

# EGU General Assembly

Towards a new surrogate model for predicting short term  $\text{NO}_x$ - $\text{O}_3$  effects from aviation using Gaussian processes

**Pratik Rao**, Richard Dwight, Deepali Singh, Jin Maruhashi, Irene Dedoussi, Volker Grewe, and Christine Frömming

23<sup>rd</sup> - 28<sup>th</sup> April 2023



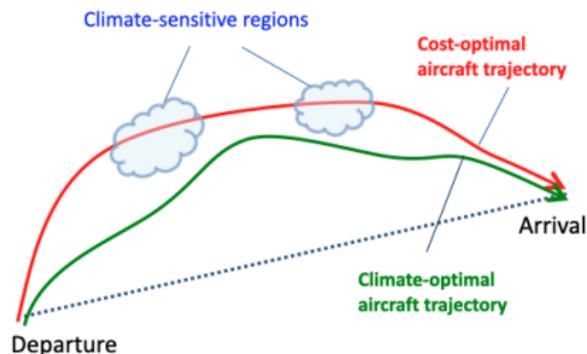
# Why?



Non-CO<sub>2</sub> aviation effects contribute to  $\sim 2/3$  of the climate impact and are characterised by **high uncertainties** [1]

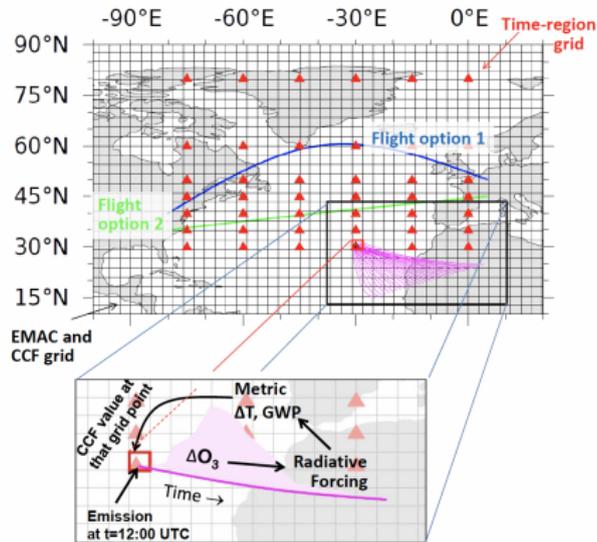


Since the impact depends strongly on emission location, what if we could get flights to avoid **climate sensitive regions**?



# Climate change functions (CCFs)

€ CCFs [2] → global climate impact due to emission at  $(x, t)$  → expensive and restrictive



## Surrogate model (aCCFs)

## Surrogate model (aCCFs)



Reproduce CCF predictions by other means?



Linearly regress CCFs against atmospheric variables  $\rightarrow$  aCCFs:

$$\text{aCCF}_{\text{O}_3} = \theta^T \mathbf{w}, \quad \theta = \langle T, \phi, T\phi \rangle$$

## Surrogate model (aCCFs)



Reproduce CCF predictions by other means?



Linearly regress CCFs against atmospheric variables  $\rightarrow$  aCCFs:

$$\text{aCCF}_{\text{O}_3} = \theta^T \mathbf{w}, \quad \theta = \langle T, \phi, T\phi \rangle$$



Regional flight planning on arbitrary days



Reasonable first estimate [3] but improvements are desirable

# Towards a new surrogate model

Expand geographical coverage of training data [4]



Objective approach to feature selection



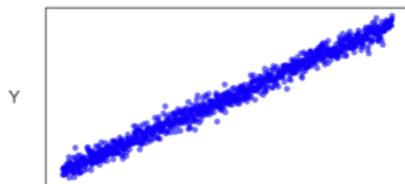
Gaussian process regression model



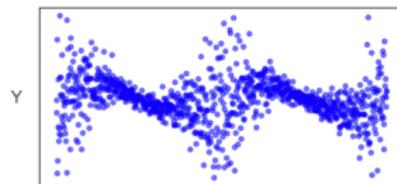
Standard [5]



Chained [6]

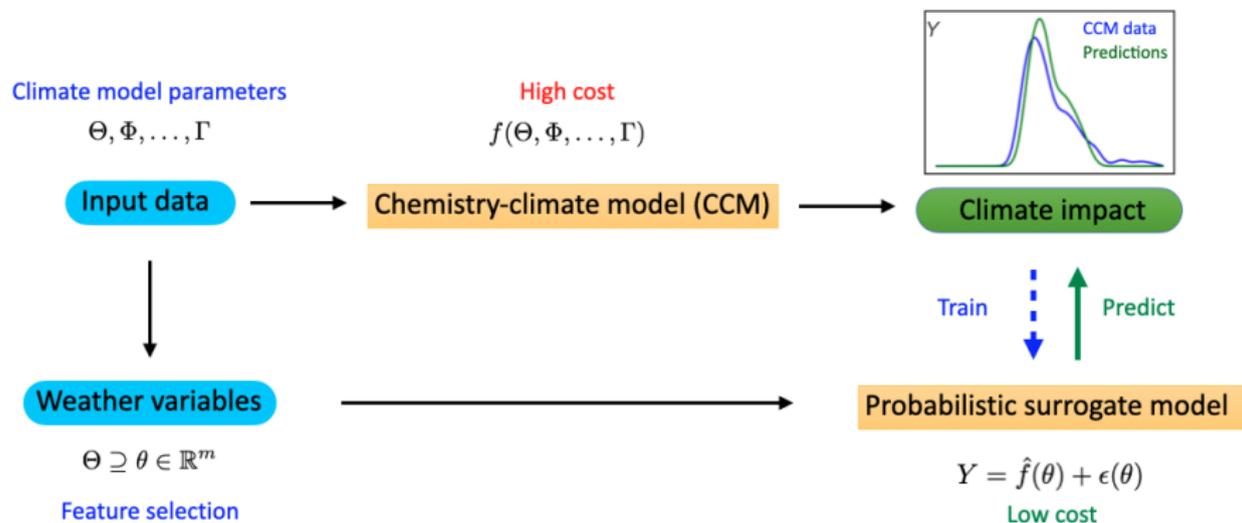


x  
Constant variance



x  
Variance is a function of x

# Towards a new surrogate model



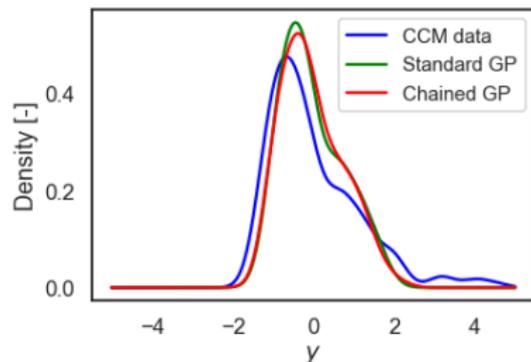
Gaussian process regression is a Bayesian nonparametric approach that can capture more information about  $\mathcal{D} = \{\theta, y\}$  with error bars as data grows:  $p(\hat{f}|\mathcal{D}) \propto p(\hat{f}) p(\mathcal{D}|\hat{f})$

## Results

- ▶ Feature selection yields  $\theta \in \mathbb{R}^6$ : Temperature, geopotential, solar irradiance, specific humidity, zonal velocity, and release location

# Results

- ▶ Feature selection yields  $\theta \in \mathbb{R}^6$ : Temperature, geopotential, solar irradiance, specific humidity, zonal velocity, and release location
- ▶ Full distribution for (predicted) climate impact  $Y$  on test space

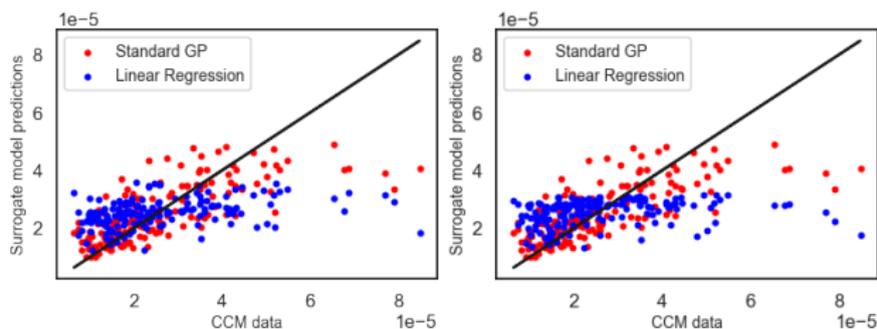


## Results

- ▶ Performs significantly better than Linear regression ( $R^2 = 0.54$ )
- ▶ Linear Regression model: Using selected features ( $R^2 = 0.13$ ) vs original features ( $R^2 = 0.05$ )

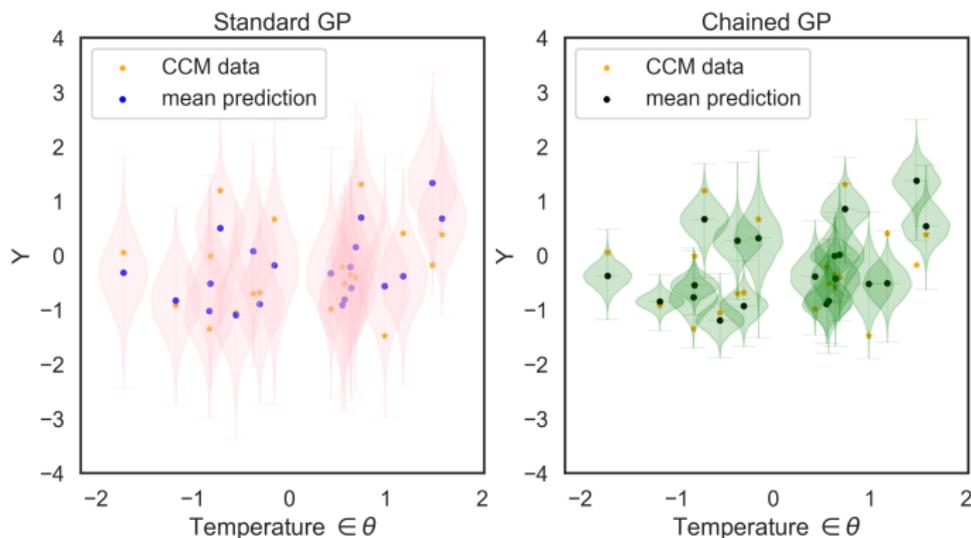
# Results

- ▶ Performs significantly better than Linear regression ( $R^2 = 0.54$ )
- ▶ Linear Regression model: Using selected features ( $R^2 = 0.13$ ) vs original features ( $R^2 = 0.05$ )

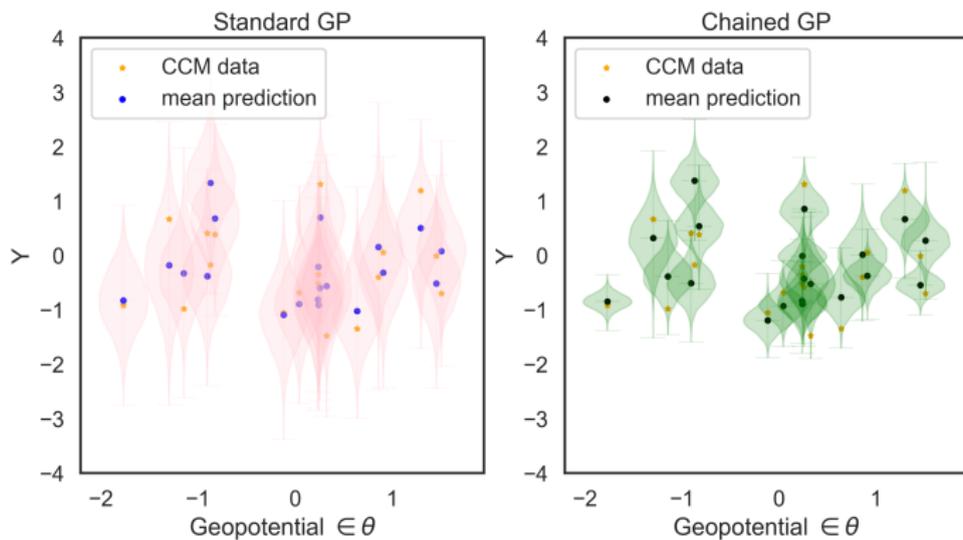


# Results

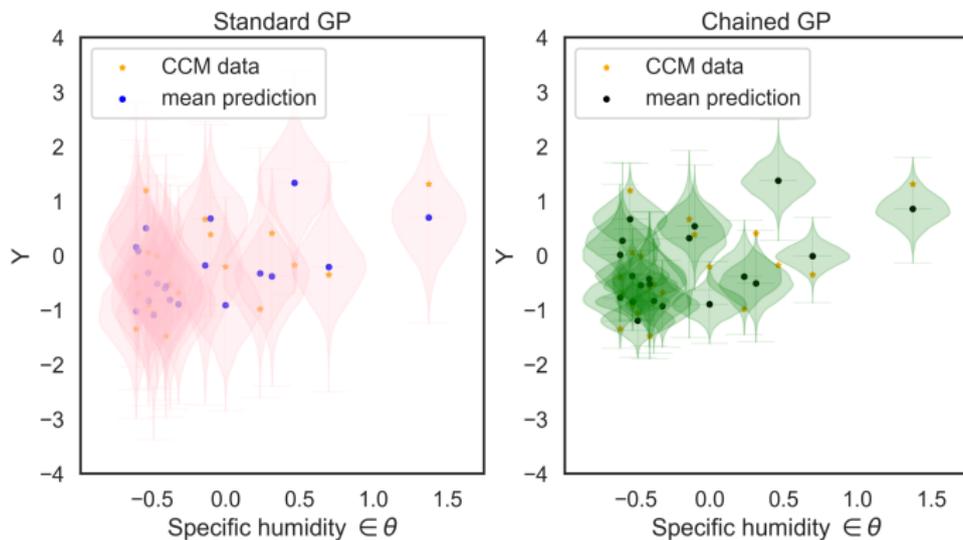
- ▶ Comparing test data and predictions  $\forall \theta$
- ▶ Violin plot shows variance of every prediction in the test space



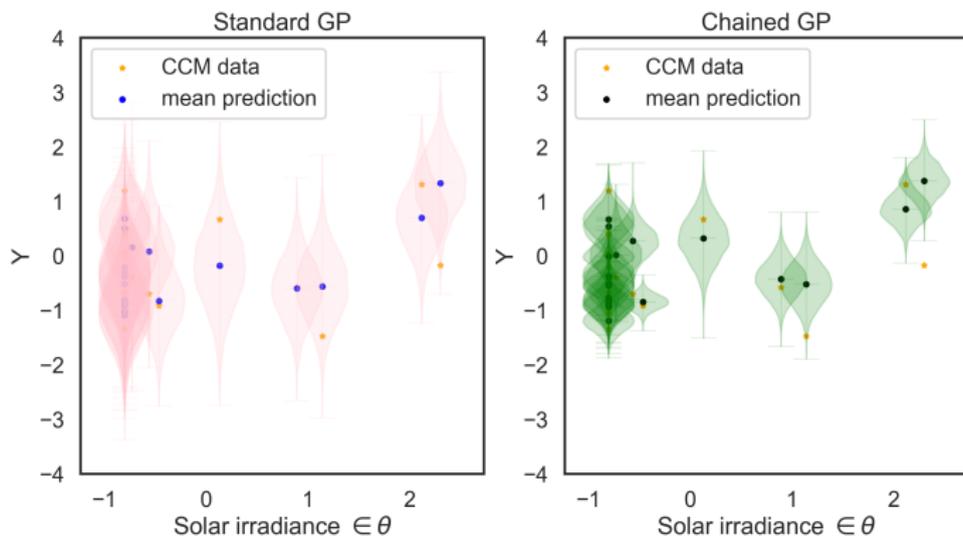
# Results



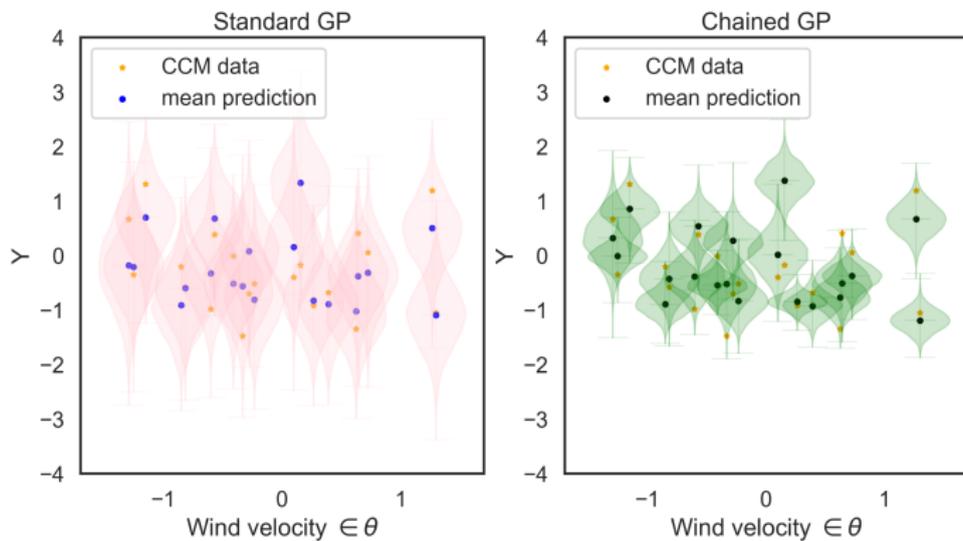
# Results



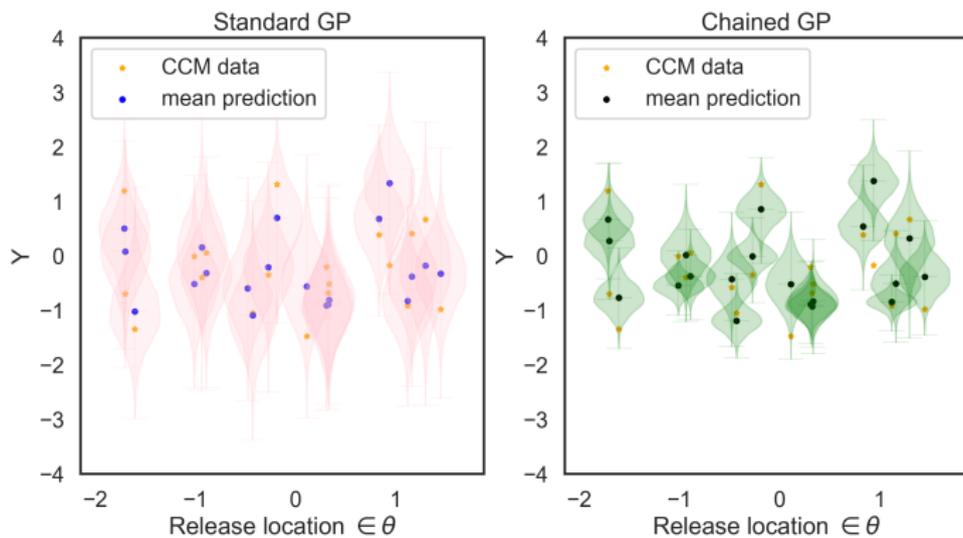
# Results



# Results



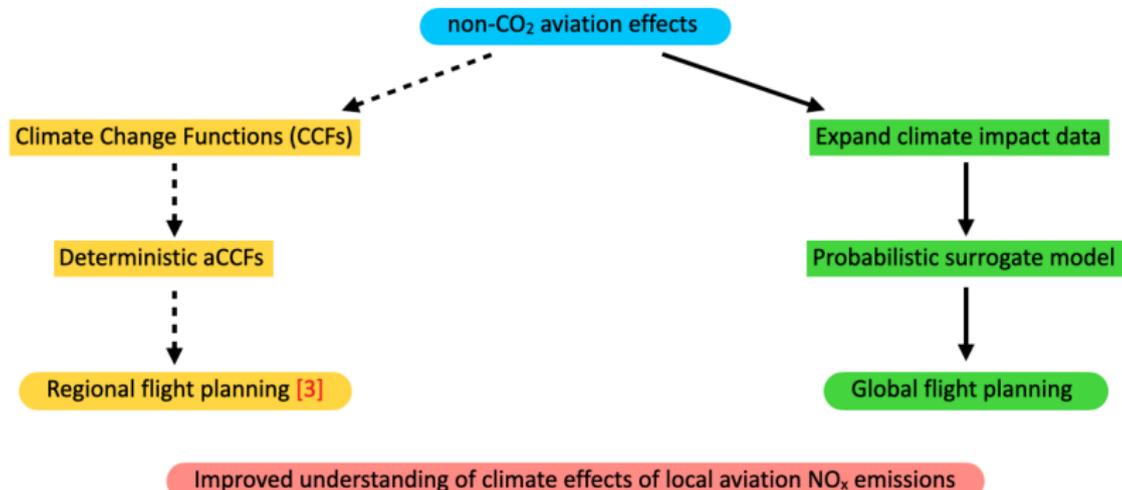
# Results



## Summary

- ▶  $R^2 > 0.50$  for GP models, while  $D_{kl}$  is lower for chained GP model
- ▶ Analyse statistical 'outliers'
- ▶ We have a model that predicts the climate impact of aviation  $\text{NO}_x$  with (varying) confidence levels

# Take away?



## References

- [1] Lee et al., 2020. The contribution of global aviation to anthropogenic climate forcing for 2000 to 2018.
- [2] Grewe et al., 2014. Aircraft routing with minimal climate impact: the REACT4C climate cost function modelling approach (V1.0).
- [3] Rao et al., 2022. Case Study for Testing the Validity of  $\text{NO}_x$ -Ozone aCCFs for Optimising Flight Trajectories.
- [4] Maruhashi et al., 2022. Transport Patterns of Global Aviation  $\text{NO}_x$  and their Short-term  $\text{O}_3$  Radiative Forcing A Machine Learning Approach.
- [5] Rasmussen & Williams, 2006. Gaussian processes for machine learning.
- [6] Saul et al., 2016. Chained Gaussian processes.

Thank you for your kind attention!



QR code for abstract