中国人民大学
RENMIN UNIVERSITY OF CHINA

高瓴人工智能学院
Gaoling School of Artificial Intelligence

Efficiently Modeling Long Sequences with Structured State Spaces

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Outline

- Introduction
- State space models (SSM) for deep sequence modeling
- Structured state spaces (S4) for long-term dependencies
- Experiments
- Conclusion

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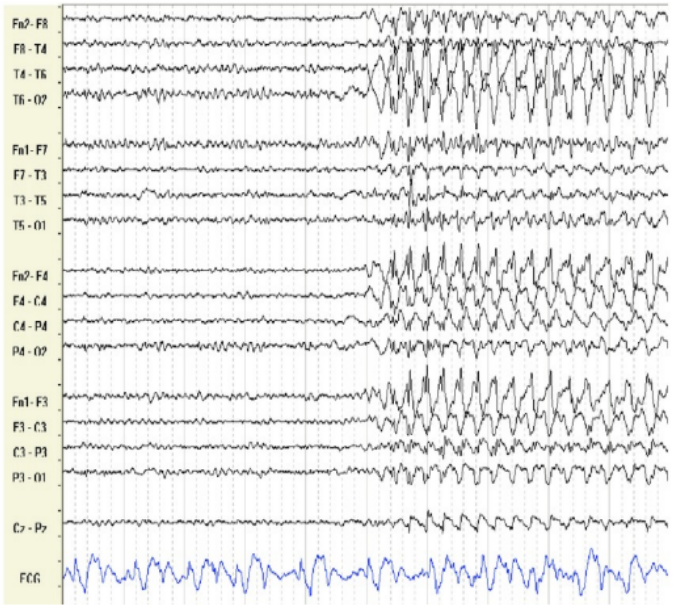
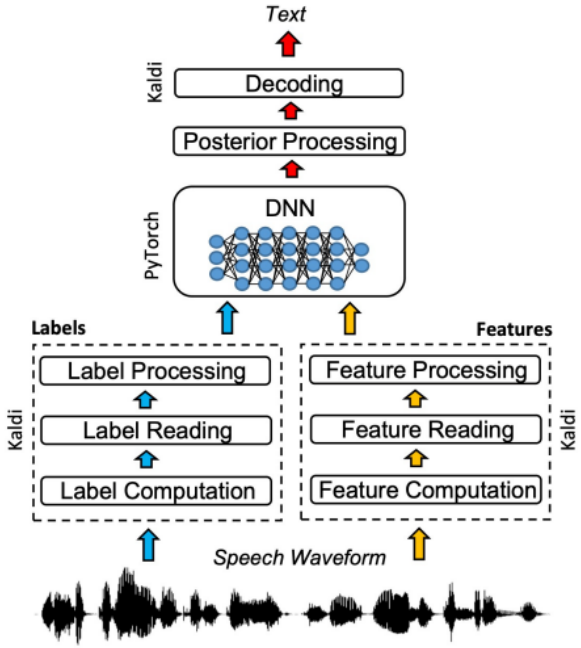
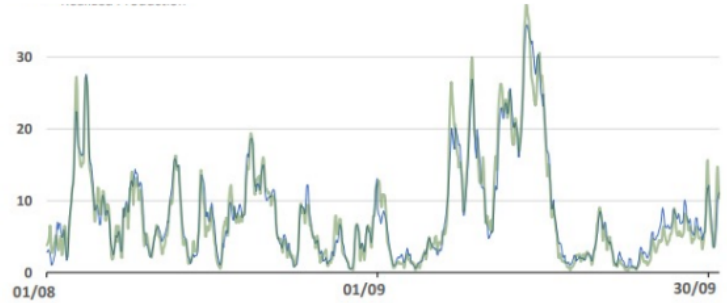
Long "Continuous" Time Series



EEG/ECG



Speech



Energy Forecasting

- Time series sampled from an underlying (continuous) physical process

Sequence Modeling Paradigms

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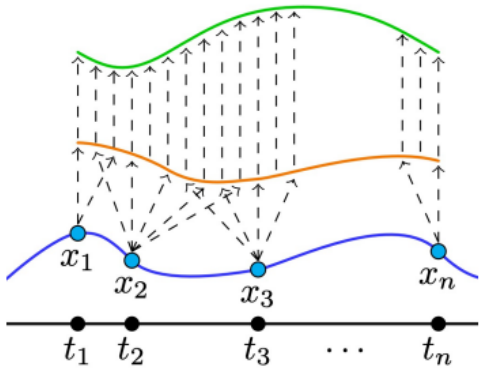
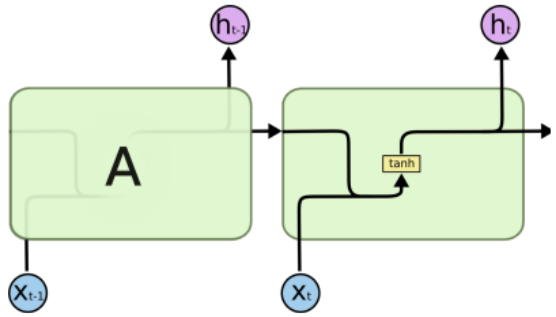
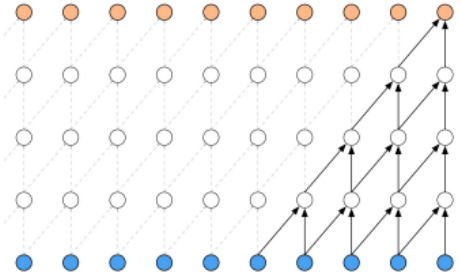
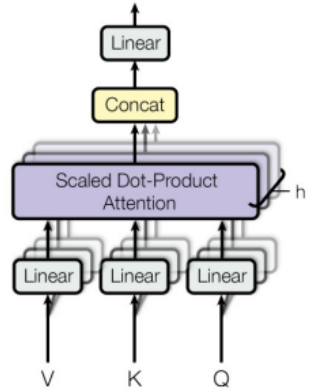
Continuous-time Model	Recurrent Neural Net.	Convolutional Neural Net.	Transformer

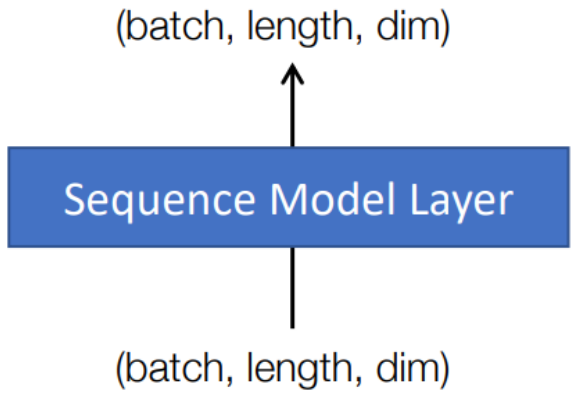




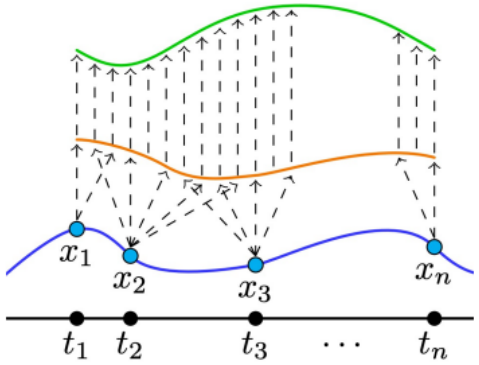




Deep Sequence Model
Sequence-to-sequence map



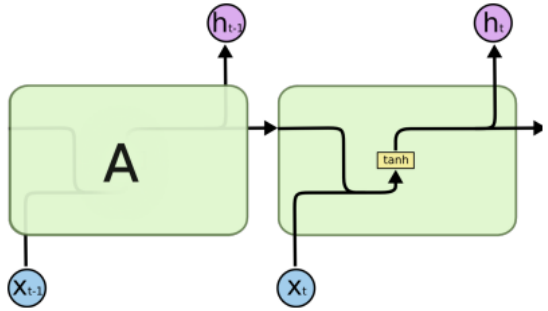
Paradigms for Long Time Series



✓ Continuous data
Irregular sampling

✗ Complex, very inefficient
Vanishing gradients

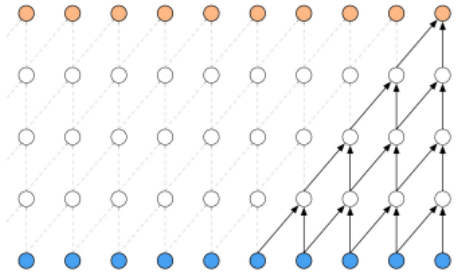
Continuous-time (CTM)



✓ Unbounded context
Stateful inference

✗ Inefficient training
Vanishing gradients

Recurrent (RNN)



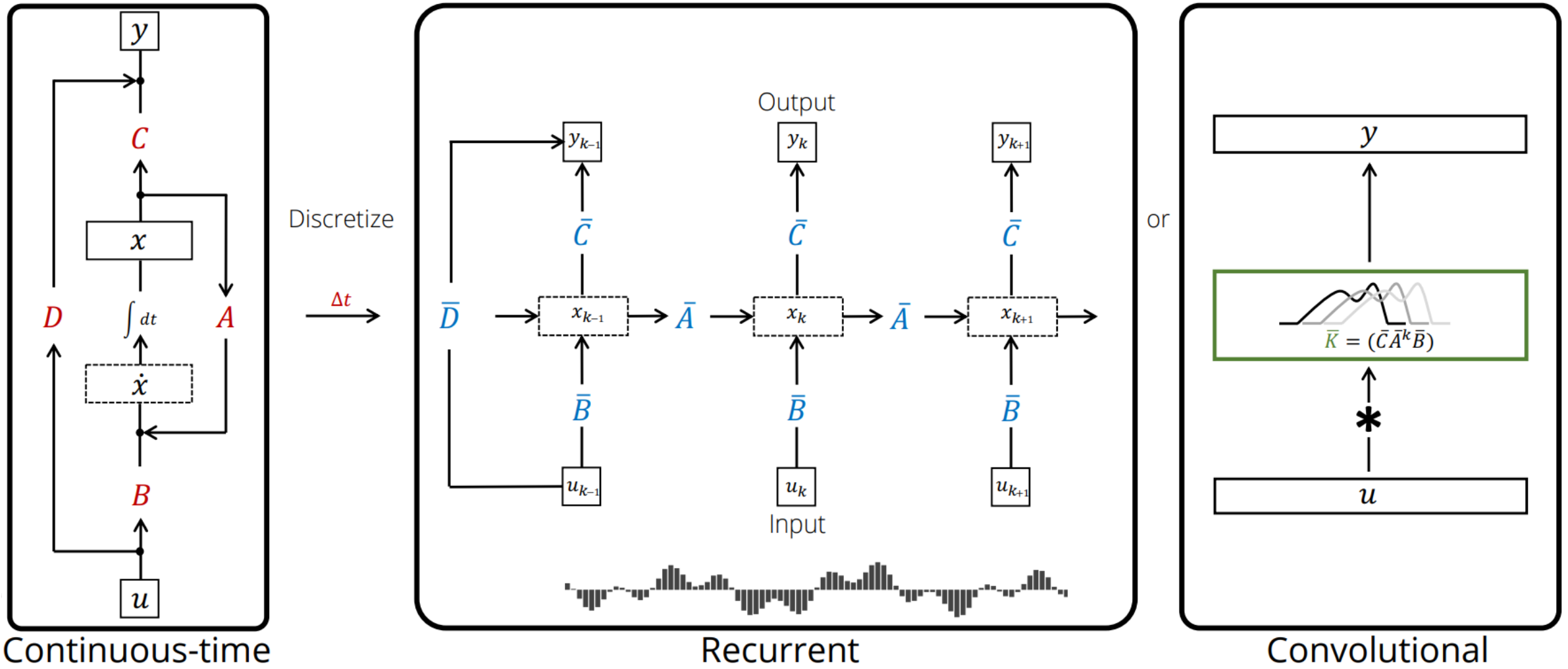
✓ Easy optimization
Parallelizable training

✗ Inefficient inference
Bounded context

Convolutional (CNN)

- Existing model families have clear tradeoffs
- All struggle with long-range dependencies (LRD)

Structured State Spaces (S4)



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Computing with SSMs: Continuous View

Input → State

$$x'(t) = \boldsymbol{A}x(t) + \boldsymbol{B}u(t)$$

$$y(t) = \boldsymbol{C}x(t) + \boldsymbol{D}u(t)$$

Parameters

$\boldsymbol{A} \in \mathbb{R}^{N \times N}$

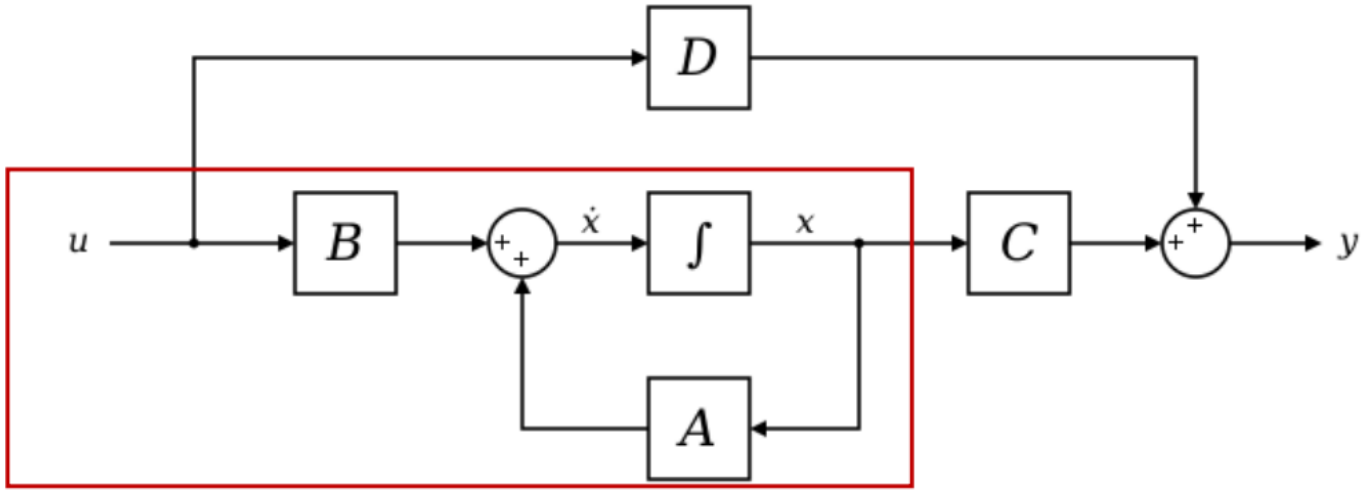
$\boldsymbol{B} \in \mathbb{R}^{N \times 1}$

$\boldsymbol{C} \in \mathbb{R}^{1 \times N}$

$\boldsymbol{D} \in \mathbb{R}^{1 \times 1}$

Function-to-function map $u(t) \mapsto y(t)$

1D input
u(t)



1D output
y(t)

Computing with SSMs: Continuous View

$$x'(t) = \boldsymbol{A}x(t) + \boldsymbol{B}u(t)$$

State → Output

$$y(t) = \boldsymbol{C}x(t) + \boldsymbol{D}u(t)$$

Parameters

$\boldsymbol{A} \in \mathbb{R}^{N \times N}$

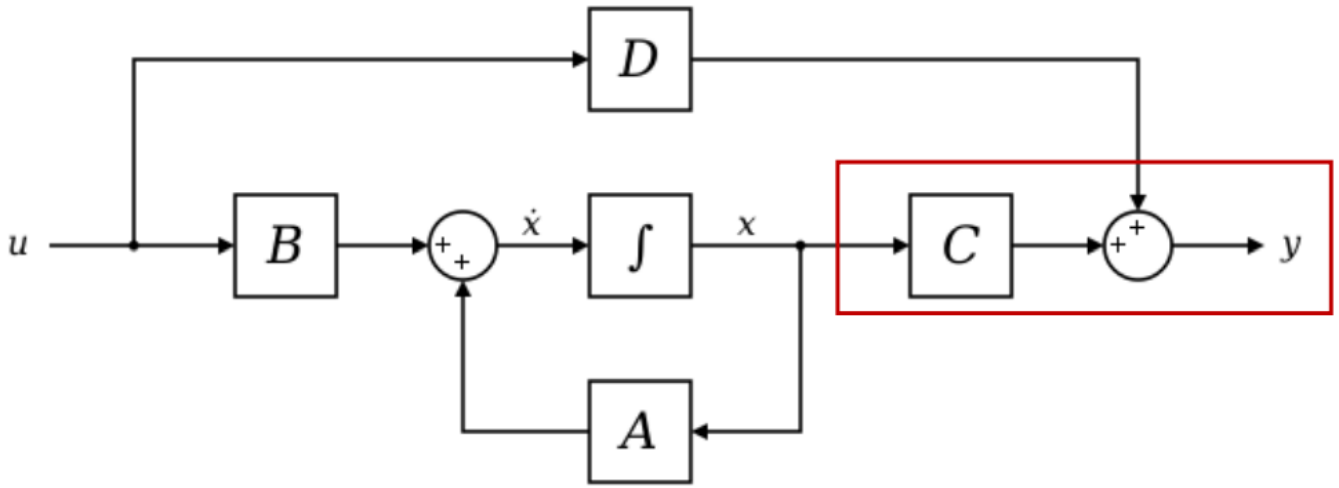
$\boldsymbol{B} \in \mathbb{R}^{N \times 1}$

$\boldsymbol{C} \in \mathbb{R}^{1 \times N}$

$\boldsymbol{D} \in \mathbb{R}^{1 \times 1}$

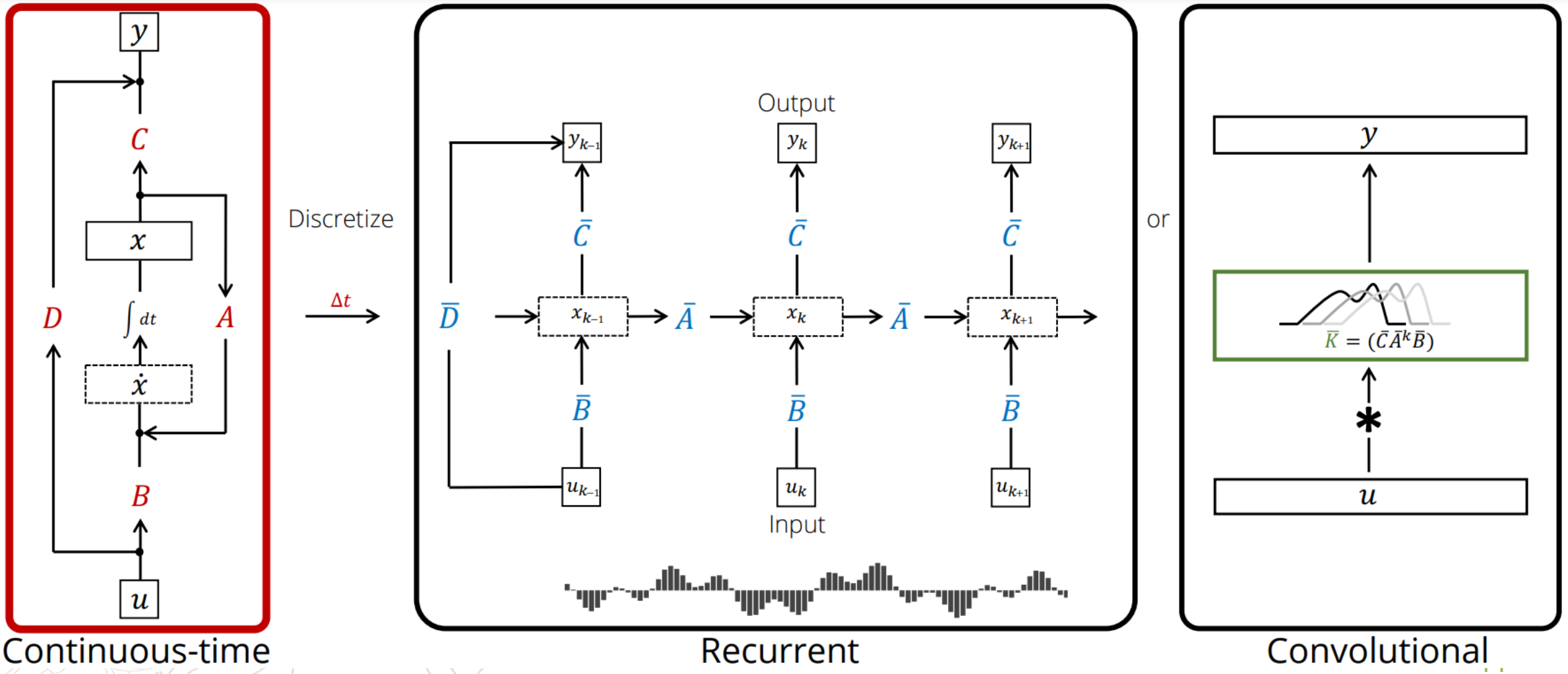
Function-to-function map $u(t) \mapsto y(t)$

1D input
u(t)



1D output
y(t)

SSM: Continuous Representation



Computing with SSMs: Recurrent View

Conceptually, the inputs u_k can be viewed as **sampling an implicit underlying continuous signal** u(t), where $u_k = u(k\Delta)$.

To discretize the continuous-time SSM, we follow prior work in using **the bilinear method**, which converts **the state matrix** $\boldsymbol{A}$ into an **approximation** $\overline{\boldsymbol{A}}$. The discrete SSM is

$$x_k = \overline{\boldsymbol{A}} x_{k-1} + \overline{\boldsymbol{B}} u_k \qquad \overline{\boldsymbol{A}} = (\boldsymbol{I} - \Delta/2 \cdot \boldsymbol{A})^{-1}(\boldsymbol{I} + \Delta/2 \cdot \boldsymbol{A})$$
$$y_k = \overline{\boldsymbol{C}} x_k \qquad \overline{\boldsymbol{B}} = (\boldsymbol{I} - \Delta/2 \cdot \boldsymbol{A})^{-1} \Delta \boldsymbol{B} \qquad \overline{\boldsymbol{C}} = \boldsymbol{C}.$$

Parameters

$\boldsymbol{A} \in \mathbb{R}^{N \times N}$

$\boldsymbol{B} \in \mathbb{R}^{N \times 1}$

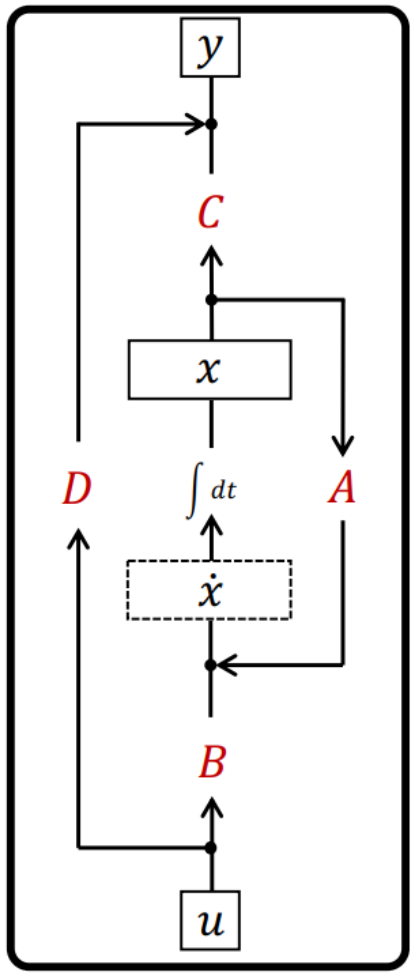
$\boldsymbol{C} \in \mathbb{R}^{1 \times N}$

$\boldsymbol{D} \in \mathbb{R}^{1 \times 1}$

$\Delta \in \mathbb{R}$

Now it's a *sequence-to-sequence* map $u(t) \mapsto y(t)$ instead of *function-to-function map*.

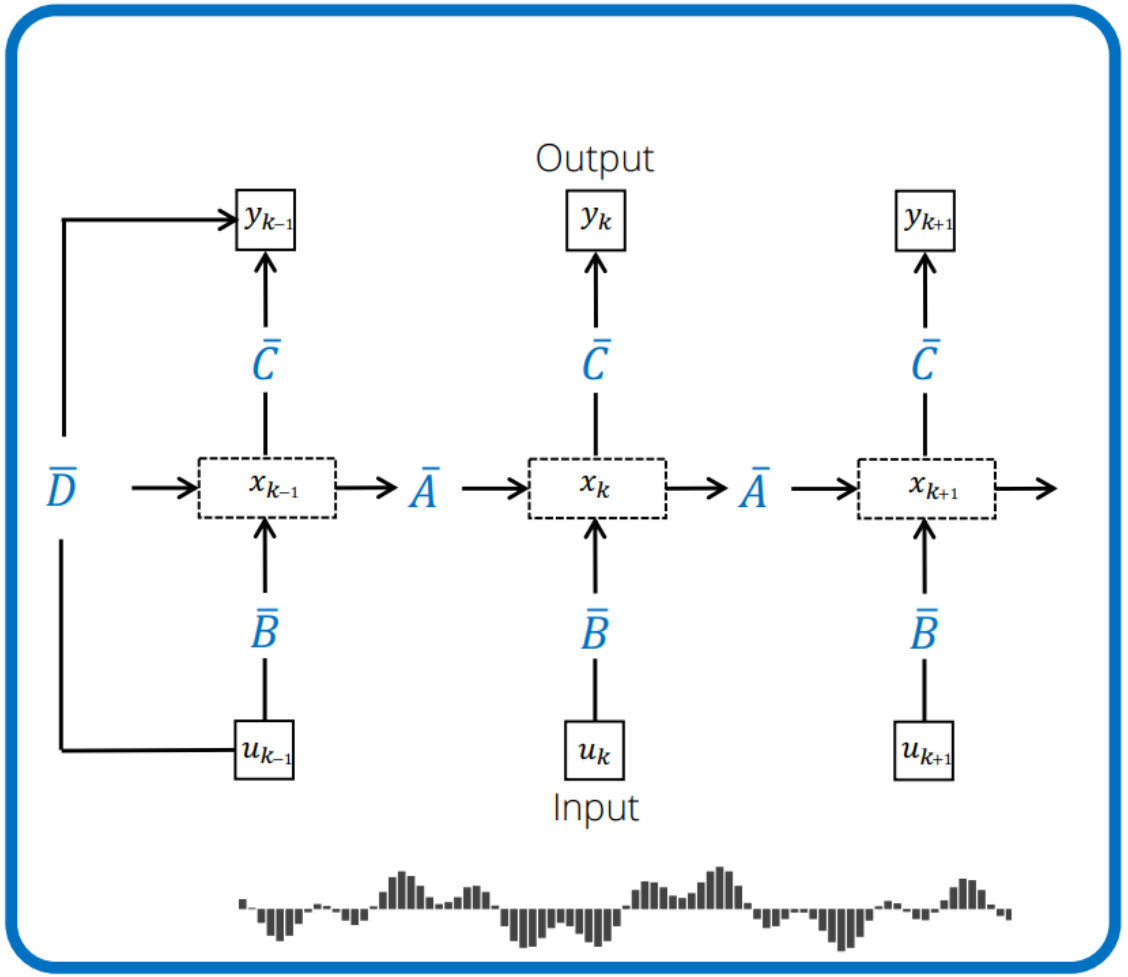
SSM: Recurrent Representation



Continuous-time

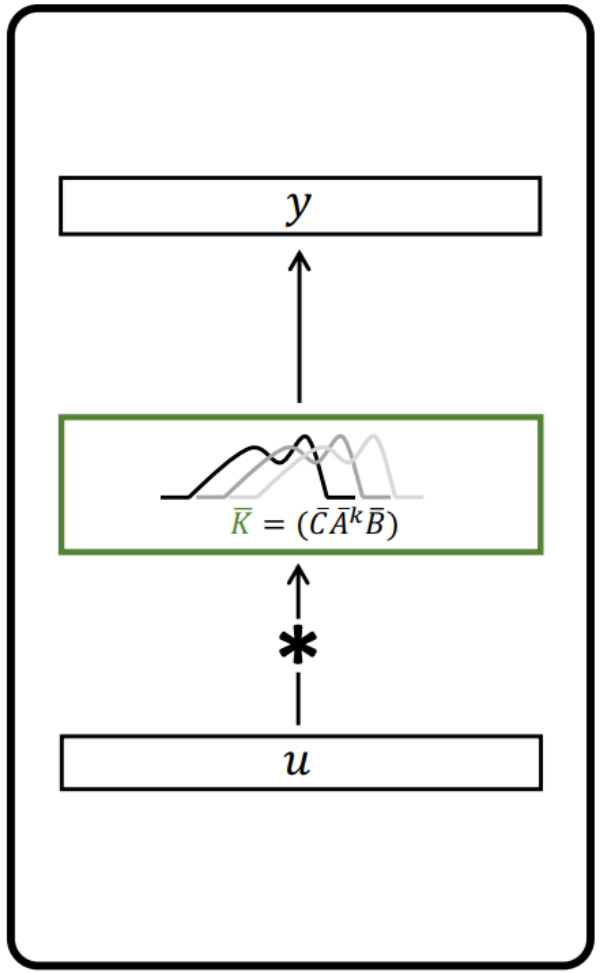
Discretize

Δt



Recurrent

or



Convolutional

Computing with SSMs: Convolutional View

$$x_k = \overline{A}x_{k-1} + \overline{B}u_k$$
$$y_k = \overline{C}x_k$$

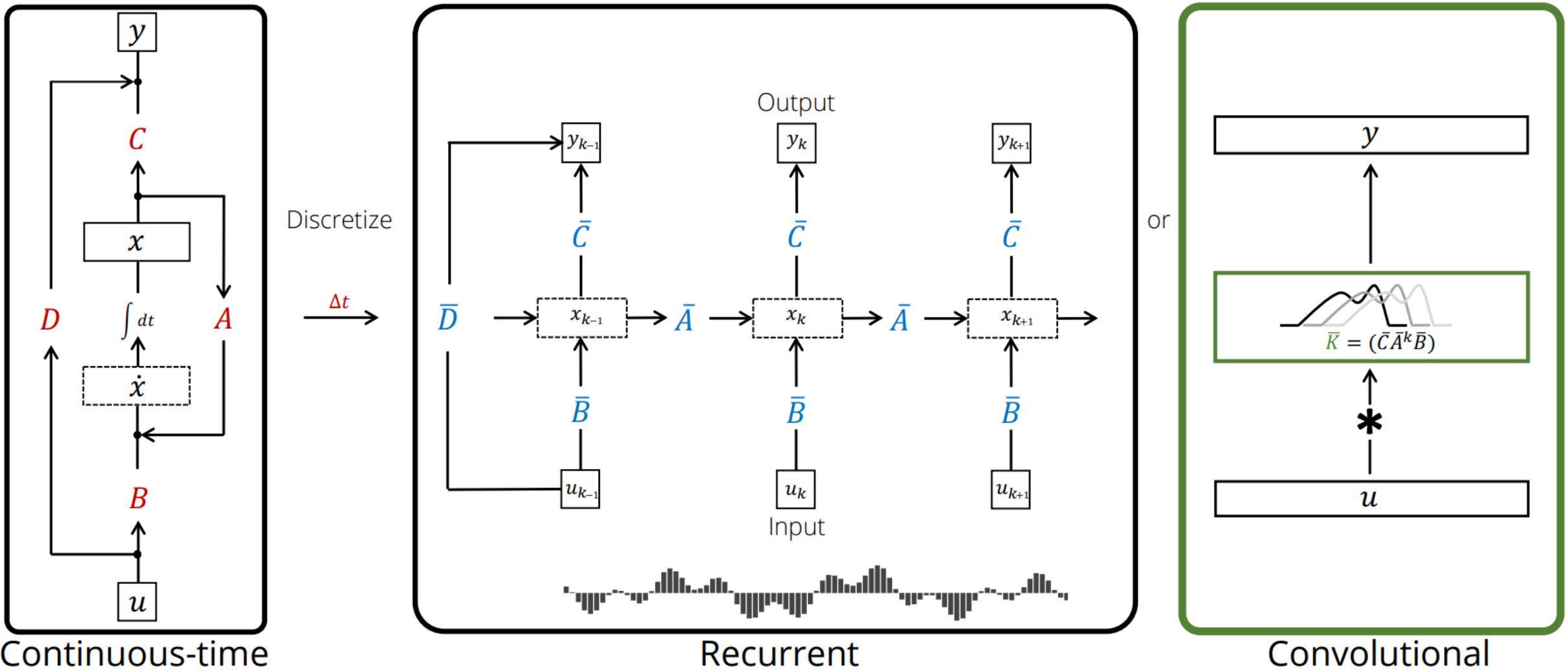
$$x_0 = \overline{B}u_0 \qquad x_1 = \overline{AB}u_0 + \overline{B}u_1 \qquad x_2 = \overline{A}^2\overline{B}u_0 + \overline{AB}u_1 + \overline{B}u_2 \qquad \dots$$
$$y_0 = \overline{CB}u_0 \qquad y_1 = \overline{CAB}u_0 + \overline{CB}u_1 \qquad y_2 = \overline{CA}^2\overline{B}u_0 + \overline{CAB}u_1 + \overline{CB}u_2 \qquad \dots$$

This can be vectorized into a **convolution** with an explicit formula for the **convolution kernel:**

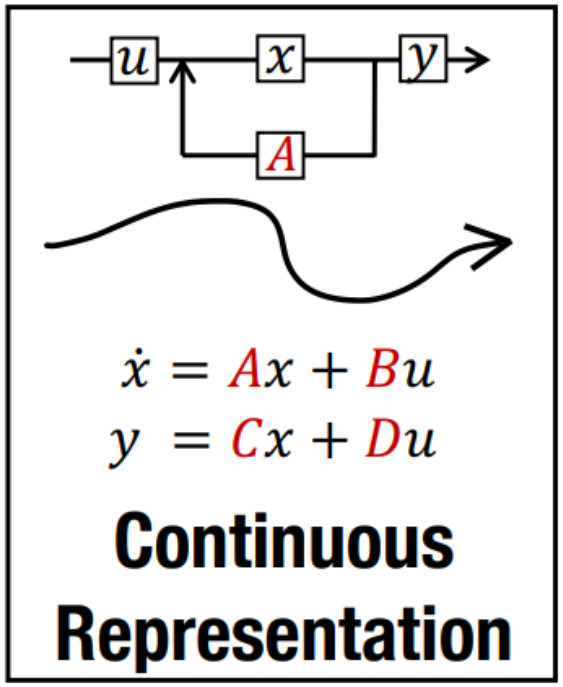
$$y_k = \overline{CA}^k\overline{B}u_0 + \overline{CA}^{k-1}\overline{B}u_1 + \cdots + \overline{CAB}u_{k-1} + \overline{CB}u_k$$
$$y = \overline{K} * u.$$

$$\overline{K} \in \mathbb{R}^L := \mathcal{K}_L(\overline{A}, \overline{B}, \overline{C}) := \left(\overline{CA}^i\overline{B}\right)_{i\in[L]} = (\overline{CB}, \overline{CAB}, \dots, \overline{CA}^{L-1}\overline{B}).$$

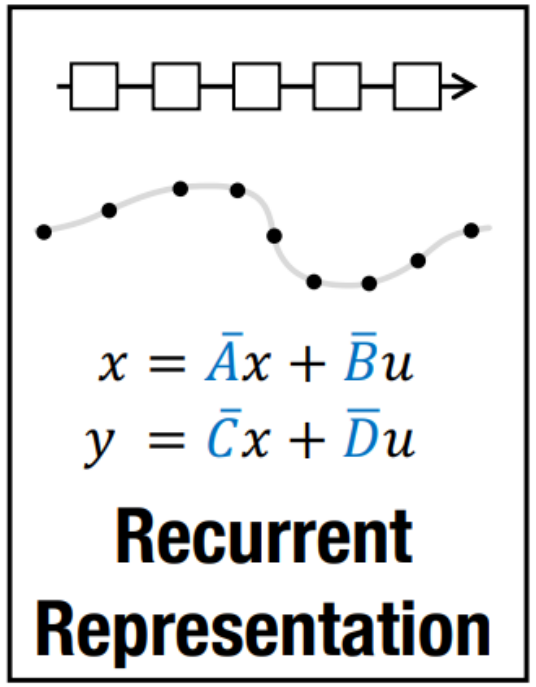
SSM: Convolutional Representation



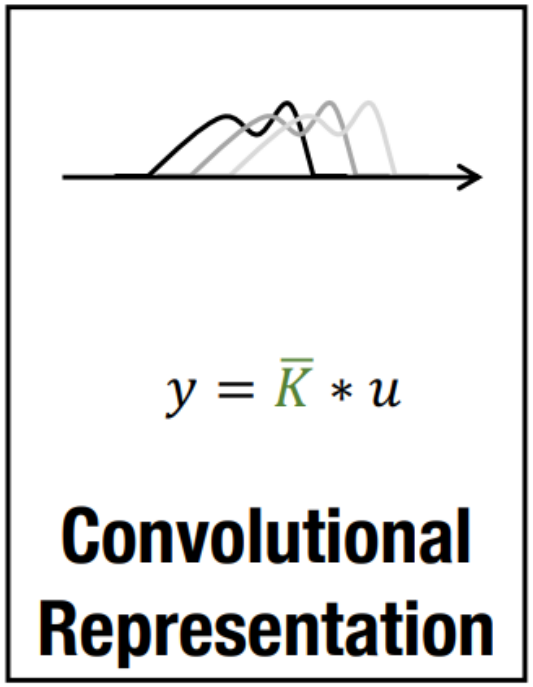
Summary: Properties of SSMs



Discretize



Unroll



- ✓ *mathematically tractable*
- ✓ *handles irregular data*

- ✓ *unbounded context*
- ✓ *efficient inference*

- ✓ *easy optimization*
- ✓ *parallelizable training*

Simple & principled... why haven't SSMs been used in deep learning?

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Challenges of Deep SSMs

- **Modeling Challenge**: SSMs inherit properties of CTMs, RNNs, CNNs... including problems with LRDs

$$x'(t) = \boldsymbol{A}x(t) + \boldsymbol{B}u(t)$$
$$y(t) = \boldsymbol{C}x(t) + \boldsymbol{D}u(t)$$

with random matrix A: 50% on MNIST

$$\overline{\boldsymbol{K}} = (\overline{\boldsymbol{C}}\overline{\boldsymbol{B}}, \overline{\boldsymbol{C}}\overline{\boldsymbol{A}}\overline{\boldsymbol{B}}, \ldots, \overline{\boldsymbol{C}}\overline{\boldsymbol{A}}^{L-1}\overline{\boldsymbol{B}})$$

Powering up $\overline{\boldsymbol{A}}$ → vanishing gradients?

Powering up $\overline{\boldsymbol{A}}$ → $O(N^2L)$ computation complexity

- **Computation Challenge**: SSMs have nice properties provided that representations $\overline{\boldsymbol{A}}$ and $\overline{\boldsymbol{K}}$ are known, but computing them is extremely hard!

Addressing Long-Range Dependencies with HiPPO Matrix

$$x'(t) = \boldsymbol{A}x(t) + \boldsymbol{B}u(t) \quad (1)$$

- HiPPO specifies a class of certain matrices $\boldsymbol{A} \in \mathbb{R}^{N \times N}$ that when incorporated into (1), allows the state x(t) to memorize the history of the input u(t).

$$A_{nk} = \begin{cases} (2n+1)^{1/2}(2k+1)^{1/2} & \text{if } n > k \\ n+1 & \text{if } n = k \\ 0 & \text{if } n < k \end{cases}, \qquad B_n = (2n+1)^{\frac{1}{2}}$$

G.*, Dao*, Ermon, Rudra, Ré. "HiPPO: Recurrent Memory with Optimal Polynomial Projections." NeurIPS 2020
G., Johnson, Goel, Saab, Dao, Rudra, Ré. "Combining Recurrent, Convolutional, and Continuous-time Models with Linear State Space Layers." NeurIPS 2021

Structured State Spaces (S4)

Computing $\overline{\boldsymbol{K}}$ is **non-trivial** and is the focus of technical contributions of this paper.

$$\overline{\boldsymbol{K}} \in \mathbb{R}^{L} := (\overline{\boldsymbol{C}}\overline{\boldsymbol{B}}, \overline{\boldsymbol{C}}\overline{\boldsymbol{A}}\overline{\boldsymbol{B}}, \ldots, \overline{\boldsymbol{C}}\overline{\boldsymbol{A}}^{L-1}\overline{\boldsymbol{B}})$$

Algorithm 1 S4 Convolution Kernel (Sketch)

Input: S4 parameters $\boldsymbol{\Lambda}, \boldsymbol{p}, \boldsymbol{q}, \boldsymbol{B}, \boldsymbol{C} \in \mathbb{C}^N$ and step size Δ
Output: SSM convolution kernel $\overline{\boldsymbol{K}} = \mathcal{K}_L(\overline{\boldsymbol{A}}, \overline{\boldsymbol{B}}, \overline{\boldsymbol{C}})$ for $\boldsymbol{A} = \boldsymbol{\Lambda} - \boldsymbol{p}\boldsymbol{q}^*$ (equation (5))

1: $\widetilde{\boldsymbol{C}} \leftarrow \left(\boldsymbol{I} - \overline{\boldsymbol{A}}^L\right)^* \overline{\boldsymbol{C}}$ ▷ Truncate SSM generating function (SSMGF) to length L

2: $\begin{bmatrix} k_{00}(\omega) & k_{01}(\omega) \\ k_{10}(\omega) & k_{11}(\omega) \end{bmatrix} \leftarrow \left[\widetilde{\boldsymbol{C}}\ \boldsymbol{q}\right]^* \left(\frac{2}{\Delta}\frac{1-\omega}{1+\omega} - \boldsymbol{\Lambda}\right)^{-1} [\boldsymbol{B}\ \boldsymbol{p}]$ ▷ Black-box Cauchy kernel

3: $\hat{\boldsymbol{K}}(\omega) \leftarrow \frac{2}{1+\omega}\left[k_{00}(\omega) - k_{01}(\omega)(1 + k_{11}(\omega))^{-1}k_{10}(\omega)\right]$ ▷ Woodbury Identity

4: $\hat{\boldsymbol{K}} = \{\hat{\boldsymbol{K}}(\omega) : \omega = \exp(2\pi i \frac{k}{L})\}$ ▷ Evaluate SSMGF at all roots of unity $\omega \in \Omega_L$

5: $\overline{\boldsymbol{K}} \leftarrow \mathsf{iFFT}(\hat{\boldsymbol{K}})$ ▷ Inverse Fourier Transform

Challenges of Deep SSMs

- **Modeling Challenge**: SSMs inherit properties of CTMs, RNNs, CNNs... including problems with LRDs

generic $\boldsymbol{A}$ → 50% on MNIST ✗

HiPPO $\boldsymbol{A}$ → 99% on MNIST ✓

- **Computation Challenge**: SSMs have nice properties provided that representations $\overline{\boldsymbol{A}}$ and $\overline{\boldsymbol{K}}$ are known, but computing them is extremely hard!

generic $\boldsymbol{A} \rightarrow O(N^2 L)$ computation ✗

HiPPO $\boldsymbol{A} \rightarrow \tilde{O}(N + L)$ computation ✓

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Long Range Arena

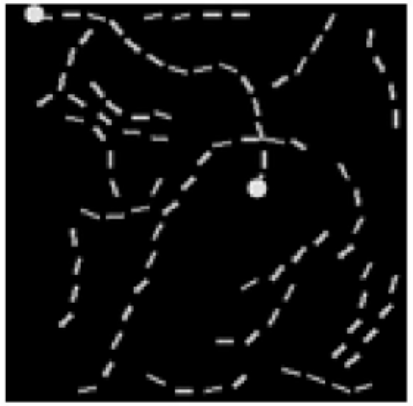
Benchmark spanning text, images, symbolic reasoning (length 1K-16K)

Model	ListOps	Text	Retrieval	Image	Pathfinder	Path-X	Avg
Random	10.00	50.00	50.00	10.00	50.00	50.00	36.67
Transformer	36.37	64.27	57.46	42.44	71.40	✗	53.66
Local Attention	15.82	52.98	53.39	41.46	66.63	✗	46.71
Sparse Trans.	17.07	63.58	59.59	44.24	71.71	✗	51.03
Longformer	35.63	62.85	56.89	42.22	69.71	✗	52.88
Linformer	35.70	53.94	52.27	38.56	76.34	✗	51.14
Reformer	37.27	56.10	53.40	38.07	68.50	✗	50.56
Sinkhorn Trans.	33.67	61.20	53.83	41.23	67.45	✗	51.23
Synthesizer	36.99	61.68	54.67	41.61	69.45	✗	52.40
BigBird	36.05	64.02	59.29	40.83	74.87	✗	54.17
Linear Trans.	16.13	65.90	53.09	42.34	75.30	✗	50.46
Performer	18.01	65.40	53.82	42.77	77.05	✗	51.18
FNet	35.33	65.11	59.61	38.67	77.80	✗	54.42
Nyströmformer	37.15	65.52	79.56	41.58	70.94	✗	57.46
Luna-256	37.25	64.57	79.29	47.38	77.72	✗	59.37
S4	**58.35**	**76.02**	**87.09**	**87.26**	**86.05**	**88.10**	**80.48**

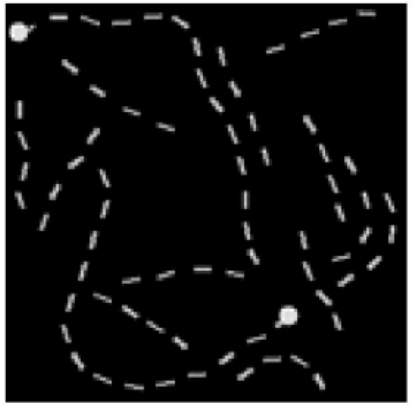
	Length 1024		Length 4096	
	Speed	Mem.	Speed	Mem.
Transformer	1×	1×	1×	1×
Performer	1.23×	0.43×	3.79×	0.086×
Linear Trans.	**1.58**×	**0.37**×	**5.35**×	**0.067**×
S4	**1.58**×	0.43×	5.19×	0.091×

Long Range Arena Path-X

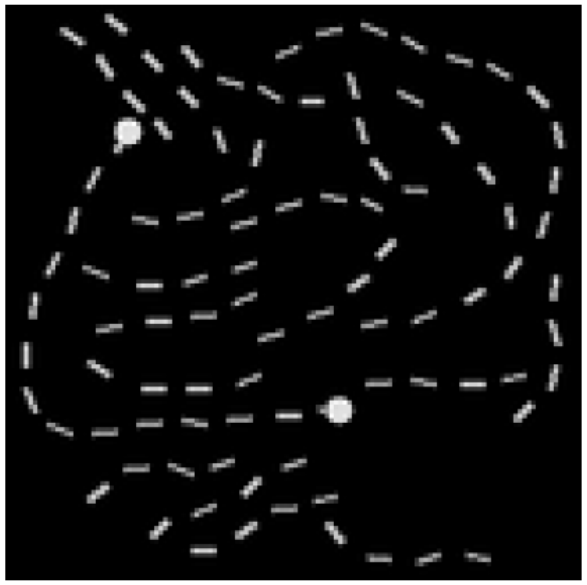
Path-X



(a) A positive example.



(b) A negative example.



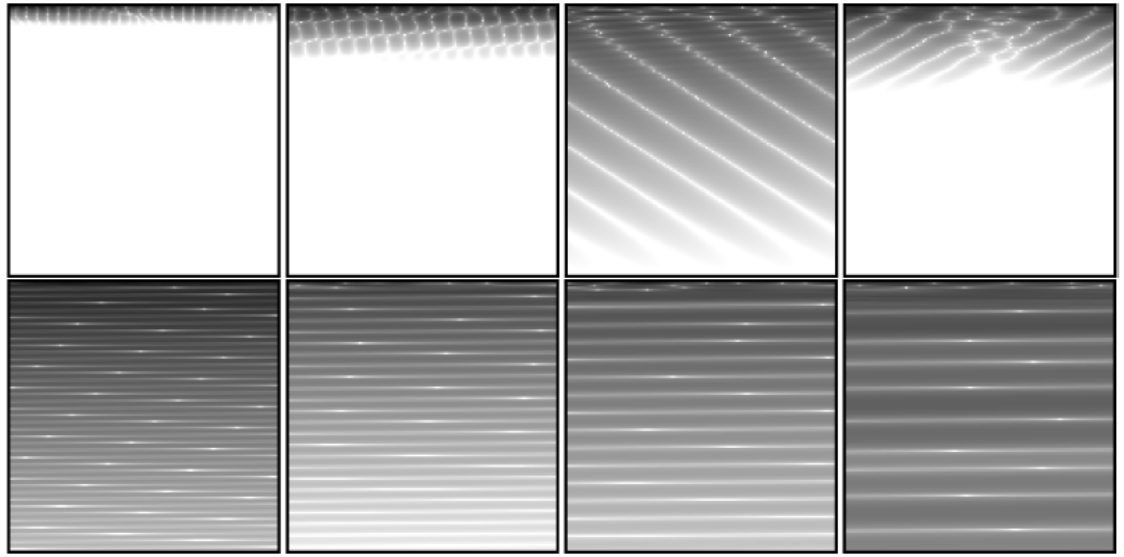


Figure 2: Visualizations of a trained S4 model on LRA Path-X. SSM convolution kernels $\overline{\boldsymbol{K}} \in \mathbb{R}^{16384}$ are reshaped into a 128×128 image. (*Left*) Example from the Path-X task, which involves deducing if the markers are connected by a path (*Top*) Filters from the first layer (*Bottom*) Filters from the last layer.

Sequential Image Classification

	Model	sMNIST	pMNIST	sCIFAR
Transformers	Transformer (Vaswani et al., 2017; Trinh et al., 2018)	98.9	97.9	62.2
CNNs	CKConv (Romero et al., 2021)	99.32	<u>98.54</u>	63.74
	TrellisNet (Bai et al., 2019)	99.20	98.13	73.42
	TCN (Bai et al., 2018)	99.0	97.2	-
RNNs	LSTM (Hochreiter & Schmidhuber, 1997; Gu et al., 2020b)	98.9	95.11	63.01
	r-LSTM (Trinh et al., 2018)	98.4	95.2	72.2
	Dilated GRU (Chang et al., 2017)	99.0	94.6	-
	Dilated RNN (Chang et al., 2017)	98.0	96.1	-
	IndRNN (Li et al., 2018)	99.0	96.0	-
	expRNN (Lezcano-Casado & Martínez-Rubio, 2019)	98.7	96.6	-
	UR-LSTM	99.28	96.96	71.00
	UR-GRU (Gu et al., 2020b)	99.27	96.51	<u>74.4</u>
	LMU (Voelker et al., 2019)	-	97.15	-
	HiPPO-RNN (Gu et al., 2020a)	98.9	98.3	61.1
	UNIcoRNN (Rusch & Mishra, 2021)	-	98.4	-
	LMUFFT (Chilkuri & Eliasmith, 2021)	-	98.49	-
	LipschitzRNN (Erichson et al., 2021)	<u>99.4</u>	96.3	64.2
SSMs	**S4**	**99.63**	**98.70**	**91.13**

Speech Classification(keywords spotting)

- Speech is difficult because LRD:

  1 second clip = length-16000

- Mel-frequency Cepstrum Coefficients (MFCC) (length 160)

	L=160 MFCC	L=16K Raw	L=8K 0.5×
Transformer	90.75	✗	✗
Performer	80.85	30.77	30.68
ODE-RNN	65.9	✗	✗
NRDE	89.8	16.49	15.12
ExpRNN	82.13	11.6	10.8
LipschitzRNN	88.38	✗	✗
CKConv	**95.3**	71.66	<u>65.96</u>
WaveGAN-D	✗	<u>96.25</u>	✗
LSSL	93.58	✗	✗
S4	<u>93.96</u>	**98.32**	**96.30**

- Introduction
- State space models (SSM) for deep sequence modeling
- Structured state spaces (S4) for long-term dependencies
- Experiments
- Conclusion

Conclusion

- This paper proposed a surprising sequence model S4, which can handle LRDs, and move between **continuous-time**, **convolutional**, and **recurrent** model representations, each with distinct capabilities.
- This approach enables SSMs to be applied successfully to a varied set of benchmarks with minimal modification.

Thank You for listening!

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