
GNNforMD
Una GNN per la predizione delle forze per la dinamica molecolare

Generazione dati

Input script

```
units real
atom_style atomic
boundary p p p

pair_style lj/cut 10.0
mass 1 39.948
pair_coeff 1 1 0.2378 3.405 10

region box block -13.14 13.14 -13.14 13.14 -13.14 13.14
create_box 1 box

variable T equal 90
variable P equal 3.0
variable N equal 400

create_atoms 1 random $N 42 NULL overlap 2.0 maxtry 50
velocity all create $T 42 dist gaussian

timestep 1
thermo 1000
fix 2 all npt temp 1 $T 1.0 iso $P $P 1000.0

run 20000       # for equilibration
dump mydmp all custom 100 data\argon.lammpstrj id type x y z fx fy fz
run 9999
```

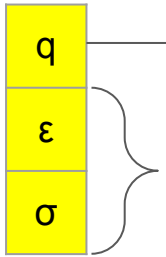
Output file

data > argon.lammpstrj

```
ITEM: TIMESTEP
20000
ITEM: NUMBER OF ATOMS
400
ITEM: BOX BOUNDS pp pp pp
-1.3559535422117442e+01 1.3559535422117442e+01
-1.3559535422117442e+01 1.3559535422117442e+01
-1.3559535422117442e+01 1.3559535422117442e+01
ITEM: ATOMS id type x y z fx fy fz
337 1 -10.8427 -10.4041 -9.6201 0.111551 -0.694874 0.816131
80 1 -11.4759 -6.92209 -8.1658 -1.2953 -1.40647 -0.520197
179 1 -12.6327 -12.299 -12.4528 -0.0491539 0.00615476 -0.348215
50 1 -10.5481 -7.81052 -11.9976 -0.829663 -0.00326355 -1.20126
1 1 -6.36677 -12.542 -10.6472 0.0330129 -0.151112 -0.0707339
89 1 -3.40216 -7.68648 -9.35792 -0.28323 -0.333796 0.509244
231 1 -6.15924 -10.0801 -7.77694 0.26985 0.0405483 -1.35934
175 1 -3.01399 -11.7082 -12.8122 0.328601 0.275039 0.126978
```

Elaborazione dati

Nodes features



Potenziale coulombiano

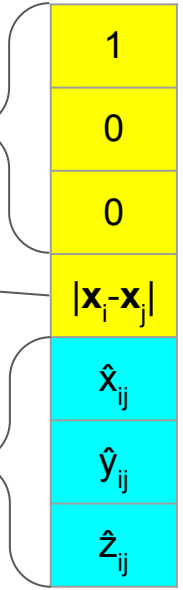
Potenziale di Lennard-Jones

Edge features

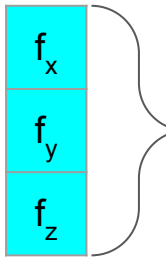
One hot vector per il tipo di legame

Modulo della distanza

Direzione legame



Target (node-level)

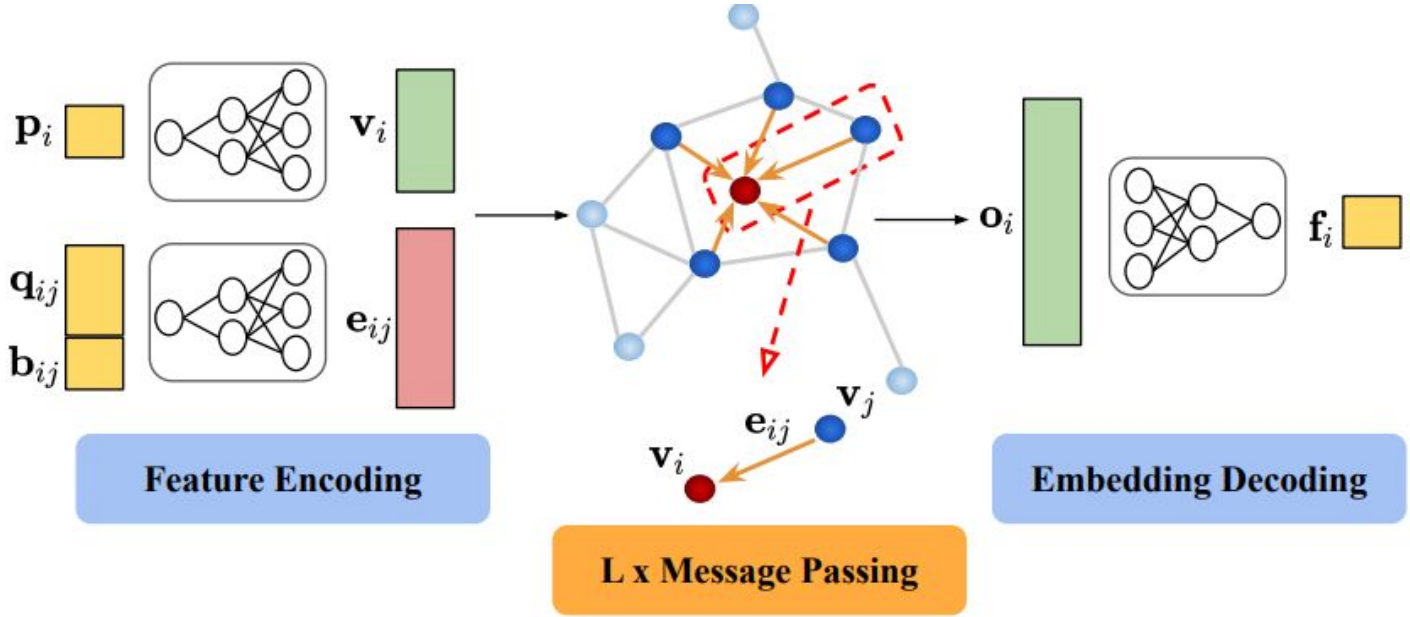


Componenti della forza

Invariante per traslazioni e rotazioni

Invariante per traslazioni e equivariante per rotazioni

Architettura



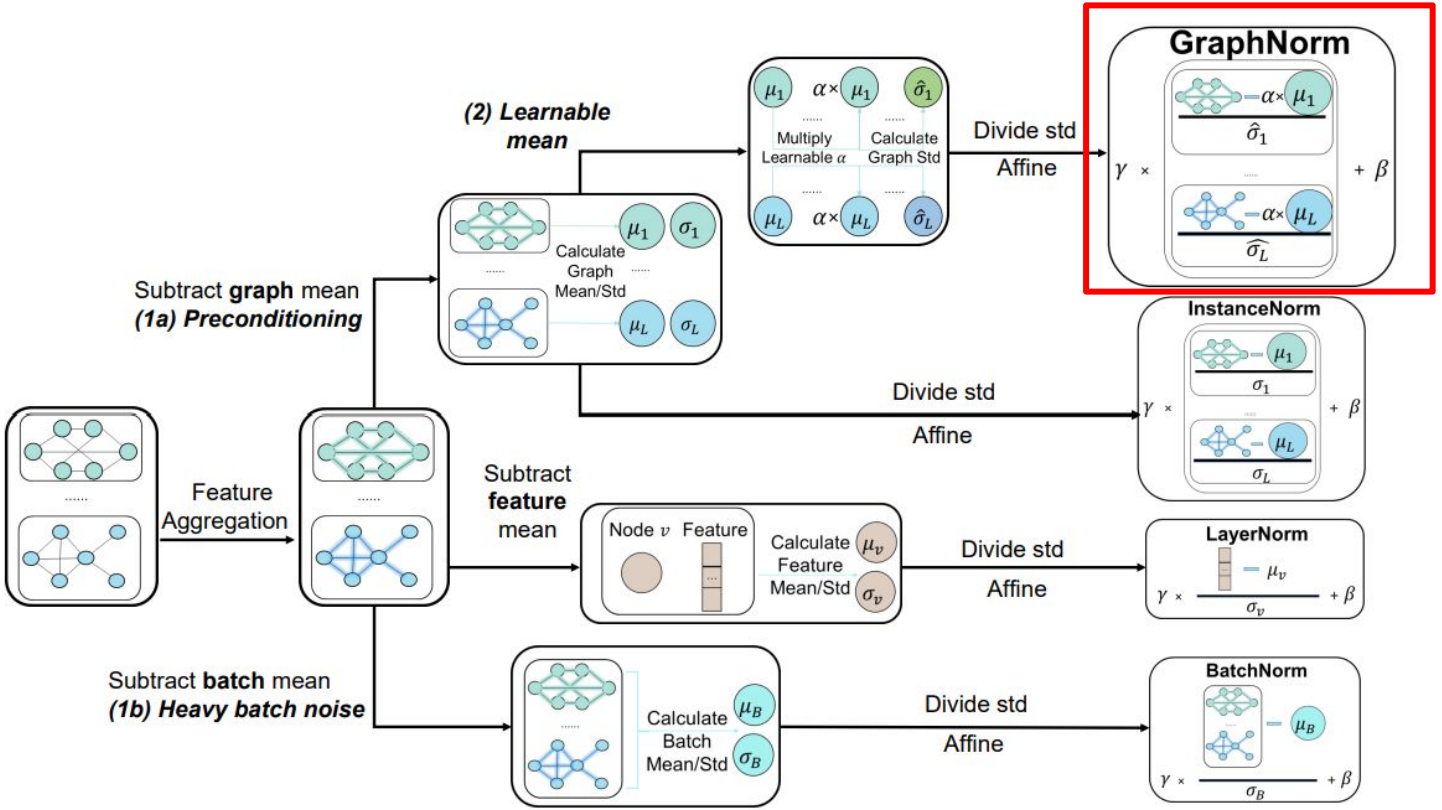
https://arxiv.org/pdf/2112.03383

Architettura - Message Passing

$$\mathbf{x}'_i = \mathrm{MLP}\left(\Sigma_{j \in \mathcal{N}(i)} \left\{\mathrm{MLP}\left((\mathbf{x}_i * \mathbf{x}_j) \,||\, \mathbf{e}_{j,i}\right)\right\}\right)$$

- Solo il primo layer usa informazioni sul legame
- Secondo e terzo layer usano residual connection

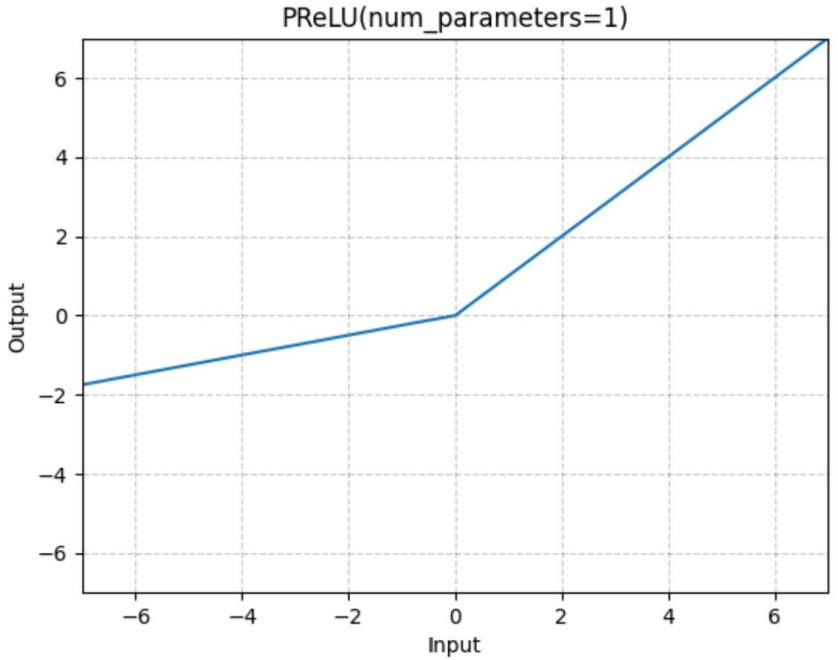
Architettura - Normalization



https://arxiv.org/pdf/2009.03294

Architettura - Activation function

L’utilizzo della PReLU (Parametric Rectified Linear Unit), assieme ad alcune epoche di warm-up, ha risolto il problema dei *dead neurons* alla fine della rete



Training

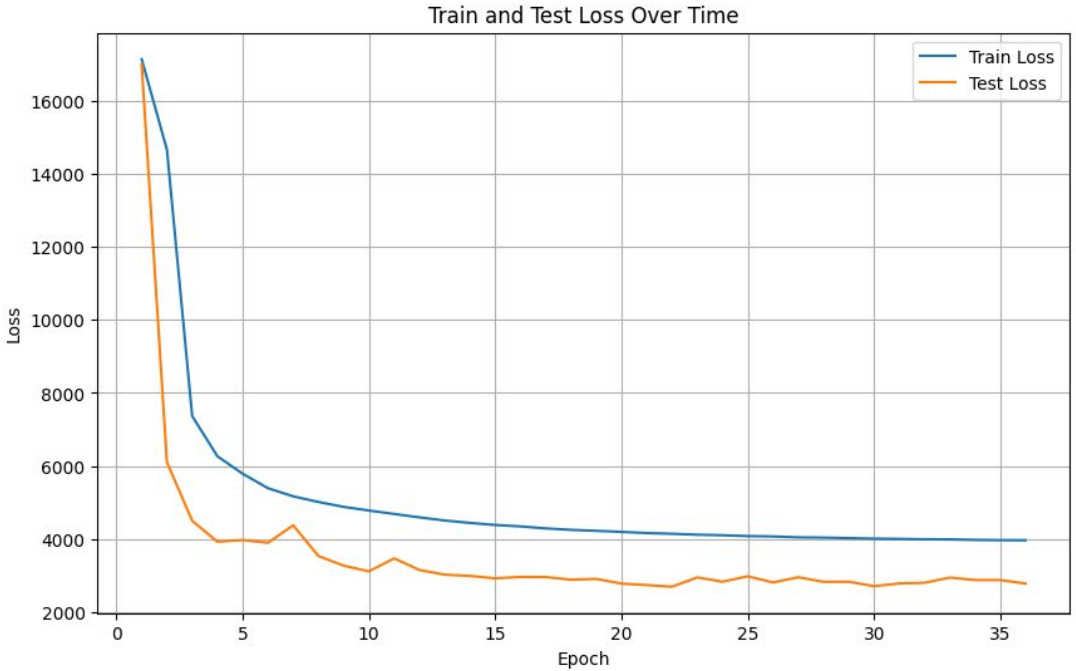
- 5 epoche di warm-up con una *loss function* modificata per favorire output diversi da 0
- *Learning rate* iniziale uguale a 10^{-3} e poi decadimento esponenziale
- Salvataggio di un checkpoint ogni sei epoche
- *Data augmentation* con rotazioni casuali 3D durante il training
- Tracking dell'errore lungo ognuna delle tre coordinate
- Miglior modello scelto a posteriori

training_log.txt

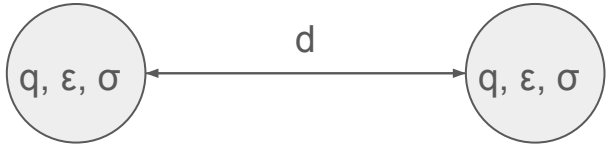
```
Epoch: 01, Train Loss: 17136.9064, Test Loss: 16993.3735, LR: 2000.00*10^(-7)
Losses: x: 5668.9822, y: 5674.6931, z: 5650.0226
Epoch: 02, Train Loss: 14662.1705, Test Loss: 6105.3166, LR: 4000.00*10^(-7)
Losses: x: 2052.6152, y: 2063.3387, z: 1989.3783
Epoch: 03, Train Loss: 7368.2516, Test Loss: 4500.1855, LR: 6000.00*10^(-7)
Losses: x: 1485.8003, y: 1517.2870, z: 1497.1134
Epoch: 04, Train Loss: 6264.9336, Test Loss: 3926.5310, LR: 8000.00*10^(-7)
Losses: x: 1255.5848, y: 1333.2477, z: 1337.7135
```

Risultati

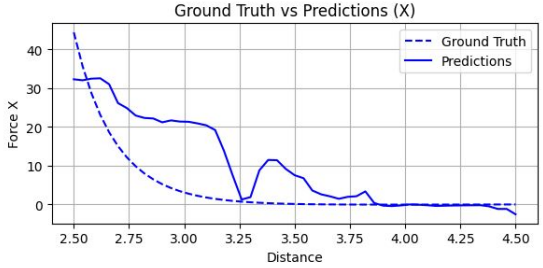
Validation error = 4,18 u/atomo (≈20%)
Test error (sistema grande di molecole d'acqua) = 4,24 u/atomo
Test error (argon) maggiore della somma dei moduli delle forze!

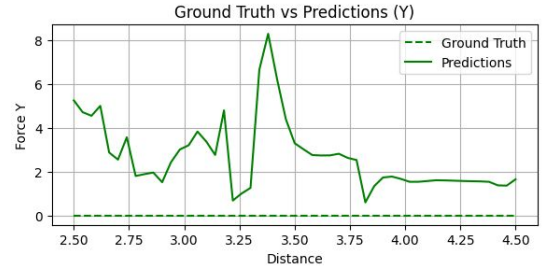


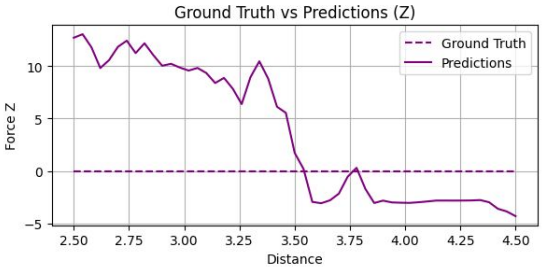
Risultati - Fit delle forze



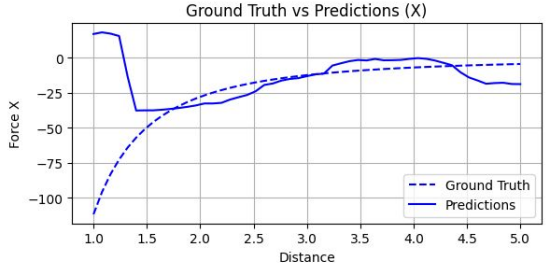
Lennard-Jones

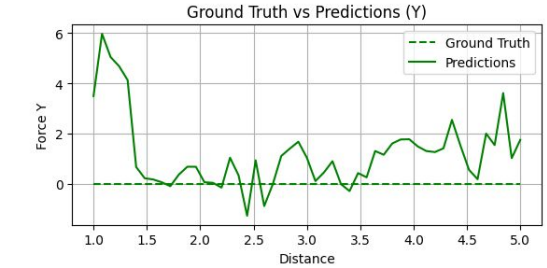


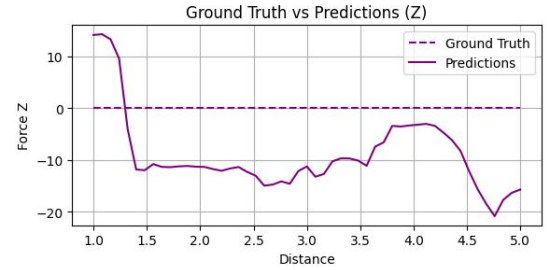




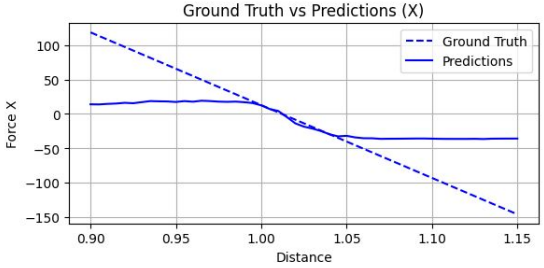
Coulomb

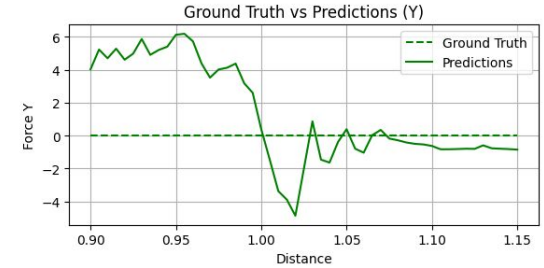


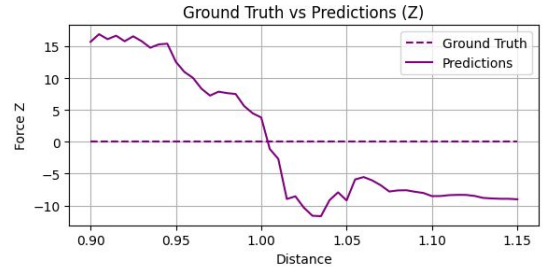




Legame armonico







Fine-tuning

Un modello davvero generalizzabile richiede dati più vari, ma almeno alcune parti della rete dovrebbe essere simili anche con input diversi (per esempio il decoder e secondo e terzo layer di Message Passing) → Il modello pre allenato sull'acqua "impara" più facilmente l'argon?