

# Distance Metrics

Mark Voorhies

4/5/2018

# List tricks

Adding data to a list:

```
mylist = []
mylist.append(3)
mylist += [4,5,6]
```

# List tricks

Adding data to a list:

```
mylist = []
mylist.append(3)
mylist += [4,5,6]
```

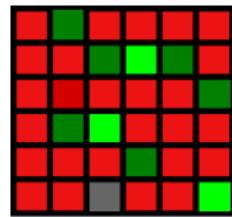
Lists of lists:

```
matrix = [[ 1 , 2 , 3 , 4] ,
           [ 5 , 6 , 7 , 8] ,
           [ 9 , 10 , 11 , 12]]
```

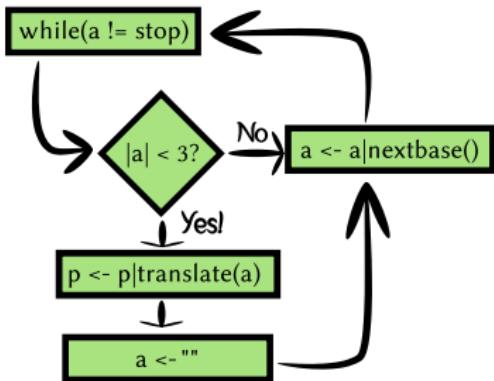
# Anatomy of a Programming Language



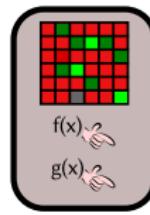
functions



data structures



control statements



objects

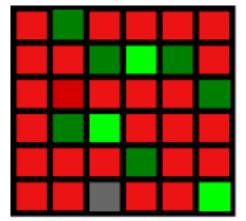
# Anatomy of a Programming Language

$f(x)$   
  
functions

```
def f(x,y):  
    return x*y  
  
from math import sqrt
```

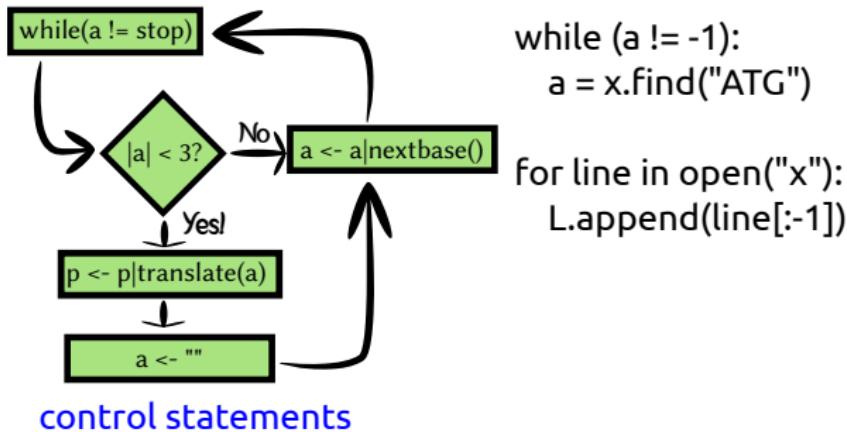
# Anatomy of a Programming Language

```
1
1.2
"my string"
["my","list"]
my_file = open("my_file.txt")
("my","tuple")
[["my","multi"],
 ["dimensional","list"]]
```



data structures

# Anatomy of a Programming Language

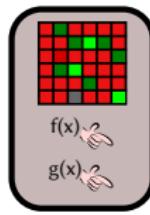


# Anatomy of a Programming Language

```
"GGGATGCATCAT".find("ATG")
```

```
L = [3,4,5]  
L.append(7)  
L += [6,7]
```

```
open("1.txt").readlines()
```

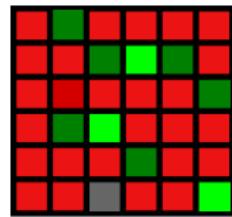


objects

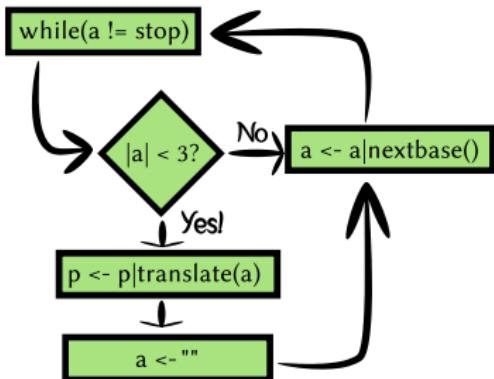
# Anatomy of a Programming Language



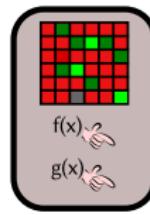
functions



data structures



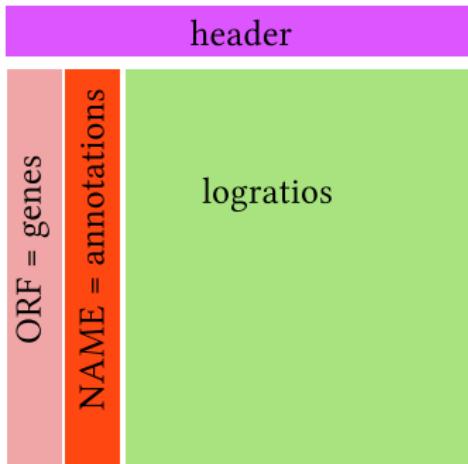
control statements



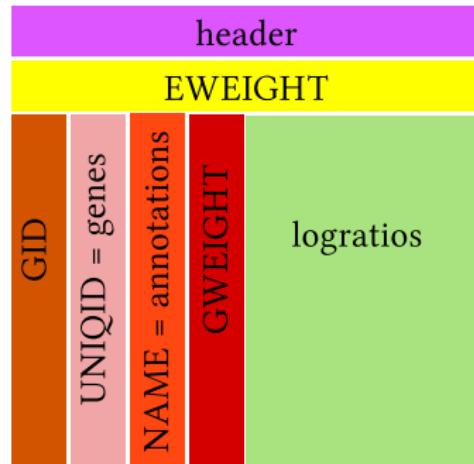
objects

# The CDT file format

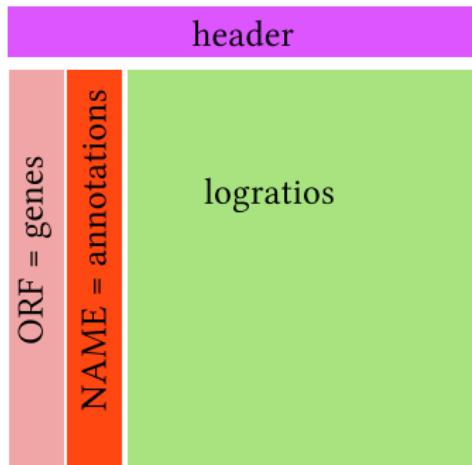
Minimal CLUSTER input



Cluster3 CDT output



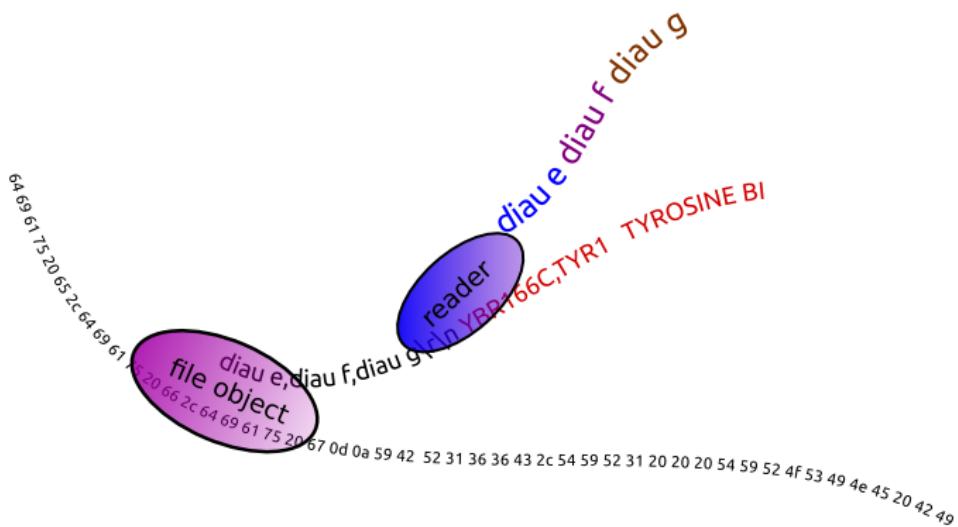
- Tab delimited (\t)
- UNIX newlines (\n)
- Missing values → empty cells



header	
ORF = genes	
NAME = annotations	logratios

```
[["YBR166C", "YOR357C", "YLR292C", ...],  
 ["TYR1 ...", "GRD19 ...", "SEC72 ...", ...],  
 [[ 0.33, -0.17,  0.04, -0.07, -0.09, ...],  
 [-0.64, -0.38, -0.32, -0.29, -0.22, ...],  
 [-0.23,  0.19, -0.36,  0.14, -0.40, ...],  
 ...]  
 ]
```

# Generators are like polymerases: iterable but not indexable



# Fun with logarithms

In log space, multiplication and division become addition and subtraction:

$$\log(xy) = \log(x) + \log(y)$$

$$\log(x/y) = \log(x) - \log(y)$$

# Fun with logarithms

In log space, multiplication and division become addition and subtraction:

$$\log(xy) = \log(x) + \log(y)$$

$$\log(x/y) = \log(x) - \log(y)$$

Therefore, exponentiation becomes multiplication:

$$\log(x^y) = y \log(x)$$

# Fun with logarithms

In log space, multiplication and division become addition and subtraction:

$$\log(xy) = \log(x) + \log(y)$$

$$\log(x/y) = \log(x) - \log(y)$$

Therefore, exponentiation becomes multiplication:

$$\log(x^y) = y \log(x)$$

Also, we can change of the base of a logarithm like so:

$$\log_A(x) = \log(x)/\log(A)$$

# Pearson distances

## Pearson similarity

$$s(x, y) = \frac{1}{N} \sum_i^N \left( \frac{x_i - x_{\text{offset}}}{\phi_x} \right) \left( \frac{y_i - y_{\text{offset}}}{\phi_y} \right)$$

$$\phi_G = \sqrt{\sum_i^N \frac{(G_i - G_{\text{offset}})^2}{N}}$$

## Pearson similarity

$$s(x, y) = \sum_i^N \left( \frac{x_i - x_{\text{offset}}}{\phi_x} \right) \left( \frac{y_i - y_{\text{offset}}}{\phi_y} \right)$$

$$\phi_G = \sqrt{\sum_i^N (G_i - G_{\text{offset}})^2}$$

# Pearson distances

Pearson similarity

$$s(x, y) = \sum_i^N \left( \frac{x_i - x_{\text{offset}}}{\sqrt{\sum_i^N (x_i - x_{\text{offset}})^2}} \right) \left( \frac{y_i - y_{\text{offset}}}{\sqrt{\sum_i^N (y_i - y_{\text{offset}})^2}} \right)$$

# Pearson distances

Pearson similarity

$$s(x, y) = \frac{\sum_i^N (x_i - x_{\text{offset}})(y_i - y_{\text{offset}})}{\sqrt{\sum_i^N (x_i - x_{\text{offset}})^2} \sqrt{\sum_i^N (y_i - y_{\text{offset}})^2}}$$

# Pearson distances

Pearson similarity

$$s(x, y) = \frac{\sum_i^N (x_i - x_{\text{offset}})(y_i - y_{\text{offset}})}{\sqrt{\sum_i^N (x_i - x_{\text{offset}})^2} \sqrt{\sum_i^N (y_i - y_{\text{offset}})^2}}$$

Pearson distance

$$d(x, y) = 1 - s(x, y)$$

# Pearson distances

Pearson similarity

$$s(x, y) = \frac{\sum_i^N (x_i - x_{\text{offset}})(y_i - y_{\text{offset}})}{\sqrt{\sum_i^N (x_i - x_{\text{offset}})^2} \sqrt{\sum_i^N (y_i - y_{\text{offset}})^2}}$$

Pearson distance

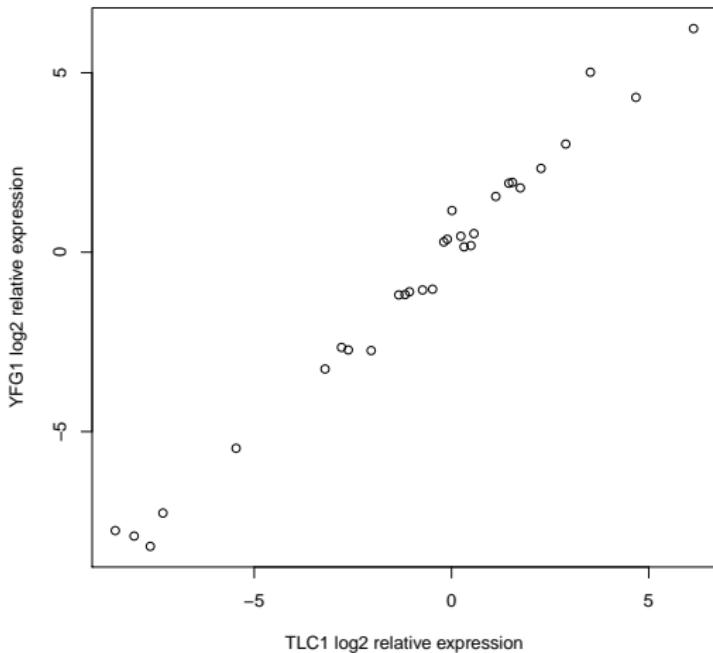
$$d(x, y) = 1 - s(x, y)$$

Euclidean distance

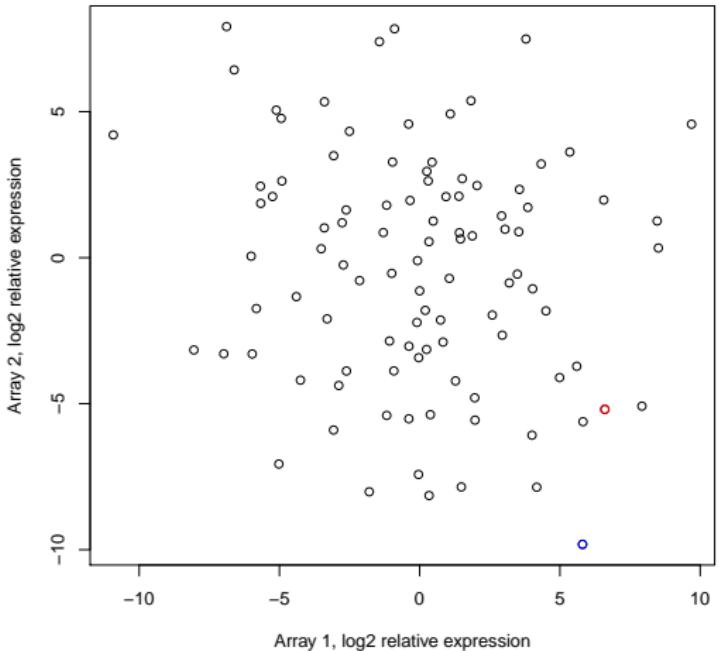
$$\frac{\sum_i^N (x_i - y_i)^2}{N}$$

## Comparing all measurements for two genes

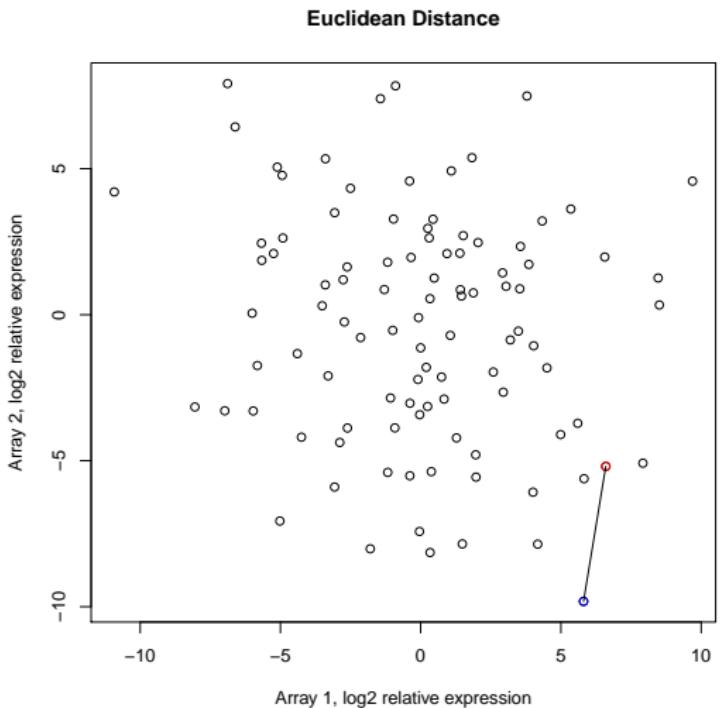
## Comparing two expression profiles ( $r = 0.97$ )



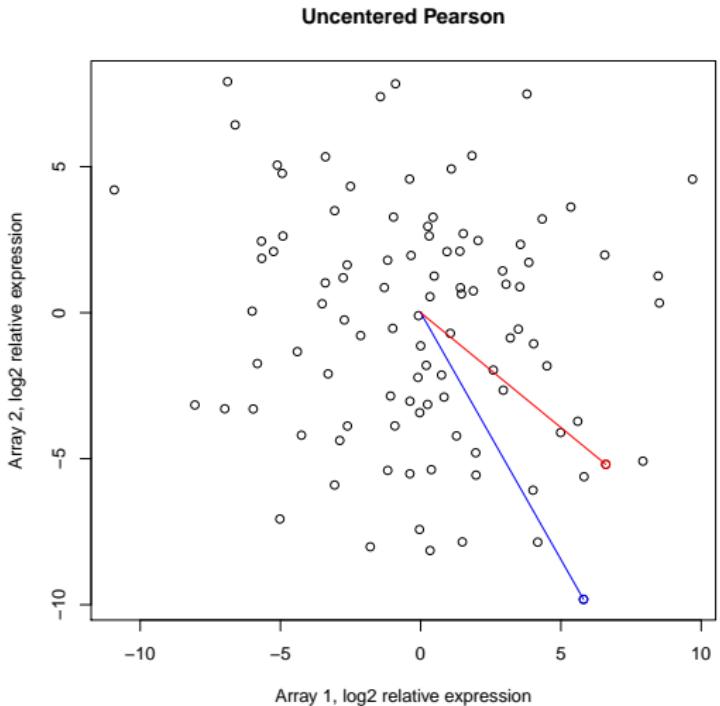
# Comparing all genes for two measurements



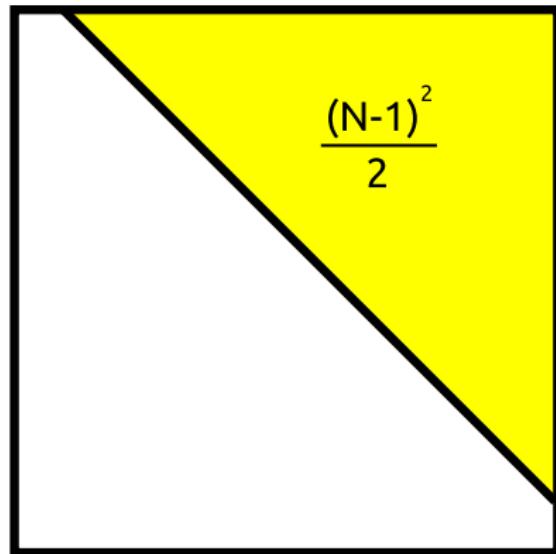
# Comparing all genes for two measurements



# Comparing all genes for two measurements



# Measure all pairwise distances under distance metric



# Homework

- ① Install biopython via Canopy (*or whatever you're using. If this doesn't work, install Cluster3*)
- ② Write a function to calculate all pairwise Pearson correlations for the yeast expression profiles.
- ③ Save the results of your pairwise correlation calculation in the CDT format described in the JavaTreeView manual.
- ④ Read PNAS 95:14863
- ⑤ Try the first two problems, replacing the Pearson correlation with the distance metric from the PNAS paper or with one of the distance metrics from the Cluster3 manual.