Deep Learning in Bioinformatics

Practice

DATA MINING & BIOINFORMATICS LAB.

HANYANG UNIVERSITY

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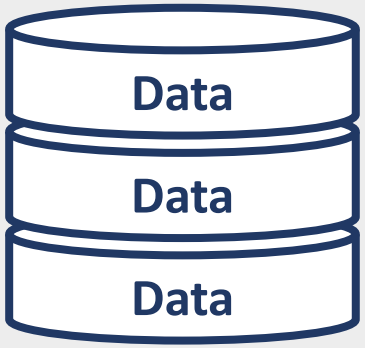
2. Sequence Classification
3. Link Prediction (Graph Neural Network)

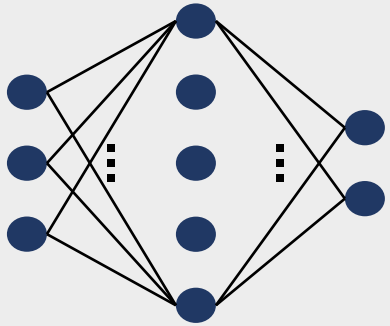
Deep Learning Process

Step1



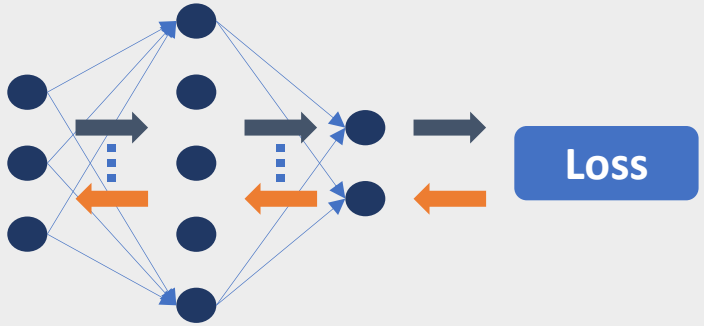
- Collecting data
- Preprocessing
- Dataset
- Data-loader

Step2



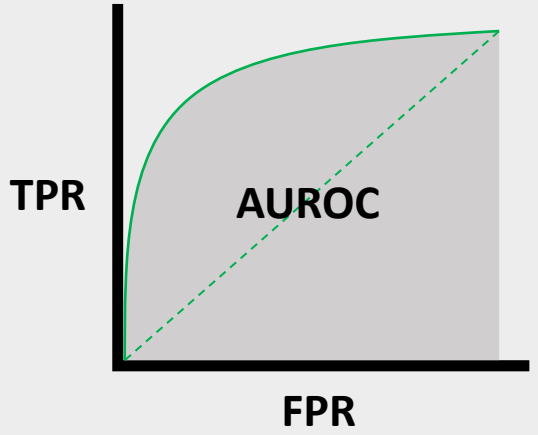
- Selecting method
- Building model

Step3



- Hyper-parameters
- Loss function
- Optimizer
- Training

Step4



- Predicting
- Evaluating

Sequence Classification

Dataset

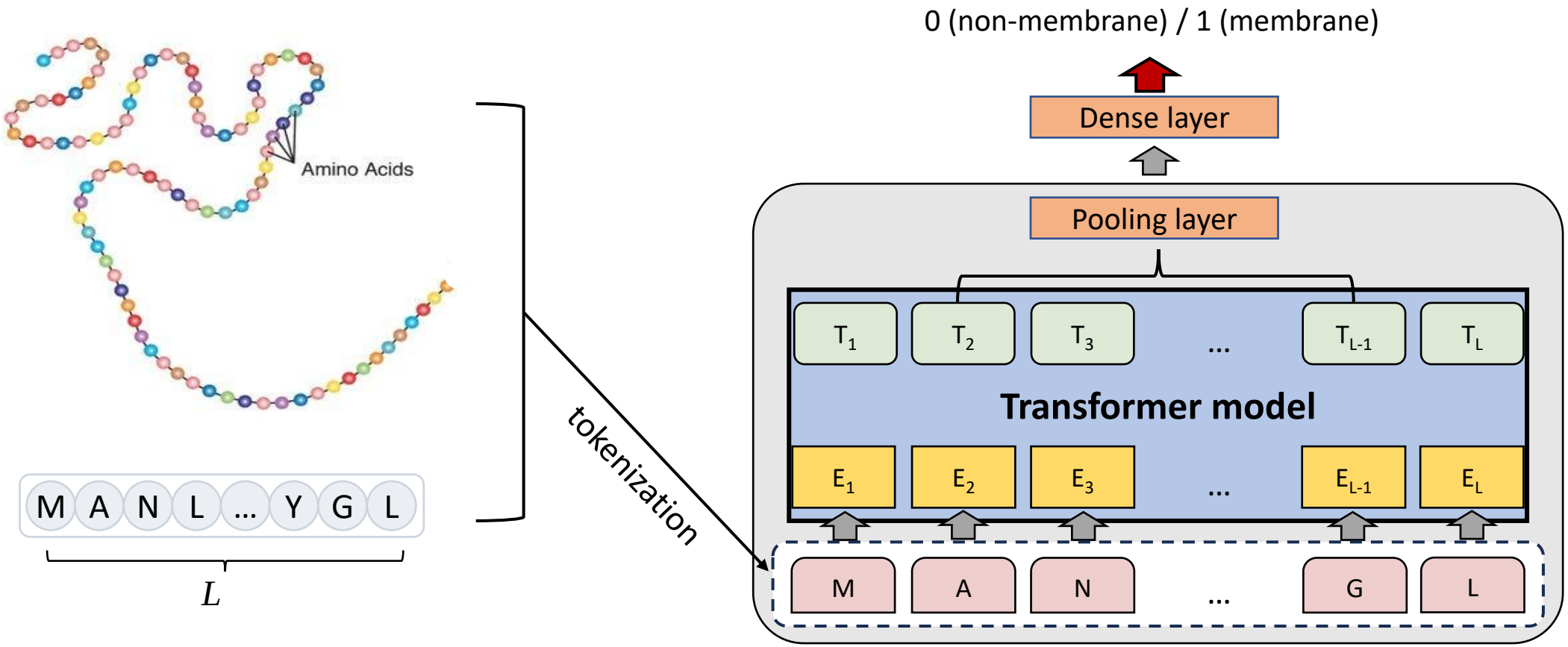
DeepLoc 2.0 provides proteins categorized into one of multiple of theses ten locations

: Cytoplasm, Nucleus, Extracellular, Cell membrane, Mitochondrion, Plastid, Endoplasmic reticulum, Lysosome/Vacuole, Golgi apparatus, Peroxisome.

ACC	Kingdom	Partition	Membrane	Cytoplasm	Nucleus	…	Sequence
Q28165	Metazoa	4	0	1	1	…	MAAAAAAAAAAGAAG…
Q86U42	Metazoa	4	0	1	1	…	MAAAAAAAAAAGAAG…
Q0GA42	Metazoa	3	1	0	0	…	MAAAAAAAAALGVRL…
P82349	Metazoa	1	1	1	0	…	MAAAAAAAAATEQQG…
Q7L5N1	Metazoa	1	0	1	1	…	MAAAAAAAAATNGTG…
Q96S94	Metazoa	0	0	0	1	…	MAAAAAAAGAAGSAA…
Q9CQ25	Metazoa	0	0	1	0	…	MAAAAAAAGGAALAV…
Q96P70	Metazoa	4	0	1	1	…	MAAAAAAGAASGLPG…
P63086	Metazoa	1	1	1	0	…	MAAAAAAGPEMVRGQ…

Model

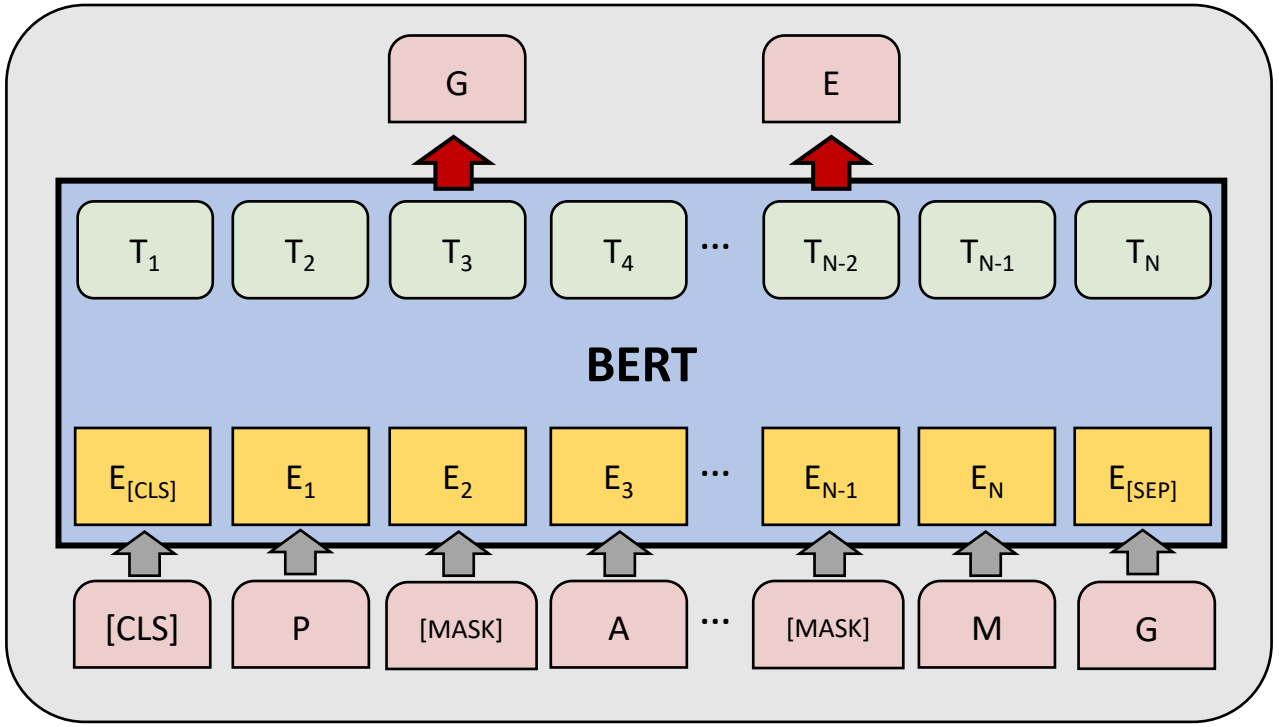
- **Protein sequence classification**
  - Sequence classification is the task of assigning a label or class to a given text.
  - Input : protein sequence
  - Target : binary classification (membrane or non-membrane)



Model

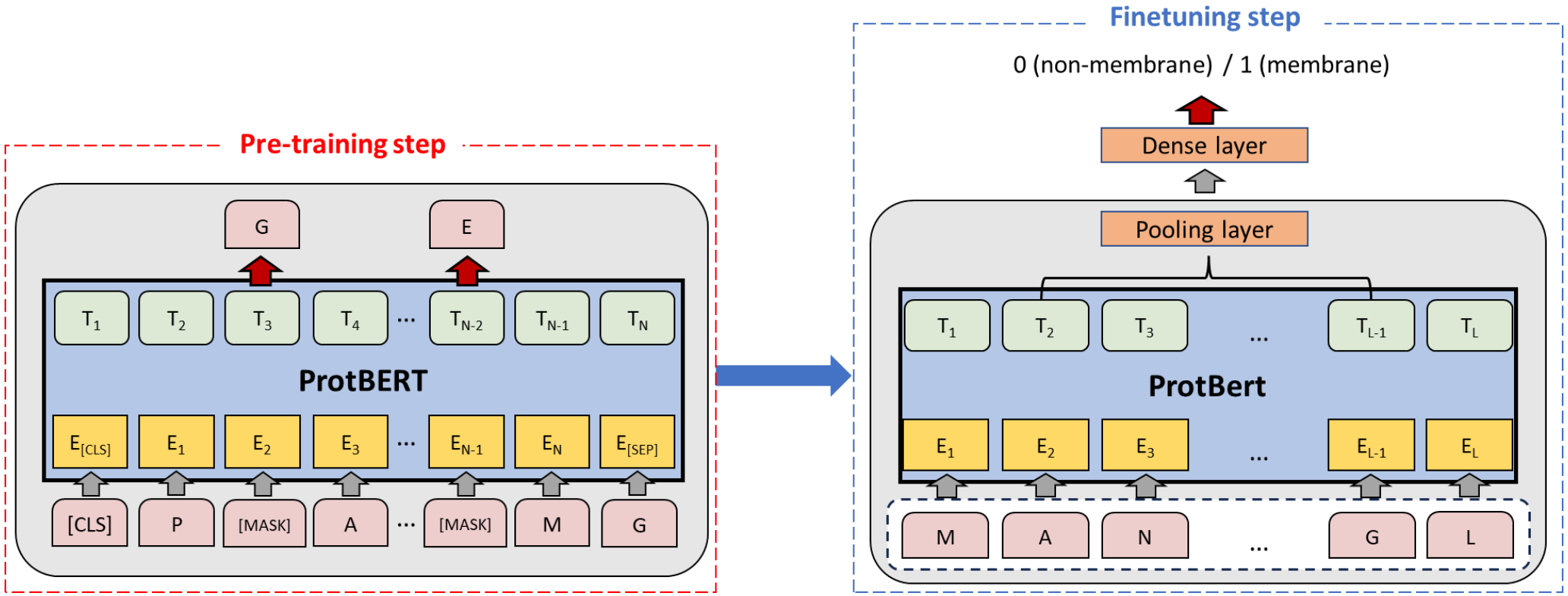
Pre-training model – ProtBERT

- *"Prottrans: Toward understanding the language of life through self-supervised learning."*
- Bert-based protein language model developed as part of the *Prottrans* project.
- ProtBERT is trained in self-supervised manner, essentially learning to predict masked amino acids (tokens) in already known sequences.



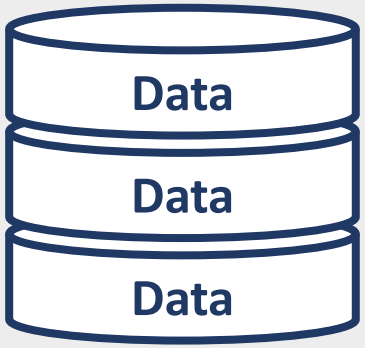
Model

- **Protein sequence classification**
  - Sequence classification is the task of assigning a label or class to a given text.
  - Input : protein sequence
  - Target : binary classification (membrane or non-membrane)
  - **Transfer learning (pretrained model : ProtBERT)**



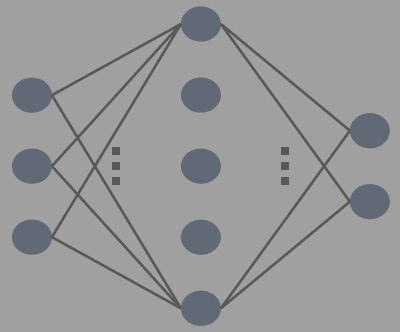
Deep Learning Process

Step1



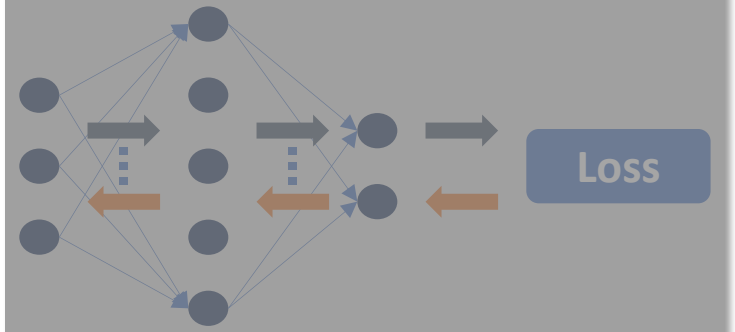
- Collecting data
- Preprocessing
- Dataset
- Data-loader

Step2



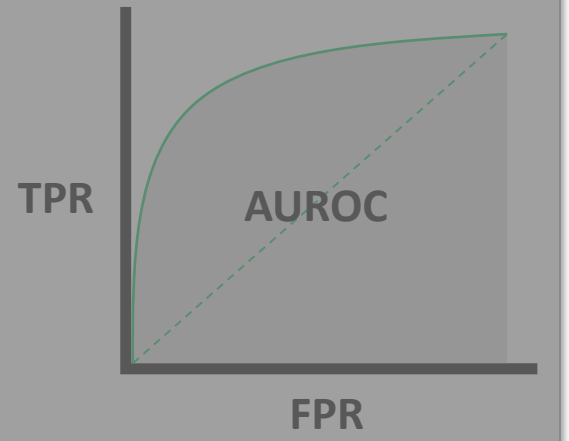
- Selecting method
- Building model

Step3



- Hyper-parameters
- Loss function
- Optimizer
- Training

Step4



- Predicting
- Evaluating

Step 1. Load dataset

```
### Load dataset ###
train_df = pd.read_csv('./toy_train.csv')
valid_df = pd.read_csv('./toy_valid.csv')

train_df.head()
```

	index	acc	sequence	labels
0	0	P63086	MAAAAAAGPEMVRGQVFDVGPRYTNLSYIGEGAYGMVCSAYDNLNK...	1
1	1	Q9UID3	MAAAAAAGPSPGSGPGDSPEGPEGEAPERRRKAHGMLKLYYGLSEG...	0
2	2	P51788	MAAAAAEEGMEPRALQYEQTLMYGRYTQDLGAFAKEEAARIRLGGP...	1
3	3	Q3UCQ1	MAAAAALSGAGAPPAGGGAGGGGSPPGGWAVARLEGREFEYLMKKR...	0
4	4	Q9NVF7	MAAAAEERMAEEGGGGQGDGGSSLASGSTQRQPPPPAPQHPQPGSQ...	0

Step 1. Load dataset

- Dataset은 데이터를 효율적으로 관리하고, 정형화된 방식으로 데이터를 가져오기 위함
- __getitem__과 __len__을 구현하여 데이터 접근과 크기 확인이 용이함
- 다양한 전처리를 쉽게 적용할 수 있음

```python
# Dataset 클래스 정의
class ProteinDataset(Dataset):
    def __init__(self, data):
        self.sequences = [" ".join(list(re.sub(r"[UZOB]", "X", sequence))) for sequence in data['sequence'].tolist()]
        self.labels = data['labels']

    def __len__(self):
        return len(self.sequences)

    def __getitem__(self, idx):
        return {
            "sequence" : self.sequences[idx],
            "label": self.labels[idx]
        }
```

```python
train_dataset = ProteinDataset(train_df)
valid_dataset = ProteinDataset(valid_df)
```

Step 1. Load dataset

- Dataloader는 Batch 단위로 데이터를 나누어 효율적인 배치 학습을 가능하게 함

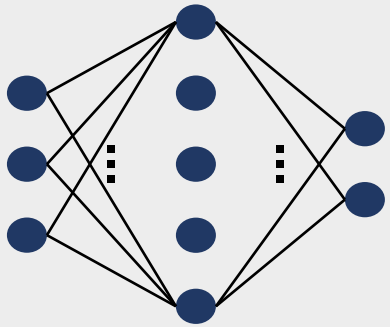
```
1 train_loader = DataLoader(train_dataset, batch_size=batch_size, shuffle=True)
2 valid_loader = DataLoader(valid_dataset, batch_size=batch_size, shuffle=False)
```

Deep Learning Process

Step1

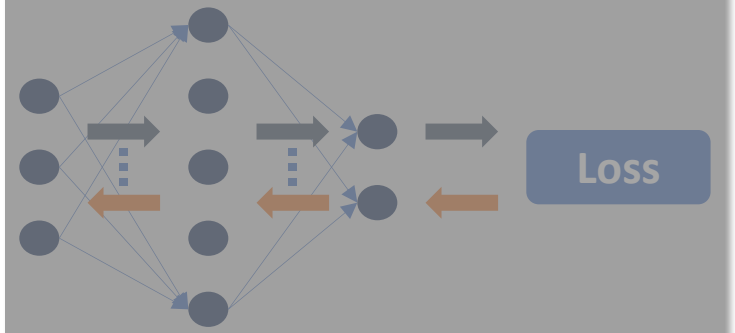
- Collecting data
- Preprocessing
- Dataset
- Data-loader

Step2



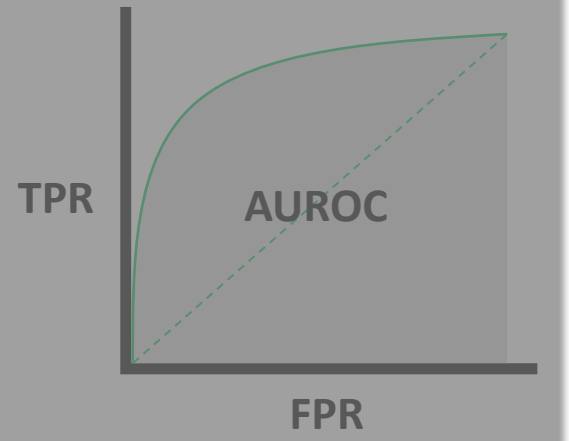
- Selecting method
- Building model

Step3



- Hyper-parameters
- Loss function
- Optimizer
- Training

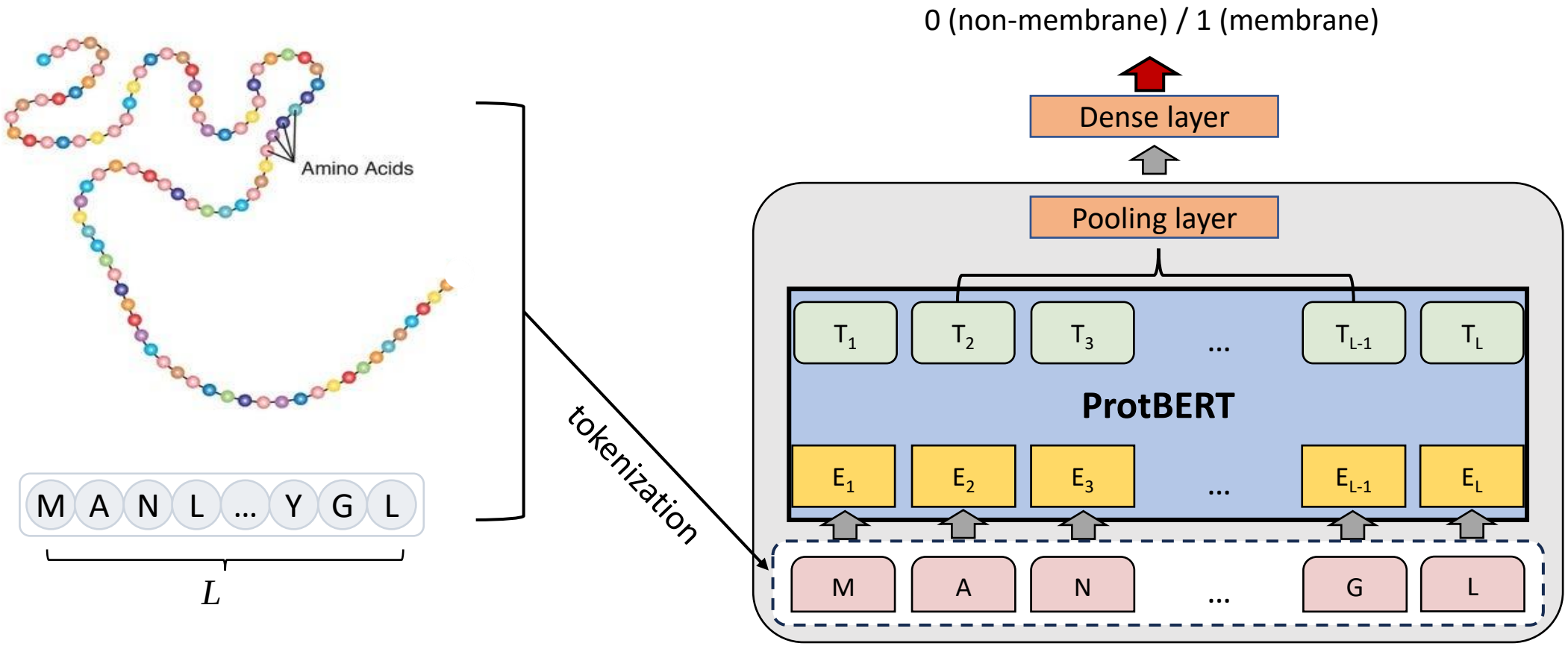
Step4



- Predicting
- Evaluating

Step 2. Build model

- Protein sequence를 tokenization 하기
- ProtBERT 네트워크 사용하기
- Protein-level embedding을 위하여 amino-acid embedding들을 pooling하기
- Dense layer 기반의 classifier 구성하여 예측하기



Step 2. Build model

- **Protein sequence를 tokenization 하기**
- ProtBERT 네트워크 사용하기
- Protein-level embedding을 위하여 amino-acid embedding들을 pooling하기
- Dense layer 기반의 classifier 구성하여 예측하기

```
5         self.tokenizer = BertTokenizer.from_pretrained(pretrained_model_name)
```

⋮

```
25      inputs = self.tokenizer.batch_encode_plus(
26          sequences, add_special_tokens = False,
27          max_length = 512,
28          padding=True,
29          truncation=True
30      )
```

Step 2. Build model

- Protein sequence를 tokenization 하기
- **ProtBERT 네트워크 사용하기**
- **Protein-level embedding을 위하여 amino-acid embedding들을 pooling하기**
- Dense layer 기반의 classifier 구성하여 예측하기

```
6         self.encoder = BertModel.from_pretrained(pretrained_model_name)
```

⋮

```
32      embeddings = self.encoder(
33          input_ids=torch.tensor(inputs["input_ids"]).to(self.device),
34          attention_mask=torch.tensor(inputs["attention_mask"]).to(self.device)
35      )
36      pooled_embeddings = torch.mean(embeddings[0], dim=1)
```

Step 2. Build model

- Protein sequence를 tokenization 하기
- ProtBERT 네트워크 사용하기
- Protein-level embedding을 위하여 amino-acid embedding들을 pooling하기
- **Dense layer 기반의 classifier 구성하여 예측하기**

```
        layers = []
        layers.append(nn.Linear(self.input_dim, hidden_dim))
        layers.append(nn.ReLU())
        layers.append(nn.Dropout(dropout))
        for _ in range(num_layers - 2):
            layers.append(nn.Linear(hidden_dim, hidden_dim))
            layers.append(nn.ReLU())
            layers.append(nn.Dropout(dropout))
        layers.append(nn.Linear(hidden_dim, num_classes))
        self.classifier = nn.Sequential(*layers)
```

⋮

```
    logits = self.classifier(pooled_embeddings)
```

Deep Learning Process

Step1

- Collecting data
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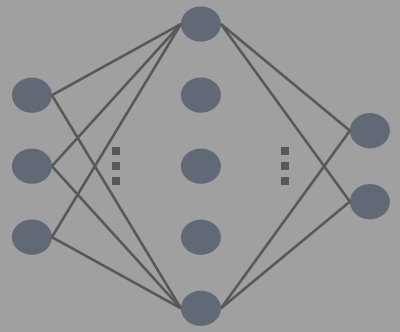
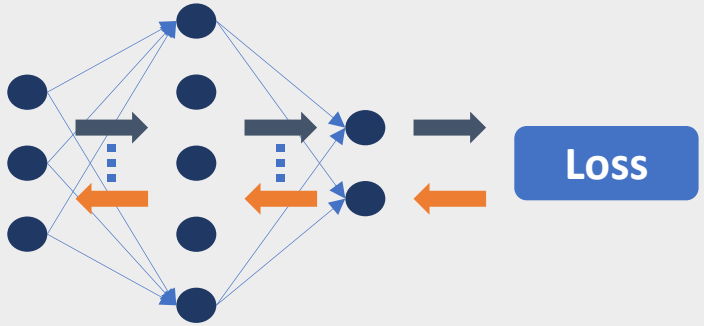
- Data-loader

Step2



- Selecting method
- Building model

Step3



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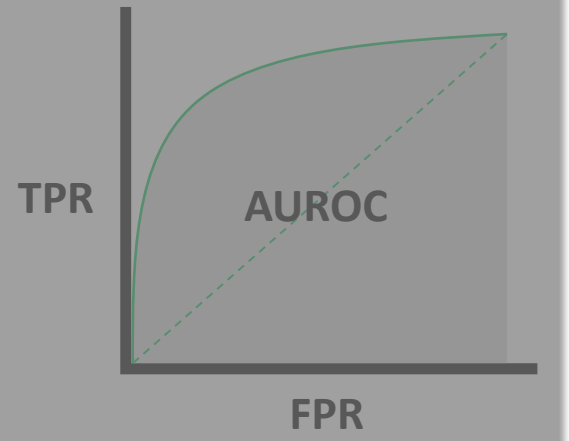

- Predicting
- Evaluating

Step 3. Training

```python
# 주요 설정
device = torch.device("cuda" if torch.cuda.is_available() else "cpu")

pretrained_model_name = "Rostlab/prot_bert"
num_classes = 2  # membrane or non-membrane
hidden_dim = 64  # 히든 레이어의 차원
num_layers = 3  # 레이어 수
batch_size = 64
epochs = 1  # 최대 에포크 수
learning_rate = 0.001
dropout = 0.0  # 드롭아웃 확률
```

```python
# 모델 초기화
model = DeeplocPredictor(pretrained_model_name, hidden_dim, num_classes, device, num_layers=num_layers, dropout=dropout).to(device)
criterion = nn.CrossEntropyLoss()
optimizer = torch.optim.AdamW(filter(lambda p: p.requires_grad, model.parameters()), lr=learning_rate)
```

Step 3. Training

- Epoch : 데이터셋 전체를 한 번 학습하는 주기
- Batch : 데이터셋을 나눈 작은 묶음
- Training loop는 각 epoch마다 모든 batch를 반복 학습하며, 각 batch마다 모델이 손실(loss)을 계산하고, 이를 통해 역전파 (backpropagation)로 가중치를 업데이트 하는 과정

```
for epoch in range(epochs) :          # 사용자가 정의한 epoch 만큼 학습 진행
  model.train()                       #  model을 training mode로 변경
  ⋮
  for batch in train_loader :         # batch 마다 모델 파라미터를 업데이트
    ⋮
    outputs = model(batch)            # 모델에 batch를 입력으로 넣어 output 계산
    loss = criterion(outputs, labels) # output과 label 사이의 오차 (loss) 계산
    loss.backward()                   # loss function의 gradient를 계산
    optimizer.step()                  # 계산된 gradient를 기반으로 하여 weight update 진행
    optimizer.zero_grad()             # 다음 step을 위하여 gradient 초기화
    ⋮
```

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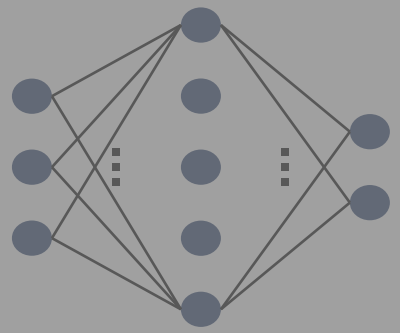

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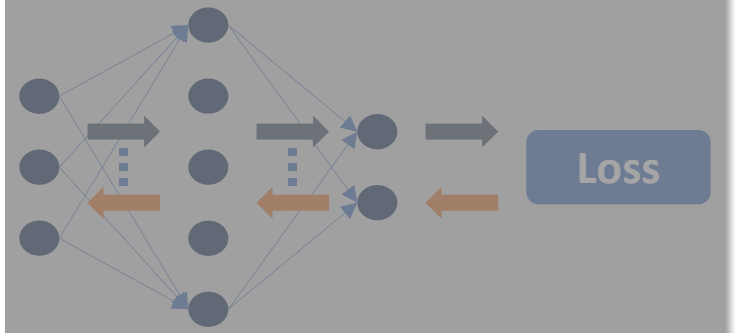

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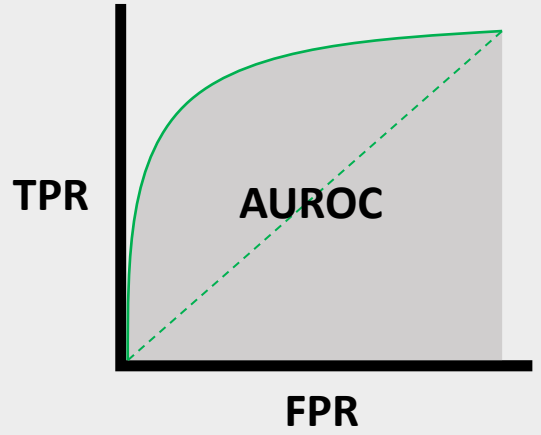


- Predicting
- Evaluating

Step 4. Evaluation

- Validation 단계에서는 모델의 성능을 평가하는 과정이므로 가중치 업데이트를 진행하지 않음
- model.eval()을 호출하여 모델을 평가모드로 전환
- With torch.no_grad()를 사용하여 미분 계산을 비활성화하여 메모리 사용을 줄이고, 계산 속도를 높임

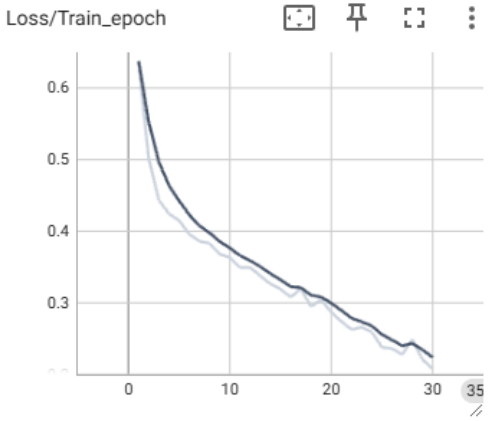
```
for epoch in range(epochs) :            # 사용자가 정의한 epoch 만큼 학습 진행
  model.eval()                          #  model을 evaluation mode로 변경
  ⋮
  with torch.no_grad():                 # gradient 계산 비활성화
    for batch in valid_loader :           # batch 마다 forward propagation 진행
      ⋮
      outputs = model(batch)            # 모델에 batch를 입력으로 넣어 output 계산
      loss = criterion(outputs, labels) # output과 label 사이의 오차 (loss) 계산
      ⋮
```

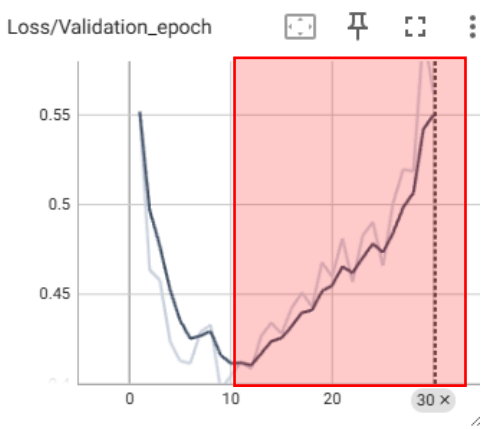
Visualization

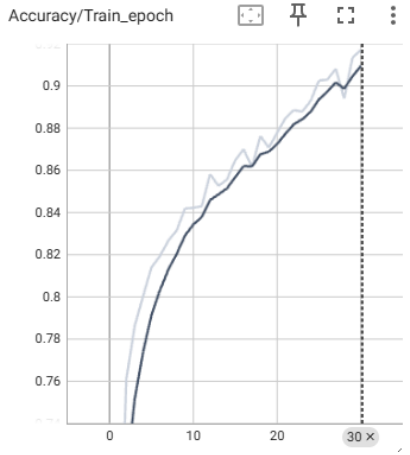
```
# TensorBoard writer 초기화
tensorboard_log_dir = "runs/deeploc_membrane_prediction"
os.makedirs(tensorboard_log_dir, exist_ok=True)
writer = SummaryWriter(tensorboard_log_dir)
```

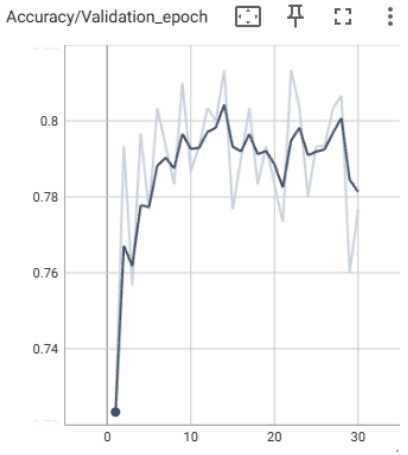
```
# TensorBoard에 Training 기록
writer.add_scalar('Loss/Train', avg_train_loss, epoch + 1)
writer.add_scalar('Accuracy/Train', train_accuracy, epoch + 1)
```

```
# TensorBoard에 Validation 기록
writer.add_scalar('Loss/Validation', avg_val_loss, epoch + 1)
writer.add_scalar('Accuracy/Validation', val_accuracy, epoch + 1)
```









Link Prediction

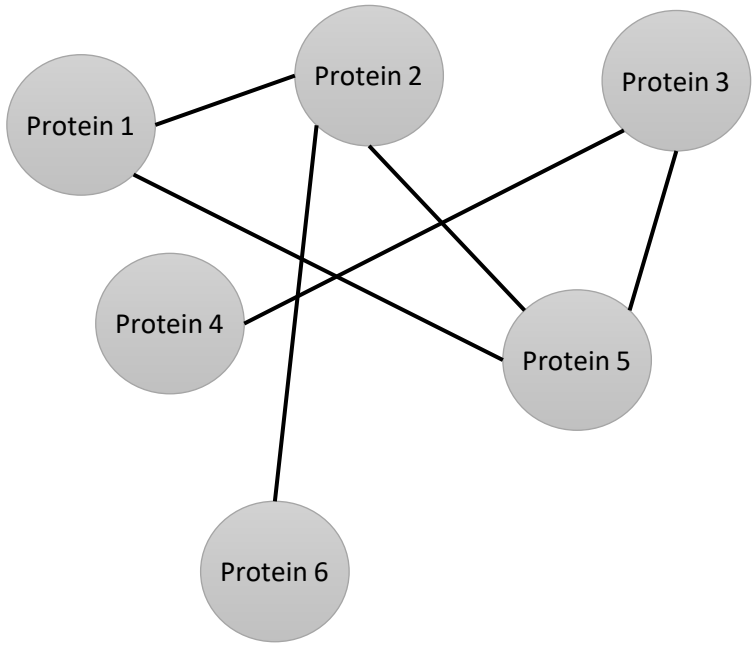
Dataset

PPI (Protein-Protein Interaction)

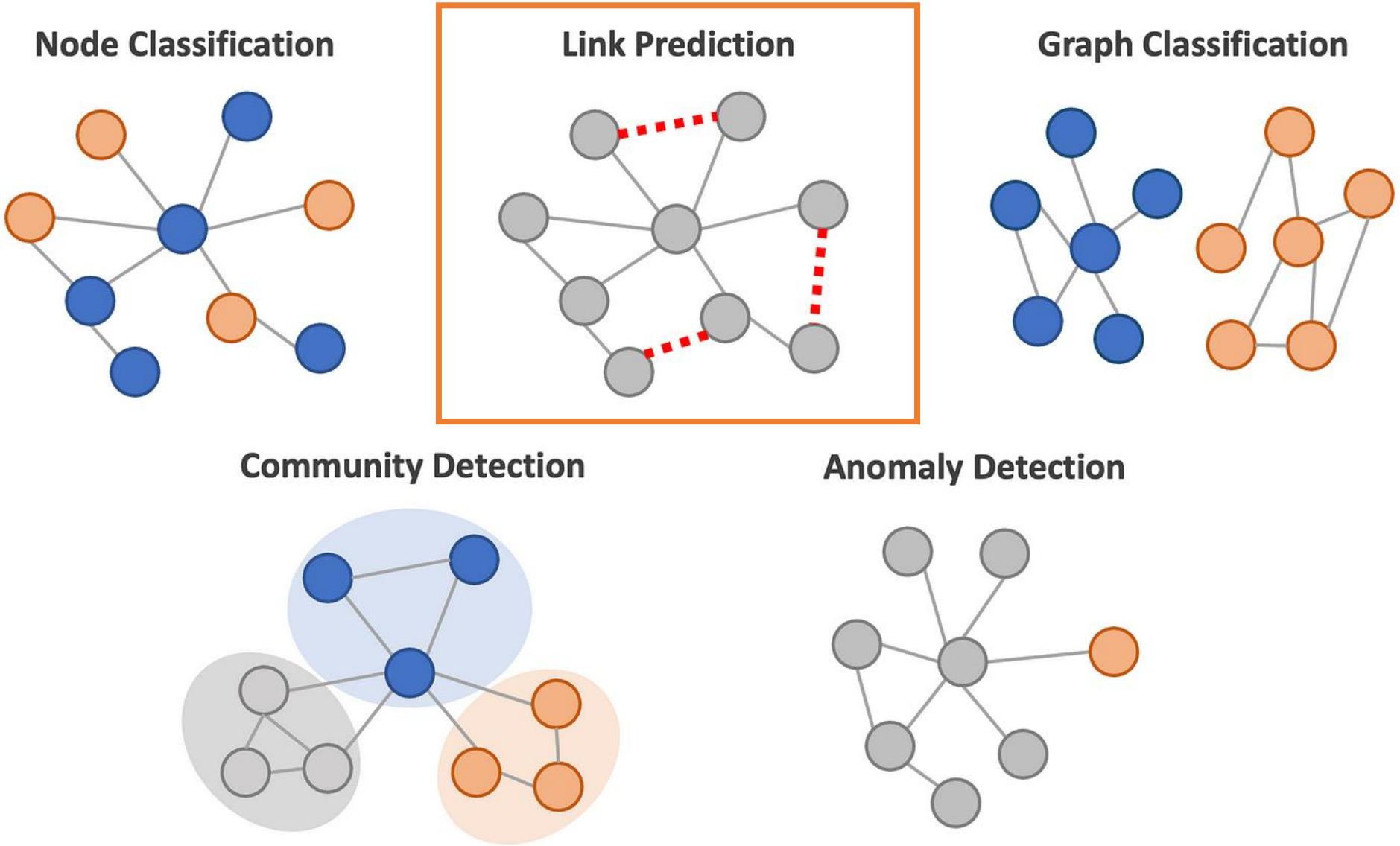
- This networks from the "Predicting Multicellular Function through Multi-layer Tissue Networks" paper
- Containing 50 features (positional gene sets, motif gene sets and immunological signatures, …)
- https://pytorch-geometric.readthedocs.io/en/stable/generated/torch_geometric.datasets.PPI.html#torch_geometric.datasets.PPI

#graphs	#nodes	#edges	#features
20	~2,245.3	~61,318.4	50

PPI Grpah Example



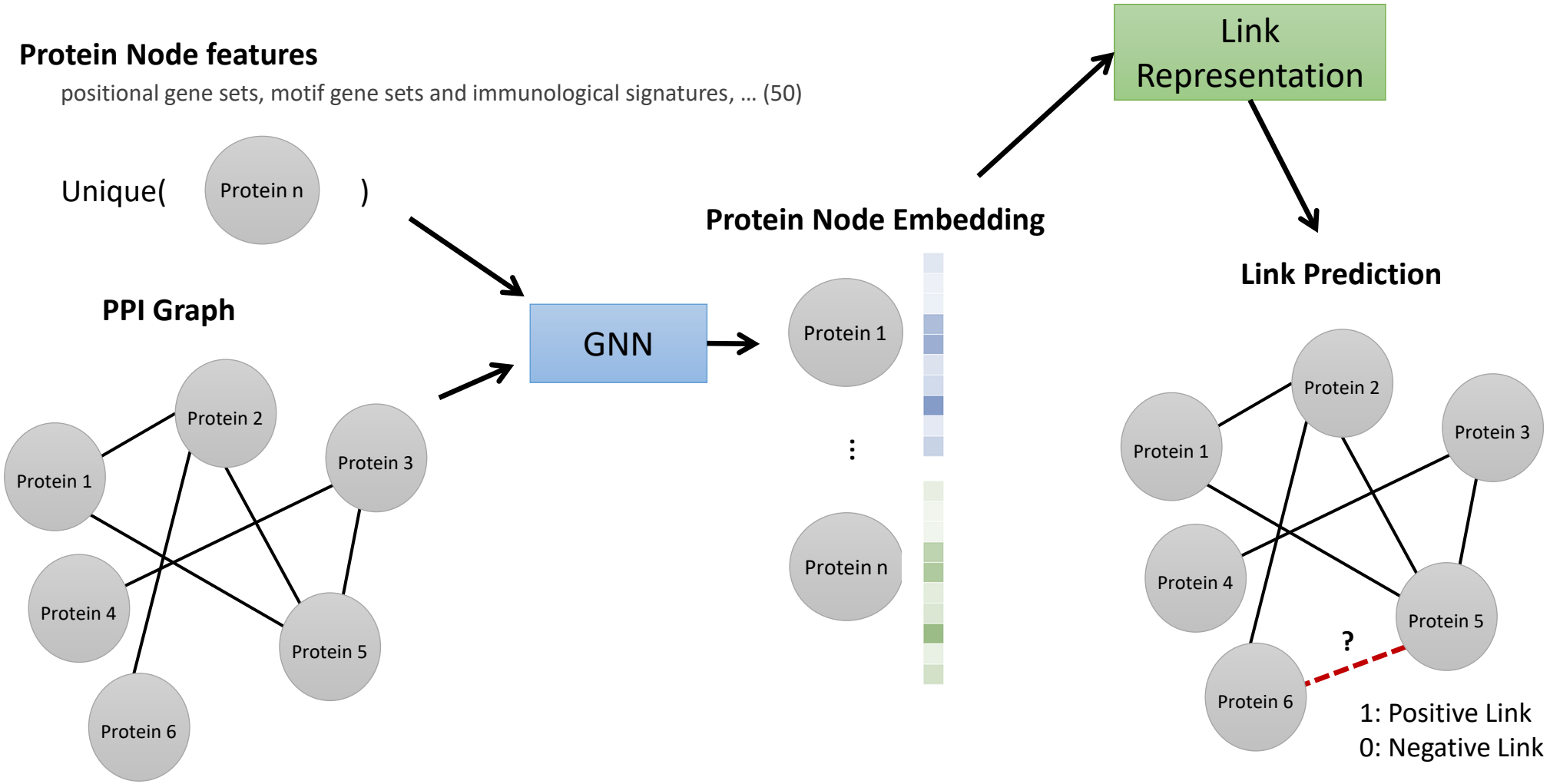
Tasks of Graph



https://towardsdatascience.com/graph-neural-networks-with-pyg-on-node-classification-link-prediction-and-anomaly-detection-14aa38fe1275

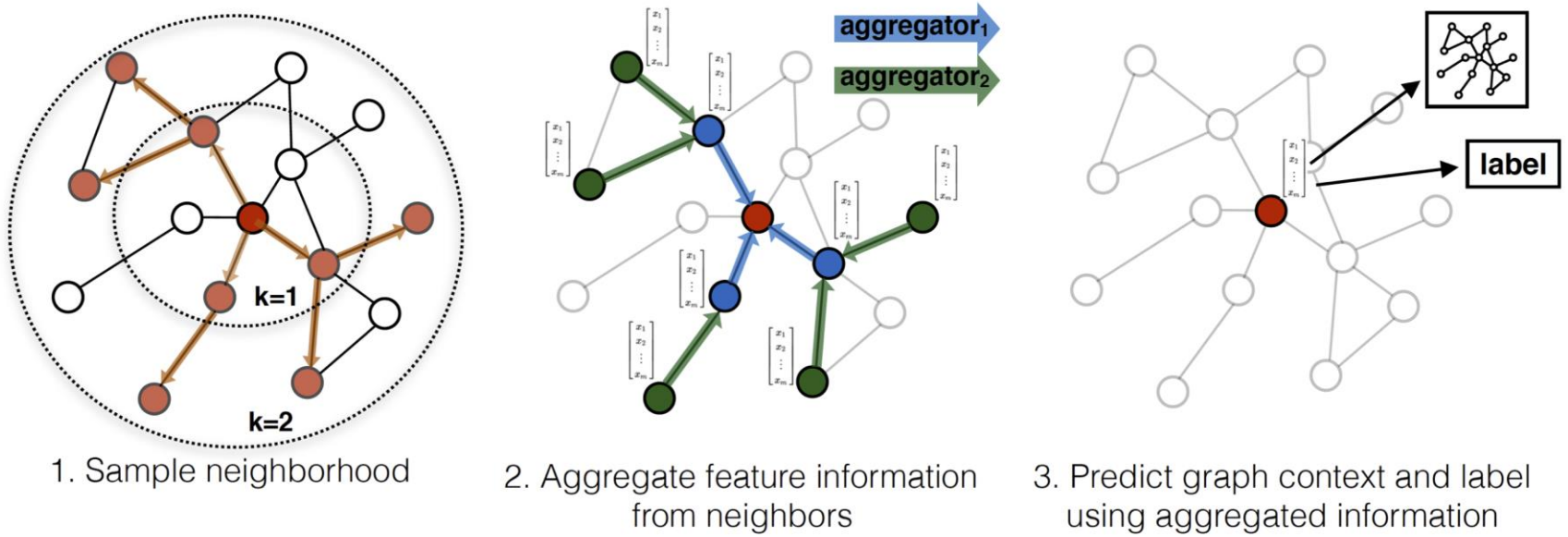
Link Prediction

Pipeline



GNN Model

GraphSAGE https://arxiv.org/pdf/1706.02216



1. Sample neighborhood
2. Aggregate feature information from neighbors
3. Predict graph context and label using aggregated information

1. **특정 단백질의 주변 이웃을 샘플링**

   사용자가 정의한 k-hop 단계의 이웃을 포함하여 정보를 추출

2. **이웃 특징 정보 집계**

   샘플링된 이웃의 특징 벡터를 학습 가능한 집계 함수(aggregator)를 사용하여 통합

   Aggregator에는 Mean, LSTM, Pooling 등이 사용될 수 있음

3. **그래프 문맥과 노드 레이블 예측**

   집계된 정보를 바탕으로 단백질의 기능 또는 소속 그룹(노드 레이블)을 예측

   전체 그래프의 문맥을 반영하여 단백질 간의 관계를 파악할 수 있음

Environment

- **Python3**
  - **Pytorch**

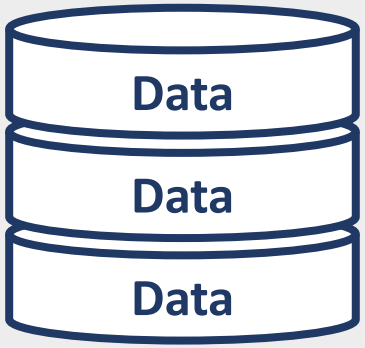
```
pip install torch
```

  - **Pytorch Geometric**

```
pip install torch-geometric
```

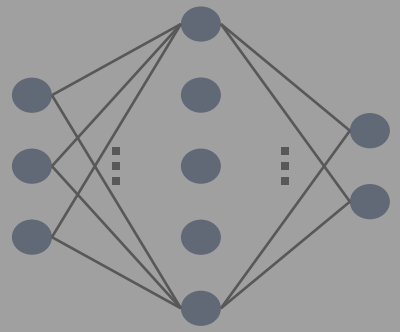
Deep Learning Process

Step1



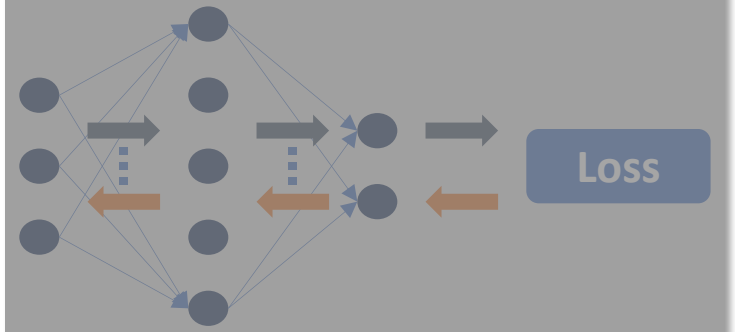
- Collecting data
- Preprocessing
- Dataset
- Data-loader

Step2



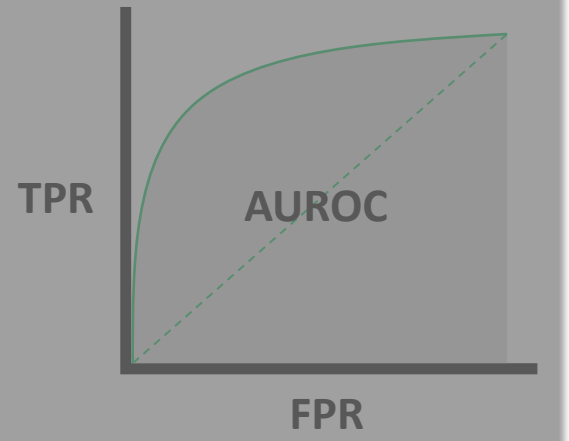
- Selecting method
- Building model

Step3



- Hyper-parameters
- Loss function
- Optimizer
- Training

Step4



- Predicting
- Evaluating

Step 1. Load dataset

```python
# Load Dataset
from torch_geometric.datasets import PPI
ppi = PPI(root="./data/PPI")  # 데이터셋 다운로드 및 로드

# 첫 번째 서브그래프 사용
data = ppi[0]

print("Number of nodes: ", data.num_nodes)  # 그래프의 노드 개수 출력
print("Number of edges: ", data.edge_index.size(1))  # 그래프의 엣지 개수 출력

print("Edges shape: ", data.edge_index.shape) #엣지 인덱스 차원
print("Edge index: \n", data.edge_index) # 엣지 인덱스 구성

print("Node feature shape: ", data.x.shape)  # 노드 특성의 차원 확인 (50차원 제공)
print("Node feature Example: \n", data.x[0]) # 노드 특성 예시

print(data) # 그래프 전체 구성
```

그래프의 노드 개수 `Number of nodes:  1767`

그래프의 엣지 개수 `Number of edges:  32318`

엣지 인덱스 차원 `Edges shape:  torch.Size([2, 32318])`

엣지 인덱스 구성

```
Edge index:
 tensor([[   0,    0,    0,  ..., 1744, 1745, 1749],
         [ 372, 1101,  766,  ..., 1745, 1744, 1739]])
```

노드 특성 차원 확인 (50차원) `Node feature shape:  torch.Size([1767, 50])`

노드 특성 예시

```
Node feature Example:
 tensor([-0.0855, -0.0884, -0.1128, -0.1719, -0.0766, -0.1003, -0.0751, -0.1149,
         -0.1212, -0.0994,  0.0000, -0.1699, -0.0428, -0.1123, -0.0760, -0.1152,
         -0.1031, -0.1120, -0.1435, -0.0975, -0.0875, -0.1457, -0.1234, -0.1242,
         -0.0976, -0.1197, -0.1161, -0.0735, -0.0667, -0.0873, -0.1797, -0.1447,
         -0.1606, -0.1582, -0.1477, -0.4350, -0.1617, -0.1556, -0.1526, -0.1396,
         -0.1281, -0.1539, -0.1593, -0.1546, -0.1466, -0.1449, -0.1568, -0.1399,
         -0.1494, -0.1481])
```

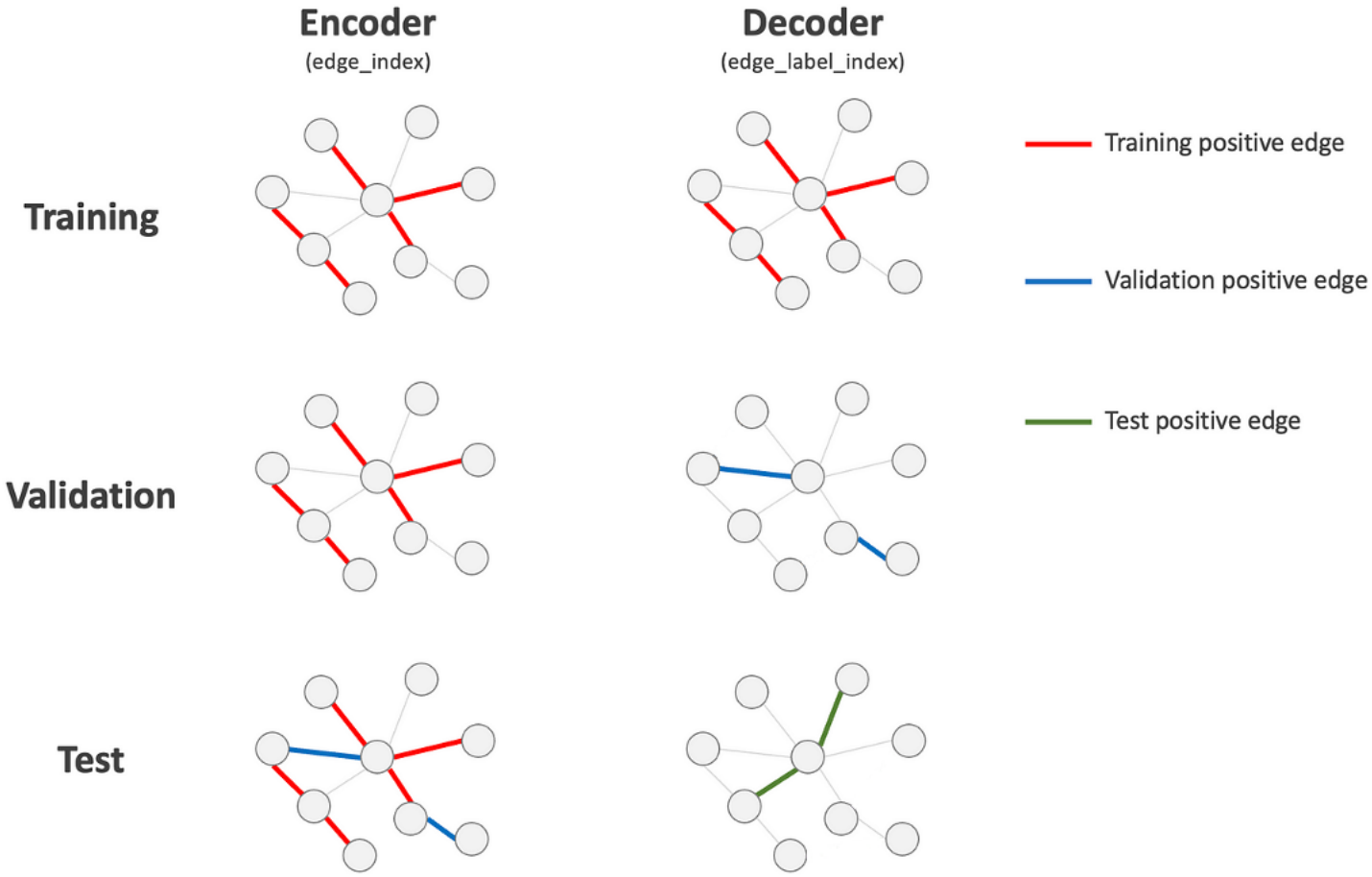
그래프 전체 구성 `Data(x=[1767, 50], edge_index=[2, 32318], y=[1767, 121])`

Step 1. Load dataset

```python
from torch_geometric.transforms import RandomLinkSplit

# 데이터셋 분리 (학습, 검증, 테스트)
# RandomLinkSplit은 데이터를 학습, 검증, 테스트 세트로 나눕니다.
# 엣지의 70%를 학습용, 10%를 검증용, 20%를 테스트용으로 사용합니다.
transform = RandomLinkSplit(
    num_val=0.1,
    num_test=0.2,
    add_negative_train_samples=False,
    disjoint_train_ratio=0.3,
    neg_sampling_ratio=0)

train_data, val_data, test_data = transform(data)
print("Train: ", train_data)
print("Validation: ", val_data)
print("Test: ", test_data)
```



Encoder: Grpah 구조 학습을 위한 Link
Decoder: Supervision을 위해 사용하는 Link

```
Train:  Data(x=[1767, 50], edge_index=[2, 15837], y=[1767, 121], edge_label=[6787], edge_label_index=[2, 6787])
Validation:  Data(x=[1767, 50], edge_index=[2, 22624], y=[1767, 121], edge_label=[3231], edge_label_index=[2, 3231])
Test:  Data(x=[1767, 50], edge_index=[2, 25855], y=[1767, 121], edge_label=[6463], edge_label_index=[2, 6463])
```

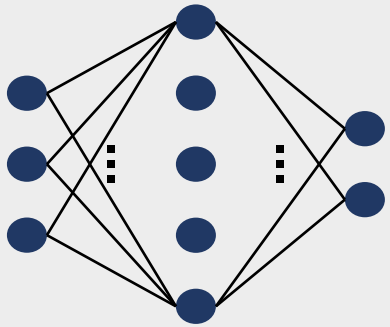
https://towardsdatascience.com/graph-neural-networks-with-pyg-on-node-classification-link-prediction-and-anomaly-detection-14aa38fe1275

Deep Learning Process

Step1

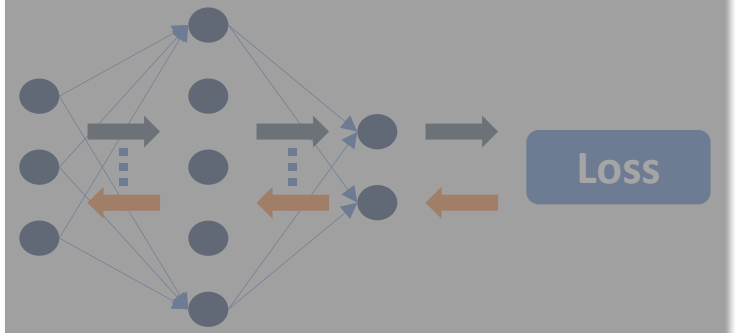
- Collecting data
- Preprocessing
- Dataset
- Data-loader

Step2



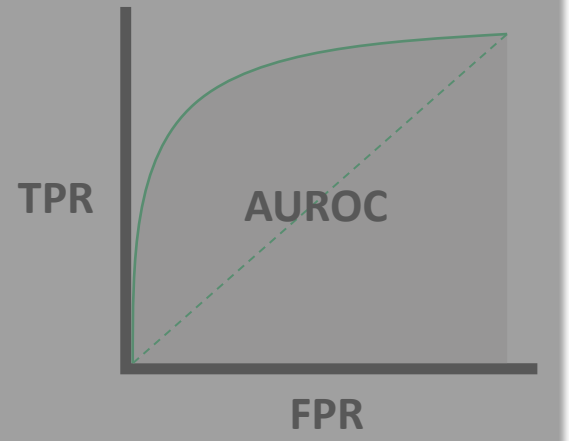
- Selecting method
- Building model

Step3



- Hyper-parameters
- Loss function
- Optimizer
- Training

Step4



- Predicting
- Evaluating

Step 2. Build model

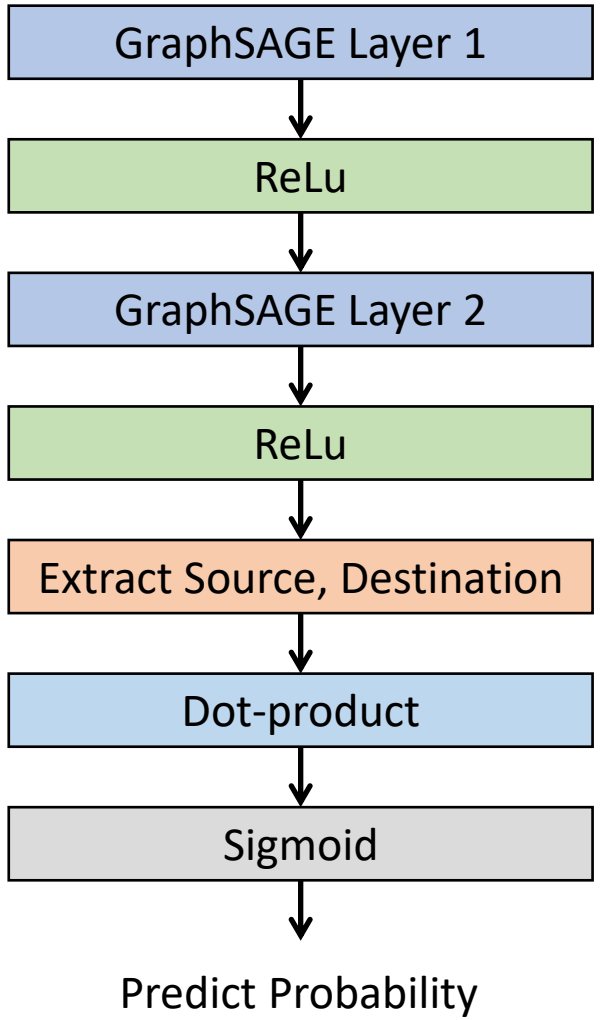
```python
import torch
import torch.nn as nn
import torch.nn.functional as F
from torch_geometric.nn import SAGEConv

# 모델 정의
# GraphSAGE 레이어를 사용하는 모델 정의
class GNNForLinkPrediction(nn.Module):
    def __init__(self, in_channels, hidden_channels):
        super().__init__()
        # SAGEConv 레이어 정의
        self.conv1 = SAGEConv((-1, -1), hidden_channels)  # 첫 번째 GraphSAGE 레이어
        self.conv2 = SAGEConv(hidden_channels, hidden_channels)  # 두 번째 GraphSAGE 레이어

    def forward(self, x, edge_index, edge_label_index):
        # 첫 번째 GraphSAGE 레이어를 통과시키고 ReLU 활성화 함수 적용
        x = F.relu(self.conv1(x, edge_index))
        # 두 번째 GraphSAGE 레이어를 통과
        x = F.relu(self.conv2(x, edge_index))
        src, dst = edge_label_index

        # 소스 및 타겟 노드의 임베딩 추출 및 점곱 계산
        src, dst = edge_label_index  # 엣지의 소스와 타겟 노드 인덱스
        edge_pred = torch.sigmoid((x[src] * x[dst]).sum(dim=-1))  # dotproduct로 스칼라 값 출력
        return edge_pred

# 모델 초기화
model = GNNForLinkPrediction(
    in_channels=train_data.num_features,
    hidden_channels=64  # 은닉층의 차원
)
```

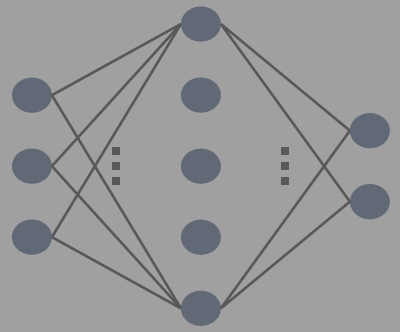


Deep Learning Process

Step1

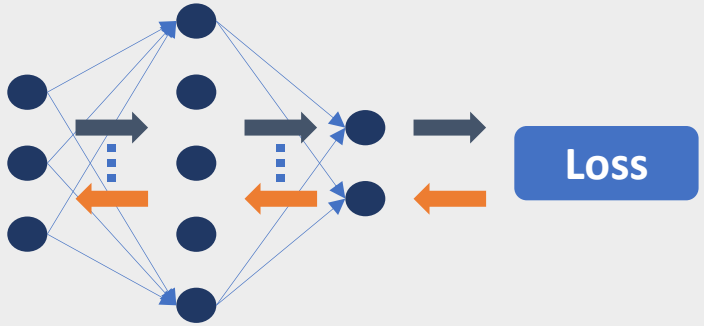
- Collecting data
- Preprocessing
- Dataset
- Data-loader

Step2



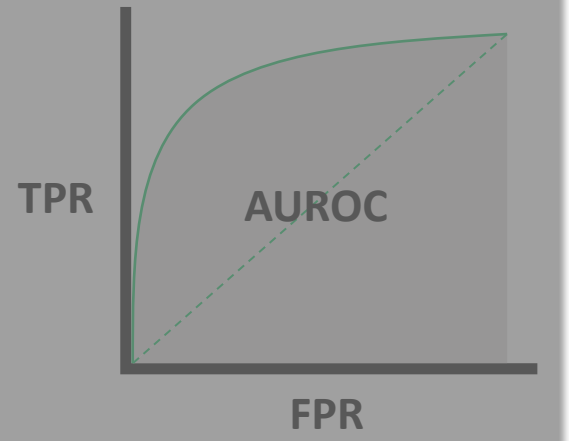
- Selecting method
- Building model

Step3



- Hyper-parameters
- Loss function
- Optimizer
- Training

Step4



- Predicting
- Evaluating

Step 3. Training

Batch 생성을 위한 Subgraph 생성하는 Loader 구성

사용하는 Data(Train, Validation, Test)에 대해 각각 모두 구성 필요

[torch geometric의 LinkNeighborLoader Option]

- batch_size : Batch 크기
- edge_label_index : Supervision에 사용하는 엣지 인덱스
- num_neighbors : 각 Layer에서 샘플링할 이웃 노드 수
- neg_sampling_ratio : negative edge를 생성할 비율 (positive edge 대비)
- shuffle : Data shuffle 여부 (Training의 경우에만, 특정 패턴 학습에 대한 overfitting 방지를 위해 True)

```python
from torch_geometric.loader import LinkNeighborLoader
# 데이터 로더 설정
# LinkNeighborLoader는 이웃 노드 샘플링을 통해 배치를 생성합니다.
train_loader = LinkNeighborLoader(
    train_data,
    batch_size=32,  # 배치 크기
    edge_label_index=train_data.edge_label_index,  # 학습용 엣지 레이블 인덱스
    num_neighbors=[10, 10],  # 각 레이어에서 샘플링할 이웃 노드 수
    neg_sampling_ratio=1.0,  # negative edge를 positive edge 수의 1배로 샘플링
    shuffle=True
)

val_loader = LinkNeighborLoader(
    val_data,
    batch_size=32,
    edge_label_index=val_data.edge_label_index,
    num_neighbors=[10, 10],
    neg_sampling_ratio=1.0,
    shuffle=False
)

test_loader = LinkNeighborLoader(
    test_data,
    batch_size=32,
    edge_label_index=test_data.edge_label_index,
    num_neighbors=[10, 10],
    neg_sampling_ratio=1.0,
    shuffle=False
)
```

Step 3. Training

Training loop는 각 epoch마다 모든 batch (앞서 생성한 subgraph)를 반복 학습하며

각 Batch 마다 모델이 손실(loss)를 계산하며, 이를 역전파(Backpropagation)로 가중치를 업데이트

```python
# 학습 및 검증
for epoch in range(10):
    print(f"\nEpoch {epoch+1}:")
    train_loss = train()  # 학습 수행
    val_loss, val_auc, _, _ = evaluate(val_loader, epoch, mode="Validation")
    print(f"Train Loss: {train_loss:.4f}, Validation Loss: {val_loss:.4f}")
```

```python
# 학습 루프 정의
def train():
    model.train()  # 모델을 학습 모드로 설정
    total_loss = 0
    loop = tqdm(train_loader, desc="Training")  # tqdm으로 학습 상태 표시
    for batch in loop:
        optimizer.zero_grad()  # 옵티마이저의 그래디언트 초기화
        edge_pred = model(batch.x, batch.edge_index, batch.edge_label_index)  # 모델 출력 계산
        loss = criterion(edge_pred, batch.edge_label.float())  # 손실 계산
        loss.backward()  # 역전파 단계
        optimizer.step()  # 가중치 업데이트

        total_loss += loss.item()
        loop.set_postfix(loss=loss.item())  # tqdm 진행 상태에 현재 손실 표시
    avg_loss = total_loss / len(train_loader)
    writer.add_scalar("Loss/Train", avg_loss, epoch)  # TensorBoard 기록
    return avg_loss
```

Step 3. Training

Validation 단계에서는 모델의 성능을 평가하는 과정으로, 가중치 업데이트를 진행하지 않음

model.eval()을 통해 모델을 평가 모드로 설정

with torch._nograd()를 사용하여 미분 계산을 비활성화하여 메모리 사용을 줄이고 계산 속도를 높임

```python
# 평가 함수 정의
def evaluate(loader, epoch, mode="Validation"):
    model.eval()  # 모델을 평가 모드로 설정
    preds, labels = [], []
    loop = tqdm(loader, desc="Evaluating")  # tqdm으로 평가 상태 표시
    with torch.no_grad():  # 그래디언트 계산 비활성화
        for batch in loop:
            edge_pred = model(batch.x, batch.edge_index, batch.edge_label_index)  # 모델 출력 계산
            preds.append(edge_pred.cpu())  # 예측값 저장
            labels.append(batch.edge_label.cpu())  # 실제 라벨 저장
    preds, labels = torch.cat(preds), torch.cat(labels)
    loss = criterion(preds, labels.float()).item()
    auc = roc_auc_score(labels, preds)
    writer.add_scalar(f"Loss/{mode}", loss, epoch)  # TensorBoard 기록
    writer.add_scalar(f"AUC/{mode}", auc, epoch)
    return loss, auc, preds, labels
```

```
Epoch 1:
Training: 100%|██████████| 213/213 [00:03<00:00, 68.09it/s, loss=0.81]
Evaluating: 100%|██████████| 101/101 [00:00<00:00, 180.07it/s]
Train Loss: 0.6756, Validation Loss: 0.6614

                                    ...

Epoch 10:
Training: 100%|██████████| 213/213 [00:03<00:00, 63.33it/s, loss=0.462]
Evaluating: 100%|██████████| 101/101 [00:00<00:00, 175.79it/s]
Train Loss: 0.5936, Validation Loss: 0.6256
```

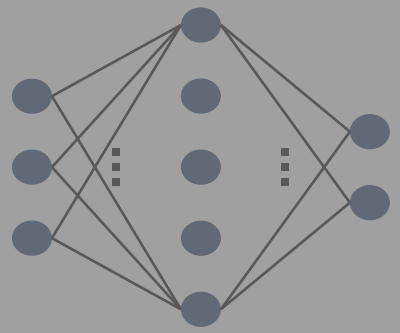
→ Validation Loss도 함께 확인하여 모델 Overfitting 정도 확인

Deep Learning Process

Step1

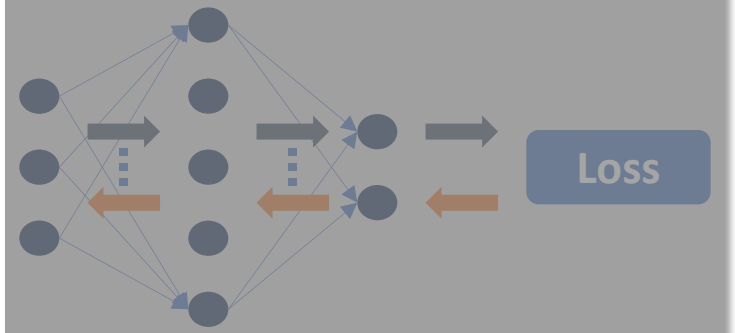
- Collecting data
- Preprocessing
- Dataset
- Data-loader

Step2



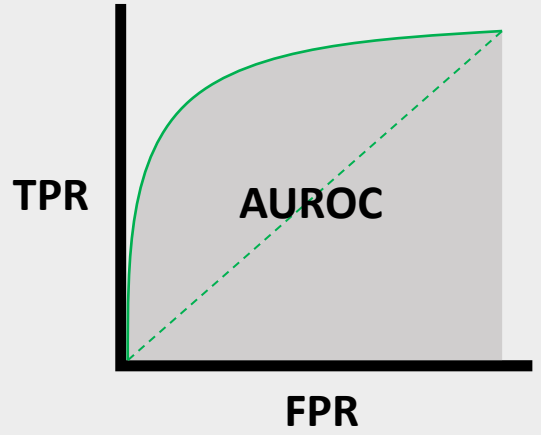
- Selecting method
- Building model

Step3



- Hyper-parameters
- Loss function
- Optimizer
- Training

Step4



- Predicting
- Evaluating

Step 4. Evaluation

모델 학습이 모두 완료된 후, 테스트 데이터에 대한 모델 성능 평가 진행

```
# 테스트
# 테스트 데이터에서 모델 성능 평가
print("\nEvaluating Test Set")
test_loss, test_auc, test_preds, test_labels = evaluate(test_loader, 10, mode="Test")
print(f"\nTest Loss: {test_loss:.4f}, Test AUC: {test_auc:.4f}")
```

```
Evaluating Test Set
Evaluating: 100%|██████████| 202/202 [00:01<00:00, 201.23it/s]
Test Loss: 0.6222, Test AUC: 0.8244
```

테스트 데이터에서 실제 예측이 어떻게 이루어졌는지 5개의 예시 확인

Positive link threshold = 0.5

```
Test Edge 1: (src: 1518, dst: 498)
Prediction Probability: 0.8915, Predicted Label: 1, Ground Truth: 1.0

Test Edge 2: (src: 1053, dst: 496)
Prediction Probability: 0.9009, Predicted Label: 1, Ground Truth: 1.0

Test Edge 3: (src: 425, dst: 366)
Prediction Probability: 0.5270, Predicted Label: 1, Ground Truth: 1.0

Test Edge 4: (src: 311, dst: 646)
Prediction Probability: 0.8610, Predicted Label: 1, Ground Truth: 1.0

Test Edge 5: (src: 1497, dst: 890)
Prediction Probability: 0.7808, Predicted Label: 1, Ground Truth: 1.0
```

```
# 테스트 데이터에서 예측 예시 출력
def print_test_examples(num_examples=5):
    #테스트 데이터에서 예측값, 실제값, 원래 엣지 정보를 출력합니다.
    for i in range(num_examples):  # num_examples만큼 출력
        # 테스트 데이터의 원래 엣지 인덱스 추출
        test_edge_index = test_data.edge_label_index[:, i]  # 원래 엣지의 (src, dst) 인덱스
        test_edge_src, test_edge_dst = test_edge_index[0].item(), test_edge_index[1].item()

        # 모델의 예측값과 실제 라벨
        test_example_pred = test_preds[i].item()
        test_example_label = test_labels[i].item()
        predicted_label = 1 if test_example_pred > 0.5 else 0  # 예측 라벨 계산 threshold 0.5

        # 결과 출력
        print(f"Test Edge {i + 1}: (src: {test_edge_src}, dst: {test_edge_dst})")
        print(f"Prediction Probability: {test_example_pred:.4f}, Predicted Label: {predicted_label}, Ground Truth: {test_example_label}\n")

# 테스트 예시 출력
print_test_examples(num_examples=5)  # 상위 5개 예시 출력
```

Visualization

```
# TensorBoard
print("To visualize results in Colab, run:")
print("%load_ext tensorboard")
print(f"%tensorboard --logdir {log_dir}")
writer.close()
```

```
%load_ext tensorboard
%tensorboard --logdir /content/runs/ppi_link_prediction
```