

Idea Factory Intensive Program #2

# 딥러닝 홀로서기

**이론강의/PyTorch실습/코드리뷰**

딥러닝(Deep Learning)에 관심이 있는 학생 발굴을 통한  
딥러닝의 이론적 배경 강의 및 오픈소스 딥러닝 라이브러리 PyTorch를 활용한 실습

# #11

# Today's Time Schedule

Assignment #1 Review

How to Parameterize Entire Code

How to Run Code with GPU!

How to Overcome Overfitting

Big Wave: Hyperparameter Tuning

1 hour?

1 hour

2 hour

How to Parametrize Entire Code (And why?)

# What is Parametrization?

```
seed = 123
np.random.seed(seed)
torch.manual_seed(seed)
args = parser.parse_args("")
```

```
##### SIZE #####
args.vocab_size = 41
args.in_dim = 59
args.out_dim = 256
args.molvec_dim = 512
```

```
##### MODEL #####
args.num_layers = 6
args.use_attn = True
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args.train_tpsa = True
```

```
##### HYPERPARAMETERS #####
args.optim = 'ADAM'
args.lr = 0.001
args.l2_coef = 0.001
args.dp_rate = 0.1
```

```
##### EXP #####
args.epoch = 100
args.batch_size = 512
args.test_batch_size = 512
args.save_every = 100
args.validate_every = 100
args.log_every = 20
```

```
##### DEVICE #####
args.device = 'cuda' if torch.cuda.is_available() else 'cpu'
```

```
##### LOGGING #####
args.log_path = 'runs'
args.model_name = 'exp_test3'
```

하이퍼파라미터  
대환장파티

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대환장파티

실험 조건(args)을 input으로 받으면  
알아서 모델 생성부터 실험 결과 리포팅까지..!



```
result = experiment(data_loader, args)
```

```
2018-12-04 02:11:42,018 [INFO] ##### Model Constructed #####
2018-12-04 02:11:42,018 [INFO] ##### Model Constructed #####
2018-12-04 02:11:42,028 [INFO] encoder : 547985 parameters
2018-12-04 02:11:42,028 [INFO] encoder : 547985 parameters
2018-12-04 02:11:42,030 [INFO] classifier: 48911 parameters
2018-12-04 02:11:42,030 [INFO] classifier: 48911 parameters
2018-12-04 02:11:42,032 [INFO] logP : 131585 parameters
2018-12-04 02:11:42,032 [INFO] logP : 131585 parameters
2018-12-04 02:11:42,034 [INFO] mr : 131585 parameters
2018-12-04 02:11:42,034 [INFO] mr : 131585 parameters
2018-12-04 02:11:42,035 [INFO] tpsa : 131585 parameters
2018-12-04 02:11:42,035 [INFO] tpsa : 131585 parameters
2018-12-04 02:11:42,036 [INFO] #####
2018-12-04 02:11:42,036 [INFO] #####
2018-12-04 02:11:48,356 [INFO] [T] E: 0. P:2.3%. Loss: 10.7. Mask Loss: 10.7. 1620.8 mol/sec. Iter: 20.
Elapsed: 6.3 sec.
2018-12-04 02:11:48,356 [INFO] [T] E: 0. P:2.3%. Loss: 10.7. Mask Loss: 10.7. 1620.8 mol/sec. Iter: 20.
Elapsed: 6.3 sec.
2018-12-04 02:11:53,104 [INFO] [T] E: 0. P:4.7%. Loss: 7.76. Mask Loss: 7.76. 2156.5 mol/sec. Iter: 40.
Elapsed: 4.7 sec.
2018-12-04 02:11:53,104 [INFO] [T] E: 0. P:4.7%. Loss: 7.76. Mask Loss: 7.76. 2156.5 mol/sec. Iter: 40.
Elapsed: 4.7 sec.
2018-12-04 02:11:57,855 [INFO] [T] E: 0. P:7.1%. Loss: 7.63. Mask Loss: 7.63. 2155.5 mol/sec. Iter: 60.
Elapsed: 4.8 sec.
2018-12-04 02:11:57,855 [INFO] [T] E: 0. P:7.1%. Loss: 7.63. Mask Loss: 7.63. 2155.5 mol/sec. Iter: 60.
Elapsed: 4.8 sec.
2018-12-04 02:12:02,694 [INFO] [T] E: 0. P:9.5%. Loss: 8.68. Mask Loss: 8.68. 2116.0 mol/sec. Iter: 80.
Elapsed: 4.8 sec.
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# Why Parametrization?

- Manage various experiment in one-place

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- Manage various experiment in one-place
- Prevent possible situation where hyperparameter is fixed inside the model
- Re-usability
- Readability
- Auto hyperparameter optimizer could conduct various experiments instead of us

Okay, Which parameter?

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Hyperparameter!

# Hyperparameter

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Determine  
Model

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Optimizer Related

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Training/Evaluation Process Related

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Saving Exp Result

Okay, Then.. How?

# Introduce Argparse

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Argparse : Dictionary like object

Import argparse!

Let's try below code to see what argparse can do!

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Argparse : Dictionary like object

Import argparse!

Let's try below code to see what argparse can do!

```
1 import argparse
2 parser = argparse.ArgumentParser()
3 args = parser.parse_args("")
4
5 print(args)
6 args.batch_size = 100
7 print(args)
8 print(args.batch_size)
9
10 args.in_dim = 256
11 print(args.in_dim)
12 args.in_dim = 128
13 print(args.in_dim)
14
```


# Experiment Manager?

## Function. Experiment

- Construct Model
- Construct Loss Function
- Construct Optimizer
- Start Training and Report Progress
- Report Evaluation Result

# Experiment Manager?

## Function. Experiment

- Construct Model  `nn.ModuleList`
- Construct Loss Function
- Construct Optimizer
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- Report Evaluation Result

# Experiment Manager?

Function. Experiment

- Construct Model
- Construct Loss Function
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Rest of parameterization is full of ‘if’ statement



# Summary

- Do not let the hyperparameter value live inside the code
- Use Argparse to gather and manage hyperparameters