Hands on NeuLat:
A Toolbox for **Neu**ral Samplers in **Lat**tice Field Theory

N E U **L** A T

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https://github.com/neulat/neulat

About me

Christopher J. Anders

PostDoc at RIKEN AIP, Tokyo

Research Interests

- Deep Learning
- Model Understanding
- Software for ML
- ML in the Sciences

Background

- B.Sc. *Computer Science* @ TU Berlin (2016)
- M.Sc. *Computer Science* @ TU Berlin (2018)
- PhD *Computer Science* @ TU Berlin (2024)

Disclaimer: I am not a physicist!

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- software framework for machine-learning-based lattice field theory

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  - trivializing maps with flows (Bacchio et al. (2023))

Benefits of Research Software Packages

- faster development of new ideas

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Existing examples:

- SchNetPack - Deep Neural Networks for Atomistic Systems
- BGFlow - Boltzmann Generators (BG) and other sampling methods

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There are already great tools available!

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But: We want to create a **highly customizable reference implementation**.

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- **Modularity and Customizability**: Swiftly incorporate new actions/theories/models/techniques

NeuLat Overview

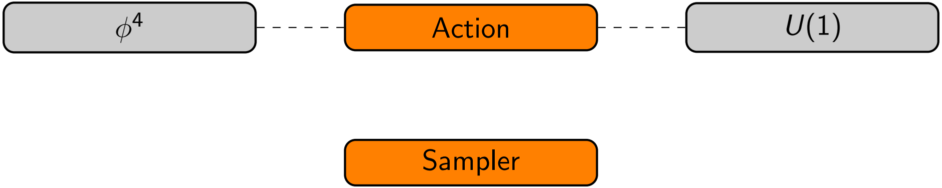
Action

Actions $S[U]$ define physical theories $p(U) \propto e^{-S[U]}$

NeuLat Overview

Actions are, e.g., ϕ^4 and $U(1)$

NeuLat Overview



Samplers are anything that can be sampled from

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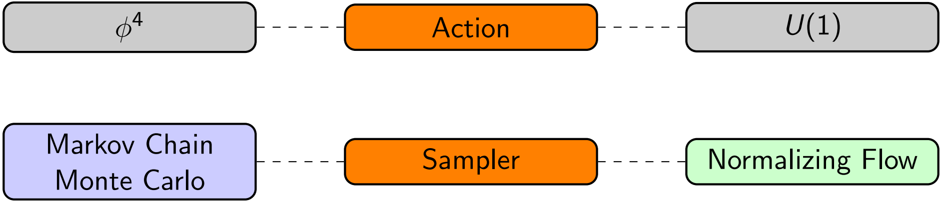

Samplers are, e.g., MCMCs, Flows, $\mathcal{N}(0, 1)$

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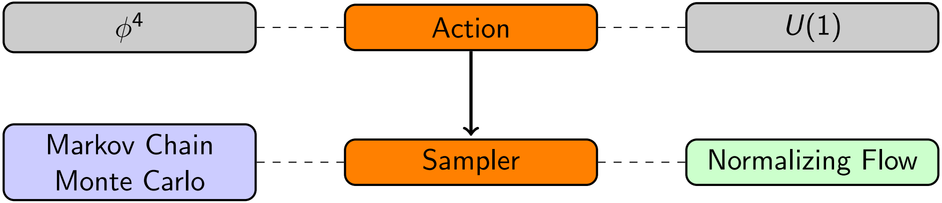
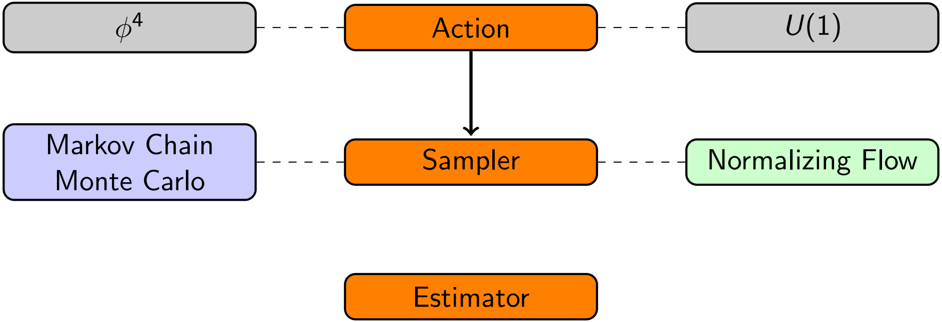


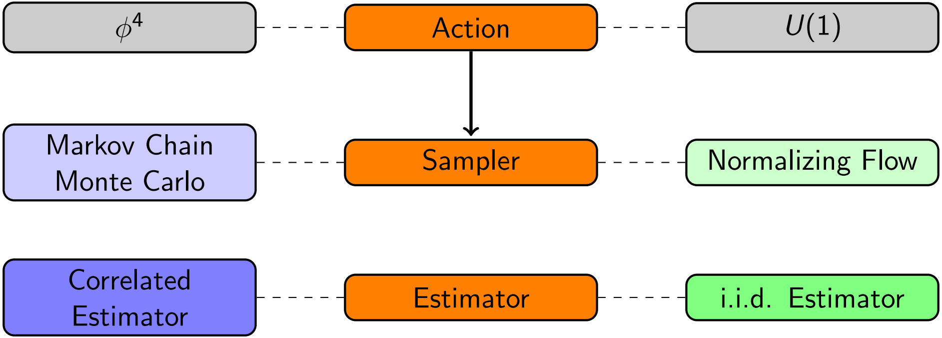
Samplers require Actions

NeuLat Overview



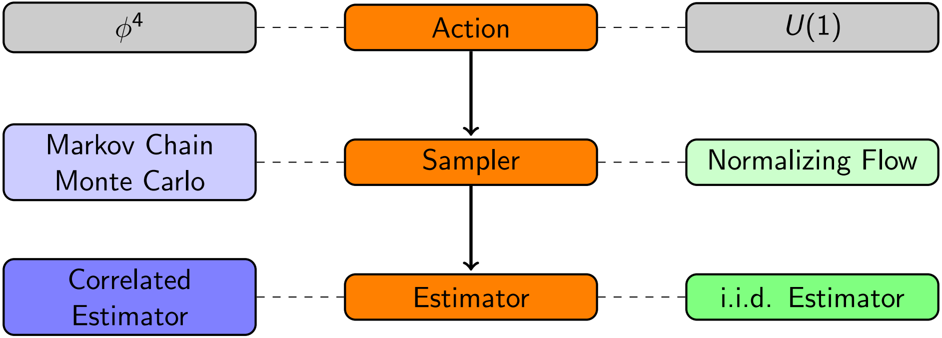
Estimators are used to estimate observables

NeuLat Overview



Estimators are, e.g., i.i.d or correlated, based on the samples

NeuLat Overview



Estimators require samples from Samplers

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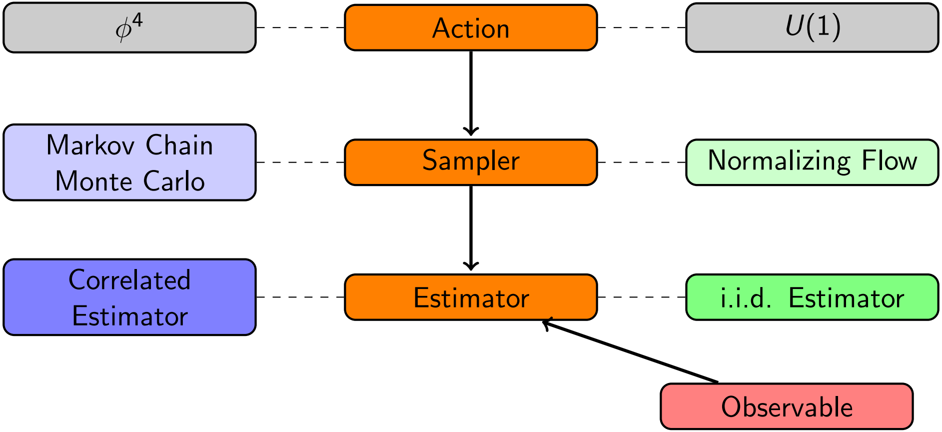

Observables, such as Magnetization in ϕ^4, are used by the Estimator

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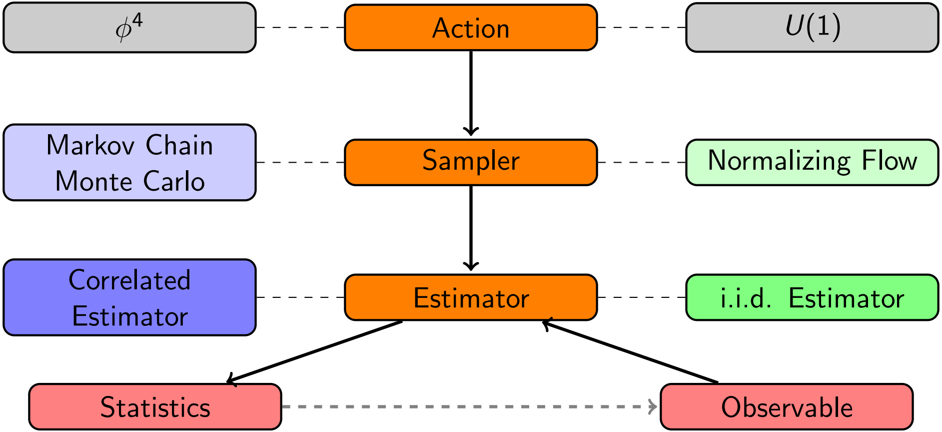

Resulting Statistics are estimations for the Observables

Actions

Actions are objects and need to be instantiated.

```
import torch
from neulat.action.phi4 import Phi4Action

# ndim_features is the number of dimensions in the lattice
action = Phi4Action(kappa=0.3, lamb=0.022, ndim_features=2)
```

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Action objects can be called to compute action values for configurations.

```python
config = torch.randn(8, 8)
unnormalized_prob = torch.exp(-action(config))
```

Defining Actions

Actions are very simple to implement, for instance ϕ^4:

```
from neulat.action.base import Action

class Phi4Action(Action):
    name = 'phi4_action'
    def __init__(self, kappa, lambd, ndim_feature=2):
        ...
    def forward(self, config):
        dims = tuple(range(-1, -self.ndim_feature, -1))
        kinetic = (-2 * self.kappa) * config * sum(
            torch.roll(config, 1, dim) for dim in dims)
        mass_inter = (1 - 2 * self.lambd) * config ** 2
        inter = self.lambd * config ** 4
        return (kinetic + mass + inter).sum(dim=dims)
```

Samplers

At the core of NeuLat are Samplers, which is anything from which can be sampled.

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For instance, the normal distribution is a Sampler in Neulat:

```
from neulat.sampler.distribution import Normal

normal = Normal(loc=0., scale=1., feature_shape=(8, 8))
```

Sampling

Samplers can be sampled from, and may or may not support probability values.

```
samples = normal.sample(sample_shape=8)
logprobs = normal.logprob(samples)

samples2, logprobs2 = normal.sample_with_logprob((2, 2))
```

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In NeuLat, we assume configurations of shape `(*sample_shape, *feature_shape)`.

- `feature_shape` is the shape of the lattice
- `sample_shape` is the number of samples, supporting arbitrary shapes

Hamiltonian Monte Carlo

A more involved Sampler is the HMC:

```
from neulat.sampler.mc.hmc import HMCMarkovChain

hmc = HMCMarkovChain(
    action, # action
    feature_shape=(8, 8),  # lattice shape
    burn_in=5000,  # equilibration steps
    skip_interval=1,  # skipped samples in chain
    overrelax_interval=50,  # steps between sign flips
    eps=0.05,  # step size along trajectory
    traj_steps=20,  # number of steps in trajectory
    bias=0.0,  # bias in initialization
)
```

HMC Sampling

The HMC can be sampled from, as any sampler

```
configs = hmc.sample(sample_shape=13)
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```

However, HMC does not implement `logprob` and by extension `sample_with_logprog`, as no normalized probabilities are available

```
# both cause exceptions:
# logprobs = hmc.logprob(sample_shape=13)
# configs2, logprobs2 = hmc.sample_with_logprob(13)
```

HMC Sampling 2

One can also iterate over HMCs to sample

```
configs = []
for n, config in zip(range(25), hmc):
    configs.append(config)
    print(f'Sampled config number {n}.')

# this gives a list of configs, combine them:
configs = torch.cat(configs)
```

HMC Sampling 2

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But be careful, HMCs are infinite iterators.

Normalizing Flows

Normalizing flows require a base distribution, and a transform.

```python
from neulat.sampler.flow import Flow, SequentialTransform

flow = Flow(
  base_distribution=Normal(feature_shape=(8, 8)),
  transform=SequentialTransform([])  # identity for demo
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Normalizing flows are (i.i.d.) Samplers supporting logprobs.

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configs, logprobs = flow.sample_with_logprob(8)
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Normalizing Flows: Base Distributions

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```

Flows themselves support logprobs, and can thus be base distributions.

```
flow2 = Flow(
  base_distribution=flow,
  transform=SequentialTransform([])  # identity for demo
)
```

Normalizing Flows: Transforms

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E.g., implementation for transform $f(\mathbf{x}) = -\mathbf{x}$, $f^{-1}(\mathbf{x}) = -\mathbf{x}$

```python
from sampler.flow.base import Transform, withlogdet

class FlipSign(Transform):
    @withlogdet
    def forward(self, input):
        return -input, 1.
    @withlogdet
    def inverse(self, input):
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The second return value is the *log absolute jacobian determinant* of the transform.

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The decorator `@withlogdet` makes sure the logdet is accumulated between transforms.

Normalizing Flows: Transforms 2

A useful transform is the `SequentialTransform`, which is used to apply transforms sequentially:

```
from sampler.flow.base import SequentialTransform

flip_a_bunch = SequentialTransform([
  FlipSign(),
  FlipSign(),
  FlipSign(),
])
```

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For common *Coupling* Flows, there is however a more convenient way.

Coupling Flows

Coupling flows like NICE consist of two parts, a `partitioner`, and a `net_factory`

```python
from neulat.sampler.flow.coupling import NICE

coupling = NICE(
    partitioner=partitioner,
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The `net_factory` is a function that constructs the *conditioner*, e.g., a neural network that acts on the partitioned input.

Coupling Flows: Partitioners

A very simple partitioner is the `AltFlatPartitioner`, which stands for *alternating flattened partitioner*

```
partitioner = AltFlatPartitioner(feature_shape=(2, 2)),
input = torch.tensor([[1., 2.],[3., 4.]])
active, passive = partitioner(input)
active += 10
output = partitioner(active, passive)
```

Coupling Flows: Partitioners

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```

This will generate an output of $\begin{pmatrix} 11 & 2 \\ 13 & 4 \end{pmatrix}$

Coupling Flows: Flipping Partitioners

Partitioners usually flip the active and pasive elements.

Such a partitioner can be created by calling `.flip()`:

```
flipped = partitioner.flip()
input = torch.tensor([[1., 2.],[3., 4.]])
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active, passive = flipped(input)
active += 1
output = flipped(active, passive)
```

This will generate an output of $\begin{pmatrix} 1 & 12 \\ 3 & 14 \end{pmatrix}$

Coupling Flows: Net Factory (Conditioner)

The `net_factory` define the *conditioner* Θ that transforms the passive input:

$$\mathbf{x}^{l+1}_{\text{active}} = h(\mathbf{x}^{l}_{\text{active}}, \Theta(\mathbf{x}^{l}_{\text{passive}})) \tag{1}$$

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```python
from functools import partial
from neulat.sampler.flow.coupling.affine import NICE, MLP

net_factory = partial(
    MLP,
    n_blocks=3,
    latent_size=1024,
    activation=torch.nn.Tanh,
    bias=False,
)
```

Coupling Flows: Defining Couplings

The coupling `Transform` itself is mostly only concerned with implementing the coupling function h. E.g. in NICE: $h(a, b) = a + b$

```
class NICE(Coupling):
    @withlogdet
    @partitioned
    def forward(self, active, passive):
        return active + self.net(passive), 1.

    @withlogdet
    @partitioned
    def inverse(self, active, passive):
        return active - self.net(passive), 1.
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Recall: `@withlogdet` makes sure the log abs jacobian det is propagated.

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```

New: `@partitioned` automates the partitioning/masking in subsequent couplings!

Coupling Flows: Completing the Flow

Putting all the previous parts together, we can create a flow in the following way:

```
flow = Flow(
  base_distribution=Normal(0.0, 1.0, feature_shape=(8, 8)),
  transform=6 * NICE(
      partitioner=AltFlatPartitioner(feature_shape=(8, 8)),
      net_factory=partial(MLP, n_blocks=3, latent_size=1024,
        activation=torch.nn.Tanh, bias=False)
)
```

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        activation=torch.nn.Tanh, bias=False)
)
```

Notice the `transform=6 * NICE`. This creates a sequential transform of 6 Couplings, with alternating masking/partitioning!

Coupling Flows: Traning

Training of the flow with ReverseKL is straight forward:

```
from neulat.loss import ReverseKLLoss

optim = torch.optim.Adam(flow.transform.parameters(), lr=5e-4)
loss_fn = ReverseKLLoss()
for _ in range(1000):
    configs, log_probs = flow.sample_with_logprob(10)
    loss = loss_fn(action(configs), log_probs)  # loss contains `mean` and `std`
    optim.zero_grad()
    loss.mean.backward()  # we train only using the loss `mean`
    optim.step()
```

Estimating Observables from i.i.d. Samples

Observables themselves are classes in NeuLat. In order to estimate them, we additionally need an `Estimator`, and configurations. For instance:

```
from neulat.observable.base import AbsMagnetization, Magnetization
from neulat.estimator.base import IidEstimator

observables = [AbsMagnetization(), Magnetization(), action]
iid_estimator = IidEstimator(observables)
configs = flow.sample(1000)
flow_statistics = iid_estimator.named_evaluate(configs)
```

The dict `flow_statistics` will contain one entry per observable, e.g.:

`{'absmag': Statistics(mean=0.6408, std=0.0473), 'mag': ...}`

Estimating Observables from Correlated Samples

Estimation of Observables from correlated samples (e.g., from HMC) requires the use of the appropriate estimator:

```python
from neulat.estimator.base import CorrelatedEstimator

correlated_estimator = CorrelatedEstimator(observables)
configs = hmc.sample(1000)
hmc_statistics = correlated_estimator.named_evaluate(configs)
```

The dict `hmc_statistics` will instead contain correlated statistics objects,

`{'absmag': CorrelatedStatistics(mean=32.82628, std=1.4674, tau_int=0.5909, tau_int_err=0.3162), ...}`

Neural Importance Sampling

To obtain an unbiased estimator, Nicoli et. al proposed to use Importance Sampling. This additionally requires the logprobs of the flow, as well as the specific action:

```
from neulat.estimator.base import ImportanceSamplingEstimator

flow_configs, flow_logprobs = flow.sample_with_logprob(1000)
iw_estimator = ImportanceSamplingEstimator(observables, action)
flow_iw_stats = iw_estimator.evaluate(flow_configs, flow_logprobs)
```

The dict `flow_iw_statistics` will contain the same Statistics object the IidEstimator returned:

`{'absmag': Statistics(mean=2.6021, std=0.4674, ...}`

Planned Features

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- **YOUR FEATURE HERE!**

We want NeuLat to be a community effort! Please reach out to us!

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Thank you for your attention!