

Deep Learning & Applied AI

Geometric deep learning

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SAPIENZA
UNIVERSITÀ DI ROMA



Audio signals



Images

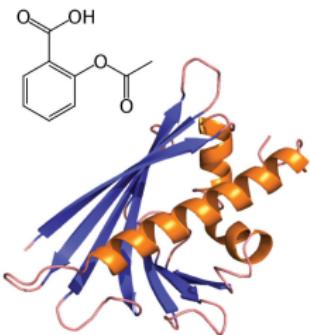
Geometric DL si occupa di estendere le capacità del DL ad altri domini non piatti come quelli qui mostrati



Audio signals



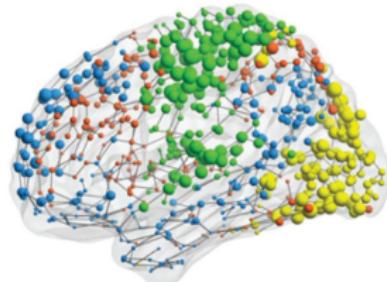
Social networks



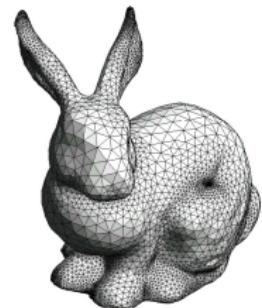
Molecules



Images

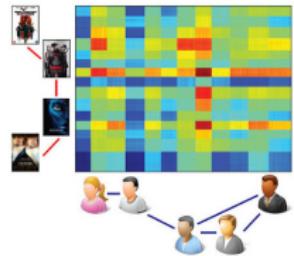


Functional networks

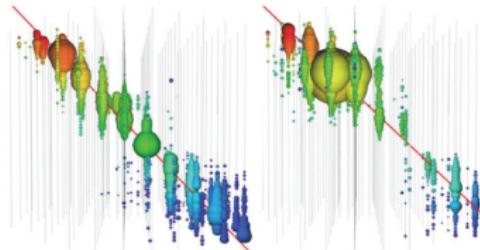


3D shapes

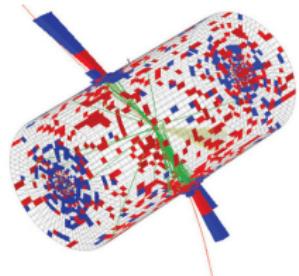
Applications of geometric deep learning



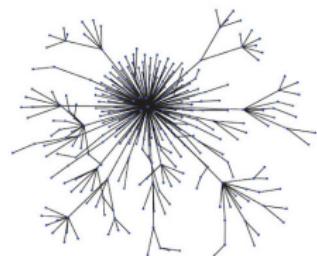
Recommender system



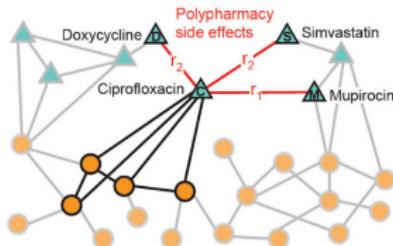
Neutrino detection



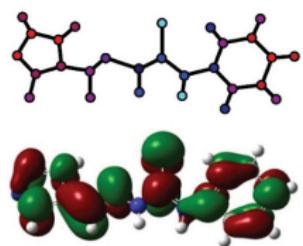
LHC



Fake news detection



Drug repurposing

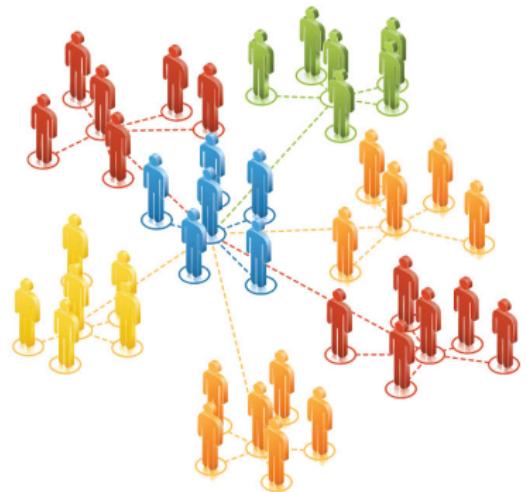


Chemistry

Prototypical non-Euclidean objects



Manifolds



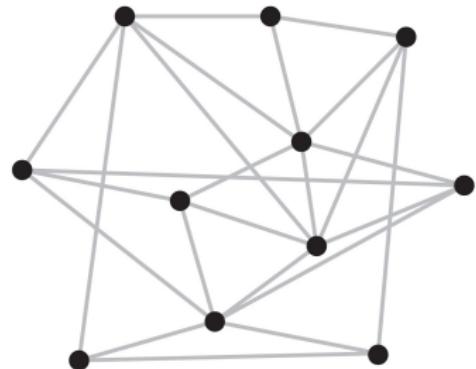
Graphs

Ci sono anche altri esempi ma questi due
sono i campi in cui il geometric DL è più utilizzato

Domain structure vs Data on a domain

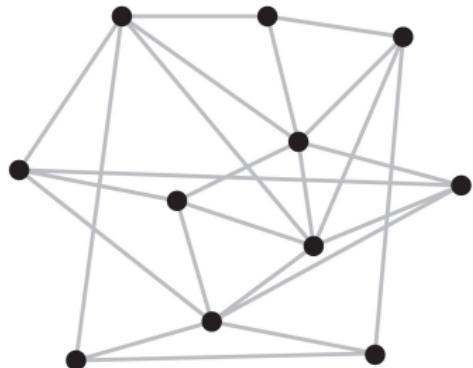


Domain structure vs Data on a domain

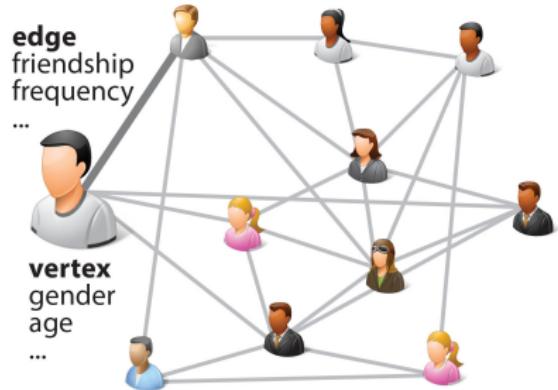


Domain structure

Domain structure vs Data on a domain

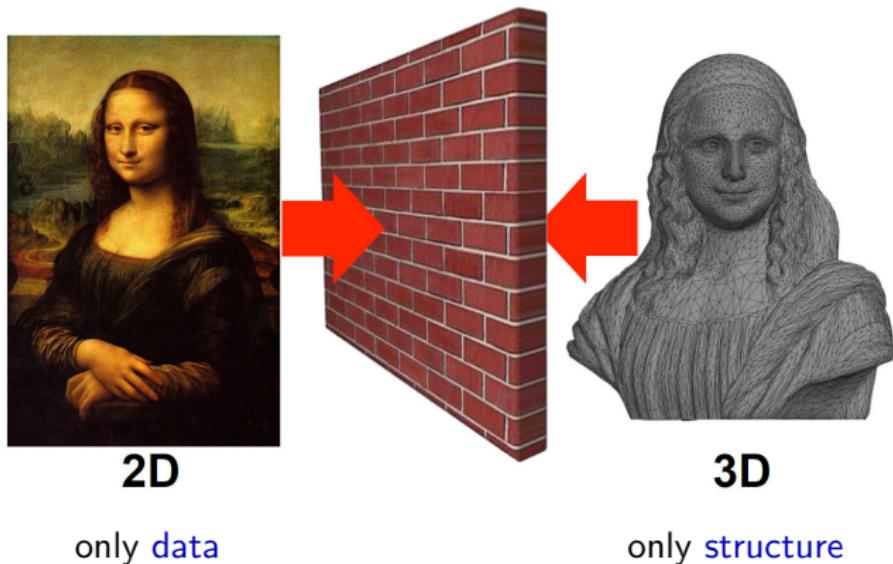


Domain structure



Data on a domain

Domain structure vs Data on a domain



Con dati 2D spesso si hanno solo informazioni riguardanti le feature. D'altra parte, spesso con dati 3D si hanno solo informazioni riguardanti la struttura. Quindi il passaggio tra questi due tipi di dato non è immediato e richiede una rimodulazione delle tecniche di DL

Fixed vs different domain



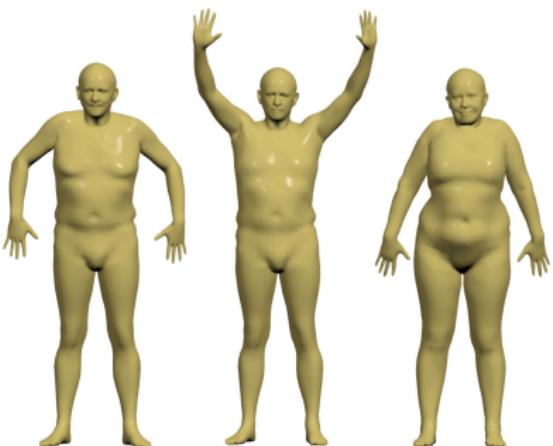
Social network
(fixed graph)

Fixed vs different domain



Social network
(fixed graph)

(idea semplificata) in un grafo il dominio
è sempre lo stesso, come in un'immagine...

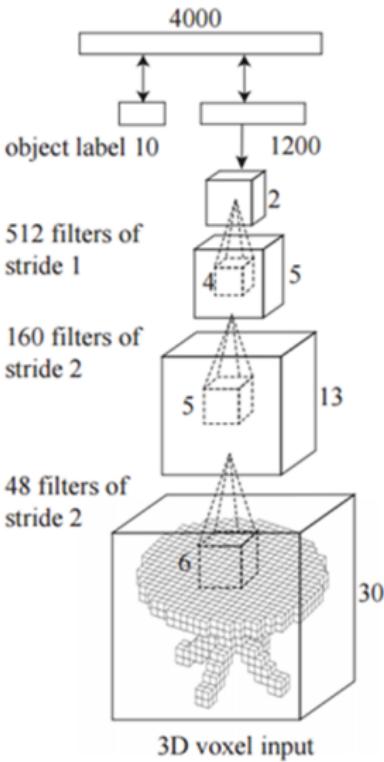


3D shapes
(different manifolds)

... mentre con le forme 3D il dominio cambia
(non esiste un dominio fisso in grado di descrivere
tutte le possibili varianti di un oggetto 3D, perché
la sua struttura cambia)

3D ShapeNets

- **Volumetric representation** (shape = binary voxels on 3D grid)

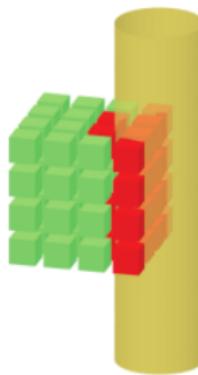


Convolutional deep belief network

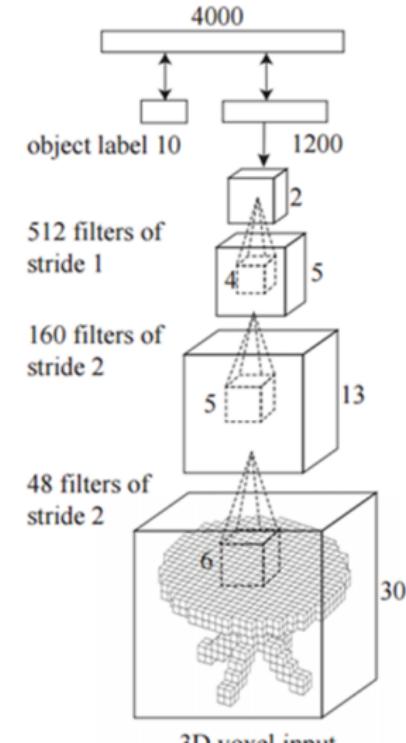
Wu et al, "3D ShapeNets: A Deep Representation for Volumetric Shapes" 2015

3D ShapeNets

- **Volumetric representation** (shape = binary voxels on 3D grid)
- 3D convolutional network

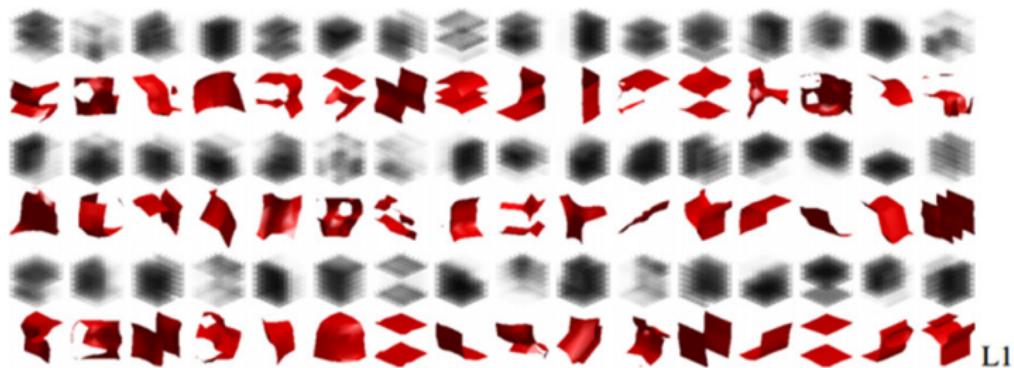


In pratica, è possibile realizzare l'operatore di convoluzione anche a forme 3D, adattando il kernel alla dimensione

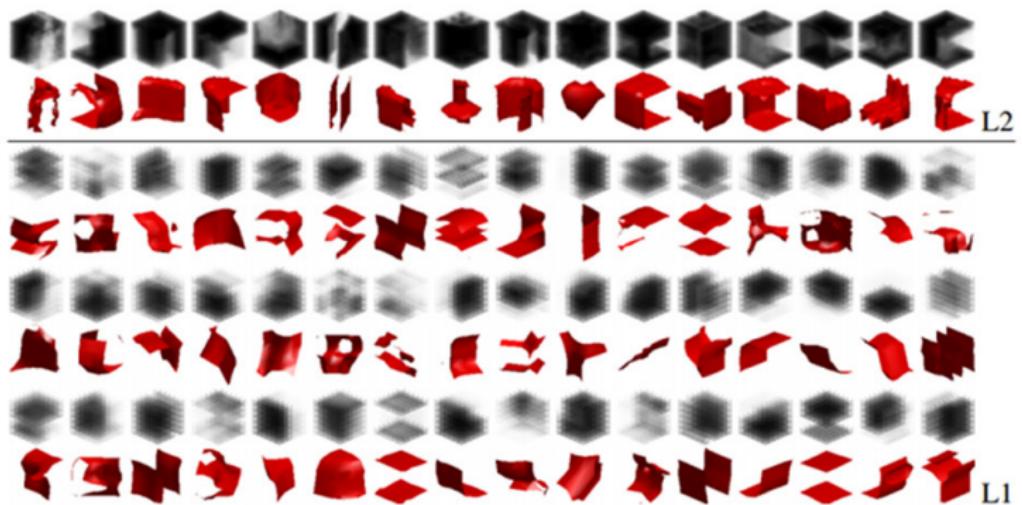


Convolutional deep belief network

Learned features: 3D primitives

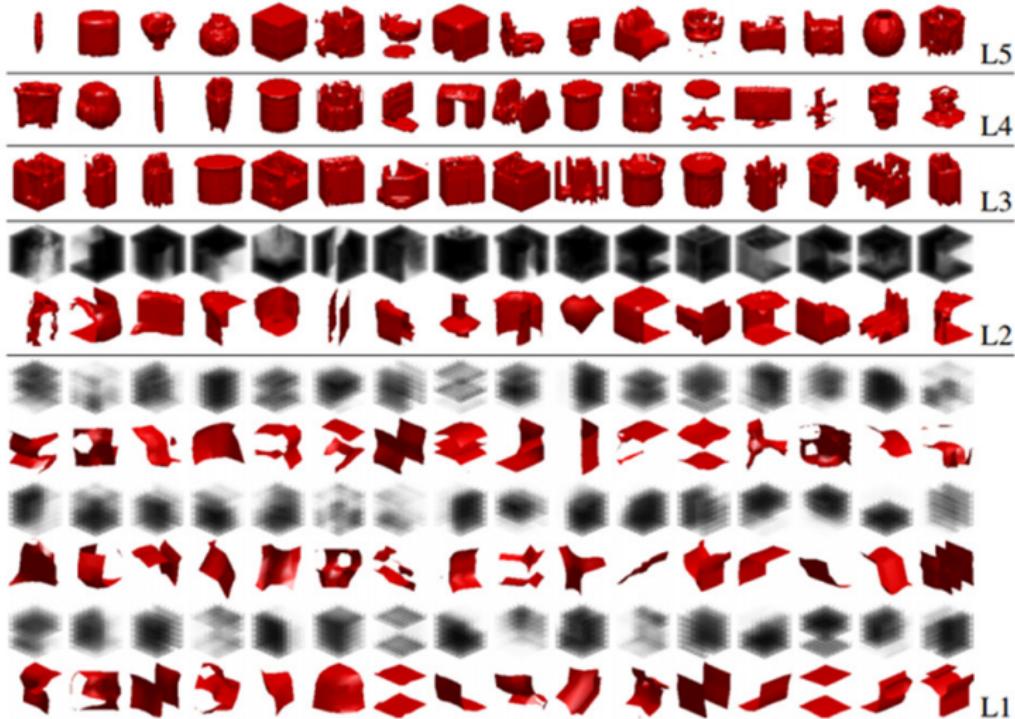


Learned features: 3D primitives

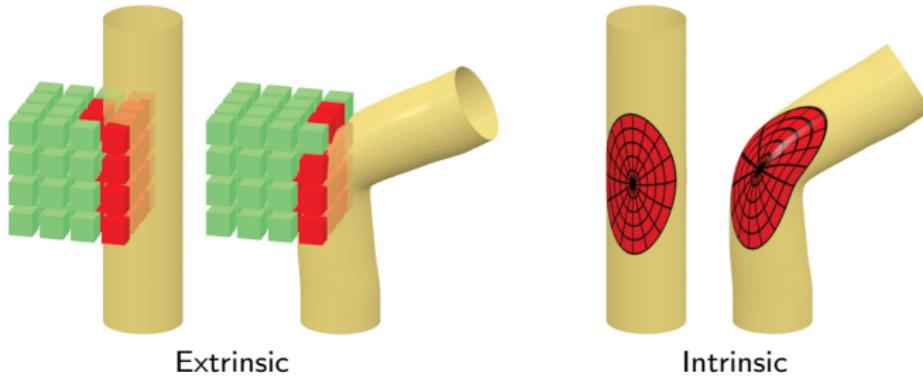


Learned features: 3D primitives

Così come in 2D, anche in 3D vengono catturate le feature su diversi piani di complessità



Challenges of geometric deep learning



Così come per il 2D, anche per il 3D vogliamo che le operazioni siano invarianti rispetto ad alcune trasformazioni. Tuttavia, in 3D sbucano fuori nuove sfide, come questa.

Nel caso di oggetti 3D deformabili (con quelli NON deformabili bastano le convoluzioni 3D), vogliamo che il kernel subisca le stesse trasformazioni/acquisisca le stesse proprietà dell'oggetto sul quale viene applicato

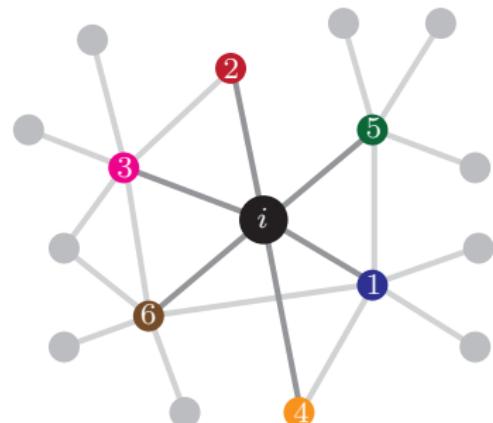
Extrinsic vs Intrinsic

Extrinsic

Intrinsic

Local ambiguity

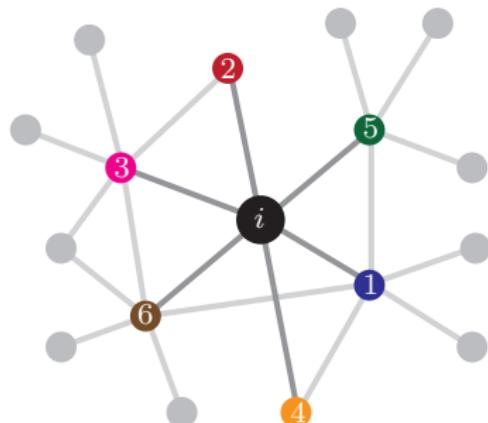
Unlike images, there is **no canonical ordering** of the domain points.



Graph (permutation)

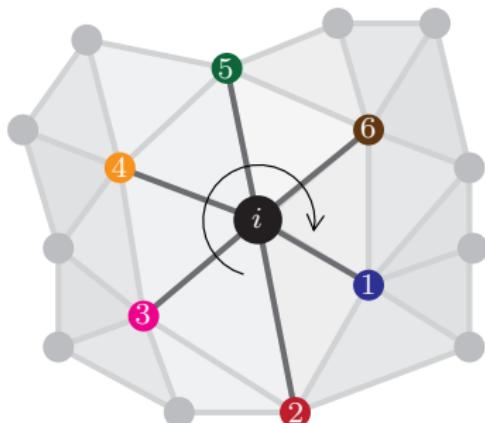
Local ambiguity

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Graph (permutation)

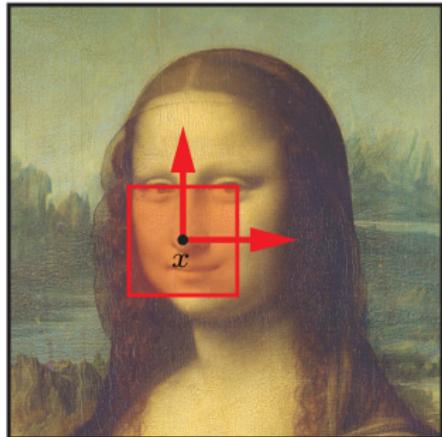
In un grafo 2D posso riordinare i nodi come voglio e così creare ogni volta un grafo diverso



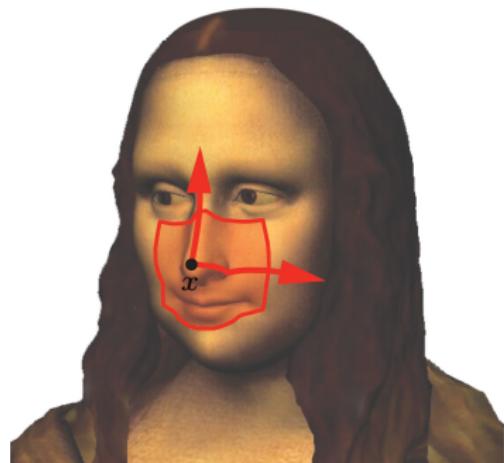
Mesh (rotation)

In un grafo 3D non posso riordinare i nodi perché il grafo possiede già una forma, ma posso cambiare il nodo iniziale e questo genera diverse orientamenti dello stesso grafo

Non-Euclidean convolution?



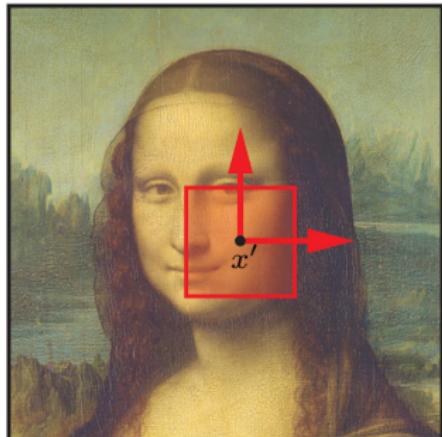
Euclidean



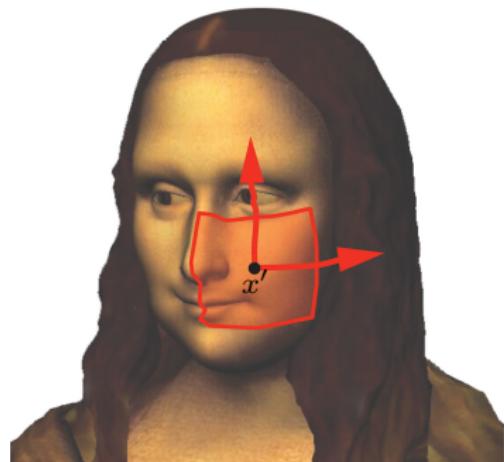
Non-Euclidean

Le coordinate 2D non funzionano su un oggetto 3D, perché un movimento base in 2D non si può tradurre in maniera universale in 3D. Ancora peggio se...

Non-Euclidean convolution?

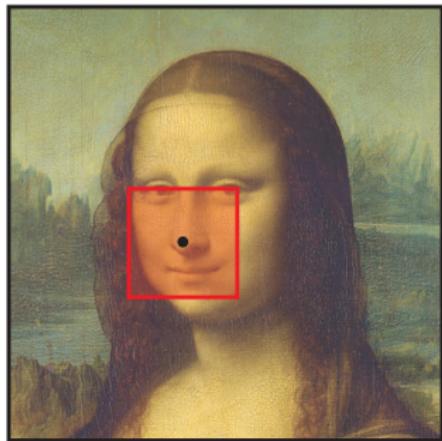


Euclidean

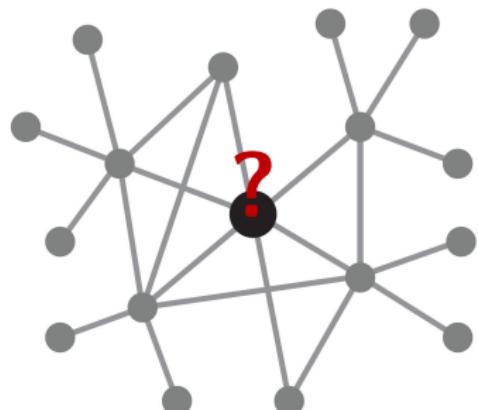


Non-Euclidean

Non-Euclidean convolution?



Image



Graph

... parliamo di grafi

Suggested reading

Bronstein et al, 2016

“Geometric deep learning: going beyond Euclidean data”

<https://arxiv.org/abs/1611.08097>