Geometric Deep Learning on Graphs and Manifolds Using Mixture Model CNNs

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JOHNS HOPKINS
WHITING SCHOOL
of ENGINEERING

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Introduction

What can CNNs handle?

→ Cat

Image: [Cat]

→ Cat

Image: [Sound]

Introduction

What can’t CNNs handle?

Graphs

Image: [SocialGraph]

Manifolds

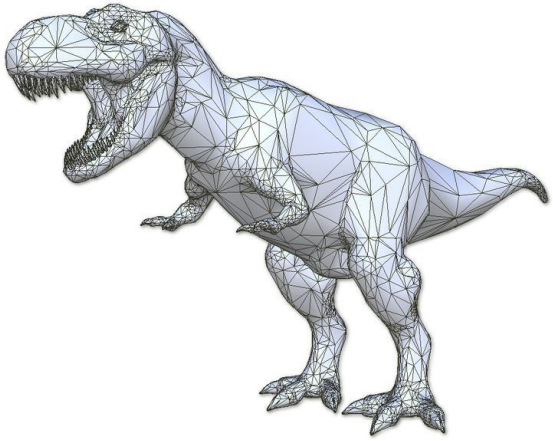


Image: [TRex]

Introduction

Why don’t classical CNNs work?

Kernels can only be applied in **Euclidean** space

1	2	1
2	4	2
1	2	1

*

= ???

Image: [SocialGraph]

Existing Approaches (Graphs) - Spectral CNN

(Bruna et al., ICLR 2013)

$$\mathrm{f}^{out} = \xi\Big(\sum_{l'=1}^{p} \Phi_k \hat{G} \Phi_k^{\top} \mathrm{f}_{l'}^{in}\Big)$$

Formula: [MoNet_Paper]

learnable "filter"

Spectral transformation

Vertex signals

Problem: Computation of the Fourier transforms is Expensive ($O(n^2)$)

Existing Approaches (Graphs) - ChebNet

(Defferrard et al., NIPS 2016)

New definition of the filter:

Formula: [MoNet_Paper]

$$g_\alpha(\Delta) = \sum_{j=0}^{r-1} \alpha_j T_j(\hat{\Delta}) = \sum_{j=0}^{r-1} \alpha_j \Phi T_j(\hat{\Lambda}) \Phi^\top$$

polynomial coefficients

Chebyshev polynomial

Laplacian

$$T_j(\lambda) = 2\lambda T_{j-1}(\lambda) - T_{j-2}(\lambda)$$

Formula: [MoNet_Paper]

→ Applying g means applying the Laplacian r times
→ O(rn)

Existing Approaches (Graphs)

Big problem:

This spectral approach can’t generalize between different graphs!

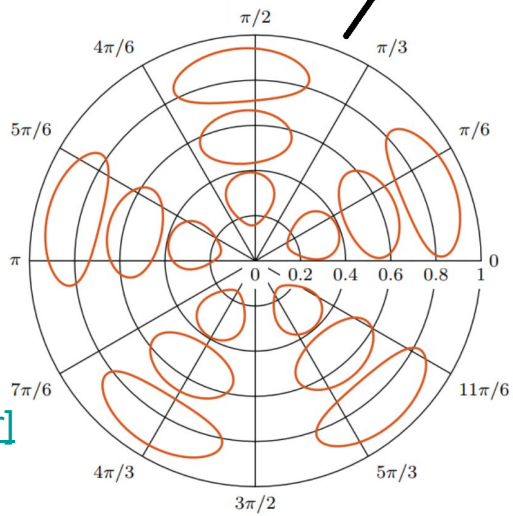
Existing Approaches (Manifolds) - GCNN

(Masci et al., 3DRR 2015)

Extracting Patches:

$$(D(x)f)(p,\theta) = \int_{\chi} w_{p,\theta}(x,y) f(y) dy$$

Formula: [MoNet_Paper]



GCNN

Image: [MoNet_Paper]

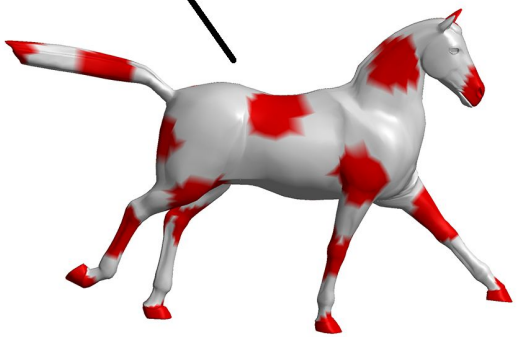


Image: [M.Bronstein]

Existing Approaches (Manifolds) - GCNN

Convolution with Patches:

$$(f \star g)(x) = \max_{\Delta\theta \in [0,2\pi)} \int_0^{2\pi} \int_0^{p_{max}} g(p, \theta + \Delta\theta)(D(x)f)(p, \theta) dp d\theta$$

Formula: [MoNet_Paper]

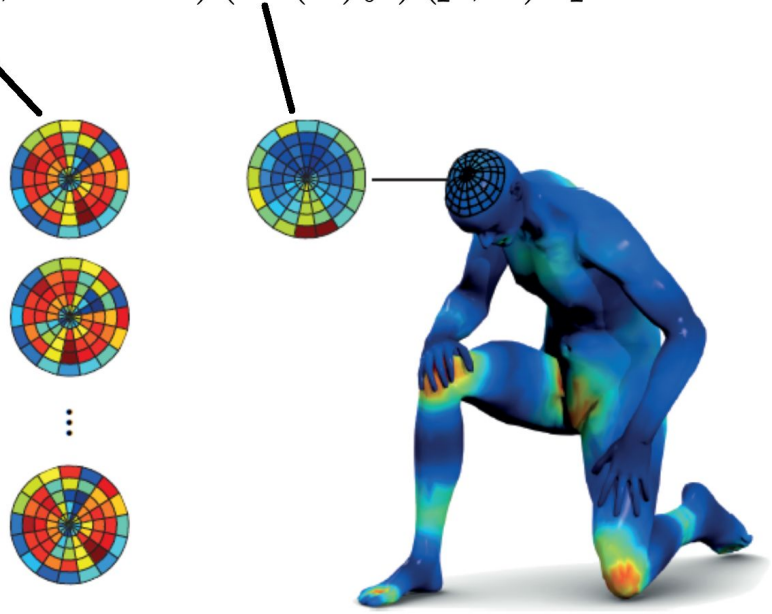


Image: [M.Bronstein]

Existing Approaches (Manifolds) - ACNN

(Boscaini et al., NIPS 2016)

Basic idea: Anisotropic patches

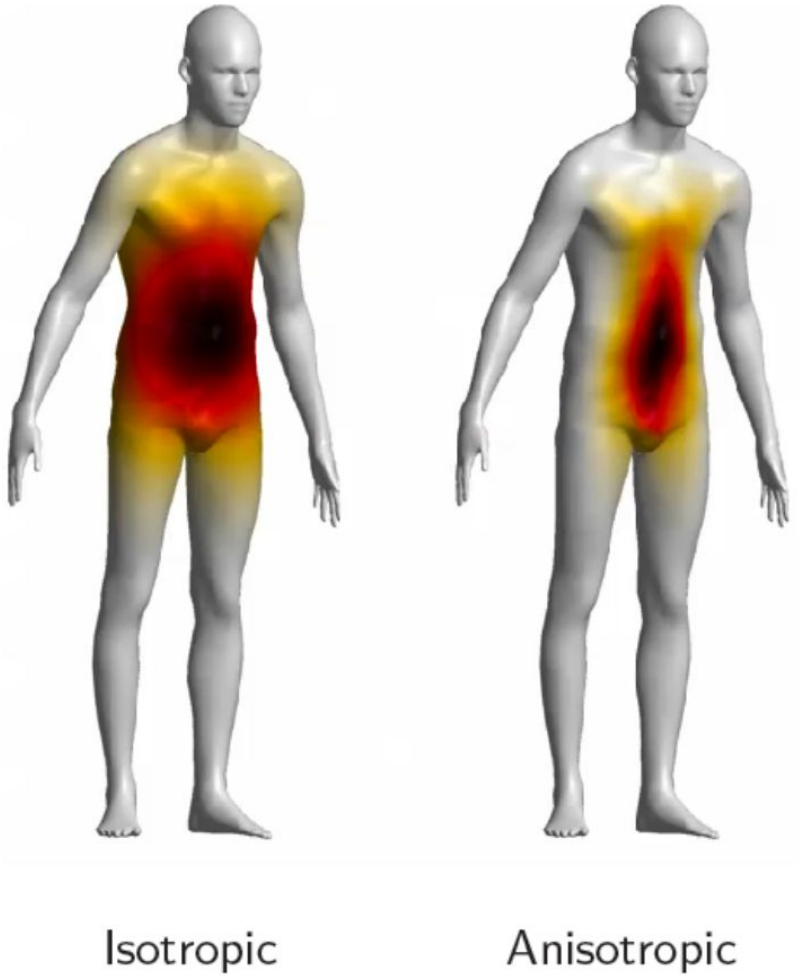


Image: [M.Bronstein]

Existing Approaches (Manifolds) - ACNN

New weighting function:

$$f_t(x,t) = -\mathrm{div}_\chi(A(x)\nabla_\chi f(x,t))$$

$$A_{\alpha\theta}(x) = R_\theta(x)\begin{pmatrix}\alpha & \\ & 1\end{pmatrix}R_\theta^\top(x)$$

rotation

elongation

Formula: [MoNet_Paper]

Formula: [MoNet_Paper]

State of the art so far:

$$(f \star g)(x) = \sum_{j=1}^{J} g_j D_j(x) f$$

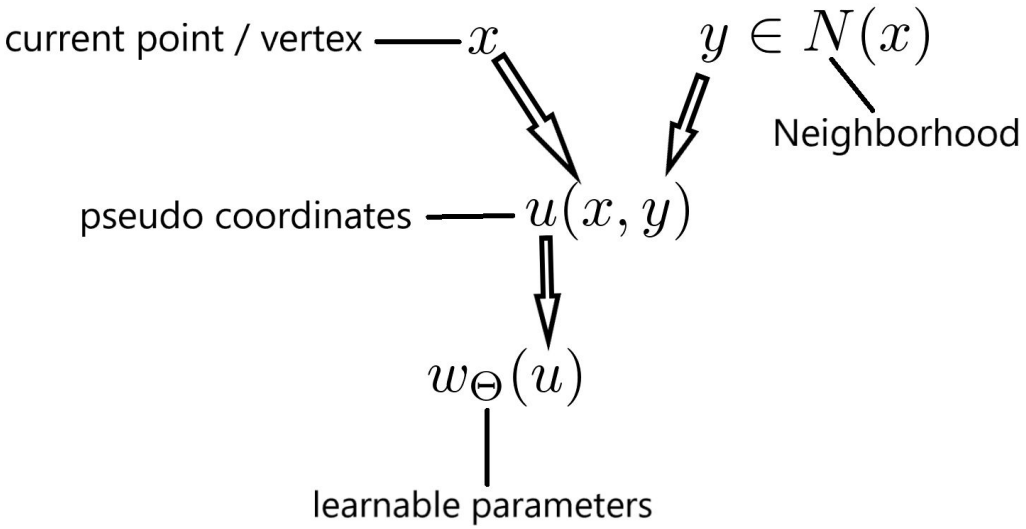
learned

not learned

→ Can’t patch operators be learned?

Monti's Framework

Approach to get machine learning into weight function:



Monti's Framework

Use the new weighting function in a patch operator:

$$D_j(x)f = \sum_{y \in N(x)} w_j(u(x,y))f(y)$$

j'th patch

j'th parameter

Formula: [MoNet_Paper]

Apply the convolution:

# of parameters

$$(f \star g)(x) = \sum_{j=1}^{J} g_j D_j(x) f$$

kernel

Patch

Formula: [MoNet_Paper]

Monti's Framework

Method	Pseudo-coordinates	$\mathbf{u}(x,y)$	Weight function $w_j(\mathbf{u}), j = 1, \dots, J$
CNN [23]	Local Euclidean	$\mathbf{x}(x,y) = \mathbf{x}(y) - \mathbf{x}(x)$	$\delta(\mathbf{u} - \bar{\mathbf{u}}_j)$
GCNN [26]	Local polar geodesic	$\rho(x,y), \theta(x,y)$	$\exp(-\frac{1}{2}(\mathbf{u} - \bar{\mathbf{u}}_j)^\top \begin{pmatrix} \bar{\sigma}_\rho^2 & \\ & \bar{\sigma}_\theta^2 \end{pmatrix}^{-1} (\mathbf{u} - \bar{\mathbf{u}}_j))$
ACNN [7]	Local polar geodesic	$\rho(x,y), \theta(x,y)$	$\exp(-\frac{1}{2}\mathbf{u}^\top \mathbf{R}_{\bar{\theta}_j} \begin{pmatrix} \bar{\alpha} & \\ & 1 \end{pmatrix} \mathbf{R}_{\bar{\theta}_j}^\top \mathbf{u})$
GCN [21]	Vertex degree	$\deg(x), \deg(y)$	$\left(1 - \lvert 1 - \frac{1}{\sqrt{u_1}} \rvert\right)\left(1 - \lvert 1 - \frac{1}{\sqrt{u_2}} \rvert\right)$
DCNN [3]	Transition probability in r hops	$p^0(x,y), \dots, p^{r-1}(x,y)$	$\mathrm{id}(u_j)$

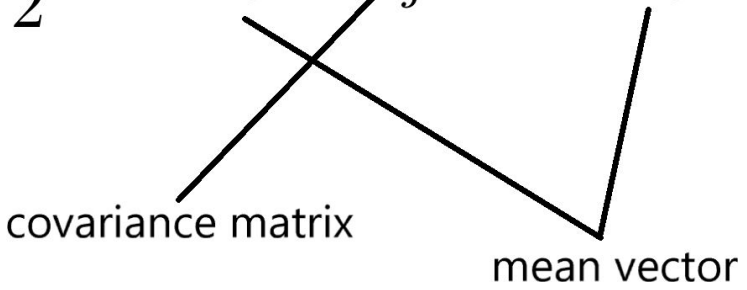
Table: [MoNet_Paper]

Existing approaches for geometric deep learning are special cases of Monti's framework!

MoNet - How it works

Formula: [MoNet_Paper]

$$w_j(u) = exp(-\frac{1}{2}(u - \mu_j)^\top \Sigma_j^{-1}(u - \mu_j))$$



→ Because of this weighting function (f ★ g)(x) can be interpreted as a **Gaussian Mixture Model**!

MoNet - Results (MNIST)

Comparing MoNet to state-of-the-art approaches for euclidean (LeNet) and graph (ChebNet) space

Dataset	LeNet5	ChebNet	**MoNet**
Full grid	99.33%	99.14%	99.19%
$\frac{1}{4}$ grid	98.59%	97.70%	98.16%
300 Superpixels	-	88.05%	**97.30%**
150 Superpixels	-	80.94%	**96.75%**
75 Superpixels	-	75.62%	**91.11%**

Table: [MoNet_Paper]

→ ChebNet fails at generalizing between different graphs

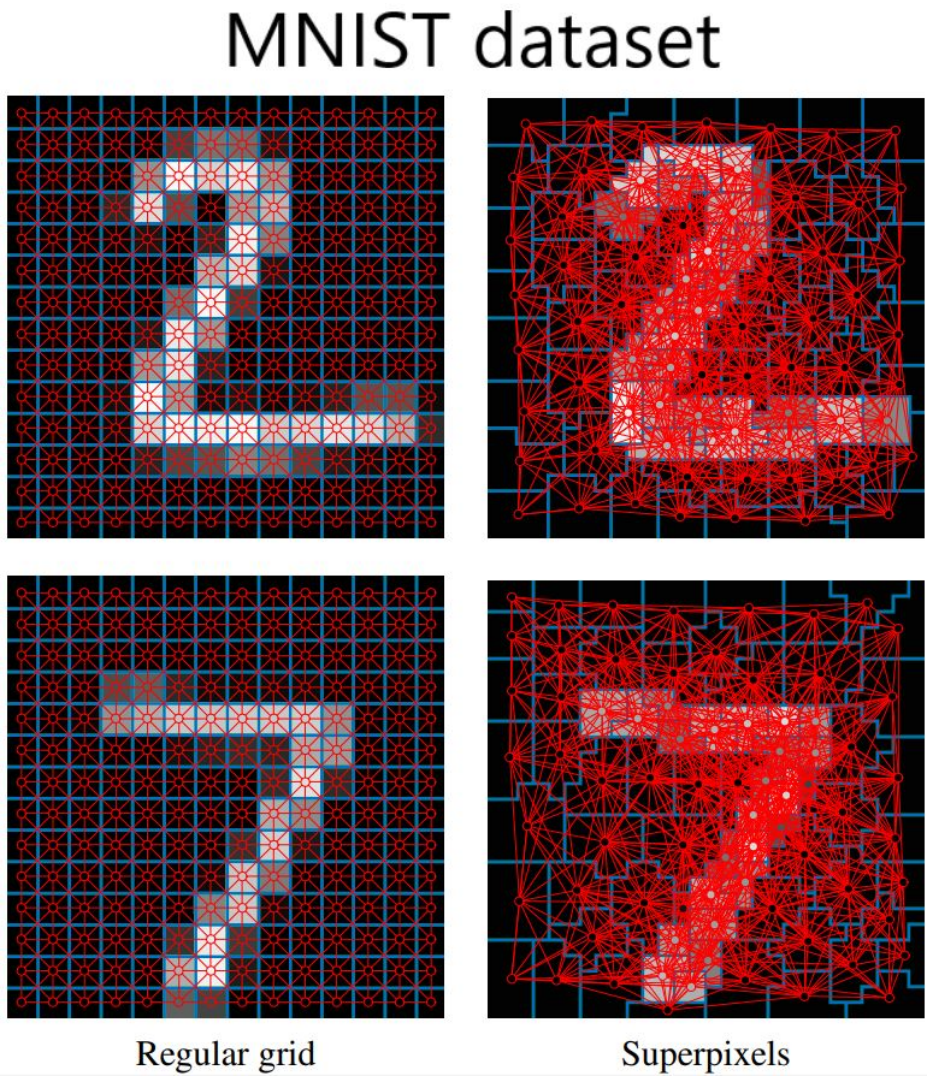


Image: [MoNet_Paper]

MoNet - Results (Cora & PubMed)

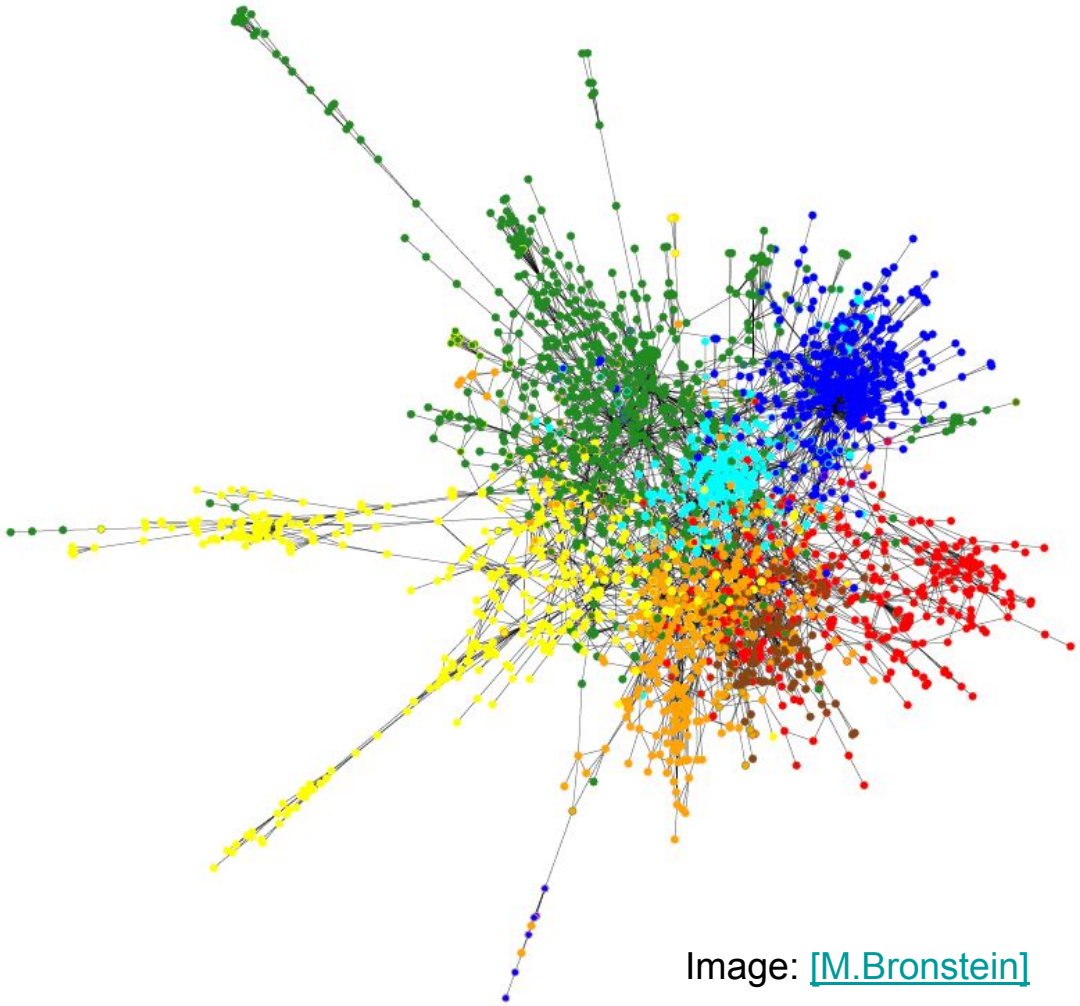


Image: [M.Bronstein]

MoNet - Results (Cora & PubMed)

MoNet was compared to GCN (simplified ChebNet) and DCNN

Task: classify papers into one of 3 (Cora) or 7 (PubMed) groundtruth classes

All approaches were trained in the same way with **20 samples** per class, **500 vertices** for validation and **1000 vertices** for testing.

	Cora	PubMed
Learning Algorithm	Adam	Adam
Number of epochs	3000	1000
Validation frequency	0.01	0.04
Learning rate	0.1	0.1
Decay rate	10^{-1}	-
Decay epochs	1500, 2500	-
Early stopping	No	No

Table: [MoNet_Paper]

MoNet - Results (Cora & PubMed)

$$u(x, y) = \left(\frac{1}{\sqrt{deg(x)}}, \frac{1}{\sqrt{deg(y)}}\right)^\top$$

Formula: [MoNet_Paper]

Patch operator was defined with their standard GMM approach

MoNet - Results (Cora & PubMed)

Table: [MoNet_Paper]

Method	Cora	PubMed
ManiReg [4]	59.5%	70.7%
SemiEmb [42]	59.0%	71.1%
LP [45]	68.0%	63.0%
DeepWalk [28]	67.2%	65.3%
Planetoid [44]	75.7%	77.2%
DCNN [3]	$76.80 \pm 0.60\%$	$73.00 \pm 0.52\%$
GCN [21]	$81.59 \pm 0.42\%$	$78.72 \pm 0.25\%$
MoNet	$\mathbf{81.69} \pm 0.48\%$	$\mathbf{78.81} \pm 0.44\%$

DCNN, GCN and MoNet were trained and tested 50 times. Shown results are average accuracy

MoNet - Results (FAUST)

FAUST dataset = 100 human bodyscans of 10 different persons

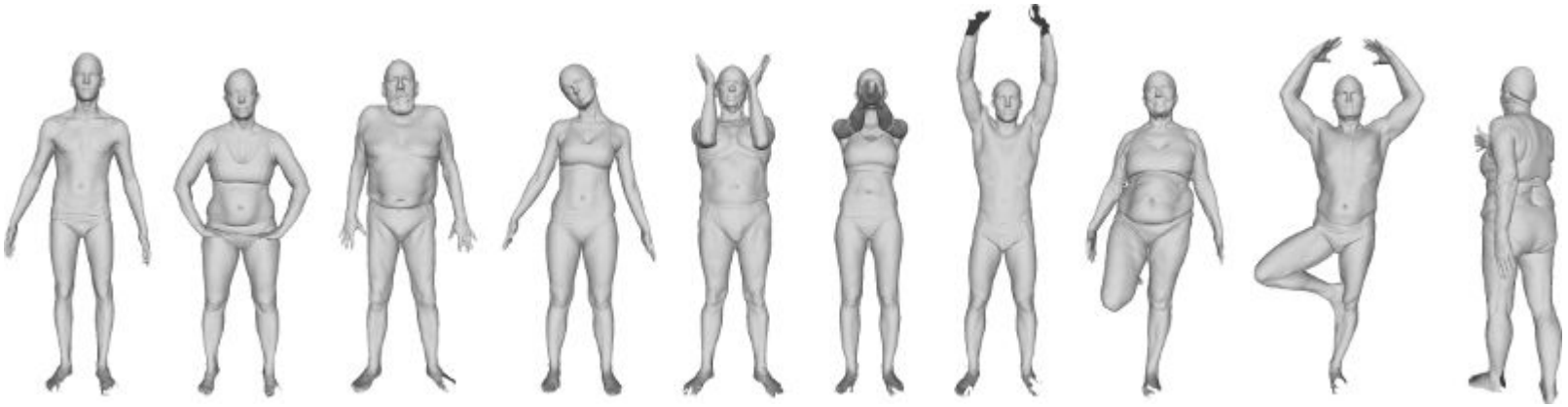


Image: [FAUST]

MoNet - Results (FAUST)

Task: find corresponding points between 3D models

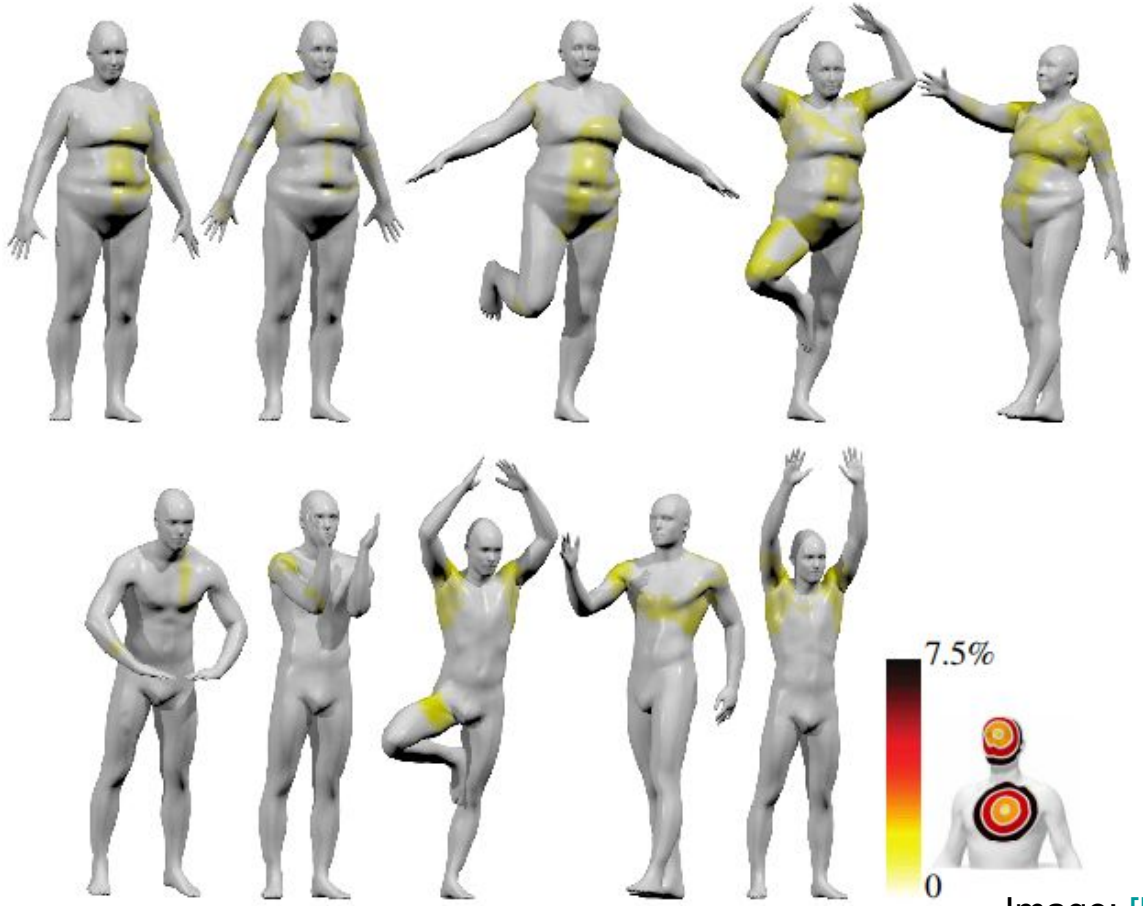


Image: [MoNet_Paper]

MoNet - Results (FAUST)

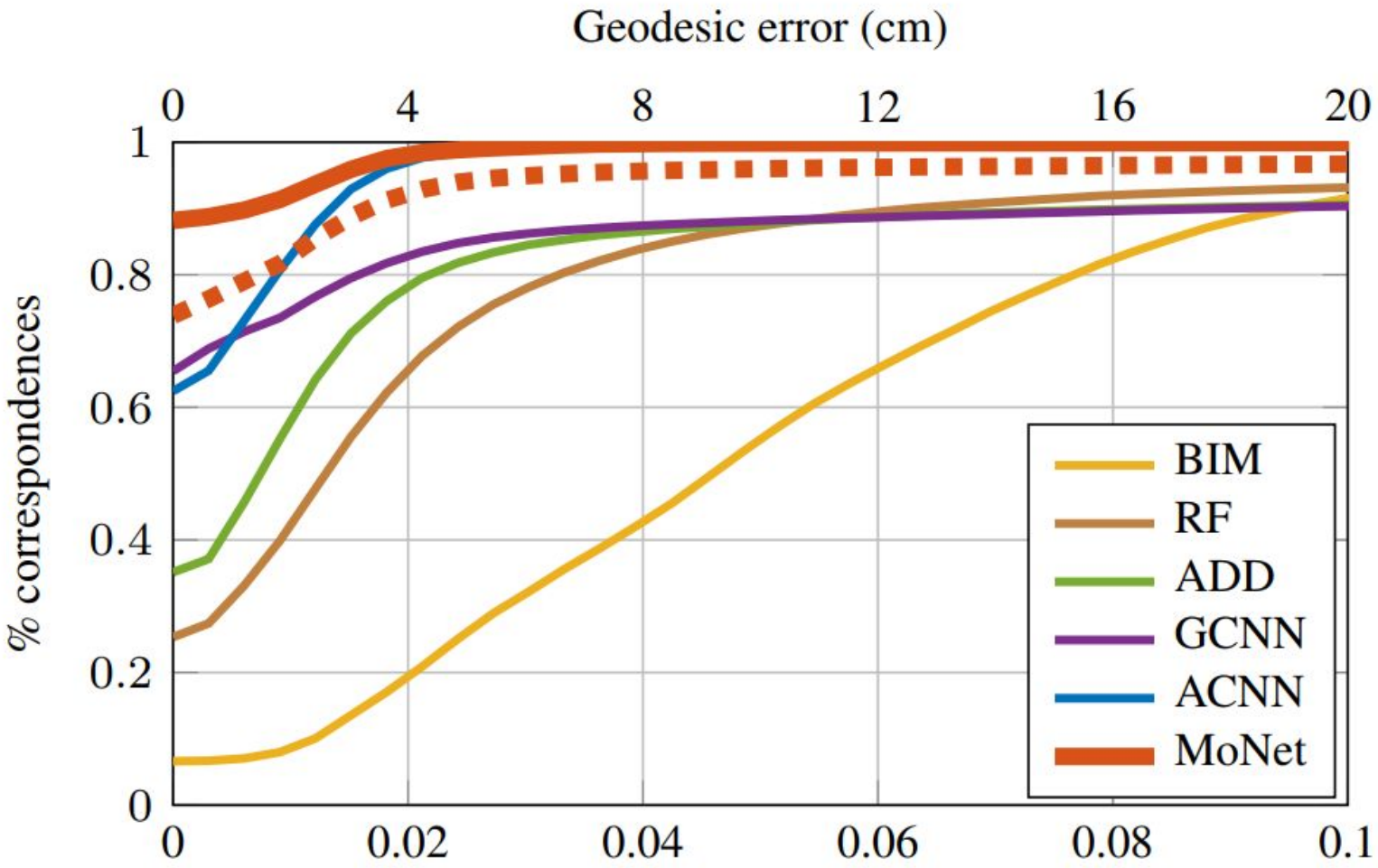


Image: [MoNet_Paper]

MoNet - Results (FAUST)

Conclusion

Positive:

+ Really powerful framework: **generic but simple**
+ Michael Bronstein held a interesting lecture at TUM last summer about geometric deep learning

Possible improvements:

- "w(u) is a convenient choice"

→ other functions might even work better!

- They could have explained more "why"

References

[Cat]: https://www.eastcottvets.co.uk/77/Kitten-Vaccination-Prices/ (26.12.2017)
[Sound]: https://pixabay.com/de/audio-musik-sfa-jazz-ton-welle-1293262/ (26.12.2017)
[SocialGraph]: http://483eclass.com/fall16/build_1/Hung/index.html (26.12.2017)
[TRex]: https://i.pinimg.com/736x/1d/b8/1b/1db81b7773c46bf3b3631a0c84b47385--quadrilateral-scripts.jpg (26.12.2017)
[M.Bronstein] https://www.dropbox.com/s/r4bzfux4ter8902/TUM%20Tutorial.pdf?dl=0 (07.01.2018)
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[MoNet_Paper] http://openaccess.thecvf.com/content_cvpr_2017/papers/Monti_Geometric_Deep_Learning_CVPR_2017_paper.pdf (16.12.2018)

Thank you

(Q&A now)