

TEST-DRIVEN DATA ANALYSIS



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

TEST-DRIVEN DATA ANALYSIS

or

Why should anyone believe your analytical results?

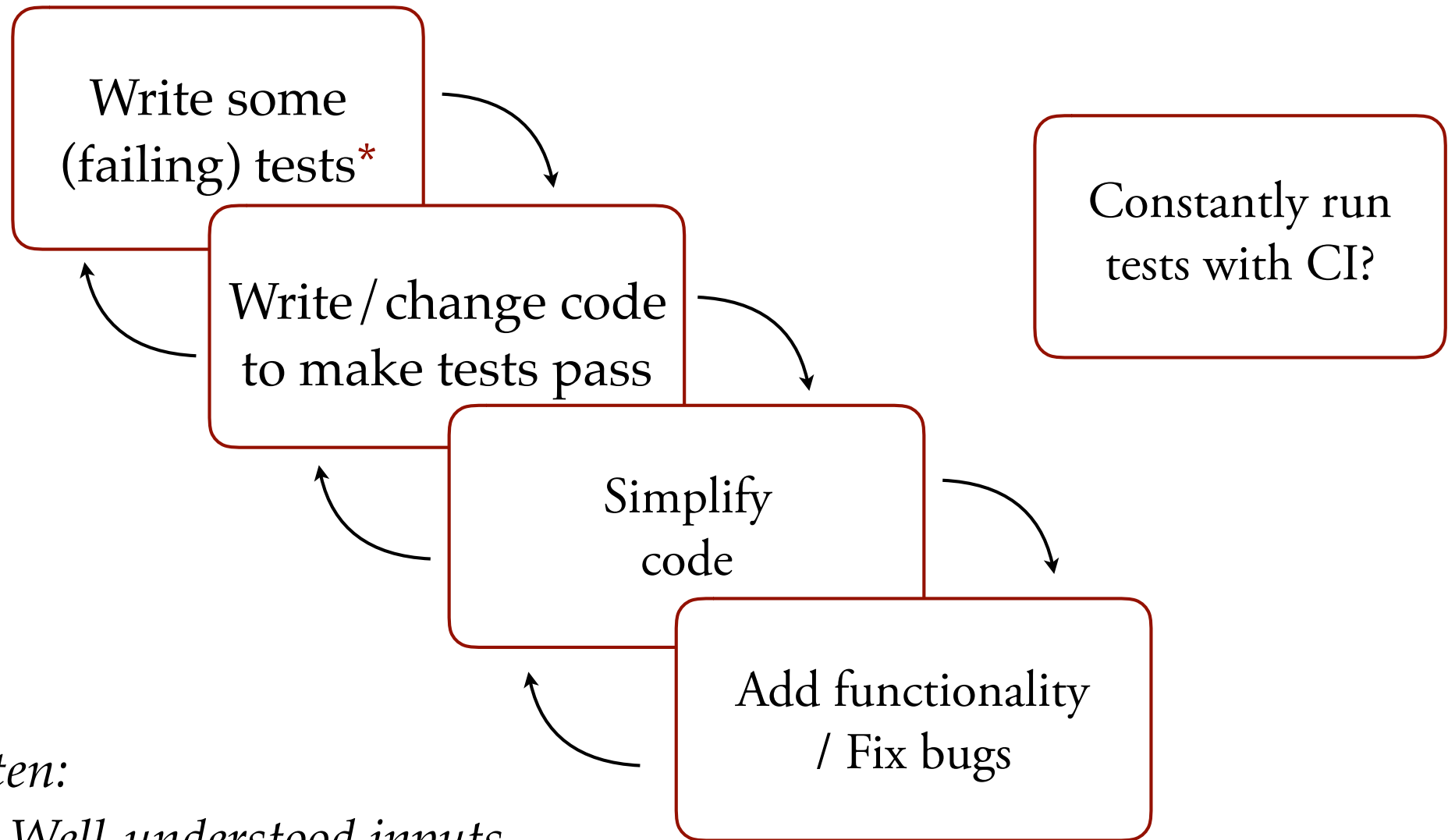
or

Data analysis as if the answers actually mattered

*“We’re not just there to help with our
sponsor’s confirmation bias:
we’re there to get it right.”*

— Edward Tufte, 26 September 2016
The Future of Data Analysis

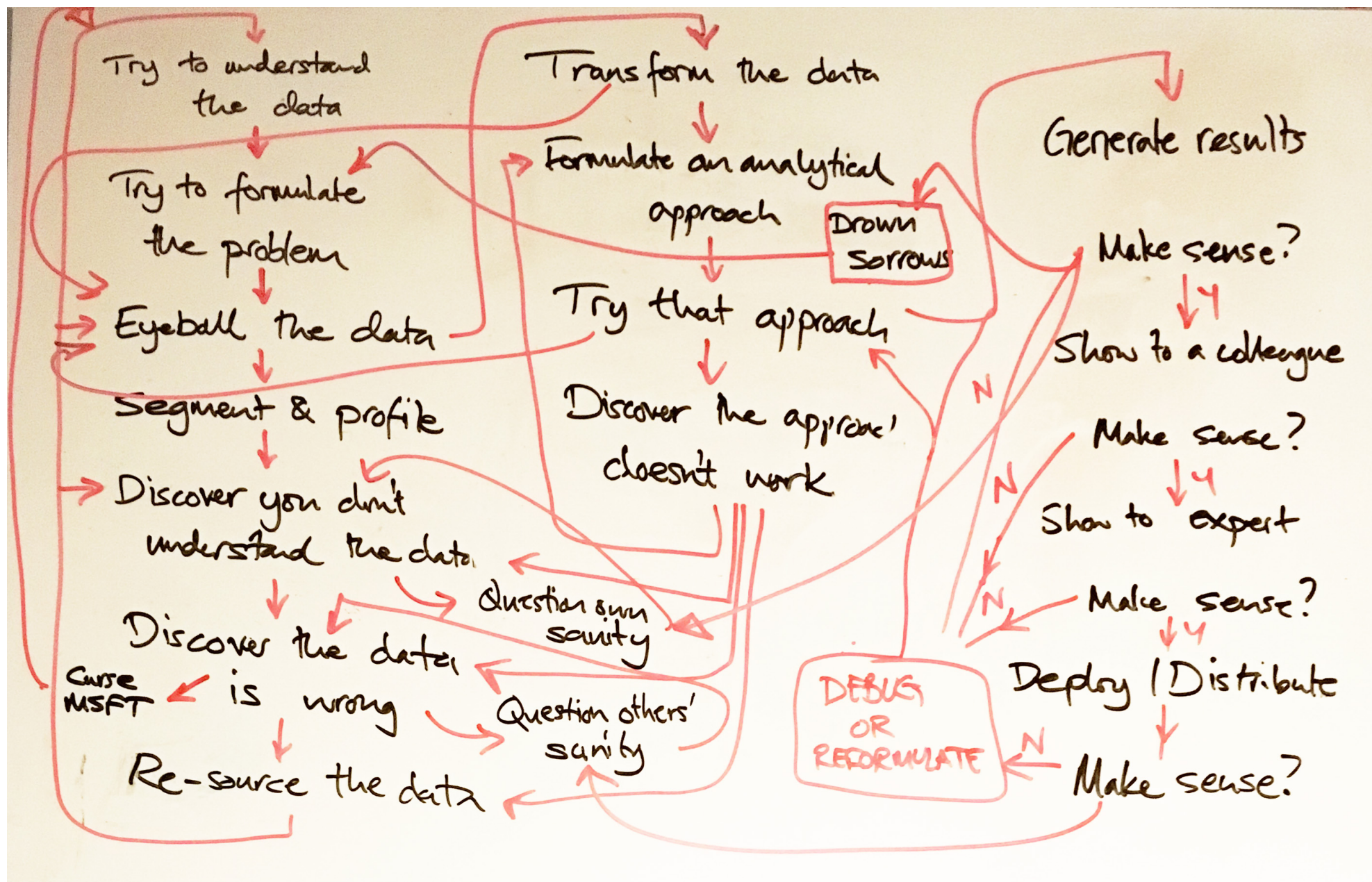
SOFTWARE DEVELOPMENT (WITH TDD)



Often:

- *Well-understood inputs*
- *Well-understood goal*
- *Many kinds of errors/failures are unmistakable*

* While mocking almost everything



*Why is this
lying bastard
lying to me?*

—Jeremy Paxman

*“Shouldn’t we do
test-driven
data analysis?”*

— Patrick Surry, c. 2010

THE BIG IDEA

*Transfer the ideas of
test-driven development
from software development
to data analysis
(mutatis mutandis*)*

**those things which need to be changed having been changed*

CORRECTNESS

STURGEON'S REVELATION

*“Ninety per cent of
everything is crap”*

— Theodore Sturgeon, Venture, 1958

TDD $\mapsto$ TDDA

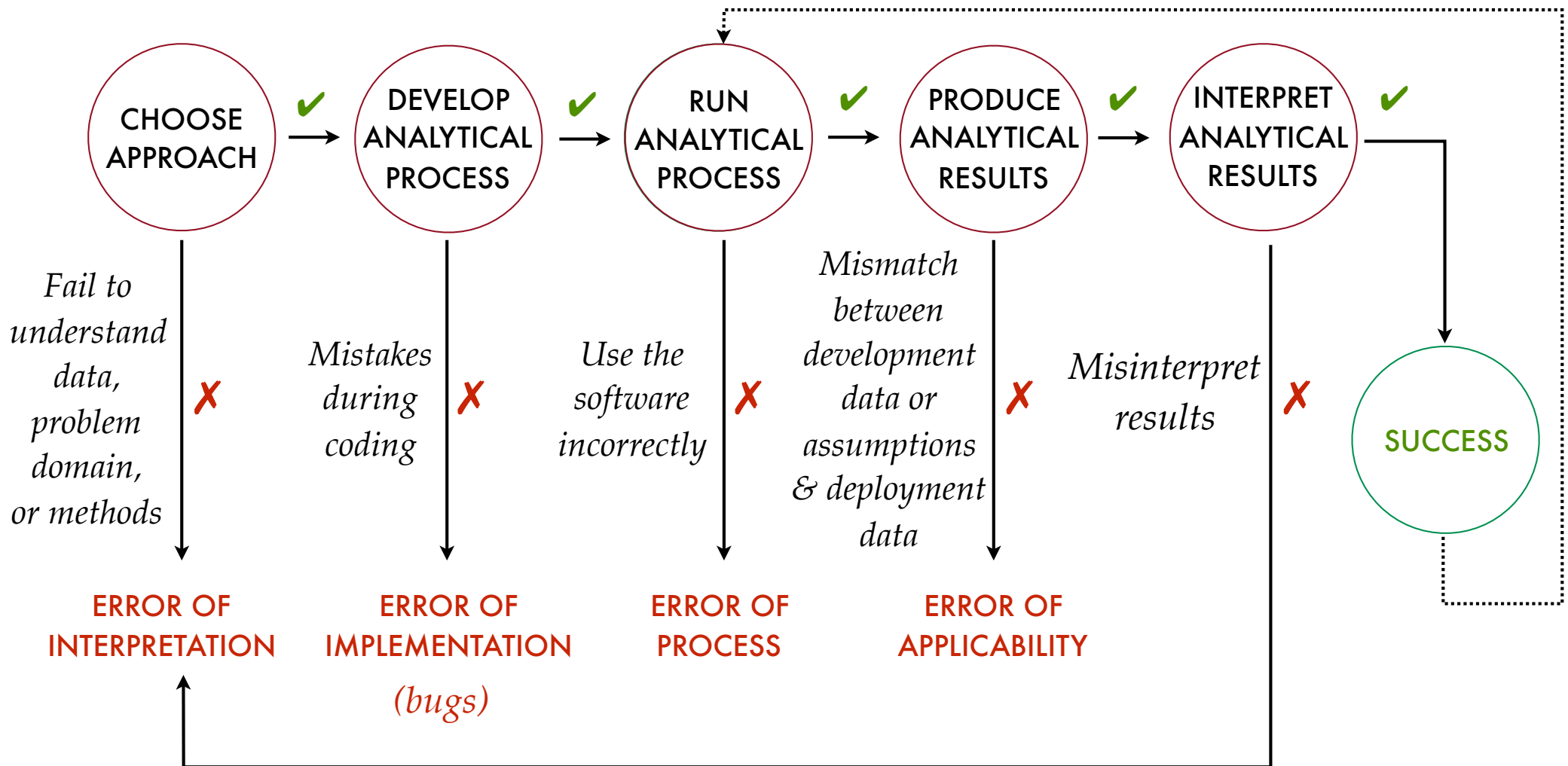
*We need to extend TDD's idea of testing for
software correctness
with the idea of testing for
meaningfulness of analysis,
correctness and validity of input data,
& correctness of interpretation.*

DEVELOPMENT PHASE

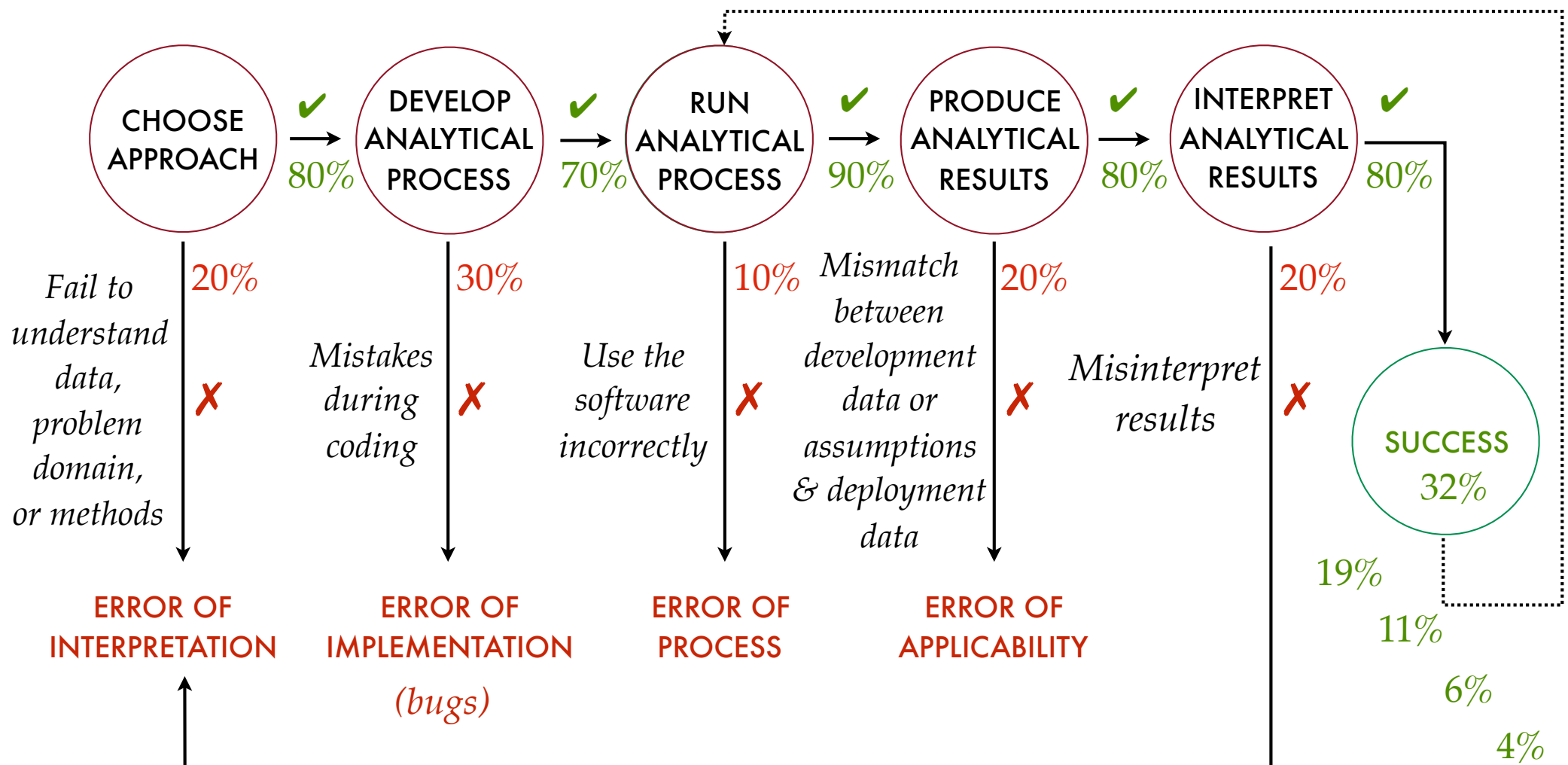
Using sample/initial datasets & inputs to develop the process

OPERATIONAL PHASE

Using the process with other datasets and inputs, possibly having different characteristics



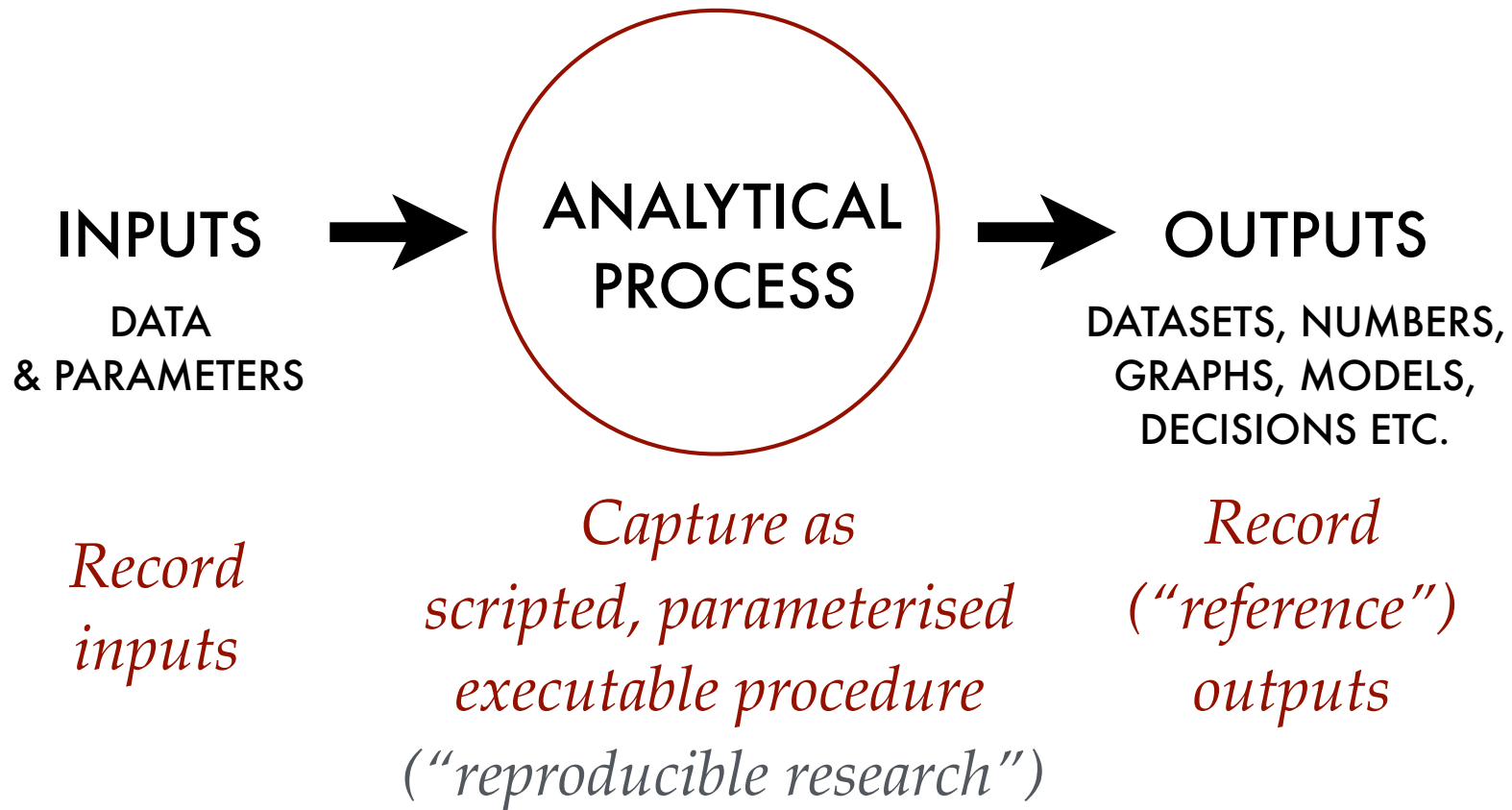
If you buy into this model, it's sobering to attach probability estimates to each transition and calculate the probability of success after a few runs . . .



TDDA: LEVEL ZERO REFERENCE TESTS

<http://github.com/tdda/writabletestcase.py>

TDDA: LEVEL ZERO



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

```
0 :$ python3 test_graphs.py
```

```
.....
```

```
File check failed.
```

```
Compare with "diff /Users/njr/pycon/testoutput/tsr-288-DS-5.svg /Users/njr/pycon/reference/tsr-288-DS-5.svg".
```

```
Note exclusions: Copyright
```

```
Compare preprocessed with "diff /tmp/actual-tsr-288-DS-5.svg /tmp/expected-tsr-288-DS-5.svg".
```

```
F
```

```
=====
```

```
=====
```

```
FAIL: testTSRGraphs (__main__.TestGraphs)
```

```
-----
```

```
Traceback (most recent call last):
```

```
File "test_graphs.py", line 111, in testTSRGraphs
    maxPermutationCases=2)
```

```
File "/Users/njr/python/tdda/writabletestcase.py", line 170, in check_file
    self.assertEqual(nFailures, 0)
```

```
AssertionError: 1 != 0
```

```
-----
```

```
Ran 9 tests in 11.320s
```

```
FAILED (failures=1)
```



```
l :$ python3 test_graphs.py -W
Written /Users/njr/pycon/reference/pndate-graph.svg.
.Written /Users/njr/pycon/reference/test-pnhbar-graph.svg.
.Written /Users/njr/pycon/reference/pnd-295-SGLD-28.svg.
Written /Users/njr/pycon/reference/pnd-295-SI-1136.svg.
Written /Users/njr/pycon/reference/pnd-295-DS-235.svg.
Written /Users/njr/pycon/reference/pnd-428-BH-44.svg.
Written /Users/njr/pycon/reference/pnd-295-SI-1139.svg.
Written /Users/njr/pycon/reference/pnd-295-SGLD-8.svg.
Written /Users/njr/pycon/reference/pnd-295-BD-97.svg.
Written /Users/njr/pycon/reference/pnd-295-BD-94.svg.
Written /Users/njr/pycon/reference/pnd-428-BH-4.svg.
...
Written /Users/njr/pycon/reference/tsr-273-DS-4.svg.
Written /Users/njr/pycon/reference/tsr-278-DS-4.svg.
Written /Users/njr/pycon/reference/tsr-282-DS-3.svg.
Written /Users/njr/pycon/reference/tsr-287-DS-3.svg.
Written /Users/njr/pycon/reference/tsr-287-PW-3.svg.
Written /Users/njr/pycon/reference/tsr-288-DS-5.svg.
.
-----
Ran 9 tests in 11.039s
```

OK

```
0 :$ python3 test_graphs.py
```

```
.....
```

```
-----  
Ran 9 tests in 11.658s
```

```
OK
```

```
0 :$
```

TDDA: LEVEL ONE CONSTRAINTS

See <http://github.com/tdda>

[/constraints/examples/pdgenerate.py](http://github.com/tdda/constraints/examples/pdgenerate.py)

EXAMPLE CONSTRAINTS

SINGLE FIELD CONSTRAINTS	DATASET CONSTRAINTS
$\text{Age} \leq 150$	The dataset must contain field CID
$\text{type}(\text{Age}) = \text{int}$	Number of records must be 118
$\text{CID} \neq \text{NULL}$	One field should be tagged 0
CID unique	Date should be sorted ascending
$\text{len}(\text{CardNumber}) = 16$	MULTI-FIELD CONSTRAINTS
$\text{Base in } \{ \text{"C"}, \text{"G"}, \text{"A"}, \text{"T"} \}$	$\text{StartDate} \leq \text{EndDate}$
$\text{Vote} \neq \text{"Trump"}$	$\text{AlmostEqual}(\text{F}, \text{m} * \text{a}, 6)$
$\text{StartDate} < \text{tomorrow}()$	$\text{sum}(\text{Favourite}^*) = 1$
$v < 2.97\text{e}10$	$\text{minVal} \leq \text{medianVal} \leq \text{maxVal}$
$\text{Height} \sim \text{N}(1.8, 0.2)$	$V \leq H * w * d$

Z	Name	Symbol	Period	Group	Chemical Series	Atomic Weight	Etymology	Relative Atomic Mass	Melting Point C	Melting Point K	Boiling Point C	Boiling Point F	Density	Description	Colour
1	Hydrogen	H	1	1	Nonmetal	1.01	Greek hydrogenes	1.01	-258.98	14.20	-252.87	-423.17	0.00	gas	colorless
2	Helium	He	1	18	Noble gas	4.00	Greek helios	4.00	∅	∅	-268.93	-452.07	0.00	noble gas	∅
3	Lithium	Li	2	1	Alkali metal	6.94	Greek lithos	6.94	180.70	453.90	1,342.00	2,448.00	0.53	0.6	silvery white/gray
4	Beryllium	Be	2	2	Alkaline earth metal	9.01	beryl	9.01	1,287.00	1,560.00	2,469.00	4,476.00	1.85	5.5	∅
5	Boron	B	2	13	Metalloid	10.81	borax	10.81	2,300.00	2,570.00	3,927.00	7,101.00	2.34	9.3	black/brown/ amorphous boron is a brown powder, metallic boron is black
6	Carbon	C	2	14	Nonmetal	12.01	Latin carbo	12.01	3,675.00	3,948.00	4,027.00	7,280.00	2.27	1-2 graphite	black
7	Nitrogen	N	2	15	Nonmetal	14.01	Greek nitron	14.01	-209.86	63.30	-195.79	-320.42	0.00	gas	∅
8	Oxygen	O	2	16	Nonmetal	16.00	Greek oxys	16.00	-222.65	50.50	-182.95	-297.31	0.00	gas	∅
9	Fluorine	F	2	17	Halogen	19.00	Latin fluo	19.00	-219.52	53.60	-188.12	-306.62	0.00	halogen gas	yellow-green or yellowish brown
10	Neon	Ne	2	18	Noble gas	20.18	Greek neos	20.18	-248.45	24.70	-246.08	-410.94	0.00	noble gas	∅
11	Sodium	Na	3	1	Alkali metal	22.99	Latin natrium	22.99	98.00	371.00	883.00	1,621.00	0.97	0.5	waxy, silvery white
12	Magnesium	Mg	3	2	Alkaline earth metal	24.31	Magnesia, Greece	24.31	650.00	923.00	1,090.00	1,994.00	1.74	2.5	silvery metallic
13	Aluminium	Al	3	13	Poor metal	26.98	Latin alumen	26.98	660.25	933.40	2,519.00	4,566.00	2.70	2.75	silvery
14	Silicon	Si	3	14	Metalloid	28.09	Latin silex	28.09	1,410.00	1,680.00	3,265.00	5,909.00	2.33	6.5 metalloid	dark gray, bluish tinge
15	Phosphorus	P	3	15	Nonmetal	30.97	Greek phosphoros	30.97	44.10	317.30	280.00	536.00	1.82	nonmetal	waxy white/ red/ black/ colorless
16	Sulfur	S	3	16	Nonmetal	32.07	Latin sulfur	32.07	115.36	388.51	444.60	832.30	2.07	2	lemon yellow
17	Chlorine	Cl	3	17	Halogen	35.45	Greek chloros	35.45	-100.84	172.00	-34.04	-29.27	0.00	halogen gas	yellowish green or greenish yellow
18	Argon	Ar	3	18	Noble gas	39.95	Greek argon	39.95	-189.19	84.00	-185.85	-302.53	0.00	noble gas	∅
19	Potassium	K	4	1	Alkali metal	39.10	Latin kalium	39.10	63.35	336.50	759.00	1,398.00	0.86	0.4	silvery white
20	Calcium	Ca	4	2	Alkaline earth metal	40.08	Latin calx	40.08	839.00	1,112.00	1,484.00	2,703.00	1.54	1.75	gray



This is Miro version 2.7.80, running under Dalí 1.0.31.

Copyright © Stochastic Solutions Limited 2008–2016.

Seed: 1520109300

Logs started at 2016/10/31 16:00:40 host godel.local.

Logging to /Users/njr/miro/log/2016/10/31/session005.

elements.feather elements.miro elements92.feather elements92.miro

[1]> load elements92

elements92.feather: 92 records; 92 (100%) selected; 16 fields.

[2]> discover -t -o /tmp/elements92

Individual Field Constraints							
Name	Type Allowed	Min Allowed	Max Allowed	Sign Allowed	Nulls Allowed	Duplicates Allowed	Values Allowed
Z	int	1	92	positive	0	no	
Name	string	length 3	length 12		0	no	
Symbol	string	length 1	length 2		0	no	
Period	int	1	7	positive	0	-	
Group	int	1	18	positive		-	
ChemicalSeries	string	length 7	length 20		0	-	"Actinoid" "Alkali metal" "Alkaline earth metal" "Halogen" "Lanthanoid" "Metalloid" "Noble gas" "Nonmetal" "Poor metal" "Transition metal"
AtomicWeight	real	1.007946	238.028913	positive	0		
Etymology	string	length 4	length 39		0	-	
RelativeAtomicMass	real	1.007946	238.028913	positive	0		
MeltingPointC	real	-258.975000	3675.0		1		
MeltingPointKelvin	real	14.200000	3948.0	positive	1		
BoilingPointC	real	-268.930000	5596.0		0		
BoilingPointF	real	-452.070000	10105.0		0		
Density	real	0.000089	22.610000	positive	0		
Description	string	length 1	length 83			-	
Colour	string	length 4	length 80			-	

/tmp/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}
  }
}
```



This is Miro version 2.7.80, running under Dalí 1.0.31.

Copyright © Stochastic Solutions Limited 2008–2016.

Seed: 1507023627
 Logs started at 2016/10/31 16:27:05 host godel.local.
 Logging to /Users/njr/miro/log/2016/10/31/session015.

[1]> load elements92

elements92.feather: 92 records; 92 (100%) selected; 16 fields.

[2]> verify -f /tmp/elements92.tdda

No failures

[3]> load elements

elements.feather: 118 records; 118 (100%) selected; 16 fields.

[4]> verify -f /tmp/elements92.tdda

Miro Warning: 15 failures during constraint verification for dataset elements.feather

Name	Failures	Type			Minimum			Maximum			Sign			Max Nulls			Duplicates			Values		
		Allowed	Actual		Allowed	Actual		Allowed	Actual		Allowed	Actual		Allowed	Actual		Allowed	Actual	Non-Null Values	Allowed	Actual	
AtomicWeight	2	real	real	✓	1.01	1.01	✓	238.03	294.00	x	positive	positive	✓	0	1	x	-	-	-	-	-	-
Etymology	2	string	string	✓	length 4	length 4	✓	length 39	length 53	x	-	-	-	0	1	x	-	3	117	-	-	-
RelativeAtomicMass	2	real	real	✓	1.01	1.01	✓	238.03	294.00	x	positive	positive	✓	0	1	x	-	-	-	-	-	-
Density	2	real	real	✓	0.00	0.00	✓	22.61	41.00	x	positive	positive	✓	0	5	x	-	-	-	-	-	-
Z	1	int	int	✓	1	1	✓	92	118	x	positive	positive	✓	0	0	✓	no	0	118	✓	-	-
Name	1	string	string	✓	length 3	length 3	✓	length 12	length 13	x	-	-	-	0	0	✓	no	0	118	✓	-	-
Symbol	1	string	string	✓	length 1	length 1	✓	length 2	length 3	x	-	-	-	0	0	✓	no	0	118	✓	-	-
MeltingPointC	1	real	real	✓	-258.98	-258.98	✓	3,675.00	3,675.00	✓	-	-	-	1	20	x	-	-	-	-	-	-
MeltingPointKelvin	1	real	real	✓	14.20	14.20	✓	3,948.00	3,948.00	✓	positive	positive	✓	1	20	x	-	-	-	-	-	-
BoilingPointC	1	real	real	✓	-268.93	-268.93	✓	5,596.00	5,596.00	✓	-	-	-	0	20	x	-	-	-	-	-	-
BoilingPointF	1	real	real	✓	-452.07	-452.07	✓	10,105.00	10,105.00	✓	-	-	-	0	20	x	-	-	-	-	-	-

15 failures


```
0 godel:$ python pdverify.py -f /miro/datasets/elements92.feather /tmp/elements92.tdda
```

```
SUMMARY:
```

```
Passes: 72
```

```
Failures: 0
```

```
0 godel:$
```

```
0 godel:$ python pdverify.py -f /miro/datasets/elements.feather /tmp/elements92.tdda
```

FIELDS:

AtomicWeight: 2 failures 3 passes type ✓ min ✓ max ✗ sign ✓ max_nulls ✗

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 ✓

BoilingPointF: 1 failure 3 passes type ✓ min ✓ max ✓ max_nulls ✗

Etymology: 2 failures 2 passes type ✓ min_length ✓ max_length ✗ max_nulls ✗

RelativeAtomicMass: 2 failures 3 passes type ✓ min ✓ max ✗ sign ✓ max_nulls ✗

MeltingPointC: 1 failure 3 passes type ✓ min ✓ max ✓ max_nulls ✗

Z: 1 failure 5 passes type ✓ min ✓ max ✗ sign ✓ max_nulls ✓ no_duplicates ✓

BoilingPointC: 1 failure 3 passes type ✓ min ✓ max ✓ max_nulls ✗

SUMMARY:

Passes: 57

Failures: 15

0 godel:\$

pdverifyelements1.py

```
# pdverifyelements1.py
```

```
from __future__ import print_function
from tdda.constraints.pdconstraints import verify_df
from pmmif.featherpmm import read_dataframe
```

```
ds = read_dataframe('/miro/datasets/elements92.feather')
v = verify_df(ds.df, '/tmp/elements92.tdda')
print('Passes:', v.passes, 'Failures:', v.failures)
```

OUTPUT

```
$ python pdverifyelements1.py
Passes: 72 Failures: 0
```

pdverifyelements2.py

```
# pdverifyelements2.py

from __future__ import print_function
from tdda.constraints.pdconstraints import verify_df
from pmmif.featherpmm import read_dataframe

ds = read_dataframe('/miro/datasets/elements.feather')
v = verify_df(ds.df, '/tmp/elements92.tdda', report='fields')
print(str(v))

dfv = v.to_frame()
print(dfv[dfv.failures > 0])
```

\$ python pdverifyelements2.py

FIELDS:

OUTPUT 1

AtomicWeight: 2 failures 3 passes type ✓ min ✓ max ✗ sign ✓ max_nulls ✗

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 ✓

BoilingPointF: 1 failure 3 passes type ✓ min ✓ max ✓ max_nulls ✗

Etymology: 2 failures 2 passes type ✓ min_length ✓ max_length ✗ max_nulls ✗

RelativeAtomicMass: 2 failures 3 passes type ✓ min ✓ max ✗ sign ✓ max_nulls ✗

MeltingPointC: 1 failure 3 passes type ✓ min ✓ max ✓ max_nulls ✗

Z: 1 failure 5 passes type ✓ min ✓ max ✗ sign ✓ max_nulls ✓ no_duplicates ✓

BoilingPointC: 1 failure 3 passes type ✓ min ✓ max ✓ max_nulls ✗

SUMMARY:

Passes: 57

Failures: 15

OUTPUT 2 (DataFrame)

	field	failures	passes	type	min	min_length	max	\
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	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

OUTPUT of to_frame()

	field	failures	passes	type	min	min_length	max	\
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	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

True *Satisfied*

FALSE *Not satisfied*

NaN *No constraint*

pdgenerate.py

```
# pdgenerate.py
```

```
from __future__ import print_function
import pandas as pd
```

```
from tdda.constraints.pdconstraints import discover_constraints
```

```
df = pd.read_csv('../testdata/elements92.csv')
constraints = discover_constraints(df)
with open('elements92.tdda', 'w') as f:
    f.write(constraints.to_json())
print('Written elements92.tdda')
```

```
print(verify_df(df, 'elements92.tdda'))
```


OUTPUT of pdgenerate.py

```
{  
  "fields": {  
    "AtomicWeight": {  
      "type": "real",  
      "min": 1.0079469999999999,  
      "max": 238.02891299999999,  
      "sign": "positive",  
      "max_nulls": 0  
    },  
    "Group": {  
      "type": "real",
```

.
.
.

SUMMARY:

Passes: 72

Failures: 0

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.

SUMMARY

- LEVEL ZERO** *Reference tests (writabletestcase.py)*
- *Support for sophisticated checking*
 - *Useful differences*
 - *Rewriting output verified as (now) correct*
- LEVEL ONE** *Input/Intermediate/Output Dataset Constraints*
- *Automatic constraint discovery*
 - *Systematic constraint verification*

 njr@StochasticSolutions.com

 <http://tdda.info>

 <http://github.com/tdda>

 @tdda0 @njr0

Correct interpretation: Zero

Error of interpretation: Letter "Oh"

OK, everything you need to know about T_EX has been explained—unless you happen to be fallible. If you don't plan to make any errors, don't bother to read this chapter.

— Donald E. Knuth, author T_EX

Chapter 27, The T_EXbook,

Recovery from Errors

ANALYTICAL SNAFU

Situation normal

— *analysis fouled* up.*

