

Automatic Dynamic Relevance Determination for Gaussian process regressions with functional inputs

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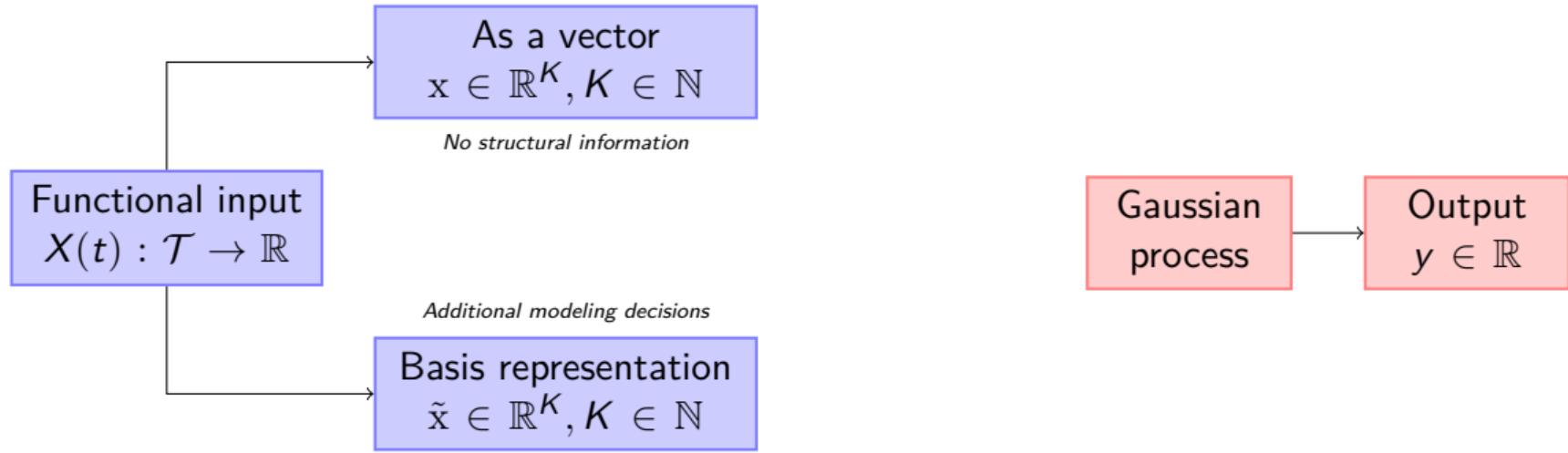
Overview & motivation

Gaussian process with functional input

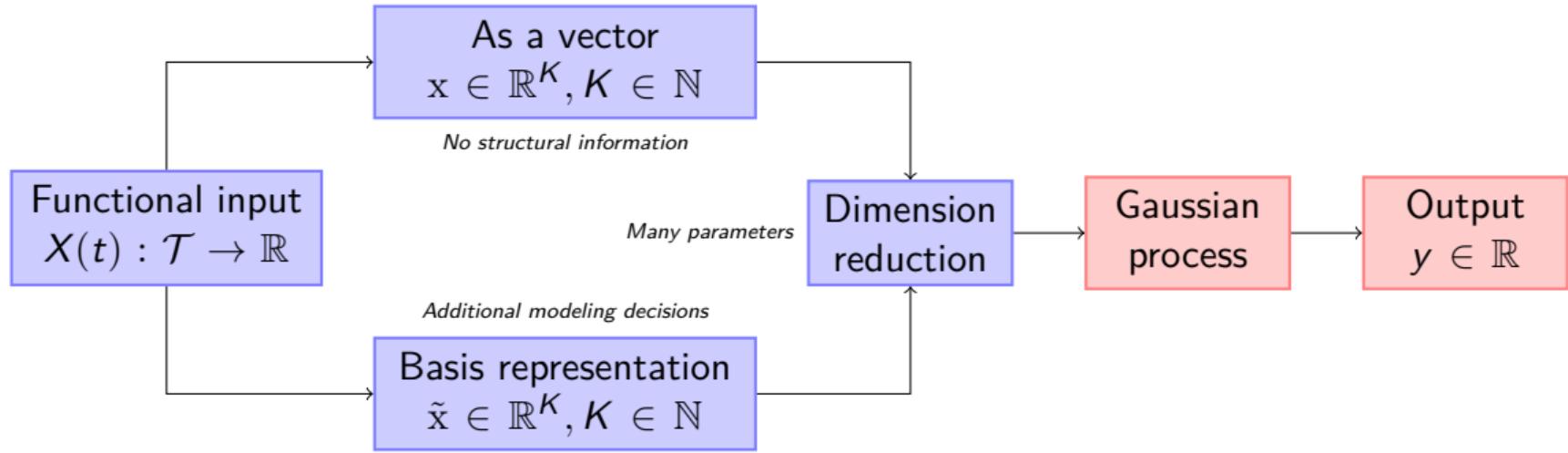
Functional input
 $X(t) : \mathcal{T} \rightarrow \mathbb{R}$

Gaussian process → Output
 $y \in \mathbb{R}$

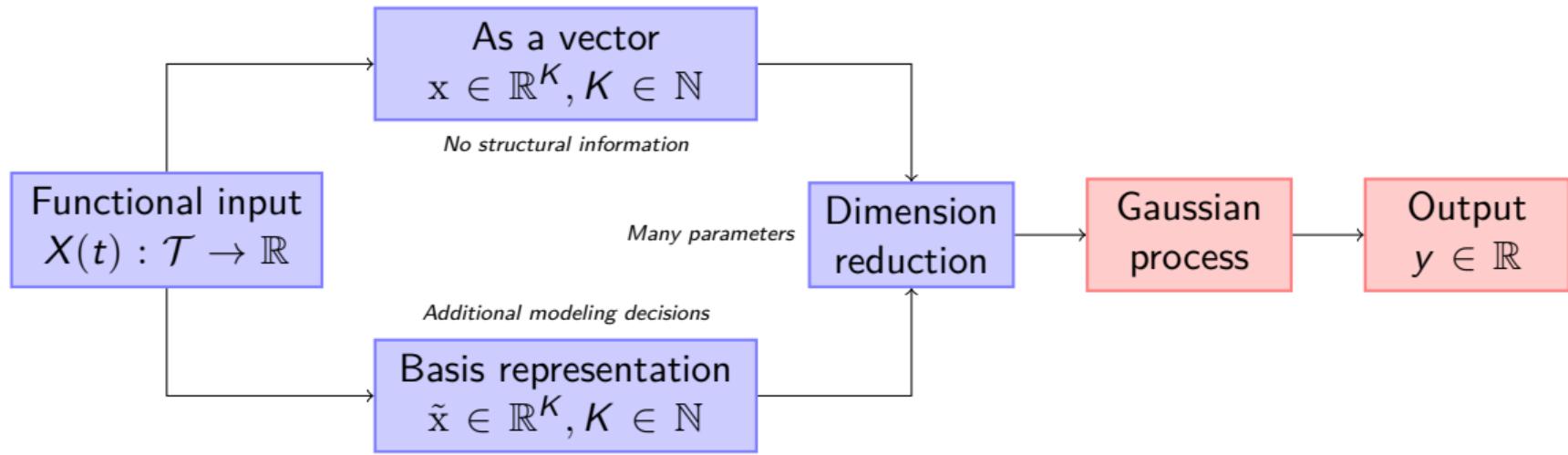
Gaussian process with functional input



Gaussian process with functional input

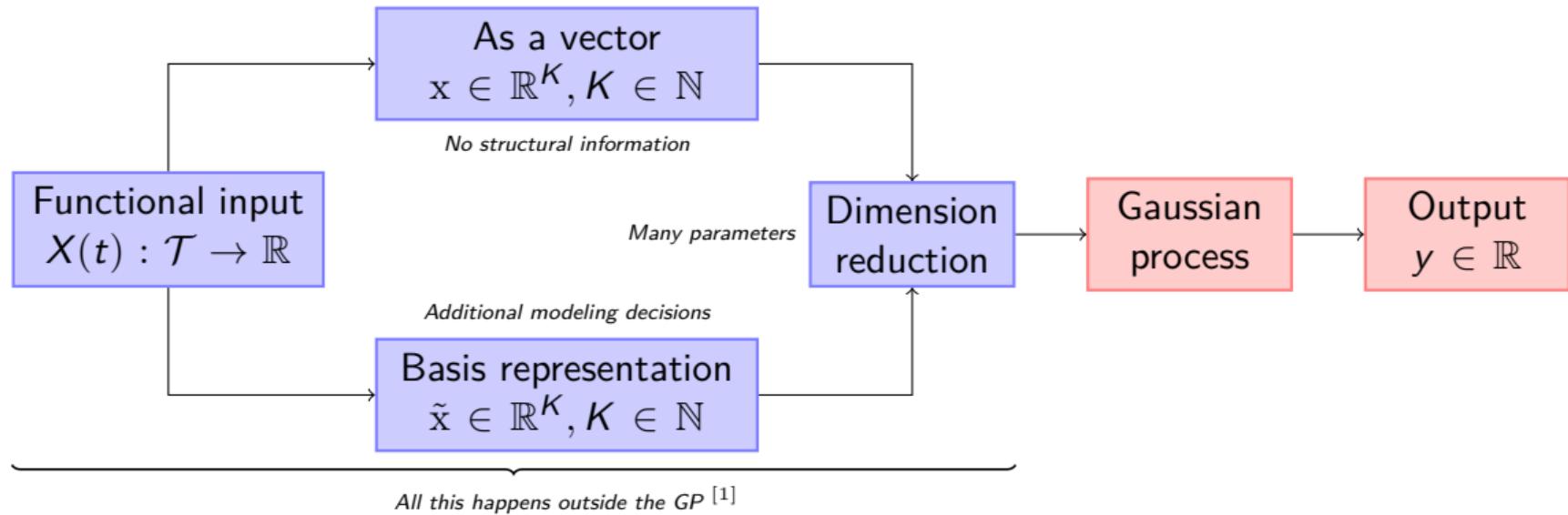


Gaussian process with functional input



- Can we connect the functional input structure to a physical mechanism?

Gaussian process with functional input

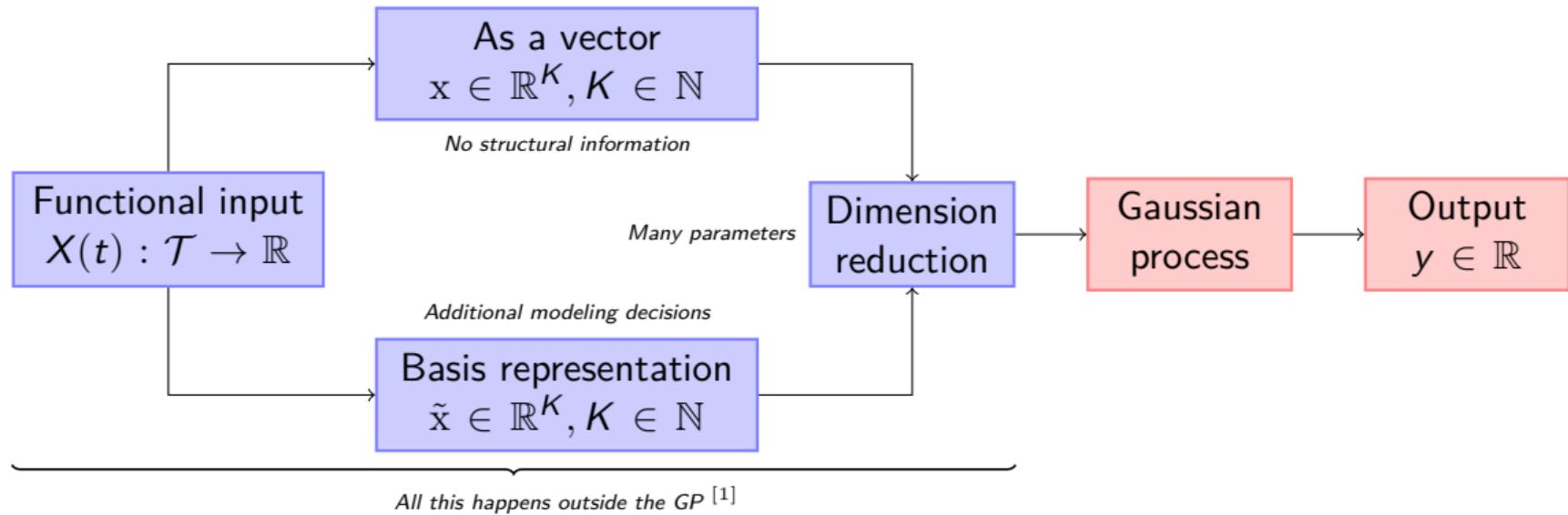


- Can we connect the functional input structure to a physical mechanism?
- Can we incorporate the functional input structure into the GP? [2]

[1][1, 2, 3, 4, 5, 6, 7, 8]

[2][9, 10]

Gaussian process with functional input



- Can we connect the functional input structure to a physical mechanism?
- Can we incorporate the functional input structure into the GP? [2]
- Can we circumvent input dimension reduction?

[1][1, 2, 3, 4, 5, 6, 7, 8] [2][9, 10]

Input structure information

Output	Input $X(t) : \mathcal{T} \rightarrow \mathbb{R}$	Index $t \in \mathcal{T}$	Index subspaces $t \in \mathcal{T}_u$	Mechanism

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Can we establish an explicit link $X(t) \xrightarrow{f} y$ for UQ?

From relevance to *dynamic* relevance

Extending relevance

Some inputs
matter more than others

x_1 vs x_2

Screening
*(exploration
& diagnostics)*

Permutation
Feature
Importance [1]

Model tuning
(learning)

Automatic
Relevance
Determination [2]

[1] [11, 12, 13, 14, 15, 16]

[2] [17, 18]

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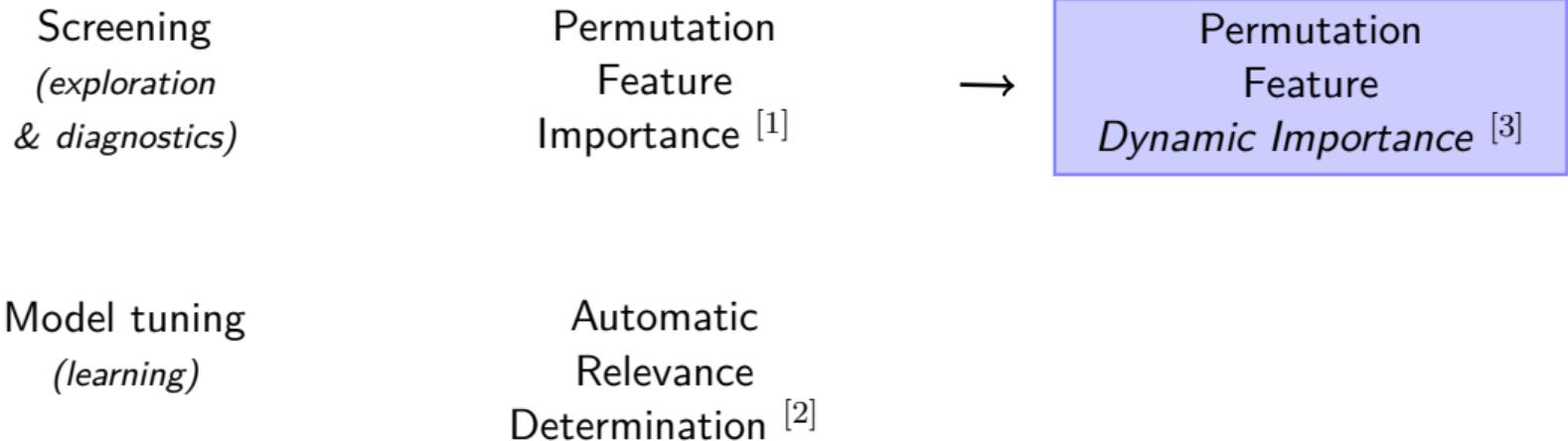
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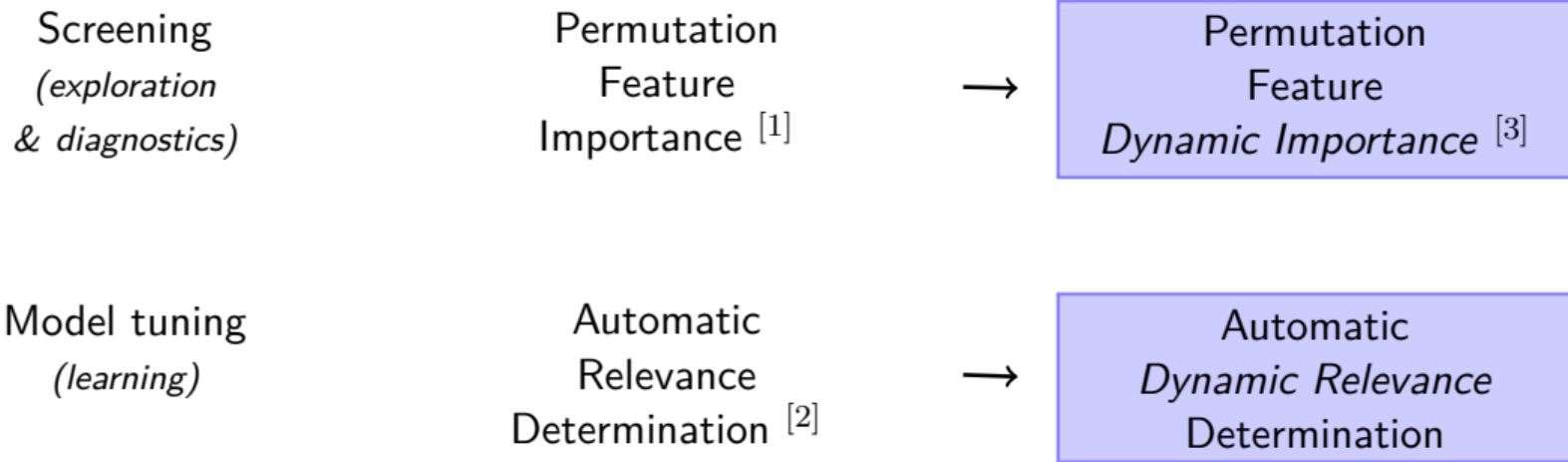
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[3] Forthcoming paper

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Modeling *dynamic* relevance

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Distance
 $d(X_i, X_j)$

$$\sum_{k=1}^K \frac{(x_{i,k} - x_{j,k})^2}{\ell_k^2}$$

Weights
(relevance)

$$\ell_1^{-2}, \dots, \ell_K^{-2} > 0$$

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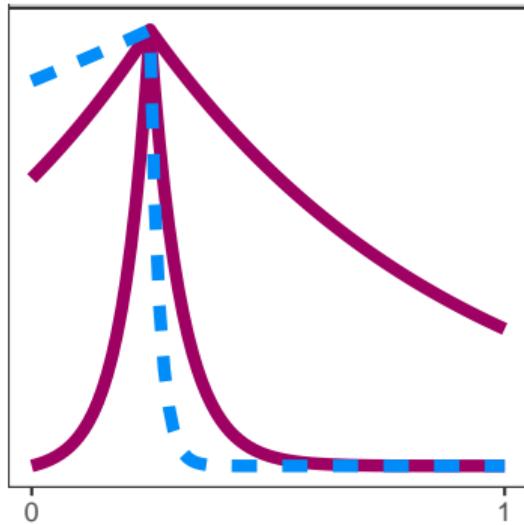
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$$\omega(t) : \mathcal{T} \rightarrow \mathbb{R}^+$$

Asymmetric Laplace function

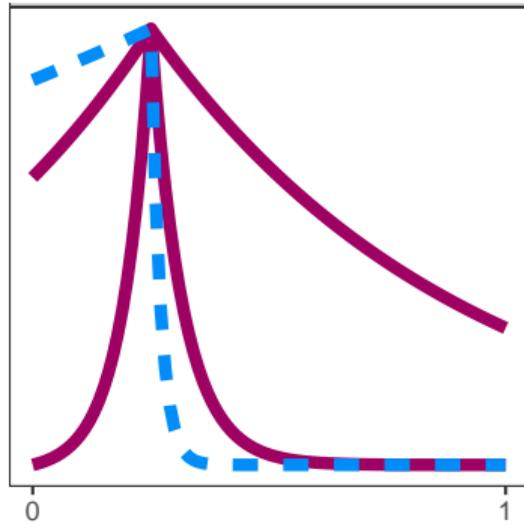
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$$\omega(t) : \mathcal{T} = [0, 1] \rightarrow (0, 1], s = \text{sign}(t - \tau), \tau > 0, \lambda > 0, \kappa > 0$$

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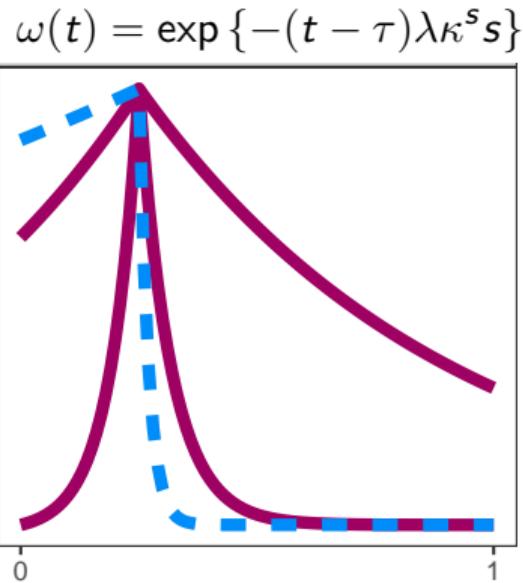
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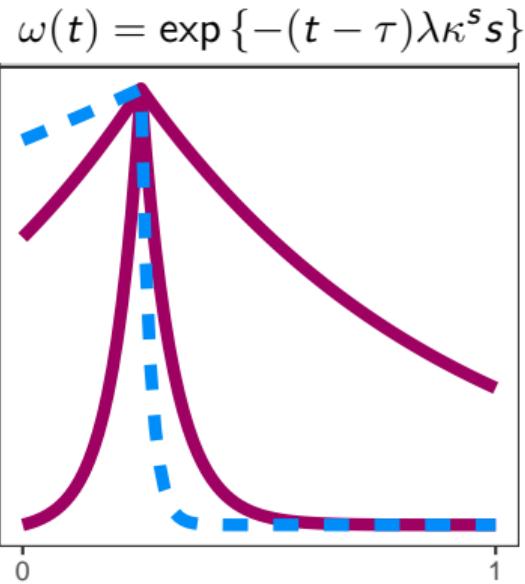
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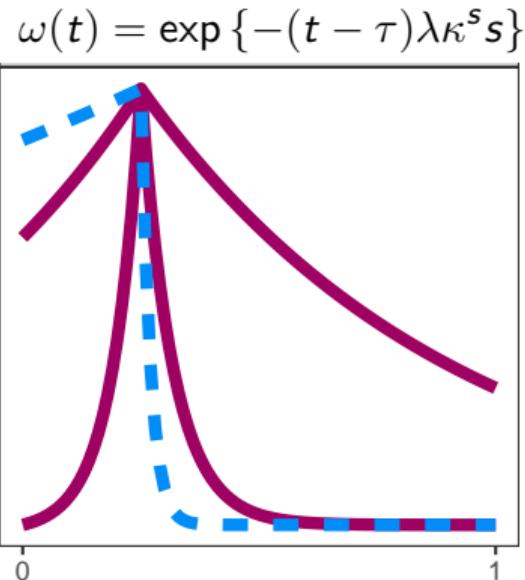
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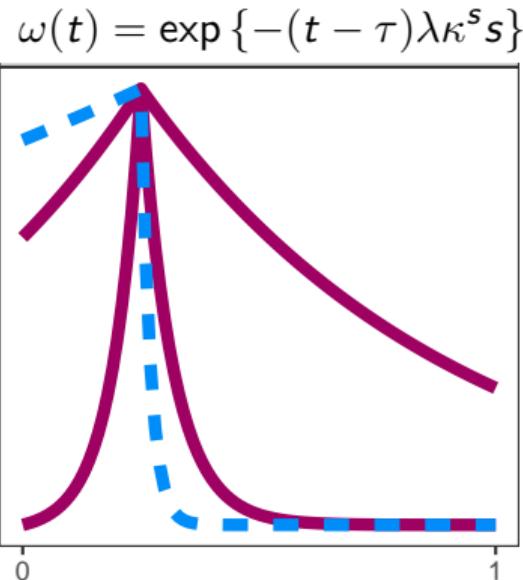
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Functional Input Gaussian Process (fiGP)

$$\mathbf{y} \sim \mathcal{N}(0, \sigma_f^2 \mathbf{R}_f + \sigma_\varepsilon^2 \mathbf{I}) \quad (1)$$

$$(\mathbf{R}_f)_{ij} = \exp\left\{-0.5\phi^{-2} d_f(X_i, X_j)\right\} \quad (2)$$

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Flexibility no need to match input-output structure nor index space

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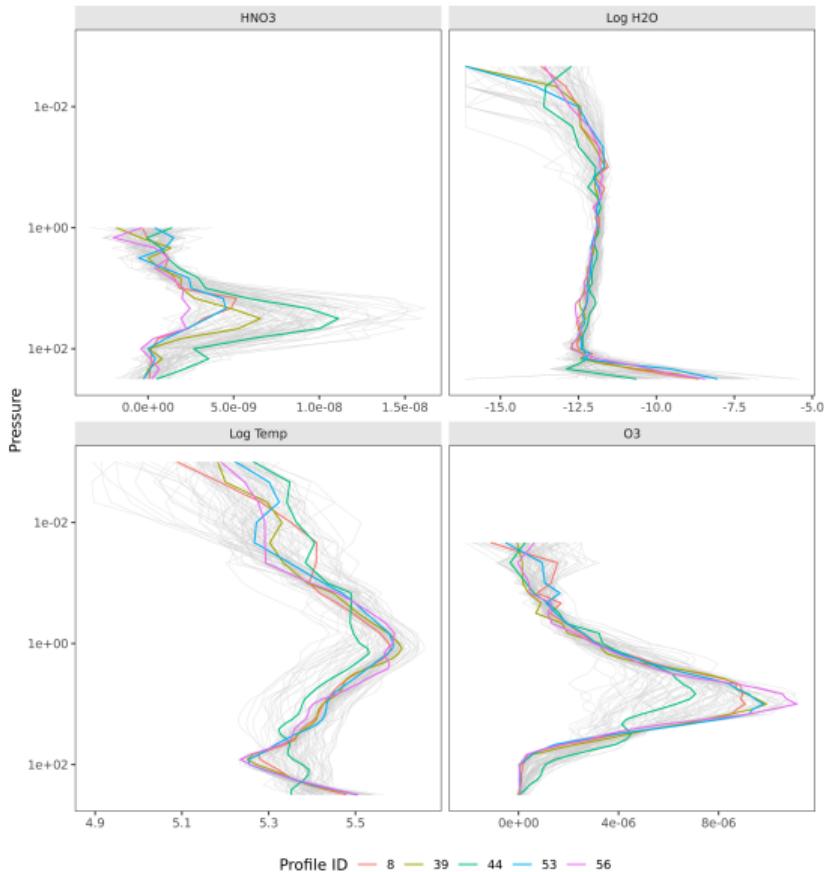
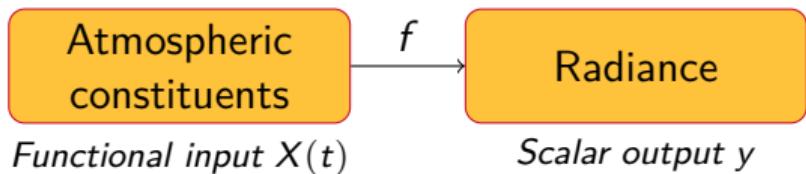
NASA's Microwave Limb Sounder

a case study

Data structure



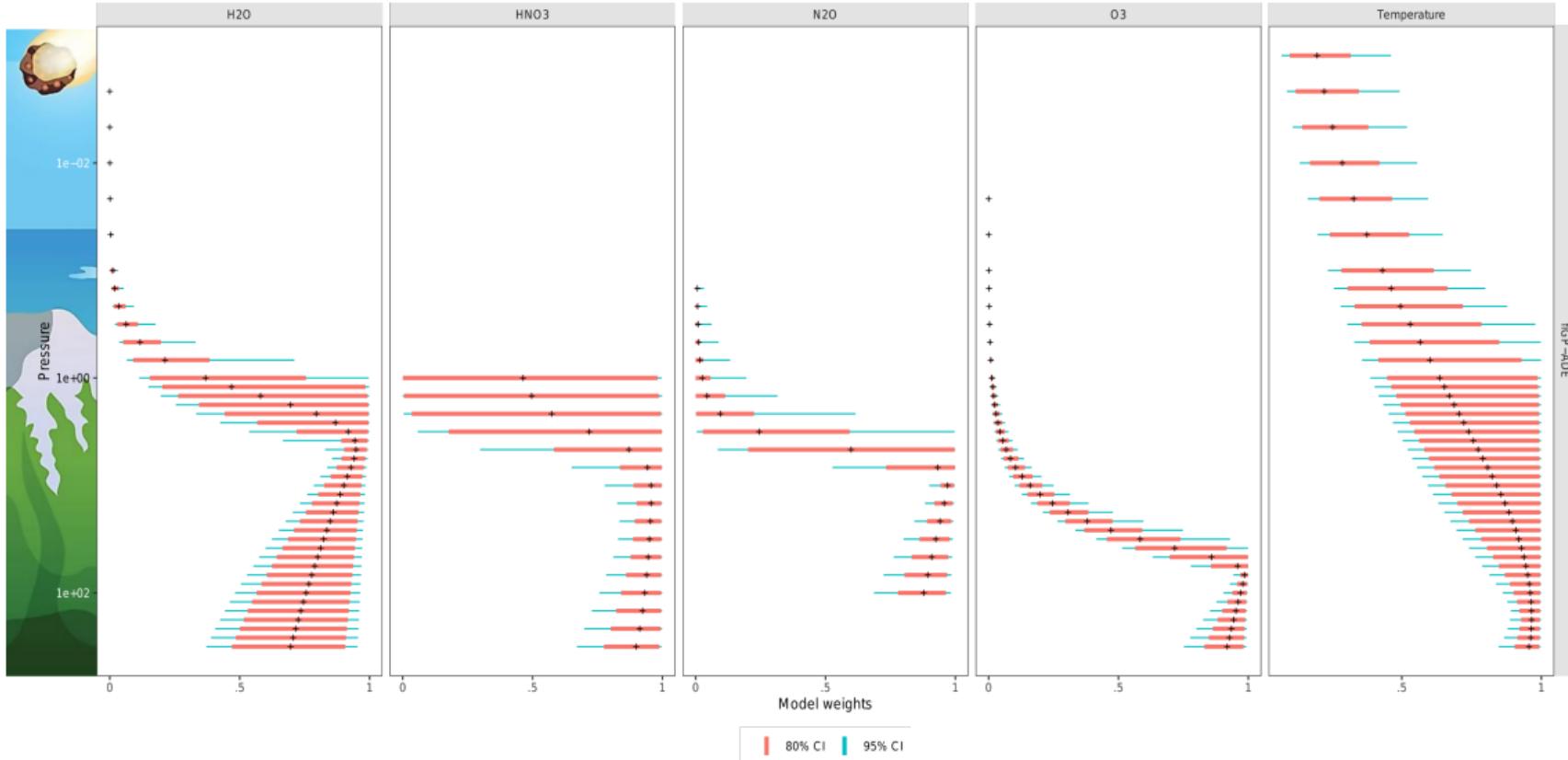
Credit: NASA Aura



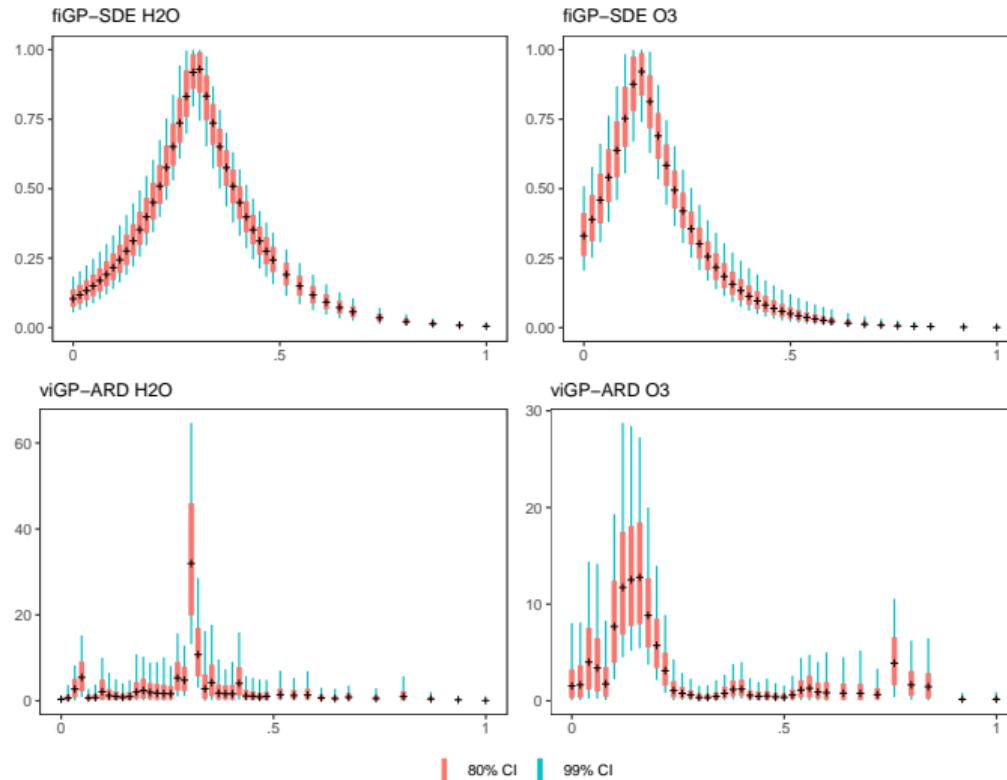
Implementation

- 8 training, 8 test complementary sets
- 1,000 soundings each
- One model fit separately per input-output pair
- Fully Bayesian inference
- Hamiltonian Monte Carlo using Stan
- 1 long chain
- Extensive search for an initial value
- 500 post-warmup iterations
- 1,500 posterior samples

Weight function posterior samples



fiGP vs a vector-input GP



Why a fiGP?

- + High dimensional inputs with no dimension reduction
 - ▶ Reduce unknowns $3 \ll K$
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[1] Appendix slides and forthcoming paper

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- ++ Extensible to **complex index spaces**, e.g., spatio-temporal spectral inputs [2]

[1] Appendix slides and forthcoming paper [2] Future research

Acknowledgments

The MLS team at JPL, California Institute of Technology

Thank you!

References and extra slides on the back

▶ mail ldamiano@iastate.edu

▶ repo <https://github.com/luisdamiano/SIAMUQ22>

Appendix

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Notation

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Index vector t with the vertical pressure level

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State vector x_i characterizing an atmospheric vertical profile

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Output scalar y_i is the radiance first functional principal component [19]

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Sounding a collection of an observed radiance, retrieved state and pressure vectors

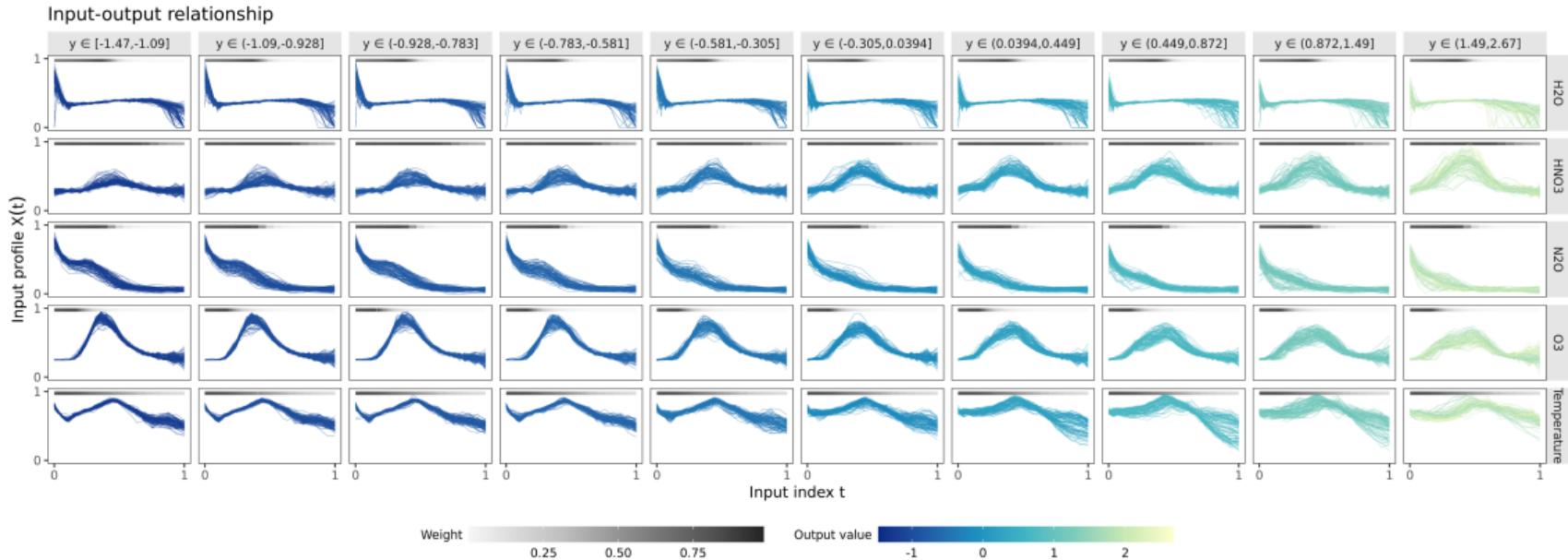
Trapezoidal approximation

$$\int_{\mathcal{T}} \omega(t) (X_i(t) - X_j(t))^2 dt \approx \sum_{k=2}^K (t_k - t_{k-1}) \frac{\Delta_{i,j,k} + \Delta_{i,j,k-1}}{2} \quad (5)$$

$$\Delta_{i,j,k} = \omega(t_{k-1})(x_{i,k} - x_{j,k})^2 \quad (6)$$

See [1] for a B-spline approach

Weights, inputs and output



Panes: profiles grouped by input variable (row) and output decile (column). Color: dark (light) for low (high) output values. Background: dark (light) for large (small) weights.

Out-of-sample prediction

	H2O	HNO3	N2O	O3	Temp	Mean		H2O	HNO3	N2O	O3	Temp	Mean
SE	.34	.48	.44	.32	.25	.37	SE	273	614	585	138	-7	323
ARD	.31	.47	.43	.30	.25	.35	ARD	196	619	581	92	-13	295
FPCA	.67	.91	.99	.46	.54	.71	FPCA	1024	1320	1406	637	802	1038
FFPCA	.46	.54	.46	.38	.33	.44	FFPCA	535	646	630	295	268	475
EDN	.33	.47	.44	.29	.25	.36	EDN	261	623	585	90	4	312
SDE	.31	.47	.44	.29	.25	.35	SDE	202	623	585	85	4	300
ADE	.31	.47	.43	.29	.25	.35	ADE	202	610	581	87	2	297
Mean	.39	.55	.52	.33	.31	.42	Mean	385	722	708	204	152	434

Mean validation statistics: RMSE (left) and negative posterior predictive log-density (right). Smaller values are better. Bold: best in column. EDN $\tau = 0, \kappa = 1$; SDE $\tau = 0$; ADE τ, κ, λ all free; ARD as many free parameters as measurements per vertical profile.