Automatic Dynamic Relevance Determination
for Gaussian process regressions with functional inputs

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Overview & motivation

Gaussian process with functional input

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

$$\boxed{\text{Gaussian process}} \longrightarrow \boxed{\text{Output } y \in \mathbb{R}}$$

Gaussian process with functional input

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

As a vector
$\mathrm{x} \in \mathbb{R}^K, K \in \mathbb{N}$

No structural information

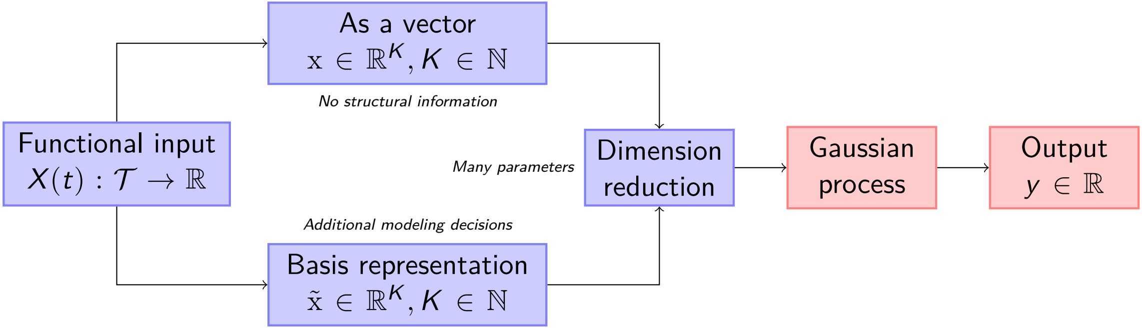
Additional modeling decisions

Basis representation
$\tilde{\mathrm{x}} \in \mathbb{R}^K, K \in \mathbb{N}$

Gaussian process

Output
$y \in \mathbb{R}$

Gaussian process with functional input



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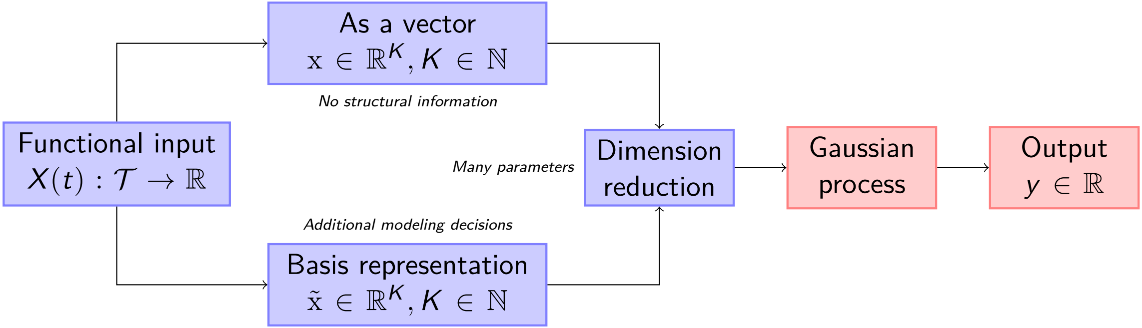
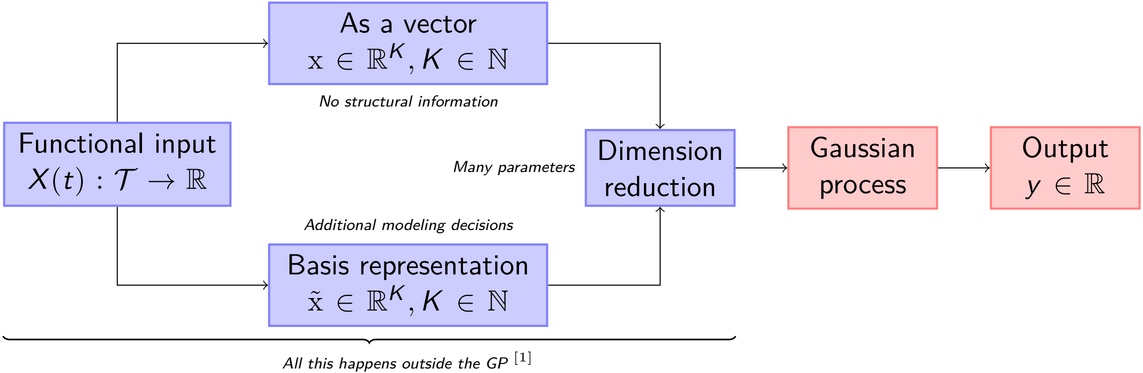


- Can we connect the functional input structure to a physical mechanism?

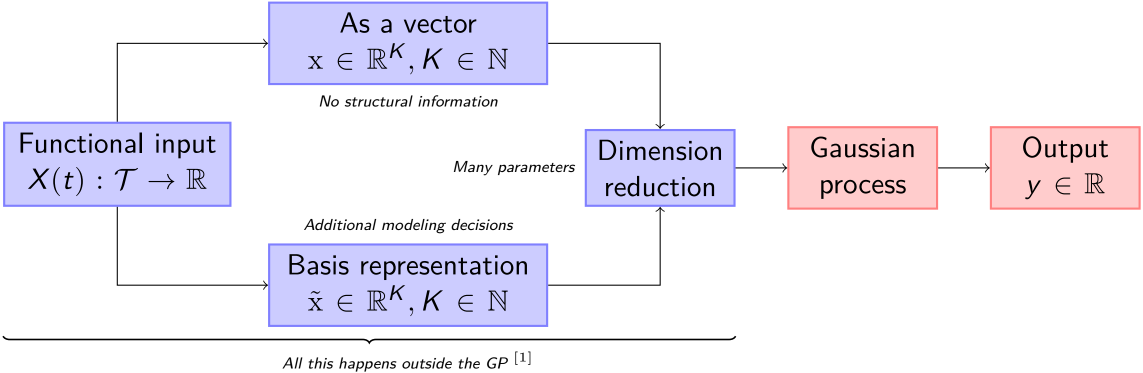
Gaussian process with functional input



- 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?

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Input structure information

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

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Index subspaces can provide a meaningful representation of the physical process

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]

Extending relevance

Some inputs matter more than others
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$\longrightarrow$

Some index subspaces matter more than others
$X(t_1)$ *vs* $X(t_2)$

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Screening *(exploration & diagnostics)*	Permutation Feature Importance [1]	$\longrightarrow$	Permutation Feature *Dynamic Importance* [3]
Model tuning *(learning)*	Automatic Relevance Determination [2]		

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Modeling *dynamic* relevance

Model tuning *(learning)*	Automatic Relevance Determination
Distance $d(X_i, X_j)$	$\sum_{k=1}^{K} \frac{(x_{i,k} - x_{j,k})^2}{\ell_k^2}$
Weights *(relevance)*	$\ell_1^{-2}, \cdots, \ell_K^{-2} > 0$

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Distance $d(X_i, X_j)$	$\sum_{k=1}^{K} \frac{(x_{i,k}-x_{j,k})^2}{\ell_k^2}$		$\int_{\mathcal{T}} \omega(t)(X_i(t) - X_j(t))^2 \mathrm{d}t$
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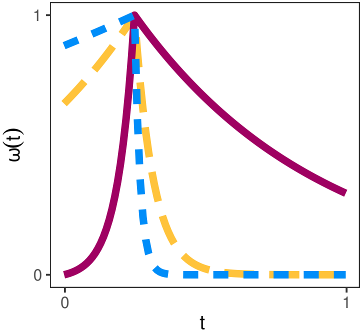
Weights *(relevance)*	$\ell_1^{-2}, \cdots, \ell_K^{-2} > 0$		$\omega(t) : \mathcal{T} \to \mathbb{R}^+$

Asymmetric Laplace function

$$\omega(t) = \exp\{-(t-\tau)\lambda\kappa^s s\}$$



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

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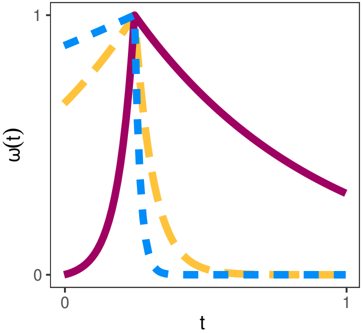

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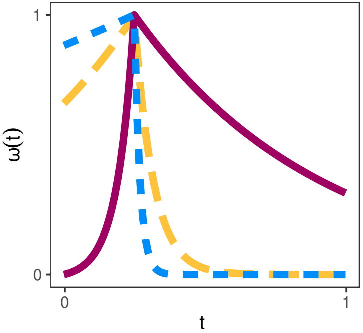

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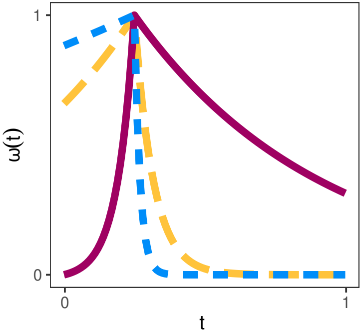

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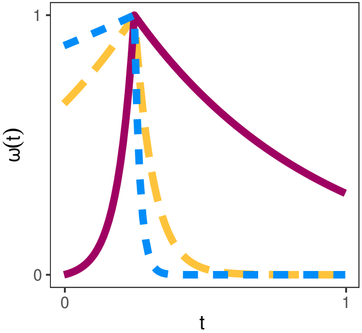

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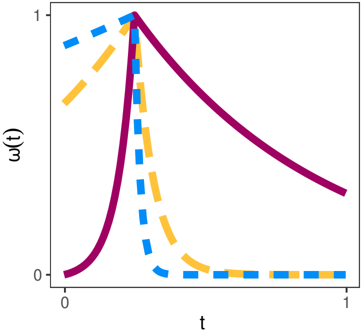

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circumvent input dimension reduction

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

Functional Input Gaussian Process (fiGP)

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

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

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(4)

$\sigma_\varepsilon^2 > 0$, $\sigma_f^2 > 0$, $\phi > 0$, $i, j = 1, \ldots, N$

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Weakly informative priors $\phi \sim \textsc{InvGamma}$, $\tau \sim \textsc{Beta}$, $\lambda \sim \mathrm{N}^+$, $\log(\kappa) \sim \mathrm{N}$

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

---

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NASA's Microwave Limb Sounder

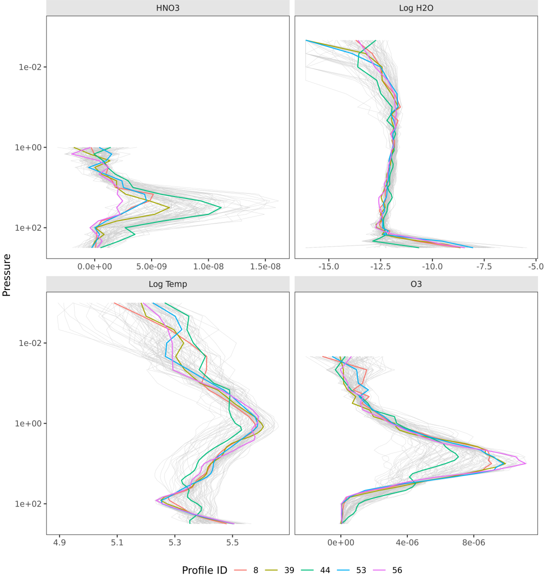
a case study

Data structure

Credit: NASA Aura

Atmospheric constituents $\xrightarrow{f}$ **Radiance**

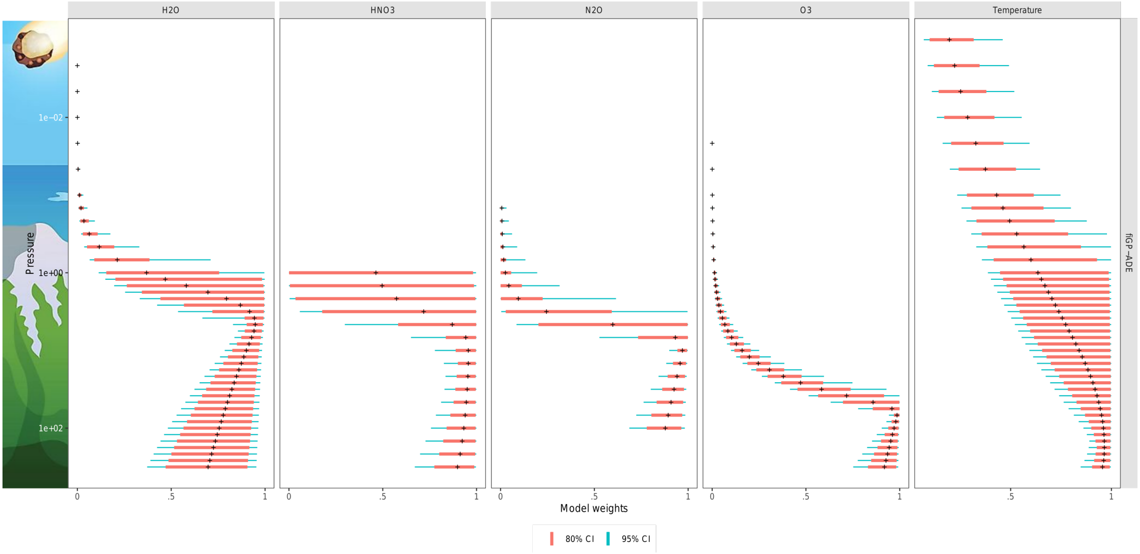
Functional input $X(t)$ — *Scalar output y*



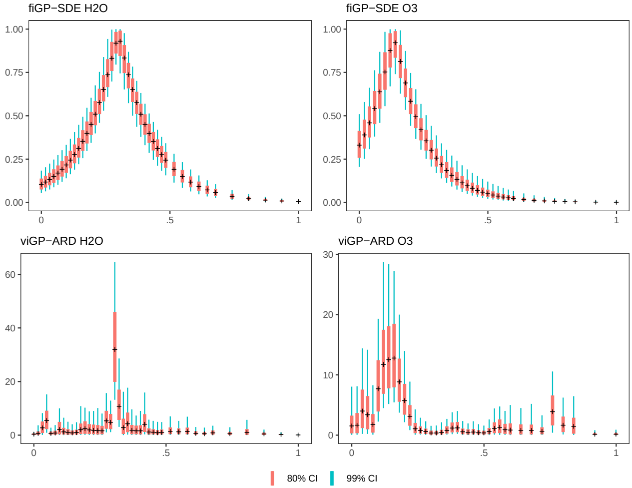
Implementation

- 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



In this slide only, we fix $\kappa = 1$ so that $\omega(t)$ is symmetrical

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  - Reduce unknowns $3 << K$
  - Scales up for applications with higher input resolution $\uparrow K$

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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

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

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State vector x_i characterizing an atmospheric vertical profile

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

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

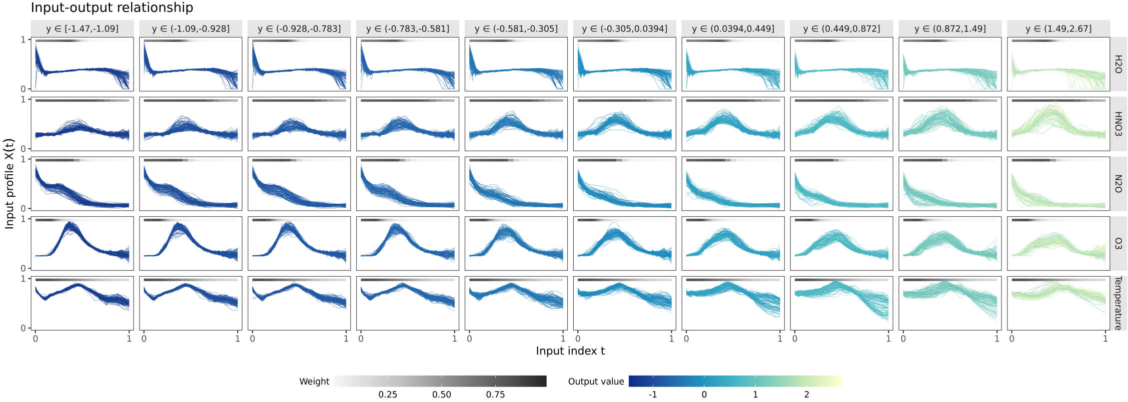
Trapezoidal approximation

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

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

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
SE	.34	**.48**	**.44**	.32	**.25**	.37
ARD	**.31**	**.47**	**.43**	**.30**	**.25**	.35
FPCA	.67	.91	.99	.46	.54	.71
FFPCA	.46	.54	**.46**	.38	.33	.44
EDN	.33	**.47**	**.44**	**.29**	**.25**	.36
SDE	**.31**	**.47**	**.44**	**.29**	**.25**	.35
ADE	**.31**	**.47**	**.43**	**.29**	**.25**	.35
Mean	.39	.55	.52	.33	.31	.42

	H2O	HNO3	N2O	O3	Temp	Mean
SE	273	**614**	**585**	138	**-7**	323
ARD	**196**	**619**	**581**	**92**	**-13**	295
FPCA	1024	1320	1406	637	802	1038
FFPCA	535	**646**	**630**	295	268	475
EDN	261	**623**	**585**	**90**	**4**	312
SDE	**202**	**623**	**585**	**85**	**4**	300
ADE	**202**	**610**	**581**	**87**	**2**	297
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.