Spline Theory of Deep Network

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Tremendous results of “AI” or Deep Learning in many fields

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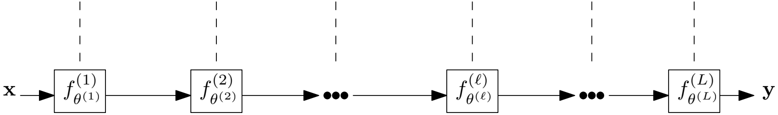
$\Rightarrow$ need of a mathematical theory of deep learning

Spline Theory of Deep Network

Work from Richard Baraniuk (ECE Dept - Rice University)
and his collaborators

Deep Learning - Notations (1/2)



Architecture:
$\mathbb{R}^C \ni \mathbf{y} = f_\Theta(\mathbf{x}) = \left(f^{(L)}_{\theta_{(L)}} \circ f^{(L-1)}_{\theta_{(L-1)}} \circ \ldots \circ f^{(\ell)}_{\theta_{(\ell)}} \circ \ldots \circ f^{(1)}_{\theta_{(1)}}\right)(\mathbf{x})\ ,\ \mathbf{x} \in \mathbb{R}^D$
where $\Theta = \{\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(L)}\}$ are the parameters (must be learned), and $f^{(l)}_{\theta^{(l)}}$ represent layer ℓ ($\in \{1, \ldots, L\}$).

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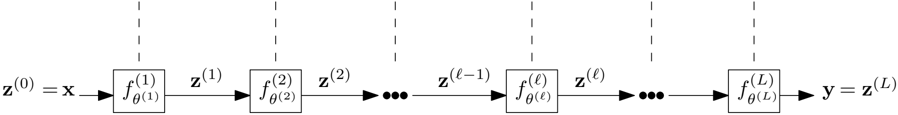

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Intermediate variables:

$\mathbf{z}^{(\ell)}(\mathbf{x})$ is the output of layer ℓ

$= \left(f^{(\ell)}_{\theta_{(\ell)}} \circ \ldots \circ f^{(1)}_{\theta_{(1)}}\right)(\mathbf{x})\ ,\ \mathbf{z}^{(0)}(\mathbf{x}) = \mathbf{x}\ ,\ \mathbf{z}^{(L)}(\mathbf{x}) = \mathbf{y}$

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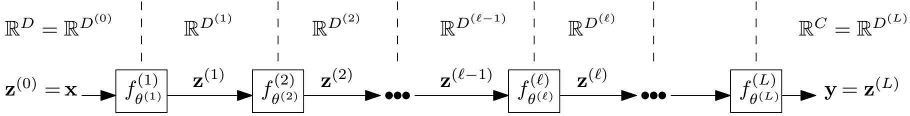

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Assume that $\mathbf{z}^{(\ell)} \in \mathbb{R}^{D^{(\ell)}}$
(take the convention that $D^{(0)} = D$ and $D^{(L)} = C$)

Deep Learning - Notations (2/2)

x can be any type of signal (audio, image,...).
Consider multichannel images: $z^{(\ell)}$ of size $C^{(\ell)} \times I^{(\ell)} \times J^{(\ell)} = D^{(\ell)}$

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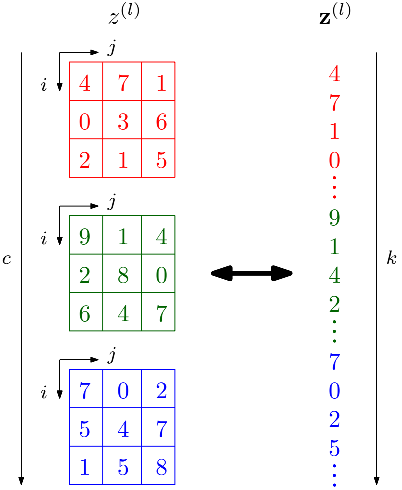
Samples can be indexed either in the tensor or flattened vector notation: $[z^{(\ell)}(x)]_{c,i,j} = [\mathbf{z}^{(\ell)}(\mathbf{x})]_k$



Deep Network (DN) basic operators (1/2)

- **fully connected operator**: $f_W^{(\ell)}(\mathbf{z}^{(\ell-1)}(\mathbf{x})) = W^{(\ell)}\mathbf{z}^{(\ell-1)}(\mathbf{x}) + b_W^{(\ell)}$ where $W^{(\ell)} \in \mathbb{R}^{D^{(\ell)} \times D^{(\ell-1)}}$ is a dense matrix and $b_W^{(\ell)} \in \mathbb{R}^{D^{(\ell)}}$ is a bias vector.

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- **activation operator**: pointwise nonlinearity σ, $\left[f_\sigma^{(\ell)}(\mathbf{z}^{(\ell-1)}(\mathbf{x}))\right]_k = \sigma([\mathbf{z}^{(\ell-1)}(\mathbf{x})]_k)$ where
  - $\sigma_{ReLU}(u) = \max(0, u)$,
  - $\sigma_{LReLU}(u) = \max(\eta u, u)\ ,\ \eta > 0$,
  - $\sigma_{abs}(u) = |u|$,
  - $\sigma_{sig}(u) = \frac{1}{1+e^{-u}}$,
  - $\sigma_{\tanh}(u) = 2\sigma_{sig}(2u) - 1$.

Deep Network (DN) basic operators (2/2)

- **pooling operator**: policy ρ to reduce dimension. Collection of indices $\left\{\mathcal{R}_k^{(\ell)}\right\}_{k=1}^{D^{(\ell)}}$.
  Example: *max pooling*: $\left[f_\rho^{(\ell)}\left(\mathbf{z}^{(\ell-1)}(\mathbf{x})\right)\right]_k = \max_{d\in\mathcal{R}_k^{(\ell)}}\left[\mathbf{z}^{(\ell-1)}(\mathbf{x})\right]_d$.

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Definition

A DN layer $f^{(\ell)}$ comprises a single nonlinear DN operator composed with any preceeding affine operator lying between it and the preceding nonlinear operator.

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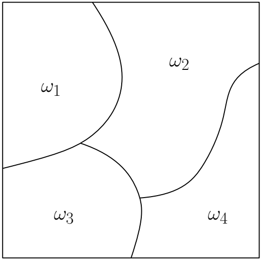
Output operator: $\mathbf{y} = g(f_\Theta(\mathbf{x}))$ where $g : \mathbb{R}^C \to \mathbb{R}^C$.
Example: *softmax* for classification problems, nothing for regression problems.

Multivariate Spline Operators

Partition $\mathbb{R}^D$ into R regions: $\Omega = \{\omega_1, \ldots, \omega_R\}$,



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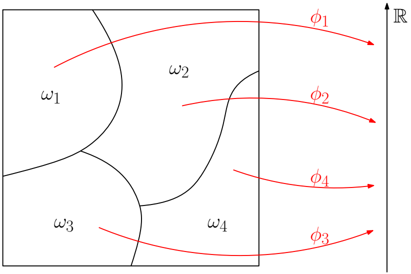
Local mappings: $\Phi = \{\phi_1, \dots, \phi_R\}, \phi_r : \omega_r \to \mathbb{R}$ s.t $\phi_r(\mathbf{x}) := \langle [\alpha]_{r,.}, \mathbf{x} \rangle + [\beta]_r$
where $\alpha \in \mathbb{R}^{R \times D}$ and $\beta \in \mathbb{R}^R$ define hyperplanes in $\mathbb{R}^D$



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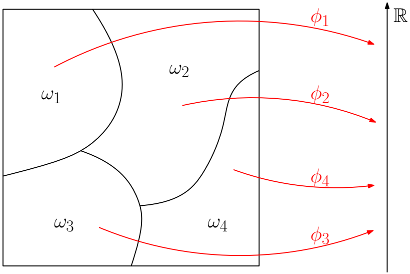

Definition (Multivariate Spline Operator)

$$s[\alpha, \beta, \Omega](\mathbf{x}) = \sum_{r=1}^{R} \left(\langle [\alpha]_{r,.}, \mathbf{x} \rangle + [\beta]_r \right) \mathbf{1}(\mathbf{x} \in \omega_r) =: \langle \alpha[\mathbf{x}], \mathbf{x} \rangle + \beta[\mathbf{x}]$$

Note: piecewise but not globally affine and convex (except for $R = 1$, degenerate spline)

Max-Affine Spline Operators (1/2)

Issue with general splines: to find the best spline approximation, we need to optimize wrt α, β and $\Omega \rightarrow$ minimizing wrt Ω is cumbersome to perform.

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Properties:

- α and β define Ω (adaptive partitioning splines) thus we simply denote them $s[\alpha, \beta](\mathbf{x})$,
- always piecewise affine and globally convex (hence continuous),
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Theorem

Any $h \in \mathcal{C}^0(\mathbb{R}^D)$ that is piecewise affine and globally convex, $\exists \alpha, \beta$ s.t $h(\mathbf{x}) = s[\alpha, \beta](\mathbf{x})$.

Max-Affine Spline Operators (2/2)

Generalization to operators: max-affine spline operators (MASO) $S[A, B] : \mathbb{R}^D \to \mathbb{R}^K$:

$$S[A, B](\mathbf{x}) = \begin{bmatrix} \max_{r=1,\dots,R} & \langle [A]_{1,r,.}, \mathbf{x} \rangle + [B]_{1,r} \\ & \vdots \\ \max_{r=1,\dots,R} & \langle [A]_{K,r,.}, \mathbf{x} \rangle + [B]_{K,r} \end{bmatrix} =: A[\mathbf{x}]\mathbf{x} + B[\mathbf{x}]$$

where $A \in \mathbb{R}^{K \times R \times D}$ and $B \in \mathbb{R}^K \times \mathbb{R}^R$.

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where $A \in \mathbb{R}^{K \times R \times D}$ and $B \in \mathbb{R}^K \times \mathbb{R}^R$.

Theorem

Any operator $H(\mathbf{x}) = [h_1(\mathbf{x}), \dots, h_K(\mathbf{x})]^T$ with $\forall k, h_k \in \mathcal{C}^0(\mathbb{R}^D)$ piecewise affine and globally convex, $\exists A, B$ s.t $H(\mathbf{x}) = S[A,B](\mathbf{x})$.

Extension: a MASO can approximate arbitrarily closely any (nonlinear) operator that is convex in each output dimension.

Simplified Max-Affine Spline Operators

Use the same bias β' for all dimension:

$$S'[A,\beta'](\mathbf{x}) = \begin{bmatrix} \max_{r=1,\dots,R} & \langle [A]_{1,r,.}, (\mathbf{x}+\beta') \rangle \\ & \vdots \\ \max_{r=1,\dots,R} & \langle [A]_{K,r,.}, (\mathbf{x}+\beta') \rangle \end{bmatrix}$$

This simplified MASO is still sufficient to model most activation functions like ReLU, leaky-ReLU, absolute value; and linearly independent filters.

Deep networks and MASOs

Basic DN operators are MASOs!

- **fully connected** $f_W^{(\ell)}$: $S[A_W^{(\ell)}, B_W^{(\ell)}]$ where $R = 1, [A_W^{(\ell)}]_{k.1,.} = [W^{(\ell)}]_{k,.}$ and $[B_W^{(\ell)}]_{k,1} = [b_W^{(\ell)}]_k$,
- **convolutional** $f_C^{(\ell)}$: $S[A_C^{(\ell)}, B_C^{(\ell)}]$ where $R = 1, [A_C^{(\ell)}]_{k.1,.} = [C^{(\ell)}]_{k,.}$ and $[B_C^{(\ell)}]_{k,1} = [b_C^{(\ell)}]_k$,
- **activation** $f_\sigma^{(\ell)}$: $S[A_\sigma^{(\ell)}, B_\sigma^{(\ell)}]$ where $R = 2, [B_\sigma^{(\ell)}]_{k,1} = [B_\sigma^{(\ell)}]_{k,2} = 0 \quad \forall k$, and
  - ReLU: $[A_\sigma^{(\ell)}]_{k,1,.} = 0 \quad ; \quad [A_\sigma^{\ell}]_{k,2,.} = \mathbf{e}_k \ \forall k$,
  - leaky-ReLU: $[A_\sigma^{(\ell)}]_{k,1,.} = \nu \mathbf{e}_k \quad ; \quad [A_\sigma^{(\ell)}]_{k,2,.} = \mathbf{e}_k \ \forall k, \nu > 0$
  - absolute value: $[A_\sigma^{(\ell)}]_{k,1,.} = -\mathbf{e}_k \quad ; \quad [A_\sigma^{(\ell)}]_{k,2,.} = \mathbf{e}_k \ \forall k$

  ($\mathbf{e}_k$ is the $k-$th canonical basis element of $\mathbb{R}^{D^\ell}$)
- **pooling** $f_\rho^{(\ell)}$: $[A_\rho^{(\ell)}, B_\rho^{(\ell)}]$
  - max-pooling: $R = \#\mathcal{R}_k, [A_\rho^{(\ell)}]_{k,.,.} = \{\mathbf{e}_i, i \in \mathcal{R}_k\}$ and $[B_\rho^{(\ell)}]_{k,r} = 0, \forall k, r$
  - average-pooling: $R = 1, [A_\rho^{(\ell)}]_{k,1,.} = \frac{1}{\#\mathcal{R}_k} \sum_{i \in \mathcal{R}_k} \mathbf{e}_i$ and $[B_\rho^{(\ell)}]_{k,1} = 0, \forall k$

Composition of MASOs

Proposition

A DN layer constructed from an arbitrary composition of fully connected/convolution operators followed by one activation or pooling operator is a MASO $S[A^{(\ell)}, B^{(\ell)}]$ such that

$$f^{(\ell)}(\mathbf{z}^{(\ell-1)}) = A^{(\ell)}[\mathbf{x}]\mathbf{z}^{(\ell-1)}(\mathbf{x}) + B^{(\ell)}[\mathbf{x}].$$

Example: fully connected operator $S[A_W^{(\ell)}, B_W^{(\ell)}]$ followed by an activation operator $S[A_\sigma^{(\ell)}, B_\sigma^{(\ell)}]$ is a MASO $S[A^{(\ell)}, B^{(\ell)}]$ where $[A^{(\ell)}]_{k,r,.} = W^{(\ell)T}[A_\sigma^{(\ell)}]_{k,r,.}$ and $[B^{(\ell)}]_{k,r} = [B_\sigma^{(\ell)}]_{k,r} + b_W^{(\ell)T}[A_\sigma^{(\ell)}]_{k,r,.}$.

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Theorem

A DN constructed from an arbitrary composition of fully connected/convolution, activation, and pooling operators of the previous types is a composition of MASOs. Moreover, the overall composition itself an ASO.

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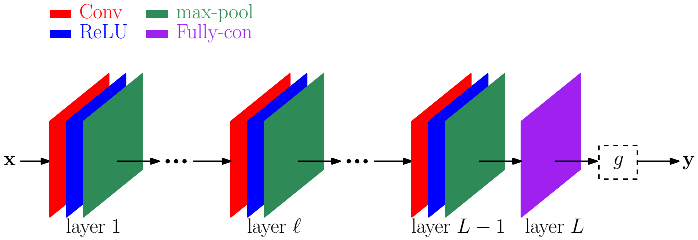
(Note that in the case we use operators which are convex but not piecewise affine, we can show that such mapping can be approximated arbitrarily closely by a MASOs. In the case, the operators are not convex then the same result hold with the use of ASOs.)

Explicit input/ouput formula (1/2)

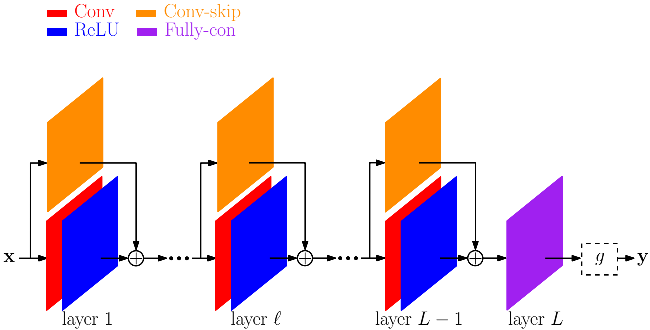
CNN affine mapping formula:



$$\mathbf{z}_{CNN}^{(L)}(\mathbf{x}) = W^{(L)} \left(\prod_{\ell=L-1}^{1} A_{\rho}^{(\ell)}[\mathbf{x}] A_{\sigma}^{(\ell)}[\mathbf{x}] C^{(\ell)} \right) \mathbf{x}$$
$$+ W^{(L)} \sum_{\ell=1}^{L-1} \left(\prod_{j=L-1}^{\ell+1} A_{\rho}^{(j)}[\mathbf{x}] A_{\sigma}^{(j)}[\mathbf{x}] C^{(j)} \right) \left(A_{\rho}^{(\ell)}[\mathbf{x}] A_{\sigma}^{(\ell)}[\mathbf{x}] b_{C}^{(\ell)} \right) + b_{W}^{(L)}$$

Explicit input/ouput formula (2/2)

ResNet affine mapping formula:



$$\mathbf{z}^{(L)}_{RES}(\mathbf{x}) = W^{(L)} \left(\prod_{\ell=L-1}^{1} \left(A_{\sigma}^{(\ell)}[\mathbf{x}] C^{(\ell)} + C_{skip}^{(\ell)} \right) \right) \mathbf{x}$$

$$+ W^{(L)} \sum_{\ell=1}^{L-1} \left(\prod_{j=L-1}^{\ell+1} \left(A_{\sigma}^{(j)}[\mathbf{x}] C^{(j)} + C_{skip}^{(\ell)} \right) \right) \left(A_{\sigma}^{(\ell)}[\mathbf{x}] b_{C}^{(\ell)} + b_{skip}^{(\ell)} \right) + b_{W}^{(L)}$$

Template Matching Machines (1/3)

The explicit formula can be rewritten in a general form:

$$\mathbf{z}^{(L)}(\mathbf{x}) = \left(W^{(L)}A[\mathbf{x}]\right)\mathbf{x} + \left(W^{(L)}B[\mathbf{x}] + b_W^{(L)}\right)$$

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- interpretation 2: hierarchical matched filters:

$$\mathbf{z}^{(L)} = W^{(L)} \max_{r^{(L-1)}} \left(A^{(L-1)}_{r^{(L-1)}} \dots \max_{r^{(2)}} \left(A^{(2)}_{r^{(2)}} \max_{r^{(1)}} \left(A^{(1)}_{r^{(1)}}\mathbf{x} + B^{(1)}_{r^{(1)}}\right) + B^{(2)}_{r^{(2)}}\right) \dots + B^{(L-1)}_{r^{(L-1)}}\right) + b_W^{(L)}$$

Template Matching Machines (1/3)

The explicit formula can be rewritten in a general form:

$$\mathbf{z}^{(L)}(\mathbf{x}) = \left(W^{(L)}A[\mathbf{x}]\right)\mathbf{x} + \left(W^{(L)}B[\mathbf{x}] + b_W^{(L)}\right)$$

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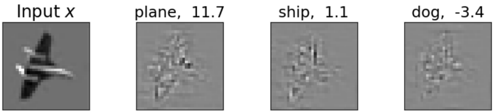
Visualization: extract (via the backpropagation algorithm) the templates

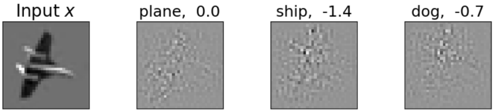
$$A[\mathbf{x}]_c = \frac{d[\mathbf{z}^{(L)}(\mathbf{x})]_c}{\mathbf{x}}$$

Template Matching Machines (2/3)

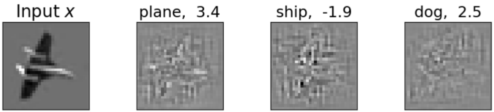


(a) *largeCNN*, ReLU activation, no BN

(b) *largeCNN*, absolute value activation, no BN

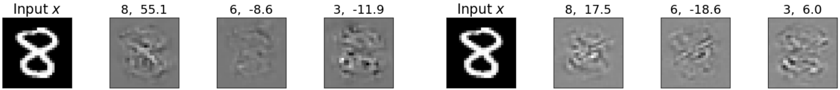


(c) *largeCNN*, ReLU activation, BN

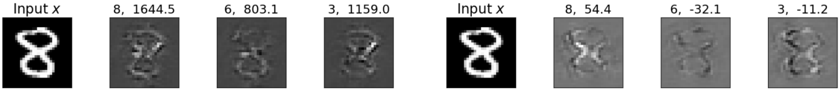


(d) *largeCNN*, absolute value activation, BN

Template Matching Machines (3/3)



(a) *smallResNet*, ReLU activation, no BN (b) *smallResNet*, ReLU activation, BN



(c) *smallResNet*, absolute value activation, no BN (d) *smallResNet*, absolute value activation, BN

See Balestriero and Baraniuk, “Mad Max: Affine Spline Insights into Deep Learning”

A simple way of boosting DN performances

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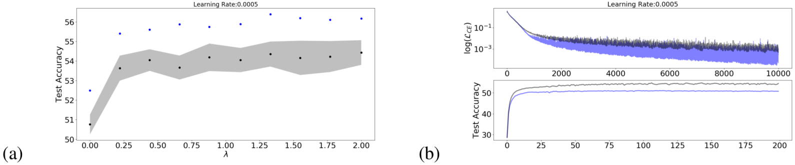
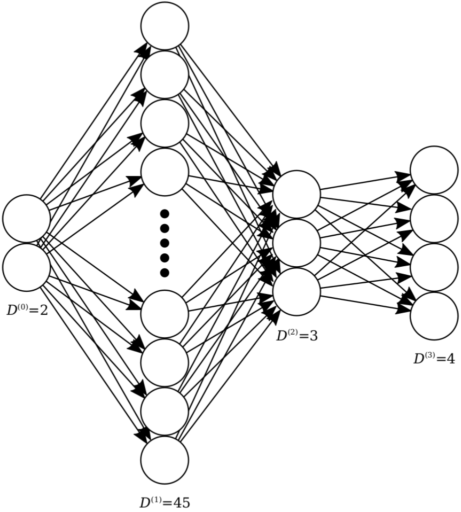
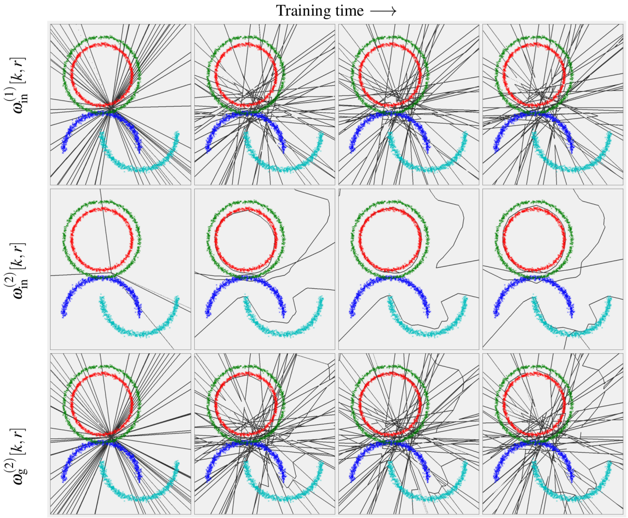


FIG. 5. Orthogonal templates significantly boost DN performance with *no change to the architecture*. (a) Classification performance of the *largeCNN* trained on CIFAR100 for different values of the orthogonality penalty λ in (5.11). We plot the average (back dots), standard deviation (gray shade), and maximum (blue dots) of the test set accuracy over 15 runs. (b, top) Training set error. The blue/black curves corresponds to $\lambda = 0/1$. (b, bottom) Test set accuracy over the course of the learning.

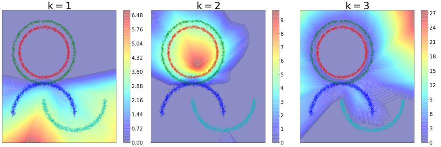
On the geometry of the partitioning



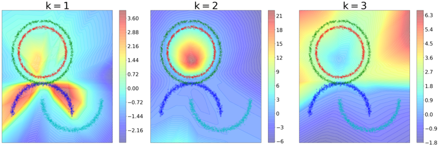
On the geometry of the partitioning



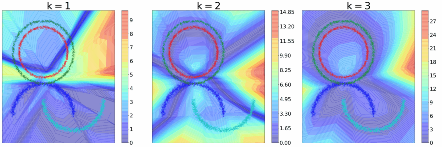
On the geometry of the partitioning



(a) ReLU



(b) Leaky ReLU



(c) Absolute value

Conclusion - Perspectives

- MASO appear to be a well-adapted tool to study DN
- Different point of views (operator, template matched filters,. . .)
- Universality of MASO DNs (i.e approximation theory)
- Stability and Lipschitz constant
- Colinear template and Data set memorization
- Multiscale partitions
- Connections with Vector Quantization (information theory), K-means (statistics) and Voronoi tiling (geometry)

- new constraints on the templates
- further study of the case of non-convex activation functions
- link with wavelet theory
- approximation theory (smoothness spaces of decision boundaries, optimal approximation)

Randall Balestriero, Richard Baraniuk, “Mad Max: Affine Spline Insights into Deep Learning,”

arxiv.org/abs/1805.06576, 2018