PyData Array Recommendations

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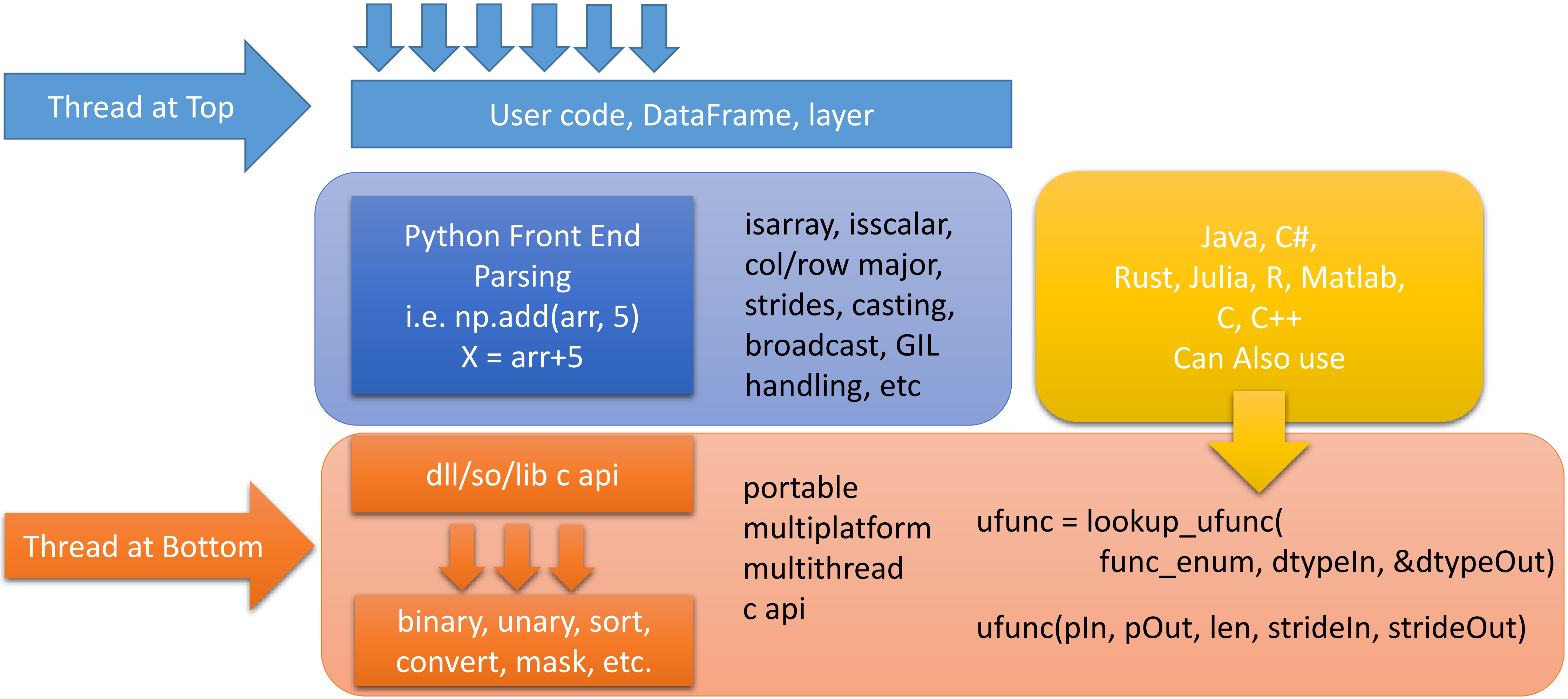
Background

- 30+ years professional software engineer – network protocols, user interfaces, compilers, file formats, pci cards, bios, trading engines, scanners, architectural software, ran 2 software companies, software patents, c/c++, java, c#, python
- 14 year consultant for SIG currently tasked with unifying large data analytics and framework
- SIG has Matlab, Python (numpy, pandas), C++/C# algos
- Desire to move towards one platform over time
- Ongoing beta solution: riptide: Uses Datasets/Structs/NumpyArrays, Multithreaded Numpy, portable FileFormat with stacking

Array Recommendations (in order of importance)

- Multithread back end engine and separate out portable c lib
- Introduce multikey categorical flavors with grouping routines
- New loops: groupby loops/ partition loops/ closer JIT coupling
- Subclass before making another dtype: Rework Date/Time classes
- Ledger + other ways to analyze performance
- Introduce new routines (hashing) + Invalids
- Dtypes for variable length string: ucs1,2,4. Bitmask.
- Hooks for display/storage/setname/getname

Threading Model



Thread at Top

User code, DataFrame, layer

Python Front End Parsing
i.e. np.add(arr, 5)
X = arr+5

isarray, isscalar, col/row major, strides, casting, broadcast, GIL handling, etc

Java, C#,
Rust, Julia, R, Matlab,
C, C++
Can Also use

Thread at Bottom

dll/so/lib c api

binary, unary, sort, convert, mask, etc.

portable
multiplatform
multithread
c api

```
ufunc = lookup_ufunc(
            func_enum, dtypeIn, &dtypeOut)

ufunc(pIn, pOut, len, strideIn, strideOut)
```

Threading Model for Arrays

- Multicore/Shared memory same computer, same process
- Possible tuning: Thread count, NUMA, Process Affinity
- Wakeup (futex) – important: selective thread wake up
  - Some routines just need 2 worker threads, more threads is not going to speed anything up for absolute value. Memory bound problem.
- Calibration of worker threads
- Array Recycling (nec for speed to reduce page faults)

NOTE: Distributed/Cloud Computing (not covered)

Portable Multithreaded C

- Gold Standard and easy to achieve with interface decoupling
- Allows other platforms or languages to call same routines with same results and performance
- Prefer C interface over C++ (a C++ layer can wrap C interface)
- In many low level routines want to get sum of Boolean mask (np.add.reduce(mask)) – should really just call SumBoolean()
- Threading while threading (have to know inside threaded routine)
- Be able to turn on “Ledger” to see what is getting called, performance

Array Routines We Threaded

- Basic Math both Unary and Binary (abs, add, sqrt, etc.)
- Comparisons (==, !=, <, >, <=, >=)
- Casting Conversions (i.e. int32 to float64)
- Boolean mask, Fancy Index mask set/get (i.e., a = b[filter])
- Reduce: all reduce functions sped up
- Sorting (espec lexsort, multithreaded multikey indirect merge sort)
- putmask, where, searchsorted, hstack, interp
- + Added Hashing, ismember, group creation

Speed ups from multi-threading

- Varies from 1.5x to 30x speedups (large arrays)
- Some users thread at top (with multiple processes), and use 2 threads at bottom for maximum performance
- Most basic math sped up by 3x
- Some reduction functions like sum,min,max,std up to 30x
- Unary functions sped up (isnotnan 10x faster than ~np.isnan())
- Many comparisons sped up by 10x
- getitem[fancyindex] sped up by 20x
- Can always turn off – thus no harm from multithreading

Example dir of FastArray
which subclasses np.ndarray (inherits)

FastArray
'abs','all','any','apply','apply_numba','argmax','argmin','argpartition','argpartition2','argsort','astype',
'base','between','byteswap','choose','clip','clip_lower','clip_upper','compress','conj','conjugate','copy','copy_invalid','count',
'crc','ctypes','cummax','cummin','cumprod','cumsum','data','describe','diagonal','diff','differs',**'display_query_property'**,
'dot','dtype','dump','dumps','duplicated','ema_decay','fill','fill_backward','fill_forward','fill_invalid','fillna','flags','flat',
'flatten',**'get_name'**,'getfield','imag','info','inv','iscomputable','isfinite','isin','isinf','isna','isnan','isnanorzero',
'isnormal','isnotfinite','isnotinf','isnotnan','isnotnormal','issorted','item','itemset','itemsize','map','map_old','max','mean',
'median','min','move_argmax','move_argmin','move_max','move_mean','move_median','move_min','move_rank','move_std','move_sum',
'move_var','nanargmax', 'nanargmin','nanmax','nanmean','nanmin','nanrankdata','nanstd','nansum','nanvar','nbytes','ndim',
'newbyteorder','nonzero','normalize_minmax', 'normalize_zscore','notna','numbastring','nunique','partition','partition2','prod','ptp',
'push','put','rankdata','ravel','real','register_function','repeat','replace','replacena','reshape','resize','rolling_mean','rolling_nanmean',
'rolling_nanstd','rolling_nansum','rolling_nanvar','rolling_std','rolling_sum',
'rolling_var','round','sample','save','searchsorted',**'set_name'**,'setfield','setflags','shape','shift','sign','size','sort',
'squeeze','std','str','str_append','strides','sum','swapaxes','take','tile','timewindow_prod','timewindow_sum','tobytes','tofile',
'tolist','tostring','trace','transitions','transpose','trunc','unique','var','view','where'

Note the added functionality for display (get_name, set_name, display_query)

Categorical Class (not a new dtype)

- Subclasses from (FastArray, GroupByOps)
  - Base array is int8/16/32/64
- Take most common categorical, of single string array
  - mycat=Cat(stringarray)
  - Often looks like string, sometimes integer bins
  - We chain ._fa or _.np to view FastArray or np.ndarray if we want to force integer bin mode
  - Can chain .str for string or .date for Dateclass to
- Creation can take two paths:
  - Via a lexsort or hashing
  - hashing (faster for low cardinality), also preserves order of first occurrence
- Once uniques are discovered, the high/low unique ratio count known important for some algorithms
- Have to be able to filter out (we reserve 0) so base 1 indexing

Categorical has Grouping object also inherits from GroupByOps

- Grouping object:

```
'apply','apply_helper','as_filter','base_index','catinstance','copy','copy_from','count','gbkeys','get_name','ifirstgroup','ifirstkey','igroup',
'igroupreverse','ikey','ilastkey','inextkey','iprevkey','iscategorical','isdirty','isdisplaysorted','isenum','isin','ismember','ismultikey','isordered',
'isortrows','issinglekey','ncountgroup','ncountkey','newclassfrominstance','newgroupfrominstance','onedict','pack_by_group','packed',
'possibly_recast','register_functions','regroup','set_dirty','set_name','shrink','sort','unique_count','uniquedict','uniquelist’
```

dir of Categorical class (inherits from FastArray and GroupByOps)

```
'abs','agg','aggregate','align','all','any','apply','apply_nonreduce','apply_numba','apply_reduce','argmax',
'argmin','argpartition','argpartition2','argsort','as_filter','as_singlekey','as_string_array','astype','auto_add_off','auto_add_on','base','base_index','between',
'byteswap','categories','categories_equal','category_add','category_array','category_codes','category_dict','category_mapping','category_mode',
'category_remove','category_replace','choose','clip',
'clip_lower','clip_upper','compress','conj','conjugate','contains_np_arrays','copy','copy_invalid','count','count_uniques','crc','ctypes','cumcount',
'cummax','cummin','cumprod','cumsum','data','describe','diagonal','diff','differs','display_convert_func','display_query_properties','doc','dot',
'dtype','dump','dumps','duplicated','ema_decay','ema_normal','ema_weighted','expand_any','expand_array','expand_dict','fill','fill_backward','fill_forward',
'fill_invalid','fillna','filter','filtered_name','filtered_set_name','filtered_string','findnth','first','first_bool','first_fancy','flags','flat','flatten',
'from_bin','from_category','gb_keychain','get_groupings','get_header_names','get_name','getfield','groupby_data','groupby_data_clear',
'groupby_data_set','groupby_reset','grouping','grouping_dict',
'groups','head','hstack','ifirstkey','ikey','ilastkey','imag','info','inv','invalid_category','invalid_set','iscomputable','isenum',
'isfiltered','isfinite','isin','isinf','ismultikey','isna','isnan','isnanorzero','isnormal','isnotfinite','isnotinf','isnotnan','isnotnormal',
'issinglekey','issorted','item','itemset','itemsize','iter_groups','key_from_bin','last','lock','map','map_old','mapping_add','mapping_new',
'mapping_remove','mapping_replace','max','mean','median','min','mode','move_argmax','move_argmin','move_max','move_mean','move_median','move_min',
'move_rank','move_std','move_sum','move_var','nan_index','nanargmax','nanargmin','nanmax','nanmean','nanmedian','nanmin','nanrankdata','nanstd',
'nansum','nanvar','nb_ema','nb_min','nb_sum','nb_sum_punt','nbytes','ndim','newbyteorder','newclassfrominstance','ngroup','nonzero','normalize_minmax',
'normalize_zscore','notna','nth','null','numbastring','nunique','ohlc','one_hot_encode','ordered','partition','partition2','prod','ptp',
'push','put','rank','rankdata','ravel','real','register_function','register_functions','repeat','replace','replacena','resample','reshape','resize',
'rolling_count','rolling_diff','rolling_mean','rolling_nanmean','rolling_nanstd','rolling_nansum','rolling_nanvar','rolling_shift','rolling_std','rolling_sum','rolling_var','round',
'sample','save','searchsorted','sem','set_name','setfield','setflags','shape','shift','shift_cat','shrink','sign','size',
'sort','sort_gb','sorted','squeeze','std','str','str_append','strides','sum','swapaxes','tail','take','tile',
'timewindow_prod','timewindow_sum','tobytes','tofile','tolist','tostring','trace','transform','transitions','transpose','trimbr','trunc','unique',
'unique_count','unique_repr','unlock','var','view','where'
```

Cat example with filter and groupbyops

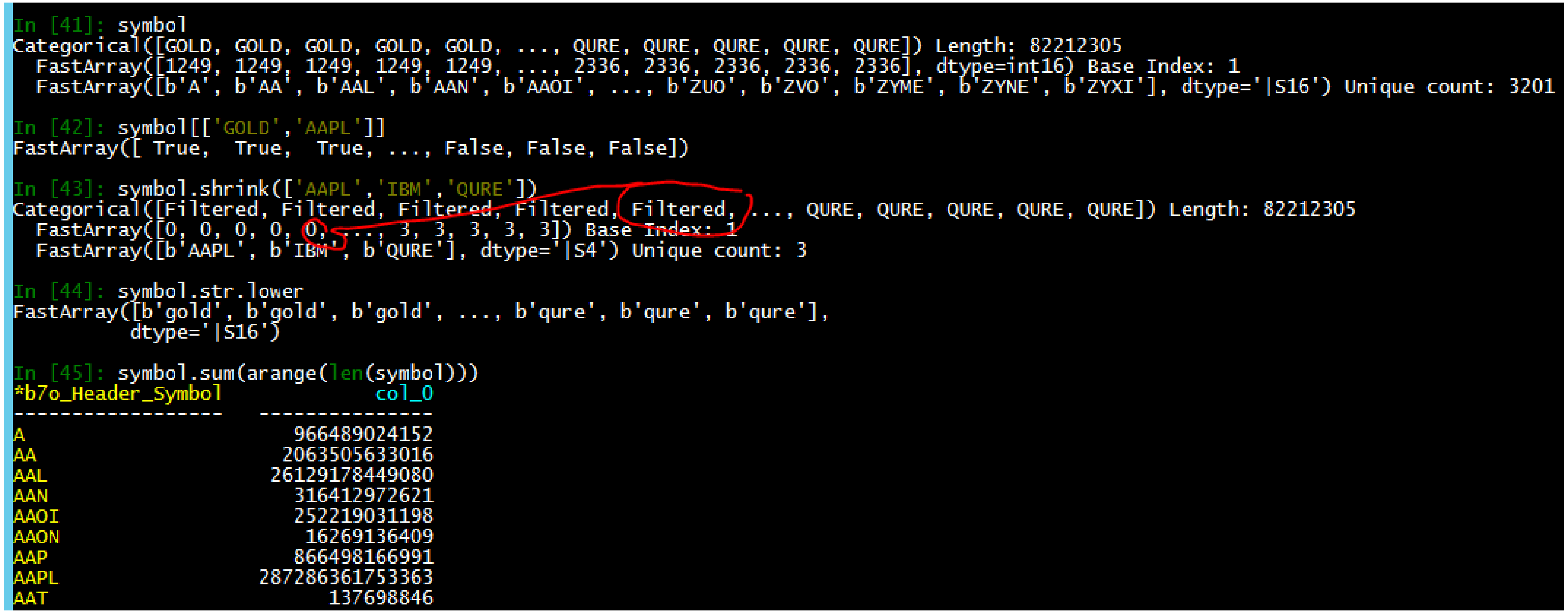
Example Cat

isin filter

can trim

very fast str ops

has groupbyops



```
In [41]: symbol
Categorical([GOLD, GOLD, GOLD, GOLD, GOLD, ..., QURE, QURE, QURE, QURE, QURE]) Length: 82212305
  FastArray([1249, 1249, 1249, 1249, 1249, ..., 2336, 2336, 2336, 2336, 2336], dtype=int16) Base Index: 1
  FastArray([b'A', b'AA', b'AAL', b'AAN', b'AAOI', ..., b'ZUO', b'ZVO', b'ZYME', b'ZYNE', b'ZYXI'], dtype='|S16') Unique count: 3201

In [42]: symbol[['GOLD','AAPL']]
FastArray([ True,  True,  True, ..., False, False, False])

In [43]: symbol.shrink(['AAPL','IBM','QURE'])
Categorical([Filtered, Filtered, Filtered, Filtered, Filtered, ..., QURE, QURE, QURE, QURE, QURE]) Length: 82212305
  FastArray([0, 0, 0, 0, 0, ..., 3, 3, 3, 3, 3]) Base Index: 1
  FastArray([b'AAPL', b'IBM', b'QURE'], dtype='|S4') Unique count: 3

In [44]: symbol.str.lower
FastArray([b'gold', b'gold', b'gold', ..., b'qure', b'qure', b'qure'],
          dtype='|S16')

In [45]: symbol.sum(arange(len(symbol)))
*b7o_Header_Symbol            col_0
------------------   ---------------
A                       966489024152
AA                     2063505633016
AAL                   26129178449080
AAN                     316412972621
AAOI                    252219031198
AAON                     16269136409
AAP                     866498166991
AAPL                 287286361753363
AAT                        137698846
```

Cat example with base array, grouping, reduction

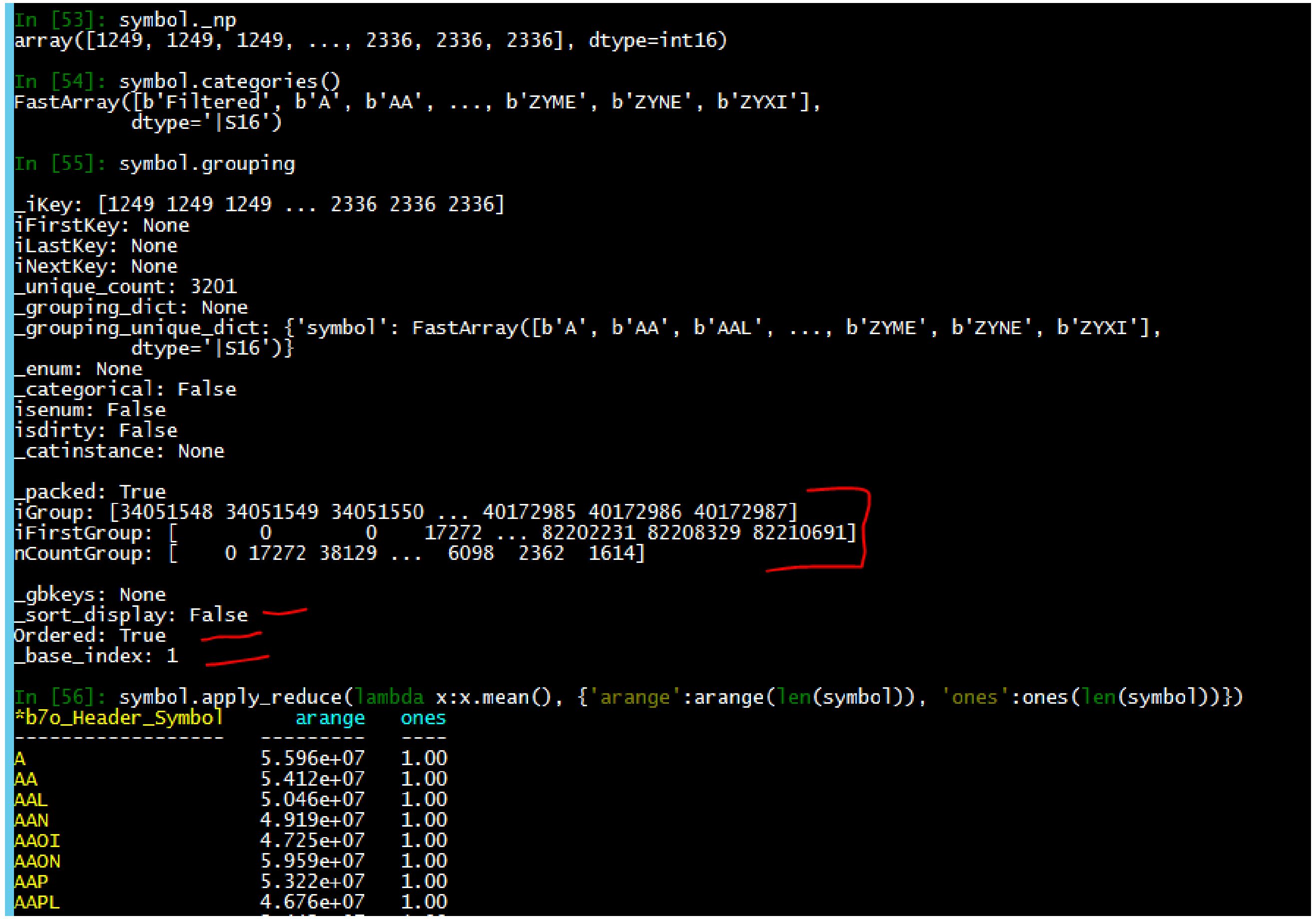
can flip view

get uniques

Grouping object

igroup is fancy index

has apply power



```
In [53]: symbol._np
array([1249, 1249, 1249, ..., 2336, 2336, 2336], dtype=int16)

In [54]: symbol.categories()
FastArray([b'Filtered', b'A', b'AA', ..., b'ZYME', b'ZYNE', b'ZYXI'],
          dtype='|S16')

In [55]: symbol.grouping

_iKey: [1249 1249 1249 ... 2336 2336 2336]
iFirstKey: None
iLastKey: None
iNextKey: None
_unique_count: 3201
_grouping_dict: None
_grouping_unique_dict: {'symbol': FastArray([b'A', b'AA', b'AAL', ..., b'ZYME', b'ZYNE', b'ZYXI'],
          dtype='|S16')}
_enum: None
_categorical: False
isenum: False
isdirty: False
_catinstance: None

_packed: True
iGroup: [34051548 34051549 34051550 ... 40172985 40172986 40172987]
iFirstGroup: [       0        0    17272 ... 82202231 82208329 82210691]
nCountGroup: [    0 17272 38129 ...  6098  2362  1614]

_gbkeys: None
_sort_display: False
Ordered: True
_base_index: 1

In [56]: symbol.apply_reduce(lambda x:x.mean(), {'arange':arange(len(symbol)), 'ones':ones(len(symbol))})
*b7o_Header_Symbol       arange   ones
------------------   ----------   ----
A                     5.596e+07   1.00
AA                    5.412e+07   1.00
AAL                   5.046e+07   1.00
AAN                   4.919e+07   1.00
AAOI                  4.725e+07   1.00
AAON                  5.959e+07   1.00
AAP                   5.322e+07   1.00
AAPL                  4.676e+07   1.00
```

Enum Cat Example (pre defined bins)

User has predefined bins

Wants to see 33 for ‘stop’

Duality: can use strings

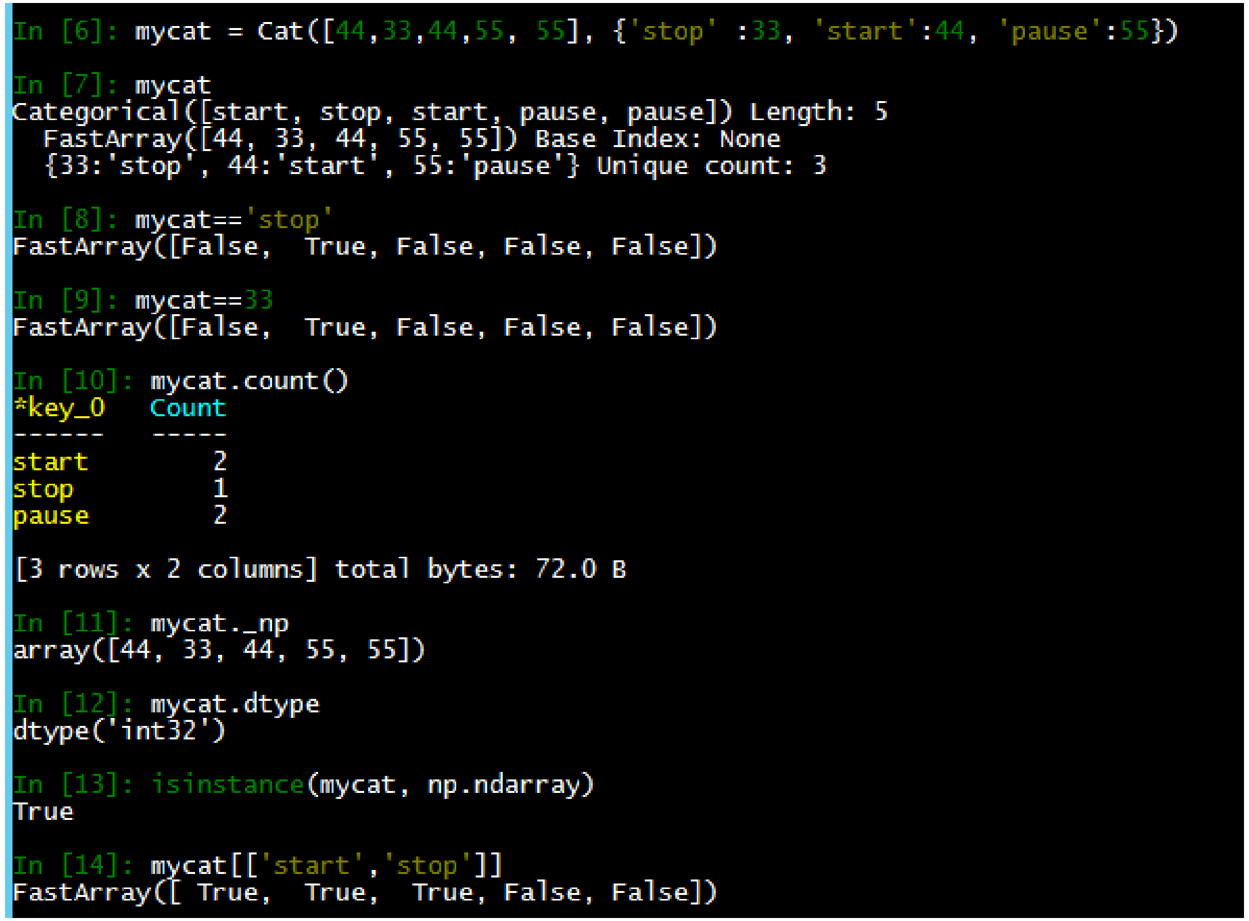
Duality: can use int

Has same functionality as normal categorical

The user bin is referenced, not copied

subclasses from np.ndarray

isin and other functionality works



```
In [6]: mycat = Cat([44,33,44,55, 55], {'stop' :33, 'start':44, 'pause':55})

In [7]: mycat
Categorical([start, stop, start, pause, pause]) Length: 5
  FastArray([44, 33, 44, 55, 55]) Base Index: None
  {33:'stop', 44:'start', 55:'pause'} Unique count: 3

In [8]: mycat=='stop'
FastArray([False,  True, False, False, False])

In [9]: mycat==33
FastArray([False,  True, False, False, False])

In [10]: mycat.count()
*key_0   Count
------   -----
start        2
stop         1
pause        2

[3 rows x 2 columns] total bytes: 72.0 B

In [11]: mycat._np
array([44, 33, 44, 55, 55])

In [12]: mycat.dtype
dtype('int32')

In [13]: isinstance(mycat, np.ndarray)
True

In [14]: mycat[['start','stop']]
FastArray([ True,  True,  True, False, False])
```

Multikey Cat Example (Date + String)
Can have many keys, ordered or not

Easy to create

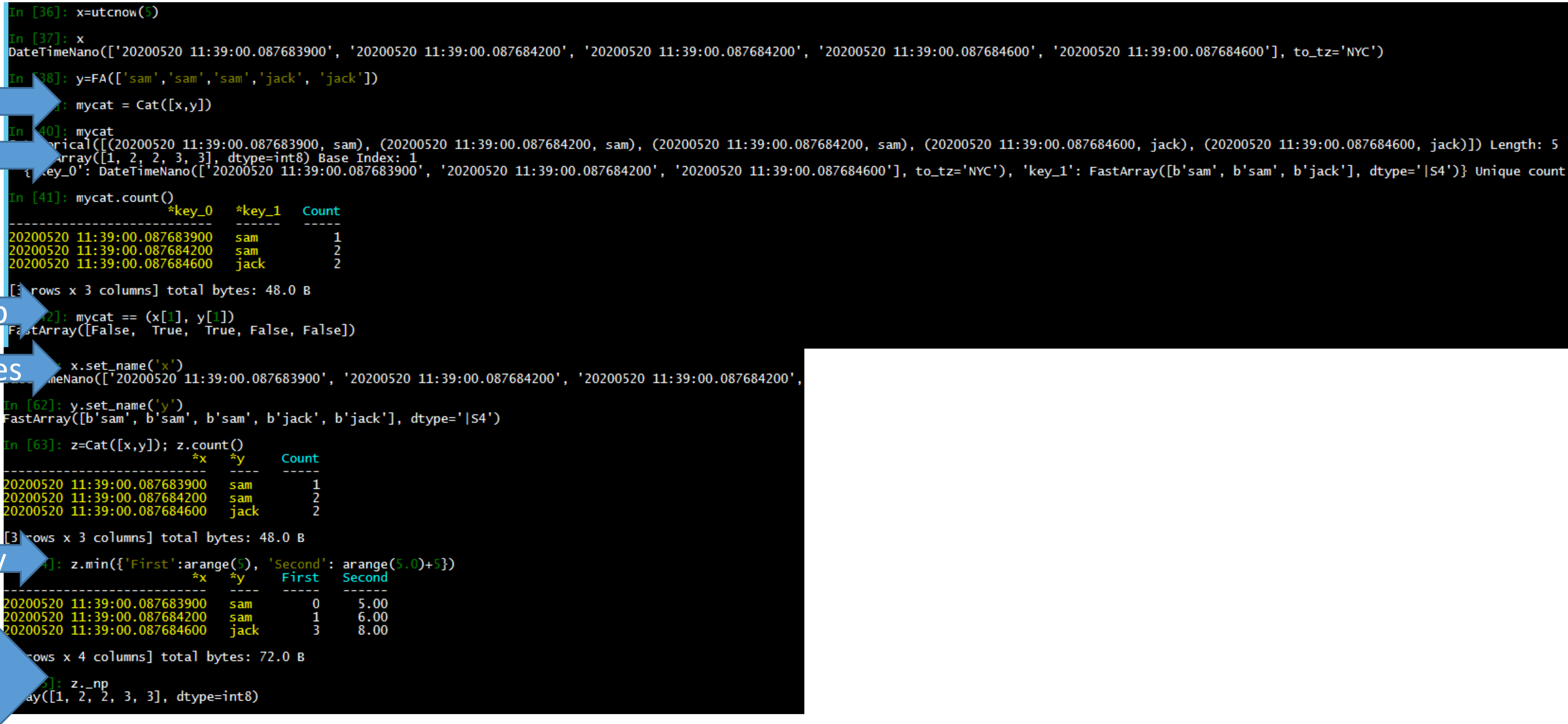
Still uses int bin

Use tuple to lookup

arrays needs names

full gb functionality

Int8/16/32/64
Based on unique



```
In [36]: x=utcnow(5)

In [37]: x
DateTimeNano(['20200520 11:39:00.087683900', '20200520 11:39:00.087684200', '20200520 11:39:00.087684200', '20200520 11:39:00.087684600', '20200520 11:39:00.087684600'], to_tz='NYC')

In  38]: y=FA(['sam','sam','sam','jack', 'jack'])

       : mycat = Cat([x,y])

In  40]: mycat
      rical([(20200520 11:39:00.087683900, sam), (20200520 11:39:00.087684200, sam), (20200520 11:39:00.087684200, sam), (20200520 11:39:00.087684600, jack), (20200520 11:39:00.087684600, jack)]) Length: 5
      rray([1, 2, 2, 3, 3], dtype=int8) Base Index: 1
  { ey_0': DateTimeNano(['20200520 11:39:00.087683900', '20200520 11:39:00.087684200', '20200520 11:39:00.087684600'], to_tz='NYC'), 'key_1': FastArray([b'sam', b'sam', b'jack'], dtype='|S4')} Unique count

In [41]: mycat.count()
                   *key_0   *key_1   Count
---------------------------   ------   -----
20200520 11:39:00.087683900   sam          1
20200520 11:39:00.087684200   sam          2
20200520 11:39:00.087684600   jack         2

[3 rows x 3 columns] total bytes: 48.0 B

     2]: mycat == (x[1], y[1])
Fa tArray([False,  True,  True, False, False])

       : x.set_name('x')
     meNano(['20200520 11:39:00.087683900', '20200520 11:39:00.087684200', '20200520 11:39:00.087684200',

In [62]: y.set_name('y')
FastArray([b'sam', b'sam', b'sam', b'jack', b'jack'], dtype='|S4')

In [63]: z=Cat([x,y]); z.count()
                         *x    *y      Count
---------------------------   ----     -----
20200520 11:39:00.087683900   sam          1
20200520 11:39:00.087684200   sam          2
20200520 11:39:00.087684600   jack         2

[3 rows x 3 columns] total bytes: 48.0 B

     4]: z.min({'First':arange(5), 'Second': arange(5.0)+5})
                         *x    *y      First   Second
---------------------------   ----     -----   ------
20200520 11:39:00.087683900   sam          0     5.00
20200520 11:39:00.087684200   sam          1     6.00
20200520 11:39:00.087684600   jack         3     8.00

    rows x 4 columns] total bytes: 72.0 B

     5]: z._np
    ay([1, 2, 2, 3, 3], dtype=int8)
```

New Loops

- Existing:
  - Contig math vector loops (stride == itemsize)
    - Able to hit mm_256_add_ routines, etc.
  - Strided loops
    - Can also use vector routines via gather intrinsic
- New: Groupby Loops
  - See “igroup” – fancy index in order of uniques
  - For example if ‘AAPL’ is first category then it might exist in 10,000 rows scattered about 1 million row array. Similar to what lexsort returns now to sum up all ‘AAPL’ can just use the index to get to the data (no need to copy or reshuffle data)
- New: Partition Loops
  - Often used after sort_inplace. Now groups are in order – might be many groups, perhaps 1 million… want to ‘fake’ slice arrays fast to do operations
- Loop over JIT kernels
  - Numba has nb.prange and threads.. Can use that to create own groupby kernel

Subclass before creating a new dtype

- Example: Datetime or ipv4 class
    - We have DateTimeNano, TimeSpan, Date, DateSpan classes
        - Date class is int32, days since epoch and is timezone agnostic
        - Subtracting two Dates produces a DateSpan
            - Also based on int32
        - Substracting two Times produces a TimeSpan
            - Can be EITHER int64 or float64 based
            - Each has pros and cons
        - Is that 5 new dtypes? Now a TimeSeries class.. 6 new dtypes? Ipv4 – 7 new dtypes? When does it end?
    - Rather just subclass
        - class Date(FastArray, otherclass):
            - def __new__(cls, arr, ..):
                - return arr.view(Date)
    - Use isinstance() to detect, may need centralized Class registry (we have a TypeRegister)
- No new ufunc loops required:
    - If I want to add 3 to DateTimeNano to add 3 nanoseconds, just +3
    - Hits sped up vectorized addition code – no new work
    - No switch(dtype):
        - case int64:
        - case datetime64: ← no need to add this new dtype everywhere anymore

Ledger

- Records all operations, can time them
- Can see when upcasting occurs, which routines take longest, order op operations, how many threads used
- Built into portable C code (so all languages can use)
- Useful for debugging performance (espec due to C code hiding from most python profilers)
- Similar info with Recycler

Suggested Additions to Array

- Hashing Class
  - Example crc
  - Like np.add.reduce… np.hash.reduce
  - ismember function (see matlab routine)
- Searchsorted with kwarg ‘exact’
  - Must be exact match or give other index, like -1
  - Searchsorted is easily multithreadable, thus it can be used in ismember
- Merge variations
  - Enrichment style
  - Left/Right Inner/Outer Join
- Think about isnot routines like isnotnan very popular
- Other ideas like fma (fused multiply add)

Hashing speed plus invalids and fancy indexing

Very common big array, 99 uniques

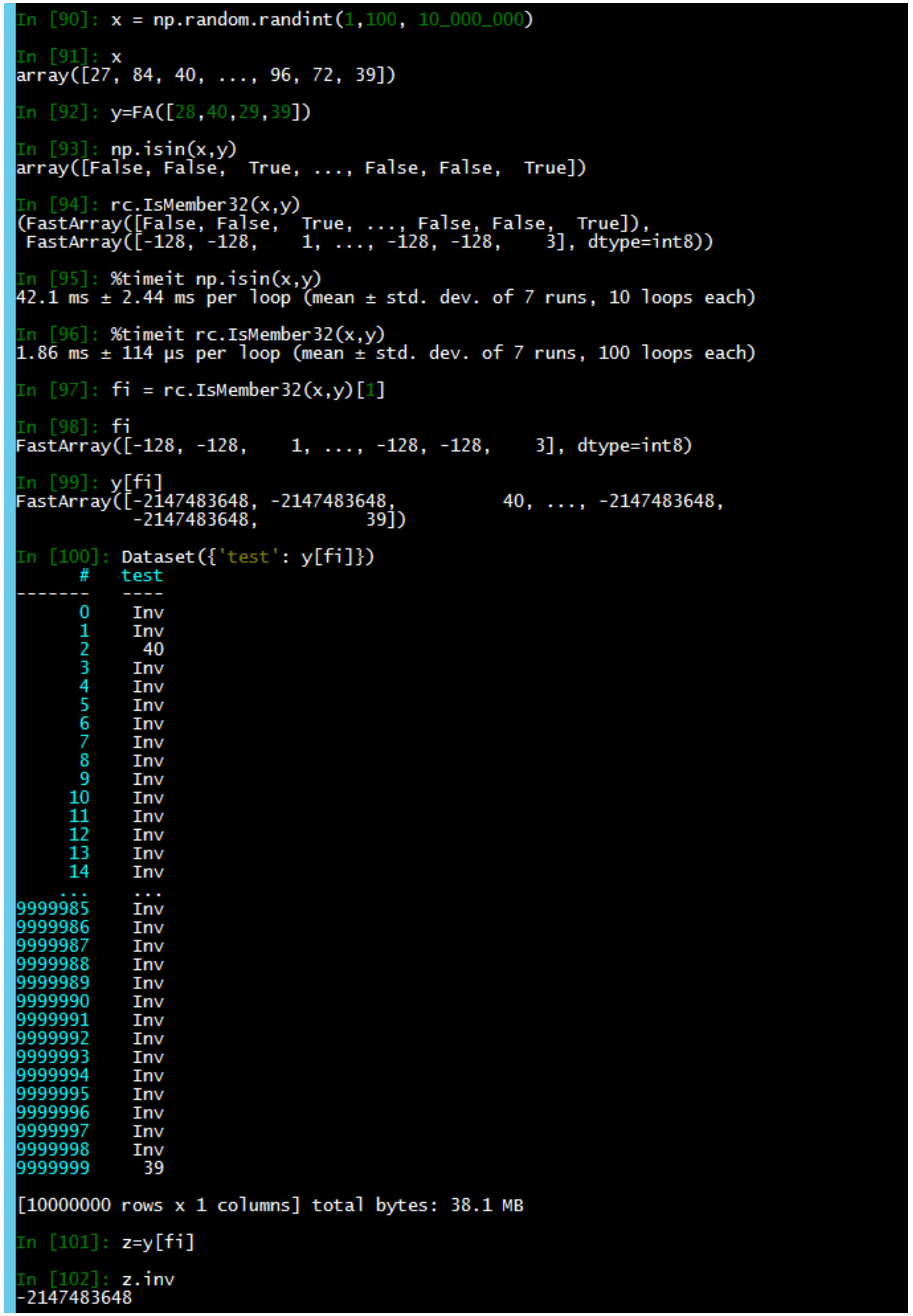
compare ismember to np.isin

ismember also returns fancy index

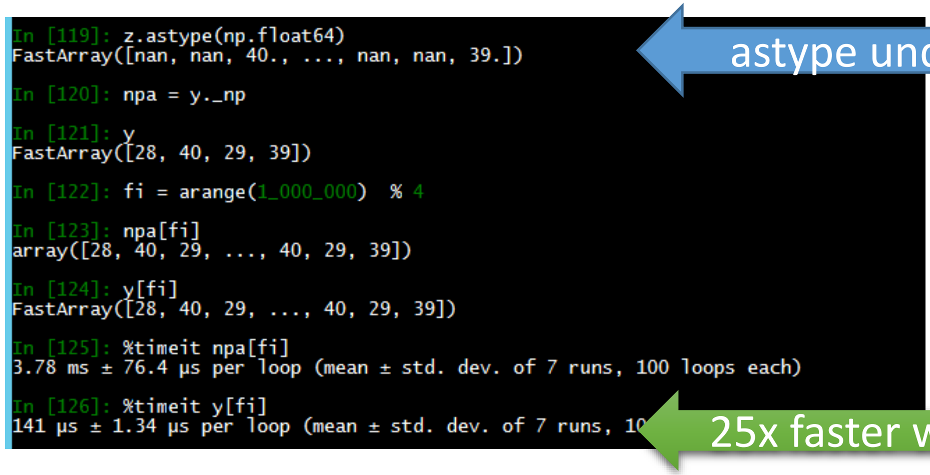
20x faster with more information

fancy idx understand invalids

Dataset/Frame understands also



```
In [90]: x = np.random.randint(1,100, 10_000_000)

In [91]: x
array([27, 84, 40, ..., 96, 72, 39])

In [92]: y=FA([28,40,29,39])

In [93]: np.isin(x,y)
array([False, False,  True, ..., False, False,  True])

In [94]: rc.IsMember32(x,y)
(FastArray([False, False,  True, ..., False, False,  True]),
 FastArray([-128, -128,    1, ..., -128, -128,    3], dtype=int8))

In [95]: %timeit np.isin(x,y)
42.1 ms ± 2.44 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)

In [96]: %timeit rc.IsMember32(x,y)
1.86 ms ± 114 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)

In [97]: fi = rc.IsMember32(x,y)[1]

In [98]: fi
FastArray([-128, -128,    1, ..., -128, -128,    3], dtype=int8)

In [99]: y[fi]
FastArray([-2147483648, -2147483648,          40, ..., -2147483648,
           -2147483648,          39])

In [100]: Dataset({'test': y[fi]})
      #   test
-------   ----
      0    Inv
      1    Inv
      2     40
      3    Inv
      4    Inv
      5    Inv
      6    Inv
      7    Inv
      8    Inv
      9    Inv
     10    Inv
     11    Inv
     12    Inv
     13    Inv
     14    Inv
    ...    ...
9999985    Inv
9999986    Inv
9999987    Inv
9999988    Inv
9999989    Inv
9999990    Inv
9999991    Inv
9999992    Inv
9999993    Inv
9999994    Inv
9999995    Inv
9999996    Inv
9999997    Inv
9999998    Inv
9999999     39

[10000000 rows x 1 columns] total bytes: 38.1 MB

In [101]: z=y[fi]

In [102]: z.inv
-2147483648
```



```
In [119]: z.astype(np.float64)
FastArray([nan, nan, 40., ..., nan, nan, 39.])

In [120]: npa = y._np

In [121]: y
FastArray([28, 40, 29, 39])

In [122]: fi = arange(1_000_000)  % 4

In [123]: npa[fi]
array([28, 40, 29, ..., 40, 29, 39])

In [124]: y[fi]
FastArray([28, 40, 29, ..., 40, 29, 39])

In [125]: %timeit npa[fi]
3.78 ms ± 76.4 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)

In [126]: %timeit y[fi]
141 µs ± 1.34 µs per loop (mean ± std. dev. of 7 runs, 10
```

astype understands invalids

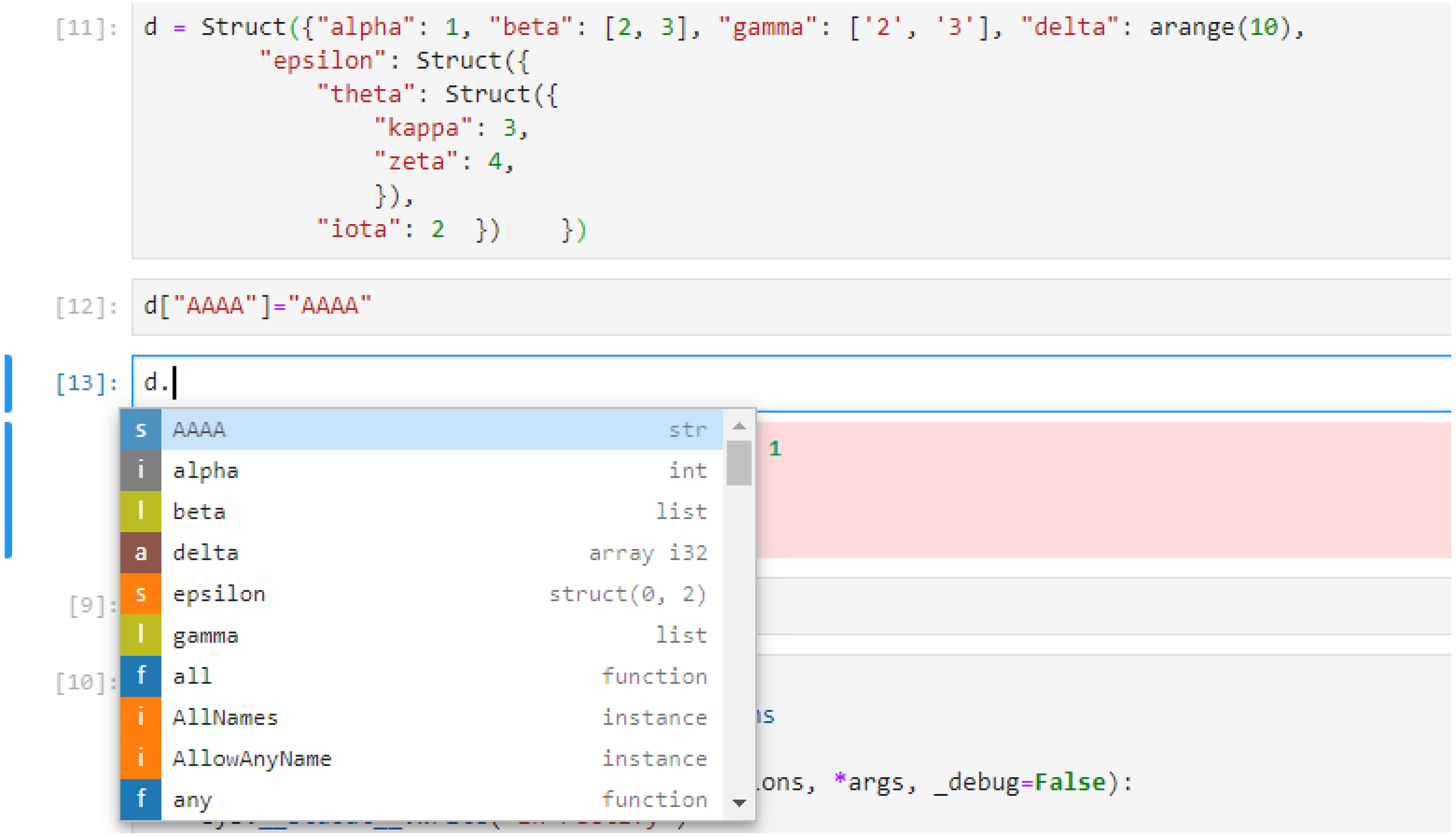
25x faster with invalid capability

New dtypes

- Variable length strings
- Bitmask Boolean
- Otherwise subclass from common dtypes
    - Use isinstance() checks
    - May want central “TypeRegister” to hold all known types
    - Class has to know how to save itself and reload itself so can be serialized to any file format
    - Class has to know how to display itself, right/left

Display/Serialization Hooks

- Known __ attributes to get/set meta data for serialization
- Hooks to help with autocomplete
- Or other display – left justified, abbreviated, etc.



```
[11]: d = Struct({"alpha": 1, "beta": [2, 3], "gamma": ['2', '3'], "delta": arange(10),
              "epsilon": Struct({
                  "theta": Struct({
                      "kappa": 3,
                      "zeta": 4,
                      }),
                  "iota": 2  })    })
```

```
[12]: d["AAAA"]="AAAA"
```

```
[13]: d.
```

```
s  AAAA                str
i  alpha               int
l  beta               list
a  delta         array i32
s  epsilon   struct(0, 2)
l  gamma              list
f  all            function
i  AllNames       instance
i  AllowAnyName   instance
f  any            function
```

```
1
[9]:
[10]:
ns
.ons, *args, _debug=False):
```