advestis
one step ahead

JCAD2022

Execution of a feature engineering algorithm in Python on a supercomputer with Dask

Agenda

Context

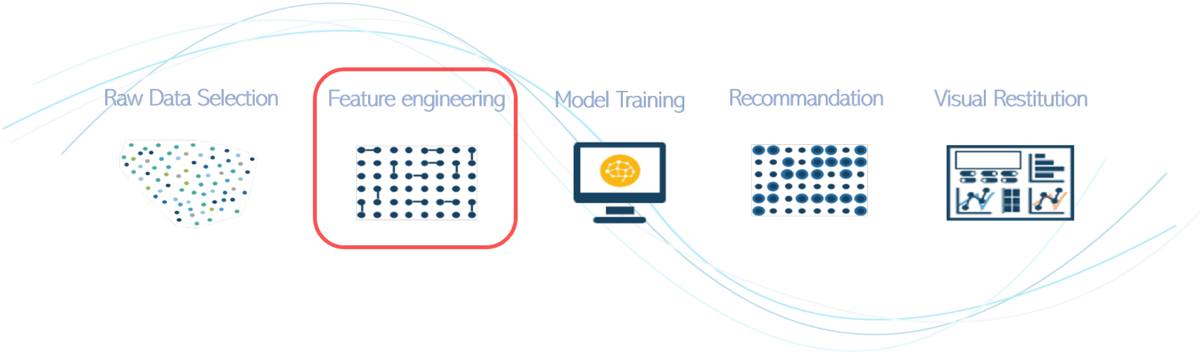
- Introduction to the problematic : derivation
- Dask
- Derivation toy model
- Chaining futures

Dask on Myria

- CRIANN Presentation
- Supercomputer *Myria*
- Dask on Myria

Conclusion

Introduction to the problematic : derivation



Primary data used in our data pipeline

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Example : ESG scores

1000 shares

10 years (2600 business days)

	Share 1	Share 2	Share 3	Share 4	Share 5	Share 6	Share 7	Share 8
2010-09-30	1	2	1	1	0	0	1	
2010-10-01	1	2	1	1	0	0	1	
2010-10-04	1	2	1	1	0	0	1	
2010-10-05	1	2	1	1	0	0	1	
2010-10-06	1	2	1	1	0	0	1	
2010-10-07	1	2	1	1	0	0	1	
2010-10-08	1	2	1	1	0	0	1	
2010-10-11	1	2	1	1	0	0	1	
2010-10-12	1	2	1	1	0	0	1	
2010-10-13	1	2	1	1	0	0	1	
2010-10-14	1	2	1	1	0	0	1	
2010-10-15	1	2	1	1	0	0	1	
2010-10-18	1	2	1	1	0	0	1	
2010-10-19	1	2	1	1	0	0	1	
2010-10-20	1	2	1	1	0	0	1	
2010-10-21	1	2	1	1	0	0	1	
2010-10-22	1	2	1	1	0	0	1	
2010-10-25	1	2	1	1	0	0	1	
2010-10-26	1	2	1	1	0	0	1	
2010-10-27	1	2	1	1	0	0	1	
2010-10-28	1	2	1	1	0	0	1	

x276 of such dataframes (scores, prices, sectors, marketcap ...) $>700\times10^{6}$ cells

Feature engineering

A set of transformations/combinations called ”derivations” is applied to the primary data in order to feed the learnings.

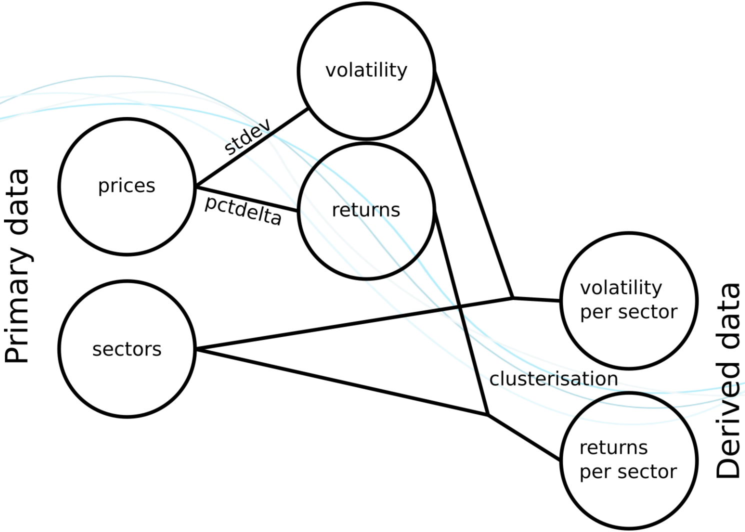
Relative positioning
For sectoral comparisons
. . .

Correlations

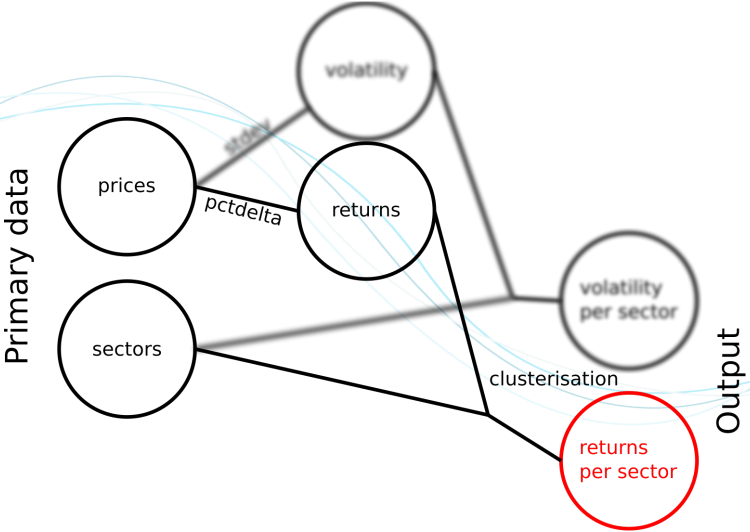
Temporal Z-Scores
To highlight the variability at different horizons.

Temporal shifts

Ex. : volatility & returns in sectors



Ex. : compute only the returns



What is Dask?

Dask

- Python library for parallel data processing
- Fully integrated in the PyData Stack (NumPy, SciPy, Scikit-Learn, Pandas, ...)

Main parts

1. Dynamic task scheduling optimized for computation
2. Big Data collections for parallel data management

How dask work?

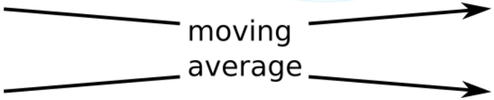
- Processing instructions on data generates a task graph
- The graph is scheduled by a cluster of workers
- Several solutions to manage the cluster: python multiprocessing (for single node only), k8s cluster, job scheduler like Slurm or PBS, MPI communicator, ...

Operators

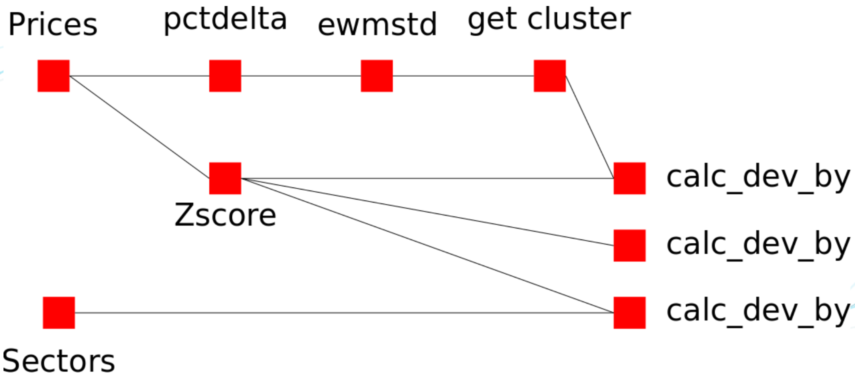
Unary operator

generic operator

Map



Derivation toy model : full graph



Derivation toy model : code

```
class Basic(AbstractDerivation):
    """The basic class to read data from data base"""

    all_prices = FileVar('all_prices.csv')
    marketcap = FileVar('marketcap.csv')
    sectors_isin = FileVar('Sectors.csv')


class Temporary(AbstractDerivation):
    """Temorary data for compute Y and X and others for the trading"""
    fin_rdt_1d_all = Var(op.pctdelta, Basic.all_prices, {'period': 1})
    fin_rdt_1d_std = Var(op.ewmstd, fin_rdt_1d_all, {'span': 260, 'min_periods': 260,
                                                     'annulize': True})

    clustervol = Var(op.get_clusters, fin_rdt_1d_std, {'levels': 5,
                                                       'dend': DATE_END_CLUSTERIZATION})

    fin_pricez1d = Var(op.zscore, Basic.all_prices, {'h': 1, 'minp': 60, 'inpct': True})
    fin_pricedevz1d_byvol = Var(op.calc_dev_by, [fin_pricez1d, clustervol],
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    fin_std260d_Z1d_bysectors = Var(op.calc_dev_by, [fin_pricez1d, Basic.sectors_isin],
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    fin_pricedevz1d_byuniver = Var(op.calc_dev_by, [fin_pricez1d], {'do_reduce': False})
    a = Var(op.wait_for_dask, fin_pricez1d, {})
```
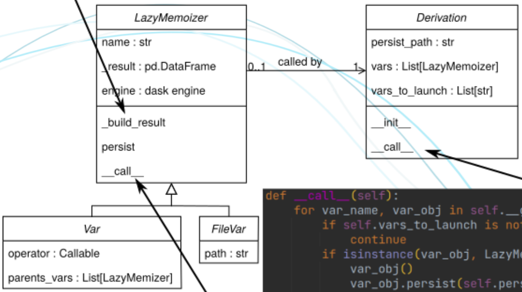

Chaining futures

```python
def _build_result(self):
    parent_inputs = list(map(self.engine.var_to_input, self.parent_vars))
    self._result.obj = self.engine.submit(self.name, self.operator, parent_inputs, self.params)
```




```python
def __call__(self):
    for var_name, var_obj in self.__get_vars():
        if self.vars_to_launch is not None and var_name not in self.vars_to_launch:
            continue
        if isinstance(var_obj, LazyMemoizer):
            var_obj()
            var_obj.persist(self.persist_path)
```

```python
def __call__(self):
    assert self.name, 'name should be set first from the derivation class'
    logger.info(f'Calling {self.name}')
    assert self._result is not None, 'self._result has not been built'
    if self._result.is_empty():
        self._build_result()
    return self._result
```

Chaining futures : _build_result

```python
def _build_result(self):
    parent_inputs = list(map(self.engine.var_to_input, self.parent_vars))
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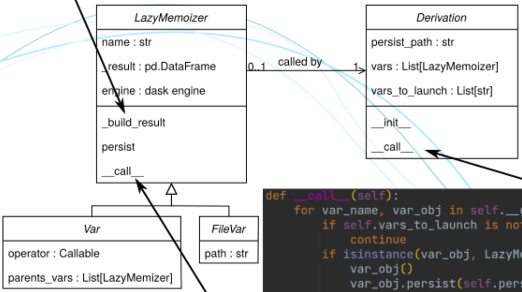


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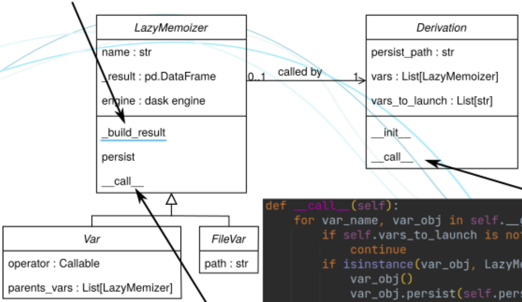


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    return self._result
```

Chaining futures : run a graph subset

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```python
def _build_result(self):
    parent_inputs = list(map(self.engine.var_to_input, self.parent_vars))
    self._result.obj = self.engine.submit(self.name, self.operator, parent_inputs, self.params)
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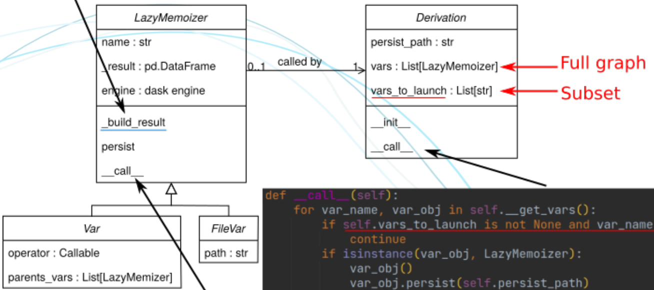


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    if self._result.is_empty():
        self._build_result()
    return self._result
```

Chaining futures : feature *calls* its parents

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```
def _build_result(self):
    parent_inputs = list(map(self.engine.var_to_input, self.parent_vars))
    self._result_obj = self.engine.submit(self.name, self.operator, parent_inputs, self.params)
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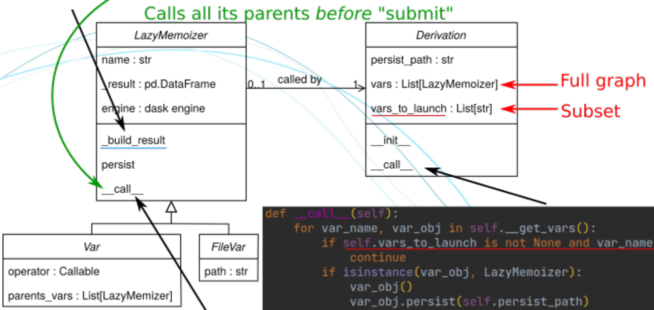


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    if self._result.is_empty():
        self._build_result()
    return self._result
```
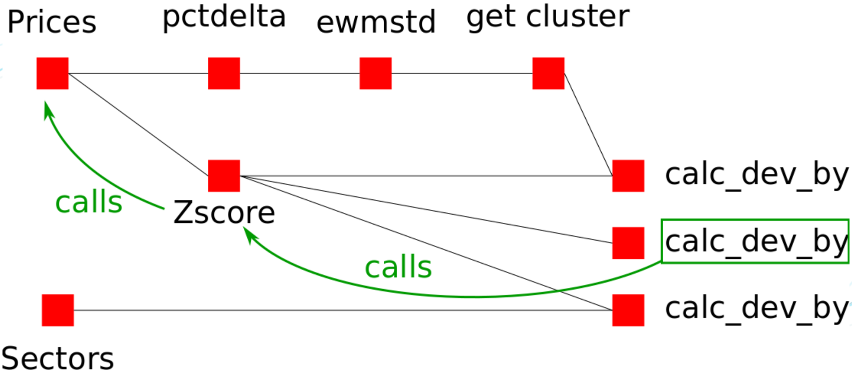
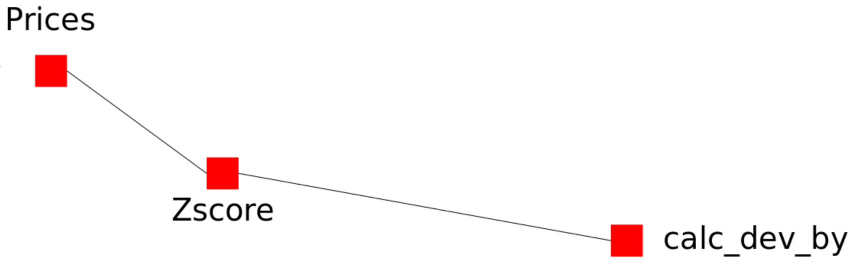
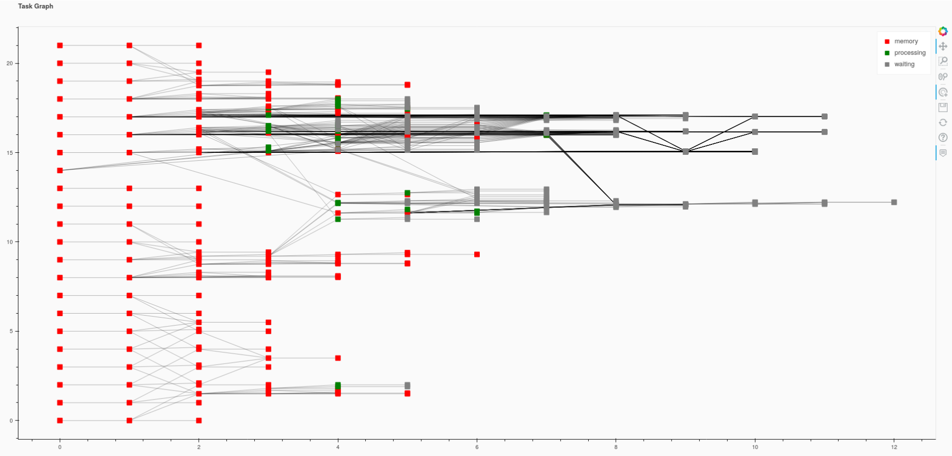

Derivation toy model : subset graph



Derivation toy model : subset graph

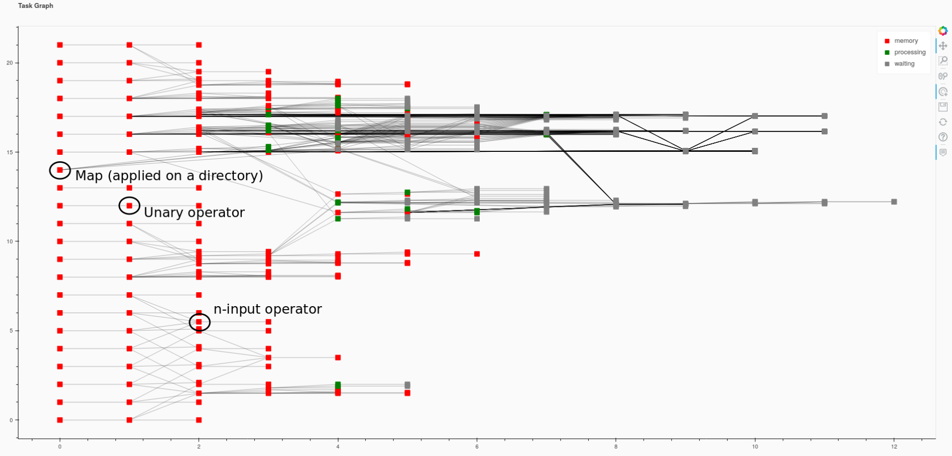


Real derivation graph subset



View execution

Real derivation graph subset



Normandy Regional Computing Center

- Created in 1991 as a Non Profit Organisation by Higher Educations Institutions & Universities
  - HPC center and regional network
- Located in Rouen Engineering Campus
- 13 employees (9 engineers or PhD)
- Funding is mainly public
  - Running costs supported by Normandy Region
  - Projects / investments funded by projects with EU, French State & Normandy Region
  - A small self-financing part
- HPC for public research, also open to private

Supercomputer *Myria*

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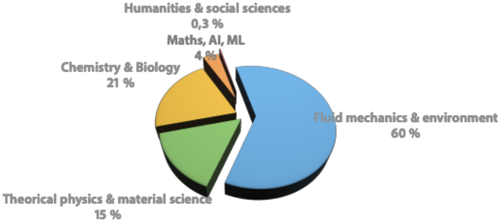

773 TFlop/s (Peak)
(419 Xeon + 327 GPU + 27 KNL)

Compute nodes

366 Broadwell Nodes (10248 cores)
28 cores@2.4 GHz - 128 GB RAM

Specialised nodes
- **26** GPUs (**48** K80, **17** P100, **20** V100)
- **13/ I/O**

SMP node Haswell
256 cores@2.2 GHz
4 To RAM DDR4

10 Xeon Phi KNL (640 cores)

Intel OmniPath
100 Gbit/s

DDN Storage
2,5 Po (HDD)

Access 4x10Gbit/s & 1x40Gbit/s
5 front-end & 3 visu. nodes

Cent OS - Slurm - GPFS

Dask on Myria: History

Since 2020

- Criann context: experimental works for growing competence
- Goal: service available for the next production machine (2023)

2020: 1 user project

- Techno watch for project users (workflow full redesign)
- Distributed data processing
- Mainly dask.dataframe features
- Results: efficient on a single node; dataframe partitioning inefficient in multinode

2022: Advestis

- Production code using Dask
- Distributed data processing
- Mainly dask.distributed features

Dask on Myria

Versions

- available only for privilegied users
- specific version for Advestis
  - resctricted access
  - in-house packages
- several versions for experimentation
  - Criann only

Dashboard unavailable

web access prohibited

Cluster technologies

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LocalCluster

- Uses Python multiprocessing/multithreading to deploy dask workers

```
cluster = LocalCluster()
client = Client(cluster)
```

- Pros
  - Easy to setup
  - In a slurm job, automatically adapt workers with the cgroups resources
- Cons
  - For single node only: no scalability

K8S Cluster

- Uses K8S cluster to deploy dask workers

```
from dask_kubernetes import KubeCluster
cluster = KubeCluster.from_dict(self.
     get_dask_kube_worker_spec())
cluster.adapt(minimum=1, maximum=self.
     dask_kube_max_pods)
client = Client(cluster)
```

- Pros
  - Easy to scale up
  - Standard approch for Advestis
- Cons
  - Unavailable on Myria (Slurm cluster without container)

Job scheduler

- Uses job scheduler (Slurm, PBS, ...) to deploy dask workers
- Configuration file (*jobqueue.yaml*) specific to the cluster
- Pros
  - Fully integrated with HPC clusters
  - Easy to scale up
- Cons
  - Dask workers run in jobs independent of the main Python process: if resources are busy the main process can wait a long time
  - Slurm jobs submitted by slurm jobs: beware side effects

jobqueue.yaml

```yaml
jobqueue:
    slurm:
        cores: 28
        memory: '120GB'
        processes: 7
        queue: 'tcourt_intra'
        walltime: '02:00:00'
```

Main python process

```python
from dask_jobqueue import SLURMCluster
cluster = SLURMCluster()
```

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MPI Cluster (dask_mpi)

- Uses MPI to deploy dask workers
- Workers are MPI processes
- Two ways:
  - MPI for main Python process and dask workers
  - MPI only for dask workers
- Pros
  - Easy to scale up
  - Adapted for HPC clusters
- Cons
  - Dysfunctions with real use case (import error, unknown variables)

same MPI context

```python
from dask_mpi import initialize
initialize()
from dask.distributed import Client
client = Client()
```

```
mpirun -np 4 python my_client_script.py
```

Warning: n - 2 workers

MPI for dask workers only

```
mpirun -np 4 dask-mpi --scheduler-file
    scheduler.json
```

```python
from dask.distributed import Client
client = Client(scheduler_file='./scheduler.
    json')
```

Can run in a heterogenous job

Conclusion

Computation graph ran on

- Local machine (Intel Core i9-9900K CPU @ 3.60GHz × 16, 32 GB RAM)
- Kubernetes on a Google Cloud Platform cluster (up to 50 workers, one worker is a 16-core VM)
- Myria

	full derivation (5327)	**medium derivation (1383)**
Local machine - Memory	120 minutes	20 minutes
Local machine - Dask	30 minutes	5 minutes
K8s on GCP - Dask	9 minutes	4 minutes
Myria - Memory	155 minutes	7 minutes
Myria - Dask	37 minutes	3 minutes

Computation time

Thank you !

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Backup slides

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With a graph of +1000 nodes:

- How to automatically cache intermediate results to avoid running same nodes multiple times?
- How to run a subset of graph by selecting a subset of final nodes?

$\Rightarrow$ Dask future or Dask delayed?

Pros:

- Visualize is pretty cool
- Delayed are lazy objects. It means the complete graph may be configured but not executed. Thus it is possible to trigger a subset of this graph.

Cons:

- Persistence has to be implemented explicitly. For complex graphs it is not sufficient.

Dask Future

Pros:

- persistence happens as long as their is at least one python object referencing the future.

Cons:

- Future is triggered without delay
- There is no visualize method

Conclusion:

- Dask primary components are not sufficient. Thus a thin wrapper is mandatory in order to manage a lazy behavior
- We opted for **Dask Futures** because they automatically persist

AbstractDerivation

```
class AbstractDerivation(ABC):
    def __init__(self, persist_folder, vars_to_launch_file=None, fs=None):
        self.persist_path = settings.DERIVED_PATH / persist_folder
        self.vars_to_launch = None
        if isinstance(vars_to_launch_file, Path):
            self.vars_to_launch = vars_to_launch_file.read()
        elif vars_to_launch_file is not None:
            if not isinstance(vars_to_launch_file, list):
                vars_to_launch_file = Path(vars_to_launch_file, fs=fs)
                self.vars_to_launch = vars_to_launch_file.read()
            else:
                self.vars_to_launch = vars_to_launch_file
        if isinstance(self.vars_to_launch, str):
            self.vars_to_launch = self.vars_to_launch.split("\n")
        self.__add_name()
```

AbstractDerivation

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```python
def __get_vars(self):
    for var_name in filter(lambda x: not x.startswith('_'), dir(self)):
        var_obj = getattr(self, var_name)
        yield var_name, var_obj

def __add_name(self):
    for var_name, var_obj in self.__get_vars():
        if any(map(lambda x: isinstance(var_obj, x), [Var, Map, FileVar])):
            logger.debug(f'adding name to {var_name}')
            var_obj.name = var_name

def __call__(self):
    for var_name, var_obj in self.__get_vars():
        if self.vars_to_launch is not None and var_name not in self.vars_to_launch:
            continue
        if isinstance(var_obj, LazyMemoizer):
            var_obj()
            var_obj.persist(self.persist_path)
```

LazyMemoizer : Abstract class

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```python
class LazyMemoizer(ABC):
    """
    Build a callable object and store the result through an engine
    """

    def __init__(self, *args, **kwargs):
        self._result = None
        self._writer = None
```

```python
    def __call__(self):
        assert self.name, 'name should be set first from the derivation class'
        logger.info(f'Calling {self.name}')
        assert self._result is not None, 'self._result has not been built'
        if self._result.is_empty():
            self._build_result()
        return self._result
```

FileVar : Base feature class

```
class FileVar(LazyMemoizer):
    """
    Setup a Var object from a dataframe stored as a csv file. It is inherited
    from Var class
    """
    def __init__(self, filename, reader=Reader, folder=settings.BASE_PATH):
        """

        params: filename: used be the reader to get the file
        """
        super().__init__()
        self._result = Result()
        self.reader = reader(folder)
        self.filename = filename
        self.__name = None

    @property
    def name(self):
        return self.__name

    @name.setter
    def name(self, value):
        self.__name = value

    def _build_result(self):
        self._result.obj = self.engine.submit(self.name, self.reader, dfs=(),
                                              params={'name': self.filename})
```

Var : Derived feature class

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```python
class Var(LazyMemoizer):
    """
    Setup a var as a transformation from another var
    """

    def __init__(self, operator, parent_vars=(), params=None):
```

```python
        super().__init__()
        self._result = Result()
        assert callable(operator)
        self.operator = operator
        if isinstance(parent_vars, Iterable):
            self.parent_vars = parent_vars
        else:
            self.parent_vars = [parent_vars]
        self.params = params if params else {}
        self.__name = None
```

```python
    def _build_result(self):
        parent_inputs = list(map(self.engine.var_to_input, self.parent_vars))
        self._result.obj = self.engine.submit(self.name, self.operator, parent_inputs, self.params)

    def persist(self, path):
        writer = Writer(path)
        self._writer = Var(writer, self, params={'name': self.name})
        self._writer.name = f'writer_{self.name}'
        self._writer()
```

Derivation

```
class Basic(AbstractDerivation):
    """The basic class to read data from data base"""

    all_prices = FileVar('all_prices.csv')
    marketcap = FileVar('marketcap.csv')
    sectors_isin = FileVar('Sectors.csv')


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    clustervol = Var(op.get_clusters, fin_rdt_1d_std, {'levels': 5,
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    fin_pricez1d = Var(op.zscore, Basic.all_prices, {'h': 1, 'minp': 60, 'inpct': True})
    fin_pricedevz1d_byvol = Var(op.calc_dev_by, [fin_pricez1d, clustervol],
                               {'do_reduce': False, 'clusterishito': True})
    fin_std260d_Z1d_bysectors = Var(op.calc_dev_by, [fin_pricez1d, Basic.sectors_isin],
                                   {'do_reduce': False})
    fin_pricedevz1d_byuniver = Var(op.calc_dev_by, [fin_pricez1d], {'do_reduce': False})
    a = Var(op.wait_for_dask, fin_pricez1d, {})
```

Derivation

```python
def main(vars_to_launch=None, fs=None):
    make_directories()
    derivations = [Basic(settings.S_FOLDER),
                   Temporary(settings.T_FOLDER)]
    for d in derivations:
        d()
    get_engine().wait()
```

Derivation

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```python
import click

from adoptim3.derivation.append import update_db
# from adoptim3.derivation import deriv_ia_stoxx600
from adoptim3.derivation import deriv_toy_model
# from adoptim3.derivation import deriv_darling


@click.group()
def cli():
    # override me
    pass
```

```python
@click.command()
@click.option("-l", "--vars_to_launch", default=None)
@click.option("-f", "--fs", default=None)
def derivtoymodel(vars_to_launch, fs):
    deriv_toy_model.main(vars_to_launch, fs)
```

```python
cli.add_command(derivtoymodel)


if __name__ == '__main__':
    cli()
```