

Extraction des entités nommées

ÉTAPE 1: Importer les librairies

```
In [1]: import numpy as np
import pandas as pd
import torch
import torch.nn as nn
import torch.optim as optim
from torch.utils.data import Dataset, DataLoader
import re
import os
from typing import List, Dict, Tuple, Optional
import importlib
import models
import utils
importlib.reload(models)
importlib.reload(utils)
from models.models import *
from utils.datasetloader import NERDataset
from utils.fonctions import (
    load_jnlpba_dataset, load_ncbi_dataset, prepare_ncbi_for_ner, create_embedding
)
from utils.creation_vocabulaire import create_vocab, create_char_vocab, preprocess

import matplotlib.pyplot as plt
import seaborn as sns
from sklearn.metrics import confusion_matrix, classification_report

import warnings
warnings.filterwarnings("ignore", category=UserWarning)
warnings.filterwarnings("ignore", category=RuntimeWarning)

print("Utilisation du dispositif : ", "gpu" if torch.cuda.is_available() else "cp
```

Utilisation du dispositif : gpu

ÉTAPE 2: DATA PREPROCESSING

```
In [2]: jnlpba_sentences, jnlpba_classes = load_jnlpba_dataset("./datasets/JNLPBA")
print(jnlpba_sentences[1])
```

Chargement du dataset JNLPBA depuis: ./datasets/JNLPBA
- sentences: 22402 phrases
- 11 Classes: ['B-DNA', 'I-DNA', 'B-cell_line', 'I-cell_line', 'B-protein', 'I-protein', 'B-cell_type', 'I-cell_type', 'B-RNA', 'I-RNA', 'O']
[('Activation', 'O'), ('of', 'O'), ('the', 'O'), ('CD28', 'B-protein'), ('surface', 'I-protein'), ('receptor', 'I-protein'), ('provides', 'O'), ('a', 'O'), ('major', 'O'), ('costimulatory', 'O'), ('signal', 'O'), ('for', 'O'), ('T', 'O'), ('cell', 'O'), ('activation', 'O'), ('resulting', 'O'), ('in', 'O'), ('enhanced', 'O'), ('production', 'O'), ('of', 'O'), ('interleukin-2', 'B-protein'), ('IL-2', 'B-protein'), ('', 'O'), ('and', 'O'), ('cell', 'O'), ('proliferation', 'O'), ('.', 'O')]

```
In [3]: ncbi_data = load_ncbi_dataset("./datasets/NCBI-Corpus")
ncbi_sentences = prepare_ncbi_for_ner(ncbi_data)
print(ncbi_sentences[1])
```

```
Chargement du dataset NCBI depuis: ./datasets/NCBI-Corpus
Documents chargés: 793
Exemple d'entités dans le premier document: 2
Total de phrases générées (format JNLPBA): 7524
```

Vérification du format:

```
Type du premier élément: <class 'tuple'>
Longueur du tuple: 2
Type tokens: <class 'list'> (longueur: 16)
Type labels: <class 'list'> (longueur: 16)
Exemple tokens[:5]: ['Germline', 'mutations', 'in', 'BRCA1', 'are']
Exemple labels[:5]: ['O', 'O', 'O', 'O', 'O']
(['However', ',', 'the', 'function', 'of', 'the', 'BRCA1', 'protein', 'has', 'remained', 'elusive', '.'], ['I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'O', 'O', 'O', 'O', 'O'])
Total de phrases générées (format JNLPBA): 7524
```

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Type du premier élément: <class 'tuple'>
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Exemple tokens[:5]: ['Germline', 'mutations', 'in', 'BRCA1', 'are']
Exemple labels[:5]: ['O', 'O', 'O', 'O', 'O']
(['However', ',', 'the', 'function', 'of', 'the', 'BRCA1', 'protein', 'has', 'remained', 'elusive', '.'], ['I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'I-CompositeMention', 'O', 'O', 'O', 'O', 'O'])
```

Création de dataset JNLPBA

```
In [4]: def create_jnlpba_dataloaders(jnlpba_sentences, batch_size=32, max_seq_len=100,
    """
    Crée les Dataloaders avec Word2Vec
    """
    # 1. Créer les vocabulaires
    vocab = create_vocab(jnlpba_sentences, min_freq=2)
    char_vocab = create_char_vocab(jnlpba_sentences)

    # 2. Créer le mapping des tags
    tag_to_idx, idx_to_tag = create_tag_mapping(jnlpba_sentences)

    # 3. Diviser en train/dev/test
    total = len(jnlpba_sentences)
    train_size = int(0.7 * total)
    dev_size = int(0.15 * total)

    train_sentences = jnlpba_sentences[:train_size]
    dev_sentences = jnlpba_sentences[train_size:train_size + dev_size]
    test_sentences = jnlpba_sentences[train_size + dev_size:]

    print(f"JNLPBA - Train: {len(train_sentences)}, Dev: {len(dev_sentences)}, T
    # 4. Entrainer ou charger Word2Vec
```

```

word2vec_model = None

if word2vec_path:
    print(f"Tentative de chargement du modèle Word2Vec depuis: {word2vec_path}")
    word2vec_model = load_word2vec_model(word2vec_path)

if word2vec_model is None:
    print("Entraînement d'un nouveau modèle Word2Vec...")

    # Extraire les phrases pour Word2Vec
    tokenized_sentences = [
        [token.lower() for token, label in sentence]
        for sentence in jnlpba_sentences
    ]

    print(f"Nombre de phrases pour Word2Vec: {len(tokenized_sentences)}")
    print(f"Exemple: {tokenized_sentences[0][:10]}")

    # Entrainer Word2Vec
    from gensim.models import Word2Vec
    word2vec_model = Word2Vec(
        sentences=tokenized_sentences,
        vector_size=200,
        window=5,
        min_count=2,
        workers=4,
        sg=1, # Skip-gram
        epochs=10
    )

    print(f"Vocabulaire Word2Vec entraîné: {len(word2vec_model.wv)} mots")

    # Sauvegarder le modèle
    if word2vec_path:
        try:
            save_word2vec_model(word2vec_model, word2vec_path)
        except Exception as e:
            print(f"Attention: impossible de sauvegarder le modèle: {e}")
            print("Le modèle sera utilisé en mémoire seulement.")

# 5. Créer la matrice d'embeddings
pretrained_embeddings = create_embedding_matrix_from_word2vec(word2vec_model)

# 6. Créer les datasets
train_dataset = NERDataset(train_sentences, vocab, char_vocab, tag_to_idx, max_s
dev_dataset = NERDataset(dev_sentences, vocab, char_vocab, tag_to_idx, max_s
test_dataset = NERDataset(test_sentences, vocab, char_vocab, tag_to_idx, max_s

# 7. Créer les DataLoaders
train_loader = DataLoader(train_dataset, batch_size=batch_size, shuffle=True)
dev_loader = DataLoader(dev_dataset, batch_size=batch_size, shuffle=False)
test_loader = DataLoader(test_dataset, batch_size=batch_size, shuffle=False)

return {
    'train_loader': train_loader,
    'dev_loader': dev_loader,
    'test_loader': test_loader,
    'vocab': vocab,
    'char_vocab': char_vocab,
}

```

```

        'tag_to_idx': tag_to_idx,
        'idx_to_tag': idx_to_tag,
        'pretrained_embeddings': pretrained_embeddings,
        'train_sentences': train_sentences,
        'dev_sentences': dev_sentences,
        'test_sentences': test_sentences,
        'word2vec_model': word2vec_model
    }

BATCH_SIZE = 32
results_jnlpba = create_jnlpba_dataloaders(jnlpba_sentences,batch_size=BATCH_SIZE)

```

Format vocab: Liste de paires (token, label)
Vocabulaire créé: 12664 mots
Mots uniques: 22678
Mots avec fréquence >= 2: 12661
Format char vocab: Liste de paires (token, label)
Vocabulaire caractères créé: 85 caractères
Caractères uniques: 83
Format tag mapping: Liste de paires (token, label)
Mapping tags créé: 12 tags uniques
Tags: ['B-DNA', 'B-RNA', 'B-cell_line', 'B-cell_type', 'B-protein', 'I-DNA', 'I-RNA', 'I-cell_line', 'I-cell_type', 'I-protein', 'O']
JNLPBA - Train: 15681, Dev: 3360, Test: 3361
Tentative de chargement du modèle Word2Vec depuis: ./word2Vecembeddings/jnlpba_word2vec
Modèle Word2Vec chargé: ./word2Vecembeddings/jnlpba_word2vec
Mots trouvés dans Word2Vec: 12661
Mots non trouvés: 0
Couverture: 100.00%
Dataset créé: 15681 phrases valides
Dataset créé: 3360 phrases valides
Dataset créé: 3361 phrases valides

```

In [5]: train_loader = results_jnlpba['train_loader']

# Récupérer un batch
for batch in train_loader:
    word_ids, char_seqs, tag_ids, lengths = batch
    break # on prend juste le premier batch pour l'exemple

# Afficher les shapes
print("word_ids shape:", word_ids.shape) # [batch_size, max_seq_len]
print("char_seqs shape:", char_seqs.shape) # [batch_size, max_seq_len, max_char_
print("tag_ids shape:", tag_ids.shape) # [batch_size, max_seq_len]
print("lengths:", lengths)

# Afficher un exemple de tokens/Labels pour le premier élément du batch
idx_to_word = {v:k for k,v in results_jnlpba['vocab'].items()} # optionnel si t
idx_to_tag = results_jnlpba['idx_to_tag']

print("\nPremier exemple du batch:")
print("Word IDs :", word_ids[0])
print("Char IDs :", char_seqs[0])
print("Tag IDs : ", tag_ids[0])
print("Longueur réelle:", lengths[0])

# Pour afficher les mots et labels décodés
decoded_words = [idx_to_word.get(w.item(), '<UNK>') for w in word_ids[0][:length
decoded_tags = [idx_to_tag[t.item()] for t in tag_ids[0][:lengths[0]]]

```

```
print("\nDécodé (mots, tags) : ", list(zip(decoded_words, decoded_tags)))
```

```
word_ids shape: torch.Size([32, 100])
char_seqs shape: torch.Size([32, 100, 20])
tag_ids shape: torch.Size([32, 100])
lengths: tensor([38, 36, 27, 19, 44, 9, 38, 34, 25, 29, 27, 34, 24, 24, 37, 28, 34,
36, 30,
               26, 20, 22, 16, 14, 33, 16, 26, 19, 29, 25, 14, 27, 23])
```

Premier exemple du batch:

Décodé (mots, tags) : [('the', '0'), ('mechanisms', '0'), ('involved', '0'), ('in', '0'), ('the', '0'), ('inhibition', '0'), ('of', '0'), ('growth', '0'), ('of', '0'), ('a', '0'), ('human', 'B-cell_line'), ('b', 'I-cell_line'), ('lymphoma', 'I-cell_line'), ('cell', 'I-cell_line'), ('line', 'I-cell_line'), (',', '0'), ('b104', 'B-cell_line'), (',', '0'), ('by', '0'), ('anti-mhc', 'B-protein'), ('class', 'I-protein'), ('ii', 'I-protein'), ('antibodies', 'I-protein'), ('(', '0'), ('ab', 'B-protein'), (')', '0'), ('were', '0'), ('compared', '0'), ('with', '0'), ('those', '0'), ('in', '0'), ('anti-igm', 'B-protein'), ('ab', 'I-protein'), ('-induced', '0'), ('b104', '0'), ('growth', '0'), ('inhibition', '0'), ('.', '0')]

```
In [6]: def create_ncbi_dataloaders(ncbi_sentences, batch_size=32, max_seq_len=200, word
      """
      Crée les DataLoaders pour NCBI avec Word2Vec
      """
      # 1. Créer les vocabulaires
      vocab = create_vocab(ncbi_sentences, min_freq=2)
      char_vocab = create_char_vocab(ncbi_sentences)

      # 2. Créer le mapping des tags
      tag_to_idx, idx_to_tag = create_tag_mapping(ncbi_sentences)

      # 3. Diviser en train/dev/test
      total = len(ncbi_sentences)
```

```

train_size = int(0.7 * total)
dev_size = int(0.15 * total)

train_sentences = ncbi_sentences[:train_size]
dev_sentences = ncbi_sentences[train_size:train_size + dev_size]
test_sentences = ncbi_sentences[train_size + dev_size:]

print(f"NCBI - Train: {len(train_sentences)}, Dev: {len(dev_sentences)}, Test: {len(test_sentences)}")

# 4. Entrainer ou charger Word2Vec
if word2vec_path and os.path.exists(word2vec_path):
    print(f"Chargement du modèle Word2Vec depuis: {word2vec_path}")
    word2vec_model = load_word2vec_model(word2vec_path)
else:
    print("Entraînement d'un nouveau modèle Word2Vec...")
    # Entrainer sur toutes les données
    word2vec_model = train_word2vec_embeddings(ncbi_sentences)

# Sauvegarder le modèle
if word2vec_path:
    save_word2vec_model(word2vec_model, word2vec_path)

# 5. Créer la matrice d'embeddings
pretrained_embeddings = create_embedding_matrix_from_word2vec(word2vec_model)

# 6. Créer les datasets
train_dataset = NERDataset(train_sentences, vocab, char_vocab, tag_to_idx, max_s)
dev_dataset = NERDataset(dev_sentences, vocab, char_vocab, tag_to_idx, max_s)
test_dataset = NERDataset(test_sentences, vocab, char_vocab, tag_to_idx, max_s)

# 7. Créer les DataLoaders
train_loader = DataLoader(train_dataset, batch_size=batch_size, shuffle=True)
dev_loader = DataLoader(dev_dataset, batch_size=batch_size, shuffle=False)
test_loader = DataLoader(test_dataset, batch_size=batch_size, shuffle=False)

return {
    'train_loader': train_loader,
    'dev_loader': dev_loader,
    'test_loader': test_loader,
    'vocab': vocab,
    'char_vocab': char_vocab,
    'tag_to_idx': tag_to_idx,
    'idx_to_tag': idx_to_tag,
    'pretrained_embeddings': pretrained_embeddings,
    'train_sentences': train_sentences,
    'dev_sentences': dev_sentences,
    'test_sentences': test_sentences,
    'word2vec_model': word2vec_model
}

results_ncbi = ncbi_data_loaders = create_ncbi_dataloaders(
    ncbi_sentences,
    batch_size=BATCH_SIZE,
    word2vec_path="./word2Vecembeddings/ncbi"
)

```

Format vocab: Tuple (tokens, labels)
 Vocabulaire créé: 5925 mots
 Mots uniques: 10845
 Mots avec fréquence >= 2: 5922
 Format char vocab: Tuple (tokens, labels)
 Vocabulaire caractères créé: 86 caractères
 Caractères uniques: 84
 Format tag mapping: Tuple (tokens, labels)
 Mapping tags créé: 10 tags uniques
 Tags: ['B-CompositeMention', 'B-DiseaseClass', 'B-Modifier', 'B-SpecificDisease',
 'I-CompositeMention', 'I-DiseaseClass', 'I-Modifier', 'I-SpecificDisease', 'O']
 NCBI - Train: 5266, Dev: 1128, Test: 1130
 Entraînement d'un nouveau modèle Word2Vec...
 Nombre de phrases pour Word2Vec: 7524
 Première phrase: ['germline', 'mutations', 'in', 'brca1', 'are', 'responsible',
 'for', 'most', 'cases', 'of']...
 Entraînement du modèle Word2Vec...
 Vocabulaire Word2Vec: 5922 mots
 Taille des vecteurs: 200
 Modèle Word2Vec sauvegardé: ./word2Vecembeddings/ncbi.model
 Mots trouvés dans Word2Vec: 5922
 Mots non trouvés: 0
 Couverture: 100.00%
 Dataset créé: 5266 phrases valides
 Dataset créé: 1128 phrases valides
 Dataset créé: 1130 phrases valides

```
In [7]: train_loader = results_ncbi['train_loader']

# Récupérer un batch
for batch in train_loader:
    word_ids, char_seqs, tag_ids, lengths = batch
    break # on prend juste le premier batch pour l'exemple

# Afficher les shapes
print("word_ids shape:", word_ids.shape) # [batch_size, max_seq_len]
print("char_seqs shape:", char_seqs.shape) # [batch_size, max_seq_len, max_char]
print("tag_ids shape:", tag_ids.shape) # [batch_size, max_seq_len]
print("lengths:", lengths)

# Afficher un exemple de tokens/labels pour le premier élément du batch
idx_to_word = {v:k for k,v in results_ncbi['vocab'].items()} # optionnel si tu
idx_to_tag = results_ncbi['idx_to_tag']

print("\nPremier exemple du batch:")
print("Word IDs :", word_ids[0])
print("Char IDs :", char_seqs[0])
print("Tag IDs : ", tag_ids[0])
print("Longueur réelle:", lengths[0])

# Pour afficher les mots et labels décodés
decoded_words = [idx_to_word.get(w.item(), '<UNK>') for w in word_ids[0][:length]]
decoded_tags = [idx_to_tag[t.item()] for t in tag_ids[0][:lengths[0]]]

print("\nDécodé (mots, tags) :", list(zip(decoded_words, decoded_tags)))
```

```
Décodé (mots, tags) : [(['a', '0'], ('new', '0'), ('molecular', 'B-DiseaseClass'), ('lesion', 'I-DiseaseClass'), ('has', 'I-DiseaseClass'), ('been', 'I-DiseaseClass'), ('identified', 'I-DiseaseClass'), ('in', 'I-DiseaseClass'), ('exon', 'I-DiseaseClass'), ('<UNK>', 'I-DiseaseClass'), ('of', 'I-DiseaseClass'), ('the', '0'), ('pah', '0'), ('gene', '0'), ('in', '0'), ('a', '0'), ('hungarian', '0'), ('pku', 'B-Modifier'), ('patient', 'I-Modifier'), ('by', 'I-Modifier'), ('direct', 'I-Modifier'), ('sequencing', 'I-Modifier'), ('of', 'I-Modifier'), ('pcr-amplified', '0'), ('dna', '0'), ('.', '0')]
```

Model architecture

```
In [8]: from tqdm import tqdm
def train_epoch(model, dataloader, optimizer, device):
    """
    Entrainement pour une epoch avec CRF
```

```

"""
model.train()
total_loss = 0.0

for batch in tqdm(dataloader, total=len(dataloader), desc="Training"):
    word_ids, char_seqs, tag_ids, lengths = batch

    word_ids = word_ids.to(device)
    char_seqs = char_seqs.to(device)
    tag_ids = tag_ids.to(device)

    mask = (word_ids != 0)
    optimizer.zero_grad()
    # Passer les tags -> forward retourne la loss directement
    loss = model(word_ids, char_seqs, mask, tag_ids)

    loss.backward()
    optimizer.step()

    total_loss += loss.item()

return total_loss / len(dataloader)

def evaluate(model, dataloader, device, idx_to_tag):
"""
Evaluate model (CRF)
"""

model.eval()
total_loss = 0
all_predictions = []
all_targets = []

with torch.no_grad():
    for batch in dataloader:
        word_ids, char_seqs, tag_ids, lengths = batch

        word_ids = word_ids.to(device)
        char_seqs = char_seqs.to(device)
        tag_ids = tag_ids.to(device)

        mask = (word_ids != 0)

        # Calculer la loss (tags fournis)
        loss = model(word_ids, char_seqs, mask, tag_ids)
        total_loss += loss.item()

        # Décoder les séquences pour obtenir les prédictions
        predictions = model(word_ids, char_seqs, mask, tags=None) # renvoie

        # Stocker les prédictions et targets
        for preds_seq, tag_seq, seq_len in zip(predictions, tag_ids, lengths):
            preds_seq = preds_seq[:seq_len] # découper au vrai leng
            tag_seq = tag_seq[:seq_len].cpu().numpy() # tag_ids tensor -> n

            pred_tags = [idx_to_tag.get(idx, 'O') for idx in preds_seq]
            target_tags = [idx_to_tag.get(idx, 'O') for idx in tag_seq]

            all_predictions.extend(pred_tags)
            all_targets.extend(target_tags)

```

```
    return total_loss / len(dataloader), all_predictions, all_targets
```

```
def calculate_metrics(predictions, targets):
    """
    Calculate precision, recall, F1-score
    """
    from sklearn.metrics import precision_recall_fscore_support

    # Filter out '0' tags for entity-specific metrics
    entity_preds = []
    entity_targets = []

    for pred, target in zip(predictions, targets):
        if target != '0':
            entity_preds.append(pred)
            entity_targets.append(target)

    precision, recall, f1, _ = precision_recall_fscore_support(
        entity_targets, entity_preds, average='macro', zero_division=0
    )

    return precision, recall, f1
```

JNLPBA Dataset

```
In [12]: def run_pipeline(
    dataset_name: str,
    loaders: dict,
    use_char_cnn: bool = False,
    use_char_lstm: bool = False,
    use_attention: bool = False,
    use_fc_fusion: bool = False,
    embedding_url: str = None,
    lstm_hidden_dim: Optional[int] = None,
    epochs: int = 40,
    patience: int = 4,
    checkpoints_dir=".//checkpoints",
):
    train_loader = loaders['train_loader']
    dev_loader = loaders['dev_loader']
    test_loader = loaders['test_loader']

    vocab = loaders['vocab']
    char_vocab = loaders['char_vocab']
    tag_to_idx = loaders['tag_to_idx']
    idx_to_tag = loaders['idx_to_tag']
    comb_name = "WE"
    if use_char_cnn and use_char_lstm:
        comb_name += "_char_bilstm_cnn"
    elif use_char_cnn:
        comb_name += "_char_cnn"
    elif use_char_lstm:
        comb_name += "_char_bilstm"

    if use_attention:
        comb_name += "_attention"
```

```

if use_fc_fusion:
    comb_name += "_fc"

checkpoints_path = f"{checkpoints_dir}/{comb_name}/best_model.pt"
os.makedirs(os.path.dirname(checkpoints_path), exist_ok=True)
# Chargement des embeddings
if embedding_url:
    pretrained_embeddings = load_word2vec_model(embedding_url)
elif 'pretrained_embeddings' in loaders and loaders['pretrained_embeddings']:
    pretrained_embeddings = loaders['pretrained_embeddings']
else:
    print("Embedding nul")
    return
if lstm_hidden_dim is None:
    lstm_hidden_dim = 256 if dataset_name == 'JNLPBA' else 128
device = "cuda" if torch.cuda.is_available() else "cpu"
model = CombinatorialNER(
    vocab_size=len(vocab),
    char_vocab_size=len(char_vocab),
    tag_to_idx=tag_to_idx,
    use_char_cnn=use_char_cnn,
    use_char_lstm=use_char_lstm,
    use_attention=use_attention,
    use_fc_fusion=use_fc_fusion,
    pretrained_embeddings=pretrained_embeddings,
    word_embed_dim=200,
    lstm_hidden_dim=lstm_hidden_dim,
    dropout=0.5
).to(device)

print(f"Model parameters: {sum(p.numel() for p in model.parameters()):,}")

optimizer = optim.Adam(model.parameters(), lr=0.001, weight_decay=5e-4)

# Scheduler: ReduceLROnPlateau (réduit le LR quand le plateau est atteint)
scheduler = optim.lr_scheduler.ReduceLROnPlateau(
    optimizer,
    mode='max',           # On maximise le F1-score
    factor=0.5,            # Réduction de 50%
    patience=2,             # Attendre 2 epochs sans amélioration
    threshold=0.0001,       # Seuil d'amélioration minimum
    min_lr=1e-6             # Learning rate minimum
)

best_f1 = 0.0
patience_counter = 0

# Pour suivre l'historique
history = {
    'train_loss': [],
    'dev_loss': [],
    'dev_f1': [],
    'lr': []
}

for epoch in range(epochs):
    # Entraînement
    train_loss = train_epoch(model, train_loader, optimizer, device)

```

```

# Évaluation
dev_loss, dev_preds, dev_targets = evaluate(model, dev_loader, device, i
precision, recall, f1 = calculate_metrics(dev_preds, dev_targets)

# Mettre à jour le scheduler avec le F1-score
scheduler.step(f1)

# Sauvegarder l'historique
history['train_loss'].append(train_loss)
history['dev_loss'].append(dev_loss)
history['dev_f1'].append(f1)
history['lr'].append(optimizer.param_groups[0]['lr'])

print(
    f"Epoch {epoch+1:02d}/{epochs} | "
    f"Train loss: {train_loss:.4f} | "
    f"Dev loss: {dev_loss:.4f} | "
    f"P: {precision:.4f} R: {recall:.4f} F1: {f1:.4f} | "
    f"LR: {optimizer.param_groups[0]['lr']:.6f}"
)

if f1 > best_f1:
    best_f1 = f1
    patience_counter = 0
    torch.save({
        'epoch': epoch,
        'model_state_dict': model.state_dict(),
        'optimizer_state_dict': optimizer.state_dict(),
        'scheduler_state_dict': scheduler.state_dict(),
        'best_f1': best_f1,
    }, checkpoints_path)
    print(f"Meilleur modèle sauvé dans {checkpoints_path} : (F1: {f
else:
    patience_counter += 1

if patience_counter >= patience:
    print(f"\nEarly stopping triggered après {epoch+1} epochs.")
    break


# Charger le meilleur modèle
checkpoint = torch.load(checkpoints_path)
model.load_state_dict(checkpoint['model_state_dict'])

test_loss, test_preds, test_targets = evaluate(
    model,
    test_loader,
    device,
    idx_to_tag
)

precision, recall, f1 = calculate_metrics(test_preds, test_targets)

print("\n" + "*50)
print("RÉSULTATS FINAUX SUR LE TEST SET")
print("*50)
print(f"Loss: {test_loss:.4f}")
print(f"Precision: {precision:.4f}")
print(f"Recall: {recall:.4f}")
print(f"F1-score: {f1:.4f}")

```

```

print("*"*50)

# Afficher l'historique des Learning rates
print("\nHistorique des learning rates:")
for i, lr in enumerate(history['lr']):
    if i == 0 or lr != history['lr'][i-1]:
        print(f" Epoch {i+1}: LR = {lr:.6f}")

return model, history

```

Cobinaison WE

```
In [ ]: model_jnlpba_we, history_jnlpba_we = run_pipeline(
    dataset_name='JNLPBA',
    loaders=results_jnlpba,
    use_char_cnn=None,
    use_char_lstm=None,
    use_attention=None,
    use_fc_fusion=None,
    embedding_url=None,
    epochs=40,
    patience=4,
    checkpoints_dir = "./checkpoints/JNLPBA",
)
```

Model parameters: 2,873,972

```
Training: 100%|██████████| 491/491 [01:20<00:00, 6.07it/s]
Epoch 01/40 | Train loss: 320.0335 | Dev loss: 172.4923 | P: 0.7993 R: 0.6633 F1: 0.7215 | LR: 0.001000
Meilleur modèle sauvegardé dans ./checkpoints/JNLPBA/WE/best_model.pt : (F1: 0.7215)
```

```
Training: 19%|█| 91/491 [00:12<00:56, 7.05it/s]
```

```
In [12]: import pickle
import os

def save_vocabularies(data_dict, save_dir):
    """Sauvegarde les vocabulaires et mappings"""
    os.makedirs(save_dir, exist_ok=True)

    with open(os.path.join(save_dir, 'vocab.pkl'), 'wb') as f:
        pickle.dump(data_dict['vocab'], f)

    with open(os.path.join(save_dir, 'char_vocab.pkl'), 'wb') as f:
        pickle.dump(data_dict['char_vocab'], f)

    with open(os.path.join(save_dir, 'tag_to_idx.pkl'), 'wb') as f:
        pickle.dump(data_dict['tag_to_idx'], f)

    with open(os.path.join(save_dir, 'idx_to_tag.pkl'), 'wb') as f:
        pickle.dump(data_dict['idx_to_tag'], f)

    print(f"Vocabulaires sauvegardés dans {save_dir}")

save_vocabularies(results_jnlpba, './vocab/jnlpba')
```

Vocabulaires sauvegardés dans ./vocab/jnlpba

```
In [ ]: def plot_training_history(history, dataset_name):
    """
```

```

Visualise l'historique d'entraînement
"""
fig, axes = plt.subplots(2, 2, figsize=(15, 10))
fig.suptitle(f'Training History - {dataset_name}', fontsize=16, fontweight='bold')

epochs = range(1, len(history['train_loss']) + 1)

# Plot 1: Train vs Dev Loss
axes[0, 0].plot(epochs, history['train_loss'], 'b-', label='Train Loss', linewidth=2)
axes[0, 0].plot(epochs, history['dev_loss'], 'r-', label='Dev Loss', linewidth=2)
axes[0, 0].set_xlabel('Epoch')
axes[0, 0].set_ylabel('Loss')
axes[0, 0].set_title('Train vs Dev Loss')
axes[0, 0].legend()
axes[0, 0].grid(True, alpha=0.3)

# Plot 2: F1-Score
axes[0, 1].plot(epochs, history['dev_f1'], 'g-', linewidth=2)
axes[0, 1].set_xlabel('Epoch')
axes[0, 1].set_ylabel('F1-Score')
axes[0, 1].set_title('Dev F1-Score')
axes[0, 1].set_ylim(0, 1)
axes[0, 1].grid(True, alpha=0.3)

# Plot 3: Learning Rate
axes[1, 0].step(epochs, history['lr'], 'purple', linewidth=2)
axes[1, 0].set_xlabel('Epoch')
axes[1, 0].set_ylabel('Learning Rate')
axes[1, 0].set_title('Learning Rate Schedule')
axes[1, 0].set_yscale('log')
axes[1, 0].grid(True, alpha=0.3)

# Plot 4: Combined (Loss + F1)
ax2 = axes[1, 1].twinx()
line1, = axes[1, 1].plot(epochs, history['dev_loss'], 'r-', label='Dev Loss', linewidth=2)
line2, = ax2.plot(epochs, history['dev_f1'], 'g-', label='Dev F1', linewidth=2)
axes[1, 1].set_xlabel('Epoch')
axes[1, 1].set_ylabel('Loss', color='r')
ax2.set_ylabel('F1-Score', color='g')
axes[1, 1].set_title('Dev Loss & F1-Score')
lines = [line1, line2]
labels = [l.get_label() for l in lines]
axes[1, 1].legend(lines, labels, loc='upper right')
axes[1, 1].grid(True, alpha=0.3)

plt.tight_layout()
plt.show()
print(f"STATISTIQUES FINALES - {dataset_name}")

print(f"Meilleur F1-score (dev): {max(history['dev_f1']):.4f}")
print(f"Final train loss: {history['train_loss'][-1]:.4f}")
print(f"Final dev loss: {history['dev_loss'][-1]:.4f}")
print(f"Final learning rate: {history['lr'][-1]:.6f}")

plot_training_history(history_jnlpba, dataset_name="JNLPBA")

```



STATISTIQUES FINALES - JNLPBA
Meilleur F1-score (dev): 0.6957
Final train loss: 42.1517
Final dev loss: 162.5667
Final learning rate: 0.000500

```
In [33]: def load_trained_model(model_path, dataset_name, loaders_dict):
    """
    Charge un modèle entraîné et le prépare pour les prédictions
    """
    device = "cuda" if torch.cuda.is_available() else "cpu"

    # Récupérer les paramètres du Loader
    vocab = loaders_dict['vocab']
    char_vocab = loaders_dict['char_vocab']
    tag_to_idx = loaders_dict['tag_to_idx']
    idx_to_tag = loaders_dict['idx_to_tag']

    # Déterminer les paramètres selon le dataset
    if dataset_name == 'JNLPBA':
        lstm_hidden = 256
    else: # NCBI-Disease
        lstm_hidden = 128

    # Créer le modèle
    model = CombinatorialNER(
        vocab_size=len(vocab),
        char_vocab_size=len(char_vocab),
        tag_to_idx=tag_to_idx,
        pretrained_embeddings=None, # On ne charge pas les embeddings, le modèle
        word_embed_dim=200,
        lstm_hidden_dim=lstm_hidden,
        dropout=0.5
    ).to(device)

    # Charger les poids sauvegardés
    checkpoint = torch.load(model_path, map_location=device)
```

```

model.load_state_dict(checkpoint['model_state_dict'])
model.eval() # Mode évaluation

print(f"Modèle chargé depuis: {model_path}")
print(f"Best F1 enregistré: {checkpoint.get('best_f1', 'N/A'):.4f}")
print(f"Époque: {checkpoint.get('epoch', 'N/A')}")

return model, device, idx_to_tag

def plot_confusion_matrix_by_class(predictions, targets, idx_to_tag, dataset_name,
                                    normalize=True, figsize=(12, 10)):
    """
    Affiche la matrice de confusion par classe avec des statistiques détaillées
    """
    # Vérification des types
    print(f"\nVérification des types:")
    print(f" Type predictions[0]: {type(predictions[0])}, valeur: {predictions[0]}")
    print(f" Type targets[0]: {type(targets[0])}, valeur: {targets[0]}")

    # S'assurer que tout est string
    predictions = [str(p) for p in predictions]
    targets = [str(t) for t in targets]

    # Filtrer les tags '0' pour se concentrer sur les entités
    entity_predictions = []
    entity_targets = []

    for pred, target in zip(predictions, targets):
        if target != '0': # On garde seulement les entités (pas le background)
            entity_predictions.append(pred)
            entity_targets.append(target)

    print("\nStatistiques:")
    print(f" Total tokens: {len(predictions)}")
    print(f" Entity tokens: {len(entity_targets)}")
    print(f" Unique entity tags in targets: {set(entity_targets)}")
    print(f" Unique entity tags in predictions: {set(entity_predictions)}")

    # Obtenir les classes uniques (sauf '0')
    all_unique_tags = sorted(set(entity_targets + entity_predictions))

    # Filtrer pour garder seulement les tags valides (pas les nombres)
    valid_tags = [tag for tag in all_unique_tags if not tag.isdigit()]

    # Si on a des tags numériques, c'est qu'il y a un problème de conversion
    numeric_tags = [tag for tag in all_unique_tags if tag.isdigit()]
    if numeric_tags:
        print(f"\nATTENTION: Tags numériques trouvés: {numeric_tags}")
        print("Cela indique que les prédictions sont des indices, pas des tags!")
        print(f"Mapping idx_to_tag: {dict(list(idx_to_tag.items())[:10])}")

    print(f" Tags valides à plotter: {valid_tags}")

    if not valid_tags:
        print("Aucune entité valide trouvée dans les données!")
        return

    cm = confusion_matrix(entity_targets, entity_predictions, labels=valid_tags)
    supports = cm.sum(axis=1)

```

```

if normalize:
    # Éviter la division par zéro
    with np.errstate(divide='ignore', invalid='ignore'):
        cm_normalized = cm.astype('float') / supports[:, np.newaxis]
        cm_normalized = np.nan_to_num(cm_normalized, nan=0.0)
    cm_to_plot = cm_normalized
    fmt = '.2f'
    title_suffix = '(Normalisée)'

else:
    cm_to_plot = cm
    fmt = 'd'
    title_suffix = '(Absolue)'

# Créer la figure
plt.figure(figsize=figsize)

# Si la matrice est trop grande, ajuster la taille
if len(valid_tags) > 15:
    figsize = (max(12, len(valid_tags)), max(10, len(valid_tags)))
    plt.figure(figsize=figsize)

sns.heatmap(cm_to_plot, annot=True, fmt=fmt, cmap='Blues',
            xticklabels=valid_tags, yticklabels=valid_tags,
            cbar_kws={'label': 'Proportion' if normalize else 'Count'})

plt.title(f'Matrice de Confusion - {dataset_name} {title_suffix}',
          fontsize=14, fontweight='bold')
plt.xlabel('Prédictions', fontsize=12)
plt.ylabel('Vraies labels', fontsize=12)
plt.xticks(rotation=45, ha='right')
plt.yticks(rotation=0)
plt.tight_layout()
plt.show()
filtered_targets = []
filtered_preds = []

for t, p in zip(entity_targets, entity_predictions):
    if t in valid_tags and p in valid_tags:
        filtered_targets.append(t)
        filtered_preds.append(p)

if filtered_targets:
    report = classification_report(filtered_targets, filtered_preds,
                                    labels=valid_tags, zero_division=0)
    print(report)
else:
    print("Pas assez de données pour générer le rapport")

for i, tag in enumerate(valid_tags):
    tp = cm[i, i]
    fp = cm[:, i].sum() - tp
    fn = cm[i, :].sum() - tp
    support = supports[i]

    # Éviter les divisions par zéro
    precision = tp / (tp + fp) if (tp + fp) > 0 else 0
    recall = tp / (tp + fn) if (tp + fn) > 0 else 0
    f1 = 2 * precision * recall / (precision + recall) if (precision + recall) > 0 else 0

    # Support est déjà un entier (sum de la ligne)

```

```

        print(f"\n{tag:20s}: Precision={precision:.3f}, Recall={recall:.3f}, "
              f"F1={f1:.3f}, Support={int(support)}")

def predict_on_test_set(model, test_loader, device, idx_to_tag):
    """
    Version simplifiée et robuste
    """
    model.eval()
    all_predictions = []
    all_targets = []
    for idx, tag in sorted(idx_to_tag.items()):
        print(f" {idx} -> {tag}")

    with torch.no_grad():
        for batch_idx, batch in enumerate(test_loader):
            word_ids, char_seqs, tag_ids, lengths = batch

            word_ids = word_ids.to(device)
            char_seqs = char_seqs.to(device)
            tag_ids = tag_ids.to(device)
            mask = (word_ids != 0)
            pred_sequences = model(word_ids, char_seqs, mask, tags=None)

            for i in range(len(word_ids)):
                actual_len = lengths[i]
                if isinstance(pred_sequences, list):
                    pred_seq = pred_sequences[i][:actual_len]
                else:
                    pred_seq = torch.argmax(pred_sequences[i], dim=1)[:actual_len]

                # Convertir indices -> tags
                pred_tags = []
                for idx in pred_seq:
                    if isinstance(idx, torch.Tensor):
                        idx = idx.item()
                    tag = idx_to_tag.get(int(idx), 'O')
                    pred_tags.append(tag)

                # Convertir cibles indices -> tags
                target_indices = tag_ids[i][:actual_len].cpu().numpy()
                target_tags = [idx_to_tag.get(int(idx), 'O') for idx in target_indices]

                all_predictions.extend(pred_tags)
                all_targets.extend(target_tags)

    return all_predictions, all_targets

model_path = "./checkpoints/JNLPBA/best_model_JNLPBA_full.pt"
model, device, idx_to_tag = load_trained_model(
    model_path=model_path,
    dataset_name='JNLPBA',
    loaders_dict=results_jnlpba
)

# 3. Faire des prédictions avec la version corrigée
test_loader = results_jnlpba['test_loader']
predictions, targets = predict_on_test_set(
    model=model,
    test_loader=test_loader,
)

```

```
    device=device,
    idx_to_tag=idx_to_tag
)
```

Modèle chargé depuis: ./checkpoints/JNLPBA/best_model_JNLPBA_full.pt

Best F1 enregistré: 0.6957

Époque: 31

```
0 -> <PAD>
1 -> B-DNA
2 -> B-RNA
3 -> B-cell_line
4 -> B-cell_type
5 -> B-protein
6 -> I-DNA
7 -> I-RNA
8 -> I-cell_line
9 -> I-cell_type
10 -> I-protein
11 -> O
```

```
In [32]: from sklearn.metrics import accuracy_score, classification_report

# Pour tous les tokens (y compris 'O')
accuracy = accuracy_score(targets, predictions)
print(f"\nAccuracy globale: {accuracy:.4f}")

entity_preds = [p for p, t in zip(predictions, targets) if t != 'O']
entity_targets = [t for p, t in zip(predictions, targets) if t != 'O']

if entity_targets:
    entity_accuracy = accuracy_score(entity_targets, entity_preds)
    print(f"Accuracy sur les entités: {entity_accuracy:.4f}")
    print(f"Nombre d'entités: {len(entity_targets)}")
    print("\nRapport de classification (entités seulement):")
    print(classification_report(entity_targets, entity_preds, zero_division=0))
else:
    print("Aucune entité trouvée dans les cibles!")

if set(predictions) == set(targets) or all(isinstance(p, str) for p in predictions):
    plot_confusion_matrix_by_class(
        predictions=predictions,
        targets=targets,
        idx_to_tag=idx_to_tag,
        dataset_name='JNLPBA (Test Set)',
        normalize=True,
        figsize=(12, 10)
)
else:
    print("\nERREUR: Les prédictions et cibles n'ont pas les mêmes types!")
    print(f"Types prédictions: {set(type(p) for p in predictions[:10])}")
    print(f"Types cibles: {set(type(t) for t in targets[:10])}")
```

Accuracy globale: 0.9163
Accuracy sur les entités: 0.7491
Nombre d'entités: 16,829

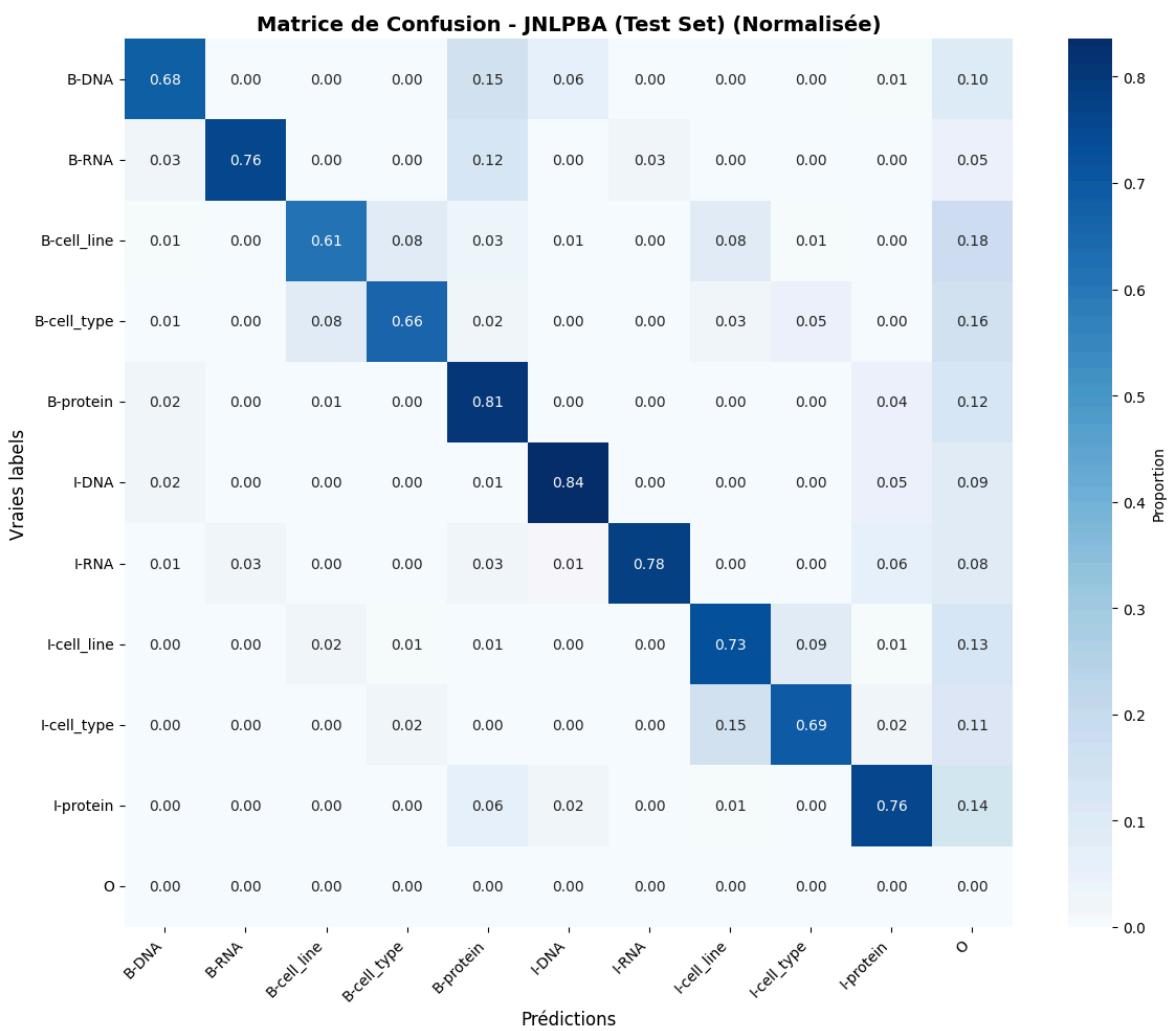
Rapport de classification (entités seulement):				
	precision	recall	f1-score	support
B-DNA	0.82	0.68	0.74	855
B-RNA	0.84	0.76	0.80	96
B-cell_line	0.54	0.61	0.57	393
B-cell_type	0.92	0.66	0.77	1729
B-protein	0.88	0.81	0.84	4505
I-DNA	0.88	0.84	0.86	1393
I-RNA	0.90	0.78	0.84	156
I-cell_line	0.53	0.73	0.61	792
I-cell_type	0.92	0.69	0.79	2690
I-protein	0.91	0.76	0.83	4220
O	0.00	0.00	0.00	0
accuracy			0.75	16829
macro avg	0.74	0.67	0.70	16829
weighted avg	0.87	0.75	0.80	16829

Vérification des types:

Type predictions[0]: <class 'str'>, valeur: 0
Type targets[0]: <class 'str'>, valeur: 0

Statistiques:

Total tokens: 87700
Entity tokens: 16829
Unique entity tags in targets: {'B-protein', 'I-cell_type', 'B-cell_type', 'B-DNA', 'I-RNA', 'I-DNA', 'B-RNA', 'I-cell_line', 'B-cell_line', 'I-protein'}
Unique entity tags in predictions: {'O', 'B-protein', 'I-cell_type', 'B-cell_type', 'B-DNA', 'I-RNA', 'I-DNA', 'B-RNA', 'I-cell_line', 'B-cell_line', 'I-protein'}
Tags valides à plotter: ['B-DNA', 'B-RNA', 'B-cell_line', 'B-cell_type', 'B-protein', 'I-DNA', 'I-RNA', 'I-cell_line', 'I-cell_type', 'I-protein', 'O']



=====

RAPPORT DE CLASSIFICATION DÉTAILLÉ - JNLPBA (Test Set)

=====

	precision	recall	f1-score	support
B-DNA	0.82	0.68	0.74	855
B-RNA	0.84	0.76	0.80	96
B-cell_line	0.54	0.61	0.57	393
B-cell_type	0.92	0.66	0.77	1729
B-protein	0.88	0.81	0.84	4505
I-DNA	0.88	0.84	0.86	1393
I-RNA	0.90	0.78	0.84	156
I-cell_line	0.53	0.73	0.61	792
I-cell_type	0.92	0.69	0.79	2690
I-protein	0.91	0.76	0.83	4220
0	0.00	0.00	0.00	0
accuracy			0.75	16829
macro avg	0.74	0.67	0.70	16829
weighted avg	0.87	0.75	0.80	16829

=====

STATISTIQUES PAR CLASSE - JNLPBA (Test Set)

=====

B-DNA	: Precision=0.816, Recall=0.684, F1=0.744, Support=855
B-RNA	: Precision=0.839, Recall=0.760, F1=0.798, Support=96
B-cell_line	: Precision=0.544, Recall=0.608, F1=0.575, Support=393
B-cell_type	: Precision=0.916, Recall=0.660, F1=0.767, Support=1729
B-protein	: Precision=0.884, Recall=0.806, F1=0.843, Support=4505
I-DNA	: Precision=0.878, Recall=0.836, F1=0.857, Support=1393
I-RNA	: Precision=0.904, Recall=0.782, F1=0.838, Support=156
I-cell_line	: Precision=0.526, Recall=0.729, F1=0.611, Support=792
I-cell_type	: Precision=0.918, Recall=0.691, F1=0.788, Support=2690
I-protein	: Precision=0.908, Recall=0.762, F1=0.829, Support=4220
0	: Precision=0.000, Recall=0.000, F1=0.000, Support=0

```
In [ ]: model_jnlpba, history_jnlpba = run_complete_pipeline_with_scheduler(  
    dataset_name='NCBI',  
    loaders=results_ncbi,  
    embedding_url=None,  
    epochs=40,  
    patience=4,  
    checkpoints_dir = "./checkpoints/NCBI"  
)
```

```
In [ ]:
```