Universität Bremen

Center for Industrial Mathematics (ZeTeM)

Faculty 03

Mathematics / Computer science

PCA-Networks

A Model Order Reduction Approach for Operator Learning

Janek Gödeke, Nick Heilenkötter, Tom Freudenberg

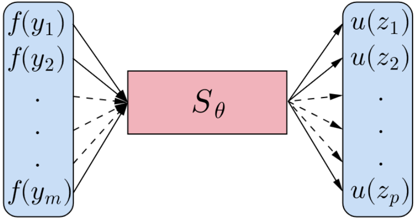
Renningen, 21.11.2025

Yesterday

One Neural Network S_θ for:

- Learning PDE-solutions u for diverse parameter functions f
- First example: solution operator $f \mapsto u$ of the problem

$$\partial_t u = f \quad \text{in } (0,1),$$
$$u(0) = 0.$$



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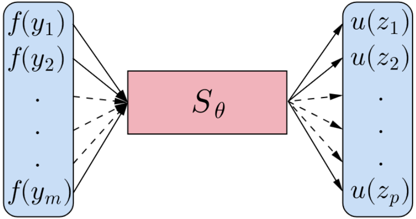

Today: PCA-Nets and FNOs
$\rightarrow$ use more information about the problem

Foundation: The Concept of a Basis

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Basis vectors

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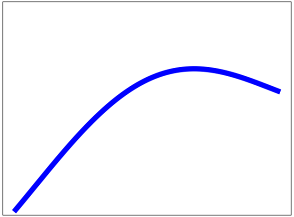
Polynomial Basis: $f(x)$



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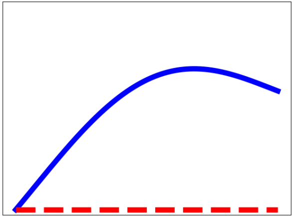

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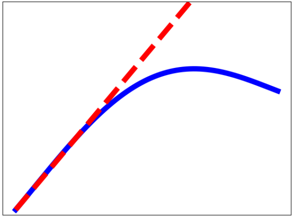

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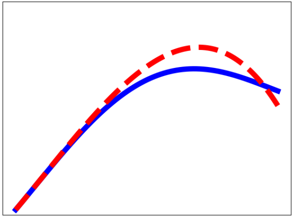

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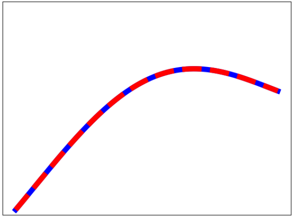

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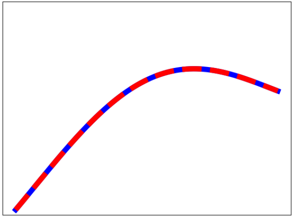
Polynomial basis:	1	x^1	x^2	x^3	$\dots$
Coefficient for f:	$f(0)$	$f'(0)$	$\frac{1}{2} f''(0)$	$\frac{1}{3!} f'''(0)$	$\dots$



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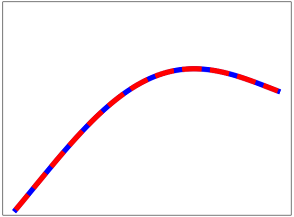
Polynomial Basis: $f(x) = f(0) \cdot 1 + f'(0)x + \frac{1}{2}f''(0)x^2 + \dots$

Fourier Basis: $f(x) = c_0 + c_1 \cos(2\pi x) + c_2 \sin(2\pi x) + \dots$



Why Bases for Functions?

Polynomial basis:	1	x^1	x^2	x^3	x^4	x^5	$\dots$
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- Given 5.000 functions f on grid of 100 points

  $\rightarrow$ Save 500.000 numbers!

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Truncated polynomial basis:	1	x^1	x^2	x^3
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Useful for compression:

- Given 5.000 functions f on grid of 100 points

  $\rightarrow$ Save 500.000 numbers!

- Use first 20 basis functions to approximate f

  $\rightarrow$ Save only *basis + coefficients* $= 20 \cdot 100 + 20 \cdot 5000 = 102.000$ numbers!

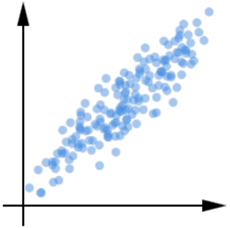
What are Good Bases?

- **Efficient compression:** Only few basis functions required
- **Computability:** Basis coefficients easy to compute
- **Noise-resilience**

Principle Component Analysis (PCA)

Given: Data functions f_j on N grid points

What is PCA?



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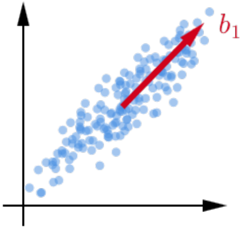

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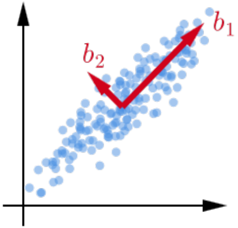

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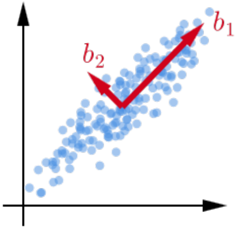

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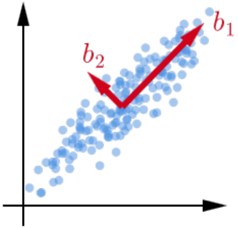

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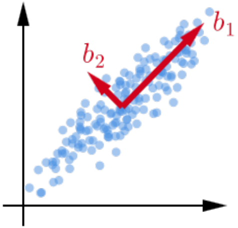

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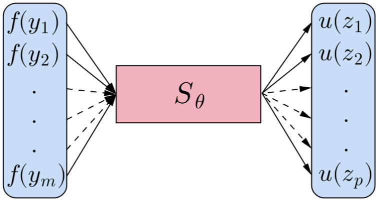
Basis coefficients easy to compute: $c_k = f \cdot b_k$

Reconstruction: $f \approx c_1 b_1 + \ldots + c_K b_K$

Benefit for Operator Learning

Reduce dimensionality of the problem:

- Given discrete input function f on a 64×64 grid
- Default FCN has $64 \cdot 64 = 4096$ input neurons



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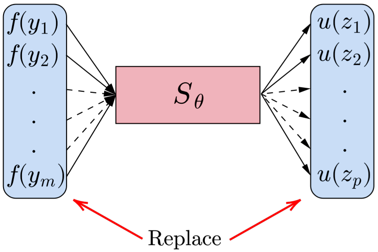

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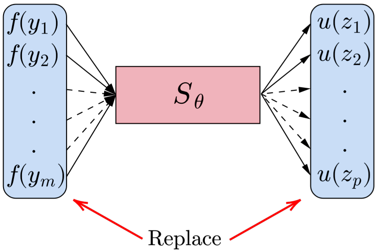
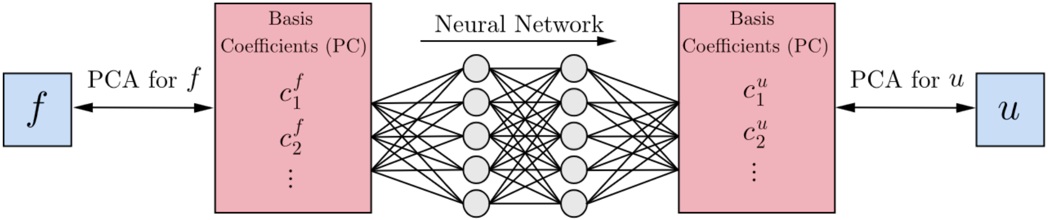
- PCA also for output u



PCA-Networks[1]



[1] Bhattacharya et al, *Model reduction and neural networks for parametric PDEs*, 2020

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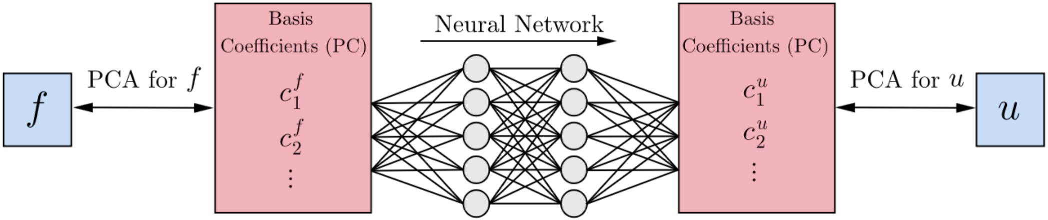

Additional advantages:

- PCA basis coeffients capture global information on f (and u)
- Reduction of noise (Exercise 7)

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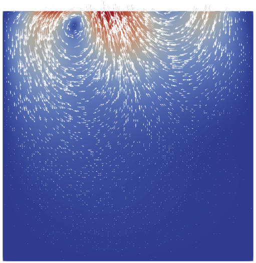
Using PCA-Networks in TorchPhysics

1. A joined exercise to see the general implementation:
   `Introduction_PCA-Nets.ipynb`
2. Solving the Stokes equations for different inflow profiles:
   `Exercise_6.ipynb`
3. Solving the inverse Allen-Cahn equation:
   `Exercise_7.ipynb`



Stokes solution