DNN based topology optimization: spatial invariance and neural tangent kernel

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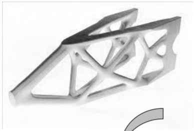
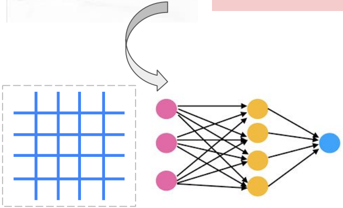
Chair of Statistical Field Theory - EPFL

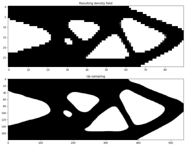
October 17, 2021

Overview



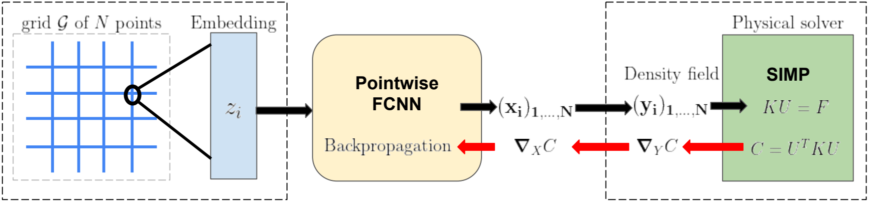
Topology optimization aims to find optimal shapes with respect to some forces and boundary conditions





- **Our goal is to use DNNs as an implicit representation of the shape**
- **We analyse it through NTK theory**
- **We suggest tools to improve coordinates-based generative models**
- **We analize an analogy between the NTK and a filter**

Algorithm



Loss function C is called the compliance.

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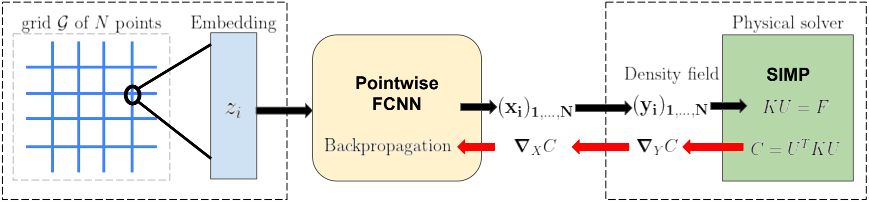

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- Embedding $z_i = \varphi(p_i)$, $\varphi : \mathbb{R}^2 \longrightarrow \mathbb{R}^{n_0}$
- Fully-connected DNN: $x_i = f_\theta(z_i)$, $f_\theta : \mathbb{R}^{n_0} \longrightarrow \mathbb{R}$

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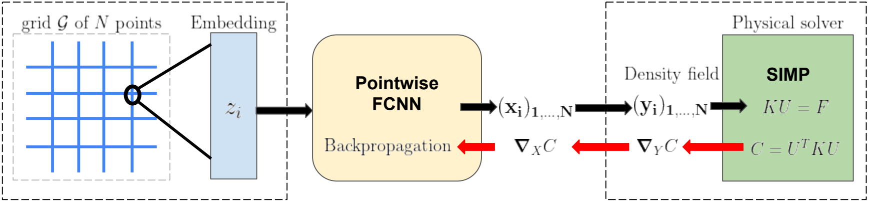

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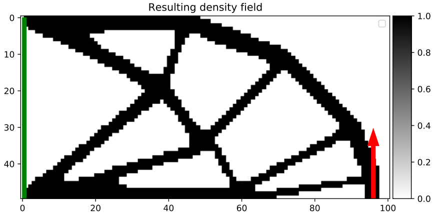
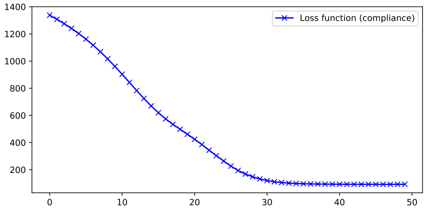
- Mass control: we find $\bar{b}$ such that $\sum_i \sigma(x_i + \bar{b}) = V_0$
- Implicit differenciation: $\nabla_X C = D_X \nabla_Y C$

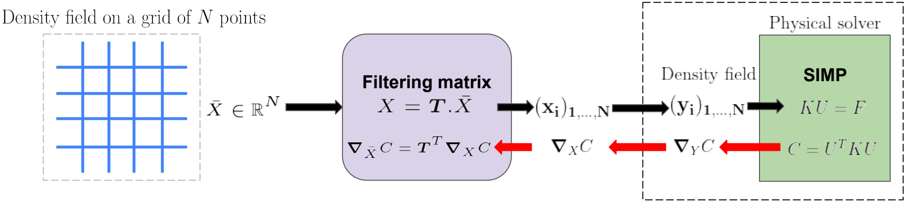
Example





- Our method achieves excellent numerical results in a small number of iterations

Comparison with traditional filtering in SIMP



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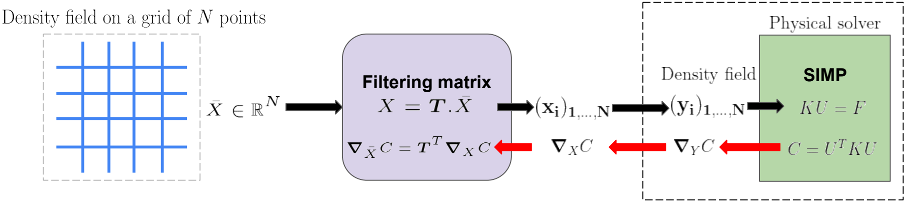
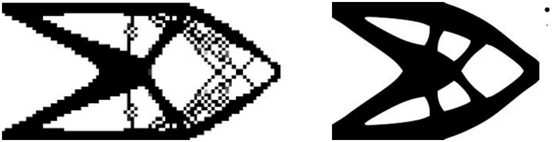


- Filtering aims to remove checkerboards but it has drawbacks



Neural Networks

- NTK parametrization of FCNNs:
  $a^0(x) = x, \quad \tilde{a}^{l+1}(x) = \frac{\alpha}{\sqrt{n_l}} W^l a^l(x) + \beta b^l, \quad a^{l+1}(x) = \mu\big(\tilde{a}^{l+1}(x)\big),$
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Gradient flow without neural network

$$\partial_t Y^{\mathrm{MF}}(t) = -D_X(t) T T^T D_X(t) \nabla_Y C(Y^{\mathrm{MF}}(t))$$

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Proposition

Let $\varphi : \mathbb{R}^d \to \mathbb{R}^{n_0}$ for $d > 2$ and any finite n_0. If φ satisfies $\varphi(x)^T\varphi(x') = K(\|x - x'\|)$ for some continuous function K then both φ and K are constant.

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- We propose embeddings ensuring spatial invariance of the NTK

Torus embedding

- The NTK is invariant under rotation (function of $z^T z'$, $\|z\|$, $\|z'\|$)
- We transfer this property to translation invariance
- $\mathbb{R}^2 \ni p = (p_1, p_2) \longmapsto \varphi(p) = r(\cos(\delta p_1), \sin(\delta p_1), \cos(\delta p_2), \sin(\delta p_2))$

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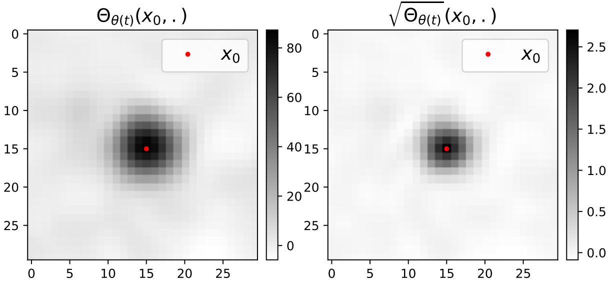

proposition

The square root of the Gram Matrix $\sqrt{\tilde{\Theta}_\infty}$ is a discrete convolution matrix

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$$\varphi(p)_i = \sqrt{2k(0)}\sin(w_i^T p + \frac{\pi}{4} + b_i)$$

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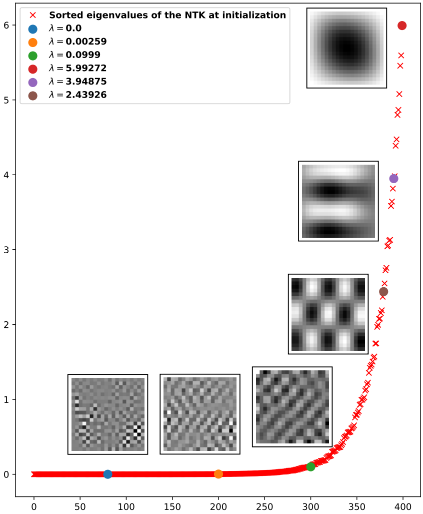
Proposition

Let φ be an embedding as described above for a positive radial kernel $k \in L^1(\mathbb{R}^d)$ with $k(0) = 1$, $k \geq 0$. There is a filter function $g : \mathbb{R} \to \mathbb{R}$ and a constant C such that for all p, p', in probability:

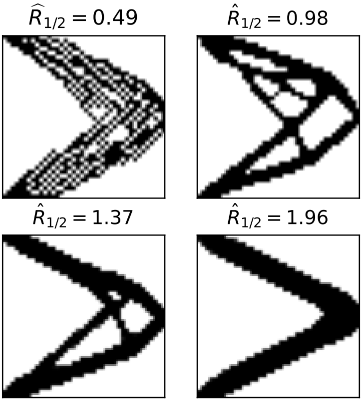
$$\lim_{n_0\to\infty} \Theta_\infty(\varphi(p), \varphi(p')) = C + (g \star g)(p - p'),$$

Experimental results - spectral decomposition of the NTK



Experimental results - Filter radius control

- We are able to define and control a "filtering radius"



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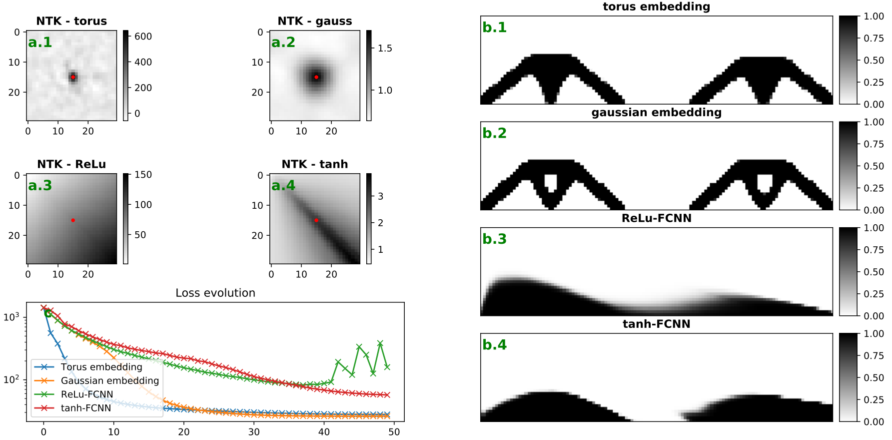
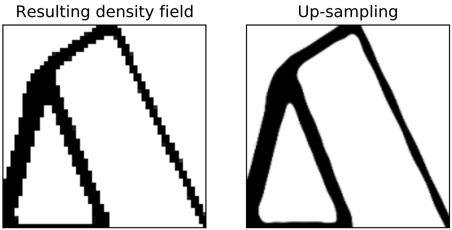


up sampling



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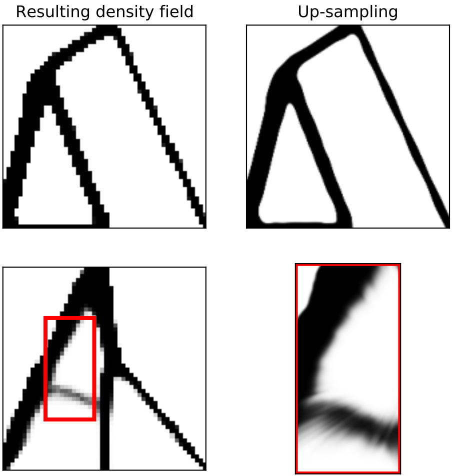

Thank you