcription
- Translation

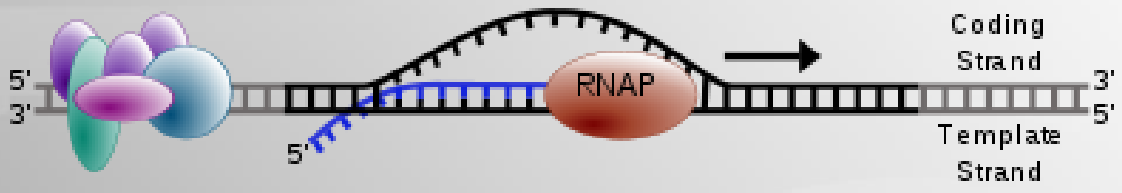


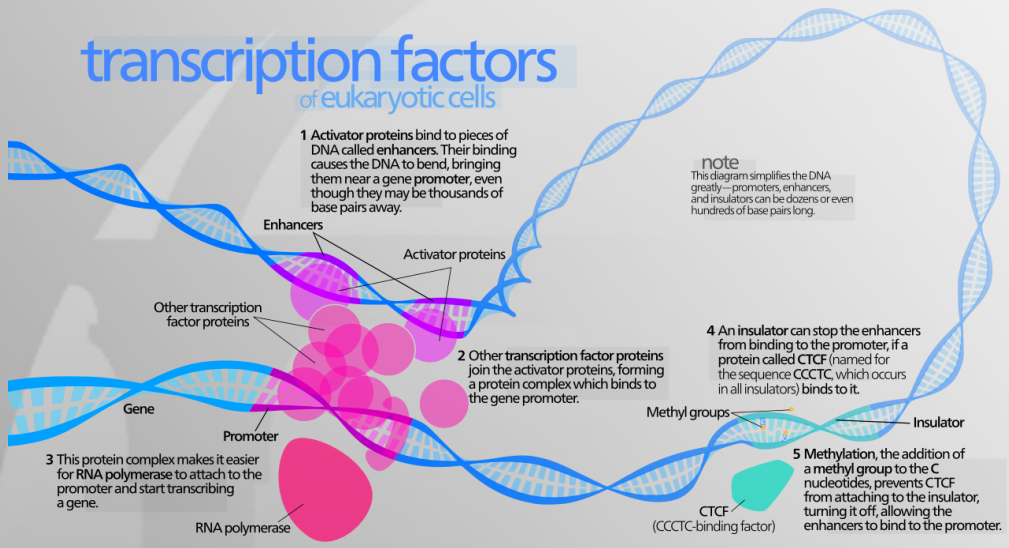


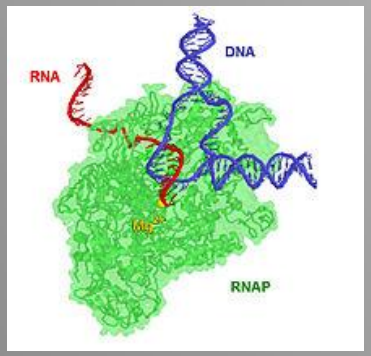


Transcription

- Double helix
- Replication
- Transcription
  - RNA Polymerase
  - Transcription Factors
  - Expression control
- Translation







Translation

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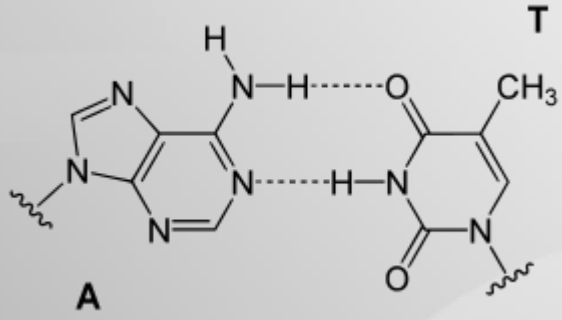
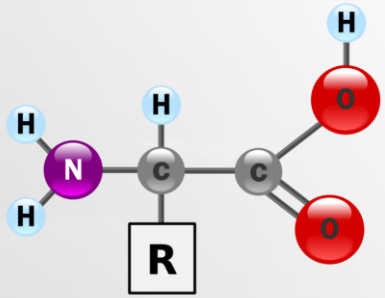
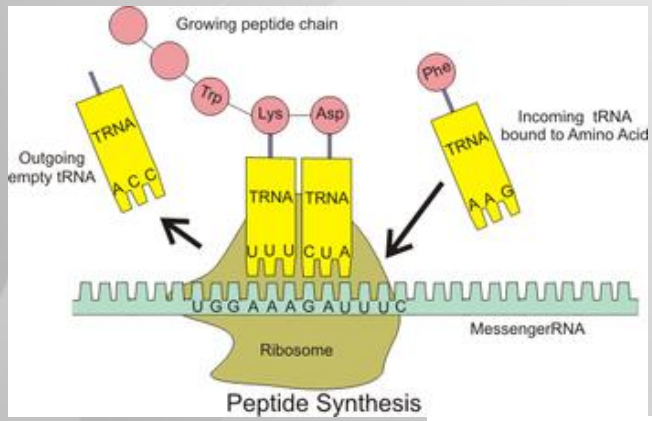
- Double helix
- Replication
- Transcription
- Translation
  - Ribosome
  - mRNA
  - tRNA
  - Nucleic acid to Amino acid







Second Codon Letter

First Codon Letter	T	C	A	G	Third Codon Letter
T	TTT – phe TTC – phe TTA – leu TTG – leu	TCT – ser TCC – ser TCA – ser TCG – ser	TAT – tyr TAC – tyr TAA – stop TAG – stop	TGT – cys TGC – cys TGA – stop TGG – trp	T C A G
C	CTT – leu CTC – leu CTA – leu CTG – leu	CCT – pro CCC – pro CCA – pro CCG – pro	CAT – his CAC – his CAA – gln CAG – gln	CGT – arg CGC – arg CGA – arg CGG – arg	T C A G
A	ATT – ile ATC – ile ATA – ile ATG – start/met	ACU – thr ACC – thr ACA – thr ACG – thr	AAT – asn AAC – asn AAA – lys AAG – lys	AGT – ser AGC – ser AGA – arg AGG – arg	T C A G
G	GTT – val GTC – val GTA – val GTG – val	GCT – ala GCC – ala GCA – ala GCG – ala	GAT – asp GAC – asp GAA – glu GAG – glu	GGT – gly GGC – gly GGA – gly GGG – gly	T C A G

Code

The University of Georgia

```
#dictionary
def main():
    f1 = open("M:\\tubulin_a.txt","r")
    seq1 = f1.readline()
    f2 = open("M:\\tubulin_b.txt", "r")
    seq2 = f2.readline()
    aa1 = {}
    aa2 = {}
-----------------------------------
```

Code

The University of Georgia

```
-------------------------------------
    for i in range(len(seq1)):
        if seq1[i] in aa1:
            aa1[seq1[i]]+=1
        else:
            aa1[seq1[i]]=1
    for i in range(len(seq2)):
        if seq2[i] in aa2:
            aa2[seq2[i]] += 1
        else:
            aa2[seq2[i]] = 1
    for i in aa1:
        print(i,aa1[i],aa1[i]/len(seq1),aa2[i],aa2[i]/len(seq2))
```

2D Array

- List = [[0]*n, for I in range(n)]


Thank You


TIME
FOR A
BREAK