Deep Ensemble predicts Exoplanets' Atmospheres Composition

Ariel Data Challenge

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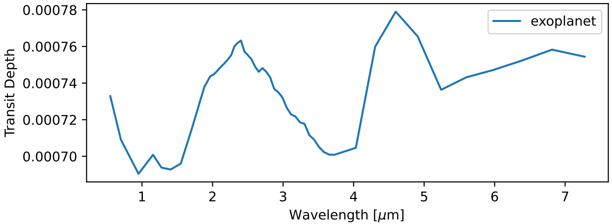
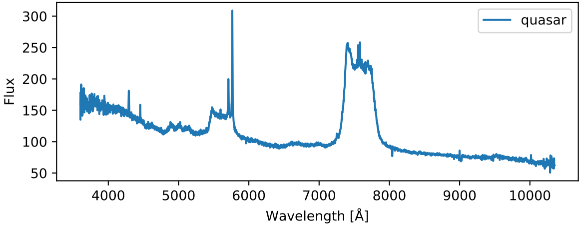
Motivation from Personal Research Perspective

- Research of **predictive uncertainty**.
- Spectra of exoplanetary atmospheres and quasars are similar.





Training Set

Training set

- Includes: annotated spectra with auxiliary data.
- Excludes: unannotated data.

My task's simplification

Predict $\mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$ where

- μ_{ij} are weighted means and σ_{ij}^2 are weighted variances,
- i indexes exoplanets and j indexes the six targets.

The Simplification

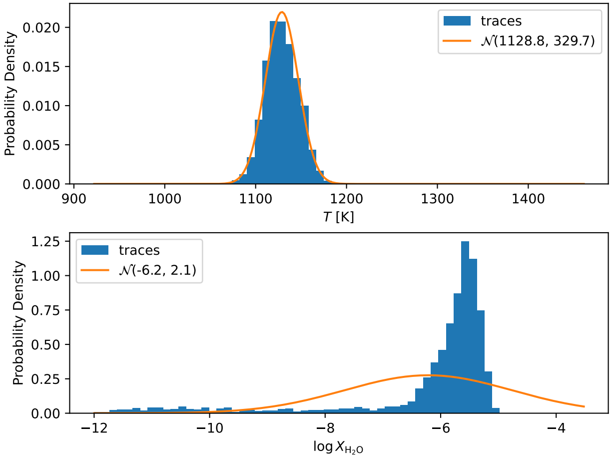


Figure: Exoplanet #2313 traces of T and $\log X_{\mathrm{H_2O}}$ with fitted $\mathcal{N}(\mu_{ij}, \sigma_{ij}^2)$.

Data Preparation

Auxiliary data

Standardisation of **each feature** (star distance, etc.).

Spectra scaling

Standardisation of **each spectrum's transit depths**.

Spectra Scaling's Effect

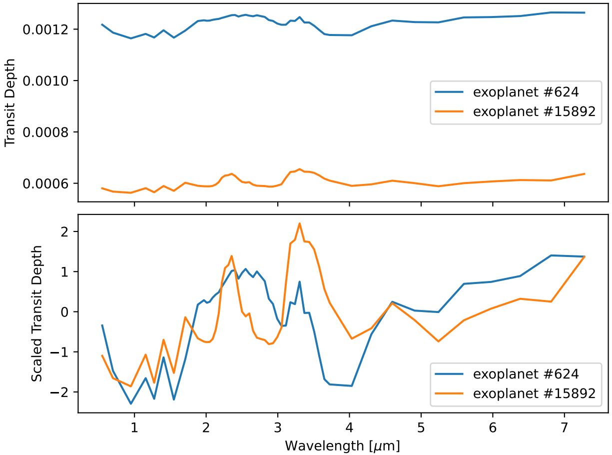


Figure: Two spectra before (top) and after (bottom) spectra scaling.

My Convolutional Neural Network (CNN)

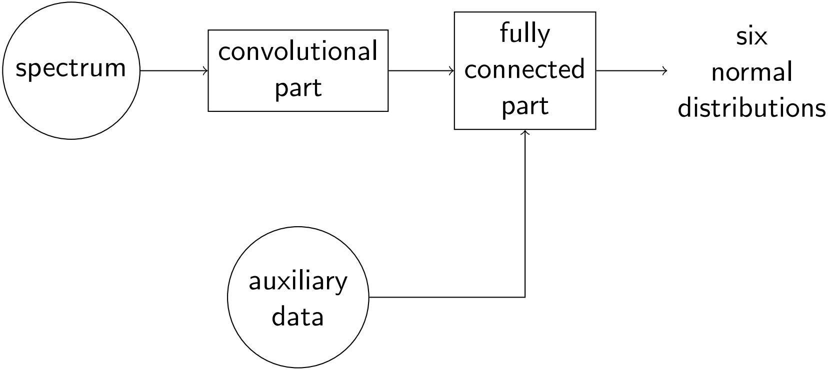


Figure: Schema of the CNN's prediction process.

CNN's Output: Six Normal Distributions

1. $\mathcal{N}(\hat{\mu}_{i1}, \hat{\sigma}^2_{i1})$ for T
2. $\mathcal{N}(\hat{\mu}_{i2}, \hat{\sigma}^2_{i2})$ for $\log X_{\mathrm{H_2O}}$
3. $\mathcal{N}(\hat{\mu}_{i3}, \hat{\sigma}^2_{i3})$ for $\log X_{\mathrm{CO_2}}$
4. $\mathcal{N}(\hat{\mu}_{i4}, \hat{\sigma}^2_{i4})$ for $\log X_{\mathrm{CH_4}}$
5. $\mathcal{N}(\hat{\mu}_{i5}, \hat{\sigma}^2_{i5})$ for $\log X_{\mathrm{CO}}$
6. $\mathcal{N}(\hat{\mu}_{i6}, \hat{\sigma}^2_{i6})$ for $\log X_{\mathrm{NH_3}}$

- Output units of $\hat{\mu}_{ij}$ are identities.
- Output units of $\hat{\sigma}^2_{ij}$: $\mathrm{softplus}(z) = \log(1 + e^z)$.

Loss Function Variants

- point value to distribution
  - negative log-likelihood (NLL)
  - continuous ranked probability score (CRPS)
- distribution to distribution
  - Kullback–Leibler (KL) divergence
  - Wasserstein distance

Final Training

- KL divergence worked best.
- The whole training set is used to train final models!

Deep Ensembles[1]

- Deep ensemble of 20 CNNs.
- Each CNN predicts six normal distributions.
- Generate 250 samples from predicted normal distributions.
- **Regular track**: Output is the 5000 samples in total.
- **Light track**: Compute quartiles of those 5000 samples.

[1] Lakshminarayanan, B., Pritzel, A., Blundell, C., 2017. Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles, in: Advances in Neural Information Processing Systems 30.

Problem: Simulated Data

- Performance will be worse on **real** data.
- Distributions of simulated and real data (likely) differ.
- Machine learning assume that data are **i.i.d.**

Active Domain Adaptation (ADA)

- ADA mitigates a difference between **source** and **target** data.

$$\begin{tikzcd}
\text{simulated spectra} \arrow[r] & \text{deep ensemble} \arrow[r] & \text{real spectra} \arrow[d] \\
& \text{annotated real spectra} \arrow[u] & \text{slow standard method} \arrow[l]
\end{tikzcd}$$

Conclusion

If you are uncertain what to do, use an uncertain deep ensemble:

- Deep ensembles are powerful at estimating **predictive uncertainty**.
- There is potential for **active domain adaptation**.

Code

See `https://github.com/podondra/ariel-data-challenge`.

Thanks

Thank the organisers for organising this challenge.

Acknowledgement

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CNN's Architecture: Modification of VGG Net-A[2]

Type of Layer	Hyperparameters
convolutional	8 kernels
max pooling	
convolutional	16 kernels
max pooling	
convolutional	32 kernels
convolutional	32 kernels
max pooling	
convolutional	64 kernels
convolutional	64 kernels
max pooling	
$6 \times$ fully connected	1024 neurons
fully connected	12 neurons

[2] Simonyan, K., Zisserman, A., 2015. Very Deep Convolutional Networks for Large-Scale Image Recognition. arXiv:1409.1556.

Loss Function Variants

- negative log-likelihood (NLL):

$$\ln \hat{\sigma}_{ij}^2 + \frac{(\mu_{ij} - \hat{\mu}_{ij})^2}{\hat{\sigma}_{ij}^2}$$

- continuous ranked probability score (CRPS):

$$\hat{\sigma}_{ij} \left\{ \frac{\mu_{ij} - \hat{\mu}_{ij}}{\hat{\sigma}_{ij}} \left[2\Phi \left(\frac{\mu_{ij} - \hat{\mu}_{ij}}{\hat{\sigma}_{ij}} \right) - 1 \right] + 2\varphi \left(\frac{\mu_{ij} - \hat{\mu}_{ij}}{\hat{\sigma}_{ij}} \right) - \frac{1}{\sqrt{\pi}} \right\}$$

- Kullback–Leibler (KL) divergence:

$$\ln \frac{\hat{\sigma}_{ij}^2}{\sigma_{ij}^2} + \frac{\sigma_{ij}^2 + (\hat{\mu}_{ij} - \mu_{ij})^2}{\hat{\sigma}_{ij}^2}$$

- Wasserstein distance:

$$(\hat{\mu}_{ij} - \mu_{ij})^2 + (\hat{\sigma}_{ij} - \sigma_{ij})^2$$