# Automatic Relevance Determination for Gaussian Processes with Functional Inputs

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## Automatic Dynamic Relevance Determination

A **framework for Gaussian Processes with functional inputs** [2]. We generalize previous work with indexed inputs [5, 7, 8] and incorporate the ideas behind automatic relevance determination for vectors [9].

Let $X(t) \in \mathcal{X} = \{X : [0,1] \to \mathbb{R}\}$, $t \in [0,1]$ be a functional input, $y \in \mathbb{R}$ a scalar output, and $f : \mathcal{X} \to \mathcal{Y}$ an unknown function with evaluations $y_i = f(X_i)$, $i = 1, \ldots, N \in \mathbb{N}$. We place a GP prior on $f$.

$$\mathbf{y} \sim \mathcal{N}\left(\mathbf{m}_f, \sigma_f^2\, \mathbf{R}_f + \sigma_\varepsilon^2 \mathbf{I}\right) \tag{1}$$

$$(\mathbf{m}_f)_i = m_f(X_i) \tag{2}$$

$$(\mathbf{R}_f)_{ij} = \exp\left\{-0.5\phi^{-2}\, d_f(X_i, X_j)\right\} \tag{3}$$

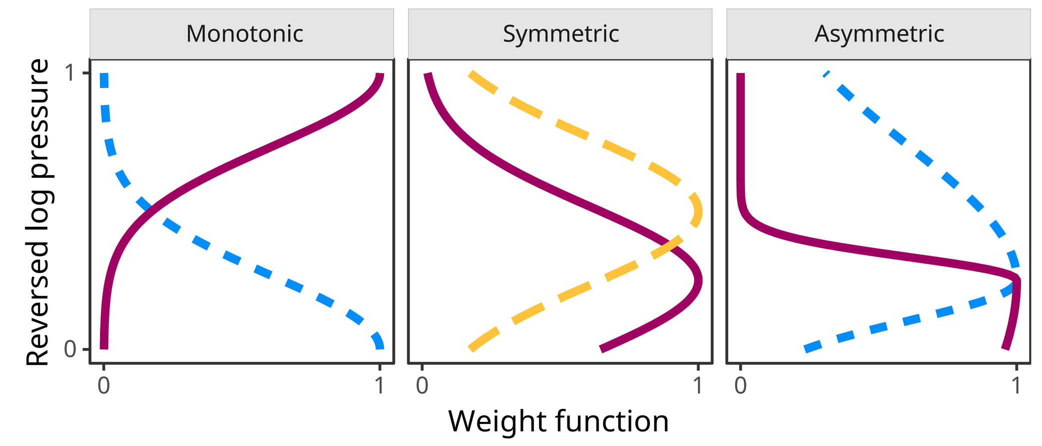
$$d_f(X_i, X_j) = \int_{\mathcal{T}} \omega(t)\big(X_i(t) - X_j(t)\big)^2 dt \tag{4}$$

$$\omega(t) : \mathcal{T} \to \mathbb{R}^+ \tag{5}$$

Space: $\sigma_\varepsilon^2 > 0$, $\sigma_f^2 > 0$, $\phi > 0$, and $m_f(\cdot)$ is left unspecified w.l.o.g.

Priors: $\phi \sim$ InvGamma, and $\sigma_f, \sigma_\varepsilon \sim$ N$^+$

## Asymmetric Squared Exponential weight function




$$\omega(t) = \begin{cases} \exp\left[-(t-\tau)^2 \lambda \kappa^{-1}\right] & \text{for } t \leq \tau \\ \exp\left[-(t-\tau)^2 \lambda \kappa\right] & \text{for } t > \tau \end{cases} \tag{9}$$

Space: $\omega(t) : \mathcal{T} = [0,1] \to (0,1]$, $\tau \in [0,1]$, $\lambda > 0$, $\kappa > 0$

Priors: $\tau \sim$ Beta, $\lambda \sim$ N$^+$, $\log(\kappa) \sim$ N

## Learning & validation

Fully Bayesian inference on the unknown quantities $\boldsymbol{\theta}$. One long chain [10] with $M \in \mathbb{N}$ post warm-up samples generated via the NUTS algorithm [3],

$$\log p(\boldsymbol{\theta}|\mathbf{y}, \mathbf{X}) = -\frac{1}{2}(\mathbf{y} - \mathbf{m}_y)^\top {\mathbf{S}_y}^{-1}(\mathbf{y} - \mathbf{m}_y) - \frac{1}{2}\log|\mathbf{S}_y| + \log p(\boldsymbol{\theta}) \tag{6}$$

where $(\mathbf{X}, \mathbf{y})$ training input and output, $(\mathbf{m}_y, \mathbf{S}_y)$ mean and covariance.

Validation statistic posterior expectation approximated using a thinned posterior parameter sample with $\tilde{M} \in \mathbb{N}$ draws,

$$\hat{v}_1 = \tilde{M}^{-1} \sum_{\tilde{m}=1}^{\tilde{M}} N^{-\frac{1}{2}} \left\| \mathrm{E}\left\langle \boldsymbol{y}_* | \boldsymbol{X}, \boldsymbol{X}_*, \boldsymbol{y}, \boldsymbol{\theta}_{\tilde{m}} \right\rangle - \boldsymbol{y}_* \right\| \tag{7}$$

$$\hat{v}_2 = \tilde{M}^{-1} \sum_{\tilde{m}=1}^{\tilde{M}} p(\boldsymbol{y}_* | \boldsymbol{X}, \boldsymbol{X}_*, \boldsymbol{y}, \boldsymbol{\theta}_{\tilde{m}}) \tag{8}$$

where $(\mathbf{X}_*, \mathbf{y}_*)$ test input and output.

## Input relevance statistics

Most relevant location

$$\tau = \underset{t \in \mathcal{T}}{\arg\max}\, \omega(t) \tag{10}$$

Global relevance

$$\Omega = \phi^{-2} \int_{\mathcal{T}} \omega(t)\, \mathrm{d}t \tag{11}$$

## Choice of weight function

Dynamic input predictive relevance varies over the index space

Smoothness irons out erratic relevance patterns over the index space

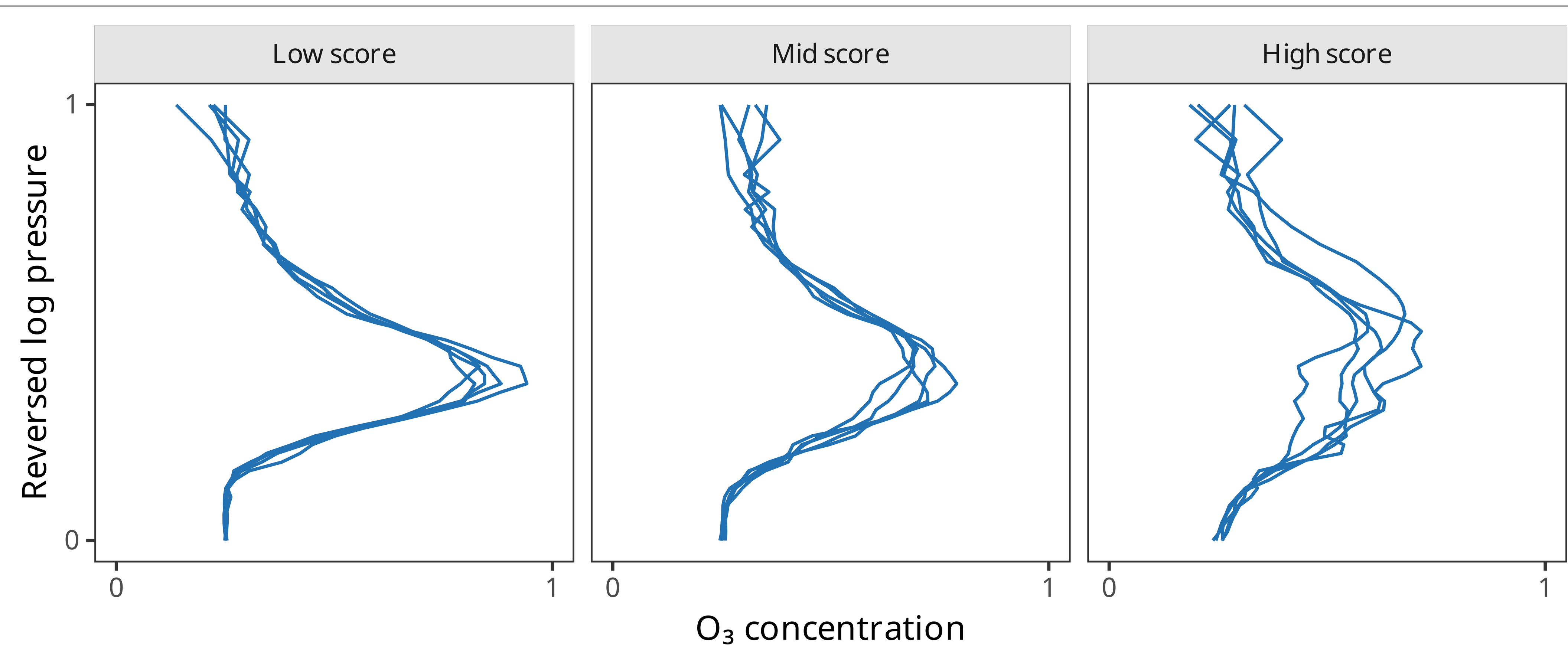
Parsimony fewer parameters than vector representations

Interpretation better physical understanding and statistical modeling

## Microwave Limb Sounder

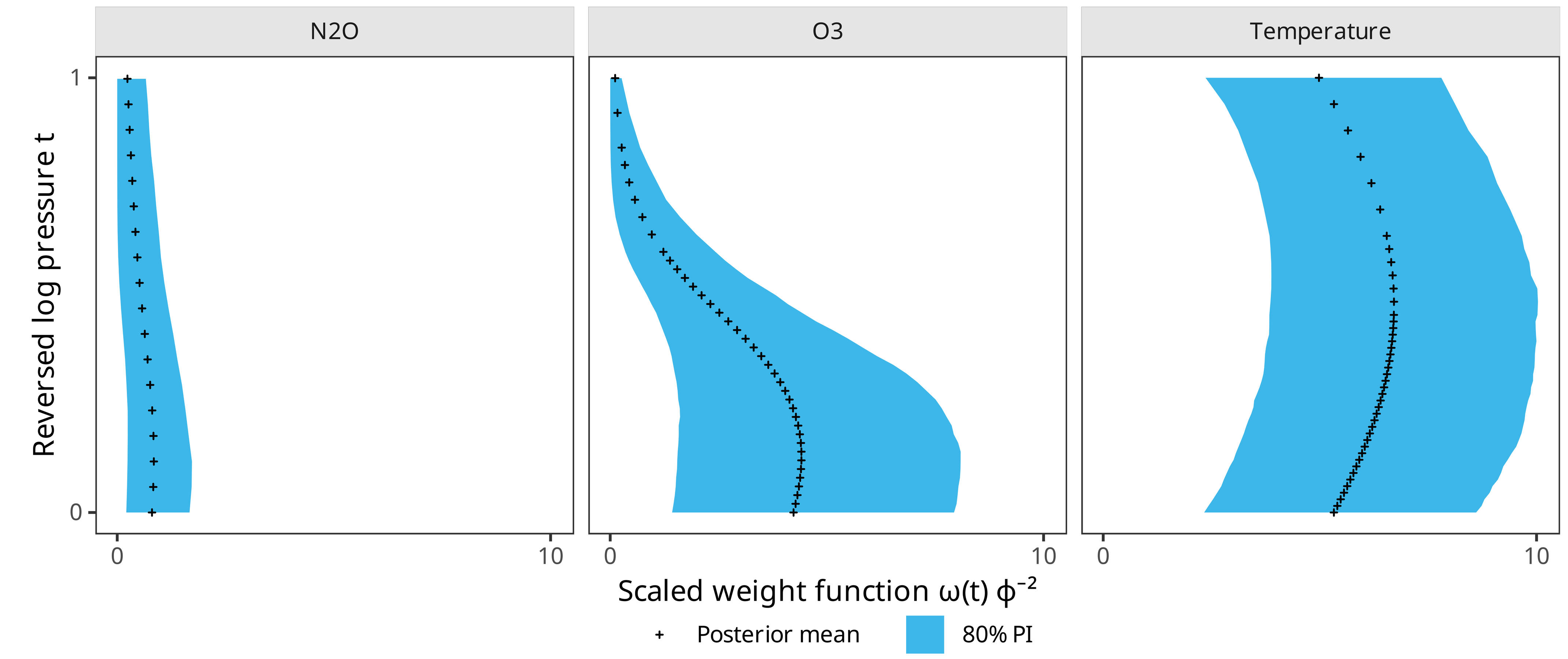
- Computer model: forward model [11, 12, 14] estimates, or *retrieves*, geophysical variables from electromagnetic radiation
- Planetwide, daily data products [6] and uncertainty experiments [1, 13] rely on a myriad of runs
- Output: score for reflected sunlight around 190GHz [4]
- Functional input: atmospheric profiles over a vertical grid
- We consider some species in pressure regions expected to be well-informed by the measurements [6]

## Data

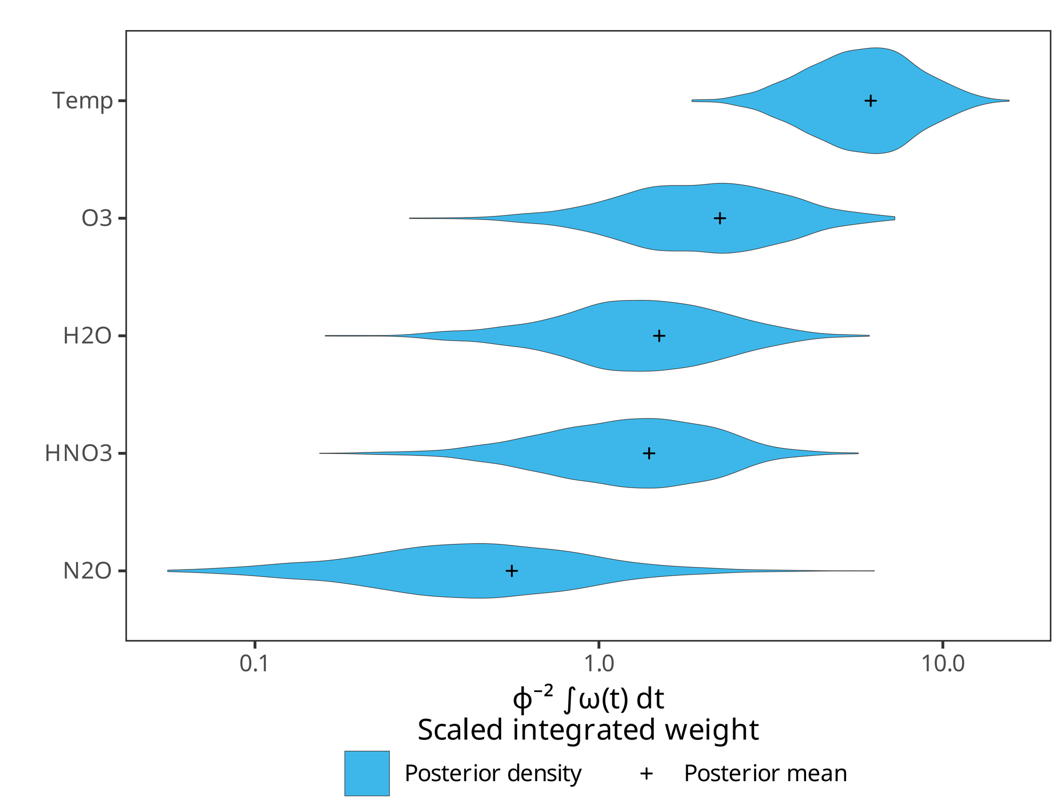



Radiance score variability seems associated with the tropopause Ozone concentration

## Are inputs equally relevant over the atmosphere?




## Are all the inputs equally relevant?




## How does ADRD compare to ARD predictionwise?

| | RMSE | $R^2$ | nCRPS | nPPLD | Cov 95% |
|---|---|---|---|---|---|
| Asym dbl exp | .18 | .97 | .10 | -.03 | .96 |
| Asym sqd exp | .18 | .97 | .10 | -.03 | .96 |
| FPCA (99%) | .34 | .88 | .19 | .03 | .95 |
| Vector SE | .23 | .95 | .13 | -.01 | .98 |
| Vector ARD | .19 | .97 | .10 | -.03 | .97 |

Underline: best in class over 8 data splits using $t_{7,.80} \approx 1.41$.

## In summary

- ADRD and ARD perform similarly predictionwise
- ADRD and ARD agree on the overall relevance patterns
- ADRD has $\sim 15$ times fewer parameters to learn
- ADRD rules out erratic patterns in relevance
- ADRD posterior patterns are consistent with the underlying science
  - Relevance within a chemical species over the vertical grid via the $\omega(t)$ function
  - Relevance between chemical species via the integrated weight statistic $\Omega$

## Onwards and upwards

Toward a framework for Gaussian processes with functional inputs $Y = f(X_1(u), X_2(v), \ldots, x_1, x_2, \ldots)$

- Multiple scalar‡, vector, and functional inputs
- Flexible functional weight forms: ADE, ASE, FEW‡
- Case studies: Microwave Limb Sounder, Water Erosion Prediction Project‡
- Exact integral for piecewise linear inputs‡

‡ Manuscript in preparation

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