DEEP NETWORKS WITH ADAPTIVE NYSTRÖM APPROXIMATION (IJCNN 2019)

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INTRODUCTION

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Take Home Message

We use an adaptive variant of the Nyström method for kernel approximation as a drop-in replacement for dense layers in Convolutional Neural Networks (CNN)

Usual CNN architecture with dense layer(s) :

Our proposed architecture with Nyström layer(s) :

Outline

- **Non-linear mappings :**
  - *Dense (Fully-connected) neural network layers*
  - *Kernel methods*

- **Adaptive Nyström Layer**
  - *Standard formulation*
  - *Multiple Kernel Learning (MKL) formulation*

- ***Experiments***
  - *Standard setting*
  - *Small sample set*
  - *Multiple Kernel Learning*

NON-LINEAR MAPPINGS

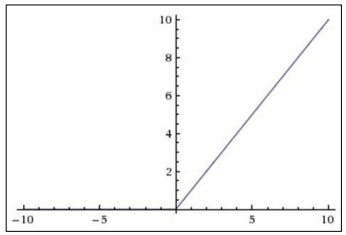
Dense (Fully-connected) layers

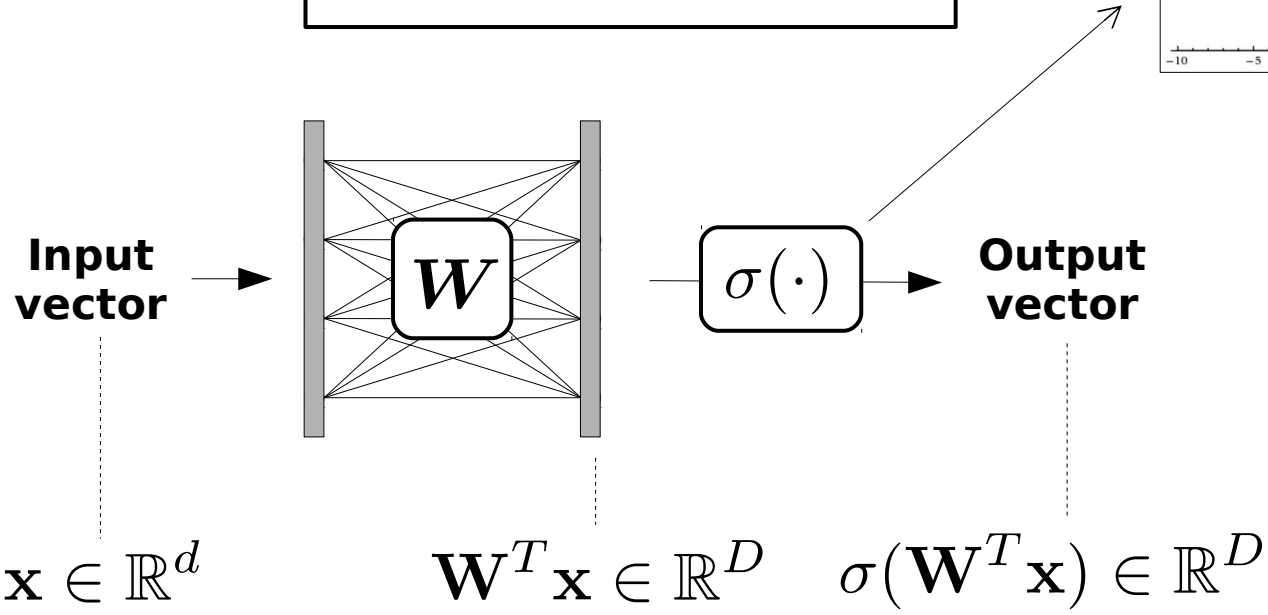
Each dense layer of a neural network learns a non-linear mapping of its input

Dense layer:

$$\phi_{dense}(\mathbf{x}) = \sigma(\mathbf{W}^T\mathbf{x})$$

Example : ReLU





Kernel methods

$$\forall i \ \mathbf{x}_i \in \mathbf{X} \qquad k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$$

$$\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j) \rangle$$

Some kernel methods can give the feature map approximation $\tilde{\phi}$ for a kernel.

$$k(\mathbf{x}, \mathbf{z}) \approx \langle \tilde{\phi}(\mathbf{x}) \cdot \tilde{\phi}(\mathbf{z}) \rangle$$

(to keep the notations light, we drop the ~ on $\tilde{\phi}$ in the rest of the presentation)

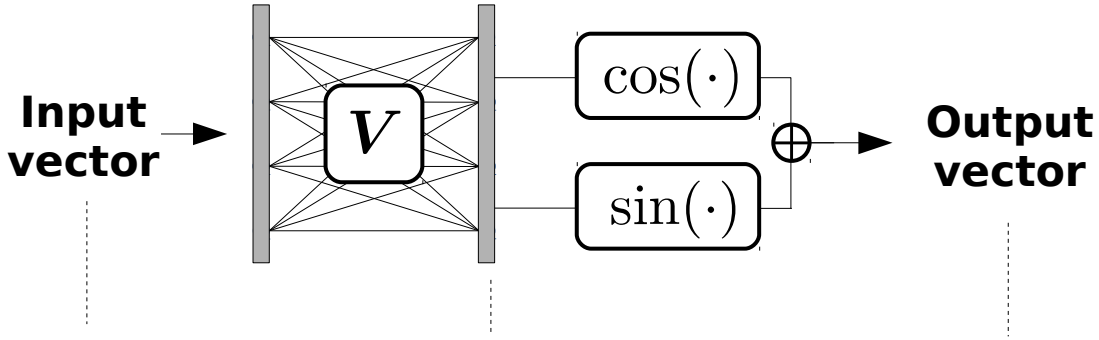
Kernel methods : Random features

Fast-Food (FF) :

FF is a fast approximation of the Gaussian kernel. It is a variant of the RKS method, a general approximation method for RBF kernels.

$$\phi_{FF}(\mathbf{x}) = [\cos(\mathbf{Vx}), \sin(\mathbf{Vx})] \qquad \mathbf{V} = \frac{1}{\sigma\sqrt{d}}\mathbf{SHG\Pi HB}$$

- **S**, **G** and **B** diagonal random
- $\mathbf{\Pi}$ random permutation
- **H** Hadamard matrix



(This mapping can be done multiple times In parallel then concatenated)

Kernel methods : Nyström method

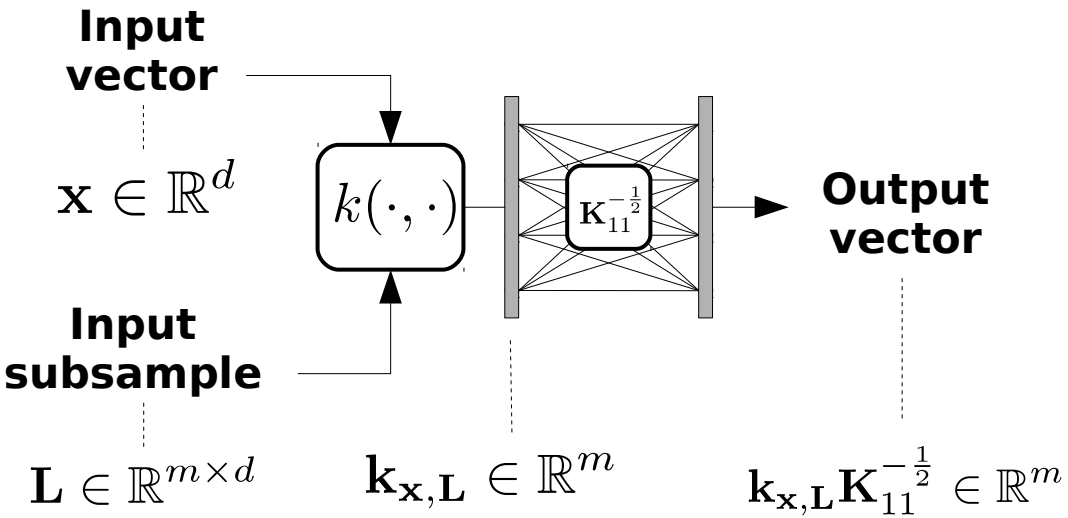
Nyström method for kernel approximation :

The Nyström method gives a low rank approximation of a Kernel matrix. For this approximation, we can extract the feature map approximation of the kernel.

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{21}^T \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \qquad \forall i,j \in 1...m \; \mathbf{K}_{11\,i,j} = k(\mathbf{L}_i, \mathbf{L}_j);\; \mathbf{L} \subset \mathbf{X};$$

$$\boxed{\phi_{nys}(\mathbf{x}) = \mathbf{k}_{\mathbf{x},\mathbf{L}} \mathbf{K}_{11}^{-\frac{1}{2}}}$$

$$\mathbf{k}_{\mathbf{x},\mathbf{L}} = [k(\mathbf{x}, \mathbf{L}_i,),\ ...,\ k(\mathbf{x}, \mathbf{L}_m)]$$



ADAPTIVE NYSTRÖM LAYER

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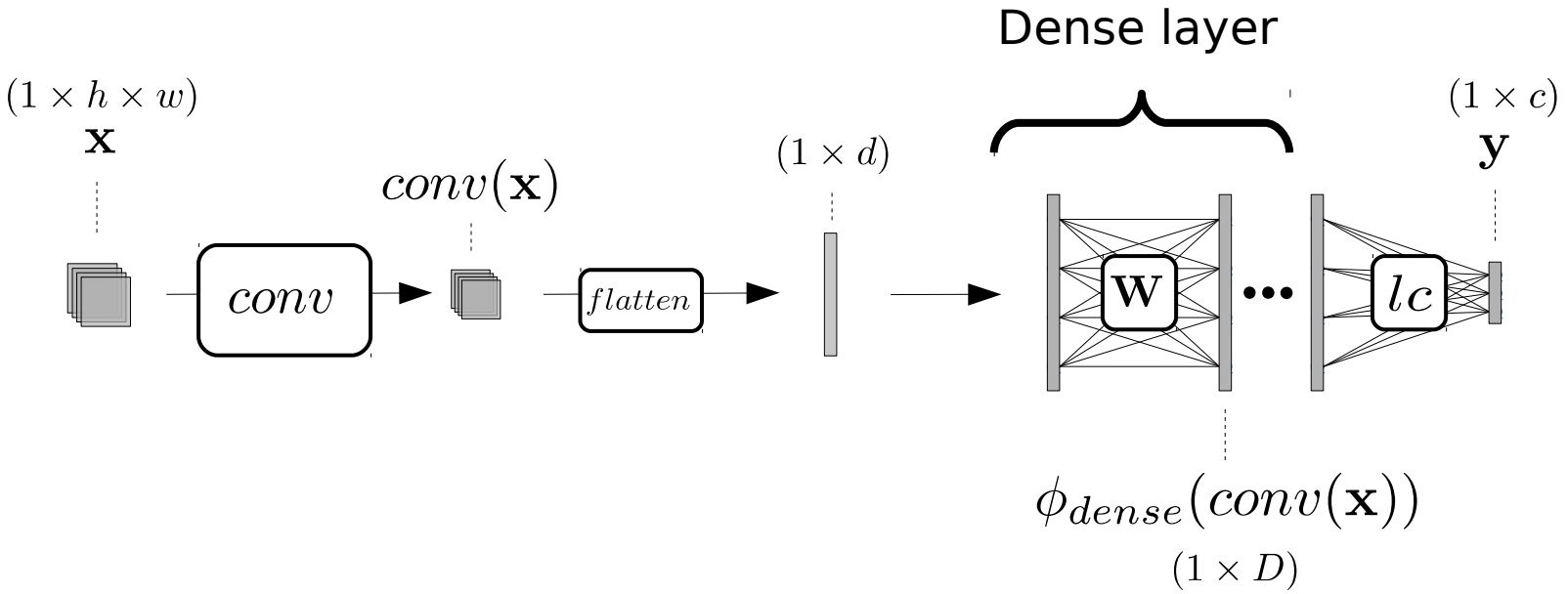
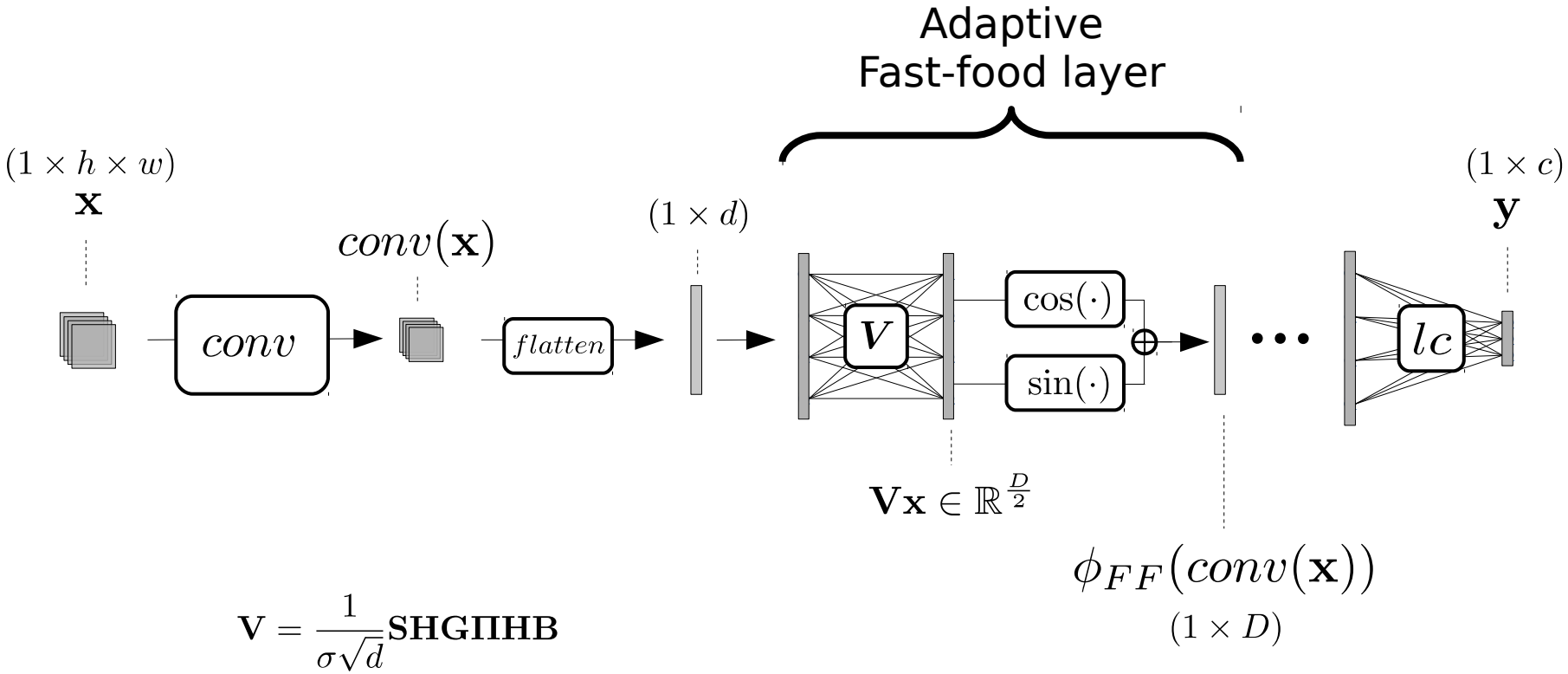
Standard formulation

CNN with Dense layer :



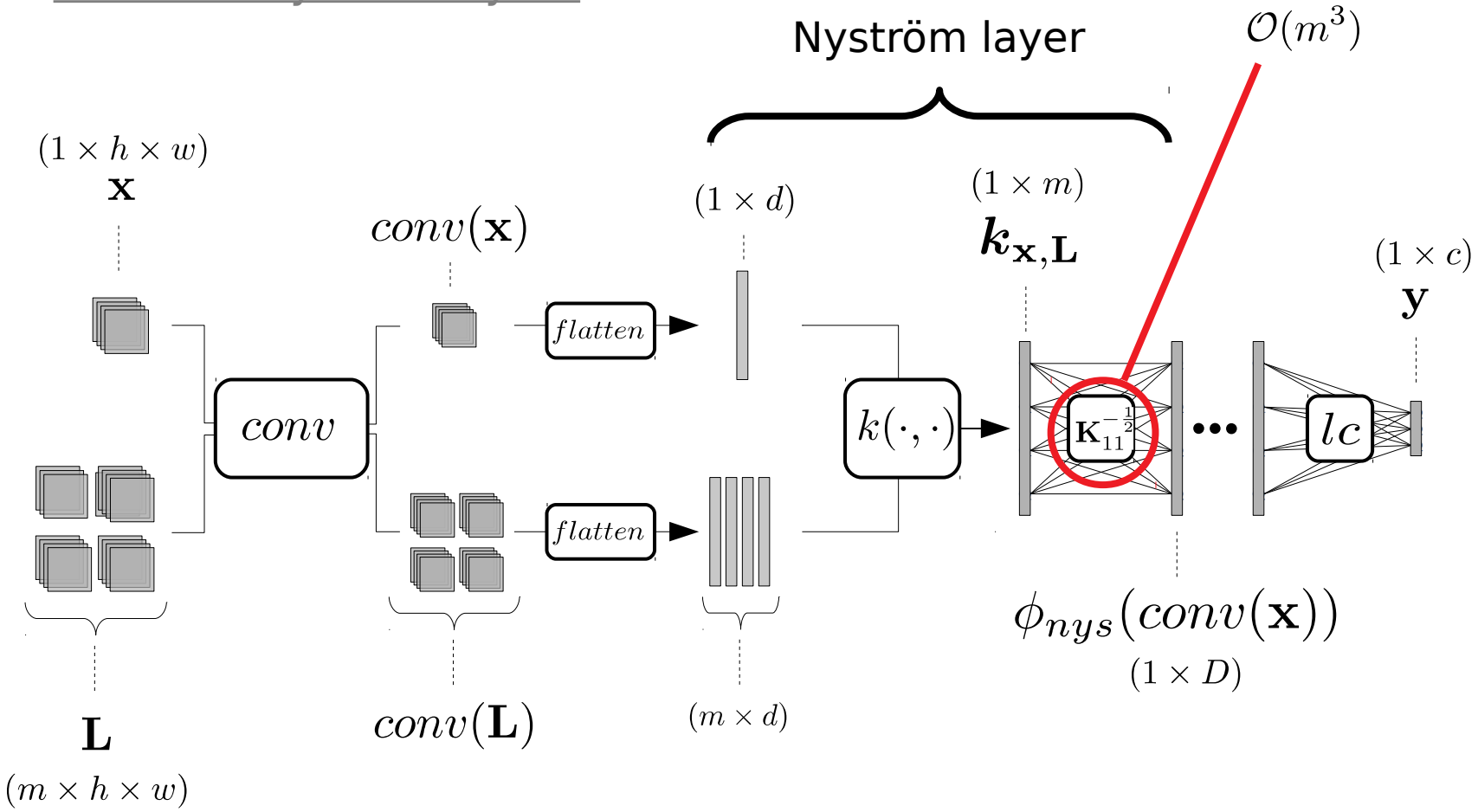
Standard formulation

CNN with Fast-food layer : *(Deep Fried Convnets – Yang et al. 2014)*



Standard formulation

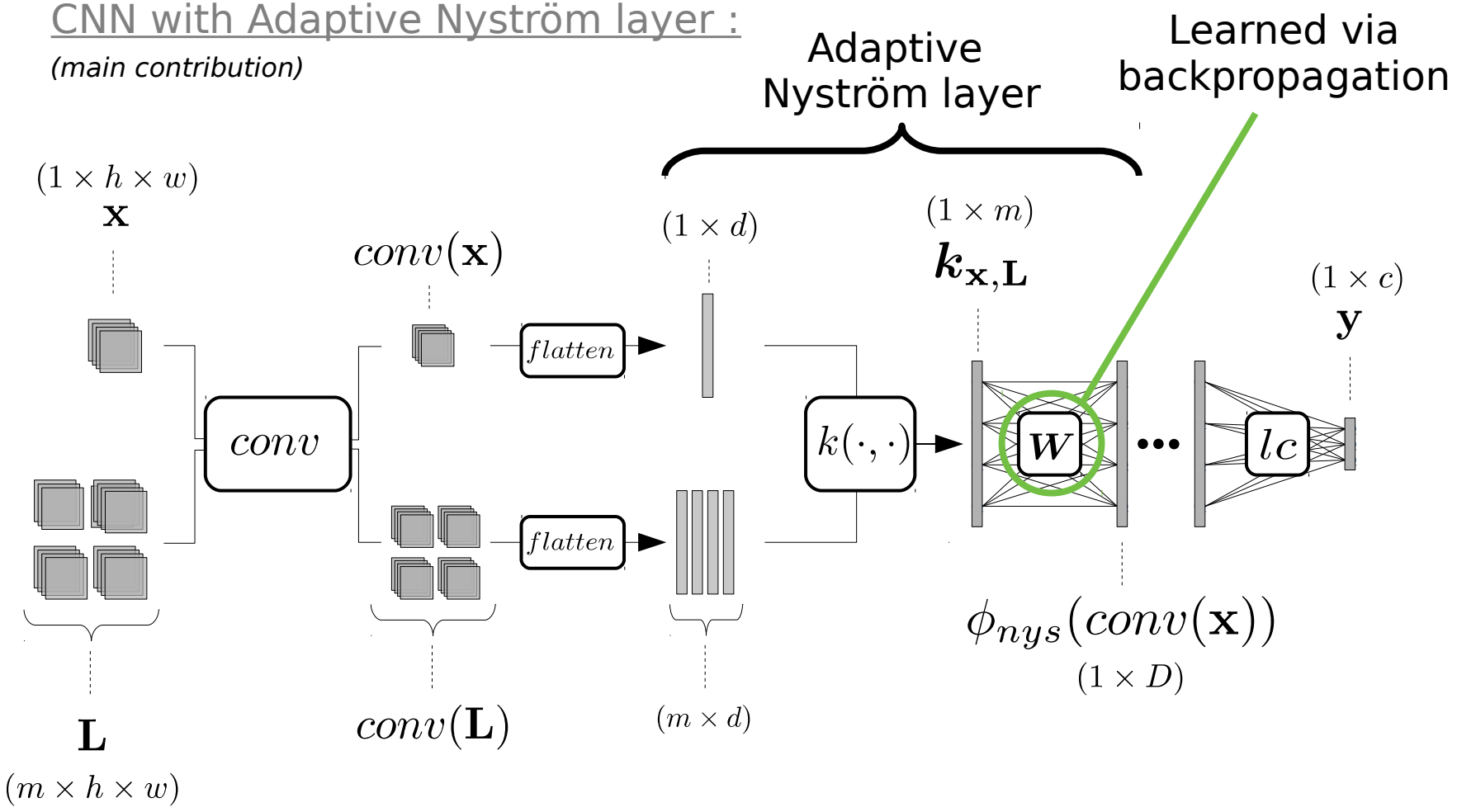
CNN with Nyström layer :



Standard formulation

CNN with Adaptive Nyström layer :

(main contribution)



Multiple Kernel Learning (MKL) formulation

In the Multiple Kernel setting, we can learn several adaptive Nyström layers in parallel then merge them by concatenation or weighted sum.

Concatenation :

$$\phi_{nys_{mkl}} = \begin{bmatrix} \mathbf{W}_1 \boldsymbol{k}^1_{\mathbf{x},\mathbf{L}} \\ \vdots \\ \mathbf{W}_l \boldsymbol{k}^l_{\mathbf{x},\mathbf{L}} \end{bmatrix}$$

Weighted sum :

$$\phi_{nys_{mkl}} = \sum_{i=1}^{l} \alpha_i \mathbf{W}_i \boldsymbol{k}^i_{\mathbf{x},\mathbf{L}}$$

Kernel function examples :

- **Chi2 kernel**

$$k(\mathbf{x}_i, \mathbf{x}_j) = \frac{||\mathbf{x}_i - \mathbf{x}_j||^2}{\mathbf{x}_i + \mathbf{x}_j}$$

- **Linear kernel**

$$k(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i \cdot \mathbf{x}_j \rangle$$

- **Gaussian kernels with different sigmas**

$$k(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{||\mathbf{x}_i - \mathbf{x}_j||^2}{\sigma^2})$$

- **Kernel on single feature map**

$$k^z(\mathbf{x}_i, \mathbf{x}_j) = k(conv(\mathbf{x}_i)_z, conv(\mathbf{x}_j)_z)$$

EXPERIMENTS

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Standard setting

- **Datasets :**

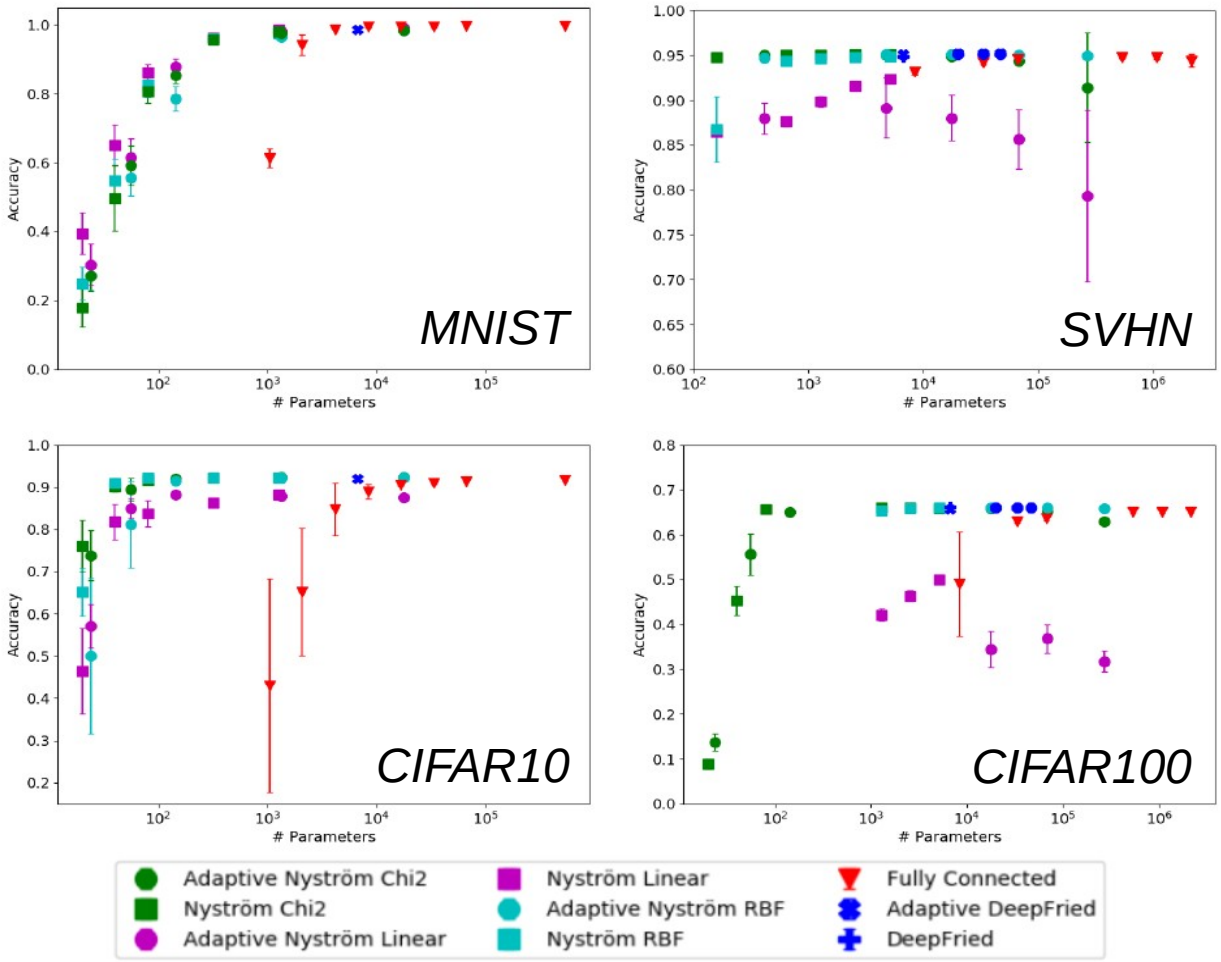
Dataset	Input shape	# classes	Training set size	Validation set size	Test set size
MNIST	$(28 \times 28 \times 1)$	10	40 000	10 000	10 000
SVHN	$(32 \times 32 \times 3)$	10	63 257	10 000	26 032
CIFAR10	$(32 \times 32 \times 3)$	10	50 000	10 000	10 000
CIFAR100	$(32 \times 32 \times 3)$	100	50 000	10 000	10 000

- **Convolutional Architectures :**
  - *LeNet for MNIST ;*
  - *VGG19 for SVHN, CIFAR10 and CIFAR100.*

- **Number of learnable parameters :**
  - *Range from 2 to 1024 hidden neurons in the dense hidden layer ;*
  - *Range from 2 to 128 subsamble size for the Nystrom layer ;*
  - *One stack of random features for the Fast-food layer.*

Standard setting

Our Nyström layer reaches dense layers accuracy with much less parameters. The adaptive variant performs better in most scenario.

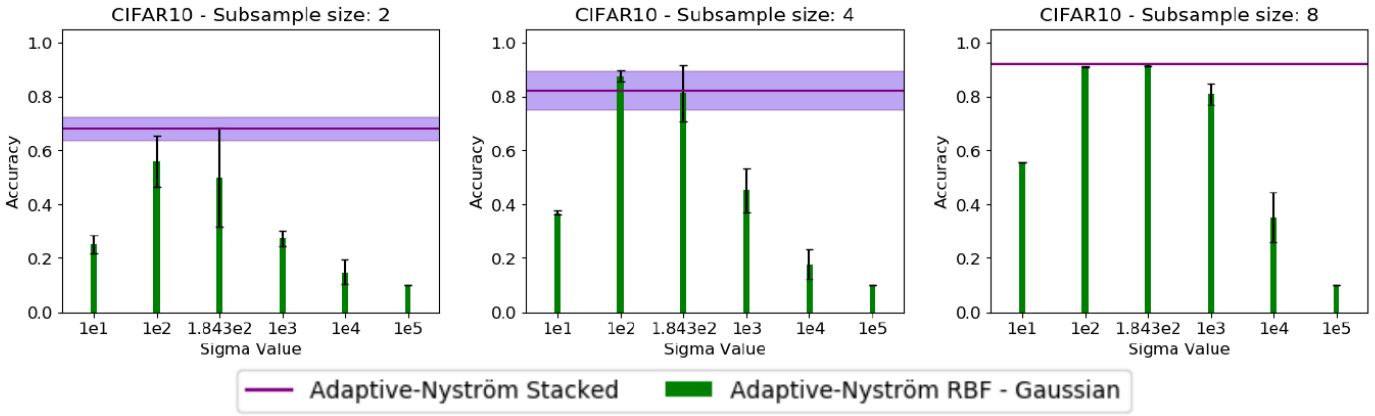


Small sample set

	MNIST		SVHN		CIFAR10		CIFAR100	
	5	20	5	20	5	20	5	20
Dense	**49.7** (4)	94.4 (0.5)	65.6 (11.6)	81.7 (3.9)	39.1 (3.3)	87.1 (3.7)	19.2 (2.2)	35.7 (2.7)
Adaptive-Deepfried	12.4 (3.3)	12.4 (1.4)	16.7 (5)	21.0 (6.4)	28.3 (9.2)	41.2 (3.6)	3.9 (1.2)	6.4 (0.8)
Adaptive-Nyström-L	48.1 (5.5)	95.0 (0.5)	22.4 (6.9)	29.6 (13.5)	12.0 (5.6)	27.8 (7.6)	1.2 (0.6)	1.9 (0.8)
Adaptive-Nyström-R	41.2 (7.7)	**95.5** (0.3)	42.1 (29.6)	53.5 (33.6)	**70.8** (4.4)	**92.2** (0.1)	**24.7** (2.6)	**62.1** (1.2)
Adaptive-Nyström-C	26.4 (7.7)	92.3 (1.8)	**89.6** (3.1)	**93.3** (1.3)	67.1 (4.7)	**92.2** (1)	20.2 (2.2)	55.4 (1.9)

Multiple Kernel Learning

Multiple Gaussian kernel :

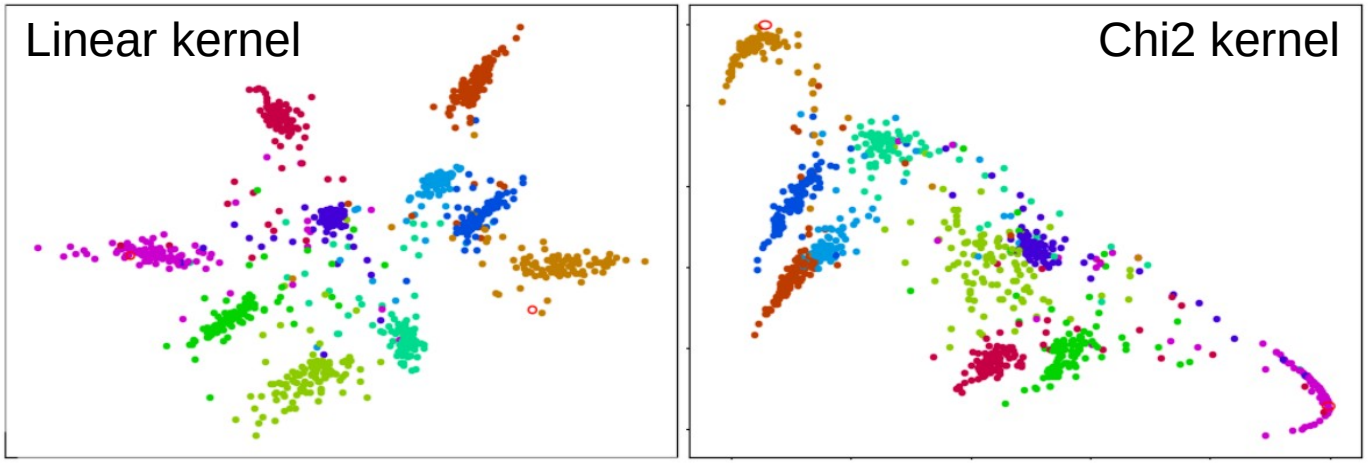


Multiple Kernel Learning

Kernel on single feature maps : CIFAR100

Model	Accuracy (std)	Architecture
Dense	68.0 (0.7)	1 hidden layer 1024 neurons
Adaptive-Deepfried	67.6 (0.5)	5 stacks
Adaptive-Nyström	**69.1** (0.2)	256 subsamples + 512 Linear Kernels
Adaptive-Nyström	67.6 (0.2)	16 subsamples + 512 Chi2 Kernels

2D representations : CIFAR10



CONCLUSION

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Conclusions

- **Learns fewer parameters than standard Dense layers while not reducing the performance ;**
- **Total flexibility in the choice of the kernel function in contrast with the Deep Fried Convnets ;**
- **Modular and able to deal with Multiple Kernel Learning paradigm ;**
- **Simple to implement with Keras or Tensorflow**

THANK YOU FOR YOUR ATTENTION

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Kernel methods : Nyström method

Nyström method for kernel approximation :

The Nyström method gives a low rank approximation of a Kernel matrix. From this approximation, we can extract the feature map approximation of the kernel.

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{21}^T \\ \mathbf{K}_{21} & \mathbf{K}_{22} \end{bmatrix} \qquad \forall i,j \in 1...m \ \mathbf{K}_{11\,i,j} = k(\mathbf{L}_i, \mathbf{L}_j);\ \mathbf{L} \subset \mathbf{X};$$

The Nyström method gives :

$$\mathbf{K} \simeq \tilde{\mathbf{K}} = \begin{bmatrix} \mathbf{K}_{11} \\ \mathbf{K}_{21} \end{bmatrix} \mathbf{K}_{11}^{-1} \begin{bmatrix} \mathbf{K}_{11} & \mathbf{K}_{21}^T \end{bmatrix} = \tilde{\mathbf{\Phi}} \tilde{\mathbf{\Phi}}^T$$

Then the Nyström feature map is :

$$\tilde{\mathbf{\Phi}} = \begin{bmatrix} \mathbf{K}_{11} \\ \mathbf{K}_{21} \end{bmatrix} \mathbf{K}_{11}^{-\frac{1}{2}} \quad \Rightarrow \quad \forall i\ \tilde{\mathbf{\Phi}}_i = \phi_{nys}(\mathbf{x}_i) = \mathbf{k}_{\mathbf{x}_i,\mathbf{L}} \mathbf{K}_{11}^{-\frac{1}{2}}$$

$$\mathbf{k}_{\mathbf{x},\mathbf{L}} = [k(\mathbf{x}, \mathbf{L}_i,),\ ...,\ k(\mathbf{x}, \mathbf{L}_m)]$$

Kernel methods : Random features

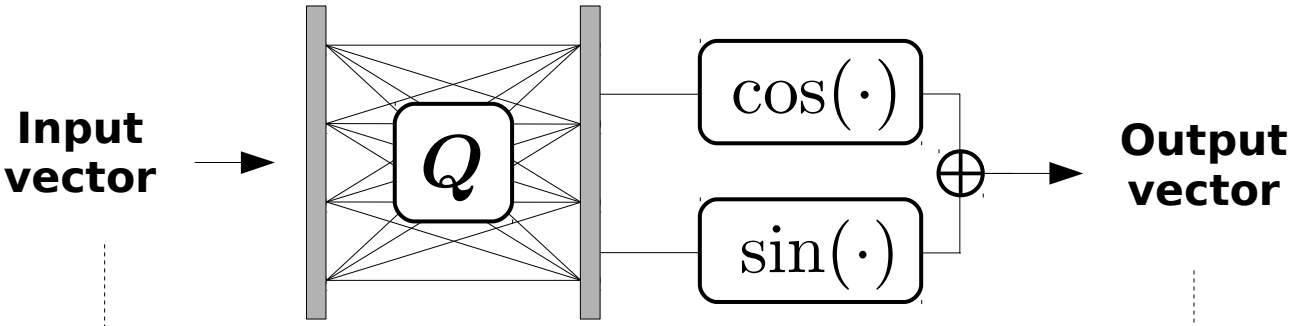
Random Kitchen Sinks (RKS) :

The RKS approximates a *Radial Basis Function* (RBF) kernel.

$$\phi_{RKS}(\mathbf{x}) = [\cos(\mathbf{Q}\mathbf{x}), \sin(\mathbf{Q}\mathbf{x})]$$

$$\mathbf{Q}_{i,j} \sim \mathcal{N}(\mu, \sigma)$$

(For the Gaussian kernel)



$\mathbf{x} \in \mathbb{R}^d$ $\quad \mathbf{Q}\mathbf{x} \in \mathbb{R}^{\frac{D}{2}}$ $\quad [\cos(\mathbf{Q}\mathbf{x}), \sin(\mathbf{Q}\mathbf{x})] \in \mathbb{R}^D$

Kernel methods

$$\forall i \ \mathbf{x}_i \in \mathbf{X} \qquad k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$$

$$\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j) = \langle \phi(\mathbf{x}_i) \cdot \phi(\mathbf{x}_j) \rangle$$

Some kernel methods can give the feature map approximation $\tilde{\phi}$ for a kernel.

$$k(\mathbf{x}, \mathbf{z}) \approx \langle \tilde{\phi}(\mathbf{x}) \cdot \tilde{\phi}(\mathbf{z}) \rangle$$

$$\mathbf{K} \approx \tilde{\mathbf{K}} = \tilde{\mathbf{\Phi}} \tilde{\mathbf{\Phi}}^T \qquad \forall i \ \tilde{\mathbf{\Phi}}_i = \tilde{\phi}(\mathbf{x}_i)$$

(to keep the notations light, we drop the ~ on $\tilde{\phi}$ in the rest of the presentation)