Learning signals defined on graphs with optimal transport and Gaussian process regression

Raphaël Carpintero Perez

Sébastien Da Veiga
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Brian Staber

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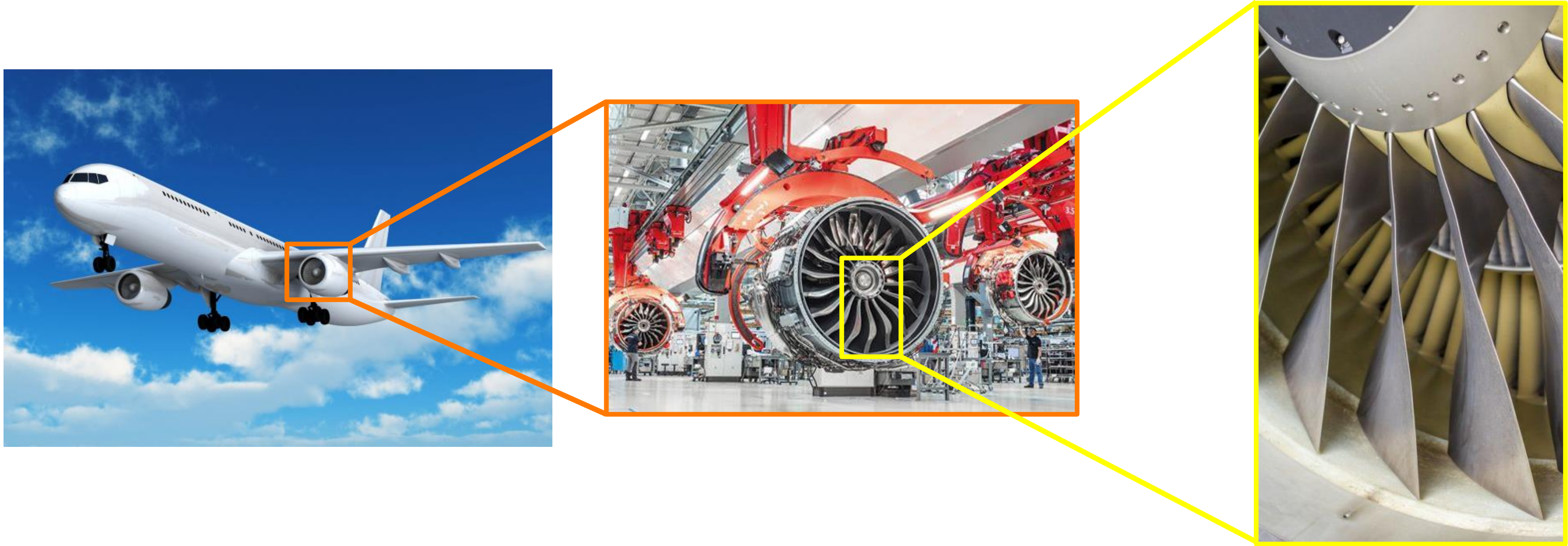
CMAP

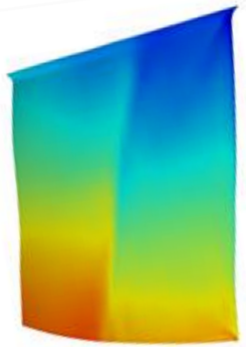
Objectives



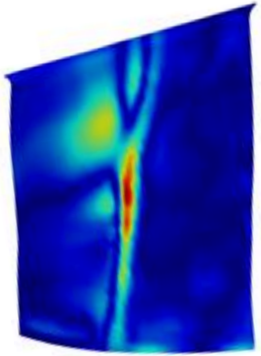
Turbine blades

Objectives

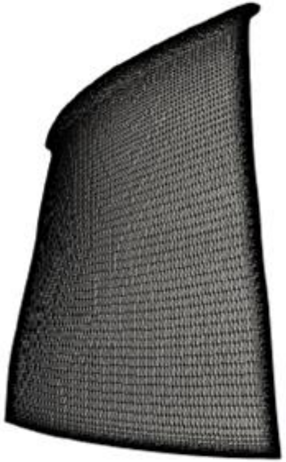
Costly numerical simulation (~4 hours)



Field



Uncertainties



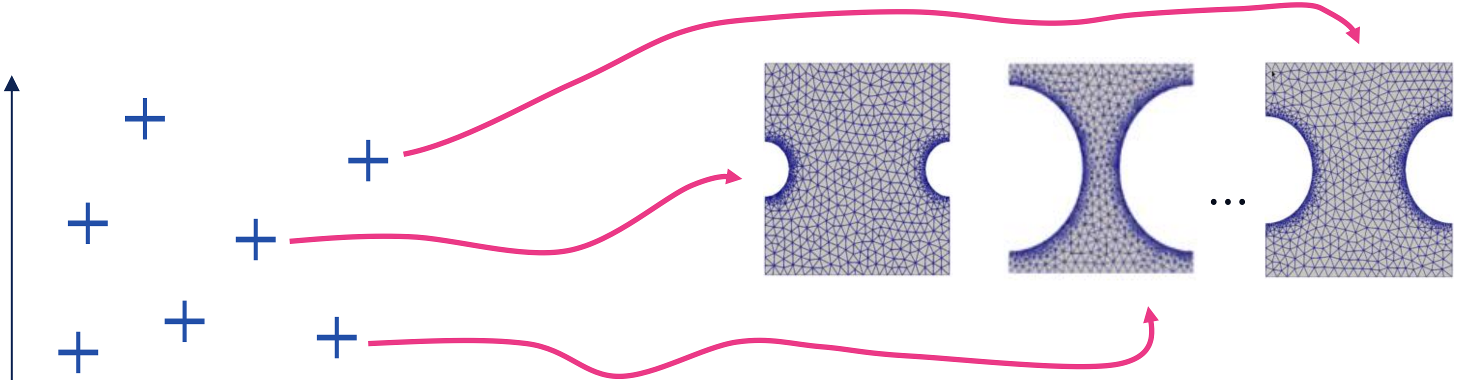
Surrogate model

Turbine blades

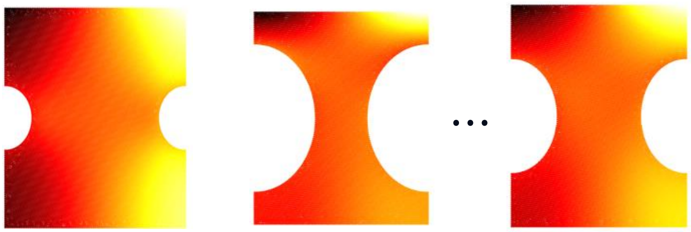
Supervised learning context

<u>Step 1</u>: Generate a design of experiments

<u>Step 2</u>: Create the meshes



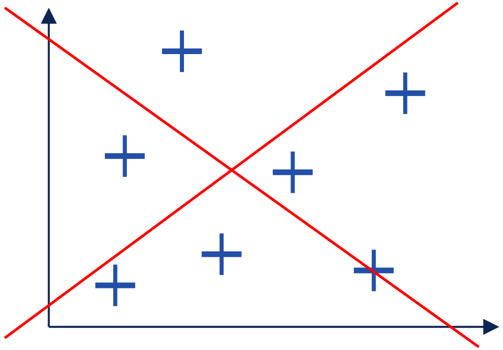
<u>Step 3</u>: Finite-element solver



c characteristic mesh parameters (curvature, cord length, $\cdots$)

b boundary/external conditions

Supervised learning context

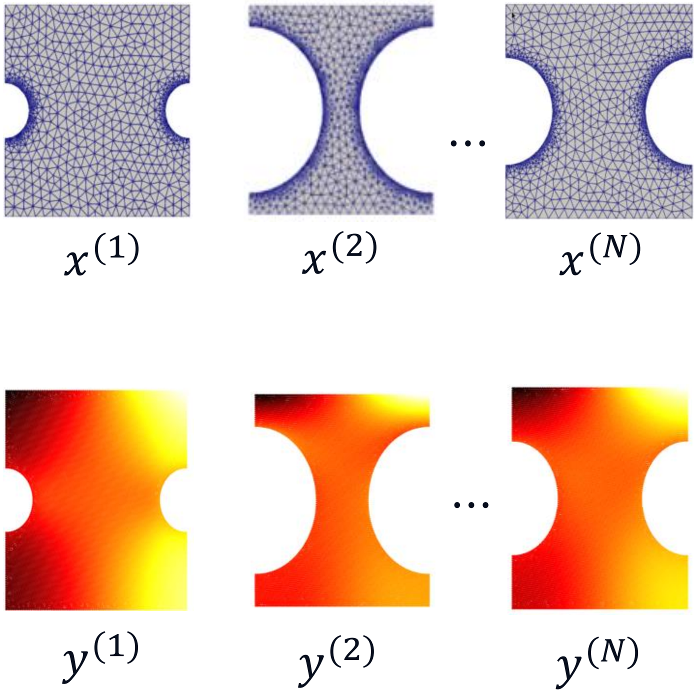


~~c characteristic mesh parameters (curvature, cord length, …)~~

b boundary/external conditions

Meshes

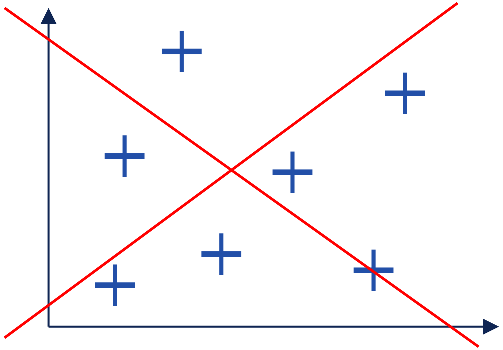
Fields



Inputs

Outputs

Supervised learning context



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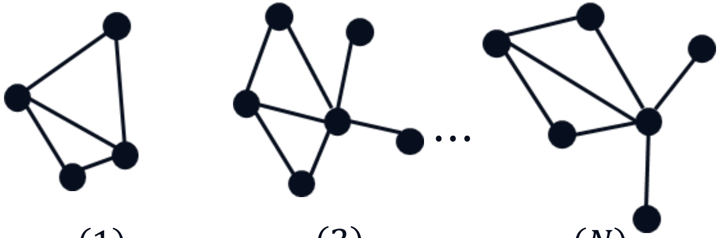
~~Meshes~~

Graphs



$x^{(1)}$ $x^{(2)}$ … $x^{(N)}$ $\in \mathcal{X}$

Inputs

<u>Step 3</u>: Finite-element solver

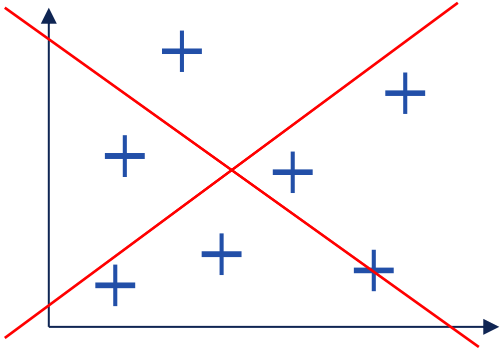
~~Fields~~

Signals

$y^{(1)}$ $y^{(2)}$ … $y^{(N)}$

Outputs

Supervised learning context



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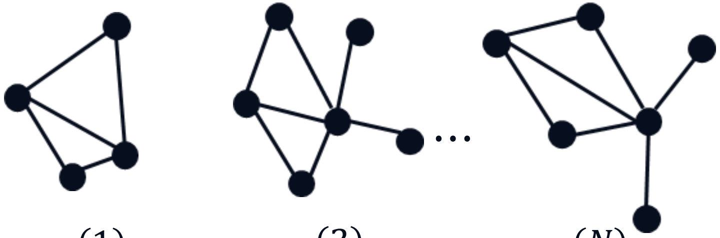
Graphs



$x^{(1)}$ $x^{(2)}$ … $x^{(N)}$ $\in \mathcal{X}$

Inputs

Scalars

$\mathbb{R}$ $\mathbb{R}$ … $\mathbb{R}$

$y^{(1)} \in \mathbb{R}$, $y^{(2)} \in \mathbb{R}$, …, $y^{(N)} \in \mathbb{R}$

Outputs

I) Scalar outputs

1- Gaussian process regression
2- SWWL graph kernel

II) Signal outputs

1- Problem statement
2- Related approaches
3- TOS-GP
4- Experiments

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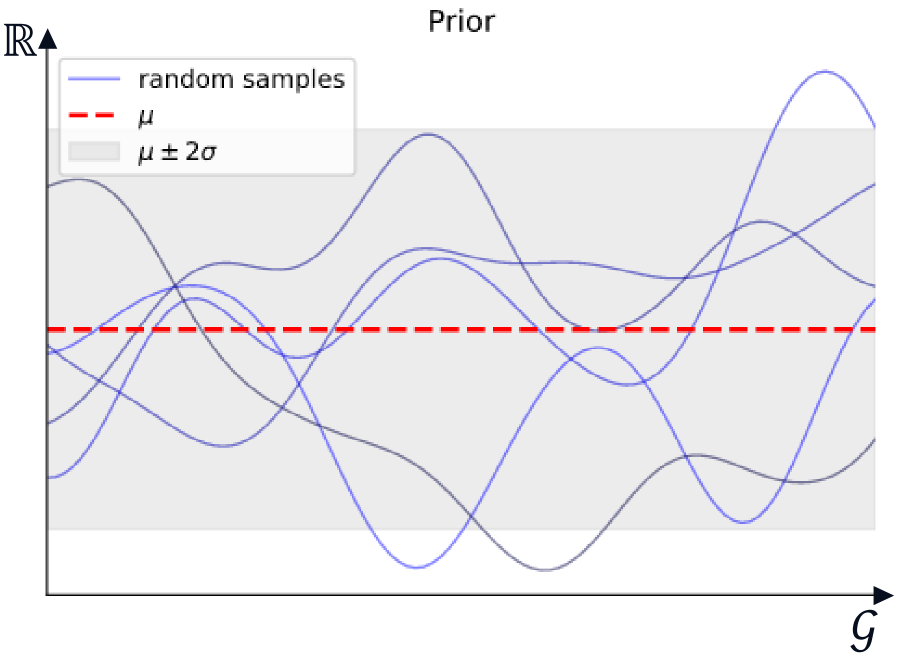
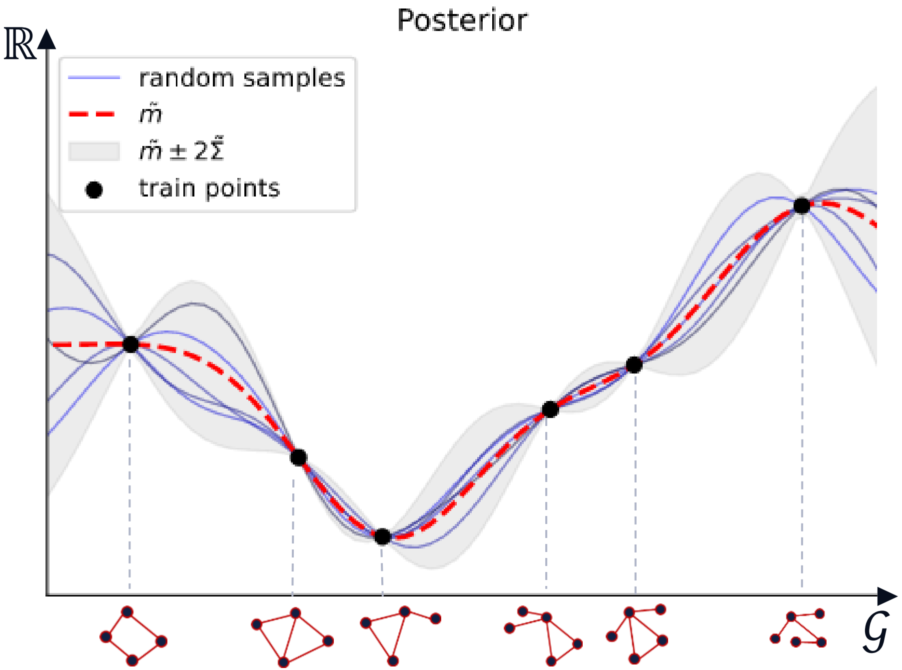
Gaussian process regression





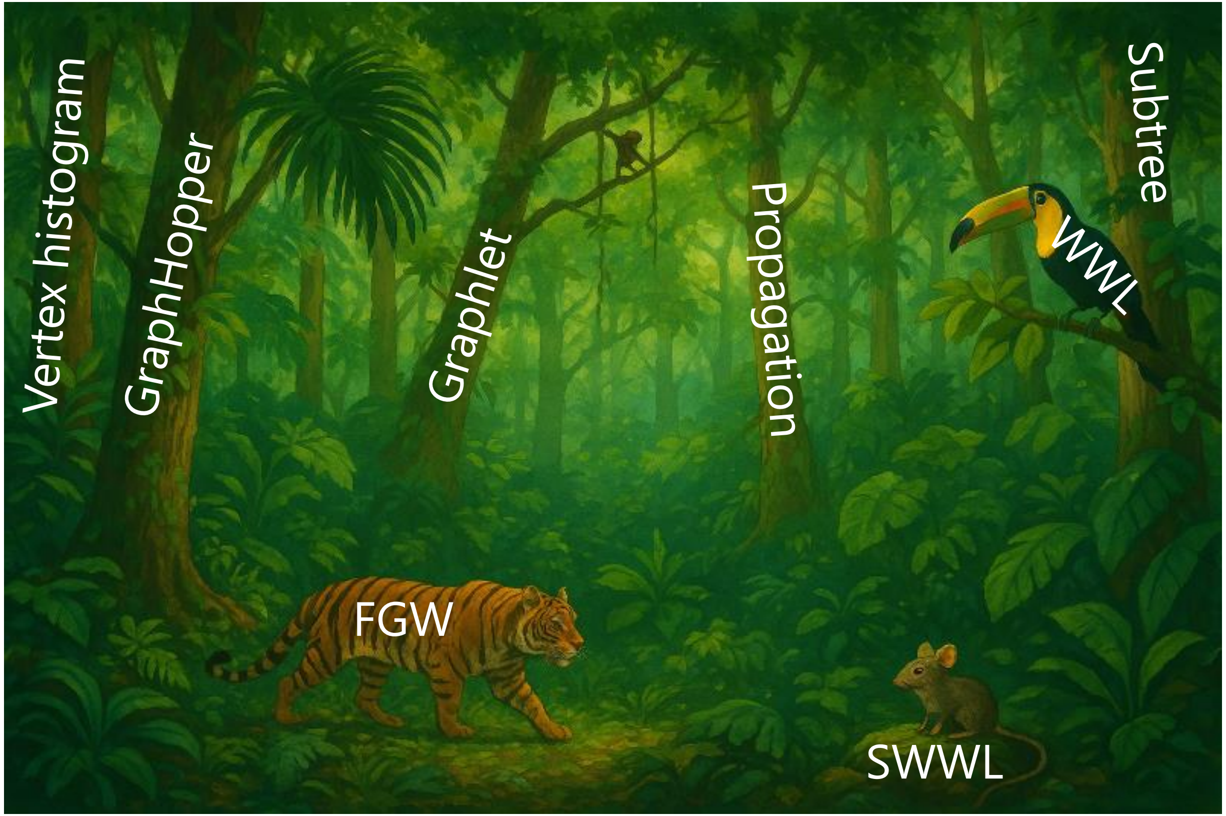
$f \sim \mathcal{GP}(\mu, k)$

$k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$?

Positive definite kernel?

$f \mid \mathcal{D} \sim \mathcal{GP}(\tilde{m}, \tilde{\Sigma})$

The kernel jungle (graph edition)



Picture generated by Chatgpt

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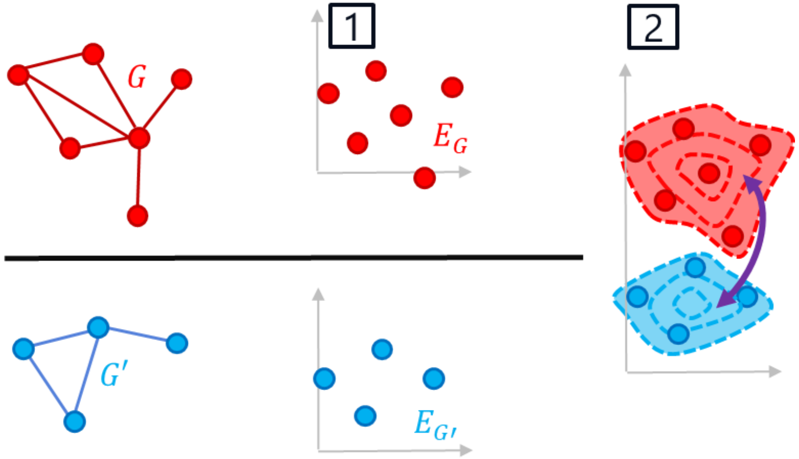
Sliced Wasserstein Weisfeiler-Lehman graph kernels

[CP, Da Veiga, Garnier, Staber, 2024]



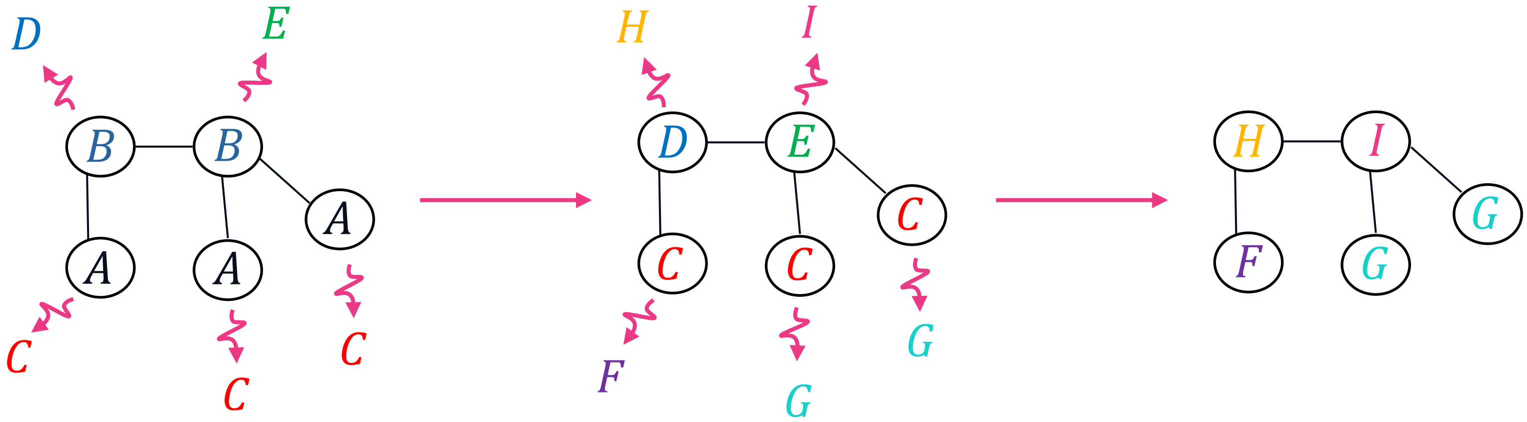
1 Embeddings of the graphs

2 Build a positive definite kernel between empirical measures

Weisfeiler-Lehman embeddings

Example from [Kriege et al., 2020]

- WL relabeling (categorical case)



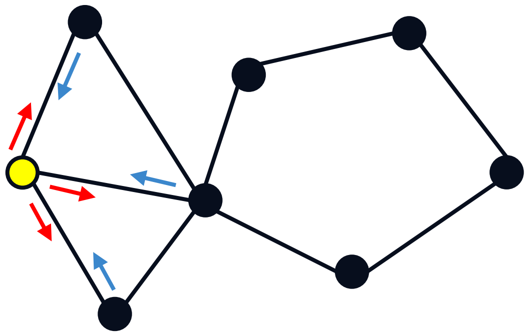
$$l^{(i+1)}(v) = Hash\left(l^i(v), \{l^i(u)\ , u \in \mathcal{N}(v)\}\right)$$

$$X_G^{(i)} = \left[l^{(i)}(v), v \in V_G\right] \qquad X_G = Concatenate(X_G^{(0)}, \cdots, X_G^{(H)})$$

Continuous Weisfeiler-Lehman embeddings

[Togninalli et al., 2019]

- WL relabeling (continuous case)



$$a^{(i+1)}(v) = \frac{1}{2}\left(a^{(i)}(v) + \frac{1}{\deg(v)} \sum_{u \in \mathcal{N}(v)} w(v,u)\, a^{(i)}(u)\right)$$

$$X_G^{(i)} = \left[a^{(i)}(v), v \in V_G\right] \qquad X_G = Concatenate(X_G^{(0)}, \cdots, X_G^{(H)})$$

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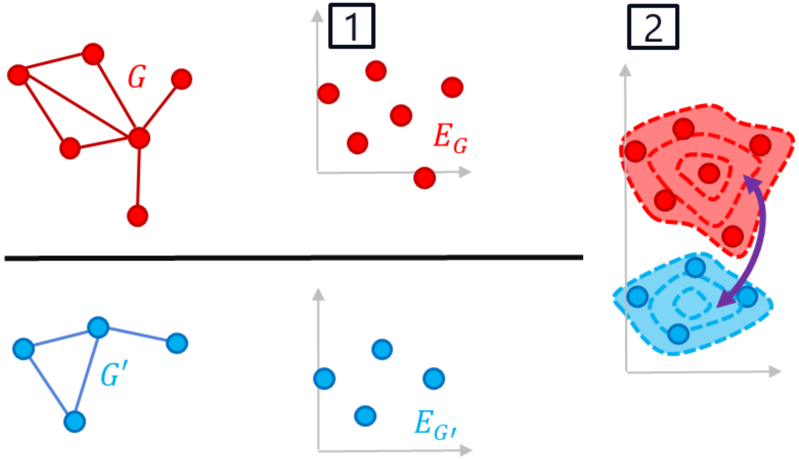
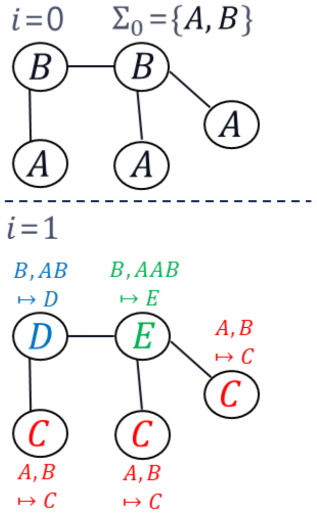
Sliced Wasserstein Weisfeiler-Lehman graph kernels

[CP, Da Veiga, Garnier, Staber, 2024]



1 Embeddings of the graphs



Continuous WL embeddings

2 Build a positive definite kernel between empirical measures

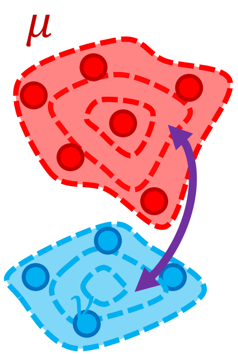
Wasserstein distance

Wasserstein distance

$$\mathcal{W}^2(\mu,\nu) = \inf_{\gamma\in\Pi(\mu,\nu)} \int_{\mathbb{R}^s\times\mathbb{R}^s} \|x-y\|^2 d\gamma(x,y),$$

Where:

- $s \in [1,+\infty)$,
- $\mathcal{P}_2(\mathbb{R}^s)$: probability measures on $\mathbb{R}^s$ with finite moments of order 2,
- $\Pi(\mu,\nu) = \{\pi \in \mathcal{P}_2(\mathbb{R}^s \times \mathbb{R}^s): \ (Proj_1)_{\#\pi} = \mu, \ (Proj_2)_{\#\pi} = \nu\}$



- ✗ $\mathcal{O}(\boldsymbol{n^3 \log(n)})$
- ✗ Substitution kernels are not positive definite in dimension $s \geq 2$

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Sliced Wasserstein distance

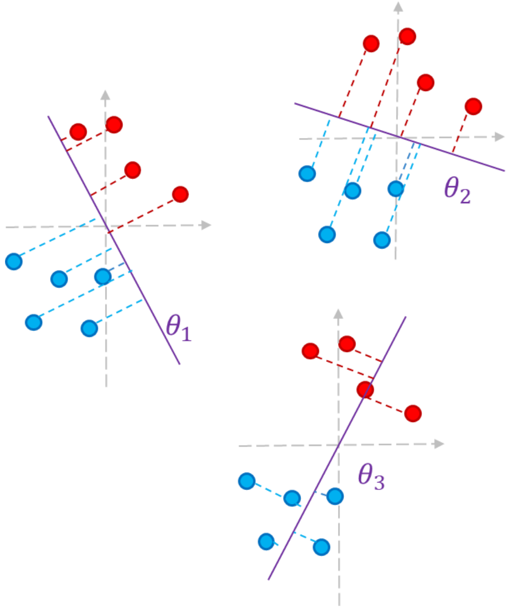
Sliced Wasserstein distance

[Bonneel et al. 2015]

$$\mathcal{SW}^2(\mu,\nu) = \int_{\mathbb{S}^{s-1}} \mathcal{W}^2(\theta^*_\#\mu, \theta^*_\#\nu)\mathrm{d}\sigma(\theta)$$

Where:

- $\mathbb{S}^{s-1}$: $(s-1)$-dimensional unit sphere,
- σ : uniform distribution on $\mathbb{S}^{s-1}$
- $\theta^*_\#\mu$: push-forward measure of $\mu \in \mathcal{P}_2(\mathbb{R}^s)$ by $\theta^*\begin{pmatrix} \mathbb{R}^s \to \mathbb{R} \\ x \mapsto \langle\theta, x\rangle \end{pmatrix}$



✓ Complexity: scales as $\boldsymbol{n}\,\mathbf{log}(\boldsymbol{n})$

✓ Positive definite substitution kernels

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Sliced Wasserstein distance

Sliced Wasserstein distance [Bonneel et al. 2015]

$$\mathcal{W}^2(\theta^*_{\#}\mu, \theta^*_{\#\nu}) = \int_0^1 |F^{-1}(\mu) - F^{-1}(\nu)|^2 \, \mathrm{d}t$$

Quantile function

Where:
- $\mathbb{S}^{s-1}$: $(s-1)$-dimensional unit sphere,
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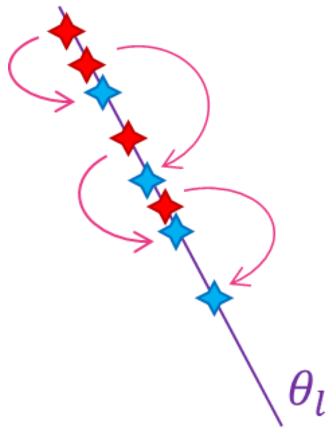

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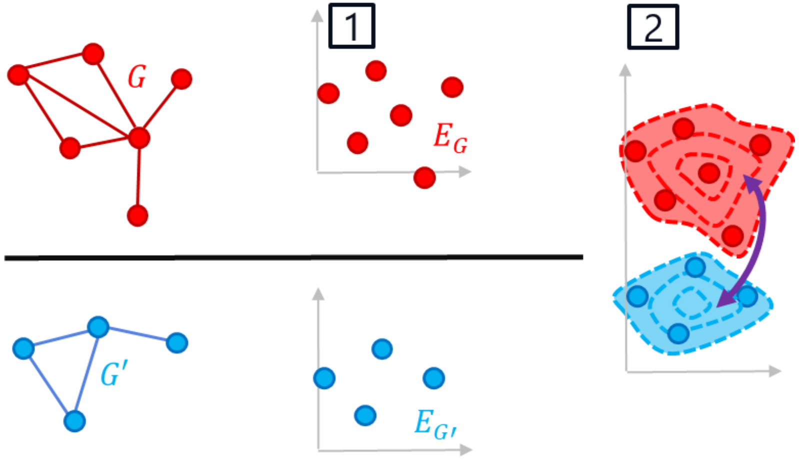

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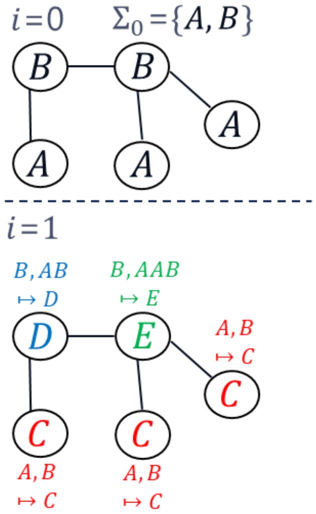
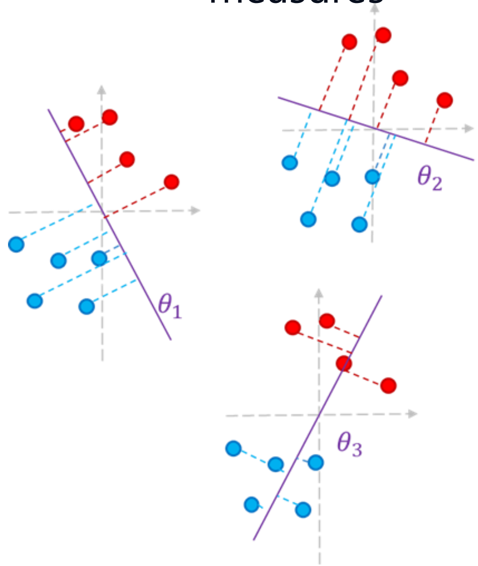
$\boxed{1}$ Embeddings of the graphs



Continuous WL embeddings

$\boxed{2}$ Build a positive definite kernel between empirical measures



Sliced Wasserstein

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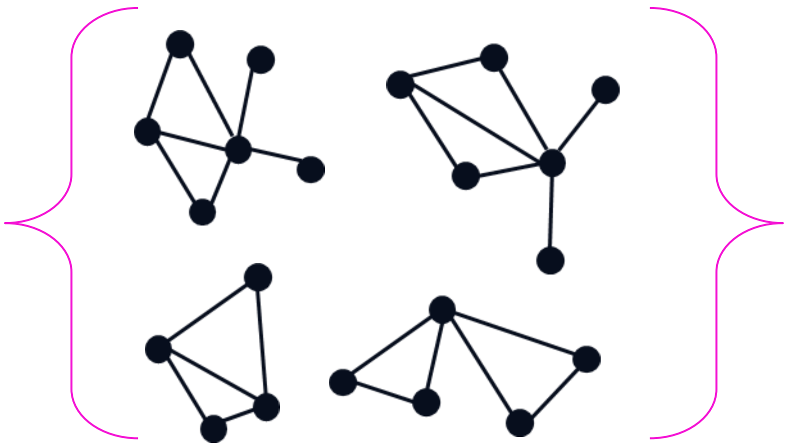
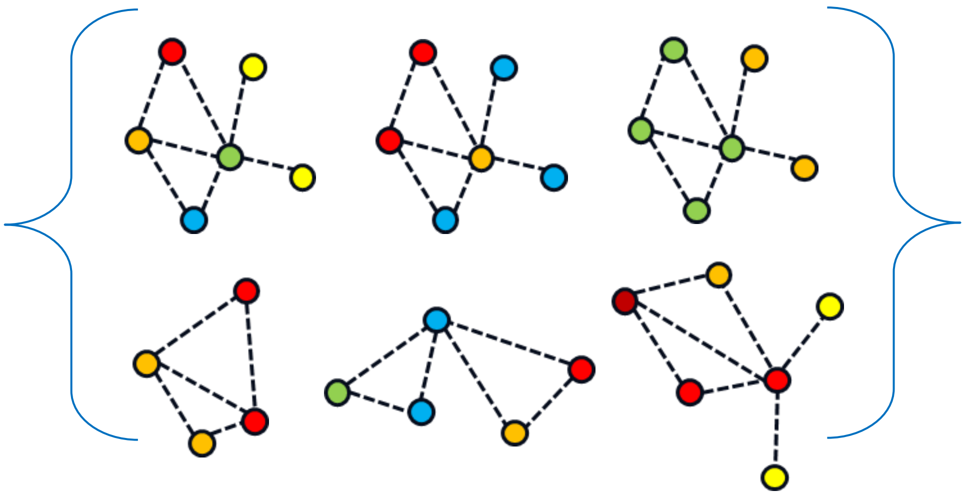
Learning output fields/signals

Learn $f : \mathcal{X} \to \mathcal{Y}$ from a train dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)})\}_{i=1,\cdots,N}$





$$\mathcal{Y} = \bigcup_{x=(V,E,w,F)\in\mathcal{X}} \{y: V \to \mathbb{R}\}$$

Learning output fields/signals

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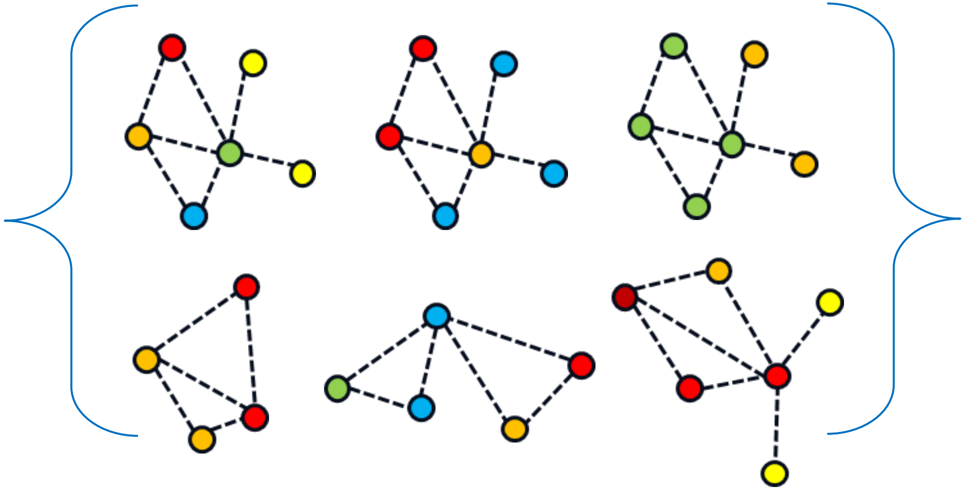
- Inputs can have different sizes, so do the outputs
- No natural ordering of the output scalar elements
- The number of output elements can be very large



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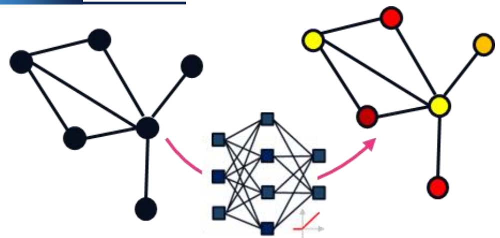
Related approaches



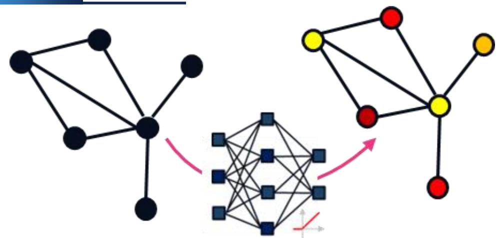
Graph Neural Networks

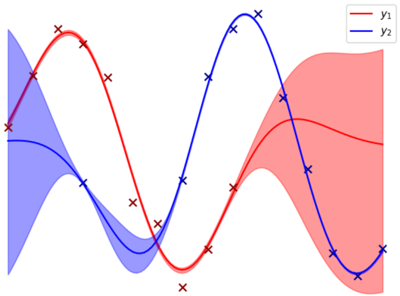
✓ Signal prediction [Pfaff, 2020]

✗ No uncertainties

✗ Training time

Related approaches





Graph Neural Networks
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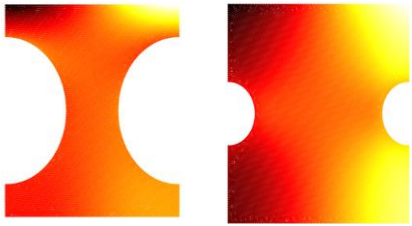
Multi/Functional Output GPs
- ✗ No ordering of the output elements
- ✗ Varying domains [Goovaerts, 1997]



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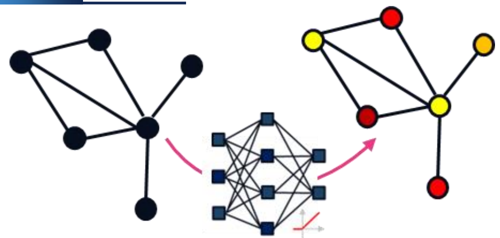

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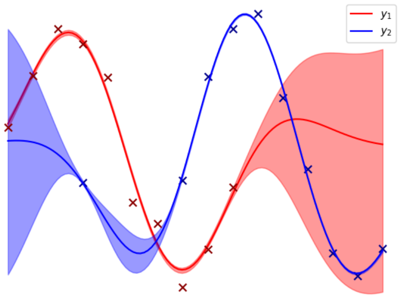

Multi/Functional Output GPs

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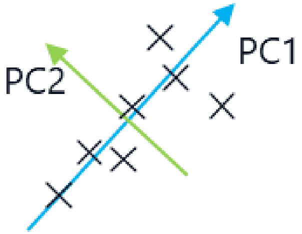

Dimension reduction

- ✗ No ordering of the output elements [Kontolati, 2022]

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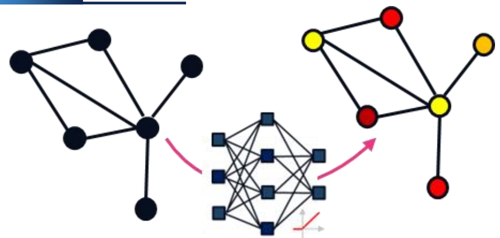
Related approaches



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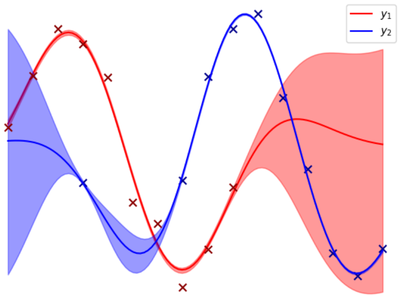

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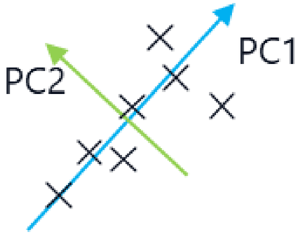

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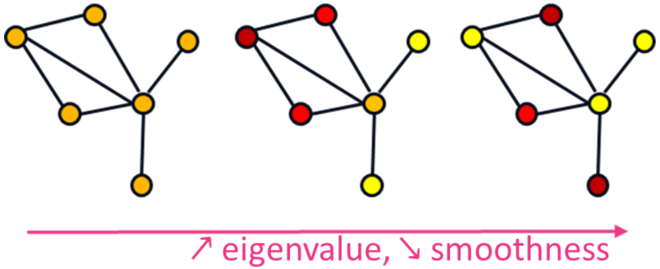

Graph signal processing [Ortega, 2018]

- ✘ Incomparable eigendecompositions

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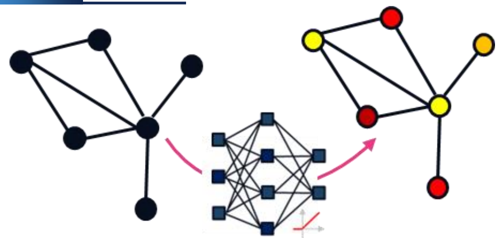
Related approaches



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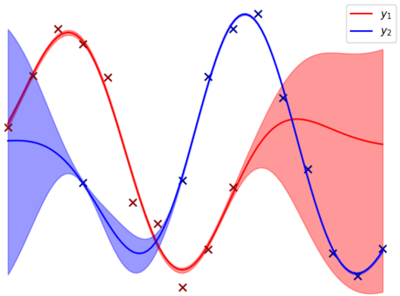

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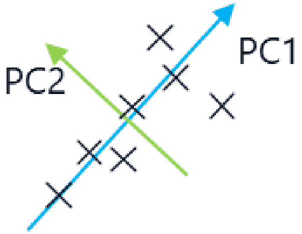

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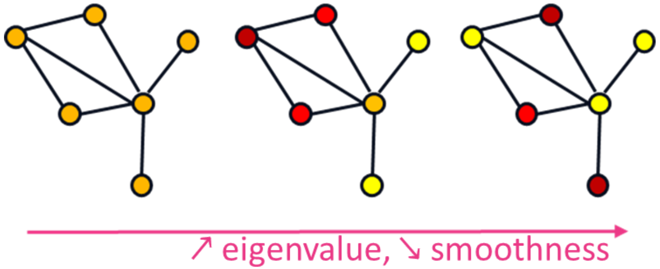

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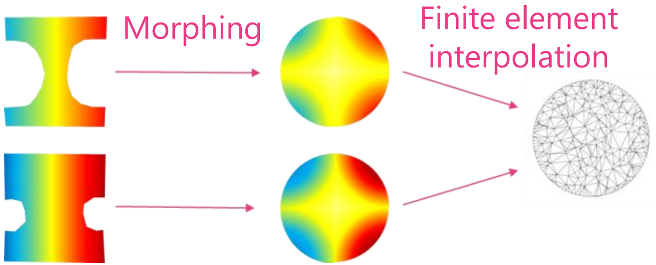

Mesh Morphing Gaussian Processes

✓ Prediction + uncertainties [Casenave, 2024]

✗ Specific to meshes + same topology

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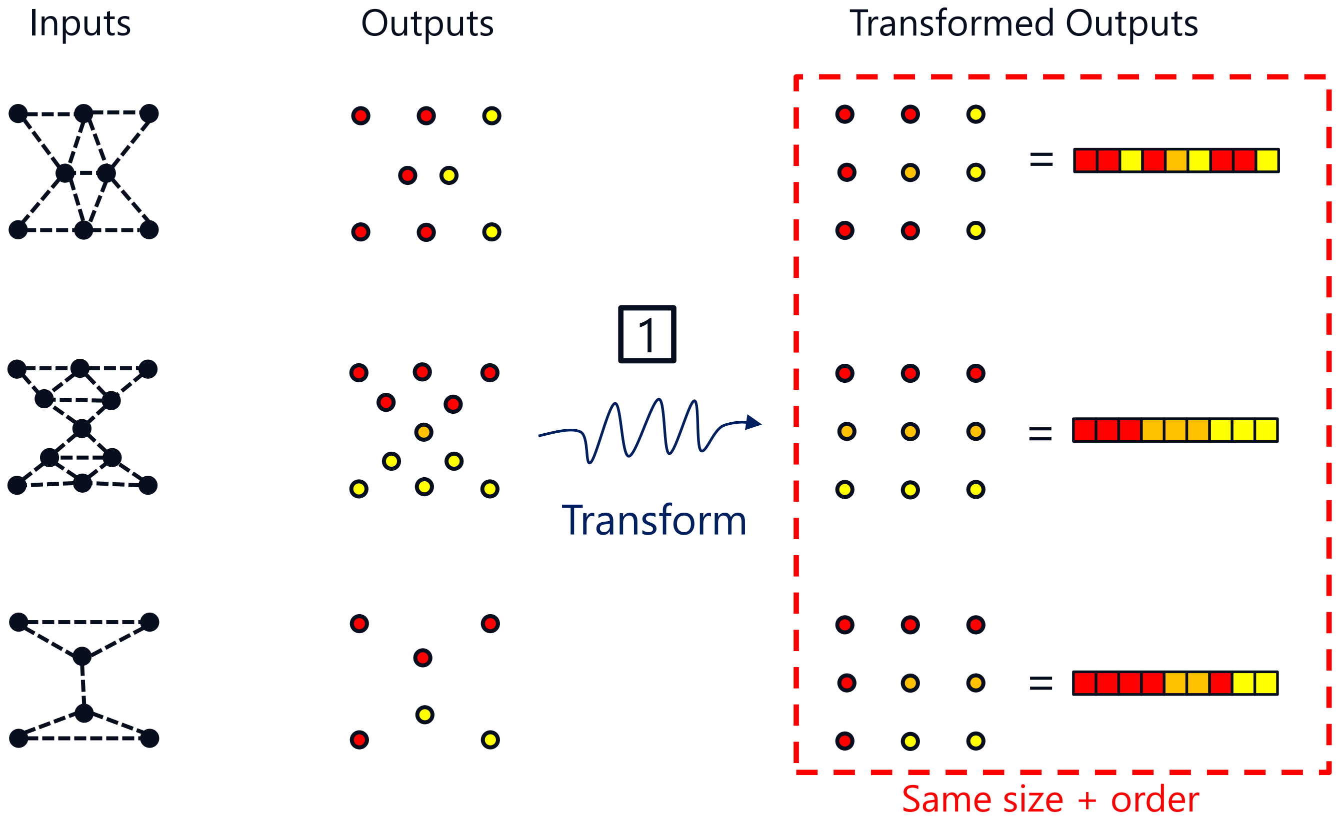
Express signals/fields in the same space?



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Wasserstein distance

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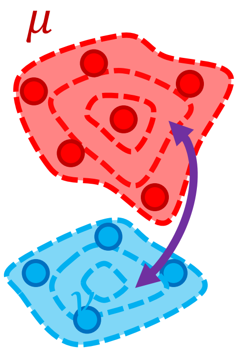

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Wasserstein distance

Wasserstein distance (discrete case)

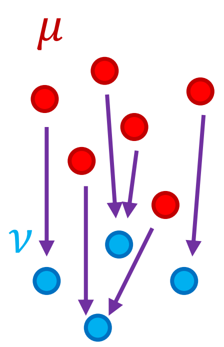
$$\mathcal{W}^2(\mu,\nu) = \min_{P \in U(n,n')} \langle C^{\mu,\nu}, P \rangle$$

Transport plan

Cost matrix

Where:

- $\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i} \qquad \nu = \frac{1}{n'}\sum_{i=1}^{n'} \delta_{z_i}$
- $U(n,n') = \left\{ P \in \mathbb{R}_+^{n \times n'} : P\mathbb{1}_{n'} = \frac{1}{n}\mathbb{1}_n, P\mathbb{1}_n = \frac{1}{n'}\mathbb{1}_{n'} \right\}$
- $C^{\mu,\nu} = \left[\left\| x_i - z_j \right\|^2 \right]_{i=1\dots n,\ j=1\dots n'}$



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Wasserstein distance

Regularized Wasserstein distance

[Peyré & Cuturi, 2019]

$$\mathcal{W}_\lambda^2(\mu,\nu) = \min_{P\in U(n,n')} \langle C^{\mu,\nu}, P\rangle - \lambda H(P), \quad \lambda > 0$$

Entropic regularization

$$L_\lambda(\mu,\nu,P) = \langle C^{\mu,\nu}, P \rangle - \lambda H(P)$$

$$\boxed{P_\lambda = \underset{P\in U(n,n')}{argmin}\ L_\lambda(\mu,\nu,P)}$$

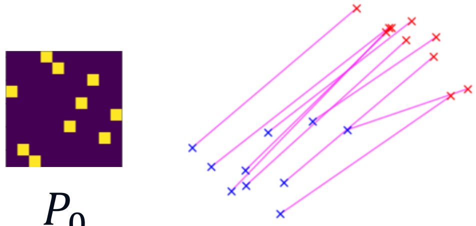
Smoothed transport plan

✓ Smoothing of the transport plans

✓ Sinkhorn: $O(n^2 \log(n))$

1- Without regularization

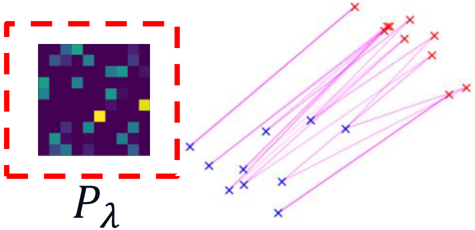
$\lambda = 0$



P_0

2- With regularization

$\lambda > 0$



P_λ

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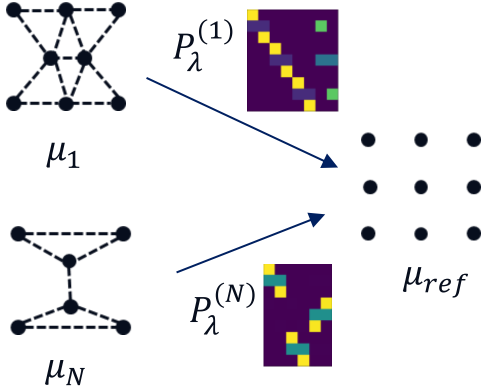
Transferring fields with transport plans

Part 1: getting transport plans (**input** space)

μ_{ref}: reference measure of size n_{ref}

$$\mu_i = \frac{1}{n_i}\sum_{j=1}^{n_i} \delta_{[\phi_{WL}(G^{(i)})]_j}$$: WL embeddings of input graph i

$$P_\lambda^{(i)} = \underset{P \in U(n_i, n_{ref})}{argmin} \; L_\lambda(\mu_i, \mu_{ref}, P) \in \mathbb{R}^{n_i \times n_{ref}}$$



Transferring fields with transport plans

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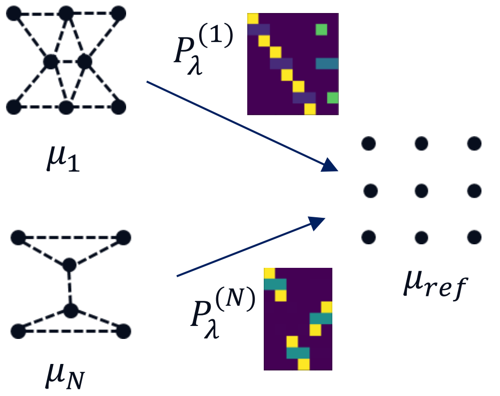
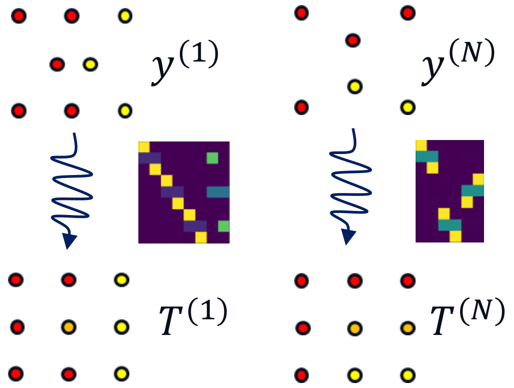
Part 2: transferring **output** signals

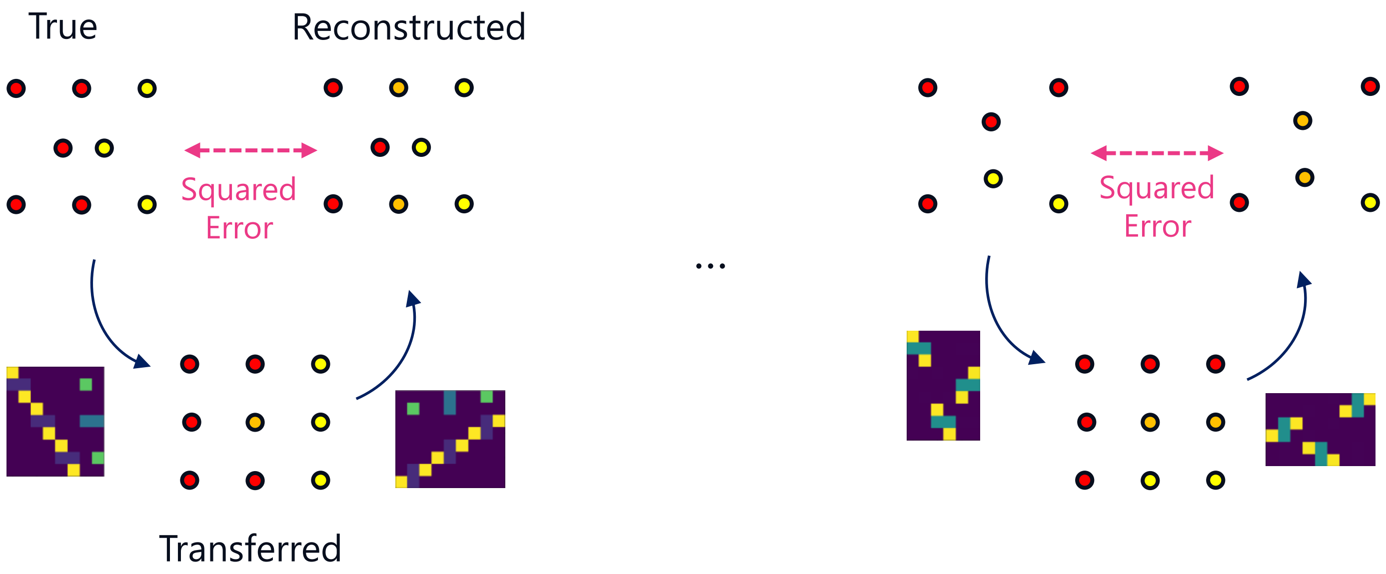
$$T^{(i)} = \left(n_{ref} P_\lambda^{(i)}\right)^{\mathsf{T}} y^{(i)} \in \mathbb{R}^{n_{ref}}$$ Transferred field

$$\tilde{y}^{(i)} = \left(n_i P_\lambda^{(i)}\right) T^{(i)} \in \mathbb{R}^{n_i}$$ Reconstructed field





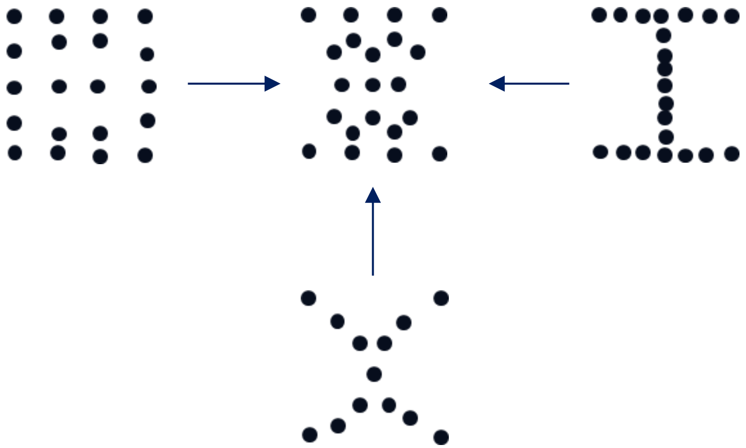
How to choose the regularization parameter ?



Choose $\lambda > 0$ that minimizes the error (RRMSE) between
- the **train** output fields and
- the **train** reconstructed fields

How to choose a reference measure ?

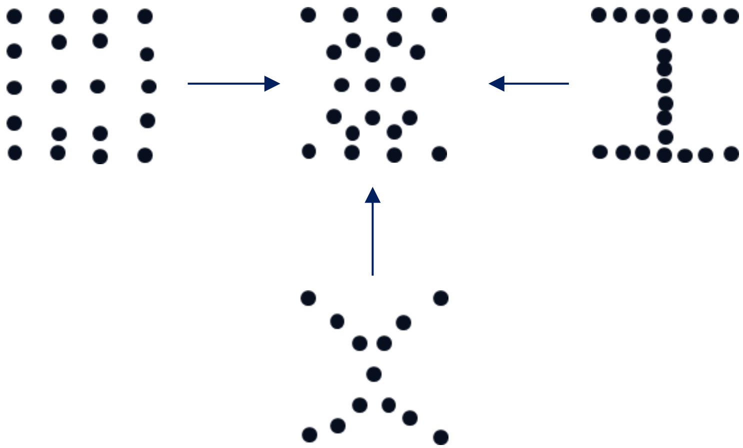
1) Optimal transport barycenter:



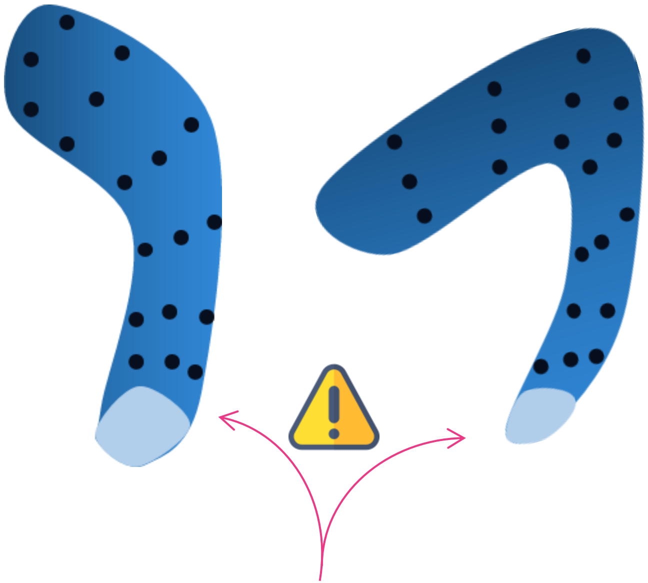
Barycenter of all train measures

How to choose a reference measure ?

1) Optimal transport barycenter:



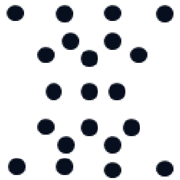
Barycenter of all train measures



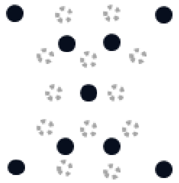
Discretizations of manifolds

How to choose a reference measure ?

2) Subsample from a train measure:

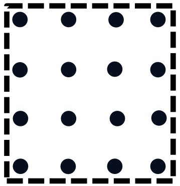


One train measure

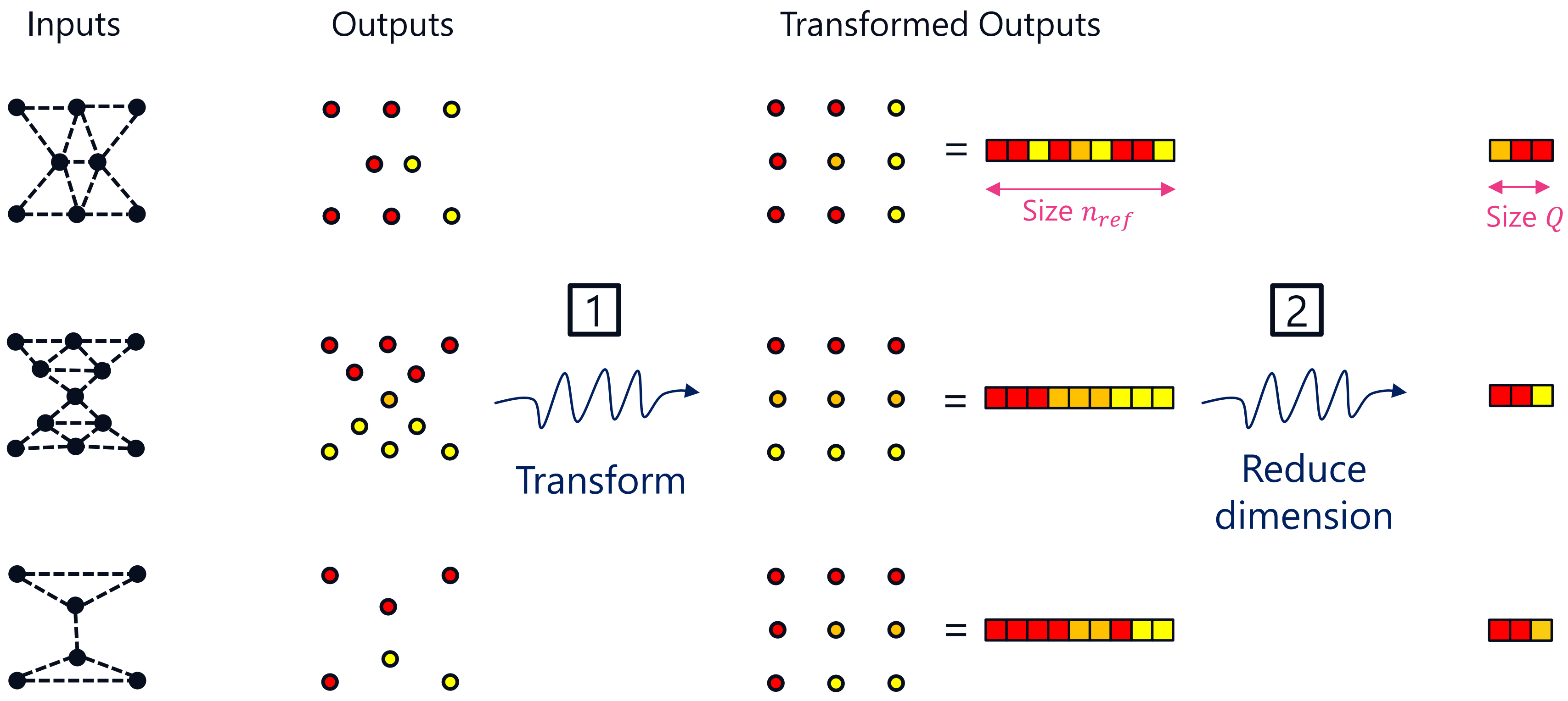


subsampled

3) Uniform grid on a reference shape:



Express signals/fields in the same space?



Dimension reduction (in practice)

Principal component analysis

[Kontolati 2022]

$$\boldsymbol{T} = (T^{(1)}, \cdots, T^{(N)}) \in \mathbb{R}^{N \times n_{ref}}$$

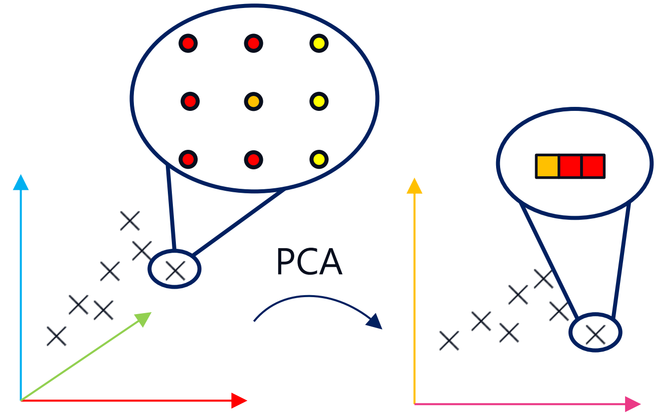
$\overline{\boldsymbol{T}} = \boldsymbol{T}$ centered

$$\frac{1}{N}\overline{\boldsymbol{T}}^{\top}\overline{\boldsymbol{T}} = E Diag(\lambda_1, \cdots, \lambda_Q) \mathrm{E}^{\top}$$

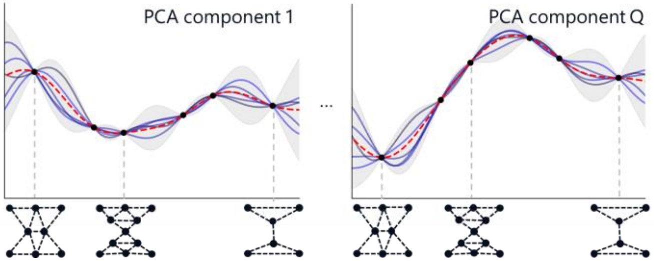
$\lambda_1 \leq \cdots \leq \lambda_Q$: eigenvalues

$\mathrm{E} \in \mathbb{R}^{n_{ref} \times Q}$: eigenvectors

Q first PCA coefficients: $C = \boldsymbol{T}E \in \mathbb{R}^{N \times Q}$



Learn Q independent GPs using SWWL graph kernels for the inputs



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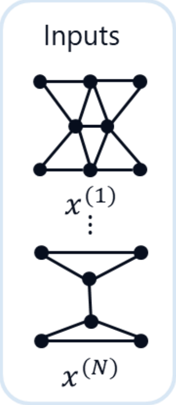
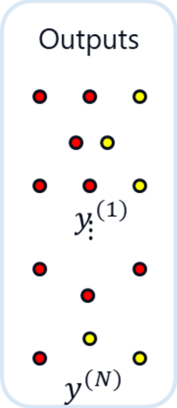
TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]

Train

Test





TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]

TOS-GP: Transported Output Signal Gaussian Processes

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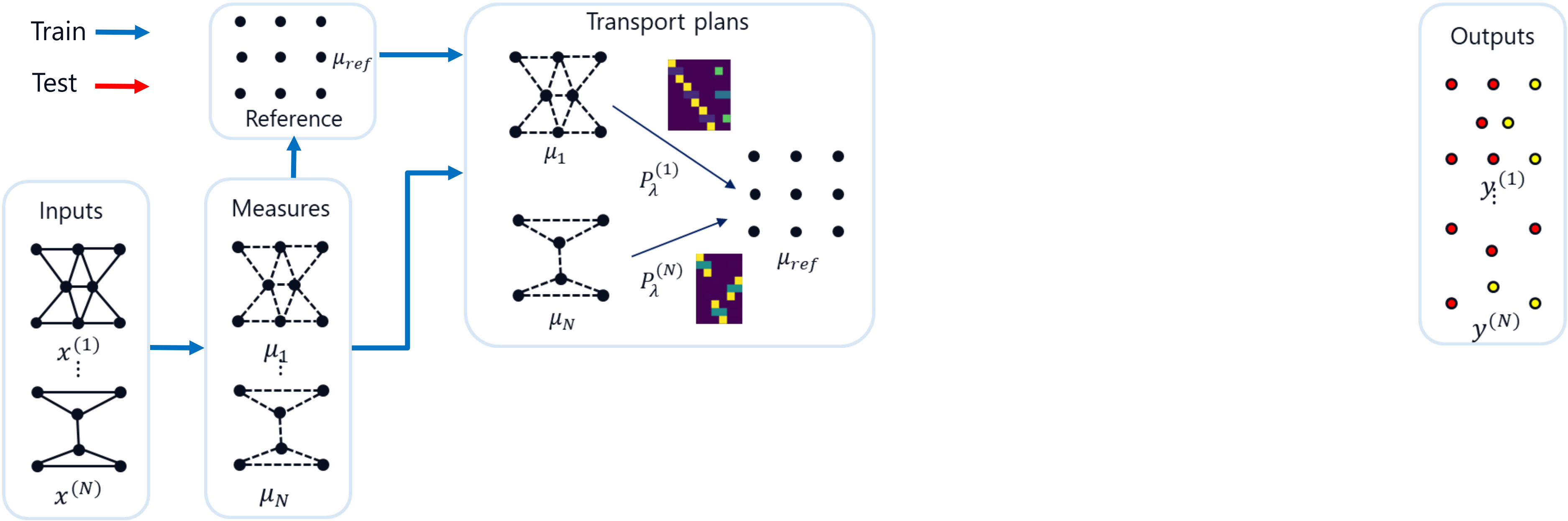

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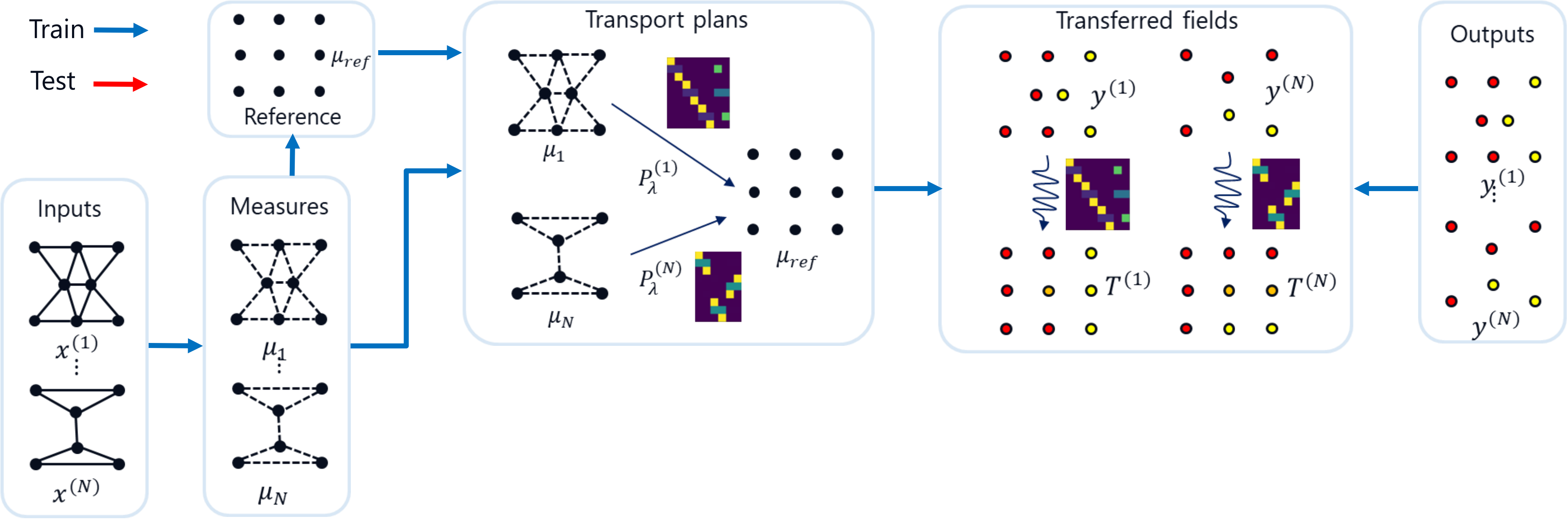
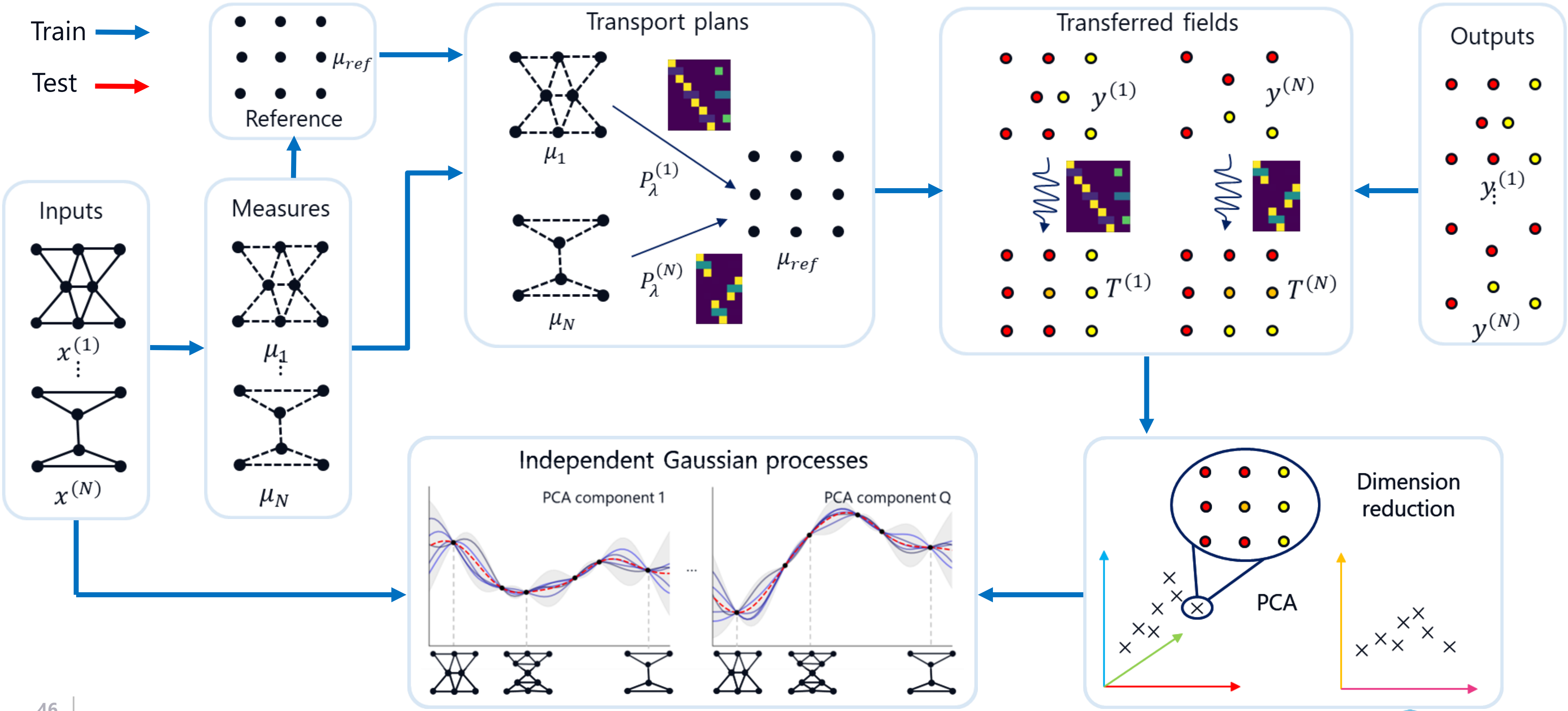
TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]



TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]



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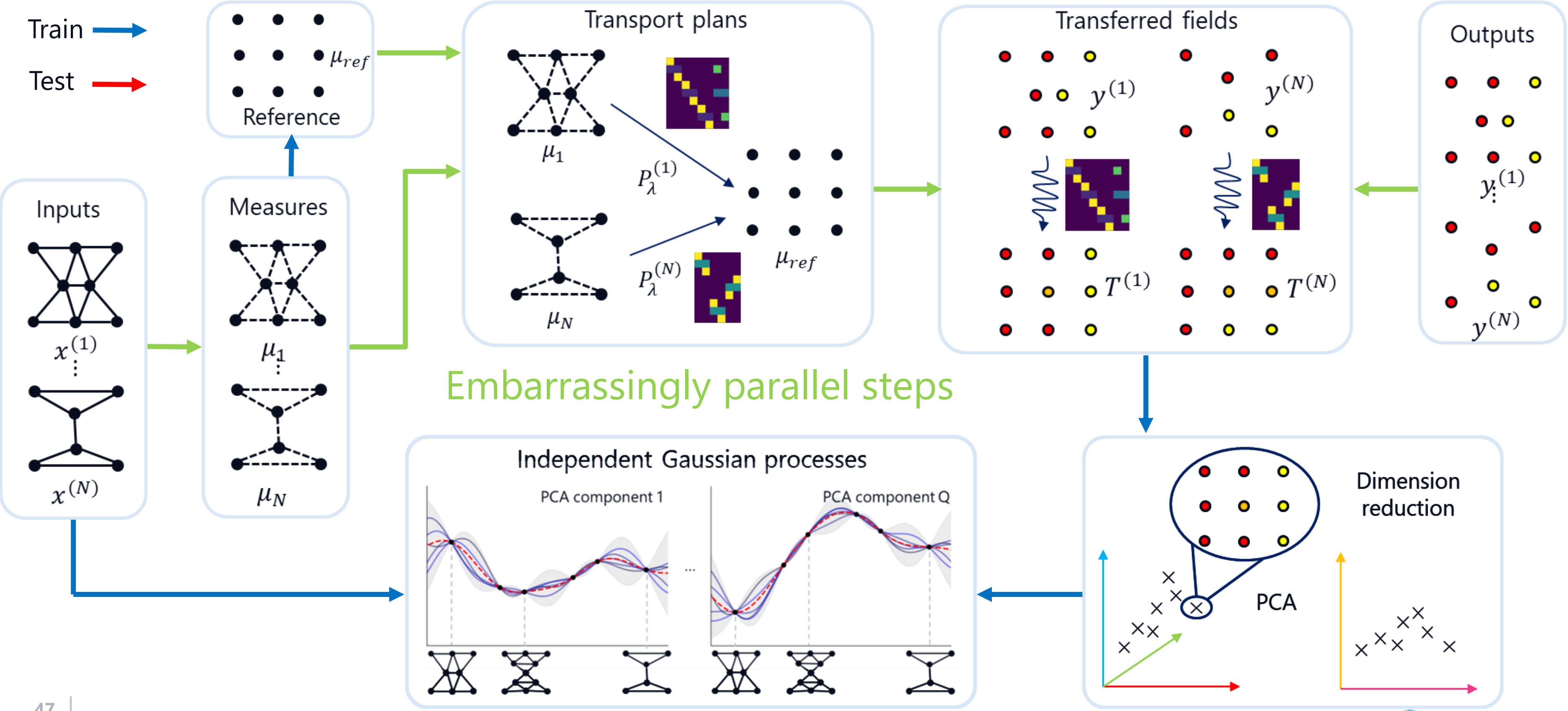
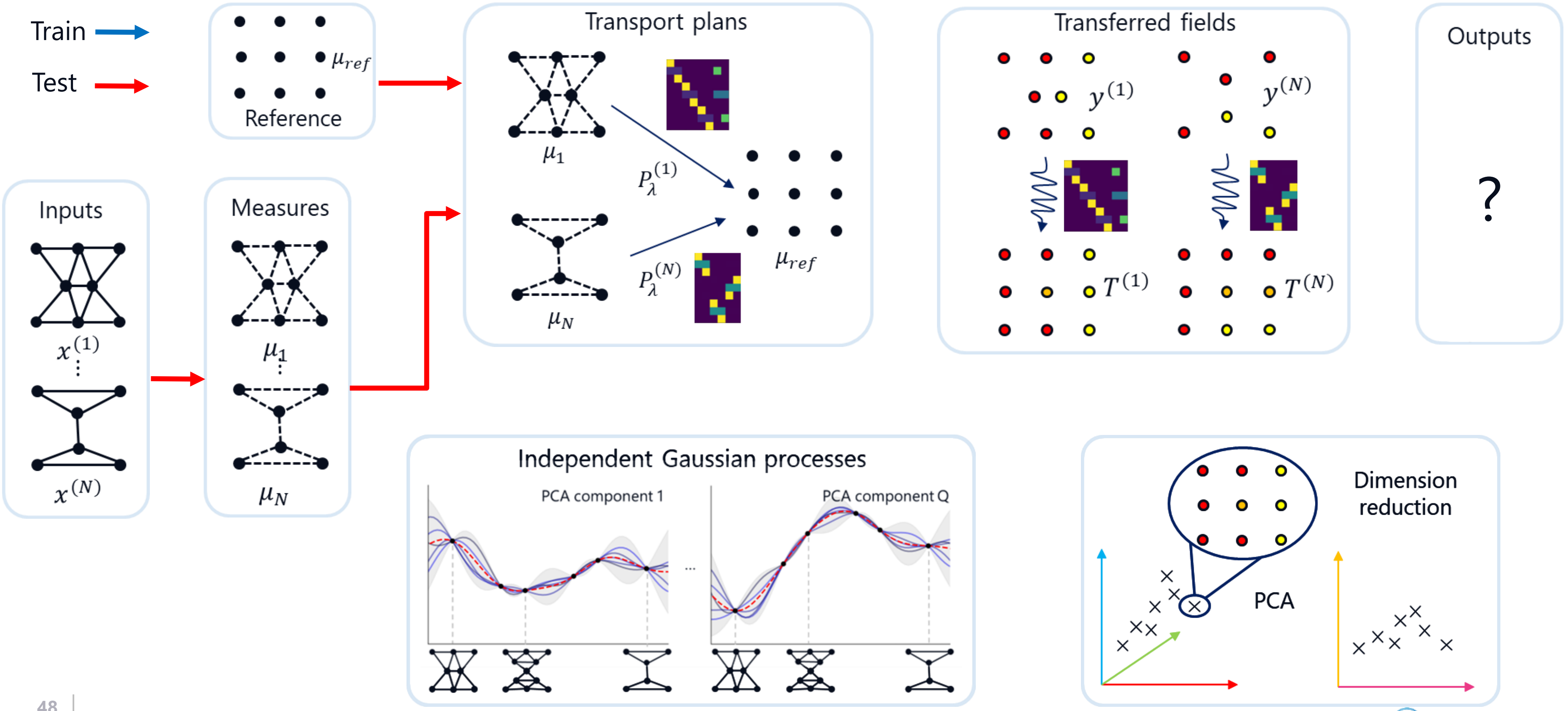
TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]



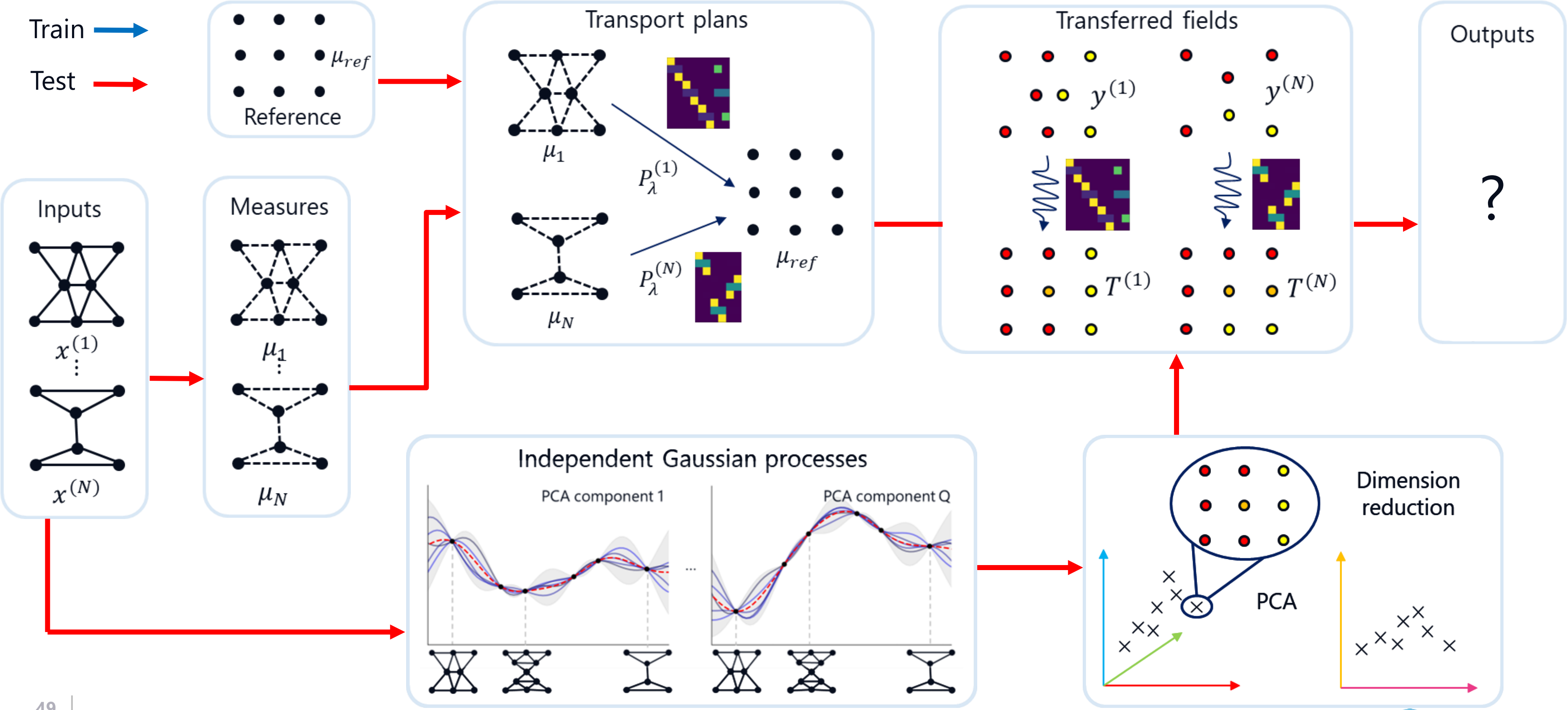
TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]



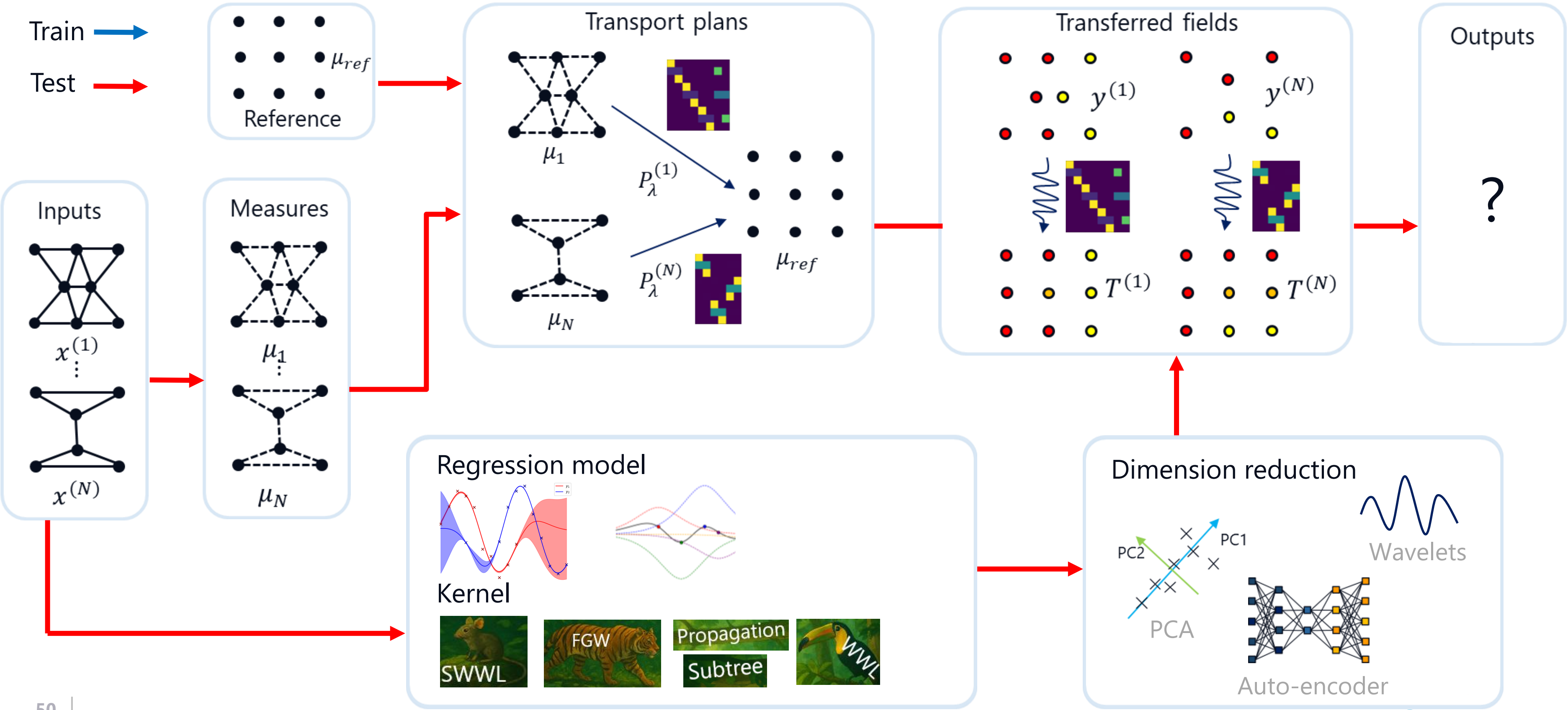
TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]



TOS-GP: Transported Output Signal Gaussian Processes

[CP, Da Veiga, Garnier, Staber, 2025]



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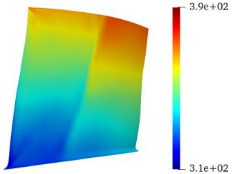
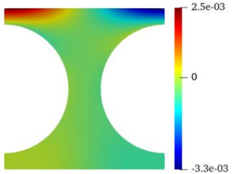
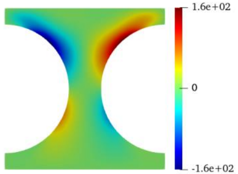
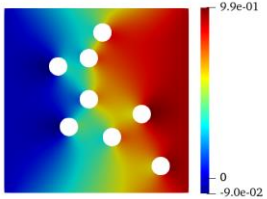
I) Scalar outputs

1- Gaussian process regression
2- SWWL graph kernel

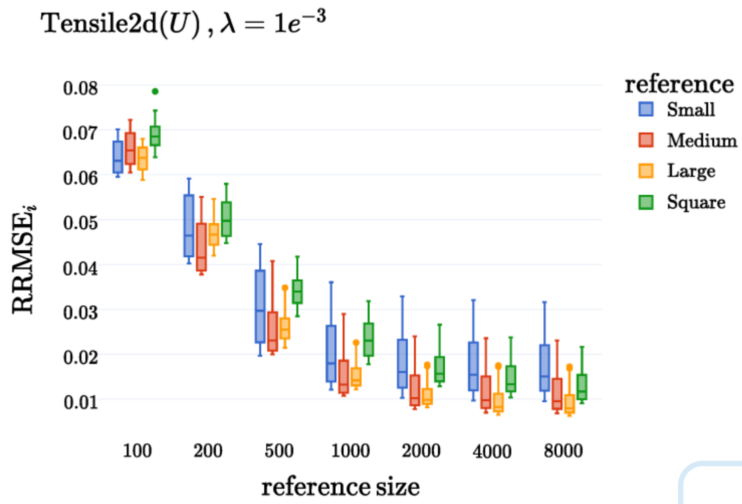
II) Signal outputs

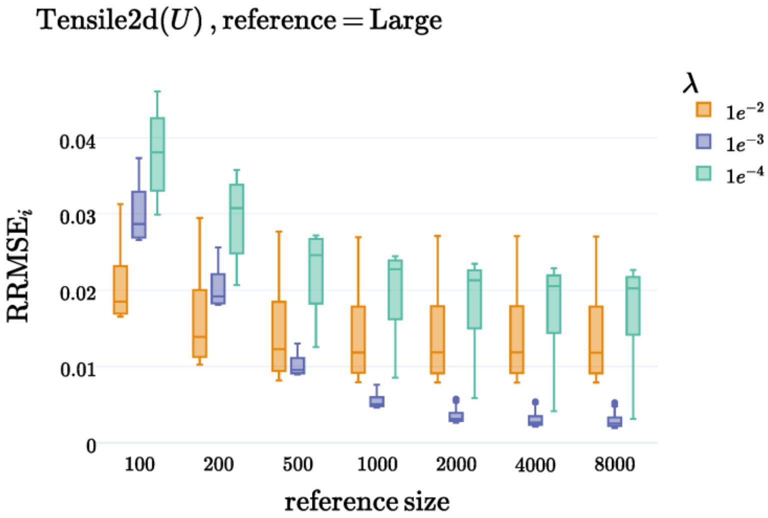
1- Problem statement
2- Related approaches
3- TOS-GP
4- Experiments

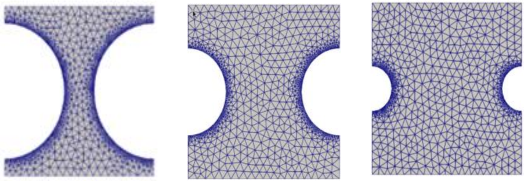
Datasets

Dataset name	Train/Test	Nodes	Output fields
Rotor37	1000 / 200	~30000	 Temperature (T)
Tensile2d	500 / 200	~9500	 H displacement (U)  Shear stress (σ12)
Multiscale	764 / 376	~4600	 H displacement (U)

TOS-GP: regression scores







Small Medium Large

- The error decreases when the size of the reference increases
- It remains close to a constant beyond 1000 points
- The choice of the reference type has little importance for this problem
- The choice of the **regularization parameter** is **critical**

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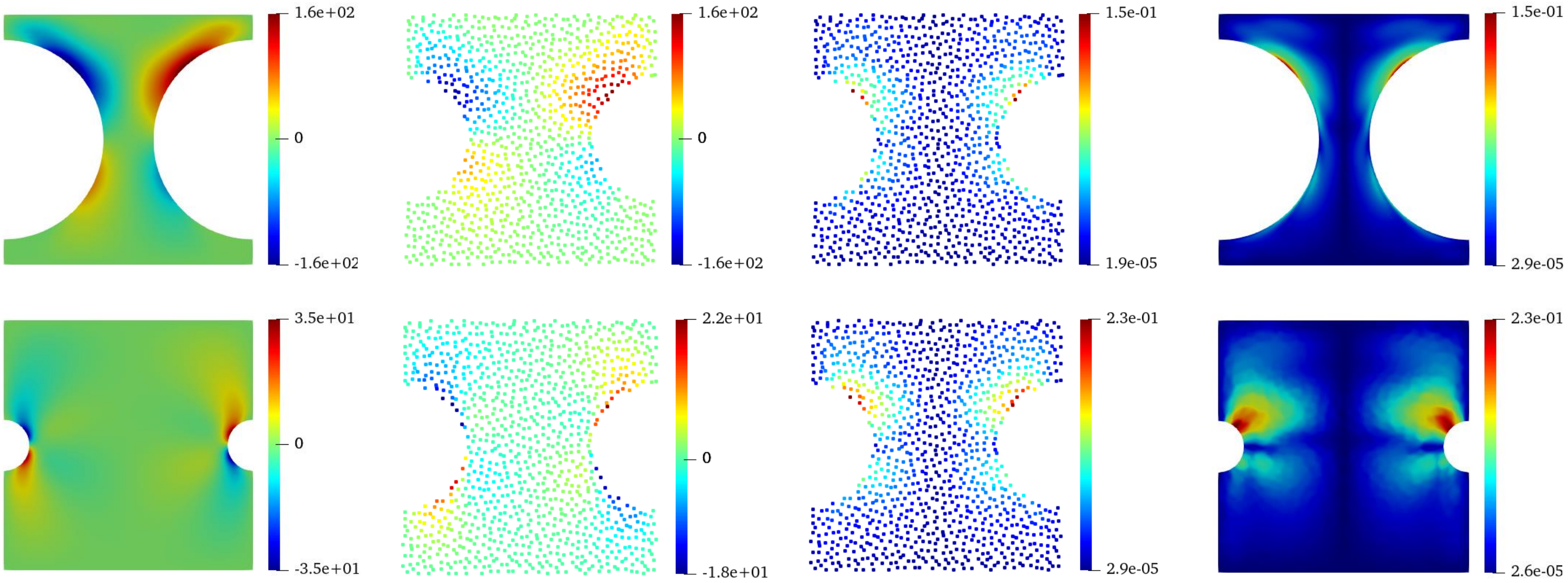
TOS-GP: uncertainty propagation (field σ_{12})



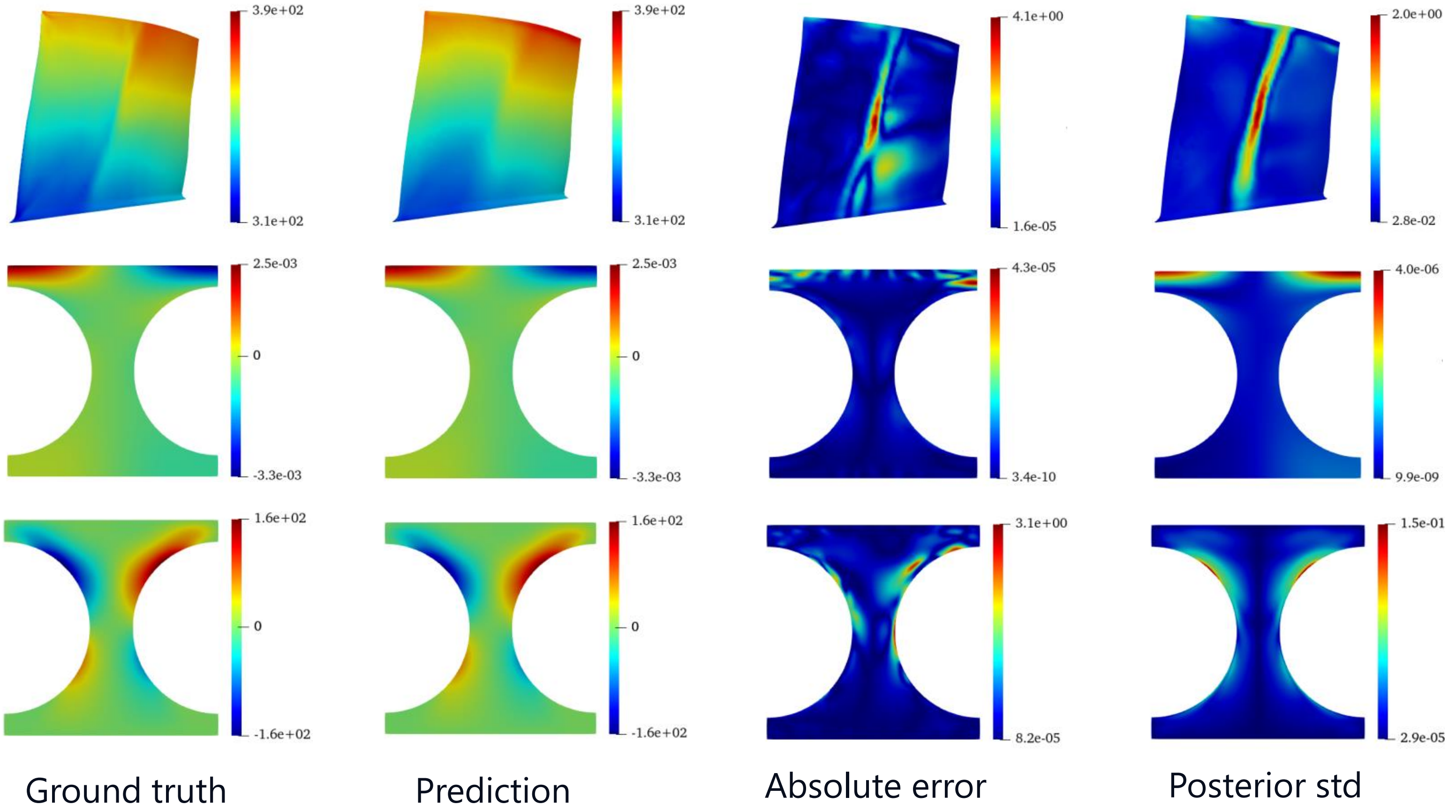
Ground truth

Prediction (transferred space)

Posterior std (transferred space)

Posterior std

TOS-GP: predictions and uncertainties



TOS-GP: regression scores

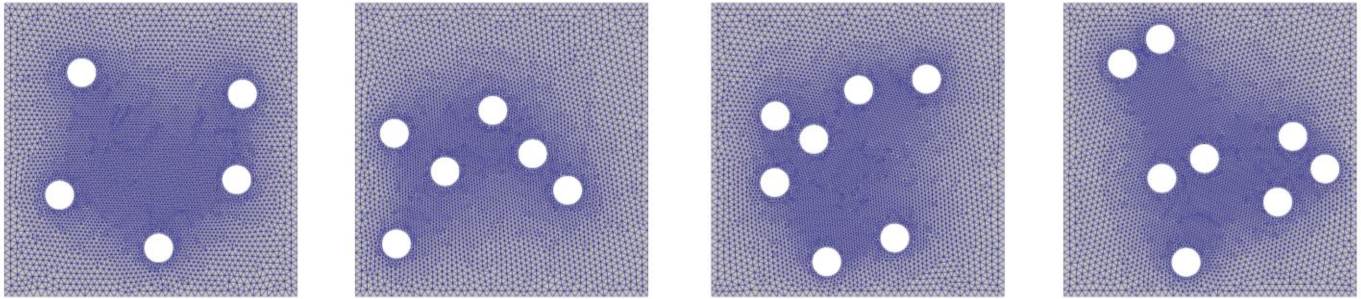
RRMSE (10 exp)

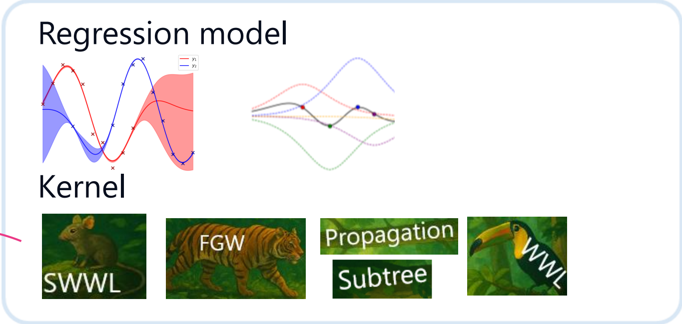
Method/Dataset	Rotor37(T)	Tensile2d(U)	Tensile2d(σ_{12})
TOS-GP	9.6e-3 (2e-5)	2.2e-3 (8e-6)	5.6e-3 (3e-6)
GCNN	3.9e-3 (1e-4)	4.5e-2 (1e-2)	4.5e-2 (4e-3)
MGN	1.4e-2 (2e-3)	1.5e-2 (1e-3)	7.5e-3 (4e-4)
MMGP	8.2e-4 (1e-5)	3.4e-3 (4e-5)	2.4e-3 (2e-5)

$$RRMSE^2\left(\{y^{(i)}\}_{i=1,\cdots,N_*},\{\hat{y}^{(i)}\}_{i=1,\cdots,N_*}\right)=\frac{1}{N_*}\sum_{i=1}^{N_*}RRMSE_i^2\left(y^{(i)},\hat{y}^{(i)}\right)$$

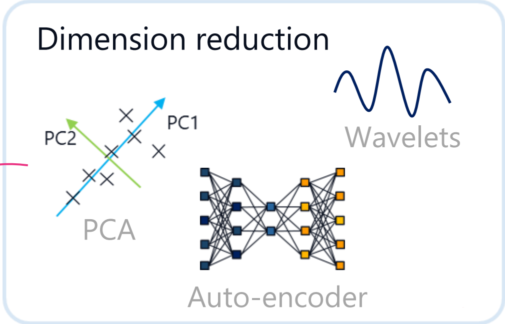
$$RRMSE_i^2\left(y^{(i)},\hat{y}^{(i)}\right)=\frac{\left\|y^{(i)}-\hat{y}^{(i)}\right\|_2^2}{n_{*i}\left\|y^{(i)}\right\|_\infty^2}$$

Varying topologies: 2D_multiscale_hyperelasticity



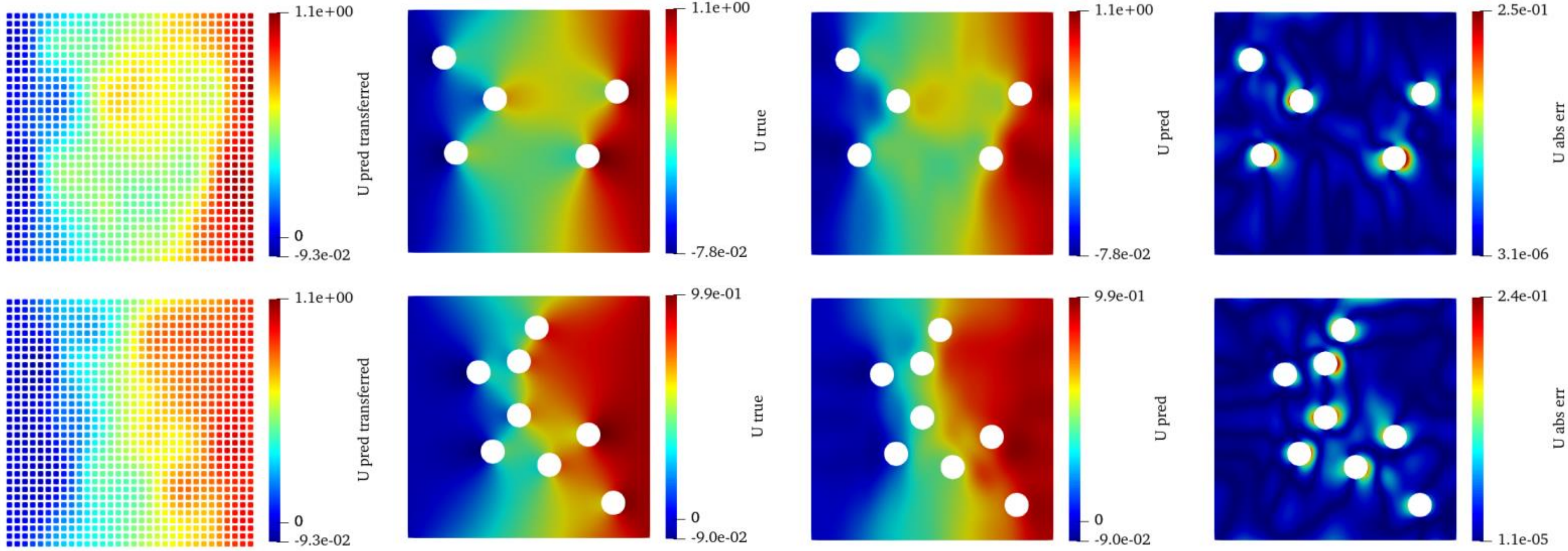


Squared-exp using the MMD distance between the centers of the pores



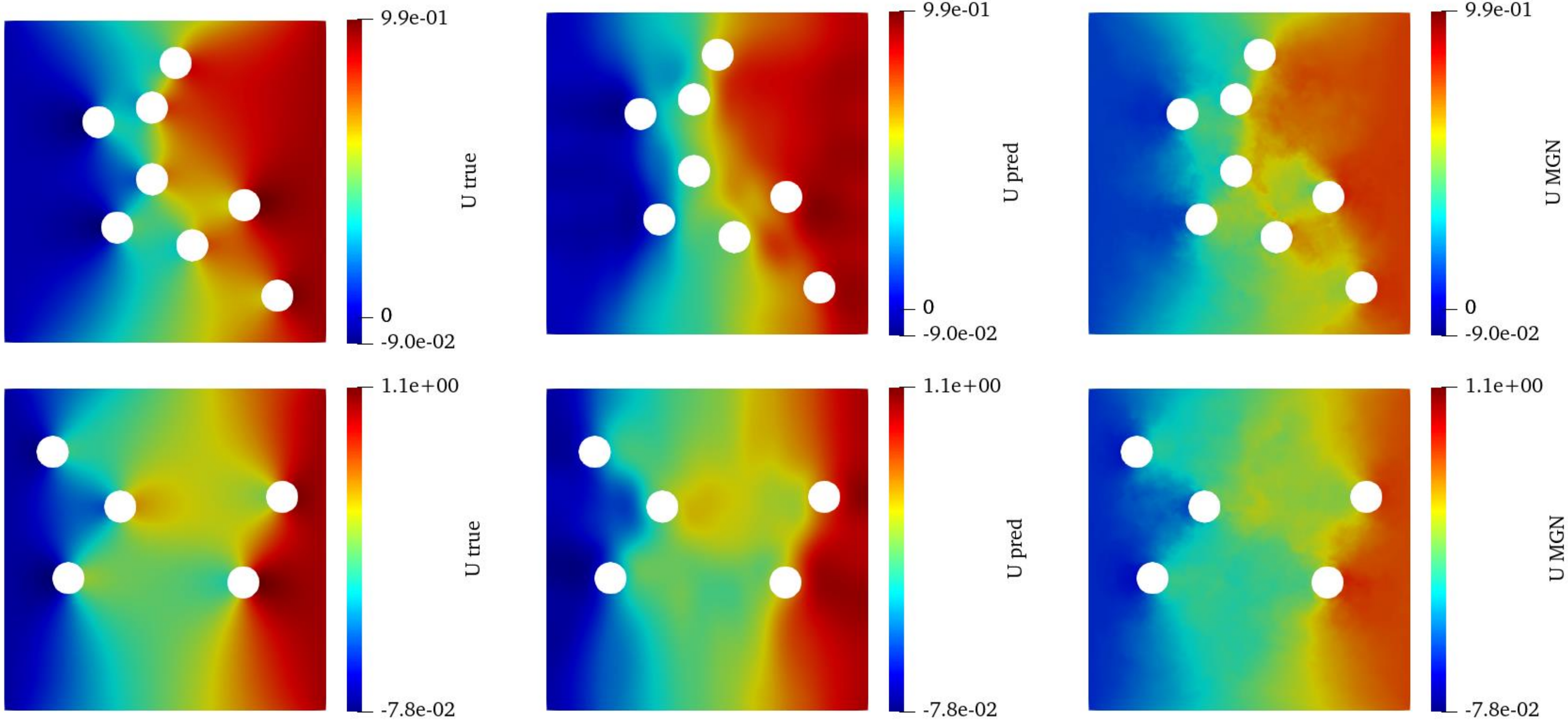
Auto-encoder with convolutional and 2D discrete Fourier layers [Li et al. 2020]

Varying topologies: 2D_multiscale_hyperelasticity



Prediction (transferred space) | Ground truth | Prediction | Absolute error

Varying topologies: 2D_multiscale_hyperelasticity

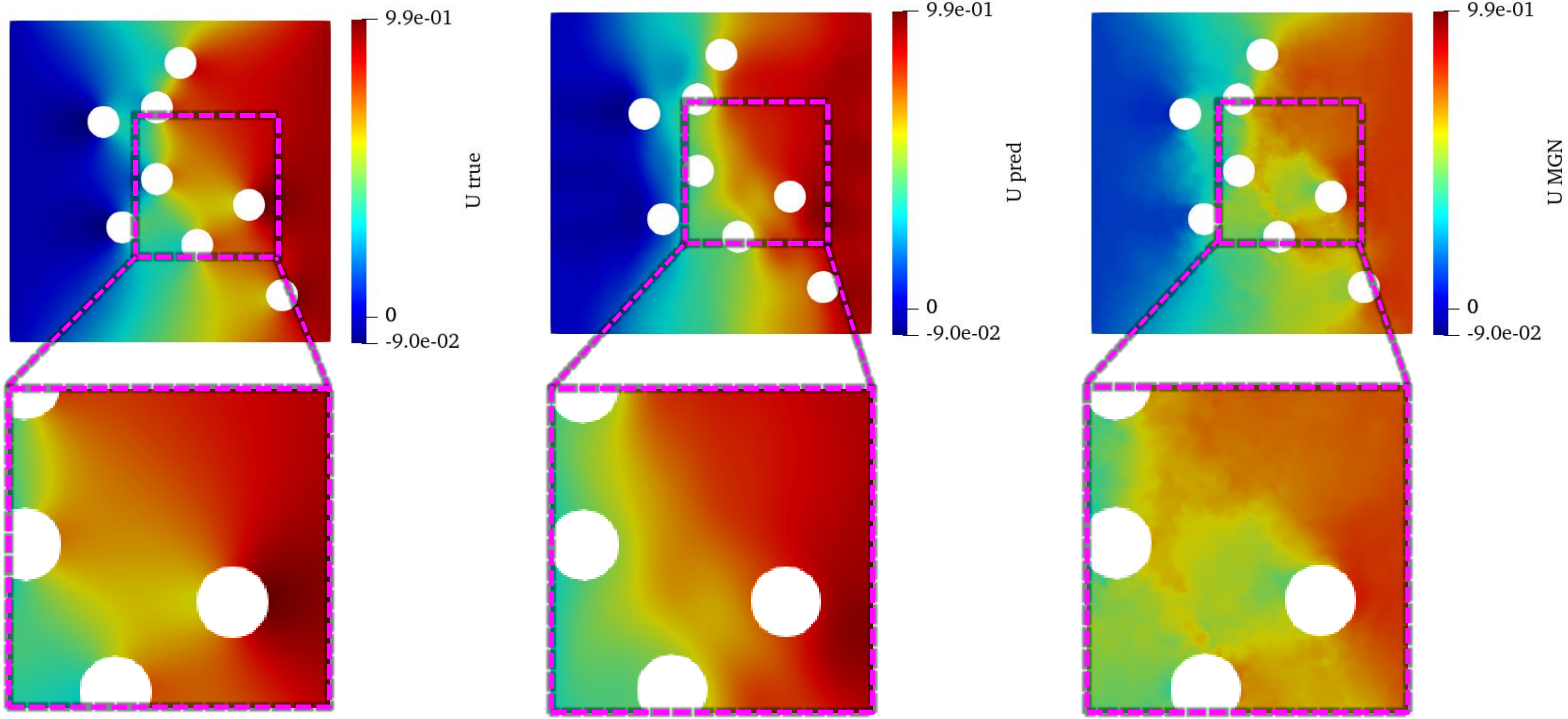


Ground truth

Prediction (TOS-GP)

Prediction (MGN)

Varying topologies: 2D_multiscale_hyperelasticity



Ground truth

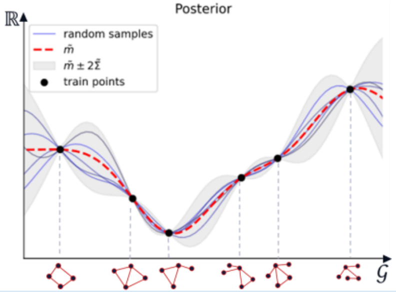
Prediction
(TOS-GP)

Prediction
(MGN)

Conclusion

Inputs = Graphs, Outputs = **Scalars**

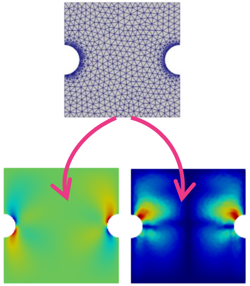
- SWWL graph kernel
  - ✓ Positive definite
  - ✓ Can consider very large graphs



Inputs = Graphs, Outputs = **Signals**

- Classical techniques impossible to use directly
  MOGP, OVGP, GSP, dimension reduction, …

- TOS-GP: Transported Output Signal GP
  Optimal transport + Dimension reduction
  - ✓ Flexible (change kernel/dimension reduction)
  - ✓ No assumption on the data (mesh/topology)
  - ✓ Few hyperparameters: λ, ref. measure, WL iter.



- Future work
  Consider more discontinuous signals
  Optimal transport variants

Acknowledgments

This work was supported by the French National Research Agency (ANR) through the SAMOURAI project under grant ANR20-CE46-0013.

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Gaussian process regression

Noisy observations:
$\mathbf{y} = (y_i)_{i=1}^N$ with $y_i = f(G_i) + \epsilon_i$ where
$\epsilon_i \sim \mathcal{N}(0, \sigma^2)$, $f: \mathcal{X} \to \mathbb{R}$

Gaussian prior over functions:

$f \sim \mathcal{GP}(0, k)$ where $k: \mathcal{G} \times \mathcal{G} \to \mathbb{R}$ is a symmetric **positive definite kernel**

Test locations:
$\boldsymbol{G}^* = (G_i^*)_{i=1}^{N^*}$
Predictions? $\boldsymbol{f}_* = (f(G_i^*))_{i=1}^{N^*}$?

$\boldsymbol{K}, \boldsymbol{K}_{**}, \boldsymbol{K}_*$: train, test, train/test Gram matrices

$$\begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{f}_* \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} \boldsymbol{K} + \sigma^2 I & \boldsymbol{K}_*^T \\ \boldsymbol{K}_* & \boldsymbol{K}_{**} \end{bmatrix}\right)$$

Posterior distribution:

$$\boldsymbol{f}_* \mid \boldsymbol{G}, \boldsymbol{y}, \boldsymbol{G}^* \sim \mathcal{N}(\overline{\boldsymbol{m}}, \overline{\boldsymbol{\Sigma}})$$

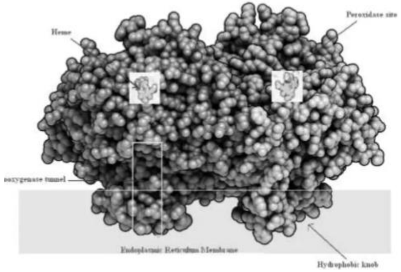
predictive mean $$\overline{\boldsymbol{m}} = \boldsymbol{K}_*(\boldsymbol{K} + \sigma^2 I)^{-1} \boldsymbol{y}$$

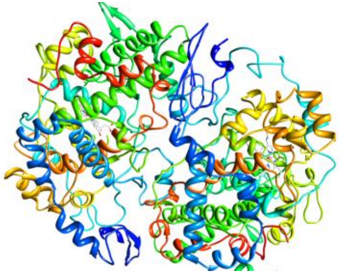
uncertainties $$\overline{\boldsymbol{\Sigma}} = \boldsymbol{K}_{**} - \boldsymbol{K}_*(\boldsymbol{K} + \sigma^2 I)^{-1} \boldsymbol{K}_*^T$$

- $\mathcal{X} = \mathcal{G}$ is a set of graphs.
-
- How to choose k ?

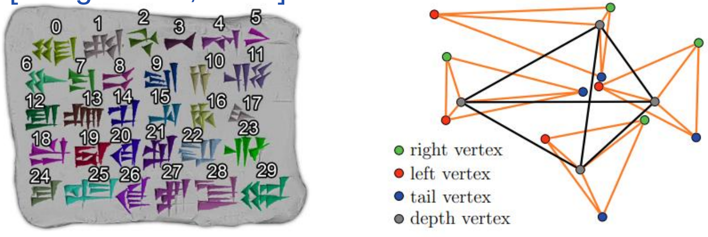
k ( , ) = ?

SWWL kernel: experiments

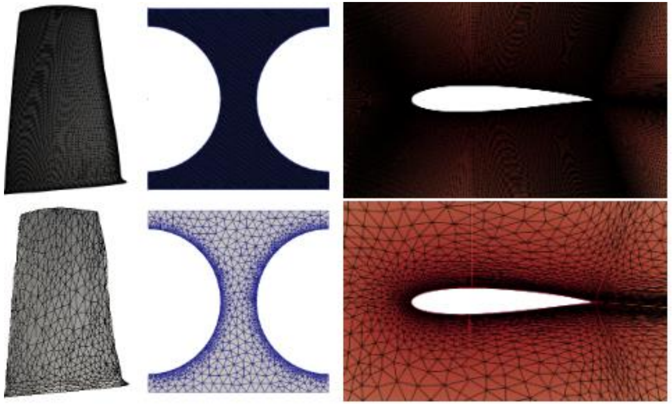


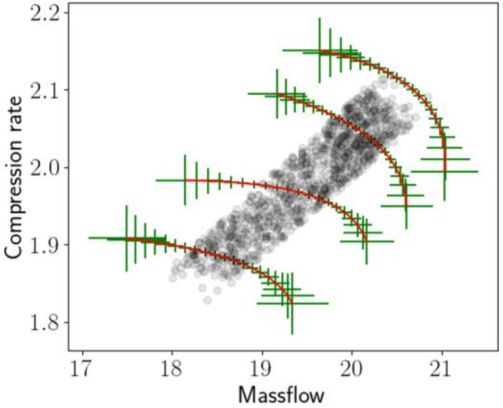


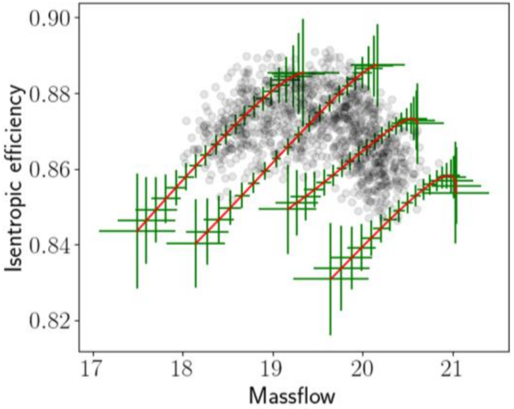
[Kriege et al., 2019]



(a) Cuneiform tablet (b) Graph representation





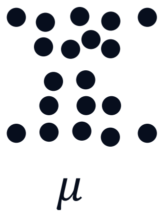


MMD subsampling procedure

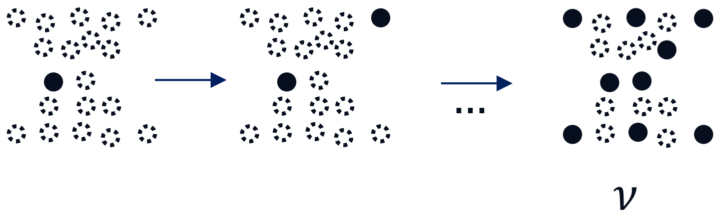
Maximum mean discrepancy:

$$MMD_k(\mu, \nu) = \mathbb{E}_{x\sim\mu, x'\sim\mu}[k(x,x')] + \mathbb{E}_{y\sim\nu, y'\sim\nu}[k(y,y')] - 2\mathbb{E}_{x\sim\mu, y\sim\nu}[k(x,y)]$$

Input: μ a given measure in the train set.
Output: ν the subsampled measure.



$\nu = \emptyset$
At each iteration, choose the point x in the support of μ that minimizes the MMD between μ and $\nu + \delta_x$, and update ν.



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