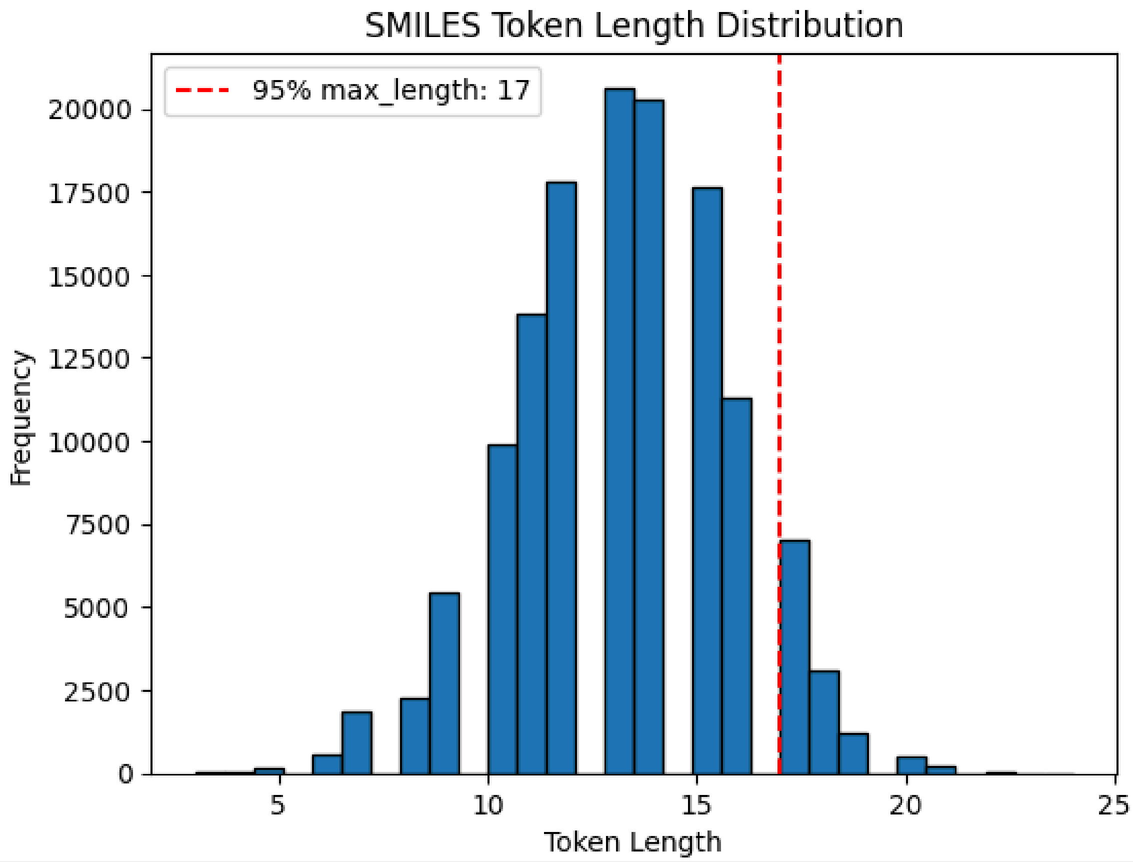
데이터 준비

max_length 계산

```
import pandas as pd
from transformers import RobertaTokenizer

# QM9 데이터셋 로드
file_path = "/content/qm9.csv"
qm9_data = pd.read_csv(file_path)

# ChemBERTa 토크나이저 로드
tokenizer = RobertaTokenizer.from_pretrained("seyonec/ChemBERTa-zinc-base-v1")

# 각 SMILES의 토큰 길이 계산 함수
def calculate_token_length(smiles):
    tokens = tokenizer(smiles, return_tensors="pt", padding=False, truncation=False)
    return len(tokens["input_ids"][0])

# 각 SMILES의 토큰 길이 계산 및 데이터프레임에 추가
qm9_data["token_length"] = qm9_data["smiles"].apply(calculate_token_length)

# 길이 분포 통계 확인
length_stats = qm9_data["token_length"].describe()
print("SMILES Token Length Statistics:")
print(length_stats)

# 95% 백분위수 계산
max_length_95 = int(qm9_data["token_length"].quantile(0.95))
print(f"95%의 SMILES는 {max_length_95} 토큰 이하의 길이를 가집니다.")

# 길이 분포 히스토그램 시각화 (선택적)
import matplotlib.pyplot as plt

plt.hist(qm9_data["token_length"], bins=30, edgecolor="k")
plt.axvline(max_length_95, color="r", linestyle="--", label=f"95% max_length: {max_length_95}")
plt.title("SMILES Token Length Distribution")
plt.xlabel("Token Length")
plt.ylabel("Frequency")
plt.legend()
plt.show()
```

```
SMILES Token Length Statistics:
count    133885.000000
mean         13.157829
std           2.571324
min           3.000000
25%          11.000000
50%          13.000000
75%          15.000000
max          24.000000
Name: token_length, dtype: float64
95%의 SMILES는 17 토큰 이하의 길이를 가집니다.
```



Canonical SMILES 변환

```
!pip install rdkit
```

```
Collecting rdkit
  Downloading rdkit-2024.3.6-cp310-cp310-manylinux_2_28_x86_64.whl.metadata (4.0 kB)
Requirement already satisfied: numpy in /usr/local/lib/python3.10/dist-packages (from rdkit) (1.
Requirement already satisfied: Pillow in /usr/local/lib/python3.10/dist-packages (from rdkit) (1
Downloading rdkit-2024.3.6-cp310-cp310-manylinux_2_28_x86_64.whl (32.8 MB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 32.8/32.8 MB
Installing collected packages: rdkit
Successfully installed rdkit-2024.3.6
```

```
# non Canonical SMILES 비율 확인

from rdkit import Chem
import pandas as pd
```

```
# QM9 데이터셋 로드
file_path = "/content/qm9.csv"  # QM9 데이터 파일 경로
qm9_data = pd.read_csv(file_path)

# Canonical SMILES 확인 함수
def is_canonical(smiles):
    try:
        mol = Chem.MolFromSmiles(smiles)  # SMILES 문자열을 Mol 객체로 변환
        if mol is None:
            return False  # 변환 실패
        canonical_smiles = Chem.MolToSmiles(mol, canonical=True)  # Canonical SMILES 생성
        return smiles == canonical_smiles  # 원본과 Canonical SMILES 비교
    except Exception as e:
        return False  # 예외 발생 시 False 반환

# Canonical SMILES 여부 확인
qm9_data["is_canonical"] = qm9_data["smiles"].apply(is_canonical)

# 결과 통계
canonical_count = qm9_data["is_canonical"].sum()
non_canonical_count = len(qm9_data) - canonical_count

print(f"Total samples checked: {len(qm9_data)}")
print(f"Canonical SMILES count: {canonical_count}")
print(f"Non-canonical SMILES count: {non_canonical_count}")
```

```
Total samples checked: 133885
Canonical SMILES count: 51287
Non-canonical SMILES count: 82598
Non-canonical SMILES samples have been saved to 'non_canonical_smiles.csv'.
```

```
from rdkit import Chem
import pandas as pd

# QM9 데이터셋 로드
qm9_data = pd.read_csv("/content/qm9.csv")

# Canonical SMILES 변환 함수
def convert_to_canonical(smiles):
    try:
        mol = Chem.MolFromSmiles(smiles)
        if mol is None:
            return None
        return Chem.MolToSmiles(mol, canonical=True)
    except Exception:
        return None

# 데이터셋에 Canonical SMILES 적용
qm9_data["canonical_smiles"] = qm9_data["smiles"].apply(convert_to_canonical)

# Canonical SMILES가 None인 데이터 제거
qm9_data = qm9_data.dropna(subset=["canonical_smiles"])

# 확인
```

```
print(qm9_data.head())

# Canonical SMILES 데이터셋 저장
qm9_data[["canonical_smiles", "gap"]].to_csv("qm9_canonical.csv", index=False)
```

```
  mol_id smiles          A           B           C      mu  alpha    homo  \
0  gdb_1      C  157.71180  157.709970  157.706990  0.0000  13.21 -0.3877
1  gdb_2      N  293.60975  293.541110  191.393970  1.6256   9.46 -0.2570
2  gdb_3      O  799.58812  437.903860  282.945450  1.8511   6.31 -0.2928
3  gdb_4    C#C    0.00000   35.610036   35.610036  0.0000  16.28 -0.2845
4  gdb_5    C#N    0.00000   44.593883   44.593883  2.8937  12.99 -0.3604

     lumo     gap  ...         u0       u298       h298       g298     cv  \
0  0.1171  0.5048  ... -40.478930 -40.476062 -40.475117 -40.498597  6.469
1  0.0829  0.3399  ... -56.525887 -56.523026 -56.522082 -56.544961  6.316
2  0.0687  0.3615  ... -76.404702 -76.401867 -76.400922 -76.422349  6.002
3  0.0506  0.3351  ... -77.308427 -77.305527 -77.304583 -77.327429  8.574
4  0.0191  0.3796  ... -93.411888 -93.409370 -93.408425 -93.431246  6.278

      u0_atom   u298_atom   h298_atom   g298_atom  canonical_smiles
0 -395.999595 -398.643290 -401.014647 -372.471772                 C
1 -276.861363 -278.620271 -280.399259 -259.338802                 N
2 -213.087624 -213.974294 -215.159658 -201.407171                 O
3 -385.501997 -387.237686 -389.016047 -365.800724               C#C
4 -301.820534 -302.906752 -304.091489 -288.720028               C#N

[5 rows x 22 columns]
```

train/test dataset 결정

```
import pandas as pd
from sklearn.model_selection import train_test_split

# QM9 데이터 로드
file_path = "/content/qm9.csv"  # QM9 데이터셋 경로
qm9_data = pd.read_csv(file_path)

# 필요한 열만 추출 (smiles와 gap)
data = qm9_data[['smiles', 'gap']].dropna()

# Train/Test 데이터셋 분리 (90% Train, 10% Test)
train_data, test_data = train_test_split(data, test_size=0.1, random_state=42)

# 결과 확인
print(f"Train dataset size: {train_data.shape[0]} rows")
print(f"Test dataset size: {test_data.shape[0]} rows")

# Train/Test 데이터셋 저장
train_data.to_csv("qm9_train.csv", index=False)
test_data.to_csv("qm9_test.csv", index=False)

print("Train/Test datasets have been saved as 'qm9_train.csv' and 'qm9_test.csv'.")
```

```
Train dataset size: 120496 rows
Test dataset size: 13389 rows
```

```
Train/Test datasets have been saved as 'qm9_train.csv' and 'qm9_test.csv'.
```

```
import pandas as pd
from sklearn.model_selection import train_test_split

# QM9 Canonical 데이터 로드
file_path = "/content/qm9_canonical.csv"  # QM9 Canonical 데이터셋 경로
qm9_data = pd.read_csv(file_path)

# 필요한 열만 추출 (canonical_smiles와 gap)
data = qm9_data[['canonical_smiles', 'gap']].dropna()

# Train/Test 데이터셋 분리 (90% Train, 10% Test)
train_data, test_data = train_test_split(data, test_size=0.1, random_state=42)

# 결과 확인
print(f"Train dataset size: {train_data.shape[0]} rows")
print(f"Test dataset size: {test_data.shape[0]} rows")

# Train/Test 데이터셋 저장
train_data.to_csv("qm9_canonical_train.csv", index=False)
test_data.to_csv("qm9_canonical_test.csv", index=False)

print("Train/Test datasets have been saved as 'qm9_canonical_train.csv' and 'qm9_canonical_test.csv'."
```

```
Train dataset size: 120496 rows
Test dataset size: 13389 rows
Train/Test datasets have been saved as 'qm9_canonical_train.csv' and 'qm9_canonical_test.csv'.
```

Training / Testing

(Non-canonical) SMILES

```
from transformers import RobertaTokenizer, RobertaForSequenceClassification, Trainer, TrainingArgumer
import torch
from torch.utils.data import Dataset
from sklearn.model_selection import train_test_split
import pandas as pd

# 모델 및 토크나이저 로드
model_name = "seyonec/ChemBERTa-zinc-base-v1"
tokenizer = RobertaTokenizer.from_pretrained(model_name)
model = RobertaForSequenceClassification.from_pretrained(model_name, num_labels=1)

# 데이터 로드
train_data = pd.read_csv("/content/qm9_train.csv")
test_data = pd.read_csv("/content/qm9_test.csv")

# SMILES 토큰화
class SMILESDataset(Dataset):
```

```
    def __init__(self, dataframe, tokenizer, target_col):
        self.data = dataframe
        self.tokenizer = tokenizer
        self.target_col = target_col

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

    def __getitem__(self, idx):
        smiles = self.data.iloc[idx]['smiles']
        target = self.data.iloc[idx][self.target_col]
        tokens = self.tokenizer(smiles, padding='max_length', truncation=True, max_length=20, return_
        item = {key: val.squeeze(0) for key, val in tokens.items()}
        item['labels'] = torch.tensor(target, dtype=torch.float)
        return item

# 데이터셋 준비
train_dataset = SMILESDataset(train_data, tokenizer, 'gap')
test_dataset = SMILESDataset(test_data, tokenizer, 'gap')

# 데이터 Collator
data_collator = DataCollatorWithPadding(tokenizer=tokenizer)

# 학습 파라미터
training_args = TrainingArguments(
    output_dir='./results',
    evaluation_strategy="epoch",
    learning_rate=5e-5,
    per_device_train_batch_size=16,  # 배치 크기 축소
    per_device_eval_batch_size=16,
    num_train_epochs=2,  # 에포크 수
    weight_decay=0.01,
    logging_dir='./logs',
    logging_steps=10,
)

# Trainer 설정
trainer = Trainer(
    model=model,
    args=training_args,
    train_dataset=train_dataset,
    eval_dataset=test_dataset,
    data_collator=data_collator,
)

# 모델 학습
trainer.train()

# 모델 저장
model.save_pretrained("./jjh/ChemBERTa-smiles-gap")
tokenizer.save_pretrained("./jjh/ChemBERTa-smiles-gap")

print("파인튜닝 완료 및 모델 저장 완료!")

# 테스트 데이터 평가
evaluation_results = trainer.evaluate()
```

```
print("테스트 데이터 평가 결과:", evaluation_results)
```

```
Some weights of RobertaForSequenceClassification were not initialized from the model checkpoint
You should probably TRAIN this model on a down-stream task to be able to use it for predictions
/usr/local/lib/python3.10/dist-packages/transformers/training_args.py:1568: FutureWarning: `eval
  warnings.warn(
wandb: WARNING The `run_name` is currently set to the same value as `TrainingArguments.output_d
wandb: Using wandb-core as the SDK backend.  Please refer to https://wandb.me/wandb-core for mo
wandb: Logging into wandb.ai. (Learn how to deploy a W&B server locally: https://wandb.me/wandb
wandb: You can find your API key in your browser here: https://wandb.ai/authorize
wandb: Paste an API key from your profile and hit enter, or press ctrl+c to quit: ········
wandb: Appending key for api.wandb.ai to your netrc file: /root/.netrc
```

Tracking run with wandb version 0.18.7
Run data is saved locally in /content/wandb/run-20241208_011606-26afhwwb
Syncing run **./results** to Weights & Biases (docs)
View project at https://wandb.ai/jangjh1907-korea-university/huggingface
View run at https://wandb.ai/jangjh1907-korea-university/huggingface/runs/26afhwwb
[15062/15062 9:15:11, Epoch 2/2]

Epoch	Training Loss	Validation Loss
1	0.000800	0.000521
2	0.000300	0.000344

```
파인튜닝 완료 및 모델 저장 완료!
```

[837/837 09:16]

```
테스트 데이터 평가 결과: {'eval_loss': 0.000344324012985453, 'eval_runtime': 557.5386, 'eval_sam
```

Canonical SMILES

```
from transformers import RobertaTokenizer, RobertaForSequenceClassification, Trainer, TrainingArgumer
import torch
from torch.utils.data import Dataset
from sklearn.model_selection import train_test_split
import pandas as pd

# 모델 및 토크나이저 로드
model_name = "seyonec/ChemBERTa-zinc-base-v1"
tokenizer = RobertaTokenizer.from_pretrained(model_name)
model = RobertaForSequenceClassification.from_pretrained(model_name, num_labels=1)

# 데이터 로드
train_data = pd.read_csv("/content/qm9_canonical_train.csv")
test_data = pd.read_csv("/content/qm9_canonical_test.csv")

# SMILES 토큰화
class SMILESDataset(Dataset):
    def __init__(self, dataframe, tokenizer, target_col):
        self.data = dataframe
        self.tokenizer = tokenizer
        self.target_col = target_col
```

```
    def __len__(self):
        return len(self.data)

    def __getitem__(self, idx):
        smiles = self.data.iloc[idx]['canonical_smiles']
        target = self.data.iloc[idx][self.target_col]
        tokens = self.tokenizer(smiles, padding='max_length', truncation=True, max_length=20, return_
        item = {key: val.squeeze(0) for key, val in tokens.items()}
        item['labels'] = torch.tensor(target, dtype=torch.float)
        return item

# 데이터셋 준비 (전체 데이터 사용)
train_dataset = SMILESDataset(train_data, tokenizer, 'gap')
test_dataset = SMILESDataset(test_data, tokenizer, 'gap')

# 데이터 Collator
data_collator = DataCollatorWithPadding(tokenizer=tokenizer)

# 학습 파라미터
training_args = TrainingArguments(
    output_dir='./results',
    evaluation_strategy="epoch",
    learning_rate=5e-5,
    per_device_train_batch_size=16,  # 배치 크기
    per_device_eval_batch_size=16,
    num_train_epochs=2,  # 에포크 수
    weight_decay=0.01,
    logging_dir='./logs',
    logging_steps=10,
)

# Trainer 설정
trainer = Trainer(
    model=model,
    args=training_args,
    train_dataset=train_dataset,
    eval_dataset=test_dataset,
    data_collator=data_collator,
)

# 모델 학습
trainer.train()

# 모델 저장
model.save_pretrained("./jjh/ChemBERTa-canonical_smiles-gap")
tokenizer.save_pretrained("./jjh/ChemBERTa-canonical_smiles-gap")

print("파인튜닝 완료 및 모델 저장 완료!")

# 테스트 데이터 평가
evaluation_results = trainer.evaluate()
print("테스트 데이터 평가 결과:", evaluation_results)
```

```
Some weights of RobertaForSequenceClassification were not initialized from the model checkpoint
You should probably TRAIN this model on a down-stream task to be able to use it for predictions
/usr/local/lib/python3.10/dist-packages/transformers/training_args.py:1568: FutureWarning: `eval
  warnings.warn(
wandb: WARNING The `run_name` is currently set to the same value as `TrainingArguments.output_d
wandb: Using wandb-core as the SDK backend.  Please refer to https://wandb.me/wandb-core for mo
wandb: Logging into wandb.ai. (Learn how to deploy a W&B server locally: https://wandb.me/wandb-
wandb: You can find your API key in your browser here: https://wandb.ai/authorize
wandb: Paste an API key from your profile and hit enter, or press ctrl+c to quit: ········
wandb: Appending key for api.wandb.ai to your netrc file: /root/.netrc
```

Tracking run with wandb version 0.18.7
Run data is saved locally in /content/wandb/run-20241208_011624-0r7ughyv
Syncing run **./results** to Weights & Biases (docs)
View project at https://wandb.ai/jangjh1907-korea-university/huggingface
View run at https://wandb.ai/jangjh1907-korea-university/huggingface/runs/0r7ughyv
[15062/15062 8:34:45, Epoch 2/2]

Epoch	Training Loss	Validation Loss
1	0.001000	0.001319
2	0.000400	0.000296

파인튜닝 완료 및 모델 저장 완료!
[837/837 08:02]
테스트 데이터 평가 결과: {'eval_loss': 0.00029595196247100083, 'eval_runtime': 483.0734, 'eval_sa

› 기타 코드

[ ] ↳ *숨겨진 셀 7개*