# Beyond the `dict`

## Python tools for data wrangling

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PyData NYC

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github.com/ihaque
github.com/counsyl

https://github.com/ihaque/pydata_nyc_2013

# Who Are You?

Counsyl performs carrier screening for
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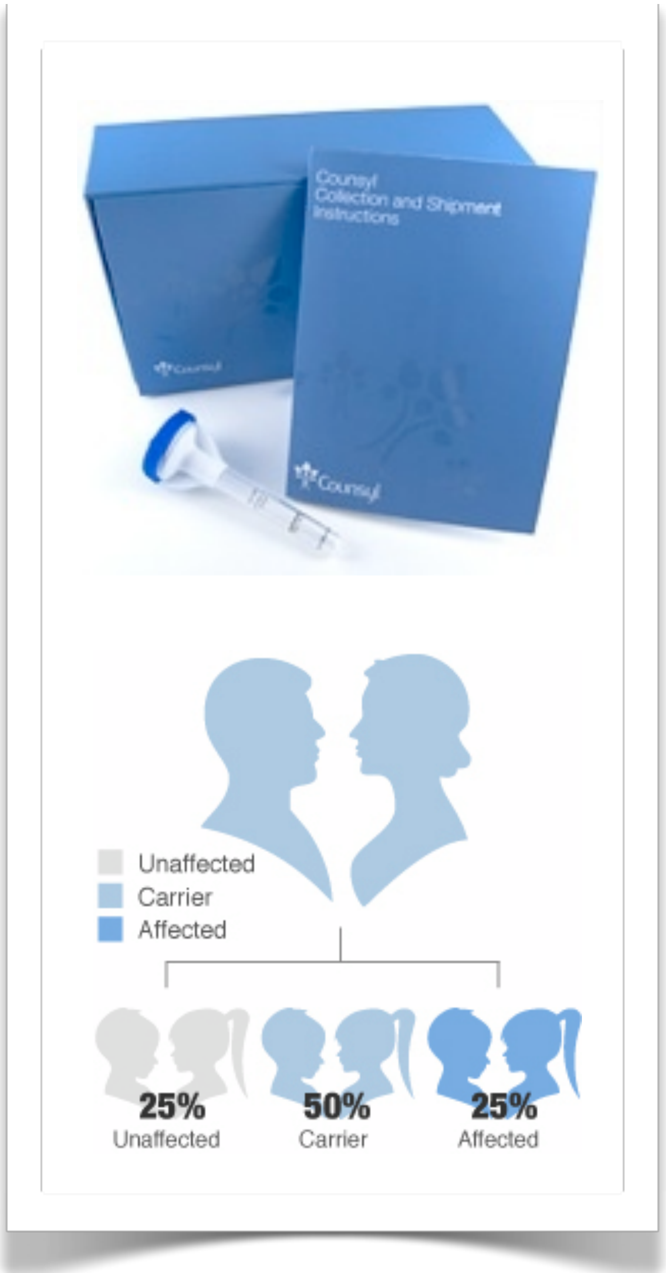

# Who Are You?

Counsyl performs carrier screening for inherited genetic disorders on >3% of all births in the USA.

Almost all backend code at Counsyl is in Python: it can do everything from hardcore numerics to webapps.

Medical genomics requires dealing with lots of structured (numerical, tabular) and semi-structured (crappy log file) data.

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Parsing

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Parsing Querying

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Parsing

Querying

Storing

# Today's Menu

Three courses:

- Literate parsing: `csv`, `sheets`
- Querying beyond the dict: `sqlite3`, `pony.orm`
- Efficient numerical storage: `tables`

# Today's Menu

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- Literate parsing: **`csv`**, **`sheets`**
- Querying beyond the dict: **`sqlite3`**, **`pony.orm`**
- Efficient numerical storage: **`tables`**

Off the menu:

- **`pandas`**
- "Real" databases: **`psycopg2`**, **`MySQLdb`**
- Heavyweight ORMs: **`django`**, **`sqlalchemy`**

# Let’s parse the One True Format.

Let’s parse the One True Format.

CSV

# hapmap.txt

```
rs# refallele_freq otherallele_freq
rs6423165 0.143 0.857
rs6608381 0.464 0.536
rs6644972 0.354 0.646
...
```

# Basic CSV

```
def read_csv(filename):
  with open(filename, 'r') as csvfile:
    for line in csvfile:
      yield line.strip().split(' ')
```

```
['rs#', 'refallele_freq', 'otherallele_freq']
['rs6423165', '0.143', '0.857']
...
```

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# Basic CSV

```
def
    w                                                    :
```


```
['rs#'                                                  freq']
['rs64
...
```

# stdlib: csv

```
import csv
def read_csv(filename):
  with open(filename, 'r') as csvfile:
    for row in csv.reader(csvfile, delimiter=' '):
      yield row
```

```
['rs#', 'refallele_freq', 'otherallele_freq']
['rs6423165', '0.143', '0.857']
...
```

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# stdlib: csv

```
import csv
def read_csv(filename):
  with open(filename, 'r') as csvfile:
    for row in csv.DictReader(csvfile,
                              delimiter=' '):
      yield row
```

```
{'rs#': 'rs6423165',
 'refallele_freq': '0.143',
 'otherallele_freq': '0.857'}
...
```

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# Intro to sheets

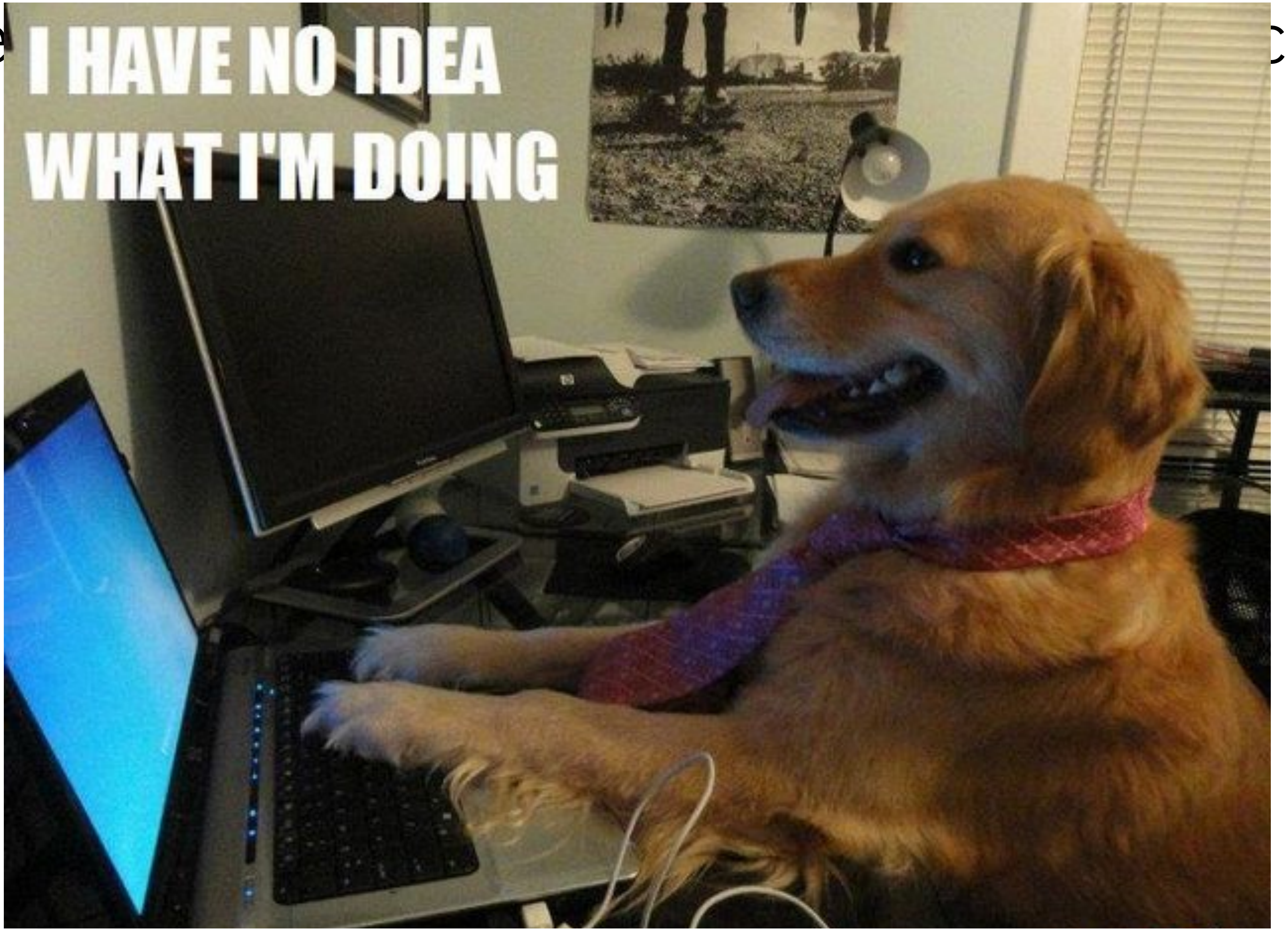
Literate schemas for text data, by Marty Alchin

*CSV* $\longleftrightarrow$ *objects*

https://github.com/gulopine/sheets

# Intro to sheets

Lite … chin




https://github.com/gulopine/sheets

# Intro to sheets

Literate schemas for text data, by Marty Alchin

*CSV ↔ objects*

```
class HapMapRow(Row):
    Dialect = Dialect(has_header_row=True,
                      delimiter=' ')
    rsid = StringColumn()
    ref_freq = FloatColumn()
    alt_freq = FloatColumn()
```

https://github.com/gulopine/sheets

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# CSV with sheets

```
def parse_csv(filename):
  with open(filename, 'r') as csvfile:
    for row in HapMapRow.reader(csvfile):
      yield row
```

```
HapMapRow(rsid='rs6423165', ref_freq=0.143,
              alt_freq=0.857)
HapMapRow(rsid='rs6608381', ref_freq=0.464,
              alt_freq=0.536)
                  ...
```

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# Let’s query the data.

# Simple Queries

```
next(row for row in rows
        if row.rsid == 'rs6423165').ref_freq
```

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# Simple Queries

```
next(row for row in rows
     if row.rsid == 'rs6423165').ref_freq
```

```
rsid2ref_freq = {
    row.rsid: row.ref_freq
    for row in read_csv('hapmap.txt')
}

rsid2ref_freq['rs6423165']
```

# Multiple-Key Queries

```
rows = read_csv('hapmap.txt')

pop2rsid2ref_freq = {
    pop: {
        row.rsid: row.ref_freq
        for row in rows
        if row.pop == pop
    } for pop in {row.pop for row in rows}
}

pop2rsid2ref_freq['YRI']['rs6423165']
```

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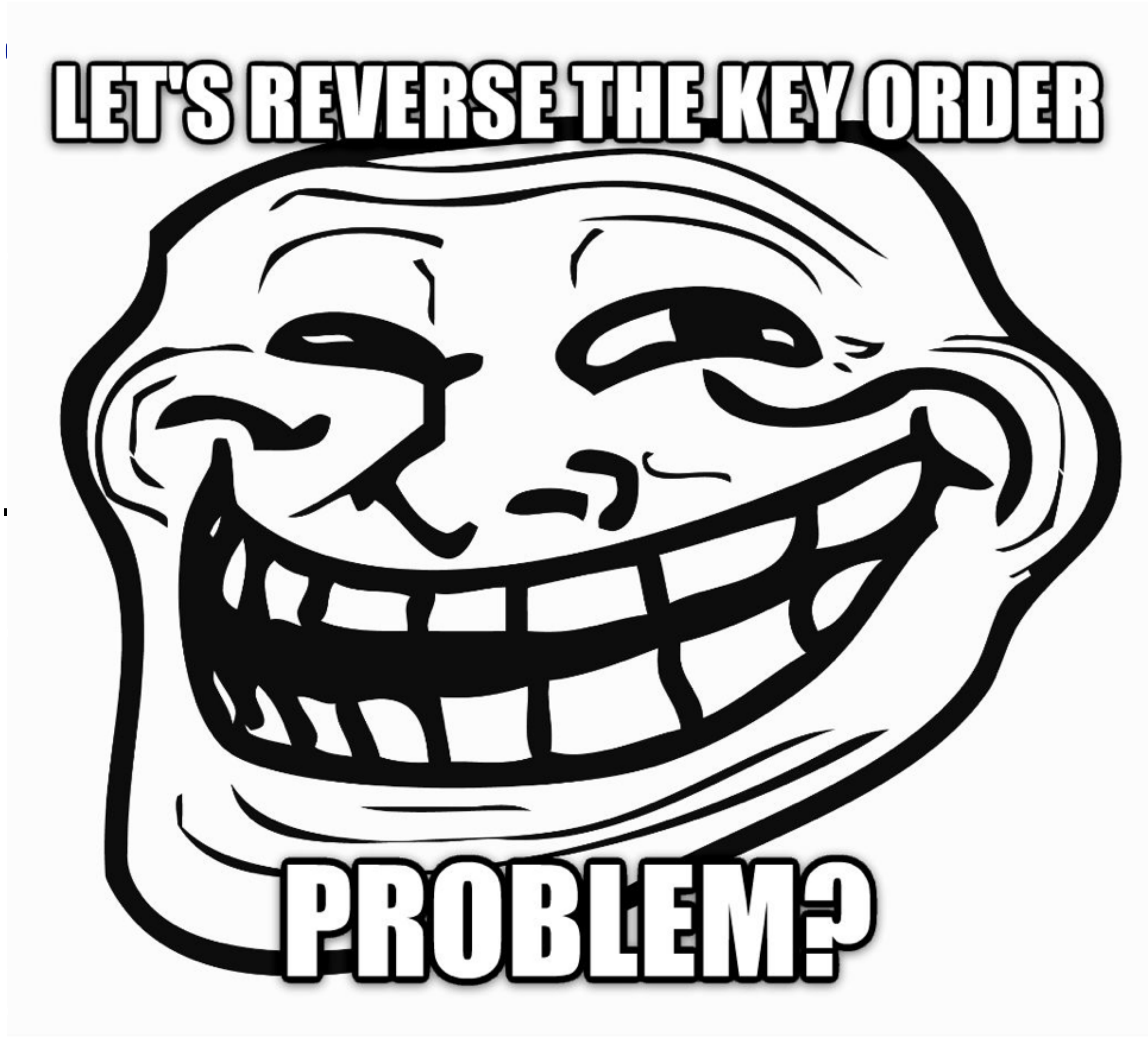
# Multiple-Key Queries

```
rows = r
pop2rsid
    pop:
    } fo                         in rows}
}
pop2rsid                         5']
```

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`dict` construction is equivalent to materializing *one* query plan.

This is fragile!

# Intro to sqlite3

Embedded, serverless SQL database
*in the Python standard library*

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Embedded, serverless SQL database

*in the Python standard library*

```python
import sqlite3
db = sqlite3.connect(':memory:')
...
for row in db.execute('SELECT * FROM ...'):
```

# sqlite3 example

```
db.execute('''CREATE TABLE hapmap
              (rsid VARCHAR,
               ref_freq REAL,
               alt_freq REAL);''')

for row in read_csv(hapmap_file):
  db.execute('''INSERT INTO hapmap
                (rsid, ref_freq, alt_freq)
                VALUES (?, ?, ?);''',
             (row.rsid, row.ref_freq, row.alt_freq))

db.execute('SELECT rsid FROM hapmap '
           'WHERE alt_freq > 0.01;')
```

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# sqlite3 example

```
db.execute('''CREATE TABLE hapmap
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for row in read_csv(hapmap_file):
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             (row.rsid, row.ref_freq, row.alt_freq))

db.execute('SELECT rsid FROM hapmap '
           'WHERE alt_freq > 0.01;')
```

# sqlite3 example

```
db.exe

for ro
   db.e
                                            freq))

db.exe
```

ORMs let you map objects into a database.

`sheets`: CSV $\leftrightarrow$ objects

ORM: objects $\leftrightarrow$ database

OR nto


C e

# pony-orm example

```
from pony.orm import Database, Required

db = Database('sqlite', ':memory:')
class HapMapAllele(db.Entity):
  rsid = Required(str)
  ref_freq = Required(float)
  alt_freq = Required(float)

...
from pony.orm import db_session, select
with db_session:
    select(allele for allele in HapMapAllele
           if allele.alt_freq > 0.01)[:]
```

# pony-orm example

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from pony.orm import Database, Required

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# pony-orm example

```
from
from

db =
clas
  rs
  re
  al

...
with
                                                lele
```

# pony-orm example

```
class HapMapAllele(db.Entity):
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  alt_freq = Required(float)
```

↕ This looks familiar!

```
class HapMapRow(Row):
  Dialect = Dialect(has_header_row=True,
                    delimiter=' ')
  rsid = StringColumn()
  ref_freq = FloatColumn()
  alt_freq = FloatColumn()
```

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# pony-blanket example

```
# ...sheets stuff up here...
from pony_blanket import csv_to_db
db, models = csv_to_db(
    {'hapmap.txt': HapMapAllele})

from pony.orm import db_session, select
with db_session:
  print len(select(x.rsid
                   for x in models[HapMapAllele]
                   if x.alt_freq > 0.01))
```

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# pony-blanket example

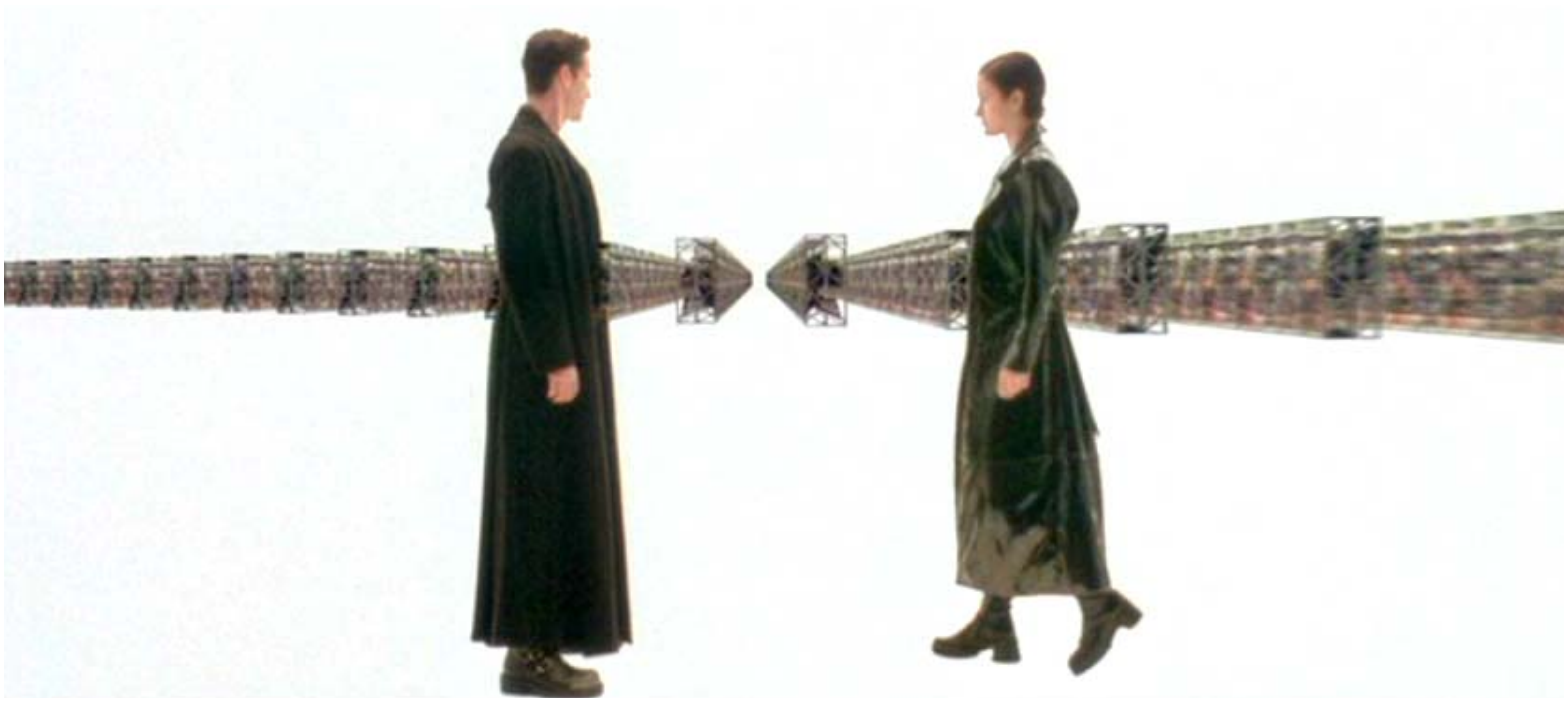
```
# ...sheets stuff up here...
from pony_blanket import csv_to_db
db, models = csv_to_db(
    {'hapmap.txt': HapMapAllele})

from pony.orm import db_session, select
with db_session:
  print len(select(x.rsid
                   for x in models[HapMapAllele]
                   if x.alt_freq > 0.01))
```

# pony-blanket example

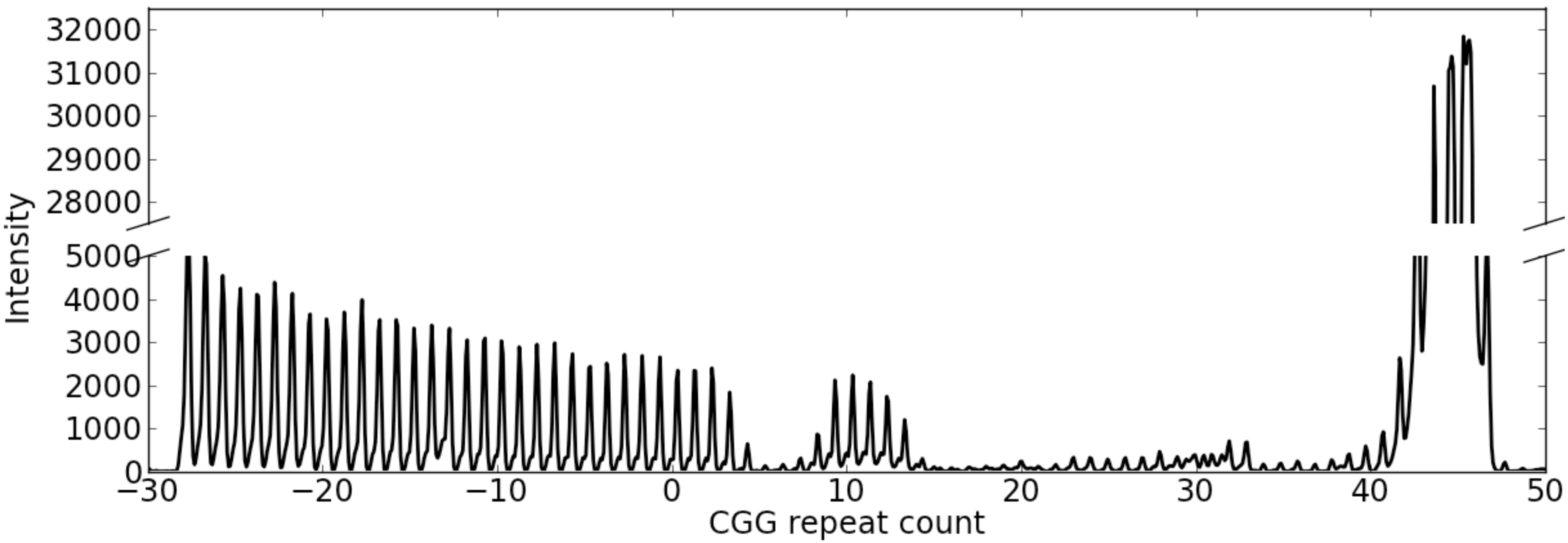
```
# ...sheets stuff up here...
from pony[redacted]
db, model[redacted]
    {'hap[redacted]

from pony[redacted]
with db_s[redacted]
  print l[redacted]
[redacted]apAllele]
                    if x.alt_freq > 0.01))
```

# Let’s talk about numbers.

# Lots of numbers.



# Like this.




$\times 10^5$

# Large-Scale Numeric Storage

- Text formats are slow to parse, bulky
- Relational DBs are not optimized for numeric storage/ops

Straw-man benchmark: read 10e6 random floats

| Format | Speed | Size | Space Overhead |
|---|---|---|---|
| CSV | 2918 ms | 144 MiB | 87.5% |
| JSON | 1410ms | 194 MiB | 153% |
| SQLite3 | 10996 ms | 166 MiB | 116% |
| HDF5 | 33 ms | 77 MiB | 0.0027% |

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# tables: A Quick Intro

```python
# data is a numpy array

import tables
h5 = tables.openFile('mydata.h5', 'w')
h5.createArray(h5.root, 'some_data', data)
h5.close()
```

# tables: A Quick Intro

```python
with tables.openFile('mydata.h5', 'r') as h5:
    data = h5.root.some_data[:]

    sampled_data = h5.root.some_data[::10]
```

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# tables: Compression

```
filters = tables.Filters(complevel=1,
                         complib='zlib',
                         fletcher32=True,
                         shuffle=True)

chunked = h5.createCArray(h5.root, 'chunked_data',
                          atom=tables.FloatAtom(),
                          shape=data.shape,
                          filters=filters)

chunked[:] = data
```

# tables: Metadata Storage

```
import numpy as np
row_type = np.dtype([('batch', 'S16'),
                     ('well', 'S3'),
                     ('idx', 'u8')])

metatable = h5.createTable(h5.root, 'metadata',
                           description=row_type)
```

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# tables: Metadata Storage

```
new_row = metatable.row

for i in xrange(10):
    new_row['batch'] = 'Batch %d' % i
    new_row['well'] = 'A01'
    new_row['idx'] = i
    new_row.append()

metatable.cols.batch.createCSIndex()
metatable.cols.well.createCSIndex()

metatable.flush()
```

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# tables: Metadata Queries

```python
def get_row_indices(batch, well):

    query = '(batch == "%s") & (well == "%s")'
    params = (batch, well)

    for row in metatable.where(query % params):
        yield row['idx']
```

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# tables: Metadata Queries

```
def get_ro

    query                        == "%s")'
    params

    for ro                       % params):
        yie
```

# Summary

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- Declarative schemas make text parsing more readable and maintainable (`sheets`)

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- In-memory databases make wrangling code more flexible and readable (`sqlite3`)
- Metaprogramming lets you use ORMs to do everything in Python, without DRY violations (`pony.orm`, `pony_blanket`)

# Summary

- Declarative schemas make text parsing more readable and maintainable (**`sheets`**)
- In-memory databases make wrangling code more flexible and readable (**`sqlite3`**)
- Metaprogramming lets you use ORMs to do everything in Python, without DRY violations (**`pony.orm`**, **`pony_blanket`**)
- HDF5 lets you store both numeric data and non-numeric metadata fast and small

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</talk>

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