Learning, geometry and PDEs, a promising interaction ?

L. Bois¹², <u>E. Franck</u>¹², C. Mengel², L. Navoret¹², G. Steimer¹², V. Vigon¹²

ITI Seminar, Strasbourg

¹Inria Nancy Grand Est, France ²IRMA, Strasbourg university, France



E. Franck



Outline

Deep learning for closure PDE problem

Reduced problem for plasma physics

Deep learning and geometry

Theory of geometric deep learning





Deep learning for closure PDE problem



Models in plasma physics

- Plasma: gas at very large temperature which is electrically charged. Coupling between compressible fluid dynamic and electromagnetic.
- Kinetic models:

$$\partial_t f + \mathbf{v} \cdot \nabla f + (\mathbf{E} + \mathbf{v} \times \frac{\mathbf{B}}{\epsilon}) \cdot \nabla_{\mathbf{v}} f = \frac{1}{\epsilon} Q(f, f)$$

with $f(t, \mathbf{x}, \mathbf{v})$ the seven dimensional particles distribution and **E**, **B** the electric and magnetic fields given by the Maxwell equations.

Large dimensional multiscale PDEs with admit geometric structures to preserve and few diffusion process (less stable). So we need reduced models and adapted numerical methods.

Fluid models:

$\partial_t \mathbf{U} + \nabla \cdot \mathbf{F}(\mathbf{U}) = \epsilon \nabla \cdot (\mathbf{G}(\mathbf{U}) \nabla \mathbf{U})$

with $\mathbf{U}(t, \mathbf{x}) \in \mathbb{R}^n$ the macroscopic quantities (density, velocity etc).

Strongly nonlinear, multiscale PDE which admits discontinuous solutions in the low diffusion regime. So we need adapted numerical methods. Tricky point: stability.



Problem of closure

Simple case:

$$\partial_t f + v \partial_x f + \partial_x \phi \partial_v f = \frac{1}{\varepsilon} (M(\rho, u, T) - f)$$

with

$$\Delta \phi =
ho - 1$$

and the moment $\rho=\int f dv, \ \rho u=\int v f dv$ and $p=\int (v-u)^2 f dv.$

• When ϵ tends to zero we are close to the equilibrium $M(\rho, u, T)$.

When we take the three first moment in velocity we obtain the **Euler equation**.

$$\begin{cases} \partial_t \rho + \partial_x (\rho u) = 0\\ \partial_t \rho u + \partial_x (\rho u^2 + p) = 0\\ \partial_t E + \partial_x (Eu + pu) + \partial_x q = 0 \end{cases}$$

with $E = \frac{1}{2}\rho u^2 + \frac{1}{2}p$, $q = \frac{1}{2}\int_v (v - u)^3 f dv$.

How to compute the reduced model: we don't know q.

Solution: closure:

 $q \approx C(\rho(.), u(.), T(.), \epsilon)$

- Classical closure: asymptotic analysis gives $q = 0 + O(\epsilon)$ (Euler), $q = -\epsilon \frac{3}{2}p\partial_x T + O(\epsilon^2)$. Harmett-Perkins nonlocal in space.
- How construct a closure for moderate e?



Supervised learning and CNN

Closure by supervised learning

Using kinetic simulation we are able to collect data:

$$D = \{\rho(.), u(.), T(.), \epsilon\}_i, q(.)_i, \quad i = 1, ..., n\}$$

We can construct closure by supervised learning where we solve

$$\min_{\theta} \sum_{i}^{n} \| \mathcal{C}_{\theta}(\rho_{i}(.), u_{i}(.), \mathcal{T}_{i}(.), \epsilon_{i}) - q_{i}(.) \|_{2}^{2}$$

- The function C_{θ} can be in large dimension (if nonlocal in space) and strongly nonlinear. For this regression problem we use a neural network.
- Neural-network:

$$\mathcal{C}_{\theta}(x) = L_m \circ N \circ \ldots \circ \delta \circ L_2 \circ N \circ \delta \circ L_1(x)$$

with $L_{\theta_i}(y) = My$ with $M \in \mathcal{M}_{n_i \times n_{i+1}}(\mathbb{R})$, $y \in \mathbb{R}^{n_{i+1}}$ and N(y) a nonlinear function apply at each component of y.

The weights θ of the neural network are the coefficients of the matrix L_i ...

Supervised learning and CNN II

Fully connected neural network: the matrices *L_i* are dense.



1D convolutional neural network: the matrices L_i are sparse Toeplitz matrices.

- This is equivalent to applying a small convolution kernel to the signal 1D.
- Apply convolution kernel = apply a filter on signal (operation of the spectrum of the signal).
- Often we apply some convolution at the signal on each layer to create several new signals.

Supervised learning and CNN III

- Important properties for a convolutional layer:
 - □ Filters localized in space,
 - □ Anisotropic filter,
 - Multiple layers,
 - \Box O(1) parameters per filter (independent of input image size n),
 - \Box O(n) complexity per layer (filtering done in the spatial domain),



The convolutional network takes into account to 2D structure of the data. Essential for good performance for signal problems.



Result for closure problem I

Average results for the prediction of *q*:

pred-eps.pdf



Result for closure problem II

Examples of simulation:



- Paper: A neural network closure for the Euler-Poisson system based on kinetic simulations, L. Bois, E. Franck, L. Navoret, V. Vigon.
- ANR Milk (2022-2025) with Max-Planck institute of Plasma-Physics on reduced models with deep-learning.

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Two years of post-doc position on the closure for more complex problems.



Reduced problem for plasma physics







Vlasov and PIC code

We consider the 1Dx1D nonlinear Vlasov-Poisson equation for plasma:

$$\partial_t f(t, x, v) + v \partial_x f + (E_{ext}(x) + E(x)) \partial_v f = 0$$

with

$$-\Delta\phi(x) = \int_{v} f(t, x, v') dv' - 1, \quad E(x) = -\nabla\phi(x)$$

f(t, x, v) is a probability density of the particles.

Solver PIC (Particle In Cells). We approximate the distribution by macro-particles

$$f(t, x, v) \approx f_N(x(t), v(t)) = \sum_{i=1}^N w_i \delta(x - x_i(t)) \delta(v - v_i(t))$$

where

$$\begin{cases} \frac{dx_i}{dt} = v_i, \\ \frac{dv_i}{dt} = \frac{q}{m}(E + E_{ext})(x_i(t)), \end{cases}$$
(1)

To compute the electric field, we compute $\int_{v} f(t, x, v') dv'$ on the mesh, solve the Poisson equation on the mesh, interpolate E(x) at the position of macro-particles.



Reduced order modeling

- After PIC discretization, we have a large ODE (d^2N with d the dimension and N the number of particles) to solve.
- PIC method converges in $O(\frac{C(f)}{\sqrt{N}})$ so $d^2N >> 1$ (like MC methods).

ROM method

Design reduced models of size $K \ll N$ for a subset of initial data and parameters. Assumption:

$$\mathbf{Y}(t) \approx A\mathbf{Z}(t)$$

with $\mathbf{Y}(t) \in \mathbb{R}^{d^2N}$, $\mathbf{Z}(t) \in \mathbb{R}^{2K}$.

- Here we consider $f(t = 0, x, v) = f_{\gamma}(\alpha, \beta)\mathcal{M}(v)$ with (α, β) the parameters.
- Classical approach: POD (see J. Hestaveen papers)
 - □ We collect some snapshots: $S = [(x(t_1), v(t_1)), \dots, (x(t_n), v(t_n))].$
 - □ By the SVD method, we compute the K dominant mods (associated to the K largest eigenvalues) and construct: $A \in \mathcal{M}_{K,N}$ (encoder) et $A^+ \in \mathcal{M}_{N,K}$ (decoder).
 - Reduction:

$$\partial_t \mathbf{Y}(t) = \mathbf{F}(\mathbf{Y}(t)) \rightarrow \partial_t \mathbf{Z}(t) = A\mathbf{F}(A^+\mathbf{Z}(t)), \text{ with } \mathbf{Z}(t) = A\mathbf{Y}(t)$$

□ The term $AF(A^+Z(t))$ can be computed and stored in the linear case and approximated in the nonlinear case.



Nonlinear reduction and Auto-encoder

Phase-space: PIC code (left), Reduction of PIC (middle), Reduced model (right)



It doesn't work. Why ?

Nonlinear assumption

For nonlinear transport equation, we can assume that

$$\mathbf{Y}(t) pprox \mathcal{G}(\mathbf{Z}(t)), \quad \mathbf{Y}(t) \in \mathbb{R}^N, \mathbf{Z}(t) \in \mathbb{R}^K$$

Idea: replace SVD by Deep - Auto encoder.

In practice: Partial fully connected neural network.

$$\left\{ \begin{array}{c} E^{\times}_{\theta_{e_{x}}}(\mathbf{x}) = \bar{\mathbf{x}} \\ E^{\vee}_{\theta_{e_{y}}}(\mathbf{v}) = \bar{\mathbf{v}} \end{array} \right., \left\{ \begin{array}{c} D^{\times}_{\theta_{e_{x}}}(\bar{\mathbf{x}}) = \mathbf{x} \\ D^{\vee}_{\theta_{e_{y}}}(\bar{\mathbf{v}}) = \mathbf{v} \end{array} \right.$$



Results

Results for the reduced model for one trajectory:



Learning with different initial conditions (varying α):



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Current step: varying randomly β and α in the learning step.



Next: structure-preserving reduced model

Question: how do you learn time models ?

$$\frac{d\mathbf{x}(t)}{dt} = F_{\theta}(\mathbf{x}(t))$$

- We can learn the flow F_{θ} using data to approximate time derivatives.
- Physical model: In general the physic admits specific structure (conservative, dissipative ...)
- Example:

$$\frac{d\mathbf{x}}{dt} = J(\mathbf{x})\nabla H(\mathbf{x}) + G(\mathbf{x})\nabla S(\mathbf{x})$$

with J skew-symmetric, G symmetric and $J(\mathbf{x})\nabla S(\mathbf{x}) = G(\mathbf{x})\nabla H(\mathbf{x}) = 0$

- We call H(.) an Hamiltonian which is conserved by structure and S(.) an entropy which is dissipative by structure.
- The ODE's solved in the PIC code are generated by an Hamiltonian.

Next step

- Keep an Hamiltonian structure on the reduced model learning the Hamiltonian and not the ODE flow.
- Advantage: Hamiltonian structure + specific time integrator (symplectic scheme) allows to assure some stability for the reduced model.



Deep learning and geometry







Unstructured data and non-euclidian domain

- Many possible applications of deep-learning for PDE's:
 - □ Modeling some terms: closure, turbulence models, reduced models,
 - □ Solve PDE,
 - □ Compute coefficients of numerical schemes: stabilization viscosity, flux limiter, dynamic splitting coefficient
 - □ Adaptive solving: shocks/interface detection, error prediction, meshes refinement.
- For these applications we need neural networks on unstructured data (cloud point, meshes ...) and non euclidean geometry (surface of Torus or sphere)





Figure: Picture from google image.





Unstructured data and non-euclidian domain II

- We consider a Graph (Mesh are include inside)
 - \Box Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
 - \Box Vertices $\mathcal{V} = \{1, \dots, n\}$
 - $\Box \quad \mathsf{Edges} \quad \mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$
 - $\ \ \Box \ \ {\sf Edge weights} \quad w_{ij} \geq 0 \ {\sf for} \ (i,j) \in {\mathcal E}$
 - $\Box \text{ Vertex fields } L^2(\mathcal{V}) = \left\{ f: \mathcal{V} \to \mathbb{R}^h \right\}, \text{ represented as } \mathbf{f} = (f_1, \dots, f_n)$
- How to define/generalize the convolution on graph/mesh ?
- No natural answer.



Figure: Picture from google.





Convolution and Fourier transform

Spatial definition of convolution: Given two functions $f, g : [-\pi, \pi] \to \mathbb{R}$ their convolution is a function

$$(f \star g)(x) = \int_{-\pi}^{\pi} f(x') g(x - x') dx'$$

Spectral definition of convolution:

$$(f \star g)(x) = \mathcal{F}^{-1}(\mathcal{F}g \star \mathcal{F}f)$$

with ${\mathcal F}$ the Fourier transform.

Discrete case:

$$(f \star g)(x) = \Phi(\Phi^t \mathbf{g} \circ \Phi^t \mathbf{f})$$

with Φ the fourier matrix. Each column corresponds to one eigenvector of the Laplacian.

- To apply filter/define convolution we use a Fourier basis (basis function with increasing frequency).
- **Example**: how to apply this on a function/signal defined on the sphere ?



Differential geometry and Laplace Beltrami

Differential geometry

- Application of differential calculus tools to the geometry.
- allows to study differential function defined on curve/surface/manifold etc ...

Riemannian geometry

differential geometry with the notion of distance and angle.



Important tools: Laplace-Beltrami

$$\Delta f = rac{1}{\sqrt{|m{g}|}} \partial_i \left(\sqrt{|m{g}|} m{g}^{ij} \partial_j f
ight)$$

with g the Riemanian metric tensor (manifold-dependent).

• Key point: the eigenvectors of Δ give a basis of function defined on the manifold with increasing frequency. Fourier basis on each Riemannian manifold.

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Example: manifold harmonics



Figure: Google images



Figure: Issue to B. Vallet and B. Lévy. Spectral Geometry Processing with Manifold Harmonics



Graph Laplacian

Question

Can we construct the same theory for graph/mesh to design specific Fourier basis and filters ? yes

The derivative operator $d : \mathcal{H}(V) = (\mathbb{R}^{|V|}, <, >_V) \rightarrow (\mathbb{R}^{|E|}, <, >_E) = \mathcal{H}(E)$ can ben defined

$$\forall e_{ij} \in \mathcal{E}, \quad d(e_{ij}) = \gamma(w_{ij})(f(j) - f(i))$$

with f(i), f(j) the value of the function f at the vertex i and j and

$$< f, g >_{V} = \frac{1}{|V|} \sum_{i=1}^{|V|} f_{i}g_{i}\chi_{i}, \quad < f, g >_{E} = \frac{1}{2|V|} \sum_{i,j}^{|V|} f_{ij}g_{ij}w_{ij}$$

We can define the dual operator with the relation

$$\langle df, g \rangle_V = \langle f, d^*g \rangle_E, \quad \forall f \in \mathcal{H}(V), g \in \mathcal{H}(E)$$

As in the exterior calculuss theory (differential geometry), the graph Laplacian $\Delta : \mathcal{H}(V) \to \mathcal{H}(V)$ is given by

$$\Delta(i) = d^*d$$



Graph Laplacian II

Explicit formula.

$$\Delta(i) = \left[f(i) \frac{1}{n} \sum_{j=1}^{n} \frac{w_{ij}}{d_i} - \frac{1}{n} \sum_{j=1}^{n} f(j) \frac{w_{ij}}{d_i} \right]$$

for specific choice of $\gamma(.)$ and $\chi(.)$.

Question

Can we link this graph Laplacian to Laplace-Beltrami operator ? yes

Result

We take \mathcal{M} a Riemanian manifold of dimension m in \mathbb{R}^d . $X = (x_1, ...x_n)$ are points of the manifold distributed with a probability law p(x) on \mathcal{M} . We construct a graph of nearest neighbors (close to mesh). On some technical assumption we have:

$$\Delta \rightarrow_{n \rightarrow \infty} C \frac{1}{p^s} \nabla \cdot (p^s \nabla f)$$

If s = 0 and p(x) an uniform law, we obtain the Laplace-Beltrami operator.

So, if the graph is "a discrete version of a manifold", the graph Laplacian can be an approximation of the Laplace-Beltrami operator.



Spectral convolution and Graph-signal process

- We consider a Graph G and the Graph Laplacian matrix L.
- We call Φ the eigenvectors of L.
- We obtain a natural definition of convolution on graph:

$$\mathbf{f} \star \mathbf{g} = \Phi(\underbrace{\Phi^t \mathbf{g}}_{K \in D_{n,n}(\mathbf{R})} \circ \Phi^t \mathbf{f}))$$

with n signal size and K the filter



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Defaults for Convolution layer of neural-network:

- No guarantee of spatial localization of filters,
- O(n) parameters per layer,
- $\Box O(n^2)$ computation of forward and inverse Fourier transforms,
- □ Filters are basis-dependent do not generalize across graphs.



Spectral convolution and Graph-signal process II

- Key reference: Geometric deep learning: going beyond Euclidean data. M. Bronstein an al (2016).
- Example (picture come from to the reference):





First GCNN: Chebnet

First problem: O(n) parameters per layer. Solution:

$$\mathbf{f} \star \mathbf{g} \approx \Phi_k \big(\underbrace{\Phi_k^t \mathbf{g}}_{K \in D_{k,k}(\mathbf{R})} \circ \Phi_k^t \mathbf{f} \big) \big)$$

with k << n a cut-off frequency. So Φ_k is the k first eigenvectors. K contains the trainable parameters.

Second problem: the filter can be non-local in space. Remark: duality smoothness-locality in fourier/spatial domain. Solution:

$$\mathcal{K}_{ii} = \sum_{j=1}^{k} heta_j \mathcal{B}_s(\lambda_i)$$

with B_s a smooth B-Splines function and λ_i eigenvalues of graph Laplacian.

- Using this we obtain a localized spatial filter with r parameters.
- **Third problem**: Computation of ϕ with complexity O(n). Idea:

$$\mathcal{K}_{ii} = \sum_{j=1}^k heta_j \lambda^i = \mathcal{P}_ heta(\Lambda)$$

We remark

$$\Phi^t P_{\theta}(\Lambda) \Phi^t \mathbf{f} = P_{\theta}(L) \mathbf{f}$$

So a polynomial of graph Laplacian gives a good candidate for convolutional layer.

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Second GCNN: GCN

ChebNet (X. Bresson and al 2016)

We define the normalized graph laplacian $\tilde{L}=2\frac{L}{\lambda_{max}}-\textit{I}_{d}$ and propose

$$P_{\theta}(\tilde{L})\mathbf{f} = \sum_{j=1}^{k} \theta_j T_j(\tilde{L})\mathbf{f}$$

with T_j a recurrent Tchebychev polynomial. So

$$T_j(\tilde{L})\mathbf{f} = 2\tilde{L}T_{j-1}(\tilde{L}) - T_{j-2}(\tilde{L})$$
, with $T_0 = \mathbf{f}$ and $T_1 = \tilde{L}\mathbf{f}$

Simple convolution layer:

□ Using another definition of graph laplacian and choosing k = 2:

$$P_{\theta} = \theta_0 + \theta_1 (L - I_d) = \theta_0 - \theta_1 D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$$

with D degree matrix and a W weight matrix. We choose $\theta = \theta_0 = -\theta_1$.

Eigenvalues are in [0, 2]. Lot of composition can generate instabilities. To finish we apply a transformation to have a spectrum in [-1, 1].

Vanilla GCN (Kipf, Welling 2016)

$$G = \theta (I_d + \tilde{D}^{-\frac{1}{2}} \tilde{W} \tilde{D}^{-\frac{1}{2}})$$

avec
$$ilde{W} = W + I_d$$
 et $ilde{D} = diag(\sum_{i
eq j} ilde{w}_{ij}).$



E. Franck

Recents GCNN

- Lot of difference convolutional layers based on spectral approach.
- Some spatial approachs have also been designed:
 - □ Geodesic CNN (G. Maskic and al 2015): based on local coordinate on tangent space. Mainly for mesh of manifold.
 - Monet (F. Monti and al 2017): generalization of GCNN based on local coordinate. Mainly for mesh of manifold.
 - □ GRAND (M. Bronstein and al 2022): the convolution layer is a spatial and time discretization of:

$$\partial_t \rho = \nabla \cdot (A(x, t) \nabla \rho)$$

with A a matrix. Use the theory which link ANN and ODE discretization (Neural ODE R. T. Cheng 2018).

Beltrami-flow(M. Bronstein and al 2021): the convolution layer is a spatial and time discretization of:

$$\partial_t \rho = \frac{1}{\sqrt{\text{Det}G(x,t)}} \nabla \cdot \left(\frac{\nabla \rho}{\text{Det}G(x,t)} \nabla \rho\right)$$

with the Riemannaian metric $G = I_d + \alpha (\nabla_x \rho)^t (\nabla_x \rho)$. Low diffusion in direction of high gradient.



Application to mesh and PDE I

- Train a neural network to make some task on varying meshes. Difficulty: Chebnet/GCN valid when we change the mesh. Not possible for general graph.
- Refinement/moving mesh cannot change the topology of the mesh and the manifold associated.
- We can hope that networks based on a spectral approach of convolution will continue to work.
- Examples: number detected on meshes.



Figure: accuracy results compare to the mesh deformation or mesh refinement



Application to mesh and PDE II

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Figure 12: The 20 random meshes.



Application to mesh and PDE III

A first application: discontinuity/shock detection and mesh refinement.

Case 1: constant by part function. Localization of discontinuity by GCN and iterative refinement.





Application to mesh and PDE IV

- Case 2: Detection of discontinuity for non piecewise constant function. Unet architecture with Chebnet and geometric pooling layers.
- Training on a single mesh (for informatic reason)





Application to mesh and PDE V

Case 3: Detection of discontinuity in Burgers simulation using previous training



A first refinement approach



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After refinement the discontinuity is always detected. Less after four refinements but training on a single mesh.



Theory of geometric deep learning







Neural Network architecture and symmetry I

Curse of dimensionality

The space generated by the neural-network function with RELU activation is dense in the $C_0(\Omega)$ functional space for the $L^{\infty}(\Omega)$ norm with $\Omega \subset \mathbb{R}^d$. If $f \in H^s(\Omega)$ then

$$\sup_{x\in\Omega} |f(x) - ANN(x)| \approx O(n^{-\frac{s}{d}})$$

with n the number of neurals.

How to explain the good performance of neural networks for some problems in high dimension (vision, translation problem).

Possible answer

- □ For some problems on structure data the neural network "encodes" some priors on the problems which allows it to break the curse of dimensionality.
- Mallat 2016, Bronstein and al, 2020
- Which structured data ? which prior. **Theory of Geometric Deep Learning** (Bronstein and al, 2020).



Neural Network architecture and symmetry II

Which data

- Grids and sequence (time series and vision problem)
- Homogeneous non-euclidean space (vision problem on sphere etc)
- General manifold and meshes (vision problem, form analysis, ...)
- Graphs and set/point cloud (many applications)

Which prior I

 $g \in G$ wth G a group of symetry, $x \in X(\Omega)$ a signal on Ω . f is the target function on Ω .

G-Invariance: $f(g.x) = f(x), \quad \forall g \in G, \forall x \in X(\Omega)$

G-Equivariance:

$$f(g.x) = \rho(g)f(x), \quad \forall g \in G, \forall x \in X(\Omega)$$

with ρ the representation of g (group representation theory).





Neural Network architecture and symmetry III

Which priors II

Stability compared to signal local deformation. We consider f(x) the target function with x the signal. It is equivalent to say that f is locally invariant compared to the group of diffeomorphism G:

$$\parallel f(g.x) - f(x) \parallel \leq c(g) \parallel x \parallel$$

with g.x an action group.

Stability compared to domain local deformation. We consider $f(x, \Omega)$ the target function with x signal and Ω the domain. It is equivalent to say that f is locally invariant compared to the group of isomorphism G:

$$\parallel f(x, \Omega) - f(x_2, \Omega_2) \parallel \leq d_D(\Omega, \Omega_2) \parallel x \parallel$$

with $x_2 = \eta^{-1} \circ x$ and η invertible mapping between the domains.

Which priors III

Scale separation. We define a coarsering operator: $P : x \in X(\Omega) \rightarrow x_2 \in X(\Omega_2)$ with x_2 the signal on the coarse domain (less degrees of freedom). We assume that

$$f \approx f_2 \circ P$$

with f the target function, and f_2 the target function on the coarse domain.

Neural Network architecture and symmetry IV

Geometric prior II

- Grids/sequence: translation invariance/equivariance,
- Homogeneous non-euclidean space: associated symmetry group. Rotation for sphere,
- Graph and set: permutation invariance/equivariance,
- Manifold and mesh: isometry or local gauge invariance/equivariance.

Geometric Deep Learning blueprint

- A "good" neural network chain:
- Convolutional layers which encode G-equivariance and stability to local deformation,
- Iocal Pooling/un-pooling layers which encode scale separation,
- global pooling layer for classification which encodes *G*-invariance.



