Graph Gym Tutorial 2

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https://gabrielesantin.github.io/

TABLE OF CONTENTS

01 A bit of background

Initial idea published as the study of the design space of GNN

First hosted on

- **Stanford Snap**: "Design Space for Graph Neural Networks"
  http://snap.stanford.edu/gnn-design/

- **GitHub**: https://github.com/snap-stanford/graphgym

[1] J. You, R. Ying, J. Leskovec, Design Space for Graph Neural Networks.. Neural Information Processing Systems (NeurIPS), 2020.
https://arxiv.org/abs/2011.08843

01 A bit of background

Now also integrated in PyG

- **Intro page:** "Managing experiments with GraphGym"
  https://pytorch-geometric.readthedocs.io/en/latest/notes/graphgym.html
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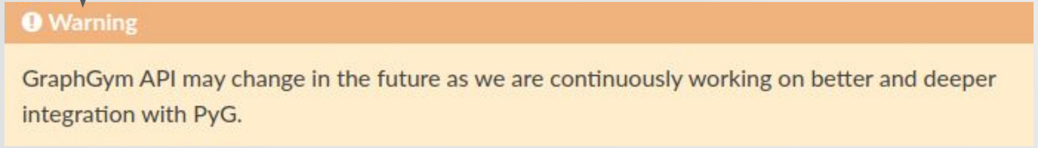
Warning → Update to the last version of the packages


Warning

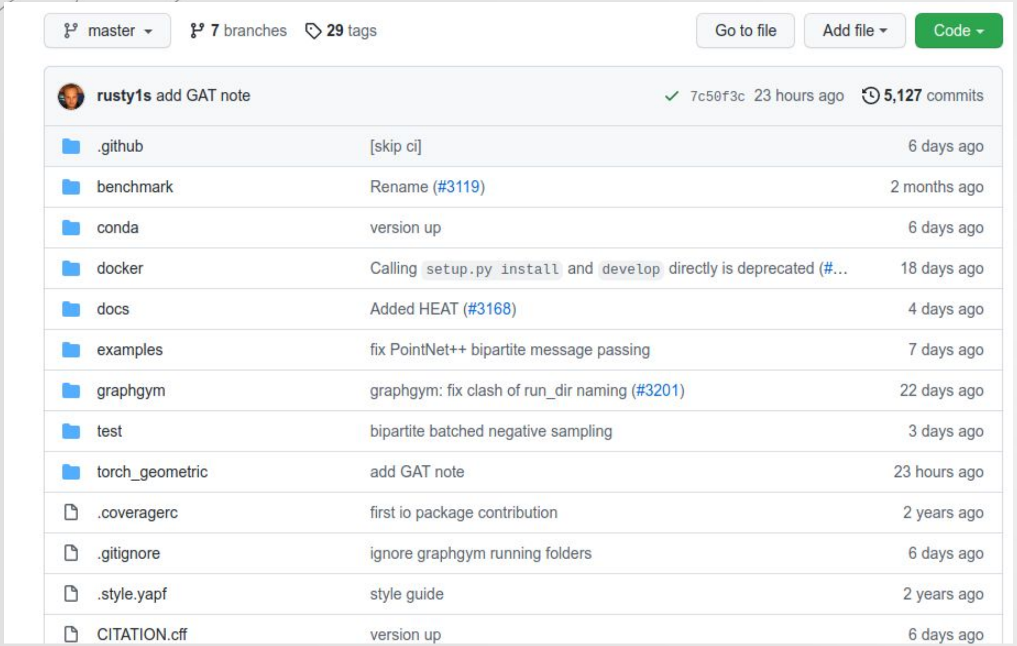
GraphGym API may change in the future as we are continuously working on better and deeper integration with PyG.

02 Goals and basic usage

Easy design and execution of experiments

- **Modularization:**
  - Pick a dataset, a model, a task, an evaluation metric, an optimizer
- **Reproducibility:**
  - Definition of simple configuration files to parametrize experiments
- **Scalability:**
  - Easy execution of multiple parallel experiments

02 Goals and basic usage



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.github	[skip ci]	6 days ago
benchmark	Rename (#3119)	2 months ago
conda	version up	6 days ago
docker	Calling `setup.py install` and `develop` directly is deprecated (#...	18 days ago
docs	Added HEAT (#3168)	4 days ago
examples	fix PointNet++ bipartite message passing	7 days ago
graphgym	graphgym: fix clash of run_dir naming (#3201)	22 days ago
test	bipartite batched negative sampling	3 days ago
torch_geometric	add GAT note	23 hours ago
.coveragerc	first io package contribution	2 years ago
.gitignore	ignore graphgym running folders	6 days ago
.style.yapf	style guide	2 years ago
CITATION.cff	version up	6 days ago

02 Goals and basic usage

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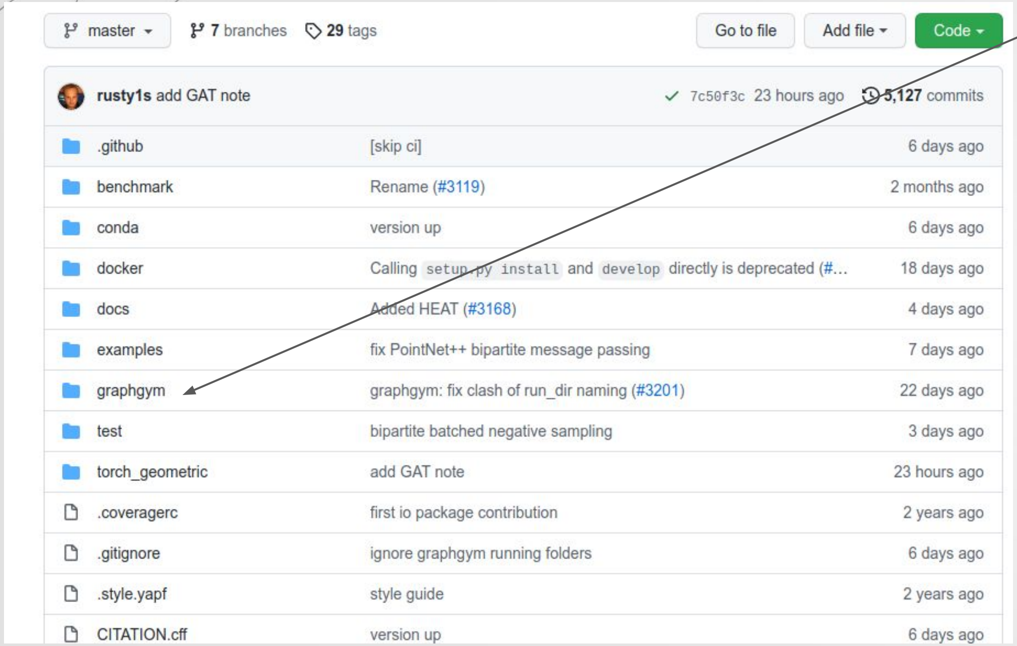

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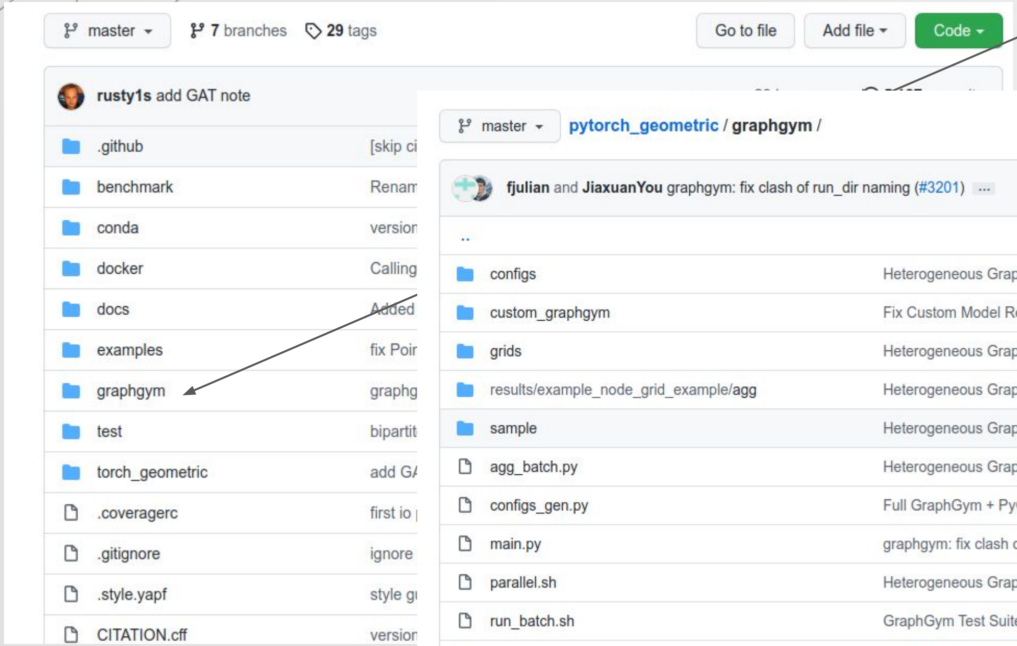

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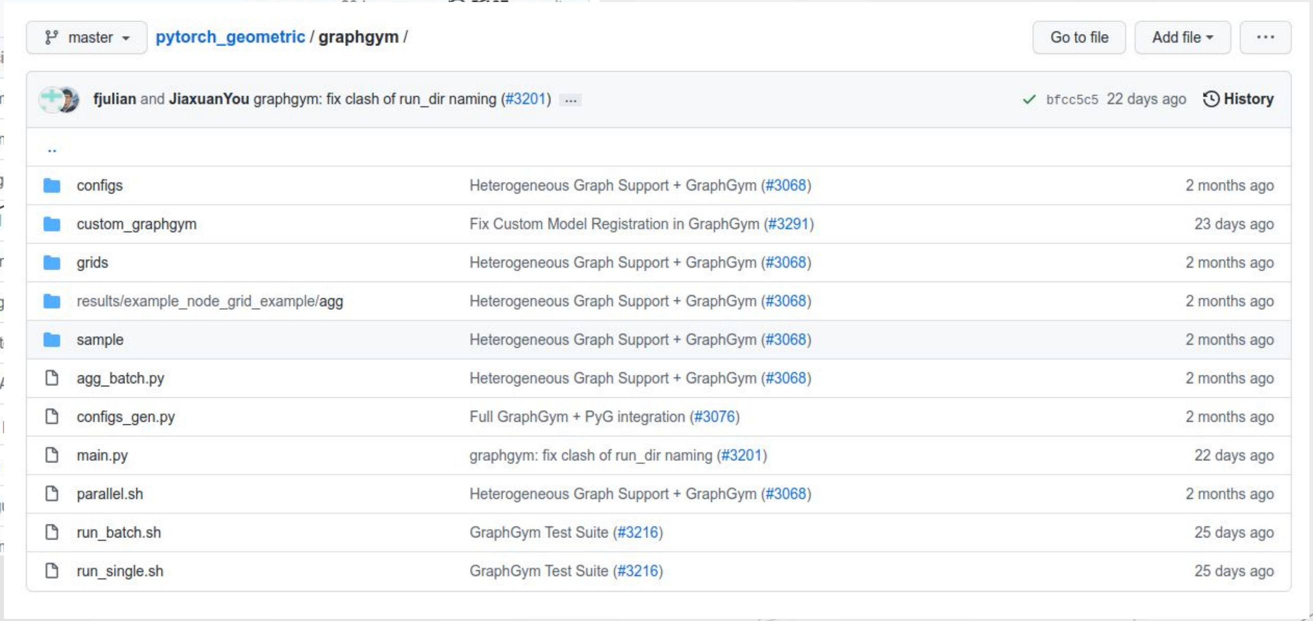

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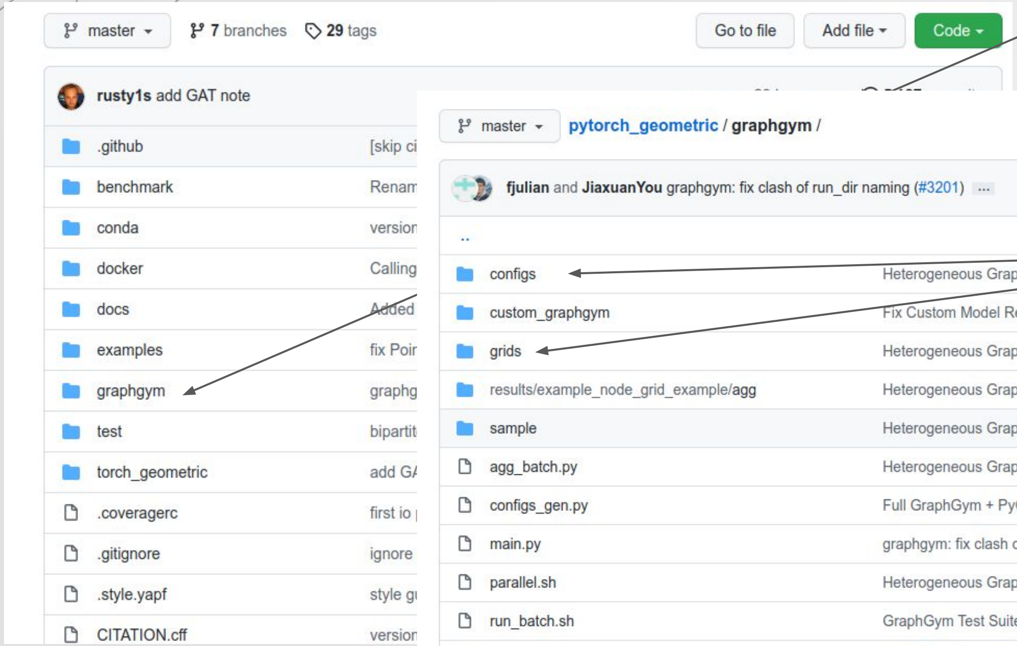
Configurations



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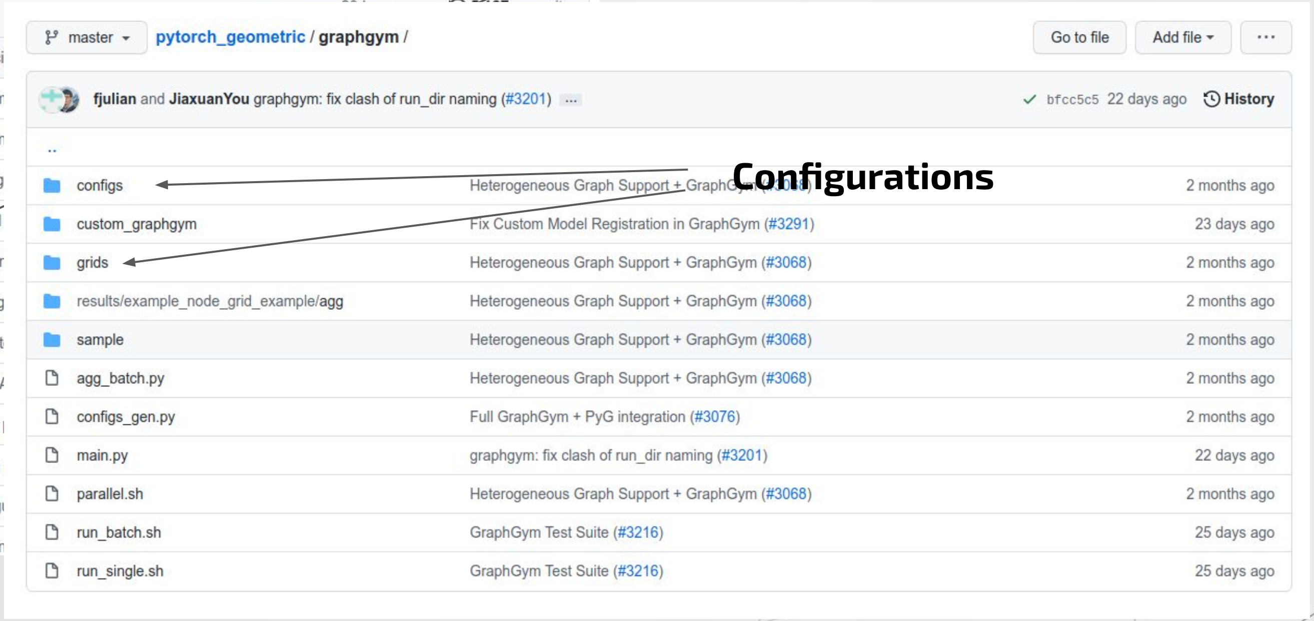

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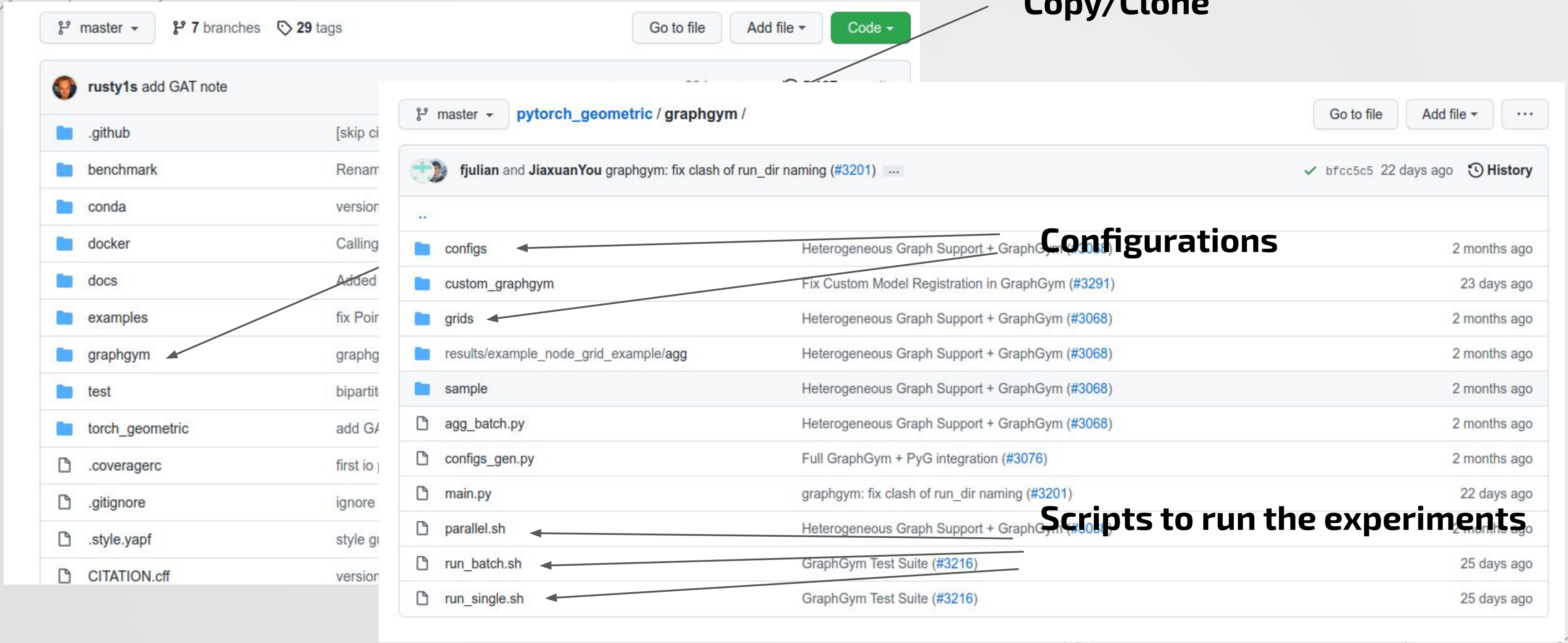

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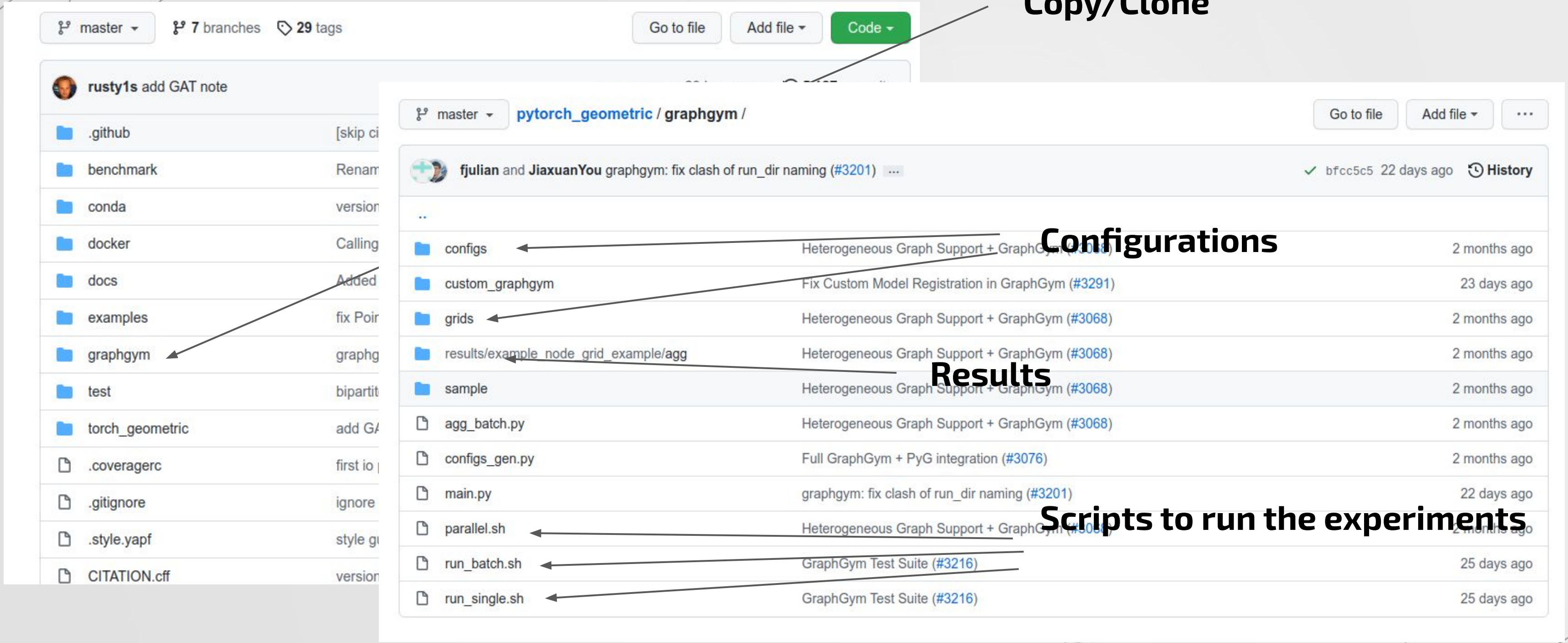
Configurations

Scripts to run the experiments

02 Goals and basic usage



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03 Example: node classification

Run run_single.sh . . .

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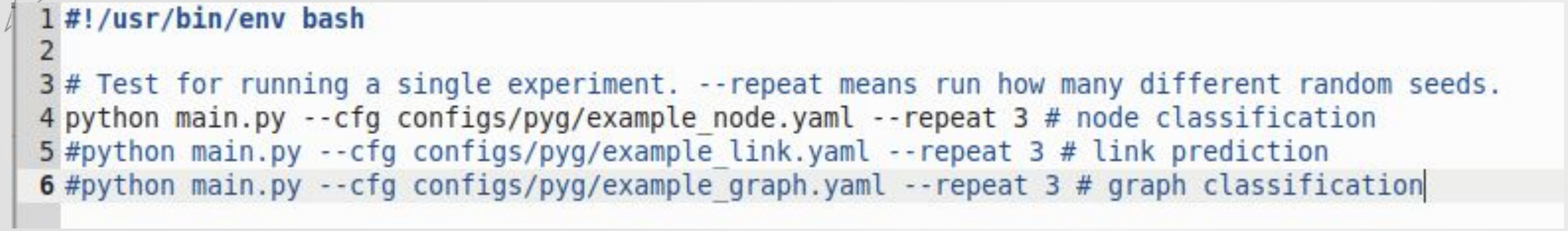

```
#!/usr/bin/env bash

# Test for running a single experiment. --repeat means run how many different random seeds.
python main.py --cfg configs/pyg/example_node.yaml --repeat 3 # node classification
#python main.py --cfg configs/pyg/example_link.yaml --repeat 3 # link prediction
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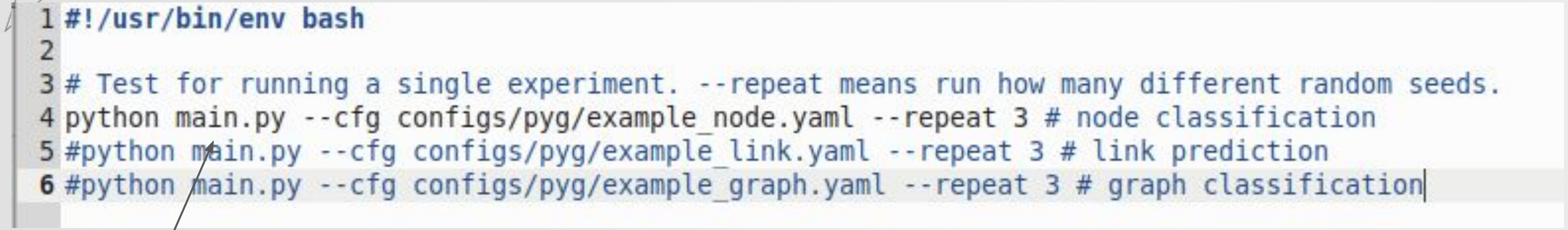

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Base Graph Gym
parsing & execution

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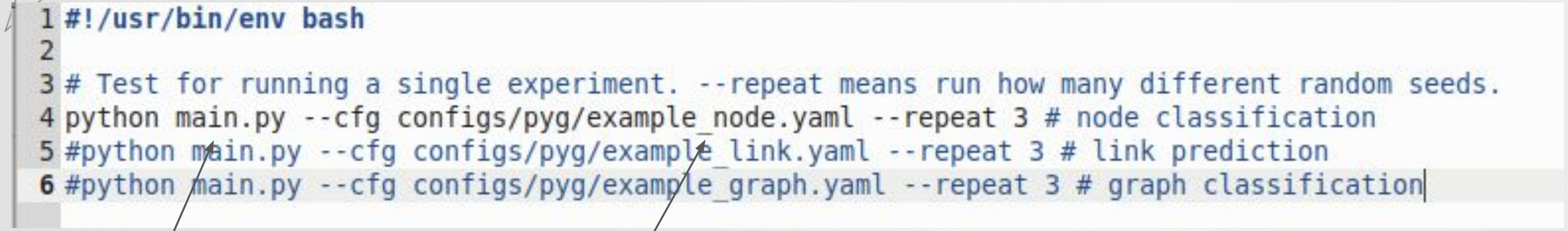

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Base Graph Gym parsing & execution

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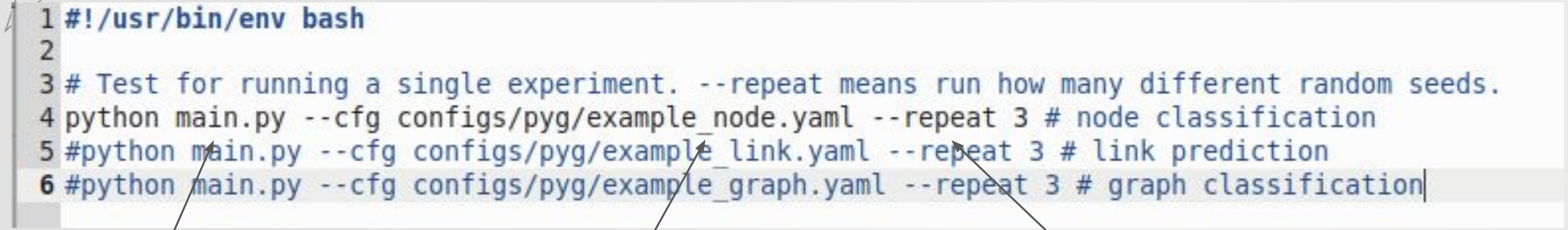

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Base Graph Gym parsing & execution

Configuration file

- define any aspect of the experiment

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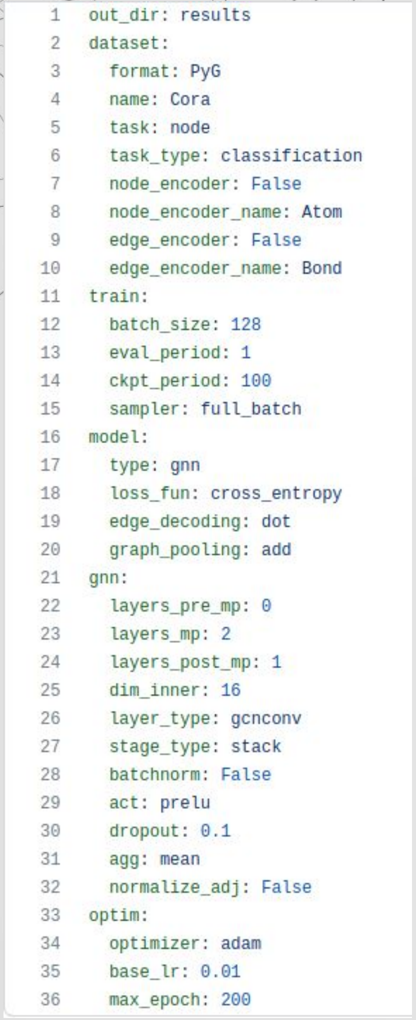
03 Example: node classification

This is configs/pyg/example_node.yaml



```yaml
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
  edge_encoder: False
  edge_encoder_name: Bond
train:
  batch_size: 128
  eval_period: 1
  ckpt_period: 100
  sampler: full_batch
model:
  type: gnn
  loss_fun: cross_entropy
  edge_decoding: dot
  graph_pooling: add
gnn:
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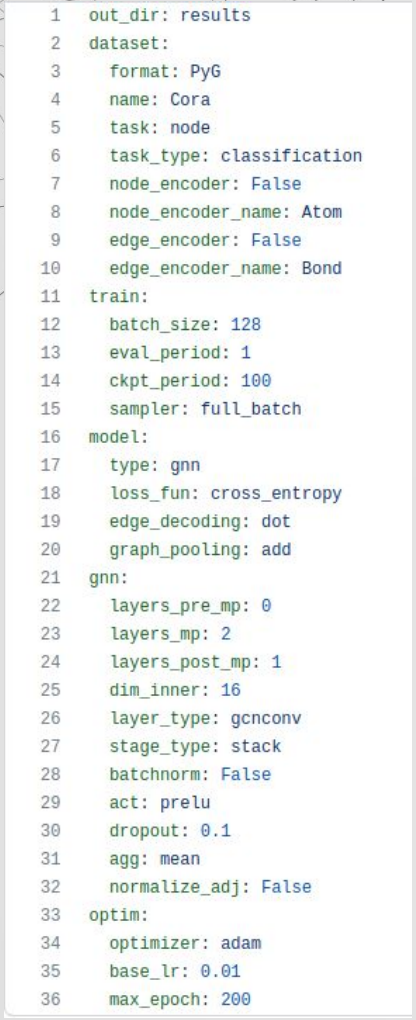

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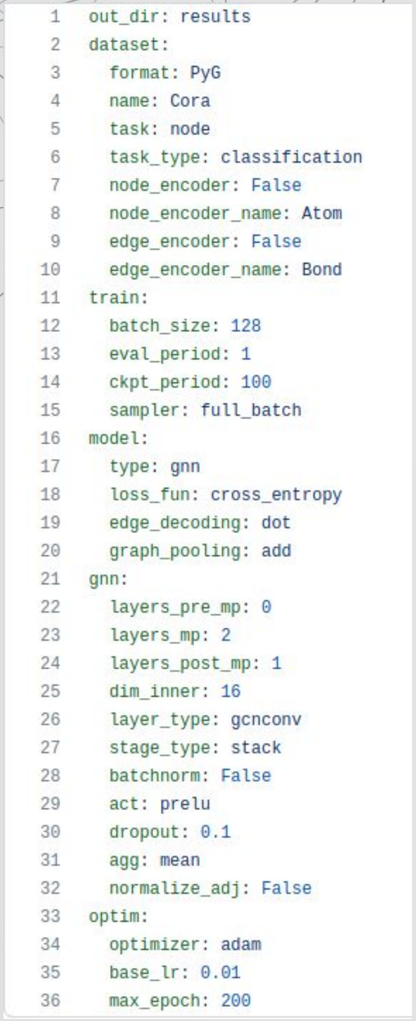

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Warning: In this example some param seem to be useless

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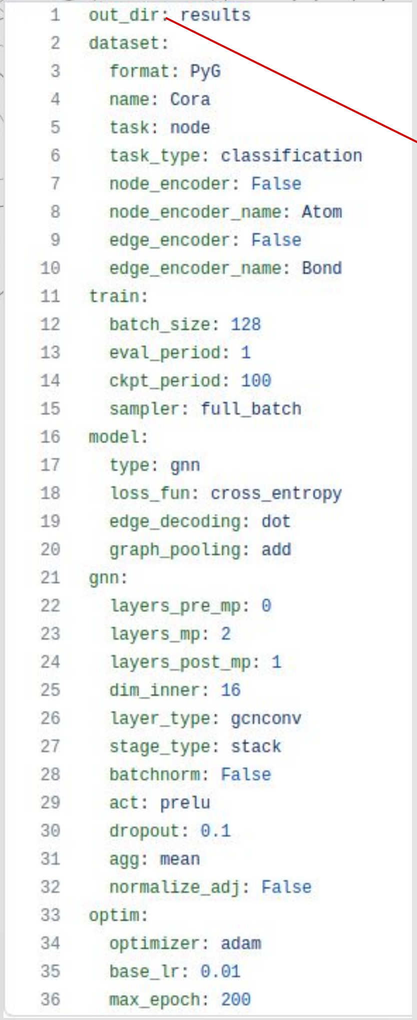

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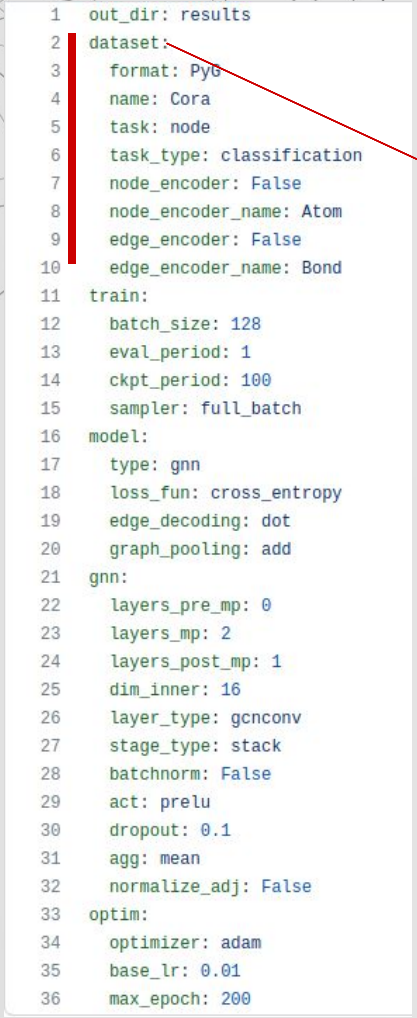
Folder to save the results

03 Example: node classification



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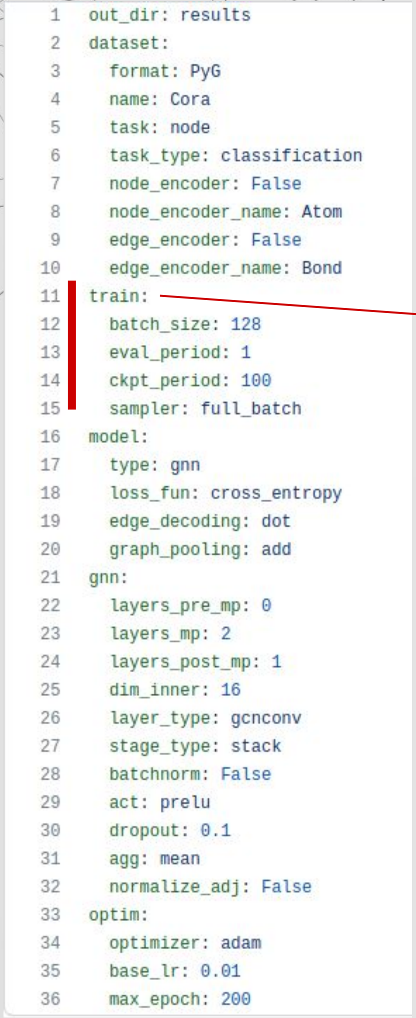
Dataset and task specification

- **format**: PyG, NetworkX
- **name**
- **task**: node, edge, graph, link_pred
- **task_type**: classification, regression, classification_binary
- **node_encoder** / **edge_encoder**: bool, use encoder for node / edge features
- **node_encoder_name**, **edge_encoder_name**

03 Example: node classification



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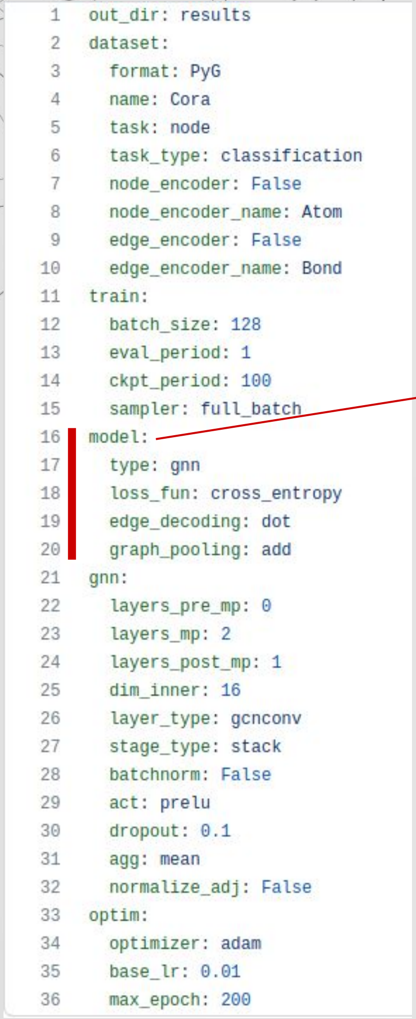
Training parameters

- **batch_size**: graph mini-batch size
- **eval_period:** evaluate on test every # epochs
- **ckpt_period**: save checkpoint every # epochs
- **sampler**: sampling strategy for the train loader

03 Example: node classification



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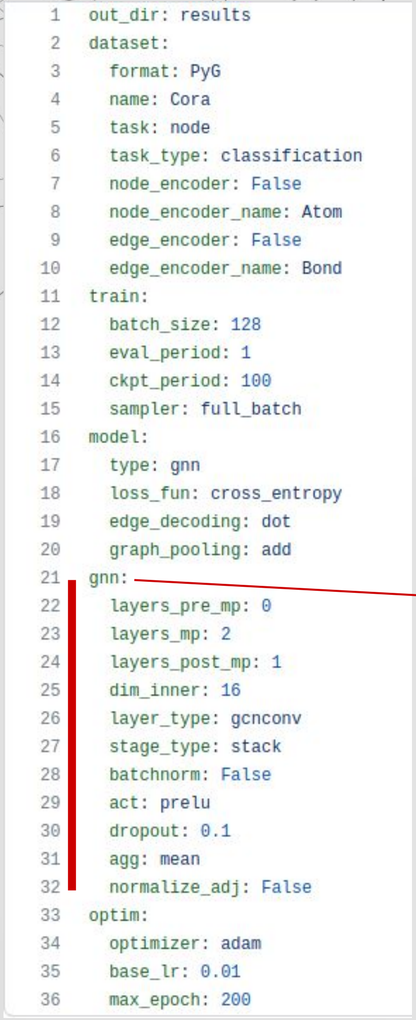
Model specification

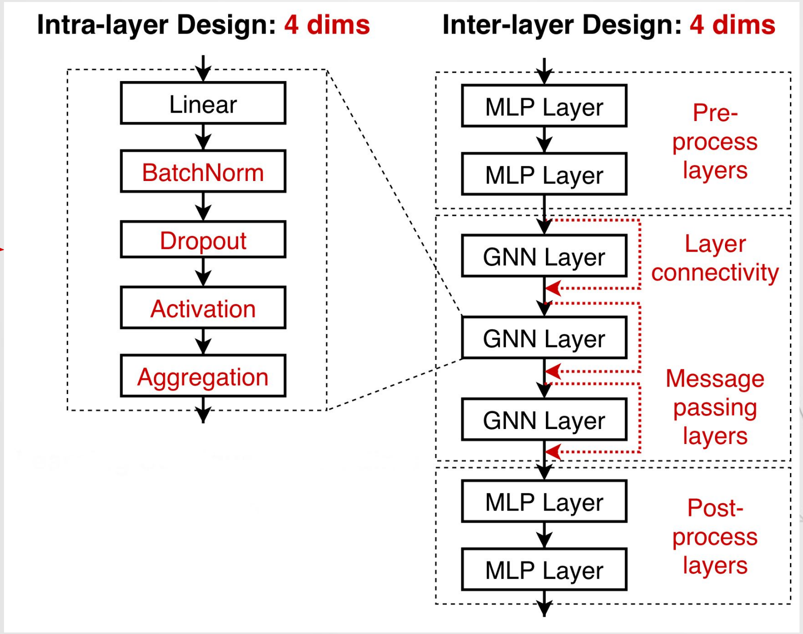
- **type:** gnn
- **loss_fun:** cross_entropy, mse
- **edge_decoding**: dot, cosine_similarity, concat
- **graph_pooling**: add, mean, max

03 Example: node classification

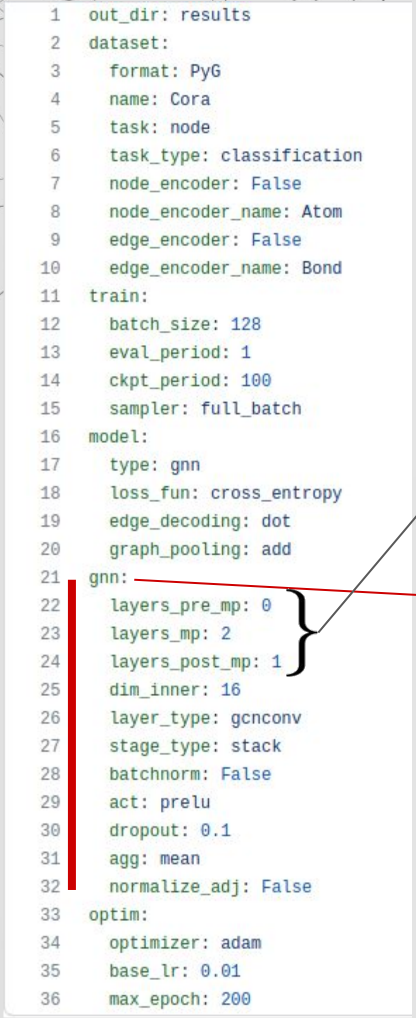


```
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
  edge_encoder: False
  edge_encoder_name: Bond
train:
  batch_size: 128
  eval_period: 1
  ckpt_period: 100
  sampler: full_batch
model:
  type: gnn
  loss_fun: cross_entropy
  edge_decoding: dot
  graph_pooling: add
gnn:
  layers_pre_mp: 0
  layers_mp: 2
  layers_post_mp: 1
  dim_inner: 16
  layer_type: gcnconv
  stage_type: stack
  batchnorm: False
  act: prelu
  dropout: 0.1
  agg: mean
  normalize_adj: False
optim:
  optimizer: adam
  base_lr: 0.01
  max_epoch: 200
```

GNN architecture specification



03 Example: node classification



```
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
  edge_encoder: False
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train:
  batch_size: 128
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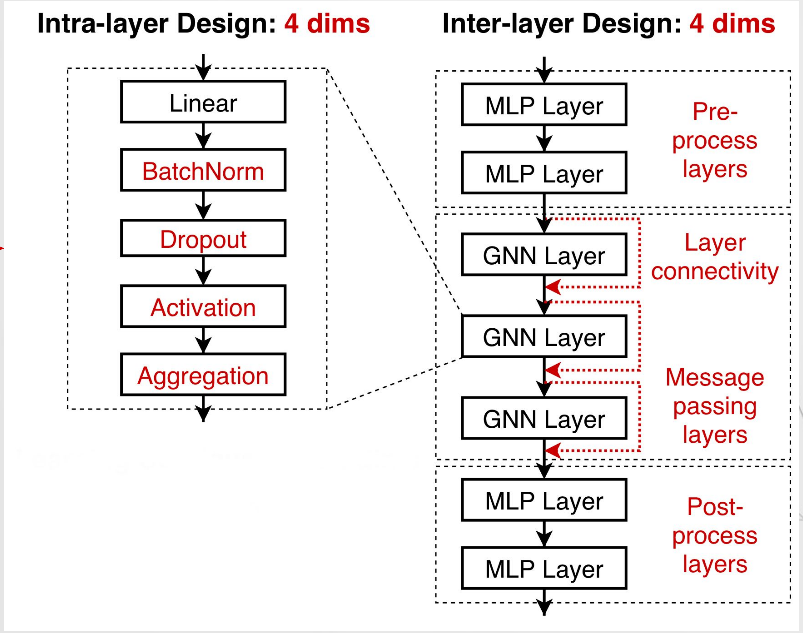
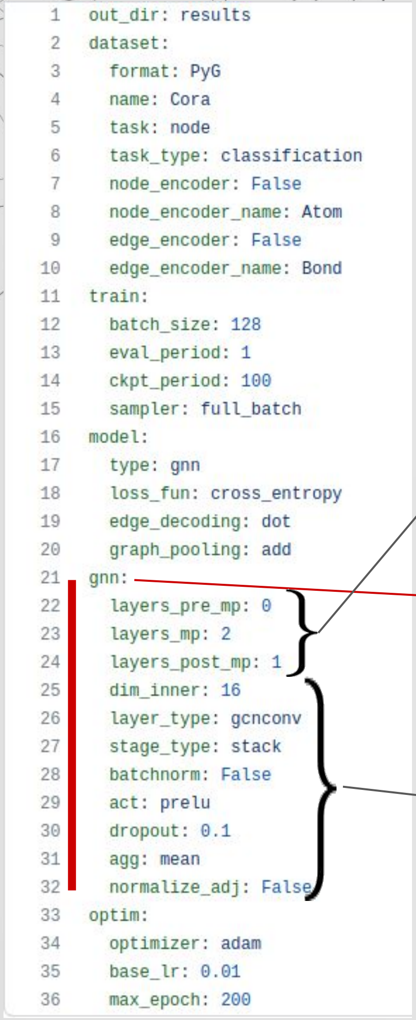
  layer_type: gcnconv
  stage_type: stack
  batchnorm: False
  act: prelu
  dropout: 0.1
  agg: mean
  normalize_adj: False
optim:
  optimizer: adam
  base_lr: 0.01
  max_epoch: 200
```

Number of layers pre/GNN/post

GNN architecture specification



03 Example: node classification



```
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
  edge_encoder: False
  edge_encoder_name: Bond
train:
  batch_size: 128
  eval_period: 1
  ckpt_period: 100
  sampler: full_batch
model:
  type: gnn
  loss_fun: cross_entropy
  edge_decoding: dot
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  layers_pre_mp: 0
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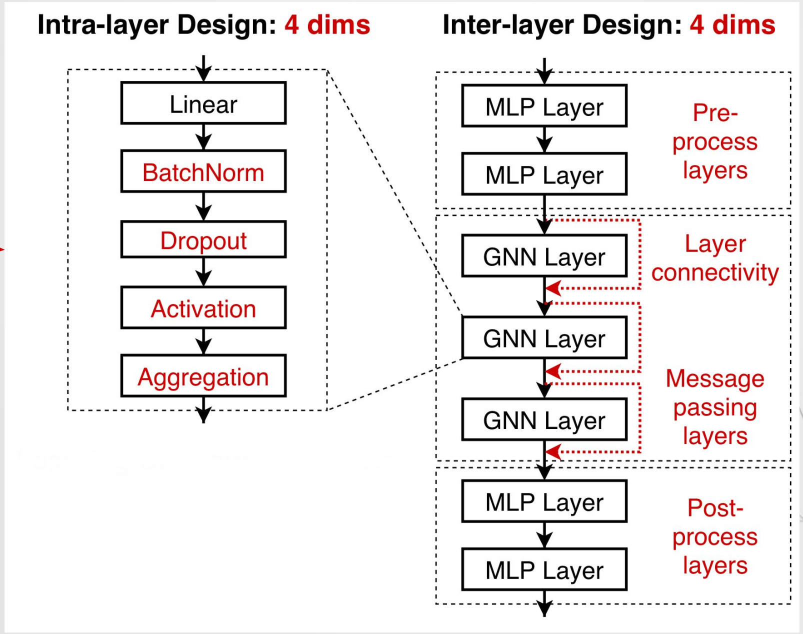
  dim_inner: 16
  layer_type: gcnconv
  stage_type: stack
  batchnorm: False
  act: prelu
  dropout: 0.1
  agg: mean
  normalize_adj: False
optim:
  optimizer: adam
  base_lr: 0.01
  max_epoch: 200
```

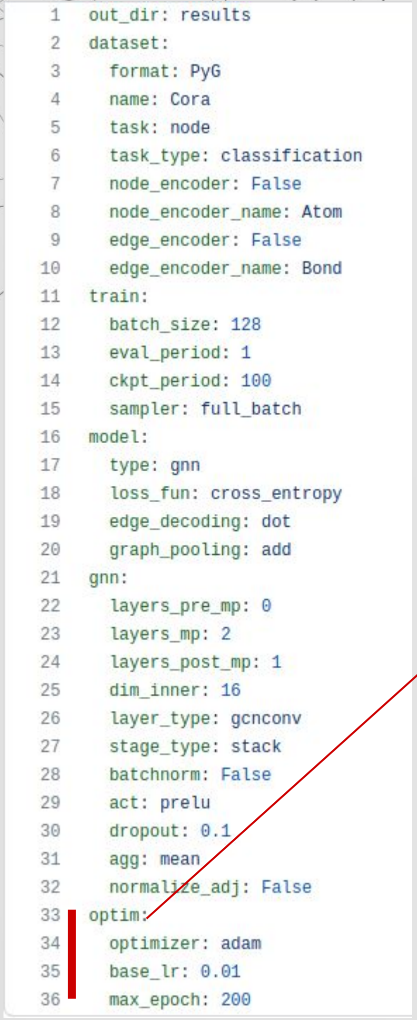
Number of layers pre/GNN/post

GNN options

GNN architecture specification



03 Example: node classification


```
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
  edge_encoder: False
  edge_encoder_name: Bond
train:
  batch_size: 128
  eval_period: 1
  ckpt_period: 100
  sampler: full_batch
model:
  type: gnn
  loss_fun: cross_entropy
  edge_decoding: dot
  graph_pooling: add
gnn:
  layers_pre_mp: 0
  layers_mp: 2
  layers_post_mp: 1
  dim_inner: 16
  layer_type: gcnconv
  stage_type: stack
  batchnorm: False
  act: prelu
  dropout: 0.1
  agg: mean
  normalize_adj: False
optim:
  optimizer: adam
  base_lr: 0.01
  max_epoch: 200
```

Optimization options

- **optimizer:** sgd, adam **CHECK**
- **base_lr**
- **max_epoch**

03 Example: node classification

A bit more work to find all the options:

03 Example: node classification

A bit more work to find all the options:

1. A **list of all** parameters, with explanation and default values is in `torch_geometric.graphgym.set_cfg()`
   - https://pytorch-geometric.readthedocs.io/en/latest/_modules/torch_geometric/graphgym/config.html#set_cfg

2. See also the single modules
   - https://pytorch-geometric.readthedocs.io/en/latest/_modules/index.html
   - https://github.com/pyg-team/pytorch_geometric/tree/master/torch_geometric/graphgym

03 Example: node classification

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There is no automated way to ensure that every option that is available in 2) is also listed in 1)

03 Example: node classification

A bit more work to find all the options:

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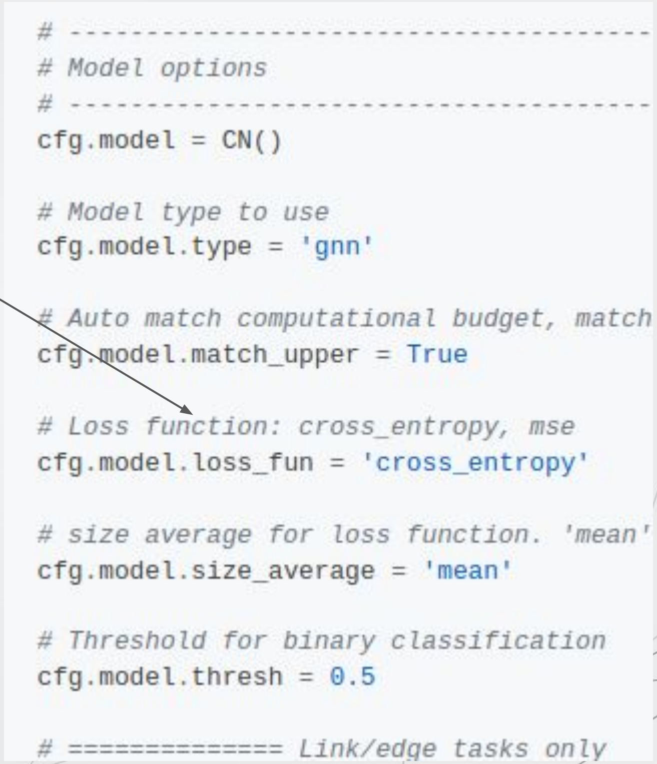
2. See also the single modules
   - https://pytorch-geometric.readthedocs.io/en/latest/_modules/index.html
   - https://github.com/pyg-team/pytorch_geometric/tree/master/torch_geometric/graphgym

There is no automated way to ensure that every option that is available in 2) is also listed in 1)



```
# ----------------------------------------
# Model options
# ----------------------------------------
cfg.model = CN()

# Model type to use
cfg.model.type = 'gnn'

# Auto match computational budget, match
cfg.model.match_upper = True

# Loss function: cross_entropy, mse
cfg.model.loss_fun = 'cross_entropy'

# size average for loss function. 'mean'
cfg.model.size_average = 'mean'

# Threshold for binary classification
cfg.model.thresh = 0.5

# ============== Link/edge tasks only
```

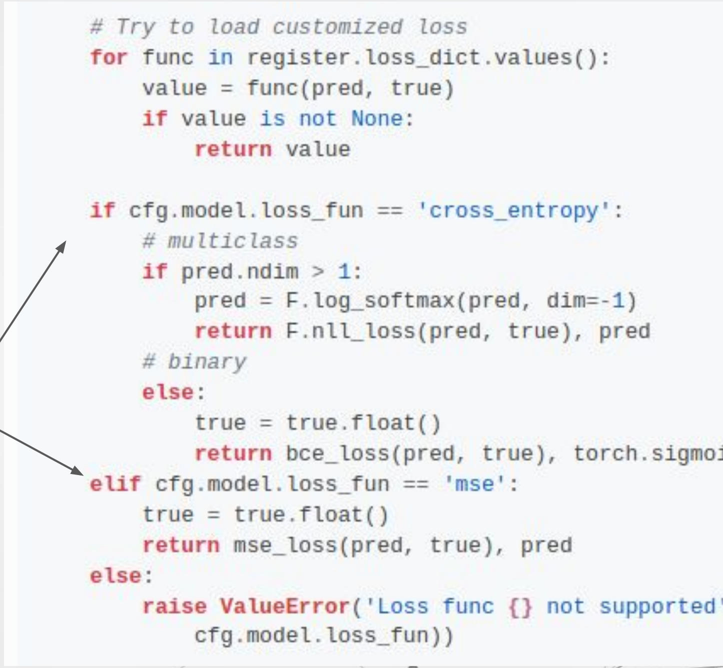
03 Example: node classification

A bit more work to find all the options:

1. A **list of all** parameters, with explanation and default values is in `torch_geometric.graphgym.set_cfg()`
   - https://pytorch-geometric.readthedocs.io/en/latest/_modules/torch_geometric/graphgym/config.html#set_cfg

2. See also the single modules
   - https://pytorch-geometric.readthedocs.io/en/latest/_modules/index.html
   - https://github.com/pyg-team/pytorch_geometric/tree/master/torch_geometric/graphgym

There is no automated way to ensure that every option that is available in 2) is also listed in 1)



```
# Try to load customized loss
for func in register.loss_dict.values():
    value = func(pred, true)
    if value is not None:
        return value

if cfg.model.loss_fun == 'cross_entropy':
    # multiclass
    if pred.ndim > 1:
        pred = F.log_softmax(pred, dim=-1)
        return F.nll_loss(pred, true), pred
    # binary
    else:
        true = true.float()
        return bce_loss(pred, true), torch.sigmoi
elif cfg.model.loss_fun == 'mse':
    true = true.float()
    return mse_loss(pred, true), pred
else:
    raise ValueError('Loss func {} not supported'
        cfg.model.loss_fun))
```

torch_geometric.graphgym.loss

03 Example: node classification

Results written in results/${CONFIG_NAME}/

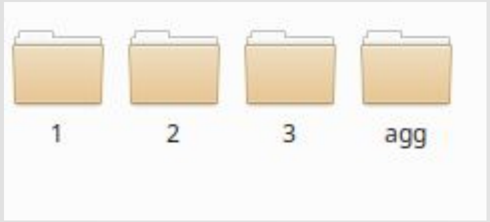
results/example_node/

03 Example: node classification

Results written in results/${CONFIG_NAME}/

$\uparrow$

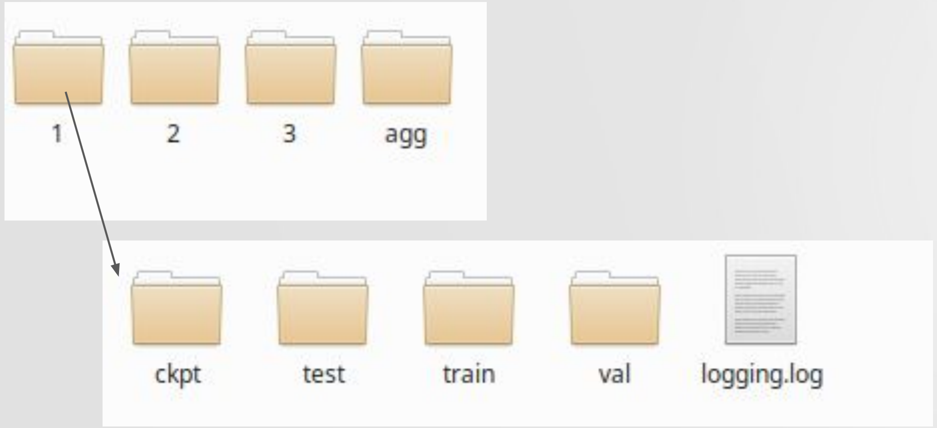
results/example_node/



03 Example: node classification

Results written in results/${CONFIG_NAME}/

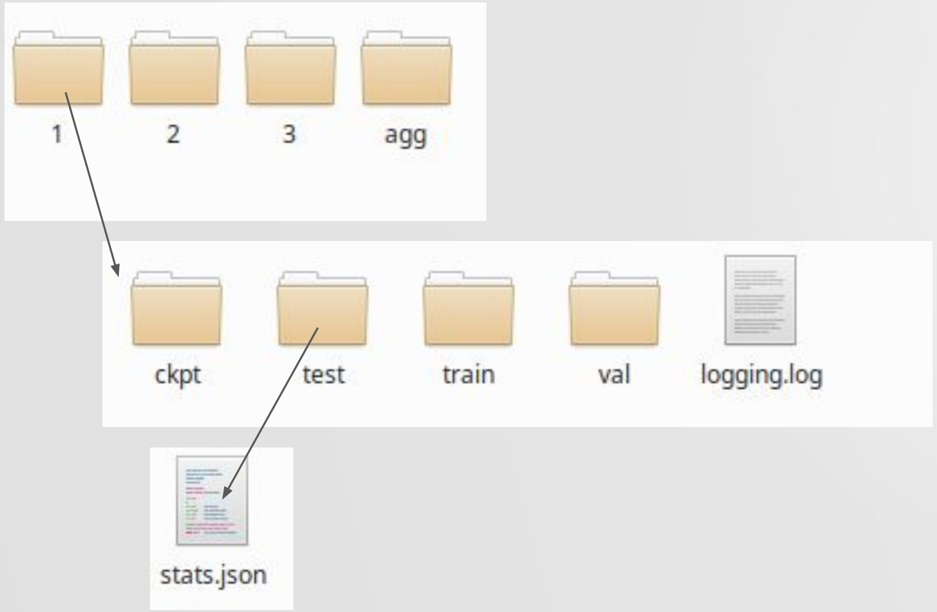
results/example_node/



03 Example: node classification

Results written in results/${CONFIG_NAME}/

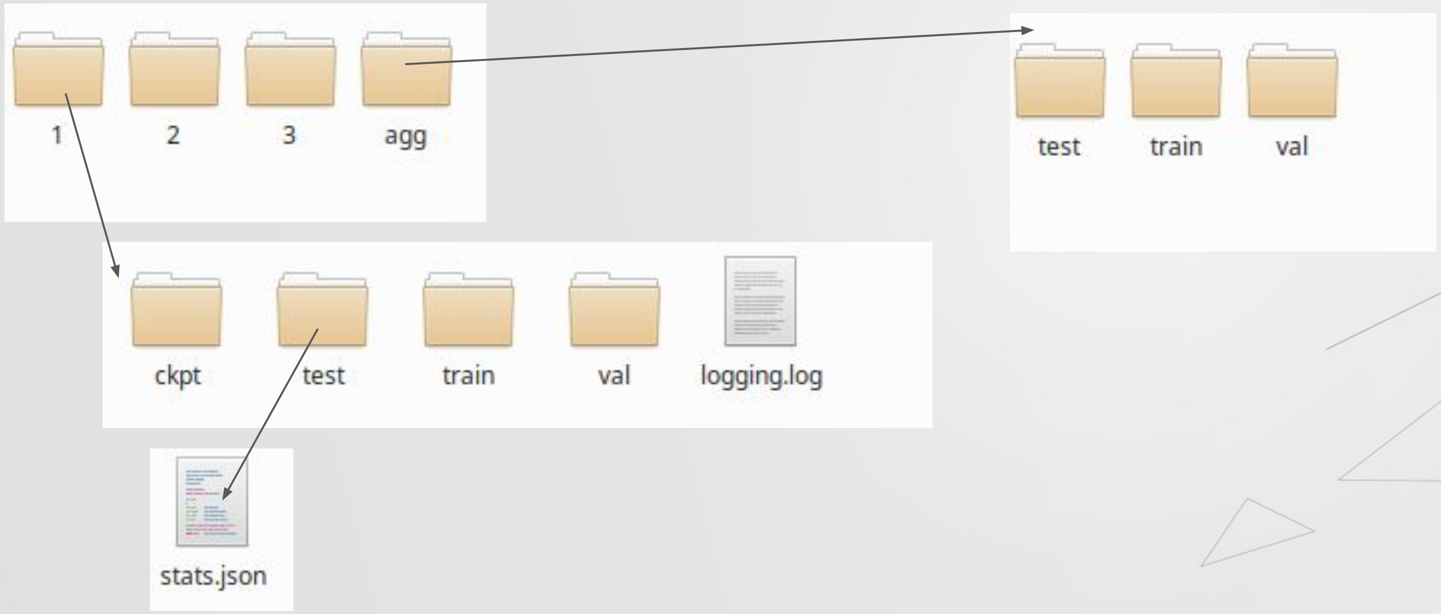
results/example_node/



03 Example: node classification

Results written in results/${CONFIG_NAME}/

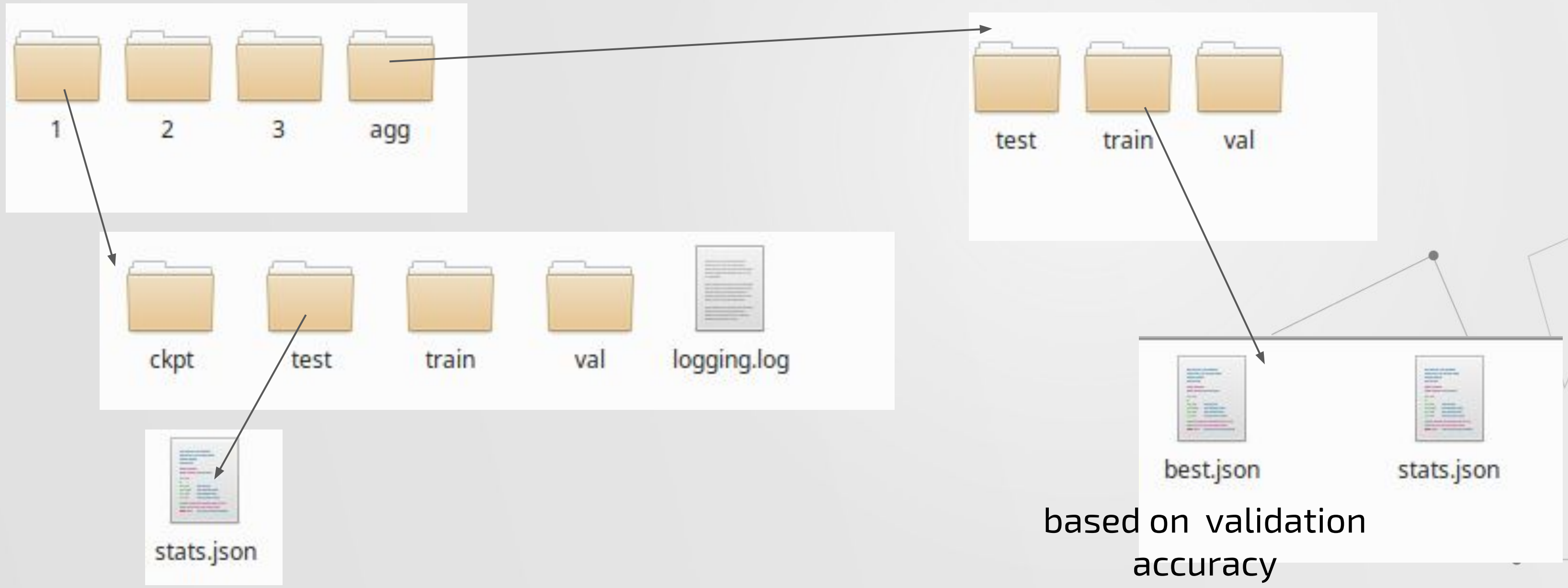
results/example_node/



03 Example: node classification

Results written in results/${CONFIG_NAME}/

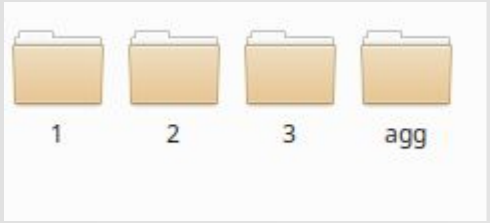
results/example_node/



03 Example: node classification

Results written in results/${CONFIG_NAME}/

results/example_node/



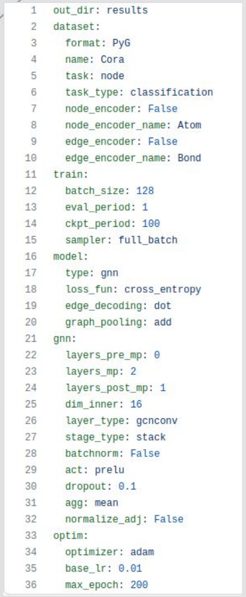
Let's **check** this . . .

04 Example: batch training

Idea define multiple experiments by perturbing a base config file

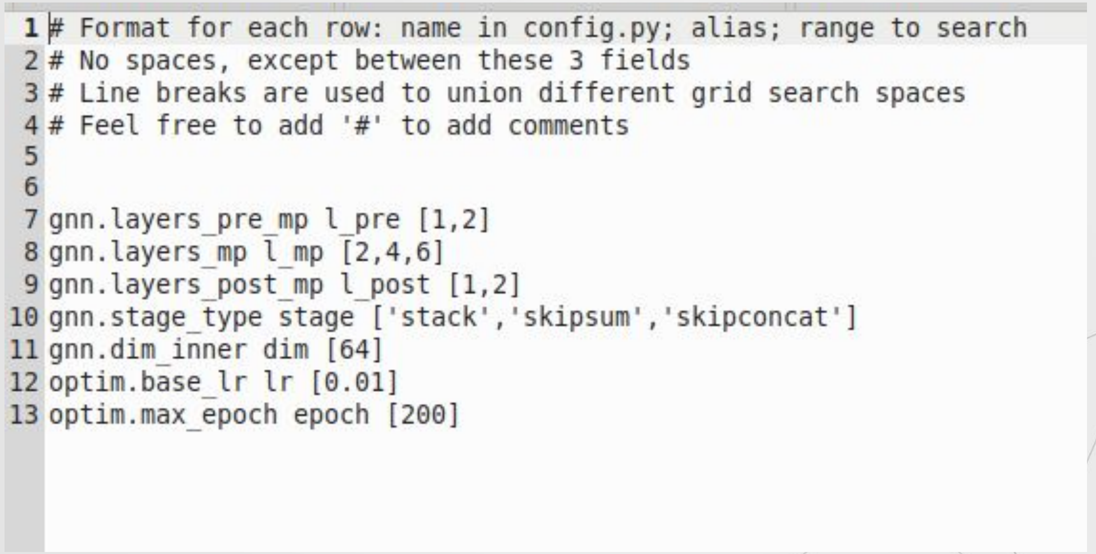
04 Example: batch training

Idea define multiple experiments by perturbing a base config file



```yaml
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
  edge_encoder: False
  edge_encoder_name: Bond
train:
  batch_size: 128
  eval_period: 1
  ckpt_period: 100
  sampler: full_batch
model:
  type: gnn
  loss_fun: cross_entropy
  edge_decoding: dot
  graph_pooling: add
gnn:
  layers_pre_mp: 0
  layers_mp: 2
  layers_post_mp: 1
  dim_inner: 16
  layer_type: gcnconv
  stage_type: stack
  batchnorm: False
  act: prelu
  dropout: 0.1
  agg: mean
  normalize_adj: False
optim:
  optimizer: adam
  base_lr: 0.01
  max_epoch: 200
```

+



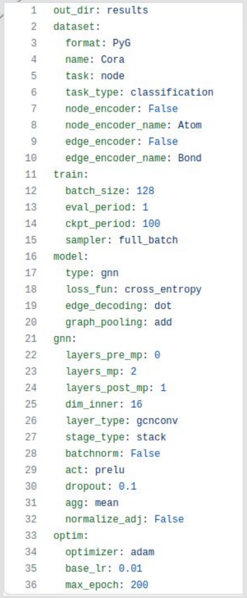
```
# Format for each row: name in config.py; alias; range to search
# No spaces, except between these 3 fields
# Line breaks are used to union different grid search spaces
# Feel free to add '#' to add comments


gnn.layers_pre_mp l_pre [1,2]
gnn.layers_mp l_mp [2,4,6]
gnn.layers_post_mp l_post [1,2]
gnn.stage_type stage ['stack','skipsum','skipconcat']
gnn.dim_inner dim [64]
optim.base_lr lr [0.01]
optim.max_epoch epoch [200]
```

configs/pyg/example_node.yaml

grids/pyg/example.txt

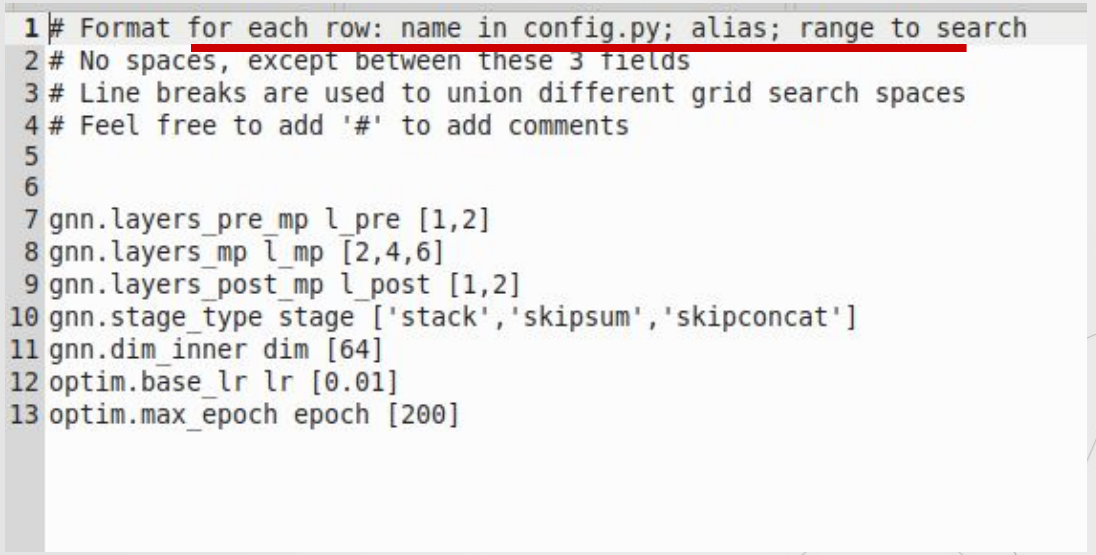
04 Example: batch training

Idea define multiple experiments by perturbing a base config file



```yaml
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
  edge_encoder: False
  edge_encoder_name: Bond
train:
  batch_size: 128
  eval_period: 1
  ckpt_period: 100
  sampler: full_batch
model:
  type: gnn
  loss_fun: cross_entropy
  edge_decoding: dot
  graph_pooling: add
gnn:
  layers_pre_mp: 0
  layers_mp: 2
  layers_post_mp: 1
  dim_inner: 16
  layer_type: gcnconv
  stage_type: stack
  batchnorm: False
  act: prelu
  dropout: 0.1
  agg: mean
  normalize_adj: False
optim:
  optimizer: adam
  base_lr: 0.01
  max_epoch: 200
```

+



```
# Format for each row: name in config.py; alias; range to search
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gnn.layers_pre_mp l_pre [1,2]
gnn.layers_mp l_mp [2,4,6]
gnn.layers_post_mp l_post [1,2]
gnn.stage_type stage ['stack','skipsum','skipconcat']
gnn.dim_inner dim [64]
optim.base_lr lr [0.01]
optim.max_epoch epoch [200]
```
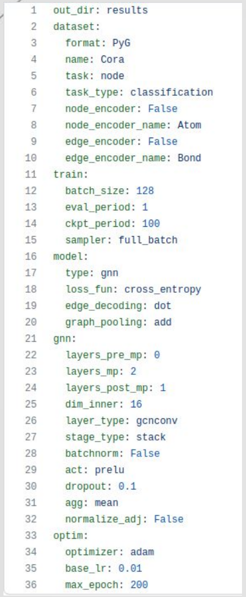

configs/pyg/example_node.yaml

grids/pyg/example.txt

04 Example: batch training

Idea define multiple experiments by perturbing a base config file



```
out_dir: results
dataset:
  format: PyG
  name: Cora
  task: node
  task_type: classification
  node_encoder: False
  node_encoder_name: Atom
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  edge_encoder_name: Bond
train:
  batch_size: 128
  eval_period: 1
  ckpt_period: 100
  sampler: full_batch
model:
  type: gnn
  loss_fun: cross_entropy
  edge_decoding: dot
  graph_pooling: add
gnn:
  layers_pre_mp: 0
  layers_mp: 2
  layers_post_mp: 1
  dim_inner: 16
  layer_type: gcnconv
  stage_type: stack
  batchnorm: False
  act: prelu
  dropout: 0.1
  agg: mean
  normalize_adj: False
optim:
  optimizer: adam
  base_lr: 0.01
  max_epoch: 200
```
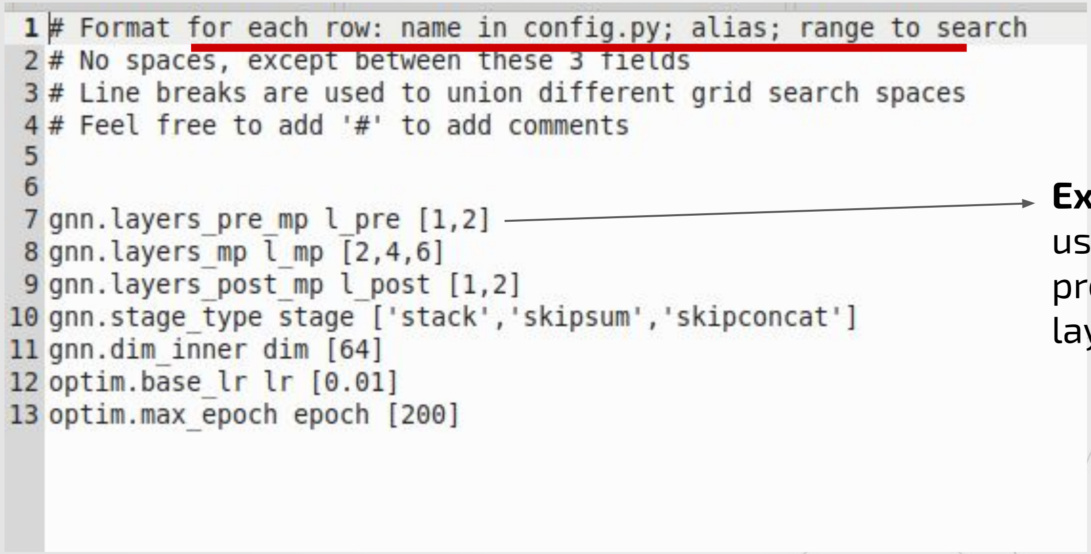

configs/pyg/example_node.yaml

+



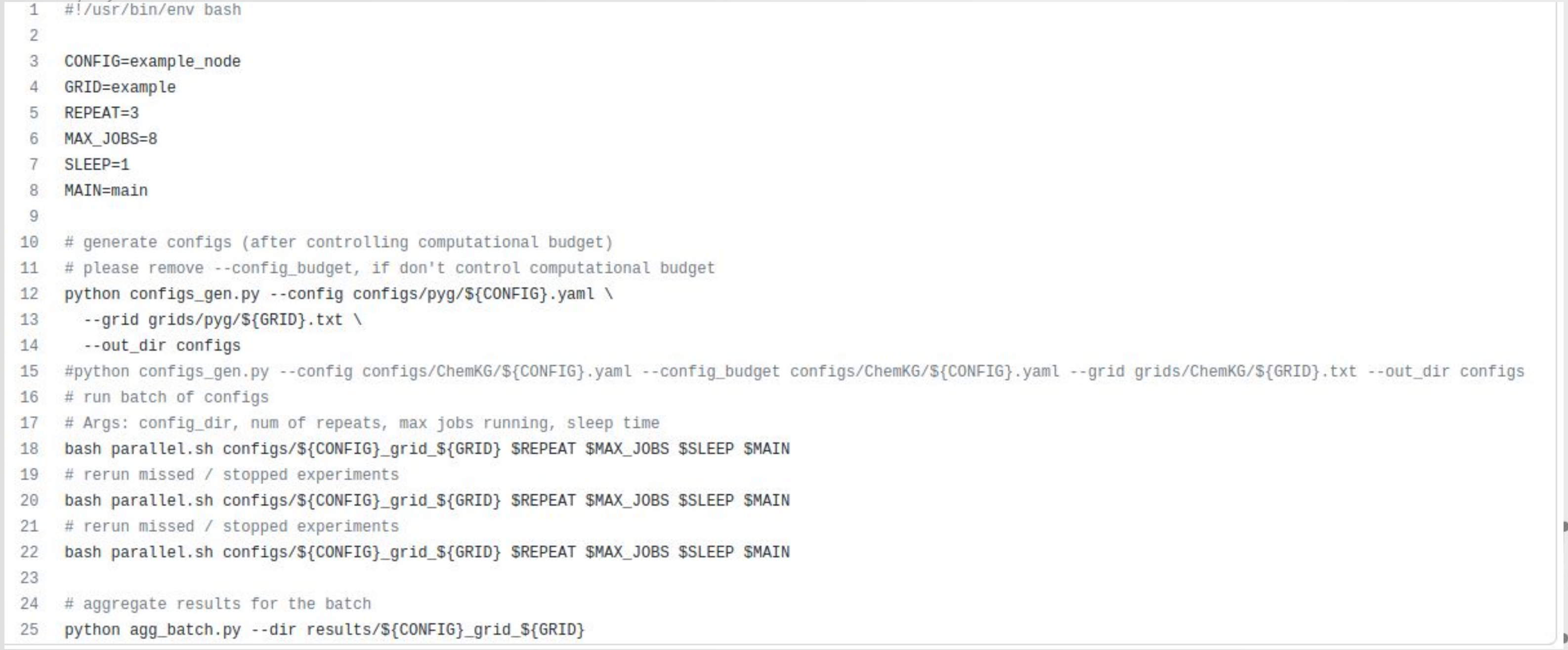
```
# Format for each row: name in config.py; alias; range to search
# No spaces, except between these 3 fields
# Line breaks are used to union different grid search spaces
# Feel free to add '#' to add comments


gnn.layers_pre_mp l_pre [1,2]
gnn.layers_mp l_mp [2,4,6]
gnn.layers_post_mp l_post [1,2]
gnn.stage_type stage ['stack','skipsum','skipconcat']
gnn.dim_inner dim [64]
optim.base_lr lr [0.01]
optim.max_epoch epoch [200]
```

Example:
use 1 or 2 preprocessing layers

grids/pyg/example.txt

04 Example: batch training

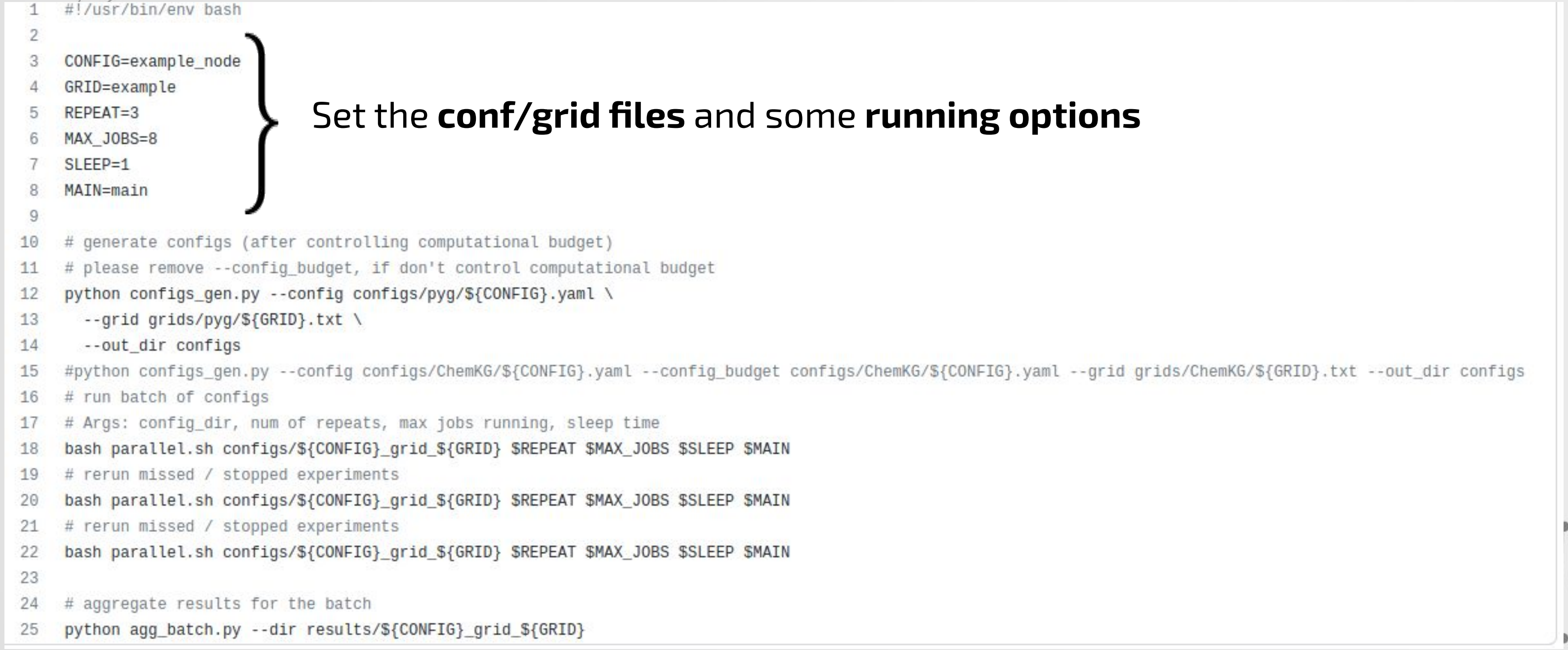
Run run_batch.sh . . .



```bash
#!/usr/bin/env bash

CONFIG=example_node
GRID=example
REPEAT=3
MAX_JOBS=8
SLEEP=1
MAIN=main

# generate configs (after controlling computational budget)
# please remove --config_budget, if don't control computational budget
python configs_gen.py --config configs/pyg/${CONFIG}.yaml \
  --grid grids/pyg/${GRID}.txt \
  --out_dir configs
#python configs_gen.py --config configs/ChemKG/${CONFIG}.yaml --config_budget configs/ChemKG/${CONFIG}.yaml --grid grids/ChemKG/${GRID}.txt --out_dir configs
# run batch of configs
# Args: config_dir, num of repeats, max jobs running, sleep time
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN

# aggregate results for the batch
python agg_batch.py --dir results/${CONFIG}_grid_${GRID}
```

04 Example: batch training

Run run_batch.sh . . .

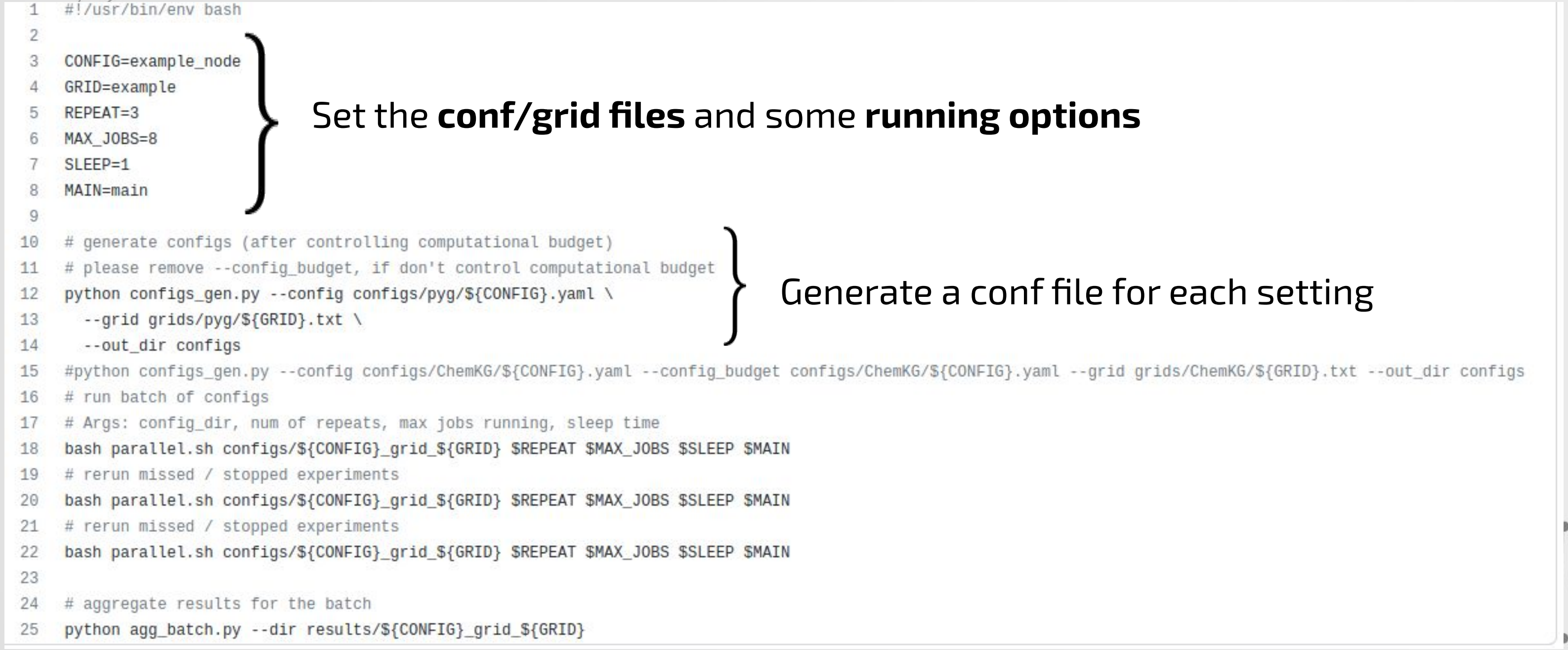


```bash
#!/usr/bin/env bash

CONFIG=example_node
GRID=example
REPEAT=3
MAX_JOBS=8
SLEEP=1
MAIN=main

# generate configs (after controlling computational budget)
# please remove --config_budget, if don't control computational budget
python configs_gen.py --config configs/pyg/${CONFIG}.yaml \
  --grid grids/pyg/${GRID}.txt \
  --out_dir configs
#python configs_gen.py --config configs/ChemKG/${CONFIG}.yaml --config_budget configs/ChemKG/${CONFIG}.yaml --grid grids/ChemKG/${GRID}.txt --out_dir configs
# run batch of configs
# Args: config_dir, num of repeats, max jobs running, sleep time
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN

# aggregate results for the batch
python agg_batch.py --dir results/${CONFIG}_grid_${GRID}
```

Set the **conf/grid files** and some **running options**

04 Example: batch training

Run run_batch.sh . . .



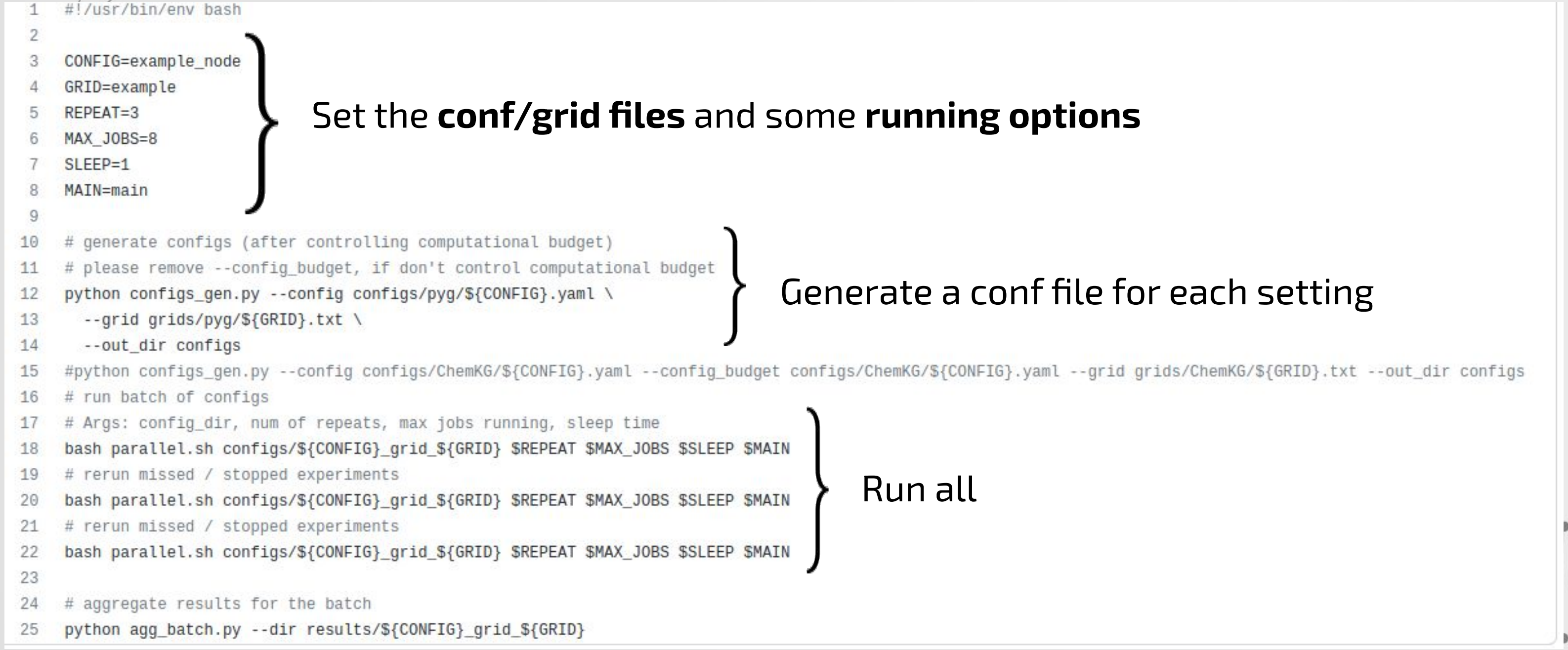
```
#!/usr/bin/env bash

CONFIG=example_node
GRID=example
REPEAT=3
MAX_JOBS=8
SLEEP=1
MAIN=main

# generate configs (after controlling computational budget)
# please remove --config_budget, if don't control computational budget
python configs_gen.py --config configs/pyg/${CONFIG}.yaml \
  --grid grids/pyg/${GRID}.txt \
  --out_dir configs
#python configs_gen.py --config configs/ChemKG/${CONFIG}.yaml --config_budget configs/ChemKG/${CONFIG}.yaml --grid grids/ChemKG/${GRID}.txt --out_dir configs
# run batch of configs
# Args: config_dir, num of repeats, max jobs running, sleep time
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN

# aggregate results for the batch
python agg_batch.py --dir results/${CONFIG}_grid_${GRID}
```

Set the **conf/grid files** and some **running options**

Generate a conf file for each setting

04 Example: batch training

Run run_batch.sh . . .



```
#!/usr/bin/env bash

CONFIG=example_node
GRID=example
REPEAT=3
MAX_JOBS=8
SLEEP=1
MAIN=main

# generate configs (after controlling computational budget)
# please remove --config_budget, if don't control computational budget
python configs_gen.py --config configs/pyg/${CONFIG}.yaml \
  --grid grids/pyg/${GRID}.txt \
  --out_dir configs
#python configs_gen.py --config configs/ChemKG/${CONFIG}.yaml --config_budget configs/ChemKG/${CONFIG}.yaml --grid grids/ChemKG/${GRID}.txt --out_dir configs
# run batch of configs
# Args: config_dir, num of repeats, max jobs running, sleep time
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN

# aggregate results for the batch
python agg_batch.py --dir results/${CONFIG}_grid_${GRID}
```

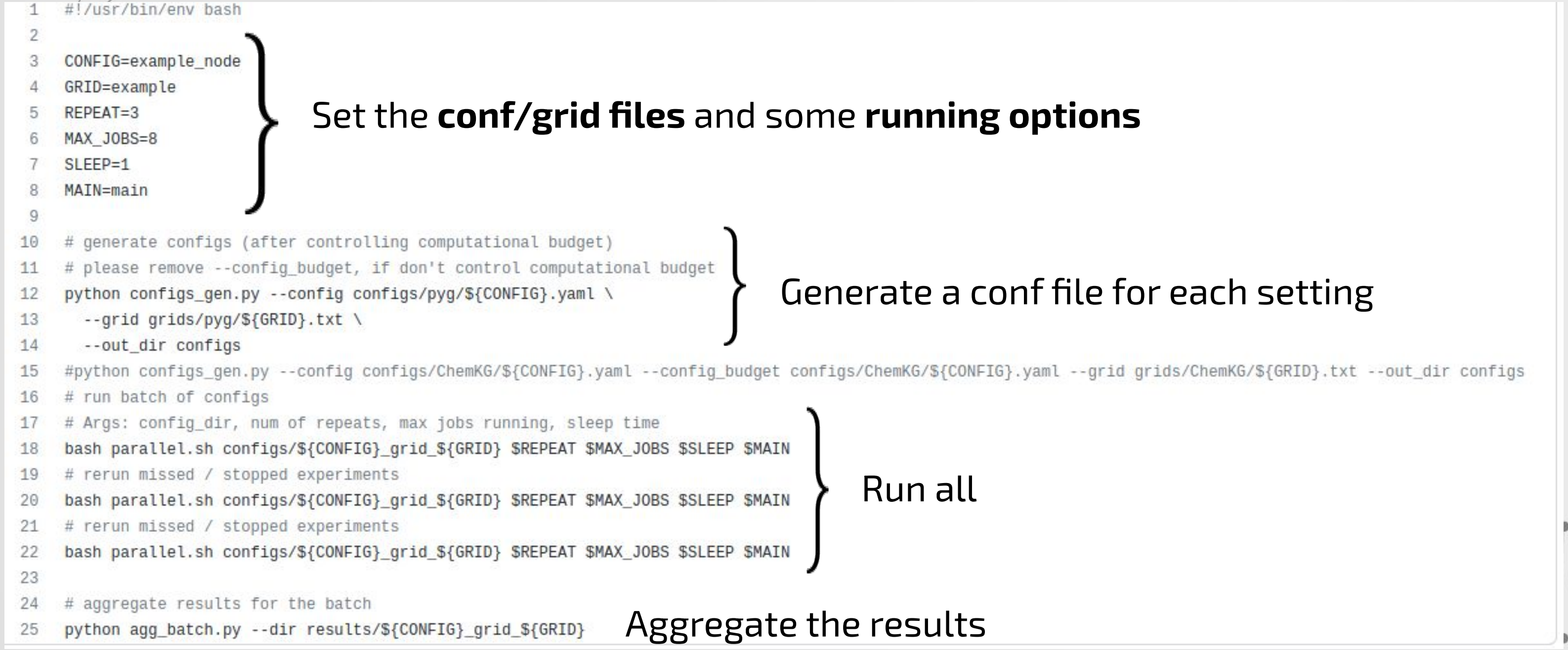
Set the **conf/grid files** and some **running options**

Generate a conf file for each setting

Run all

04 Example: batch training

Run run_batch.sh . . .



```bash
#!/usr/bin/env bash

CONFIG=example_node
GRID=example
REPEAT=3
MAX_JOBS=8
SLEEP=1
MAIN=main

# generate configs (after controlling computational budget)
# please remove --config_budget, if don't control computational budget
python configs_gen.py --config configs/pyg/${CONFIG}.yaml \
  --grid grids/pyg/${GRID}.txt \
  --out_dir configs
#python configs_gen.py --config configs/ChemKG/${CONFIG}.yaml --config_budget configs/ChemKG/${CONFIG}.yaml --grid grids/ChemKG/${GRID}.txt --out_dir configs
# run batch of configs
# Args: config_dir, num of repeats, max jobs running, sleep time
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN
# rerun missed / stopped experiments
bash parallel.sh configs/${CONFIG}_grid_${GRID} $REPEAT $MAX_JOBS $SLEEP $MAIN

# aggregate results for the batch
python agg_batch.py --dir results/${CONFIG}_grid_${GRID}
```

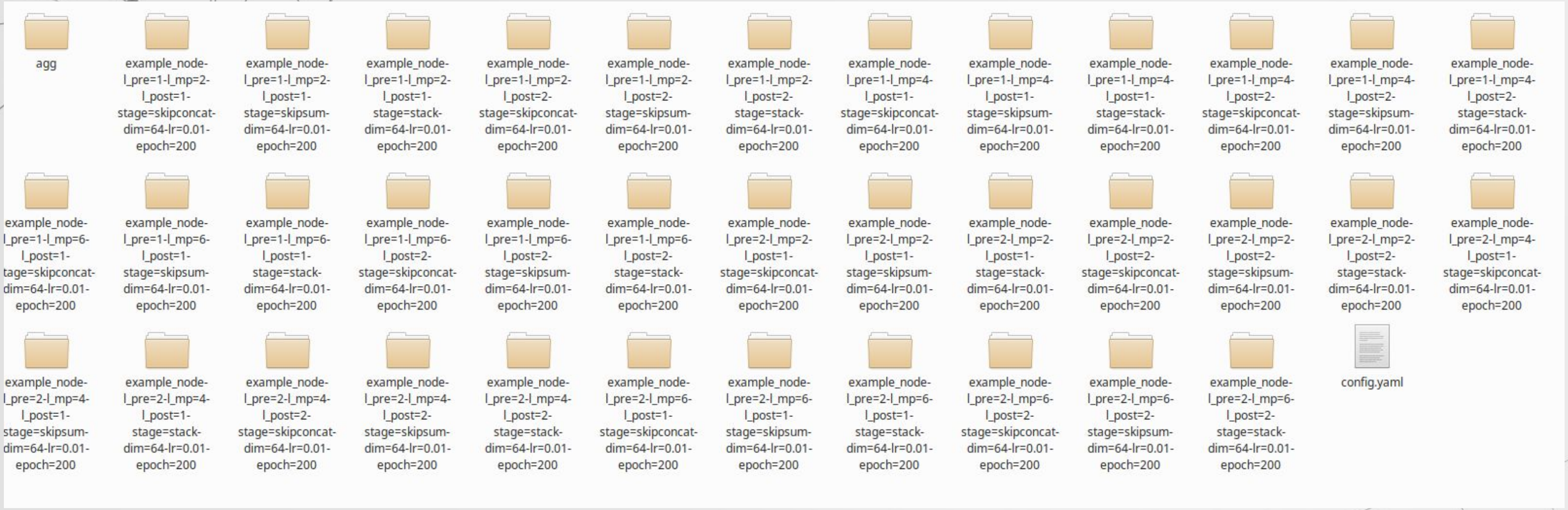
Set the **conf/grid files** and some **running options**

Generate a conf file for each setting

Run all

Aggregate the results

04 Example: batch training



agg

example_node-l_pre=1-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=4-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=6-l_post=1-tage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=1-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=4-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=6-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200

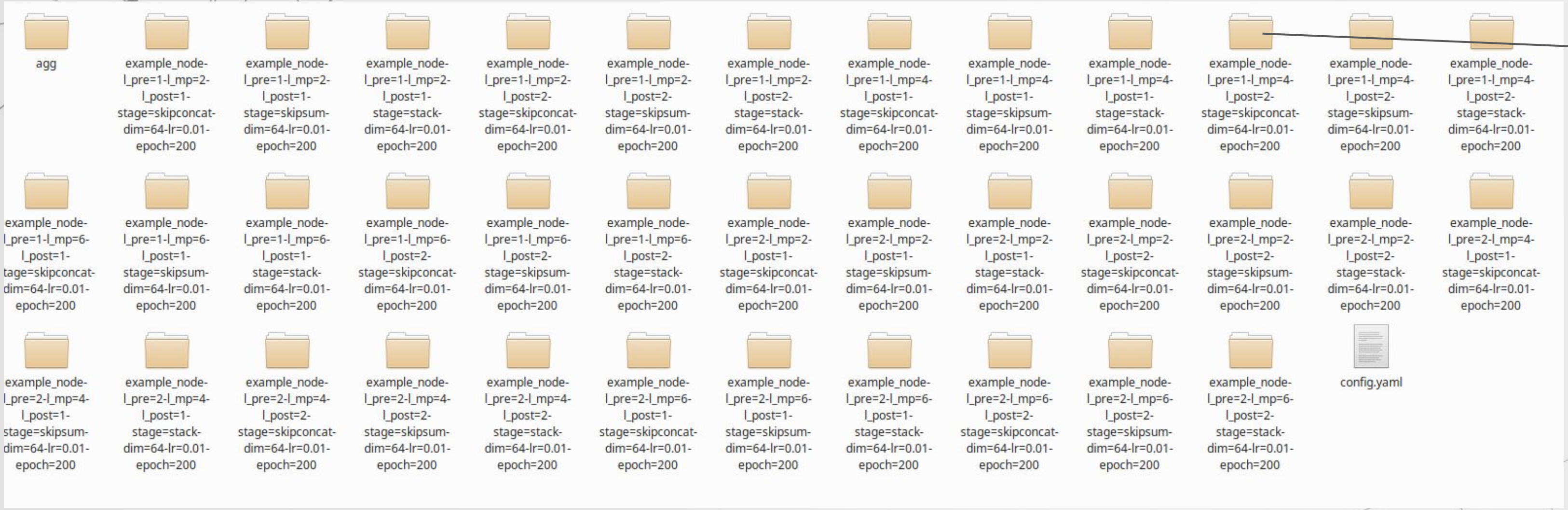
example_node-l_pre=2-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200

example_node-l_pre=2-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200

config.yaml

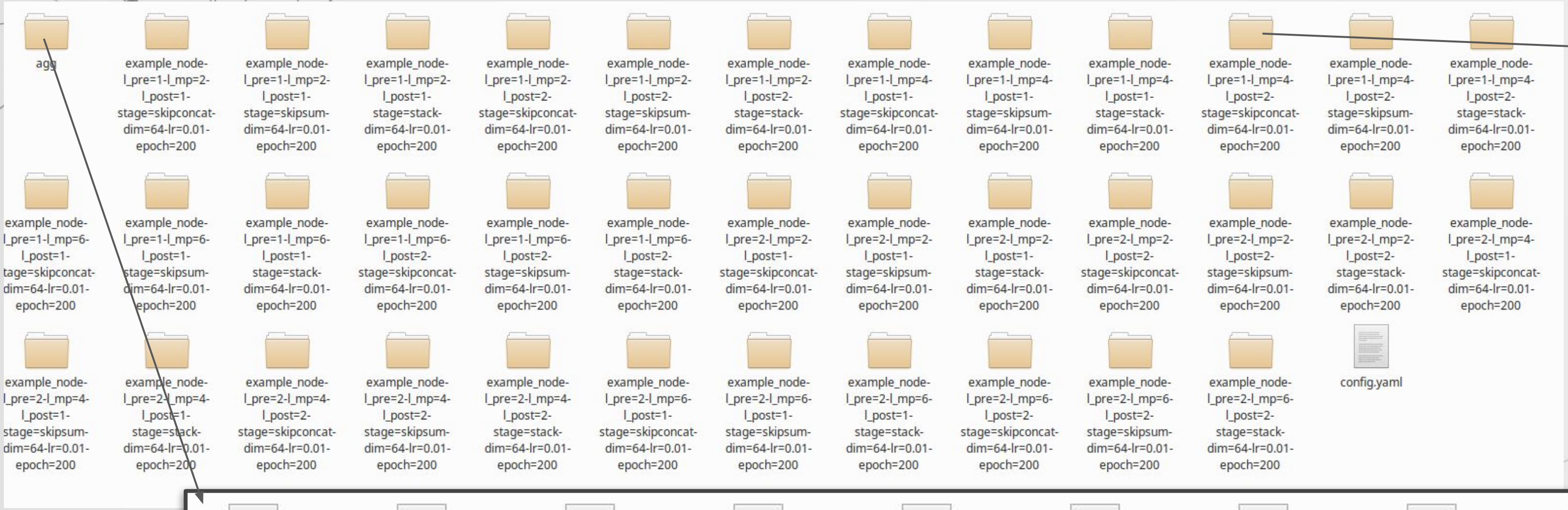
04 Example: batch training



```
agg
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-tage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
config.yaml
```

Single experiment: same as before

04 Example: batch training


agg
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
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example_node-l_pre=2-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
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example_node-l_pre=2-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
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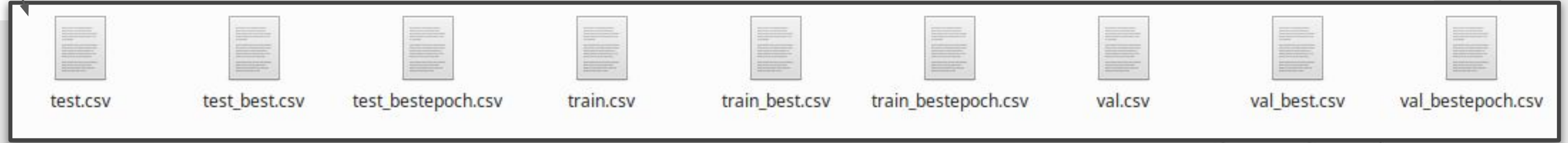
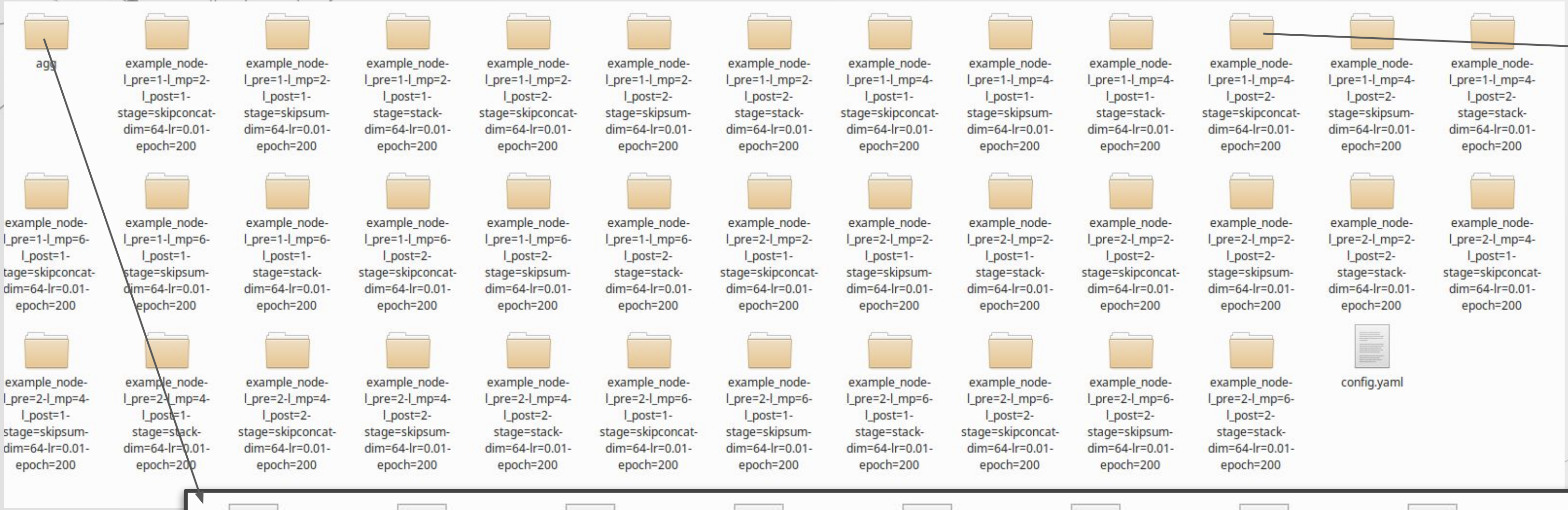
example_node-l_pre=2-l_mp=6-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
config.yaml

Single experiment: same as before

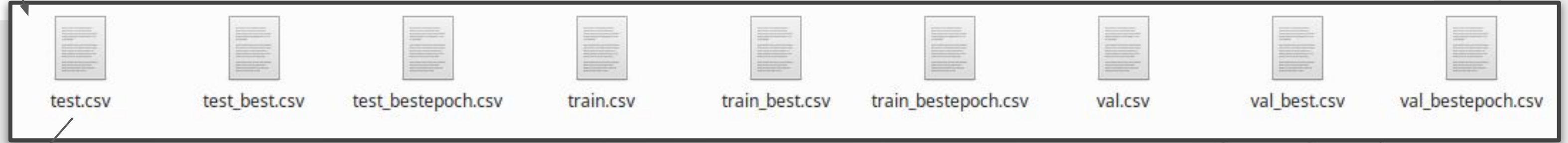

test.csv
test_best.csv
test_bestepoch.csv
train.csv
train_best.csv
train_bestepoch.csv
val.csv
val_best.csv
val_bestepoch.csv

04 Example: batch training



agg
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=4-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=4-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=2-l_mp=6-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
config.yaml

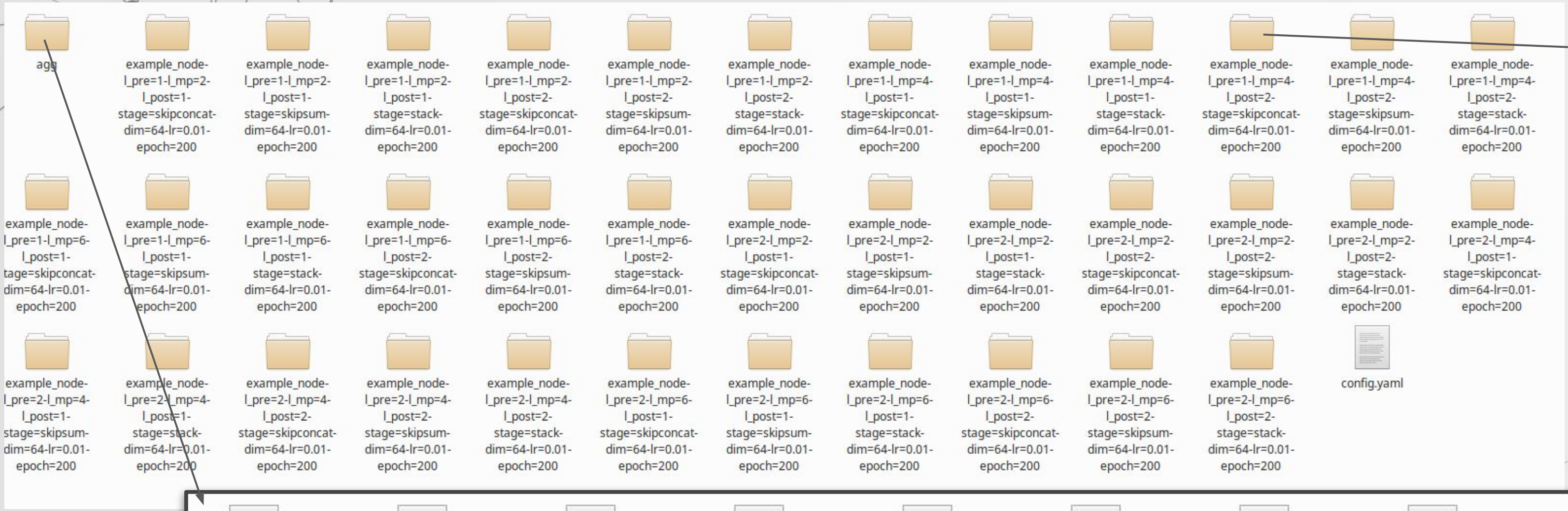
Single experiment: same as before



test.csv
test_best.csv
test_bestepoch.csv
train.csv
train_best.csv
train_bestepoch.csv
val.csv
val_best.csv
val_bestepoch.csv

Final epoch

04 Example: batch training



agg
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=1-stage=stack-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipconcat-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=skipsum-dim=64-lr=0.01-epoch=200
example_node-l_pre=1-l_mp=2-l_post=2-stage=stack-dim=64-lr=0.01-epoch=200
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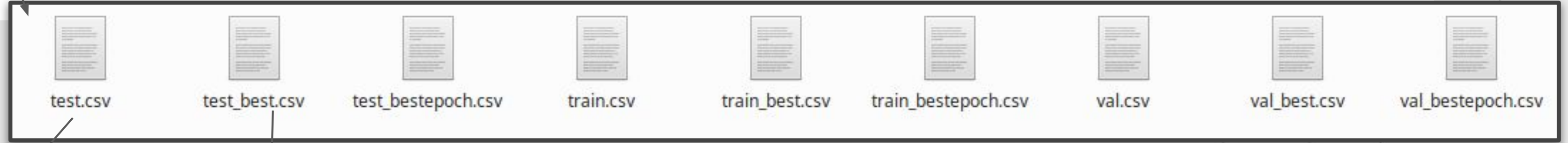
config.yaml

Single experiment: same as before

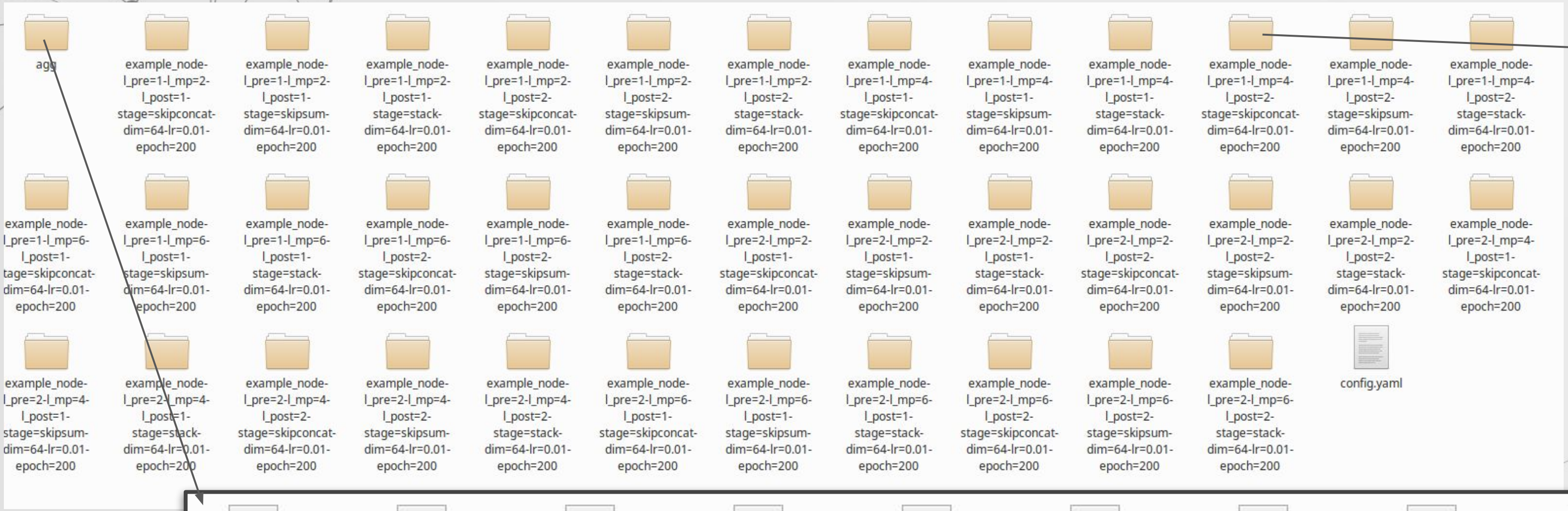


test.csv
test_best.csv
test_bestepoch.csv
train.csv
train_best.csv
train_bestepoch.csv
val.csv
val_best.csv
val_bestepoch.csv

Final epoch

Epoch with the highest average validation accuracy

04 Example: batch training



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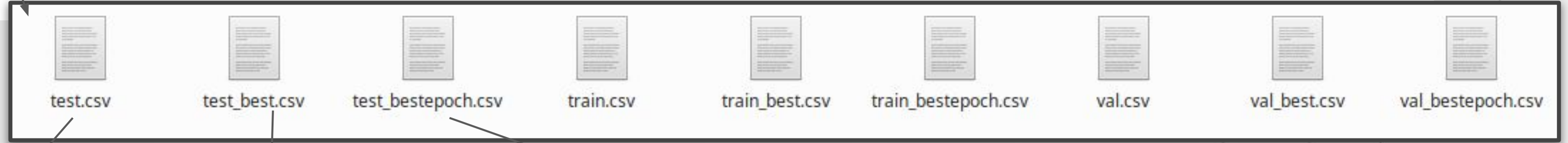

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Final epoch

Epoch with the highest average validation accuracy

Epoch with the highest validation accuracy averaged over different random seeds

04 Example: batch training

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small bug: the script run_batch.sh does not create the folder for the results. You need to create it manually if you want to run another experiment with another name

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05 Customization

Add new modules, losses, options…:

- **Personal use:** add to your local `graphgym/custom_graphgym`

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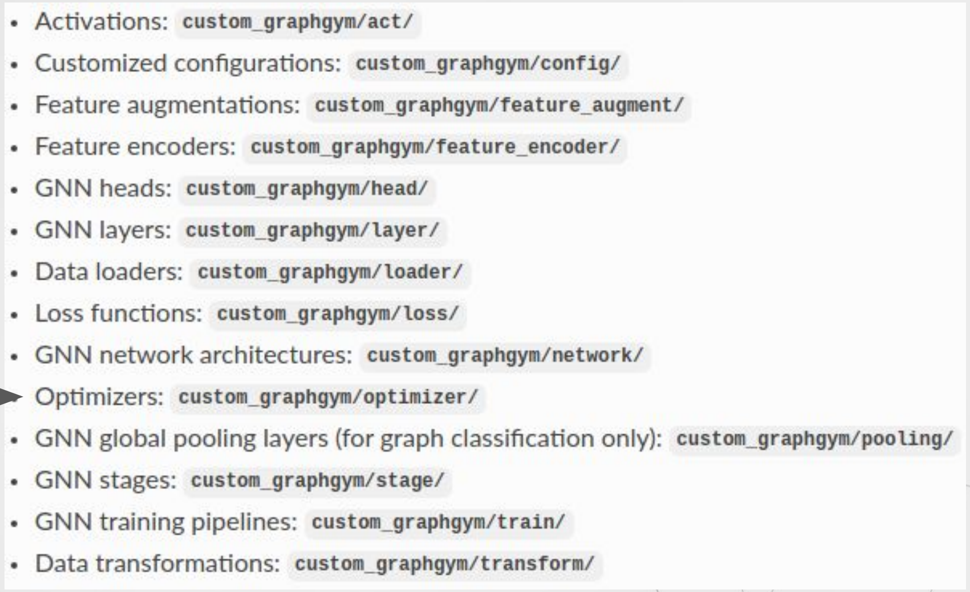

- Activations: `custom_graphgym/act/`
- Customized configurations: `custom_graphgym/config/`
- Feature augmentations: `custom_graphgym/feature_augment/`
- Feature encoders: `custom_graphgym/feature_encoder/`
- GNN heads: `custom_graphgym/head/`
- GNN layers: `custom_graphgym/layer/`
- Data loaders: `custom_graphgym/loader/`
- Loss functions: `custom_graphgym/loss/`
- GNN network architectures: `custom_graphgym/network/`
- Optimizers: `custom_graphgym/optimizer/`
- GNN global pooling layers (for graph classification only): `custom_graphgym/pooling/`
- GNN stages: `custom_graphgym/stage/`
- GNN training pipelines: `custom_graphgym/train/`
- Data transformations: `custom_graphgym/transform/`

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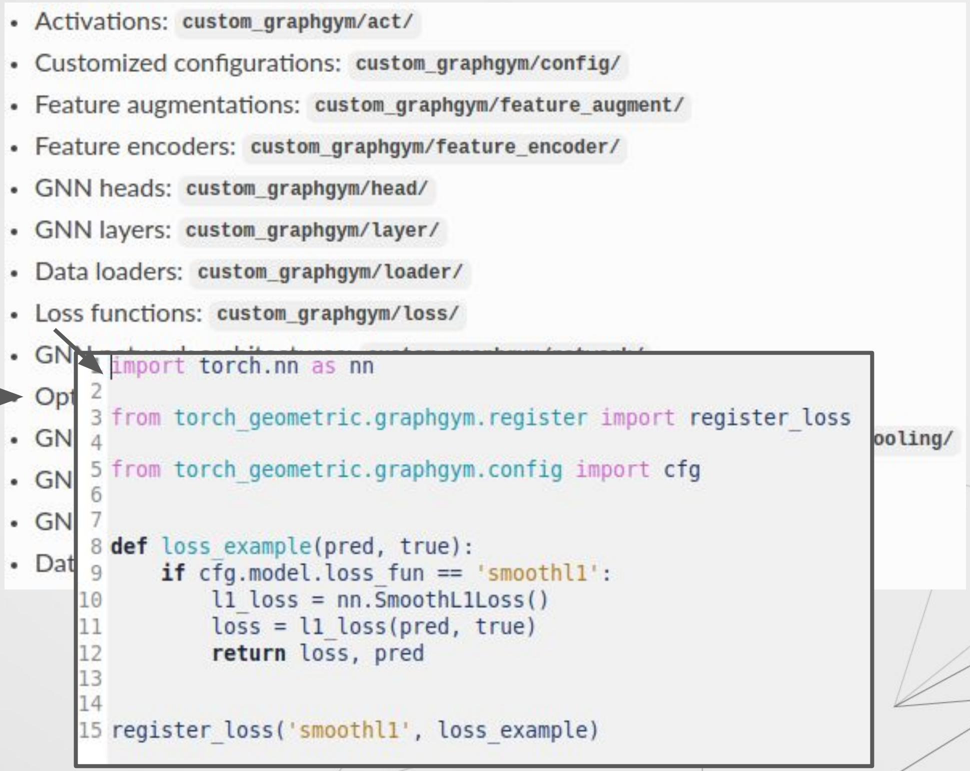

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```python
import torch.nn as nn

from torch_geometric.graphgym.register import register_loss

from torch_geometric.graphgym.config import cfg


def loss_example(pred, true):
    if cfg.model.loss_fun == 'smoothl1':
        l1_loss = nn.SmoothL1Loss()
        loss = l1_loss(pred, true)
        return loss, pred


register_loss('smoothl1', loss_example)
```

graphgym/custom_graphgym/loss/example.py

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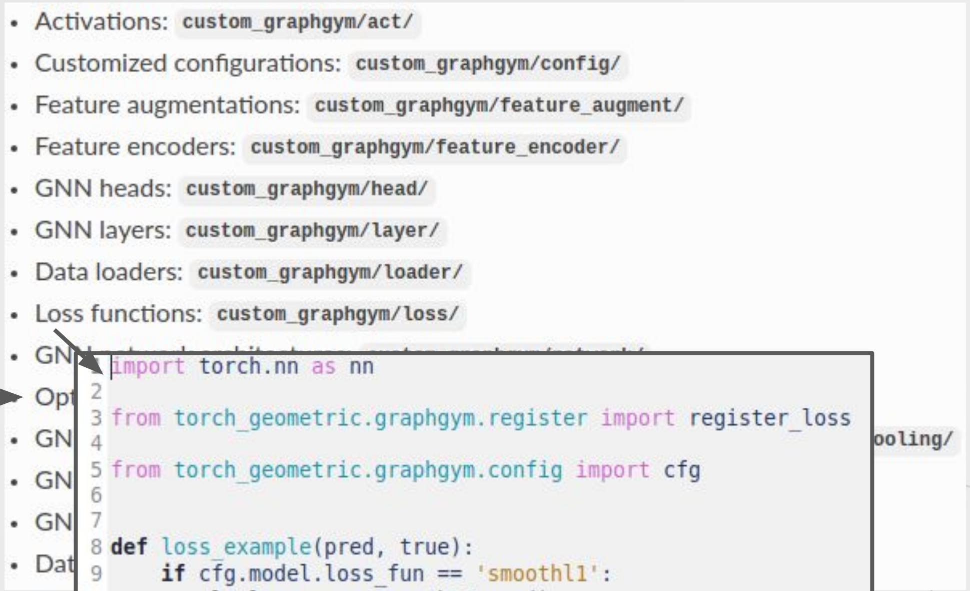
(also possible to add new config fields)



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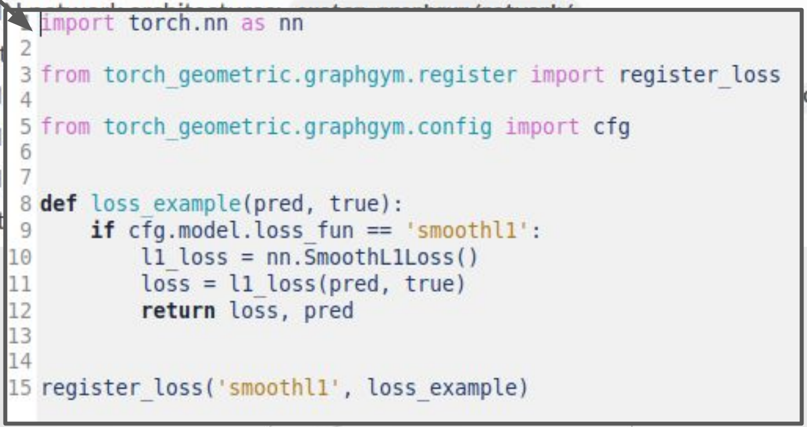

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graphgym/custom_graphgym/loss/example.py

THANKS

Questions?

gsantin@fbk.eu