Successfully installed mattergen-1.0

MODELS_PROJECT_ROOT: /content/mattergen/mattergen

Model config:

```
auto_resume: true
checkpoint_path: null
data_module:
 _recursive_: true
 _target_: mattergen.common.data.datamodule.CrystDataModule
 average_density: 0.05771451654022283
 batch_size:
  train: 32
  val: 32
 max_epochs: 2200
 num_workers:
  train: 0
  val: 0
 properties:
 - dft_bulk_modulus
 - dft_band_gap
 - dft_mag_density
 - ml_bulk_modulus
 - hhi_score
 - space_group
 - energy_above_hull
 root_dir: datasets/cache/alex_mp_20/
 train_dataset:
  _target_: mattergen.common.data.dataset.CrystalDataset.from_cache_path
  cache_path: datasets/cache/alex_mp_20/train
```

```
  properties:
  - dft_bulk_modulus
  - dft_band_gap
  - dft_mag_density
  - ml_bulk_modulus
  - hhi_score
  - space_group
  - energy_above_hull
  transforms:
  - _partial_: true
    _target_: mattergen.common.data.transform.symmetrize_lattice
  - _partial_: true
    _target_: mattergen.common.data.transform.set_chemical_system_string
transforms:
- _partial_: true
  _target_: mattergen.common.data.transform.symmetrize_lattice
- _partial_: true
  _target_: mattergen.common.data.transform.set_chemical_system_string
val_dataset:
  _target_: mattergen.common.data.dataset.CrystalDataset.from_cache_path
  cache_path: datasets/cache/alex_mp_20/val
  properties:
  - dft_bulk_modulus
  - dft_band_gap
  - dft_mag_density
  - ml_bulk_modulus
  - hhi_score
  - space_group
  - energy_above_hull
```

```
  transforms:
  - _partial_: true
    _target_: mattergen.common.data.transform.symmetrize_lattice
  - _partial_: true
    _target_: mattergen.common.data.transform.set_chemical_system_string
lightning_module:
 _target_: mattergen.diffusion.lightning_module.DiffusionLightningModule
 diffusion_module:
  _target_: mattergen.diffusion.diffusion_module.DiffusionModule
  corruption:
   _target_: mattergen.diffusion.corruption.multi_corruption.MultiCorruption
   discrete_corruptions:
    atomic_numbers:
     _target_: mattergen.diffusion.corruption.d3pm_corruption.D3PMCorruption
     d3pm:
      _target_: mattergen.diffusion.d3pm.d3pm.MaskDiffusion
      dim: 101
      schedule:
       _target_: mattergen.diffusion.d3pm.d3pm.create_discrete_diffusion_schedule
       kind: standard
       num_steps: 1000
     offset: 1
   sdes:
    cell:
     _target_: mattergen.common.diffusion.corruption.LatticeVPSDE.from_vpsde_config
     vpsde_config:
      beta_max: 20
      beta_min: 0.1
      limit_density: 0.05771451654022283
```

```
      limit_var_scaling_constant: 0.25
    pos:
     _target_: mattergen.common.diffusion.corruption.NumAtomsVarianceAdjustedWrappedVESDE
     limit_info_key: num_atoms
     sigma_max: 5.0
     wrapping_boundary: 1.0
loss_fn:
 _target_: mattergen.common.loss.MaterialsLoss
 d3pm_hybrid_lambda: 0.01
 include_atomic_numbers: true
 include_cell: true
 include_pos: true
 reduce: sum
 weights:
  atomic_numbers: 1.0
  cell: 1.0
  pos: 0.1
model:
 _target_: mattergen.denoiser.GemNetTDenoiser
 atom_type_diffusion: mask
 denoise_atom_types: true
 gemnet:
  _target_: mattergen.common.gemnet.gemnet.GemNetT
  atom_embedding:
   _target_: mattergen.common.gemnet.layers.embedding_block.AtomEmbedding
   emb_size: 512
   with_mask_type: true
  cutoff: 7.0
  emb_size_atom: 512
```

```
    emb_size_edge: 512
    latent_dim: 512
    max_cell_images_per_dim: 5
    max_neighbors: 50
    num_blocks: 4
    num_targets: 1
    otf_graph: true
    regress_stress: true
    scale_file: /scratch/amlt_code/mattergen/common/gemnet/gemnet-dT.json
  hidden_dim: 512
  property_embeddings: {}
  property_embeddings_adapt: {}
 pre_corruption_fn:
  _target_: mattergen.property_embeddings.SetEmbeddingType
  dropout_fields_iid: false
  p_unconditional: 0.2
optimizer_partial:
 _partial_: true
 _target_: torch.optim.Adam
 lr: 0.0001
scheduler_partials:
- frequency: 1
 interval: epoch
 monitor: loss_train
 scheduler:
  _partial_: true
  _target_: torch.optim.lr_scheduler.ReduceLROnPlateau
  factor: 0.6
  min_lr: 1.0e-06
```

```
    patience: 100
    verbose: true
  strict: true
load_original: false
params: {}
train: true
trainer:
 _target_: pytorch_lightning.Trainer
 accelerator: gpu
 accumulate_grad_batches: 1
 callbacks:
 - _target_: pytorch_lightning.callbacks.LearningRateMonitor
  log_momentum: false
  logging_interval: step
 - _target_: pytorch_lightning.callbacks.ModelCheckpoint
  every_n_epochs: 1
  filename: '{epoch}-{loss_val:.2f}'
  mode: min
  monitor: loss_val
  save_last: true
  save_top_k: 1
  verbose: false
 - _target_: pytorch_lightning.callbacks.TQDMProgressBar
  refresh_rate: 50
 - _target_: mattergen.common.data.callback.SetPropertyScalers
 check_val_every_n_epoch: 5
 devices: 8
 gradient_clip_algorithm: value
 gradient_clip_val: 0.5
```

```
 logger:
  _target_: pytorch_lightning.loggers.WandbLogger
  job_type: train
  project: crystal-generation
  settings:
   _save_requirements: false
   _target_: wandb.Settings
   start_method: fork
 max_epochs: 2200
 num_nodes: 2
 precision: 32
 strategy:
  _target_: pytorch_lightning.strategies.ddp.DDPStrategy
  find_unused_parameters: true



Sampling config:
sampler_partial:
 _target_:
mattergen.diffusion.sampling.classifier_free_guidance.GuidedPredictorCorrector.from_pl_module
 'N': 1000
 eps_t: 0.001
 _partial_: true
 guidance_scale: 0.0
 remove_conditioning_fn:
  _target_: mattergen.property_embeddings.SetUnconditionalEmbeddingType
 keep_conditioning_fn:
  _target_: mattergen.property_embeddings.SetConditionalEmbeddingType
 predictor_partials:
```

```
    pos:
      _target_:
mattergen.diffusion.wrapped.wrapped_predictors_correctors.WrappedAncestralSamplingPredictor
      _partial_: true
    cell:
      _target_: mattergen.common.diffusion.predictors_correctors.LatticeAncestralSamplingPredictor
      _partial_: true
    atomic_numbers:
      _target_: mattergen.diffusion.d3pm.d3pm_predictors_correctors.D3PMAncestralSamplingPredictor
      predict_x0: true
      _partial_: true
  corrector_partials:
    pos:
      _target_: mattergen.diffusion.wrapped.wrapped_predictors_correctors.WrappedLangevinCorrector
      _partial_: true
      max_step_size: 1000000.0
      snr: 0.4
    cell:
      _target_: mattergen.common.diffusion.predictors_correctors.LatticeLangevinDiffCorrector
      _partial_: true
      max_step_size: 1000000.0
      snr: 0.2
  n_steps_corrector: 1
condition_loader_partial:
  _partial_: true
  _target_: mattergen.common.data.condition_factory.get_number_of_atoms_condition_loader
  num_atoms_distribution: ALEX_MP_20
  batch_size: 16
  num_samples: 16
```

W: Skipping acquire of configured file 'main/source/Sources' as repository 'https://r2u.stat.illinois.edu/ubuntu jammy InRelease' does not seem to provide it (sources.list entry misspelt?)

ERROR: pip's dependency resolver does not currently take into account all the packages that are installed. This behaviour is the source of the following dependency conflicts.

notebook 6.5.5 requires pyzmq<25,>=17, but you have pyzmq 26.2.1 which is incompatible.

ERROR: pip's dependency resolver does not currently take into account all the packages that are installed. This behaviour is the source of the following dependency conflicts.

mattergen 1.0 requires autopep8, which is not installed.

mattergen 1.0 requires contextlib2, which is not installed.

mattergen 1.0 requires jupyterlab>=4.2.5, which is not installed.

mattergen 1.0 requires pylint, which is not installed.

mattergen 1.0 requires notebook>=7.2.2, but you have notebook 6.5.5 which is incompatible.

mattergen 1.0 requires torch==2.2.1+cu118; sys_platform == "linux", but you have torch 2.5.1+cu124 which is incompatible.

mattergen 1.0 requires torchaudio==2.2.1+cu118; sys_platform == "linux", but you have torchaudio 2.5.1+cu124 which is incompatible.

mattergen 1.0 requires torchvision==0.17.1+cu118; sys_platform == "linux", but you have torchvision 0.20.1+cu124 which is incompatible.

pymatgen 2025.2.18 requires monty>=2025.1.9, but you have monty 2024.7.30 which is incompatible.

mp-api 0.45.3 requires monty>=2024.12.10, but you have monty 2024.7.30 which is incompatible.

ERROR: pip's dependency resolver does not currently take into account all the packages that are installed. This behaviour is the source of the following dependency conflicts.

maggma 0.71.4 requires pyzmq>=25.1.1, but you have pyzmq 24.0.1 which is incompatible.

mp-api 0.45.3 requires monty>=2024.12.10, but you have monty 2024.7.30 which is incompatible.

ERROR: pip's dependency resolver does not currently take into account all the packages that are installed. This behaviour is the source of the following dependency conflicts.

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mattergen 1.0 requires monty==2024.7.30, but you have monty 2025.3.3 which is incompatible.

mattergen 1.0 requires notebook>=7.2.2, but you have notebook 6.5.5 which is incompatible.

mattergen 1.0 requires torch==2.2.1+cu118; sys_platform == "linux", but you have torch 2.5.1+cu124 which is incompatible.

mattergen 1.0 requires torchaudio==2.2.1+cu118; sys_platform == "linux", but you have torchaudio 2.5.1+cu124 which is incompatible.

mattergen 1.0 requires torchvision==0.17.1+cu118; sys_platform == "linux", but you have torchvision 0.20.1+cu124 which is incompatible.

/content/mattergen/mattergen/common/utils/data_classes.py:95: UserWarning:

The version_base parameter is not specified.

Please specify a compatability version level, or None.

Will assume defaults for version 1.1

with initialize_config_dir(str(self.model_path)):

/content/mattergen/mattergen/generator.py:324: UserWarning:

The version_base parameter is not specified.

Please specify a compatability version level, or None.

Will assume defaults for version 1.1

with hydra.initialize_config_dir(os.path.abspath(str(sampling_config_path))):

INFO:mattergen.common.utils.eval_utils:Loading model from checkpoint: /root/.cache/huggingface/hub/models--microsoft--mattergen/snapshots/17e13889818259ee9327e8d3cf58b834b528e119/checkpoints/mattergen_base/checkpoints/last.ckpt

/content/mattergen/mattergen/common/utils/data_classes.py:95: UserWarning:

The version_base parameter is not specified.

Please specify a compatability version level, or None.

Will assume defaults for version 1.1

with initialize_config_dir(str(self.model_path)):

/content/mattergen/mattergen/diffusion/lightning_module.py:109: FutureWarning: You are using `torch.load` with `weights_only=False` (the current default value), which uses the default pickle module implicitly. It is possible to construct malicious pickle data which will execute arbitrary code during unpickling (See https://github.com/pytorch/pytorch/blob/main/SECURITY.md#untrusted-models

for more details). In a future release, the default value for `weights_only` will be flipped to `True`. This limits the functions that could be executed during unpickling. Arbitrary objects will no longer be allowed to be loaded via this mode unless they are explicitly allowlisted by the user via `torch.serialization.add_safe_globals`. We recommend you start setting `weights_only=True` for any use case where you don't have full control of the loaded file. Please open an issue on GitHub for any issues related to this experimental feature.

checkpoint = torch.load(checkpoint_path, map_location=map_location)

Generating samples: 0%| | 0/1 [00:00<?, ?it/s]

0%| | 0/1000 [00:00<?, ?it/s]

0%| | 0/1000 [00:19<?, ?it/s]

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6%|▌ | 56/1000 [00:24<06:51, 2.29it/s]

7%|▋ | 68/1000 [00:29<06:41, 2.32it/s]

8%|▊ | 80/1000 [00:34<06:34, 2.33it/s]

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57%|▉▉▉▉ | 567/1000 [04:14<03:13, 2.24it/s]

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58%| | 579/1000 [04:19<03:08,  2.24it/s]
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71%| | 711/1000 [05:18<02:08,  2.25it/s]
72%| | 723/1000 [05:24<02:02,  2.26it/s]
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75%| | 747/1000 [05:34<01:51,  2.27it/s]
76%| | 759/1000 [05:39<01:46,  2.27it/s]
77%| | 771/1000 [05:45<01:40,  2.28it/s]
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81%| | 807/1000 [06:00<01:24,  2.28it/s]
82%| | 819/1000 [06:05<01:18,  2.30it/s]
83%| | 831/1000 [06:11<01:13,  2.31it/s]
84%| | 843/1000 [06:16<01:07,  2.31it/s]
86%| | 855/1000 [06:21<01:02,  2.32it/s]
87%| | 867/1000 [06:26<00:57,  2.32it/s]
88%| | 879/1000 [06:31<00:51,  2.33it/s]
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92%|▉▉▉▉▉▉▉▉▉▉| 915/1000 [06:47<00:36, 2.33it/s]

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