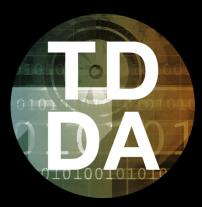
TEST-DRIVEN DATA ANALYSIS



PyData London 2018 • Tutorial • 27th April 2018

http://www.tdda.info/pdf/tdda-tutorial-pydata-london-2018.pdf

Nicholas J. Radcliffe Stochastic Solutions Limited & Department of Mathematics, University of Edinburgh

$\mathsf{TDD}\mapsto\mathsf{TDDA}$

We need to extend TDD's idea of testing for

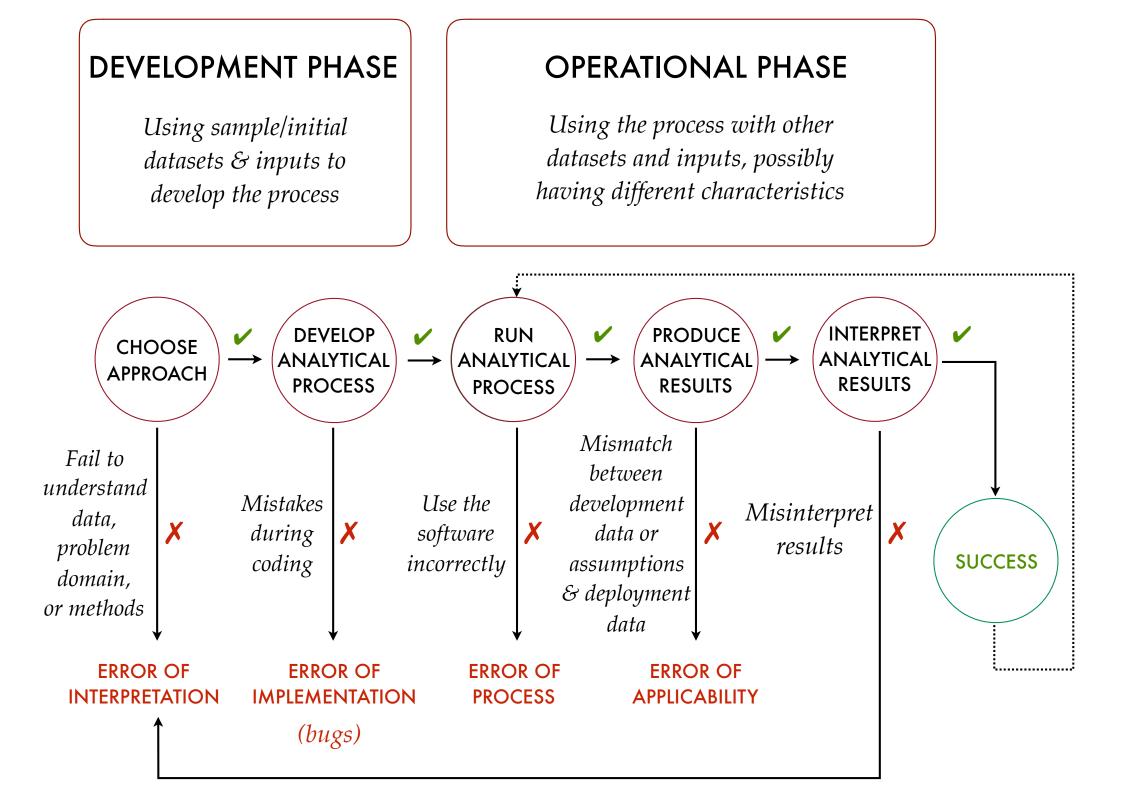
software correctness

with the idea of testing for

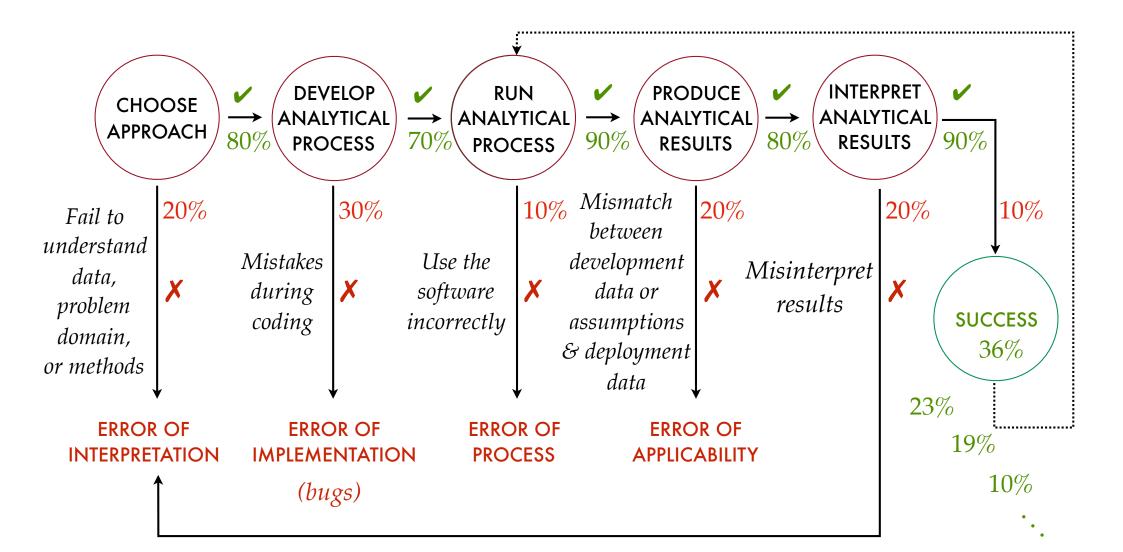
meaningfulness of analysis,

correctness and validity of input data,

& correctness of interpretation.



If you buy into this model, it's sobering to attach probability estimates to each transition and calculate the probability of success after a few runs . . .



TDDA: MAIN IDEAS

- 1. "Reference" Tests
 - *cf.* system / integration tests in TDD
 - With support for exclusions, regeneration, helpful reporting etc.
 - Re-run these tests *all the time, everywhere*
- 2. Constraint Discovery & Verification
 - a bit like unit tests for data
 - can cover inputs, outputs and intermediate results
 - automatically discovered
 - *more-or-less* including regular expressions for characterising strings (Rexpy)
 - Use as part of analysis to verify inputs, outputs and intermediates (as appropriate)

TDDA LIBRARY

1. From PyPI (recommended)

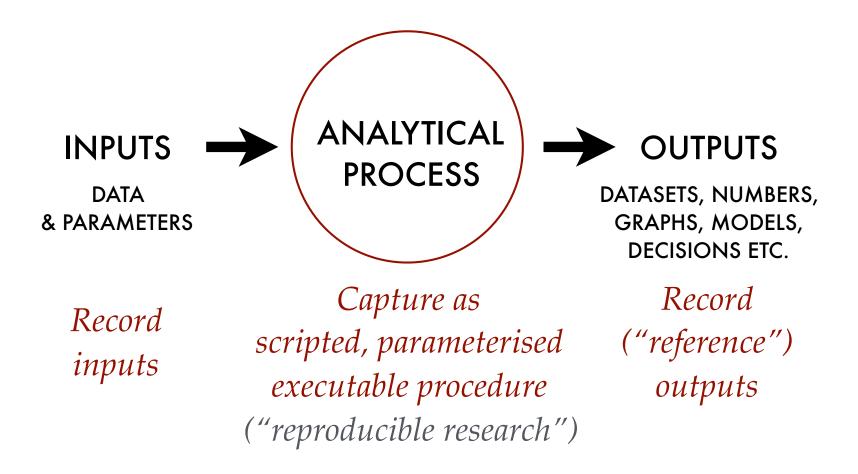
pip install tdda

2. From Github (source)

git clone https://github.com/tdda/tdda.git

- Runs on Python 2 & Python 3, Mac, Linux & Windows, under unittest and pytest
- MIT Licensed
- Documentation:
 - Sphinx source in doc subdirectory
 - Built copy at http://tdda.readthedocs.io
- Quick reference: http://www.tdda.info/pdf/tdda-quickref.pdf

REFERENCE TESTS



Develop a verification procedure (diff) *and periodically rerun: do the same inputs (still) produce the same outputs?*

REFERENCE TEST SUPPORT

1: UNSTRUCTURED (STRING) RESULTS

- Comparing actual string (in memory or in file) to reference (*expected*) string (in file)
- Exclude lines with substrings or regular expressions
- Preprocess output before comparison
- Write actual string produced to file when different
- Show specific diff command needed to examine differences
- Check multiple files in single test; report all failures
- Automatically re-write reference results after human verification.

REFERENCE TEST SUPPORT

UNSTRUCTURED (STRING) METHODS

Check a single (in-memory) string against a reference file

self.assertStringCorrect(string, ref_path, ...)

Check a single generated file against a reference file:

self.assertFileCorrect(actual_path, ref_path, ...)

Check a multiple generated files against respective reference files:

self.assertFilesCorrect(actual_paths, ref_paths, ...)

EXERCISE 1: STRING DATA REFERENCE TESTS

I. CHECK THE TESTS PASS

1. Copy examples somewhere:

```
cd ~/tmp
tdda examples
cd referencetest-examples
```

- 2. Look at reference output: reference/string_result.html reference/file_result.html

NOTE

- Although tests pass, output is *not* identical
 - version number and copyright lines in reference files are different

(*This will be clearer after next part of exercise.*)

EXERCISE 1 (CTD): STRING DATA REFERENCE TESTS

II. MODIFY THE GENERATOR, VERIFY RESULTS, RE-WRITE REFERENCE RESULTS

4. Modify generators.py

e.g. Capitalise <h1> ... </h1> contents in the generate_string function

- 5. Repeat step 3 to run tests again. Two tests should fail. cd unittest; python test_using_referencetestcase.py; cd .. or cd pytest; pytest; cd ..
- 6. Check modified results in (reported) temporary directory are as expected; run the suggested diff command or something similar (opendiff, fc, ...). Again, note that in addition to the changes you introduced, the Copyright and Version lines are different
- 7. On the assumption that these now represent the verified,* new target results, rewrite the reference output with

```
cd unittest; python test_using_referencetestcase.py -W
or cd pytest; pytest --write-all -s
```

8. Repeat step 5 to run tests again. All tests should **pass**.

* WARNING

If you habitually re-write results when tests fail without carefully verifying the new results, your tests will quickly become worthless. With great power comes great responsibility: use TDDA Reference Tests wisely!

EXERCISE 1 (CTD): STRING DATA REFERENCE TESTS

III. MODIFY THE RESULTS VERSION NUMBER; CHECK STILL OK

- 9. Modify generators.py code to change version number in output.
- 10. Repeat step 3 to run tests again. All tests should still pass since version number is excluded by ignore_substrings=['Copyright', 'Version'] parameter to assertStringCorrect.

REFERENCE TEST SUPPORT

2: STRUCTURED DATA METHODS (DATAFRAMES & CSV)

- Comparing generated DataFrame or CSV file to reference DataFrame or CSV file
- Show specific diff command needed to examine differences
- Check multiple CSV files in single test; report all failures
- Choose subset of columns (with list or function) to compare
- Choose whether to check (detailed) types
- Choose whether to check column order
- Choose whether to ignore actual data in particular columns
- Choose precision for floating-point comparisons
- Automatic re-writing of verified (changed) results.

REFERENCE TEST SUPPORT

STRUCTURED DATA METHODS (DATAFRAMES & CSV)

Check a single generated CSV file against a reference CSV file self.assertCSVFileCorrect(actual_path, ref_csv, ...)

Check multiple generated files against respective reference CSV files: self.assertCSvFilesCorrect(actual_paths, ref_csvs, . . .)
Check an (in-memory) DataFrame against a reference CSV file

self.assertDataFrameCorrect(df, ref_csv, ...)

Check an (in-memory) DataFrame against another (in-memory) DataFrame

self.assertDataFramesEqual(df, ref_df, ...)

EXERCISE 2: DATAFRAME/CSV REFERENCE TESTS I. CHECK THE TESTS PASS

- 1. If you've done Exercise 1, you already have the examples in the same directory
- 2. Look at reference output: reference/dataframe_result.csv reference/dataframe_result2.csv
- 3. Run tests (should **pass**).

```
cd unittest; python test_using_referencetestcase.py; cd ..
cd pytest; pytest; cd ..
```

NOTE

You can look at the data frame being generated with this 2-line program (save as show.py)

from dataframes import generate_dataframe

```
print(generate_dataframe())
```

EXERCISE 2: DATAFRAME/CSV REFERENCE TESTS

II. MODIFY THE DATA GENERATOR, VERIFY RESULTS, RE-WRITE REFERENCE RESULTS

4. Modify dataframes.py

e.g. Change the default precision from 3 to 2 in the generate_dataframe function. This will cause the string column s to be different.

5. Repeat step 3 to run tests again. Three tests should fail.

```
cd unittest; python test_using_referencetestcase.py; cd ..
or cd pytest; pytest; cd ..
```

- 6. Look at the way differences are reported, and check that the only material change is to column s, as expected.
- 7. On the assumption that this new output now represents the new, verified target result,* re-write the reference output with cd unittest; python test_using_referencetestcase.py -W or cd pytest; pytest --write-all -s
- 8. Repeat step 5 to run tests again. All tests should now pass.

* WARNING

If you habitually re-write results when tests fail without carefully verifying the new results, your tests will quickly become worthless. With great power comes great responsibility: use TDDA Reference Tests wisely!



NEW COOLNESS!

TAGGING TESTS TO RUN A SUBSET

With unittest (not yet pytest), you can "tag" single individual tests or whole test classes to allow only those ones to be run with when running with -1 or --tagged.

```
from tdda.referencetest import ReferenceTestCase, tag
class TestDemo(ReferenceTestCase):
    def testOne(self):
        self.assertEqual(1, 1)
                                               $ python3 tests.py -1
    @tag
    def testTwo(self):
                                               Ran 2 tests in 0.000s
        self.assertEqual(2, 2)
                                               OK
    @tag
    def testThree(self):
        self.assertEqual(3, 3)
                                               See what classes have tagged tests
                                               with -0 or --istagged
    def testFour(self):
        self.assertEqual(4, 4)
                                               $ python3 tests.py -0
                                                 main .TestDemo
if
  name == ' main ':
     ReferenceTestCase.main()
```

CONSTRAINT GENERATION & VERIFICATION

CONSTRAINTS

- Very commonly, data analysis uses data tables (e.g. DataFrames) as inputs, outputs and intermediate results
- There are many things we know (or at least expect) to be true about these data tables
- *Could* write down all these expectations as constraints and check that they are actually satisfied during analysis . . . *but life's too short!* (Also: humans are rather error-prone)

THE BIG IDEA

- Get the computer to discover constraints satisfied by example datasets automatically.
- Verify against these constraints, modifying as required
- (Humans much happier to make tweaks than start from scratch)

EXAMPLE CONSTRAINTS

SINGLE FIELD CONSTRAINTS	DATASET CONSTRAINTS		
Age ≤ 150	The dataset must contain field CID		
type(Age) = int	Number of records must be 118		
$CID \neq NULL$	One field should be tagged O		
CID unique	Date should be sorted ascending		
len(CardNumber) = 16	MULTI-FIELD CONSTRAINTS		
Base in {"C", "G", "A", T"}	StartDate \leq EndDate		
Vote ≠ "Trump"	AlmostEqual(F, m * a, 6)		
StartDate < tomorrow()	sum(Favourite*) = 1		
v < 2.97e10	$minVal \le medianVal \le maxVal$		
Height ~ N(1.8, 0.2)	$V \le H * w * d$		

CONSTRAINTS SUPPORTED BY TDDA LIBRARY

KIND	DESCRIPTION	BOOLEAN	NUMERIC	DATE	STRING	
min	<i>Minimum allowed value; on verification interpreted with proportionate tolerance</i> epsilon.	~	~	~	X	
max	<i>Maximum allowed value; on verification interpreted with proportionate tolerance</i> epsilon.	~	~	~	X	
sign	"positive", "non-negative", "zero", "non-positive" <i>or</i> "negative".	~	~	×	X	
max_nulls	0 if nulls not allowed. In principle, can be higher values (in particular, 1), but discover function does not use these at present.	~	•	~	~	
no_duplicates	true if duplicates are not allowed.	~	~	~	~	
min_length	smallest allowed string length	×	X	×	~	
max_length	largest allowed string length	×	×	X	~	
rex	list of regular expressions; strings must match at least one. (Available from version 0.4.0 on.)	×	×	×	~	

CONSTRAINT GENERATION & VERIFICATION

1. Copy examples somewhere:

```
cd ~/tmp
tdda examples (if not done already)
cd constraints-examples
```

2. Generate constraints from first 92 elements of periodic table (testdata/elements92.csv)

```
cd constraints-examples
python elements_discover_92.py
or tdda discover testdata/elements92.csv elements92.tdda
```

- 3. Examine output (elements92.tdda)
- 4. Perform verification of same data (as DataFrame). Should pass.

```
python elements_verify_92.py
or tdda verify testdata/elements92.csv elements92.tdda
```

Obviously, verifying a dataset against the constraints generated from that dataset should always work!

pip install feather-format

EXAMPLE: elements92.tdda

"fields":{

{

}

"Z": {"type": "int", "min": 1, "max": 92, "sign": "positive", "max_nulls": 0, "no_duplicates": true}, "Name": {"type": "string", "min_length": 3, "max_length": 12, "max_nulls": 0, "no_duplicates": true}, "Symbol": {"type": "string", "min length": 1, "max length": 2, "max nulls": 0, "no duplicates": true}, "Period": {"type": "int", "min": 1, "max": 7, "sign": "positive", "max nulls": 0}, "Group": {"type": "int", "min": 1, "max": 18, "sign": "positive"}, "ChemicalSeries": {"type": "string", "min_length": 7, "max_length": 20, "max_nulls": 0, "allowed_values": ["Actinoid", "Alkali metal", "Alkaline earth metal", "Halogen", "Lanthanoid", "Metalloid", "Noble gas", "Nonmetal", "Poor metal", "Transition metal"]}, "AtomicWeight": {"type": "real", "min": 1.007946, "max": 238.028914, "sign": "positive", "max nulls": 0}, "Etymology": {"type": "string", "min_length": 4, "max_length": 39, "max_nulls": 0}, "RelativeAtomicMass": {"type": "real", "min": 1.007946, "max": 238.028914, "sign": "positive", "max nulls": 0}, "MeltingPointC": {"type": "real", "min": -258.975, "max": 3675.0, "max_nulls": 1}, "MeltingPointKelvin": {"type": "real", "min": 14.2, "max": 3948.0, "sign": "positive", "max_nulls": 1}, "BoilingPointC": {"type": "real", "min": -268.93, "max": 5596.0, "max_nulls": 0}, "BoilingPointF": {"type": "real", "min": -452.07, "max": 10105.0, "max nulls": 0}, "Density": {"type": "real", "min": 8.9e-05, "max": 22.610001, "sign": "positive", "max nulls": 0}, "Description": {"type": "string", "min_length": 1, "max_length": 83}, "Colour": {"type": "string", "min_length": 4, "max_length": 80}

EXAMPLE SUCCESSFUL VERIFICATION

constraints-examples — -bash — 113×40 0 godel:\$ python elements_verify_92.py FIELDS: AtomicWeight: 0 failures 5 passes type Group: 0 failures 4 passes type </ min </ max </ sign </ Name: 0 failures 5 passes type </ min_length </ max_length </ max_nulls </ no_duplicates </ Density: 0 failures 5 passes type </ min </ max </ sign </ max_nulls </ MeltingPointKelvin: 0 failures 5 passes type Symbol: 0 failures 5 passes type </ min length </ max length </ max nulls </ no duplicates </ Period: 0 failures 5 passes type \checkmark min \checkmark max \checkmark sign \checkmark max_nulls \checkmark Description: 0 failures 3 passes type < min_length < max_length < BoilingPointF: 0 failures 4 passes type < min < max < max_nulls < Etymology: 0 failures 4 passes type ~ min_length ~ max_length ~ max_nulls ~ ChemicalSeries: 0 failures 5 passes type MeltingPointC: 0 failures 4 passes type \checkmark min \checkmark max \checkmark max_nulls \checkmark Z: 0 failures 6 passes type </ min </ max </ sign </ max_nulls </ no_duplicates </ BoilingPointC: 0 failures 4 passes type \checkmark min \checkmark max \checkmark max_nulls \checkmark Colour: 0 failures 3 passes type ~ min_length ~ max_length ~ RelativeAtomicMass: 0 failures 5 passes type SUMMARY:

Passes: 72 Failures: 0 0 godel:\$

CONSTRAINT GENERATION & VERIFICATION

5. Now run verification of larger dataset (first 118 elements of periodic table) against the same constraints. Should **fail** (because, for example, atomic number now goes to 118).

```
python elements_verify_118_against_92.py
or tdda verify testdata/elements118.csv elements92.tdda
```

6. Repeat verification of larger dataset (118 elements) against constraints generated against that same (118) data. Should **pass**.

```
python elements_verify_118.py
```

or tdda verify testdata/elements118.csv elements118.tdda

7. Finally, verify the constraints from 118 data against the 92 data. Should **pass**.

tdda verify testdata/elements92.csv elements118.tdda

Note: fewer constraints are discovered for elements118 than for elements92 (67 against 72). This is because there are nulls in some fields in the 118 data (the melting points, density etc.) but not in the 92 data.



FAILURE (ANOMALY) DETECTION

This afternoon's workshop has much more on this!

8. "Detect" the failing records

```
tdda detect testdata/elements118.csv \
    elements92.tdda \
    bads.csv \
    --per-constraint \
    --output-fields
```

- This writes out the failing records to bads.csv. (Can use .feather instead)
- The --per-constraint flag says write out a column for every constraint that ever fails, as well as an nfailures column.
- --output-fields says write all the original fields as well as the results fields (otherwise, it just writes an index/row number).

EXAMPLE UNSUCCESSFUL VERIFICATION

constraints-examples — -bash — 113×40 0 godel: \$ python elements_verify_118_against_92.py FIELDS: AtomicWeight: 2 failures 3 passes type Group: 0 failures 4 passes type </ min </ max </ sign </ Name: 1 failure 4 passes type </ min_length </ max_length </ max_nulls </ no_duplicates </ Density: 2 failures 3 passes type </ min </ max </ sign </ max_nulls </ MeltingPointKelvin: 1 failure 4 passes type ~ min ~ max ~ sign ~ max_nulls × Symbol: 1 failure 4 passes type </ min_length </ max_length </ max_nulls </ no_duplicates </ Period: 0 failures 5 passes type \checkmark min \checkmark max \checkmark sign \checkmark max_nulls \checkmark Description: 0 failures 3 passes type < min_length < max_length < BoilingPointF: 1 failure 3 passes type \checkmark min \checkmark max \checkmark max_nulls \times Etymology: 2 failures 2 passes type ChemicalSeries: 0 failures 5 passes type </ min_length </ max_length </ max_nulls </ allowed_values </ MeltingPointC: 1 failure 3 passes type Z: 1 failure 5 passes type \checkmark min \checkmark max \times sign \checkmark max_nulls \checkmark no_duplicates \checkmark BoilingPointC: 1 failure 3 passes type \checkmark min \checkmark max \checkmark max_nulls \times Colour: 0 failures 3 passes type ~ min_length ~ max_length ~ RelativeAtomicMass: 2 failures 3 passes type SUMMARY:

Passes: 57 Failures: 15 0 godel:\$

ABSENT CONSTRAINTS

Gregory (Scotland Yard detective): "Is there any other point to which you would wish to draw my attention?" Holmes: "To the curious incident of the dog in the night-time." Gregory: "The dog did nothing in the night-time." Holmes: "That was the curious incident."

> — *Silver Blaze,* in *Memoirs of Sherlock Holmes* Arthur Conan Doyle, 1892.

CONSTRAINTS API

DISCOVERY

from tdda.constraints.pdconstraints import discover_constraints

constraints = discover_constraints(df)

with open('constraints.tdda', 'w') as f:
 f.write(constraints.to_json())

VERIFICATION

from tdda.constraints.pdconstraints import verify_df

verification = verify_df(df, 'constraints.tdda') # (printable object)

constraints_df = verification.to_frame())

(Pandas DataFrame)

OUTPUT of to_frame()

	field	failures	passes	type	min	min_length	max	\setminus
0	AtomicWeight	2	3	True	True	NaN	False	
2	Name	1	4	True	NaN	True	NaN	
3	Density	2	3	True	True	NaN	False	
4	MeltingPointKelvin	1	4	True	True	NaN	True	
5	Symbol	1	4	True	NaN	True	NaN	
7	BoilingPointF	1	3	True	True	NaN	True	
8	Etymology	2	2	True	NaN	True	NaN	
9	RelativeAtomicMass	2	3	True	True	NaN	False	
11	MeltingPointC	1	3	True	True	NaN	True	
12	Z	1	5	True	True	NaN	False	
13	BoilingPointC	1	3	True	True	NaN	True	

max length sign max nulls no duplicates allowed values

	0 -	- 0			· · · · · · · · · · · · · · · · · · ·
0	NaN	True	False	NaN	NaN
2	False	NaN	True	True	NaN
3	NaN	True	False	NaN	NaN
4	NaN	True	False	NaN	NaN
5	False	NaN	True	True	NaN
7	NaN	NaN	False	NaN	NaN
8	False	NaN	False	NaN	NaN
9	NaN	True	False	NaN	NaN
11	NaN	NaN	False	NaN	NaN
12	NaN	True	True	True	NaN
13	NaN	NaN	False	NaN	NaN

CONSTRAINTS					
Satisfied					
Not satisfied					
No constraint					

1. Rexpy: Autorace String fields.

- Now in of TDDA library
- Use discover --rex to generate Regular Expression constraints
- 2. Discover & verify working in RDBMS (postgres; mysql; SQLServer; ORACLE)
- 3. Join key discovery and verification between datasets (working in proprietary version; might come over)
- 4. Characterizing distributions
- 5. "Nearly" constraint discovery (working in proprietary version; might come over)
- 6. Possibly JSON etc. (cf. JSON Schemas)
- 7. Lots of other ideas.



njr@StochasticSolutions.com

- 6
- http://tdda.info



https://github.com/tdda



#tdda*

etdda0

* tweet (DM) us email address for invitation Or email me.

Correct interpretation: Zero

Error of interpretation: Letter "Oh"

www.tdda.info/pdf/tdda-tutorial-pydata-london-2017.pdf

@njr0



Regular Expressions by Example

Source: git clone http://github.com/tdda

Package: pip install tdda

Try online: http://rexpy.herokuapp.com

Regular Expressions

212-988-0321 476 123 8829 1 701 734 9288 (617) 222 0529

 $1?[\(]?\d{3}\)?[\-]\d{3}[\-]\d{4}$

start optional of space line or open bracket

digitsoptionalspacedigits(3)closeor(3)brackethyphen

digits end (3) of line

space

0r

hyphen

Regular Expressions 212-988-0321

as before

less specific: + = 1 or more times

specific range of digits

totally specific

matches anything
 . = any char
* = 0 or more times

 $d+\sqrt{-d+}-3$

 $\ \frac{3}{-d{3}}-\frac{4}{3}$

^[1-2]+\-[8-9]+\-[0-3]+\$

^212\-988\-0321\$

^.*\$

Regular Expressions

MN 55402 OH 45202

 $[A-Z]{2} \d{5}$

Regular Expressions

MN 55402 OH 45202-7735

$[A-Z]{2} \d{5}(\-\d{4})?$

unescaped parentheses (no backslash) "tag" sub-expressions

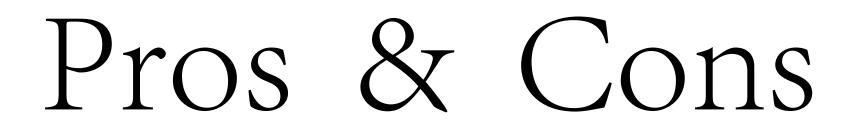
optional

You have a problem.

You think

"I know, I'll use regular expressions."

Now you have two problems



Powerful

*Ugly

Hard to write

Harder to read

Harder still to debug

Hard to quote/escape[†]

† r'...' is your friend

*Butt..

Verbal Expressions

```
verbal_expression = VerEx()
tester = (verbal_expression.
    start_of_line().
    find('http').
    maybe('s').
    find('://').
    maybe('www.').
    anything_but(' ').
    end of line()
```

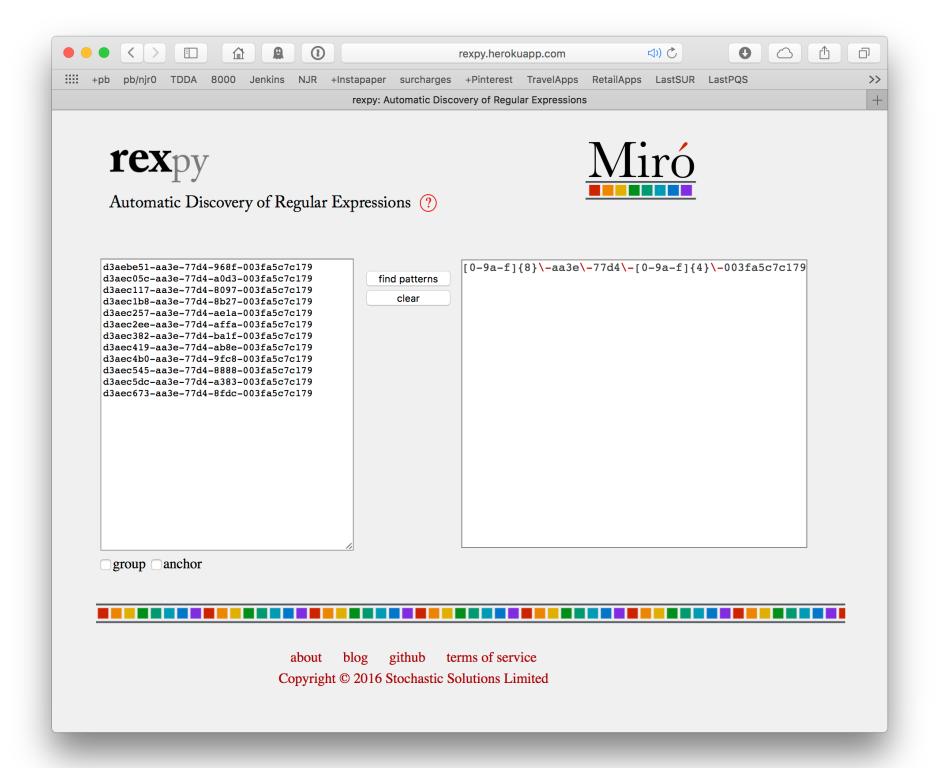
Why not let the computer do the work?



is our early attempt to let the computer find useful regular expressions from examples \$ python

```
>>> tels = ['212-988-0321', '987-654-3210', '476 123 8829', '123 456 7890',
>>> '701 734 9288', '177 441 7712', '617 222 0529', '222 111 9276']
>>> regexps = rexpy.extract(tels)
>>> for r in regexps:
... print r
^\d{3}\-\d{3}\-\d{4}$
^\d{3}\ \d{3}\ \d{4}$
```

Rexpy currently never groups white space with punctuation; but it will soon.



Command Line

\$ rexpy --help

Usage:

rexpy [FLAGS] [input file [output file]]

or

python -m tdda.rexpy.rexpy [FLAGS] [input file [output file]]

If input file is provided, it should contain one string per line; otherwise lines will be read from standard input.

If output file is provided, regular expressions found will be written to that (one per line); otherwise they will be printed.

FLAGS are optional flags. Currently::

-h,header	Discard first line, as a header.
-?,help	Print this usage information and exit (without error)
-g,group	Generate capture groups for each variable fragment of each regular expression generated, i.e. surround variable components with parentheses
	e.g. '^([A-Z]+)\-([0-9]+)\$' becomes '^[A-Z]+\-[0-9]+\$'
-u,underscore	Allow underscore to be treated as a letter. Mostly useful for matching identifiers. Also allow
-d,dot	Allow dot to be treated as a letter. Mostly useful for matching identifiers.
	Alsoperiod.
-m,minus	Allow minus to be treated as a letter. Mostly useful for matching identifiers. Alsohyphen ordash.
-v,version	Print the version number.

API: Pure Python

Get examples: python -m tdda.rexpy.examples

ids.py:

from tdda import rexpy

```
corpus = ['123-AA-971', '12-DQ-802', '198-AA-045', '1-BA-834']
results = rexpy.extract(corpus)
print('Number of regular expressions found: %d' % len(results))
for rex in results:
    print(' ' + rex)
```

RESULTS

API: Pandas

```
pandas_ids.py:
```

```
import pandas as pd
```

from tdda import rexpy

RESULTS

```
$ python pandas_ids.py
    re3: [u'^[a-z]{3}$']
    re45: [u'^[a-z]{4,5}$']
re345: [u'^[a-z]{3,5}$']
```



njr@StochasticSolutions.com

- 6
- http://tdda.info



https://github.com/tdda



#tdda*

🕑 @tddaO

* tweet (DM) us email address for invitation Or email me.

Correct interpretation: Zero

Error of interpretation: Letter "Oh"

www.tdda.info/pdf/tdda-tutorial-pydata-london-2018.pdf

@njr0