Decomposing data-fields with multiple transports using neural implicit flow

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Context

Finding low-rank structures in dynamical systems

- Derive low-rank surrogate models
  ⇝ Kolmogorov n-width problem [2]
- Separate and analyze the different components

Low-rank structures appear under certain transformations (a.k.a transports)

Applications:

- Model order reduction (e.g. wildland fire model, turbulence)
- Low-rank denoising (tomography)

sPOD: A nonlinear and low-rank decomposition

Goal: Decomposing the data $q(x,t)$ into low-rank surrogate

$$q(x,t) \approx \sum_{k=1}^{K} \mathcal{T}^k q^k(x,t).$$

where

$$q^k(x,t) \approx \sum_{r=1}^{R_k} \alpha_r^k(t)\phi_r^k(x),$$

Solution: When $\{\mathcal{T}^k\}$ are known, there exist efficient algorithm to determine $\{q^k\}$ [1].

Issues and objectives

<u>Issues:</u>
- In real-life applications, $\{\mathcal{T}^k\}$ are hard to determine
- Non-convex optimization
- Alternating optimization on $\{q^k\}$ and $\{\mathcal{T}^k\}$ fails

<u>Object:</u> Learn $\{\mathcal{T}^k\}$ and $\{q^k\}$ jointly using a dual neural network approach

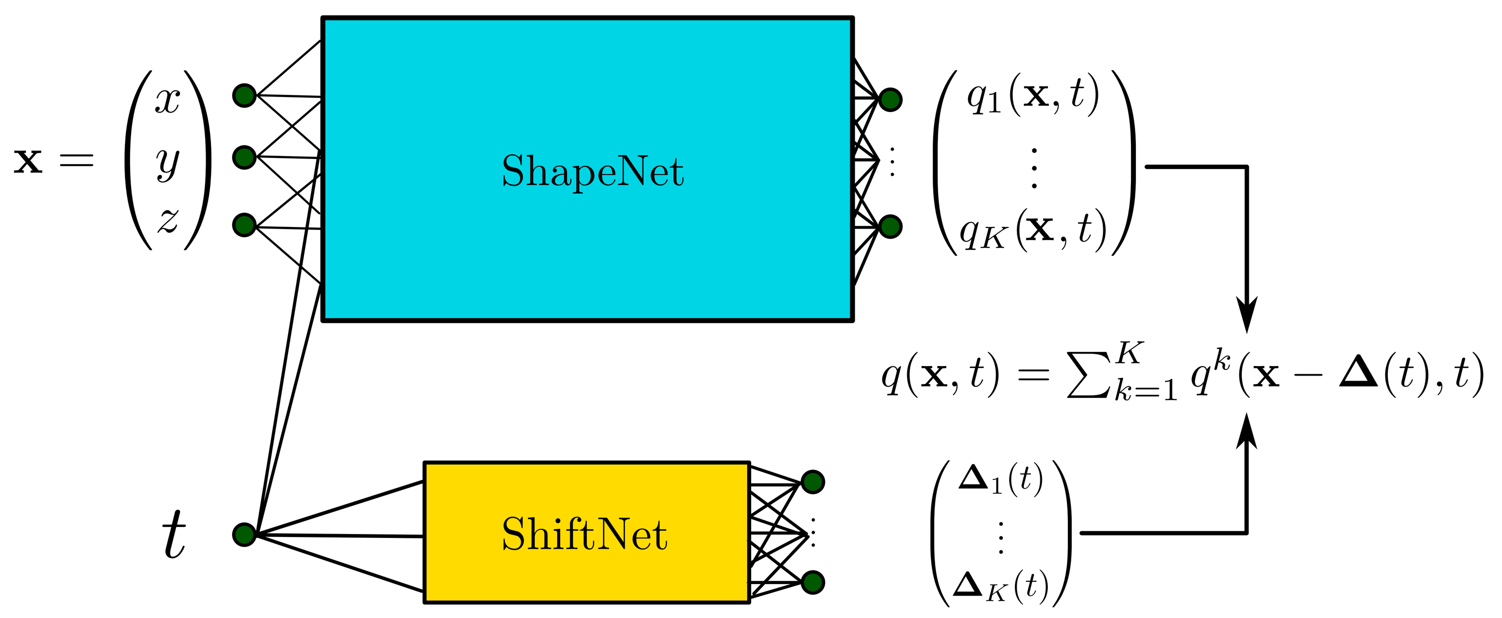
Optimization problem formulation

Minimizing the **loss function:**

$$\mathcal{L}(\{\mathbf{Q}^k\},\{\mathbf{T}^k\}) \stackrel{\text{def}}{=} \left\| \mathbf{Q} - \sum_{k=1}^{K} \mathbf{T}^k\mathbf{Q}^k \right\|_{\mathrm{F}}^2 + \lambda \sum_{k=1}^{k} \|\mathbf{Q}^k\|_* .$$

where $\mathbf{Q}^k = (q^k(x_m,t_n))_{m,n} \in \mathbb{R}^{M\times N}$ and $\mathbf{T}^k\mathbf{Q}^k = ((\mathcal{T}^k q^k)(x_m,t_n))_{m,n} \in \mathbb{R}^{M\times N}$
⇝ Discretizing the transformed data to avoid interpolation error

NsPOD: Neural sPOD using neural implicit flow



Networks = 3 Hidden fully-connected layers interleaved with ELU

Assumption: $\{\mathcal{T}^k\}$ are simple shifts $\Delta^k(t)$

Main idea: Separating spatial elements from time (or other parameters external to space)

- ShapeNet: model the output fields $\{q^k\}$ as functions of space (≈ PINNs)
- Shiftnet: model the transport $\{\mathcal{T}^k\}$ and modulate ShapeNet by changing the space parameters in ShapeNet

Training

- **Benefits of NsPOD description:**
  1. Data points = points $\{(\mathbf{x}_m, t_m, q(\mathbf{x}_m, t_m)\}$ of the discretization grid
     ⇝ Cheaper than using a full column of $\mathbf{Q}$ in the standard full discrete formulation of sPOD
     ⇝ Break the curse of dimensionality
  2. Training can be performed on points from random or irregular batches
     ⇝ Training can be performed on mesh agnostic data
- **Non-differentiable loss function**
  ⇝ Require using subgradients instead of gradients in training phase

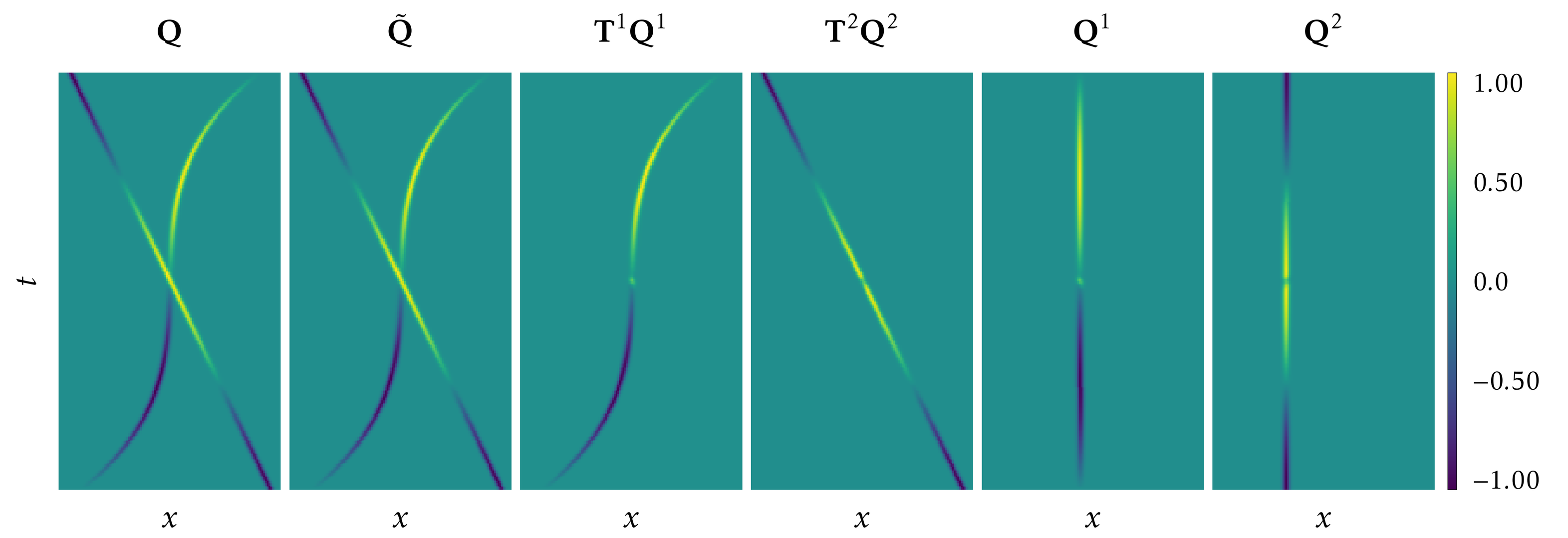
Training data are typically obtained by solving PDE or by measurements

Results

- <u>**Synthetic data:**</u> q = superposition of 2 Gaussian waves

$$q(x,t) = \sin(t) f\left(x - \Delta^1(t)\right) + \cos(t) f\left(x - \Delta^2(t)\right) \quad \text{with } f(x) = \exp(-(x-200)^2/4^2)$$

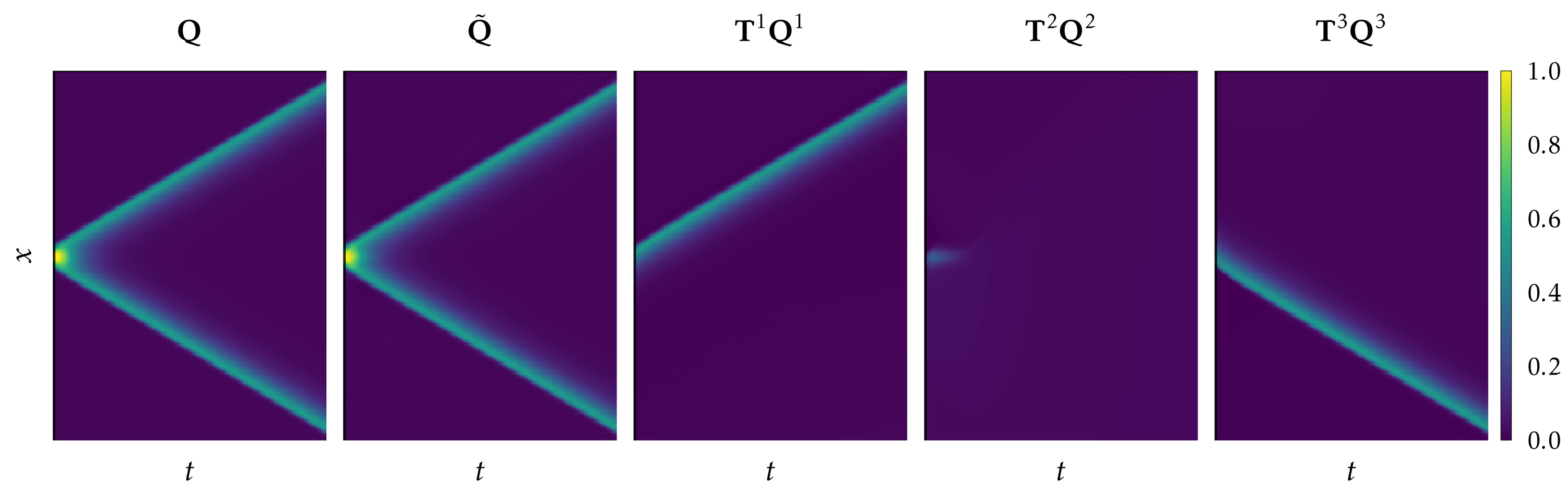
Shifts: $\Delta^1(t) = 0.15t^3 + 0.8t + 1.5$ and $\Delta^2(t) = -18t + 2$
Discretization: $M = 400$ and $N = 200$



- <u>**Wildlandfire model:**</u> q solutions of: (2 fields q ⇝ 1 for T and 1 for S)

$$\begin{cases} \partial_t T = \nabla(k\nabla T) - v\dot{\nabla} T + \alpha S r(\mu, T, T_a) - \gamma(T - T_A) \\ \partial_t S = -S\delta(T,\mu,T_a) \end{cases}$$

Discretization: $M = 500$ and $N = 500$



Conclusion

\+ Good separation capability + flexibility to the data field
\+ Continuous setting allows efficient training
\+ Do not require initialization of the shifts close to the true shifts
− NsPOD may be unstable and sensitive to initialization

Perspectives:

- Extend NsPOD to other kind of transports (not only shifts)
- Use more complex ShapeNet based on PINNs instead of fully-connected layers networks
- Demonstrate the capability of NsPOD on more complex applications and more complex discretization grids.

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References

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[2] B. Unger and S. Gugercin. Kolmogorov n-widths for linear dynamical systems, Adv Comput Math 45, 2273–2286 (2019). (doi: 10.1007/s10444-019-09701-0)

[3] B. Zorawski, S. Burela, P. Krah, A. Marmin and K. Schneider. Automated transport separation using the neural shifted proper orthogonal decomposition, ArXiV [2407.17539] (July, 2024)