Neural Representation of the Stratospheric Ozone Chemistry

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Overview: Stratospheric Ozone Chemistry in Climate Science

Lagrangian Chemistry & Transport Model ATLAS

- ☒ Computation time
- ✓ Accuracy

Neural-SWIFT

- ✓ Computation time
- ✓ Accuracy

Stratospheric Chemistry

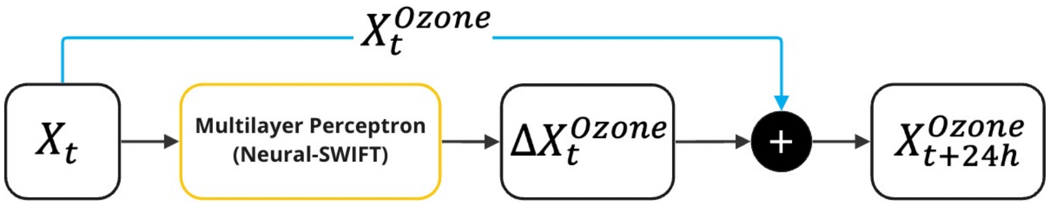
- ~ 47 chemical species
- ~ 171 chemical reactions

Prescribed Ozone tables

- ✓ Computation time
- ☒ Accuracy

How does Neural-SWIFT work?

Applying Multilayer Perceptrons in the forward Euler scheme



where

X_t are input variables at time t;

X_t^{Ozone} is the ozone variable at time t [volume mixing ratio];

ΔX_t^{Ozone} is the 24-hour ozone tendency;

X_{t+24h}^{Ozone} is the updated ozone variable;

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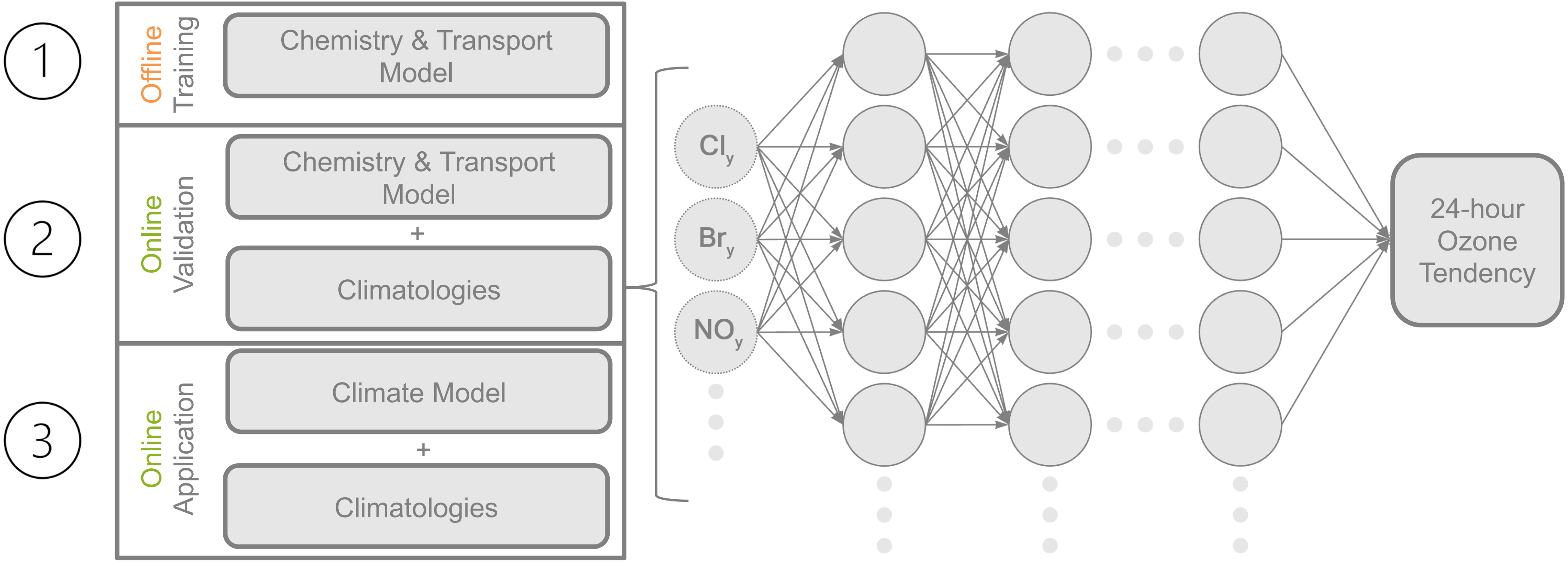
From Input-Output Data Pairs to Application

What sources of input variables (point-wise) can we consider?



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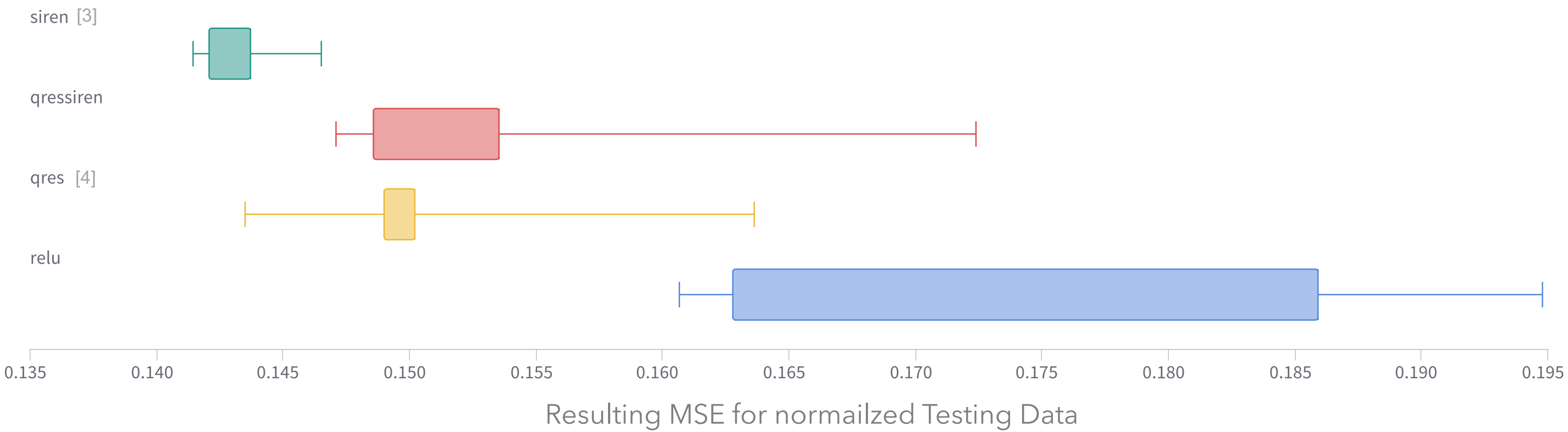
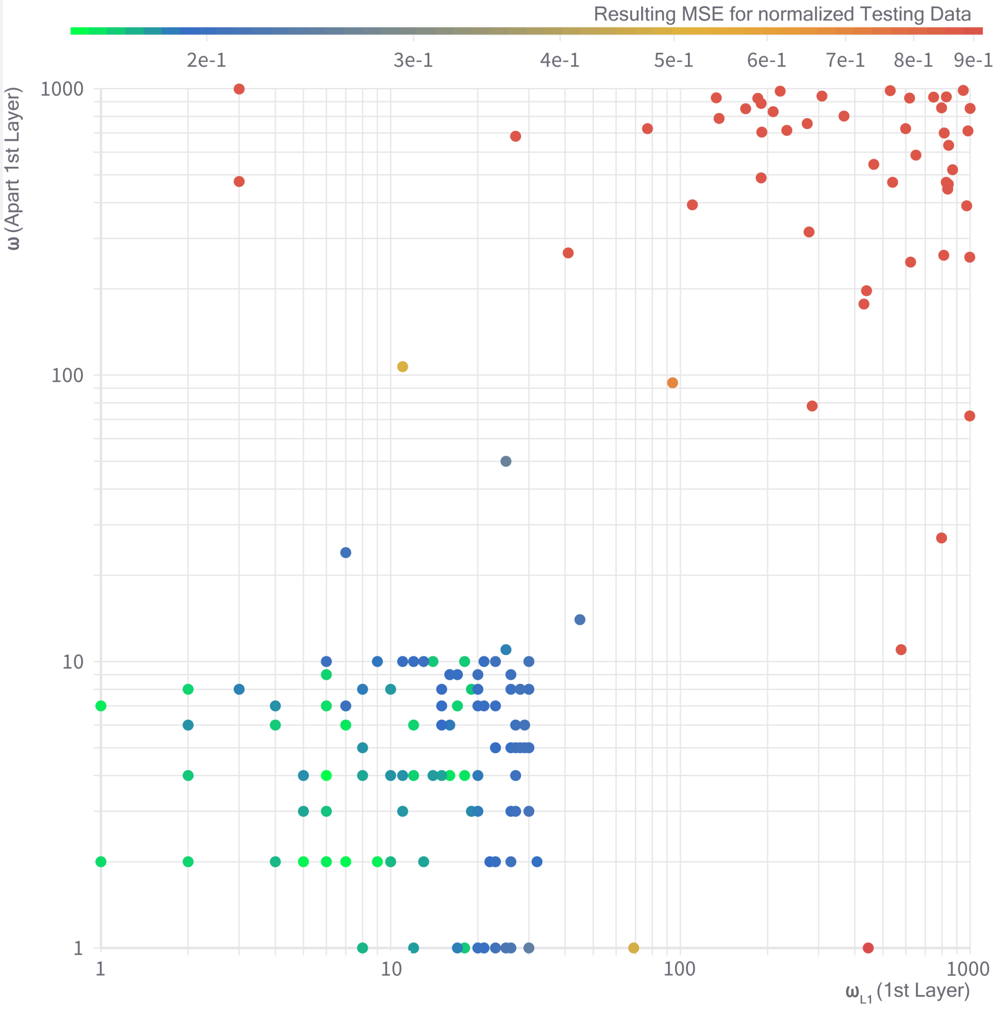
Architectures of Multilayer Perceptrons

Which available architecture performs best on our data set?



Hyperparameter Optimization

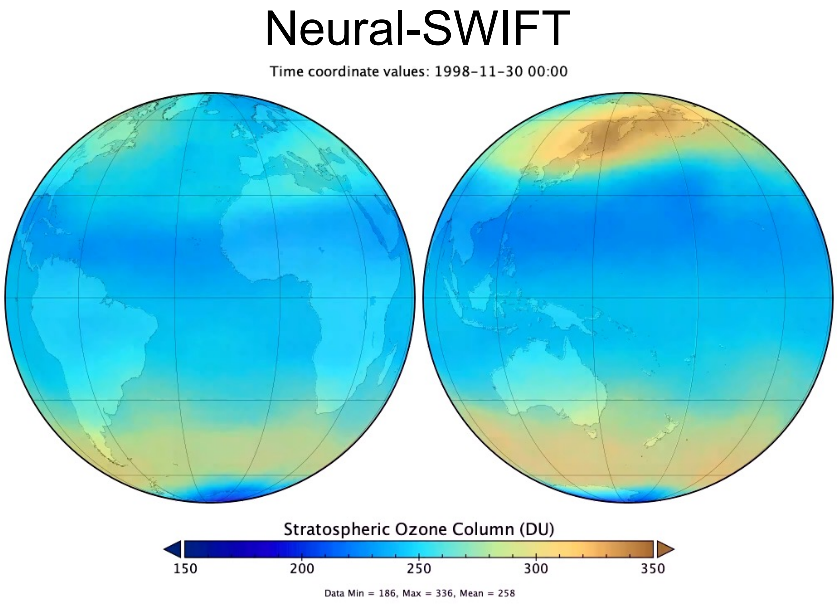
- Bayesian Hyperparameter Search
- Hyperband Early Stopping [5]
- Tuned Hyperparameters:
  1. Number of layers
  2. Number of neurons per layer
  3. Siren [3] parameter ω_{L1} for first
  4. … and one ω for other layers
  5. Learning rate
  6. Mini-Batch size

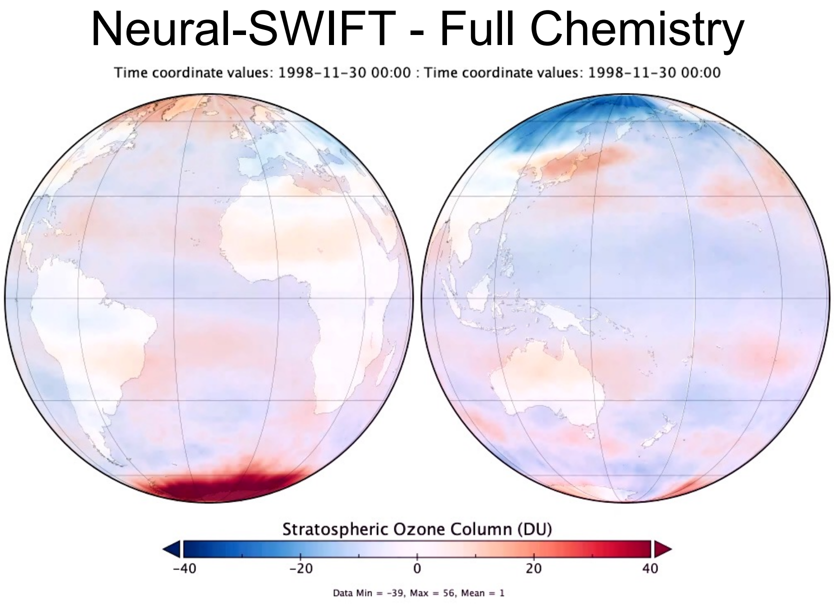


Accuracy & Stability

Is there an error accumulation?

Two-year simulation of Neural-SWIFT coupled to ATLAS:



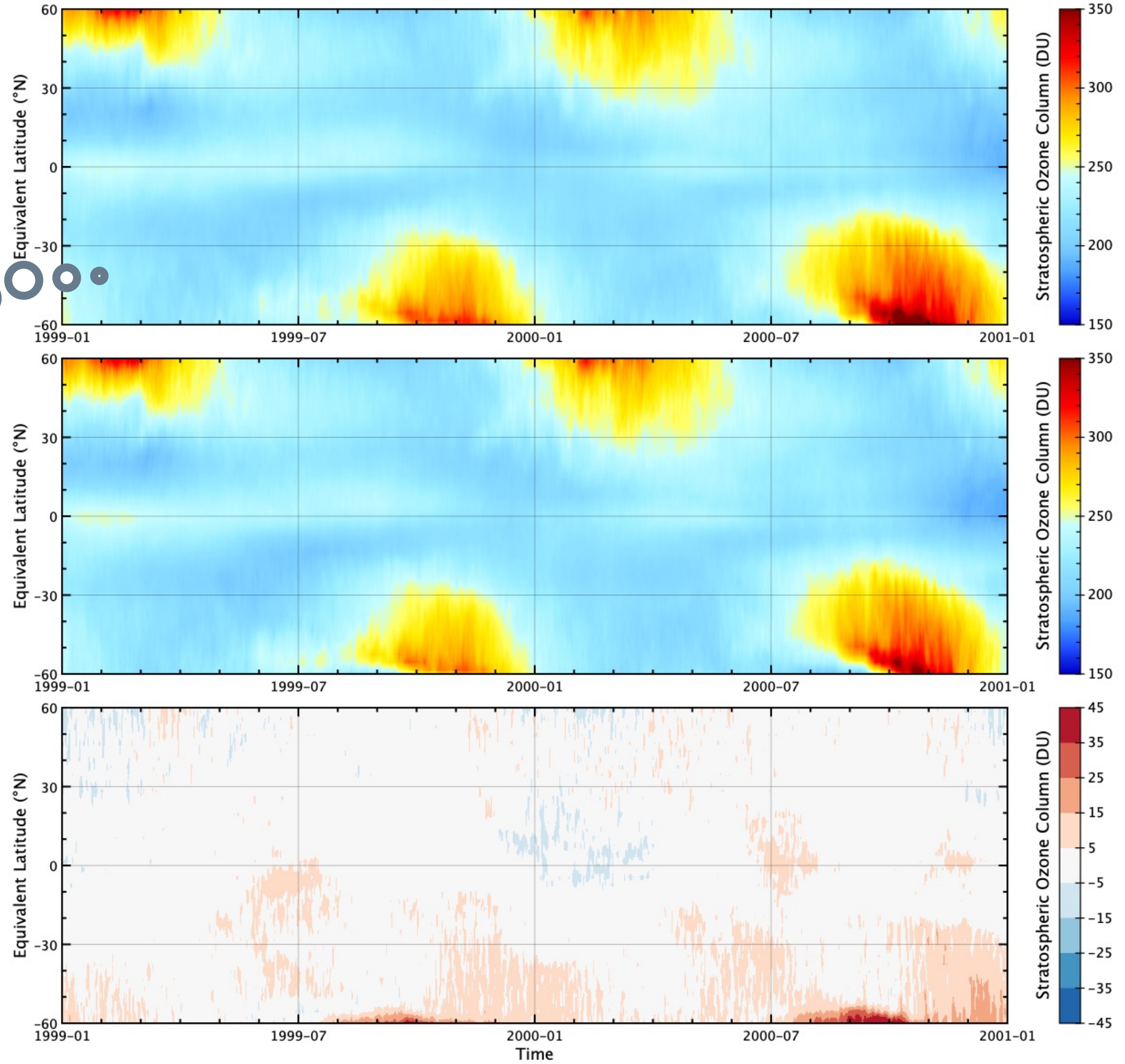


Neural-SWIFT

Accurate & stable over time

Full Stratospheric Chemistry

Difference:
[Neural-SWIFT] – [Full chemistry]



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Speed-Up

Are AI surrogate models significantly faster?

~700 x faster

Simulation	**Neural-SWIFT**	Full Chemistry [2]
1 model-day	**3.4 s**	40 min
1 model-year	**21 min**	> 10 days
100 model-years	**< 1.5 days**	> 1000 days

Note: Neural-SWIFT was coupled to the chemistry and transport model ATLAS and run on the same server with 48 CPUs 1.0-3.9 GHz, 755 GB physical memory. Calculation time refers to chemistry calculation only and does not include time required for transport and mixing in ATLAS.

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Key takeaways

- **Neural-SWIFT** is a data-driven model that enables an **interactive** representation of the **stratospheric ozone chemistry** and is intended for application in climate models.
- Benchmark Dataset open available: https://doi.org/10.1594/PANGAEA.939121
- Neural-SWIFT achieves:

✓ Speed-Up: **factor of 700**

✓ Very accurate

✓ Interactive

✓ Stable: No **significant error accumulation** within a 2-year simulation

Sources

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