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How For Loops are High Key Killing Your Code Performance

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Intros

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Hobbies: Trail running, board games, improv
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What's So Wrong With For Loops !?

What's Wrong with For Loops?

"Row-based" operations

Code patterns to look for:

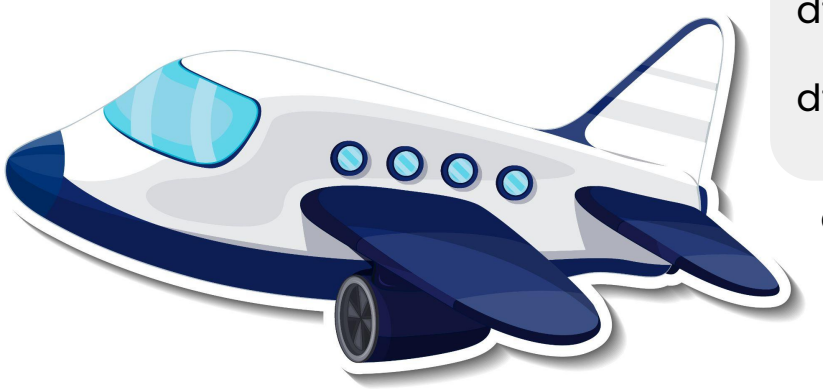
```
for i,row in df.iterrows():
    do_somthing(row['x'])

df["y"]=df["x"].apply(lambda x:my_func(x))

df.apply(lambda row:
    my_function(row["x1"],row["x2"], axis=1)
```

df: pd.DataFrame

ID	Year	Col1	Col2
ID1	2023	Y	0.342
ID2	2023	Y	0.34
ID1	2024	N	0.235
ID2	2024	Y	0.192

What To Do Instead: Vectorization

"Column-based" operations



New code patterns:

```
df["y"] = my_vec_func1(df["x1"], df["x2"])

df = my_vec_func2(df)
```

df: pd.DataFrame

ID	Year	Col1	Col2
ID1	2023	Y	0.342
ID2	2023	Y	0.34
ID1	2024	N	0.235
ID2	2024	Y	0.192

pandas

NumPy

Building Blocks: Foundations

Building Blocks: Foundational Strategies

Get data into np.array, pd.Series and/or pd.DataFrame

Use library functions with np.array & pd.Series args

Replace if/else using set theory np.isin() np.where() np.any()

np.array,
pd.Series,
pd.DataFrame

Get Everything in pd.DataFrame, pd.Series, or np.array

- **Vectorization** = element-wise operations on an entire array
- Already-optimized functions in **Numpy** and **Pandas** make this possible by leveraging LPACK, BLAS, and SIMD under the hood! 
- We can convert our data to:
  - np.array([1, 2, 3])
  - pd.Series(np.array([1, 2, 3]))
  - pd.DataFrame.from_dict(
    {“colName”: [“rowVal1”, “rowVal2”, “rowVal3”]},
    orient=”columns”
)

pandas

NumPy

Use library functions with np.array & pd.Series args

Building Blocks: Basic Operations (+ - * /) & math.log()

Replace this:

```
def slow_plus(array,inc=4):
  out=[]
  for x_i in array:
    out.append(x_i+inc)
  return np.array(out)
```

With this:

```
def vec_plus(array,inc=4):
  return array+inc
```

Performance on 10k records

```
n_reps=20; data_size= 10000 records
slow_plus_array: 0.0221s +/- 0.002s
slow_plus_df:    0.0023s +/- 0.0003s
vec_plus_df:     0.0004s +/- 0.0s
speedup:         61.2X  +/- 5.6X
```

Replace this:

```
def slow_log(array):
  out=[]
  for x_i in array:
    out.append(math.log(x_i,2))
  return np.array(out)
```

With this:

```
def vec_log(array):
  return np.log2(array)
```

Performance on 10k records

```
n_reps=20; data_size= 10000 records
slow_log_array:  0.0126s +/- 0.0027s
slow_log_df:  0.0041s +/- 0.0003s
vec_log_df:  0.0005s +/- 0.0001s
speedup:  27.8X  +/- 6.6X
```

Building Blocks: Library example (scipy.interpolate)

Use library functions with np.array & pd.Series args

```
def setup_library_fn(n: int):
    np.random.seed(12345)
    x = np.random.random(n)
    scale_fn = sp.interpolate.interp1d([0,1], [0,10], kind='linear')
```

Replace this:

```
def library_fn(x:np.array):
  y=[]
  for x_i in x:
    y.append(scale_fn(x_i))
  return y
```

With this:

```
def library_fn_vec(x:np.array):
  y = scale_fn(x)
  return y
```

Performance on 1M rows

```
tests/koans/vectorization.py::test_library_fn
for n=1000000:
time_before: 12.3905, time_vectorized: 0.0073.
improvement: 1697.3288x
```

Building Blocks: If/Else

Replace if/else using set theory

Replace this:

```
def slow_ifelse(x):
  if x['discount_code']=='SUBWAY':
    return x['subtotal']*0.85
  elif x['discount_code']=='FRIDAY':
    return x['subtotal']*0.9
  else:
    return x['subtotal']*0.95

def slow_ifelse_wrapper(X):
  return X.apply(
      lambda row: slow_ifelse(row), axis=1)
```

With this:

```
def vec_ifelse(X):
  idx_subway = X['discount_code']=='SUBWAY'
  idx_friday = X['discount_code']=='FRIDAY'
  idx_none = ~(np.any([idx_subway,idx_friday],axis=0))

  final_price = X['subtotal'].copy()
  final_price[idx_subway] = final_price[idx_subway]*0.85
  final_price[idx_friday] = final_price[idx_friday]*0.9
  final_price[idx_none] = final_price[idx_none]*0.95
  return final_price
```

Performance on 10k records

```
n_reps=20; data_size= 10000 records
slow_ifelse: 0.0973s +/- 0.0062s
vec_ifelse:  0.0068s +/- 0.001s
speedup:     14.6X  +/- 1.8X
```

Building Blocks: Set membership (np.where, np.isin)

Replace if/else using set theory

Replace this:

```
def set_membership(x, vals:set):
  y=[]
  for x_i in x:
    if x_i in vals:
      y.append(1)
    else:
      y.append(0)
  return y
```

With this:

```
def set_membership_vec(x,vals:np.array):
  # NOTE: list or np.array much faster than set
  y = np.where(np.isin(x,vals),1,0)
  return y
```

$$\text{Set Members} = \{2, 4\}$$

$$x = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}, idx = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

Performance on 10M rows

```
tests/koans/vectorization.py::test_set_membership
for n=10000000:
time_before: 1.1364, time_vectorized: 0.0619.
improvement: 18.3586x
```

Using Multiple Blocks

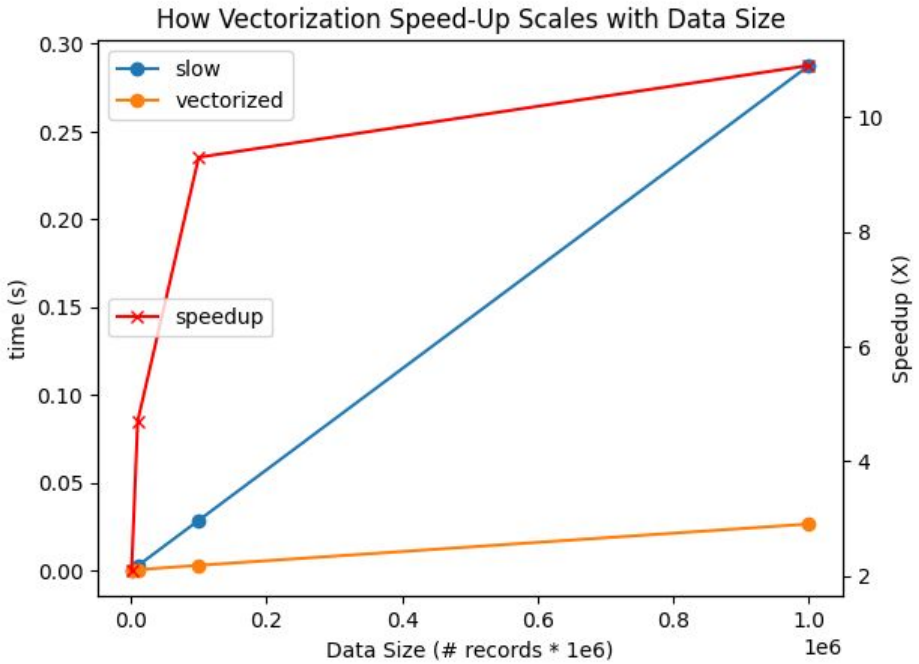
```python
def slow_esg_example(x:pd.Series , params: dict=country_params):
  if x['COUNTRY'] in params['countries_eligible_to_score']:
    if not pd.isna(x['FIELD1']):
      return sp.stats.norm.cdf(x['FIELD1'], loc=params['mu'], scale=params['scale'])
    else:
      return sp.stats.norm.cdf(x['FIELD2'], loc=params['mu'], scale=params['scale'])
  else:
    return np.nan

def slow_esg_example_on_DF(X:pd.DataFrame, params: dict=country_params):
  scores = []
  for i,row in X.iterrows():
    scores.append(slow_esg_example(row,params))
  return scores
```

1. Set theory to identify indices
2. Leverage vectorized library function (scipy.stats.norm.cdf)
3. Apply logic to select indices

```python
def vec_esg_example(X: pd.DataFrame, params: dict=country_params):
  idx_eligible = X['COUNTRY'].isin(params['countries_eligible_to_score'])
  idx_field1 = X['FIELD1'].notna()
  score = np.full(X.shape[0], np.nan, dtype=float)
  score[idx_eligible & idx_field1] = scipy.stats.norm.cdf(X.loc[idx_eligible & idx_field1]['FIELD1'], loc=params['mu'], scale=params['scale'])
  score[idx_eligible & ~idx_field1] = scipy.stats.norm.cdf(X.loc[idx_eligible & ~idx_field1]['FIELD2'], loc=params['mu'], scale=params['scale'])
  return score
```

1 3 2 3

Performance Scaling with Data Size



The bigger the data**, the more speed-up

***subject to memory constraints*

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Thank you!

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BONUS CONTENT

Building Blocks: Leveling Up

Building Blocks: Leveling Up

Broadcasting & Matrix Multiplication

Vectorized hashmap

Sort & np.argsort()

Time Series & np.roll np.nansum

Optimizing w/ Set Theory

Get data into np.array, pd.Series and/or pd.DataFrame

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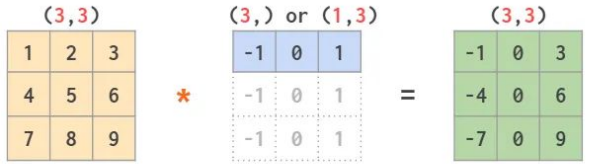
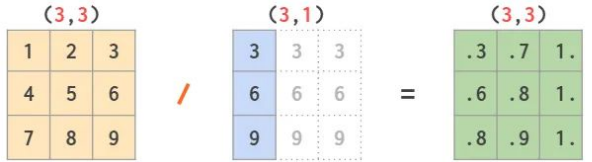
Replace if/else using set theory np.isin() np.where() np.any()

Broadcasting & Matrix Multiplication

Leveling Up: Broadcasting & Matrix Multiplication

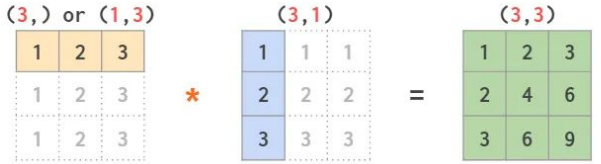
```python
def broadcasting_vec(X, c: list):
    # c is a list, numpy infers its 3x1
    # so nx3 by 3x1 multiplication works
    Y = X * c
    return Y
```





Performance on 1M rows

```
tests/koans/vectorization.py::test_broadcasting
for n=1000000: time_vec: 0.0107, time_normal: 1.5
improvement: 140.972x
```



Vectorized hashmap

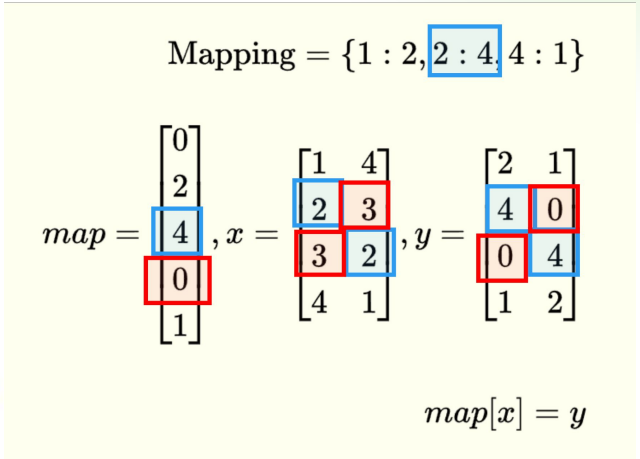
Leveling Up: Hash Lookup

Replace this:

```
def hashmap(x, params) -> list[float]:
    y = [ params.get(x_i, 0.0) for x_i in x ]
    return y
```

With this:

```
def hashmap_vec(x, params):
    # setup array of size max(dict value) + 1
    array_map = np.full(np.max(list(params.keys()))+1,0, dtype=float)
    # assign dictionary elements to array
    for key, value in params.items():
        array_map[key] = value
    # NOTE: using the array values as the index!
    y = array_map[x]
    return y
```



Performance on 10M rows

```
tests/koans/vectorization.py::test_hashmap
for n=10000000:
time_before: 4.2014, time_vectorized: 0.0309.
improvement: 135.9676x
```

Optimizing w/ Set Theory

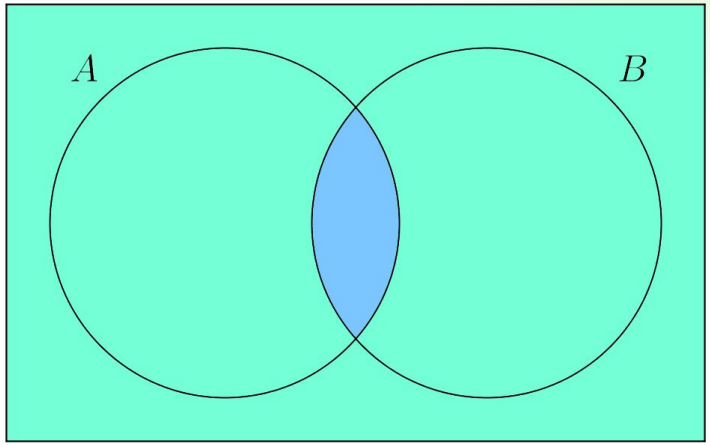
Leveling up: Optimizing Logic with Set Theory

- Use **De Morgan's Laws** (pictured: Law of Intersection) to combine & simplify all bool conditions to a single condition

- Streamline conditional logic
  - Goal 1: Refactor parentheses
  - Goal 2: One operation type (AND or OR)

- Example: (~ is NOT)
  - No error condition (A, B) occurs and input exists (C)
  - ~(A OR B) AND C
  - = (~A AND ~B) AND C
  - = ~A AND ~B AND C
  - np.any([~A, ~B, C], axis=0)

- Drawback: O(kn) where k = # conditions



$A \cap B$

$(A \cap B)^c = A^c \cup B^c$

https://brilliant.org/wiki/de-morgans-laws/

Sort & np.argsort()

Leveling Up: Vectorized Sort (np.argsort)

Replace this:

```
def argsort(x):
    y = sorted(x, key=lambda row: -row )
    return y
```

With this:

```
def argsort_vec(x):
    # make index
    idx = np.argsort(-x)
    # order vec by index
    y = x[idx]
    return y
```

```
def argsort_recover_x(x):
    # lookup and order x by index
    idx = np.argsort(-x)
    y = x[idx]
    idx_rev = np.argsort(idx)
    # x = x[idx][idx_rev]
    x_again = y[idx_rev]
    return x_again
```

Trick:
recover index!!

Performance on 1M rows

```
tests/koans/vectorization.py::test_argsort
for n=1000000:
time_before: 0.4157, time_vectorized: 0.0077.
improvement: 53.987x
```