Deep neural networks for total organic carbon prediction and data-driven sampling

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EGU Session - ESSI1.15
Towards SMART Monitoring
6.5.2020

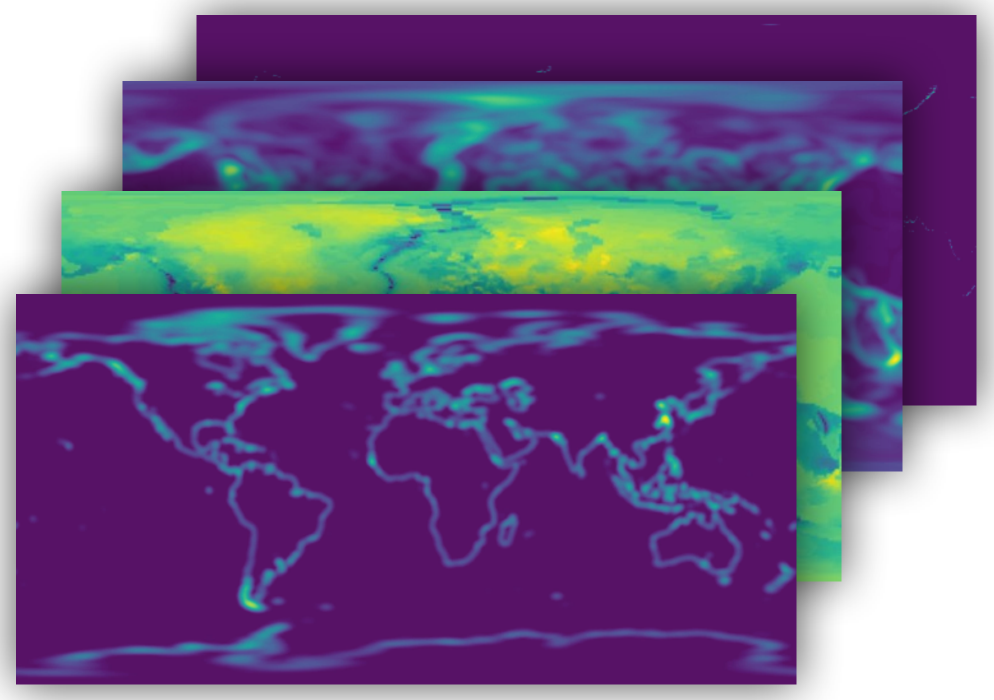
DIGITAL EARTH

1. Introduction:

An idealised Machine Learning Workflow according to a computer scientist

Idealised ML Workflow:

1. Find a set of labels and predictors for your problem



Predictors: ~600 global feature girds

https://zenodo.org/record/1471639#.XPTToCaxXGr

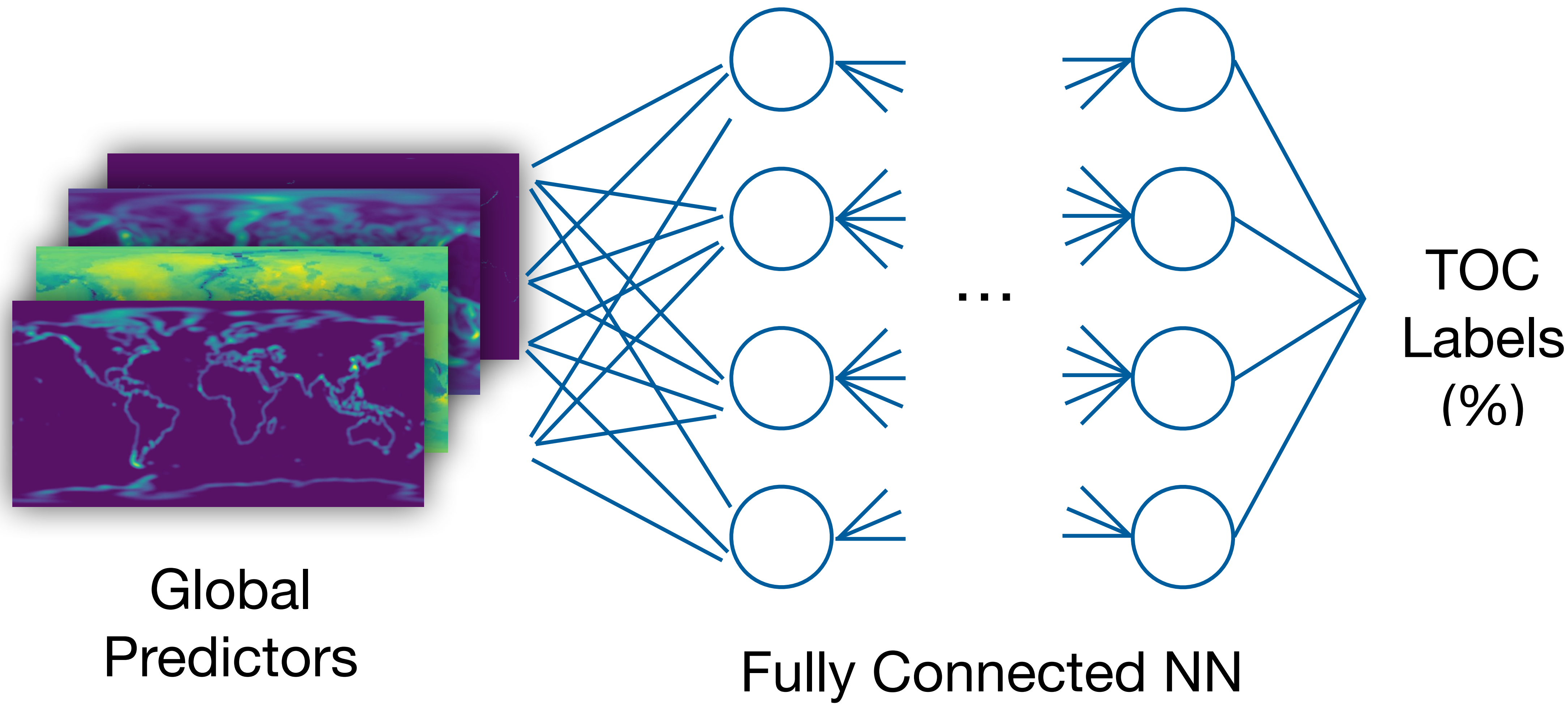
Event	Latitude	Longitude	Elevation [	Depth [m]	TOC [%]
3-14	-28.3315	-20.9410	-4343	0.0000	0.20
8-73	-1.9097	-137.4687	-4387	0.0300	0.10
10103-1B	36.1600	20.4800	-2880	0.0500	0.20
10103-8K	36.1600	20.4800	-2895	0.0150	0.30
108-663	-1.1978	-11.8785	-3706	0.0000	0.19
108-663A	-1.1978	-11.8785	-3706	0.0000	0.19
108-664	0.1073	-23.2275	-3807	0.0000	0.20
108-664B	0.1073	-23.2275	-3806	0.0000	0.20
11BC39	1.9548	-22.7830	-4210	0.0300	0.38
12BC47-2	0.0067	-22.9968	-3858	0.0300	0.58
13BCP56	-2.1083	-23.0050	-4950	0.0300	0.90
159-959	3.6276	-2.7355	-2091	0.0000	1.22
159-959C	3.6277	-2.7353	-2091	0.0250	1.22
159-962	3.2512	-3.1820	-4637	0.0000	1.22
159-962B	3.2511	-3.1820	-4637	0.0500	1.22
167-1011	31.2803	-117.6096	-2021	0.0500	1.82

Labels: ~6000 Total Organic Carbon (TOC) measurements

https://doi.pangaea.de/10.1594/PANGAEA.199835

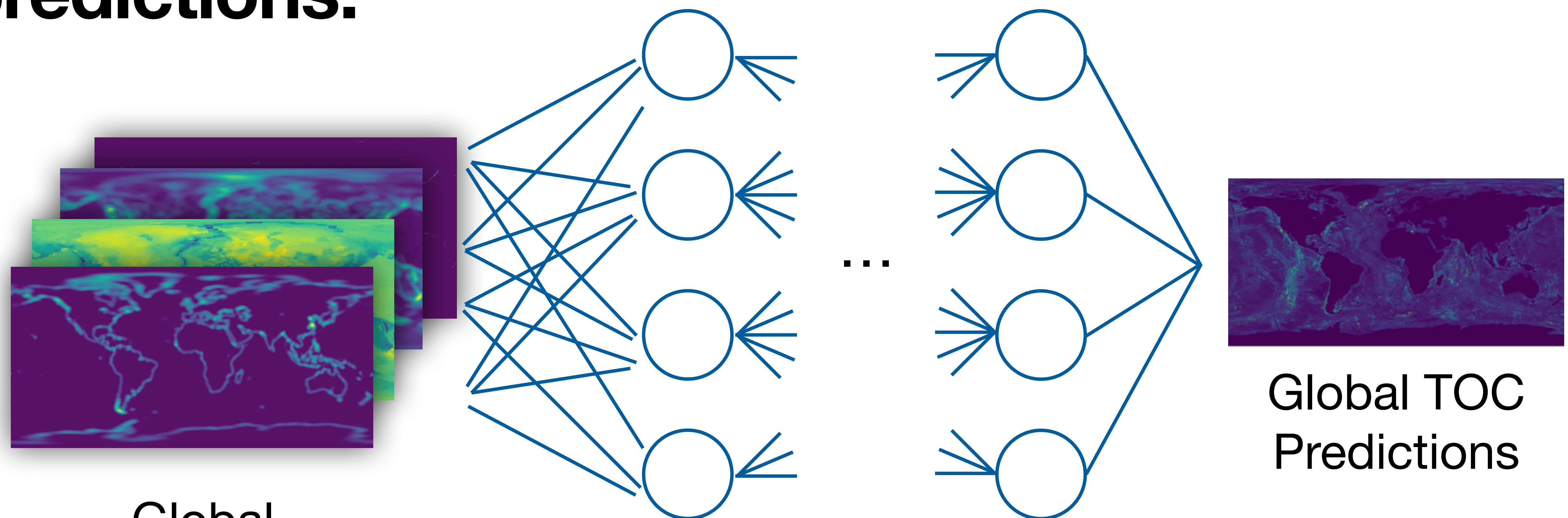
Idealised ML Workflow:

2. Use the predictors and labels to train an ML model



Idealised ML Workflow:

3. Achieve great model accuracy in test and validation datasets and make global predictions:



Global Predictors

Fully Connected NN

Global TOC Predictions

Idealised ML Workflow:

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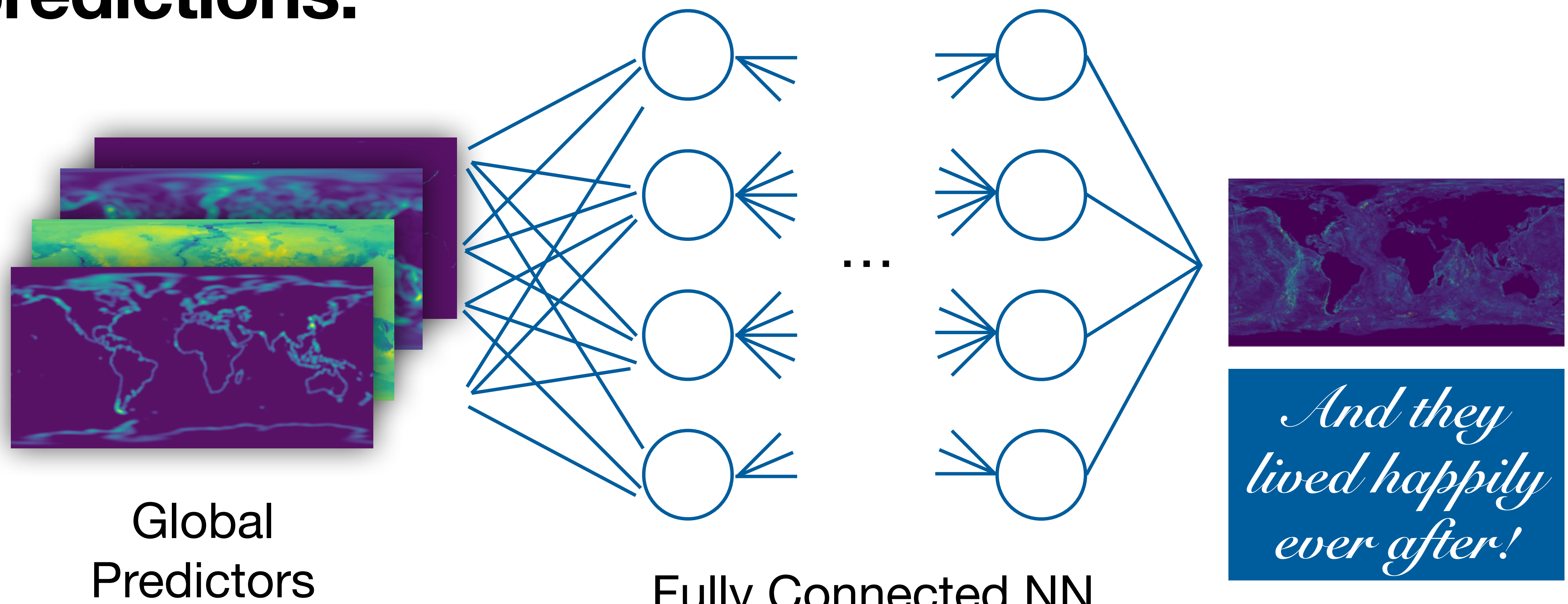

Idealised ML Workflow:

This idealised workflow contains many inaccuracies and oversimplifications incompatible with the application of machine learning to science.

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The following slides will discuss what's probably the most problematic one:

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Idealised ML Workflow:

This idealised workflow contains many inaccuracies and oversimplifications incompatible with the application of machine learning to science.

The following slides will discuss what's probably the most problematic one:

"Achieve great model accuracy, make global predictions…"

… and they lived happily ever after!

2. Data-Driven Sampling:

Neural Networks and Information Gain

Neural Networks and Information Gain

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For example, a question that good model accuracy is unable to answer is that of "data-driven sampling"…

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For example, a question that good model accuracy is unable to answer is that of "data-driven sampling"…

… that is: *assuming this model is correct, where should one sample next?*

Neural Networks and Information Gain

Information Theory can provide an answer using "Information Gain":

Entropy: $$H(P) = -\sum_{x \in X} p(x) \cdot log(p(x))$$ **"Information"**

Cross Entropy: $$H(P,Q) = -\sum_{x \in X} p(x) \cdot log(q(x))$$ **"Message Length"**

KL-Divergence: $$D_{KL}(P \,||\, Q) = H(P,Q) - H(P)$$ **"Information Gain"**

Neural Networks and Information Gain

Information Theory can provide an answer using "Information Gain":

probability distributions

Entropy: $$H(P) = -\sum_{x \in X} p(x) \cdot log(p(x))$$ **"Information"**

observed distribution predicted distribution

Cross Entropy: $$H(P,Q) = -\sum_{x \in X} p(x) \cdot log(q(x))$$ **"Message Length"**

KL-Divergence: $$D_{KL}(P||Q) = H(P,Q) - H(P)$$ **"Information Gain"**

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Neural Networks and Information Gain

Assuming sampling as a prediction with absolute certainty:

$$D_{KL}(P\,||\,Q) = H(P,Q) - H(P)$$

$$= -\sum_{x \in X} \cancel{p(x)} \cdot log(q(x)) + \sum_{x \in X} \cancel{p(x)} \cdot \cancel{log(p(x))}$$

Sampling!

$$= -\,log(q(x_i))$$

Neural Networks and Information Gain

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Sampling!

$$= -\,log(q(x_i))$$

"Information-Gain from sampling is the highest where the prediction probability is the lowest"

Neural Networks and Information Gain

… however, TOC estimation is a regression problem, and we need probability distributions:

We have: 0 50 100 %

probability distributions

We want: $$H(P,Q) = -\sum_{x \in X} p(x) \cdot log(q(x))$$

Neural Networks and Information Gain

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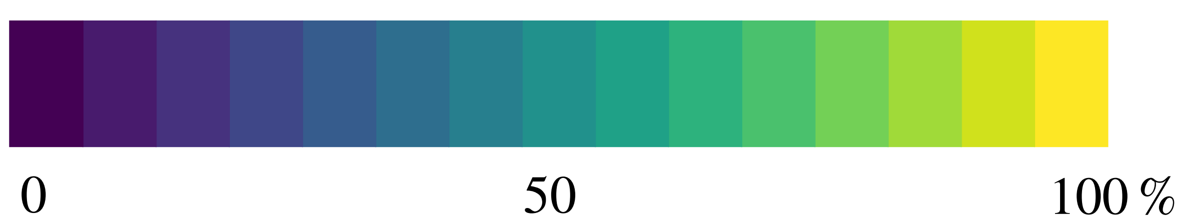
We have:

We want:

probability distributions

$$H(P, Q) = -\sum_{x \in X} p(x) \cdot log(q(x))$$

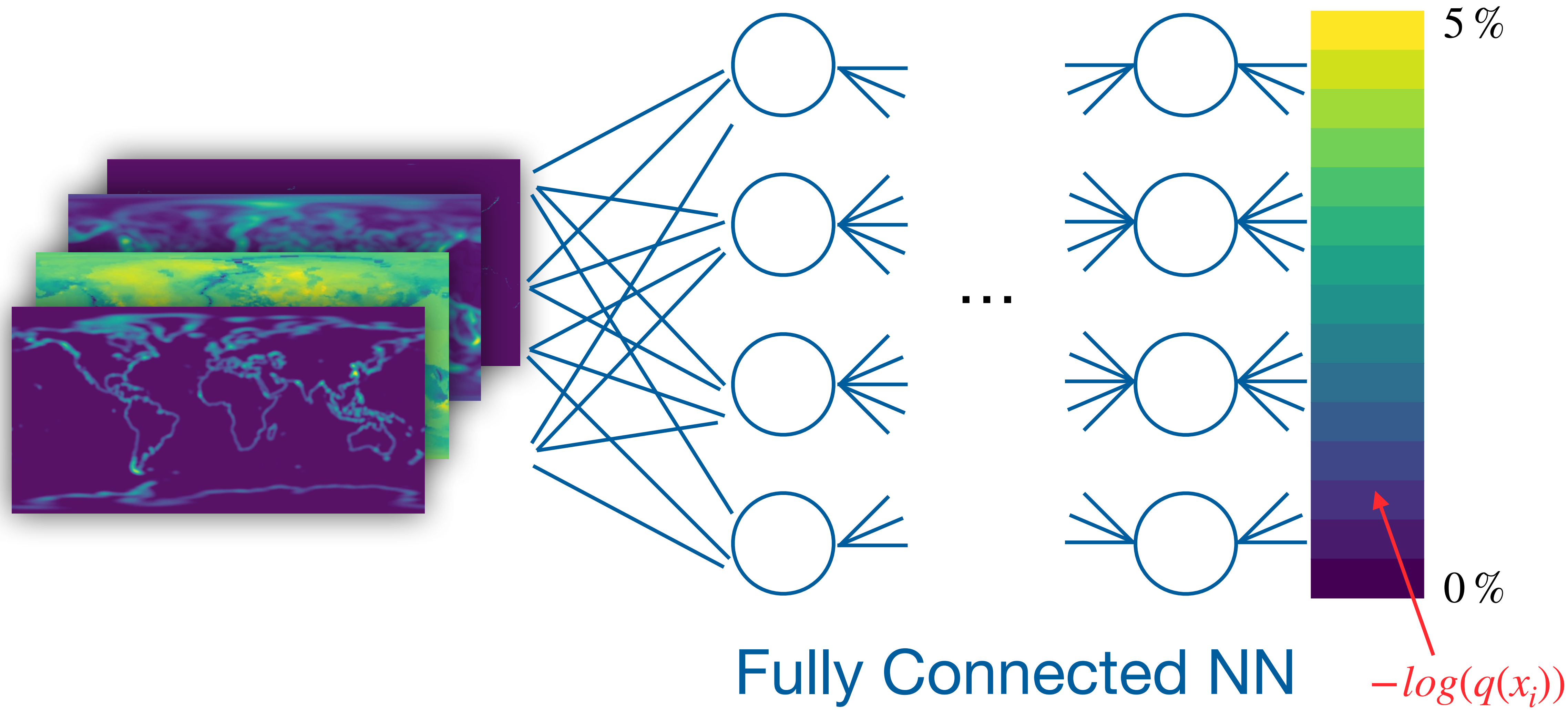
Solution:



This can be solved by digitising the output range…

Neural Networks and Information Gain

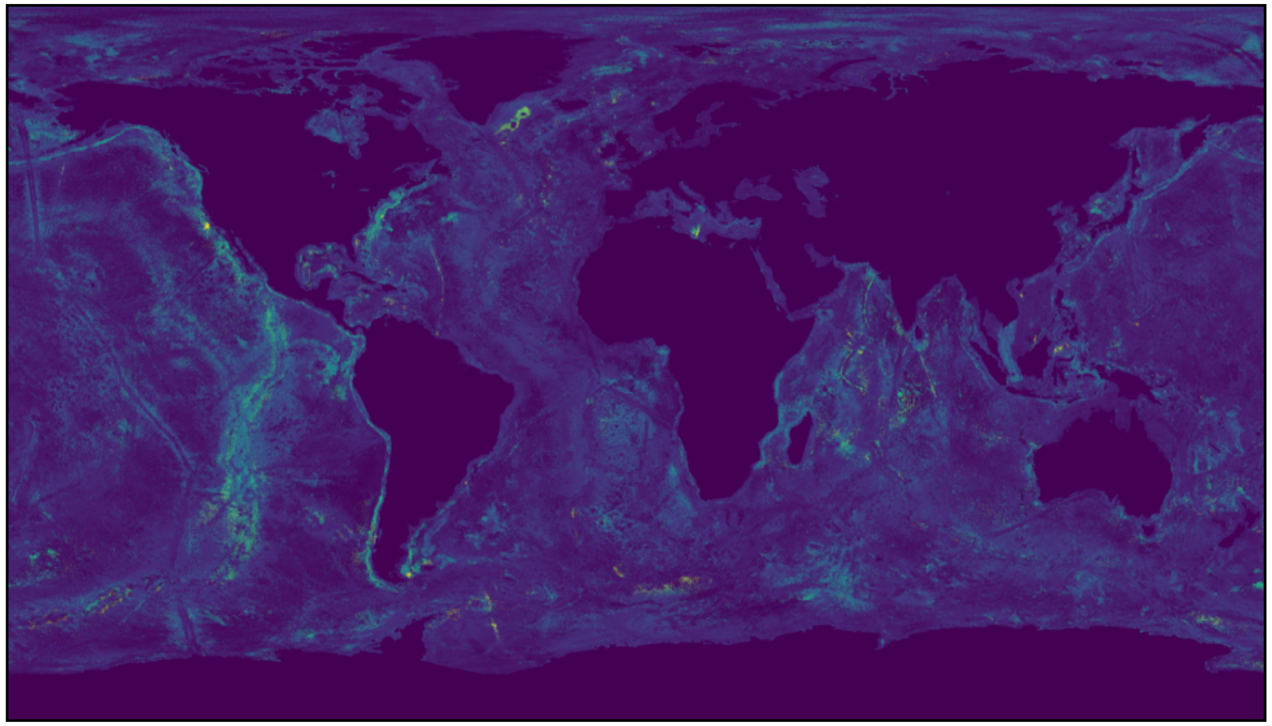
… and applying it to a *softmax* activation layer at the the of the fully connected NN:



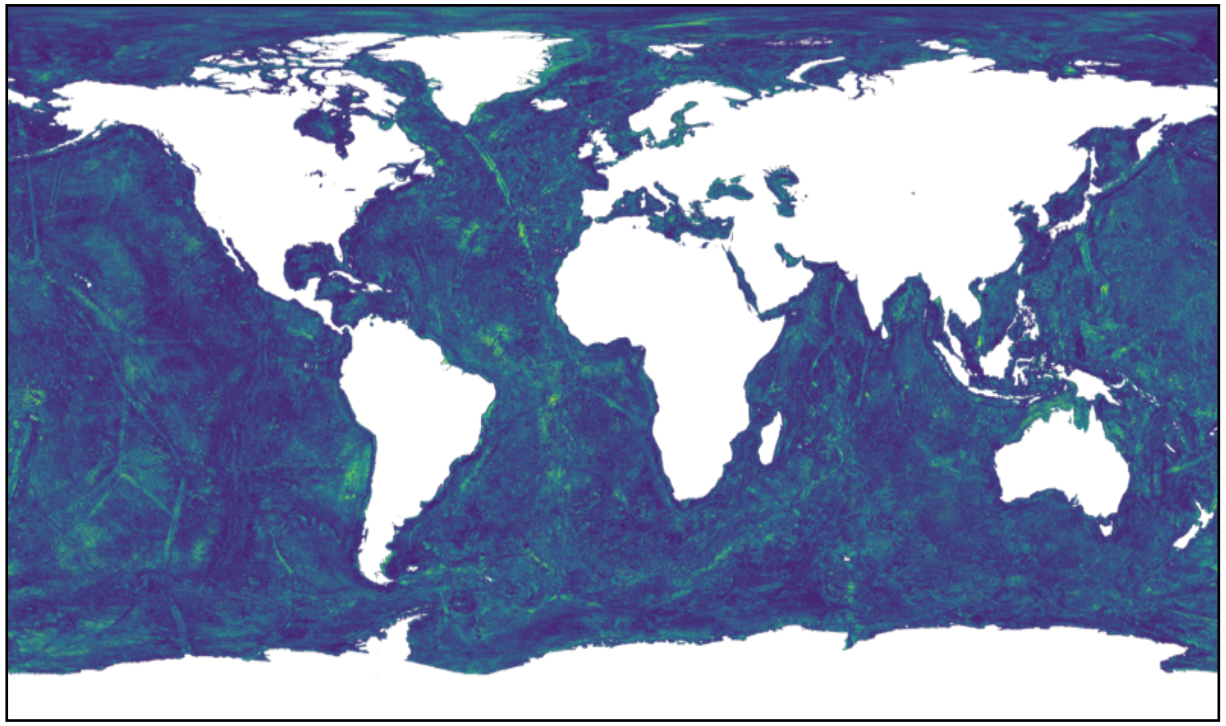
Neural Networks and Information Gain

Such a model produces a prediction along with a probability for it:

Global TOC Predictions



Global Information Gain Predictions



3. Monte Carlo Dropout

Neural Networks and Uncertainty Quantification

Uncertainty Quantification

Back to the question of data-driven sampling:

assuming this model is correct, where should one sample next?

Uncertainty Quantification

Back to the question of data-driven sampling:

***assuming this model is correct*, where should one sample next?**

**This is an uncomfortable assumption to make!
A quantification of model uncertainty would be much preferable.**

Uncertainty Quantification

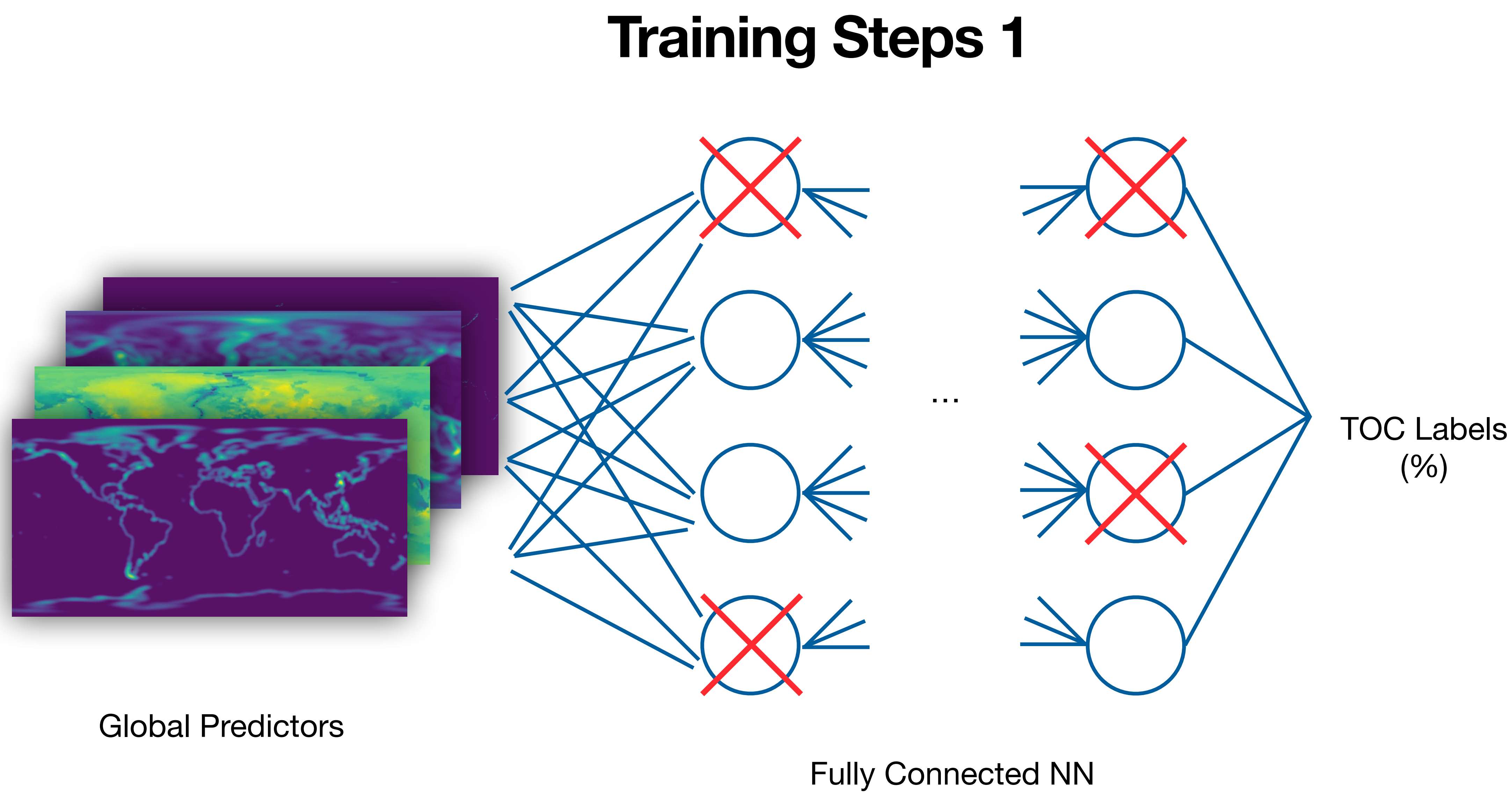
“Dropout[1]” is a standard technique for training neural networks.

It avoids overfitting by randomly deactivating connections between nodes of a neural networks during the training process.

1 https://www.cs.toronto.edu/~hinton/absps/JMLRdropout.pdf

Uncertainty Quantification

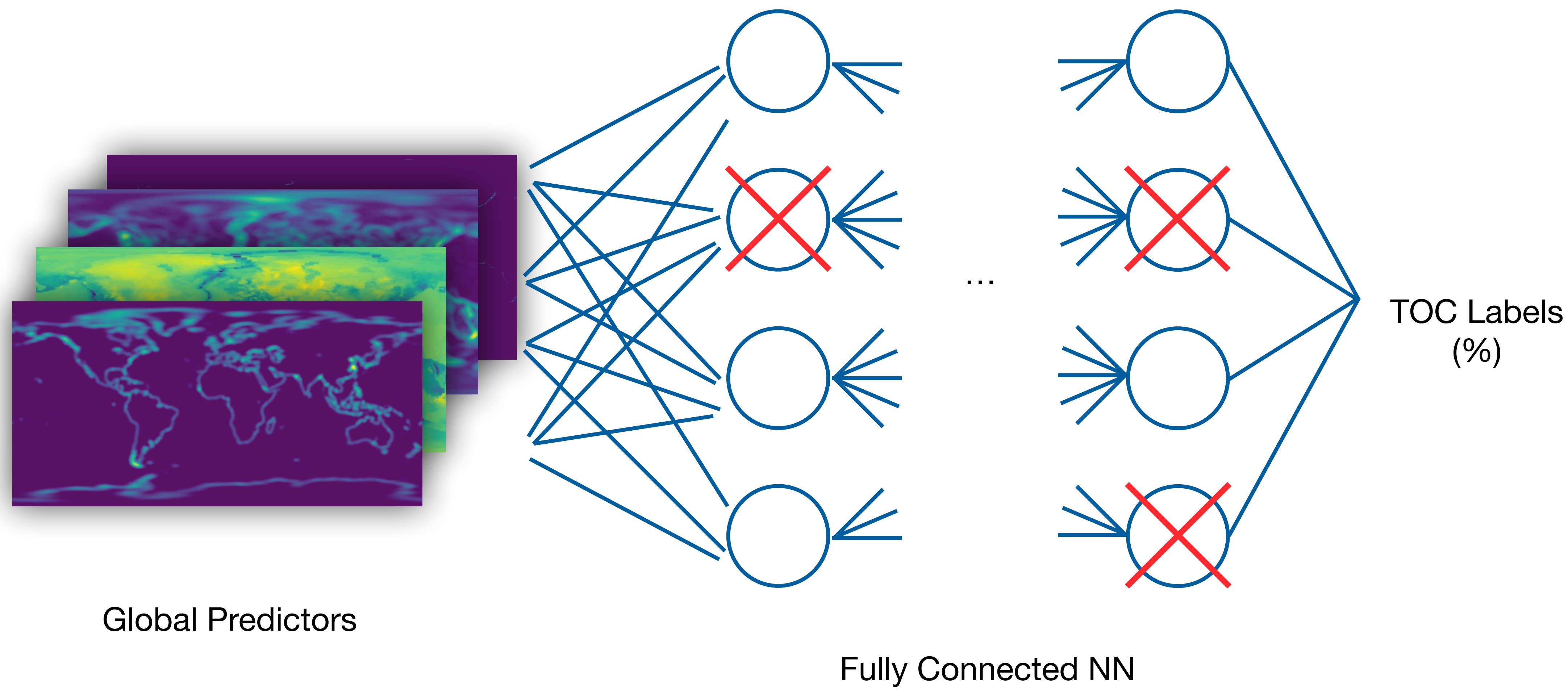
Dropout:



Uncertainty Quantification

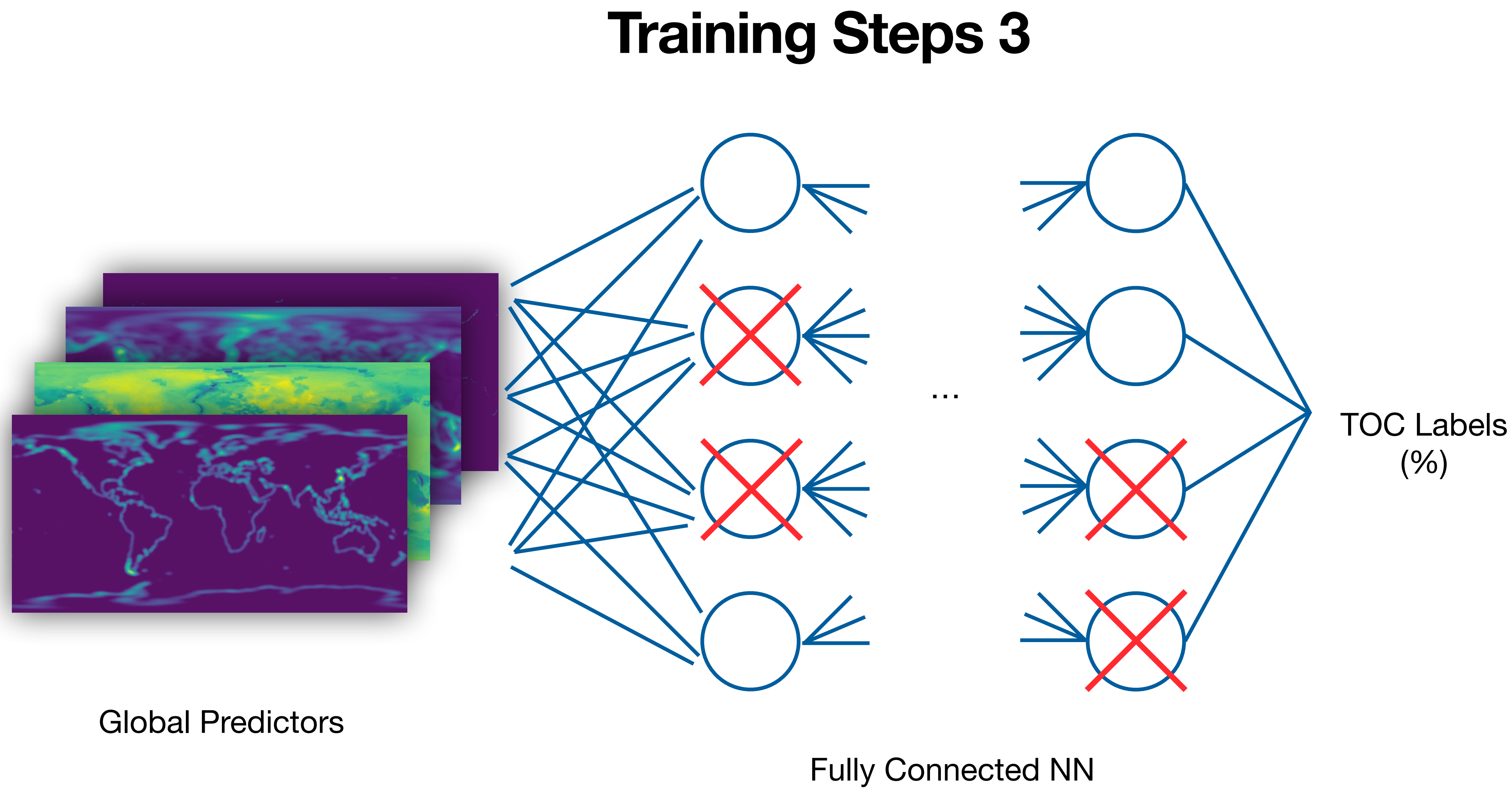
Dropout:

Training Steps 2



Uncertainty Quantification

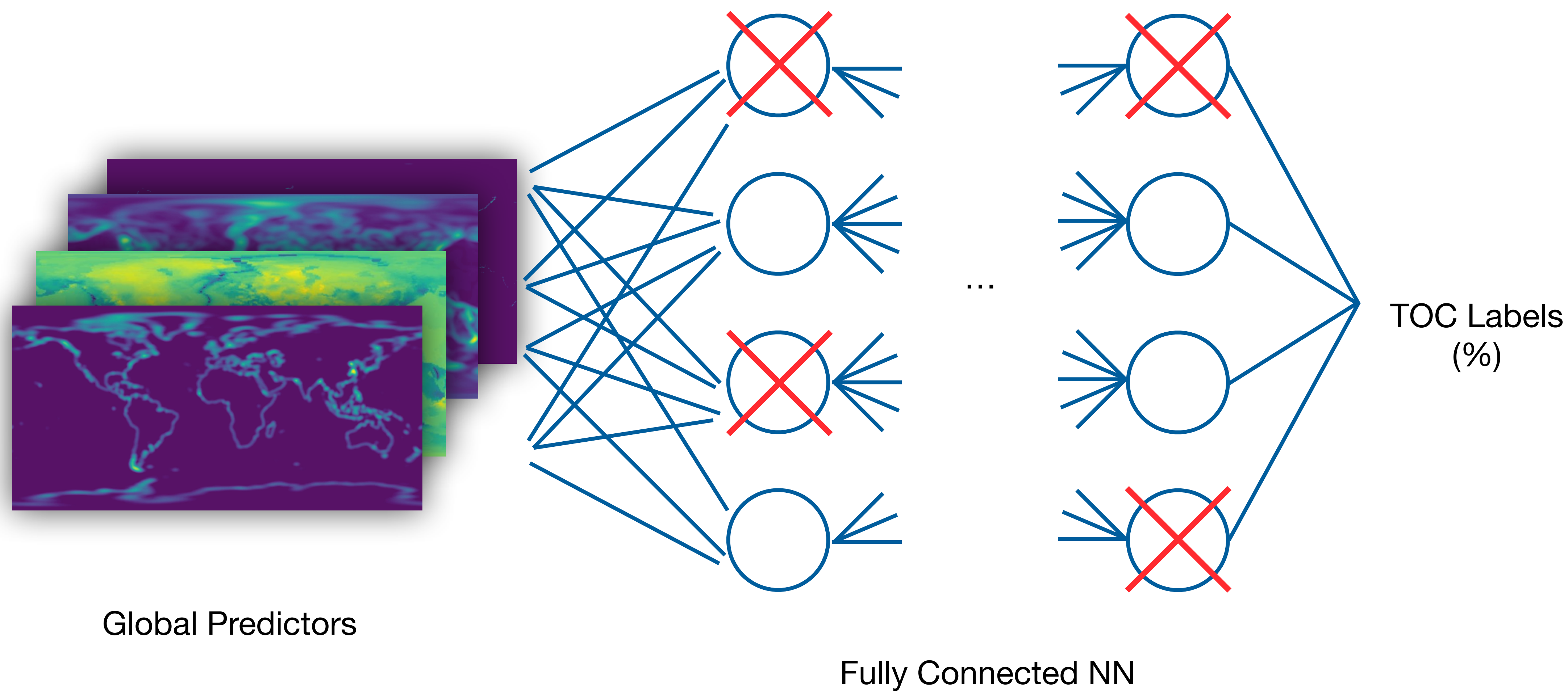
Dropout:



Uncertainty Quantification

Dropout:

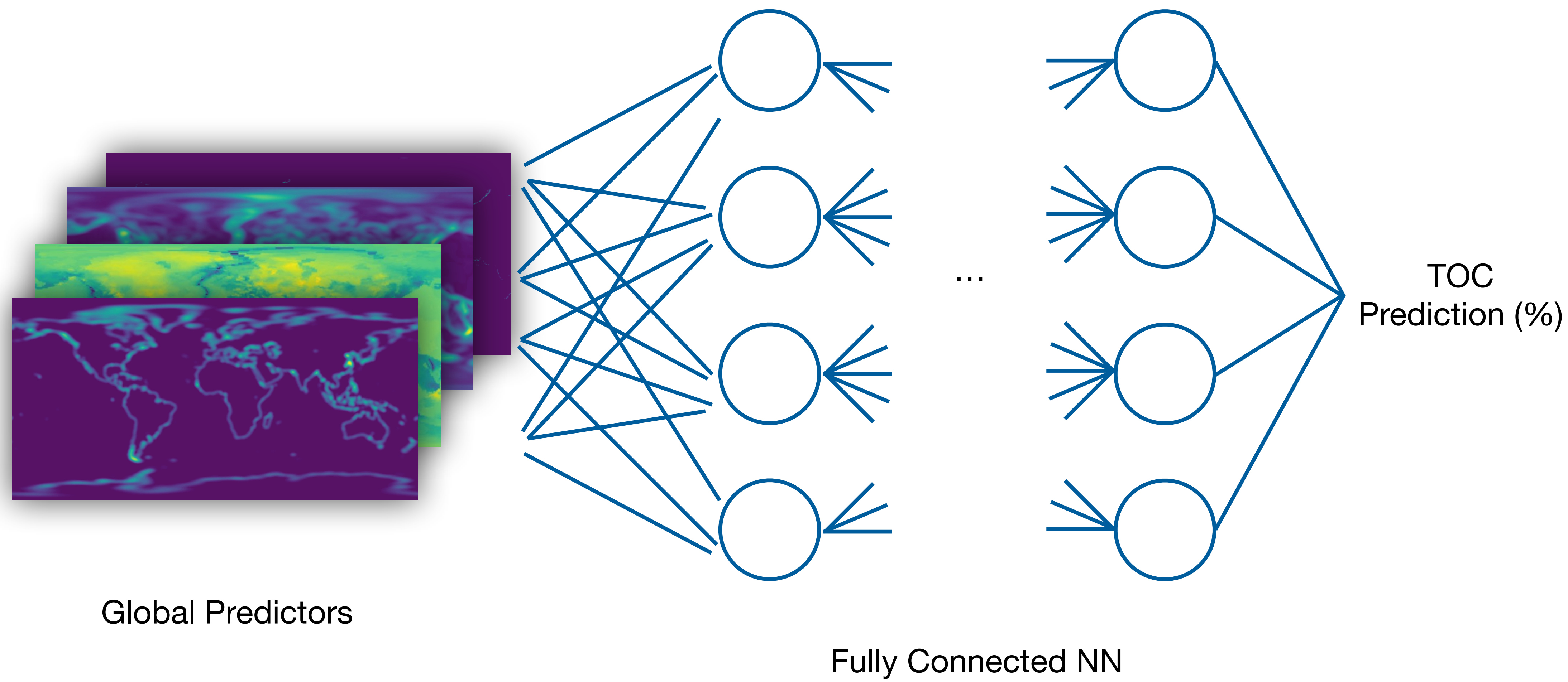
Training Steps n



Uncertainty Quantification

Dropout:

Inference Step



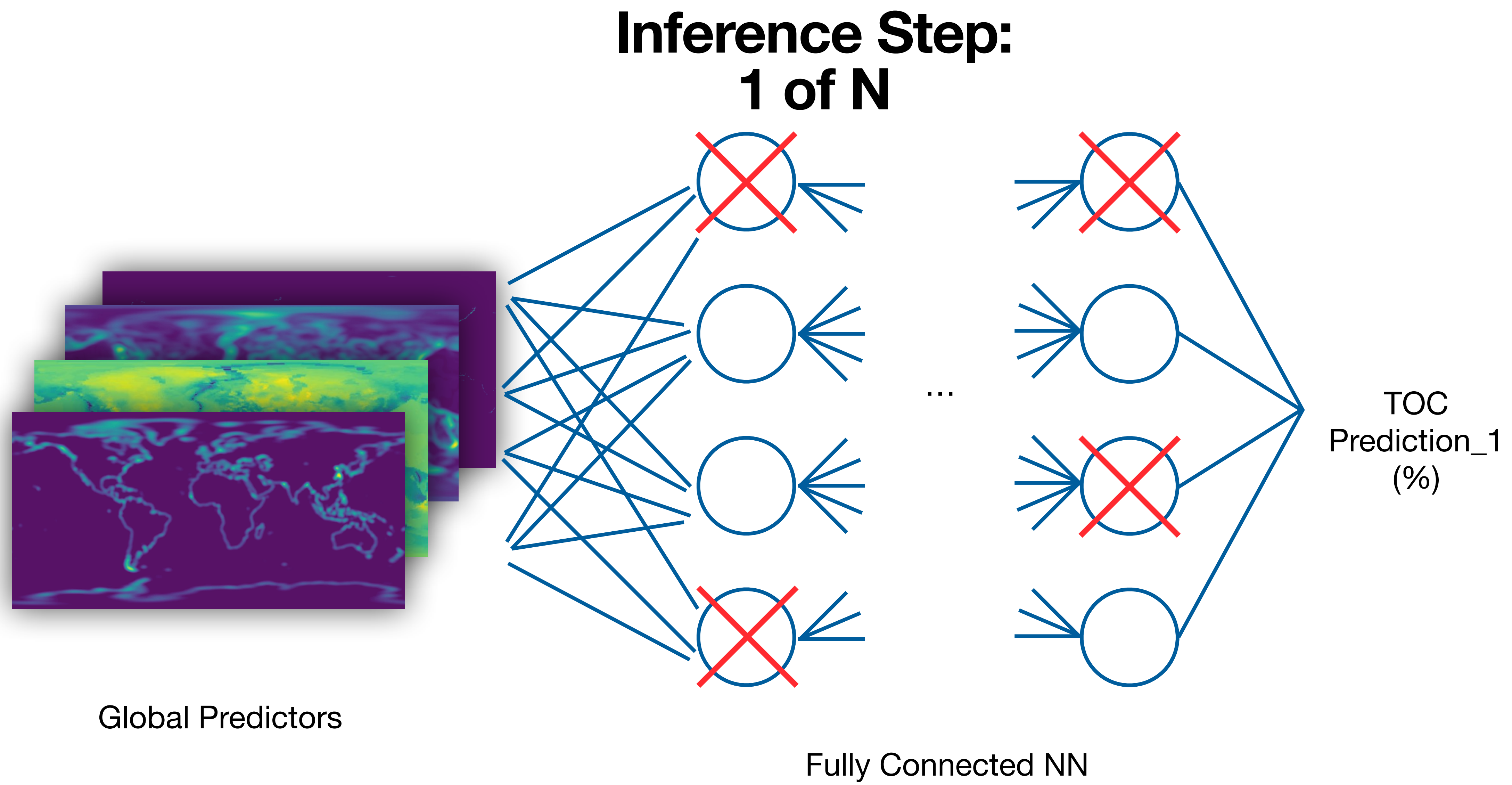
Uncertainty Quantification

Monte Carlo Dropout[1] applies dropout to several repetitions of the inference step, and averages the results to obtain a more robust estimate which also provides a way to quantify uncertainty.

1 https://arxiv.org/pdf/1506.02142.pdf

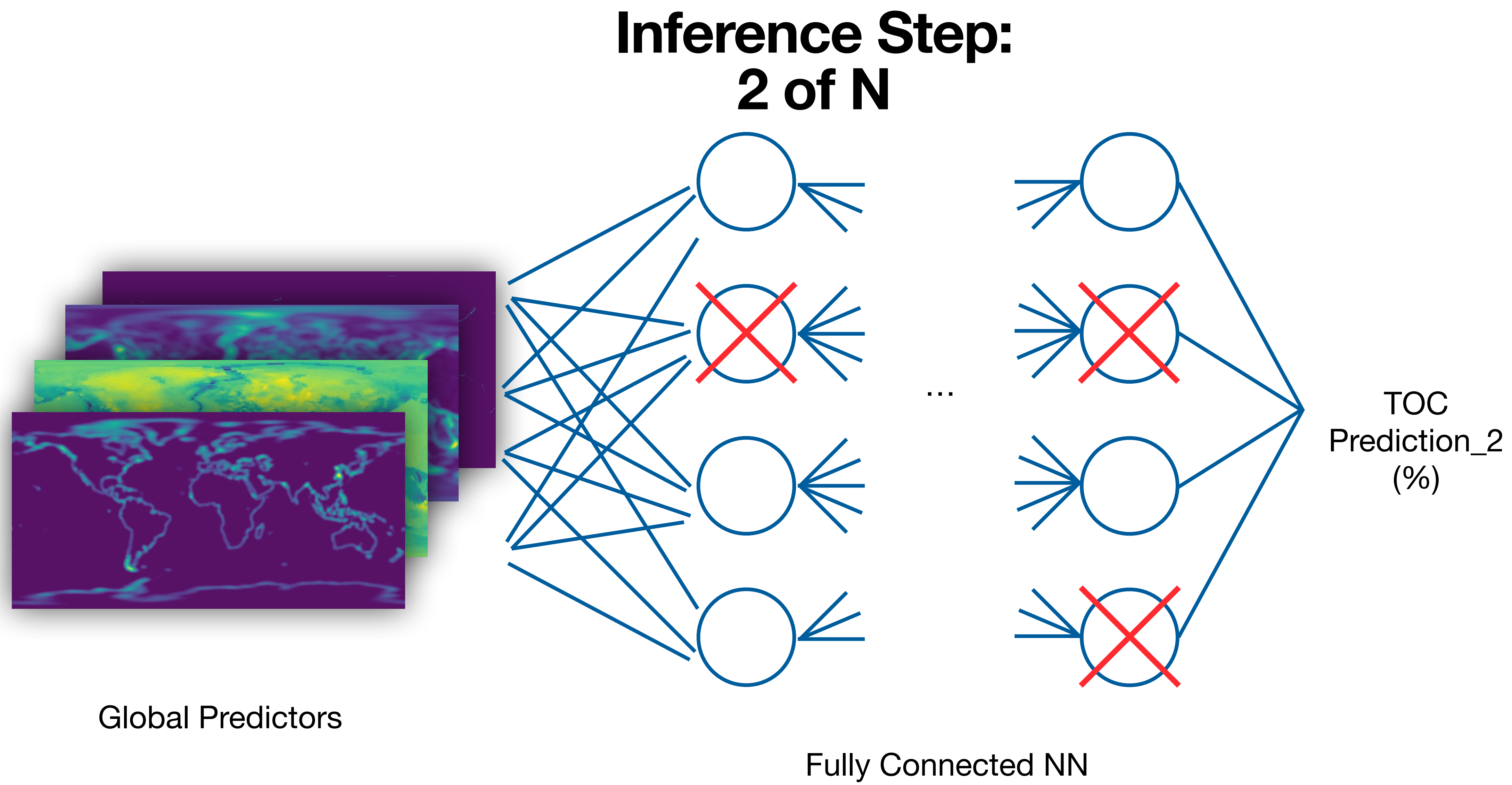
Uncertainty Quantification

Monte Carlo Dropout:



Uncertainty Quantification

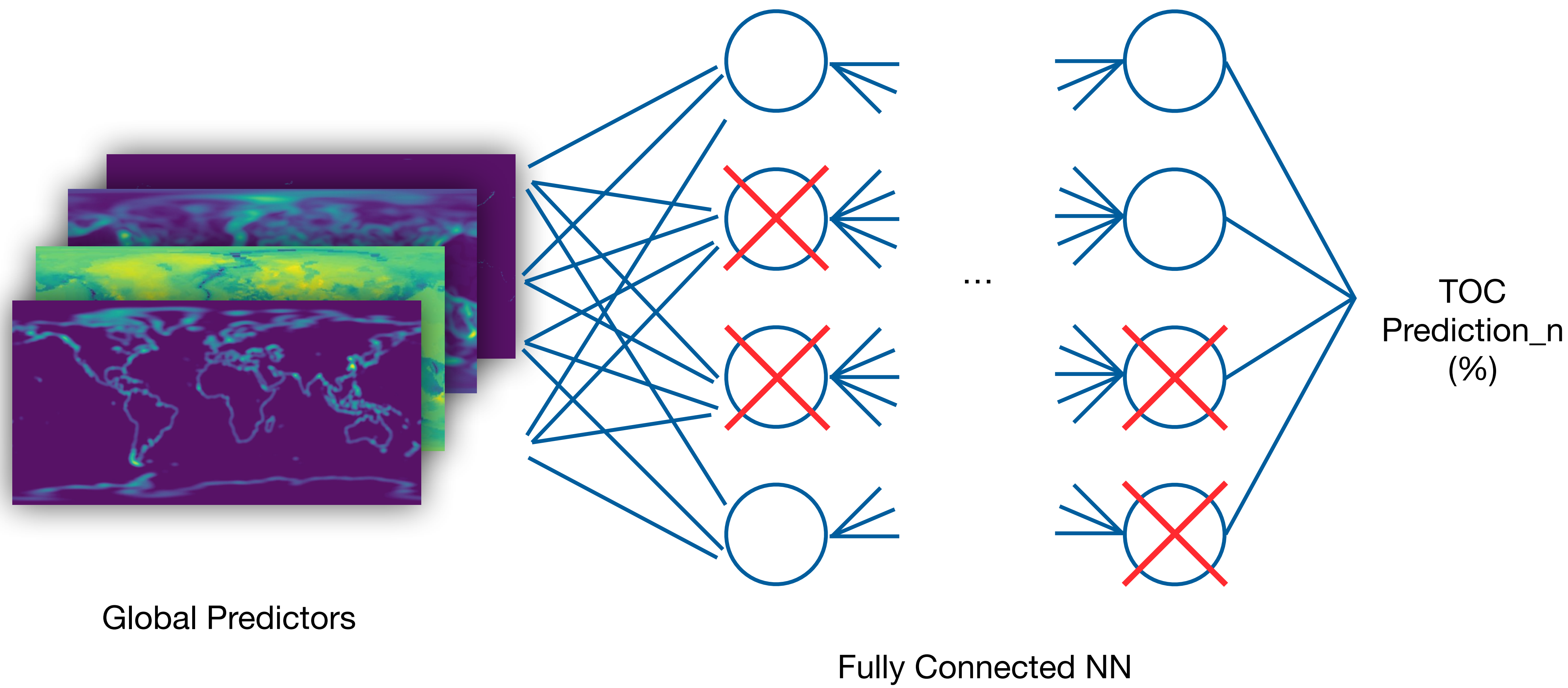
Monte Carlo Dropout:



Uncertainty Quantification

Monte Carlo Dropout:

Inference Step:
n of N



Uncertainty Quantification

Monte Carlo Dropout:

$$Pred\_val = 1/N \sum_{n \in N} Pred\_val_n$$

4. Conclusion

- **A measure for information gain was obtained by applying Softmax distributions to a discretised regression problem.**
- **A measure for model uncertainty was obtained by using MonteCarlo Dropout.**
- **Both techniques, alone or combined, are suitable to answer scientific questions other traditional neural network architectures can not.**

Questions and Comments

EGU Session - ESSI1.15 Towards SMART Monitoring
Wednesday, 6 May, 2020 10:30 - 12:45

or

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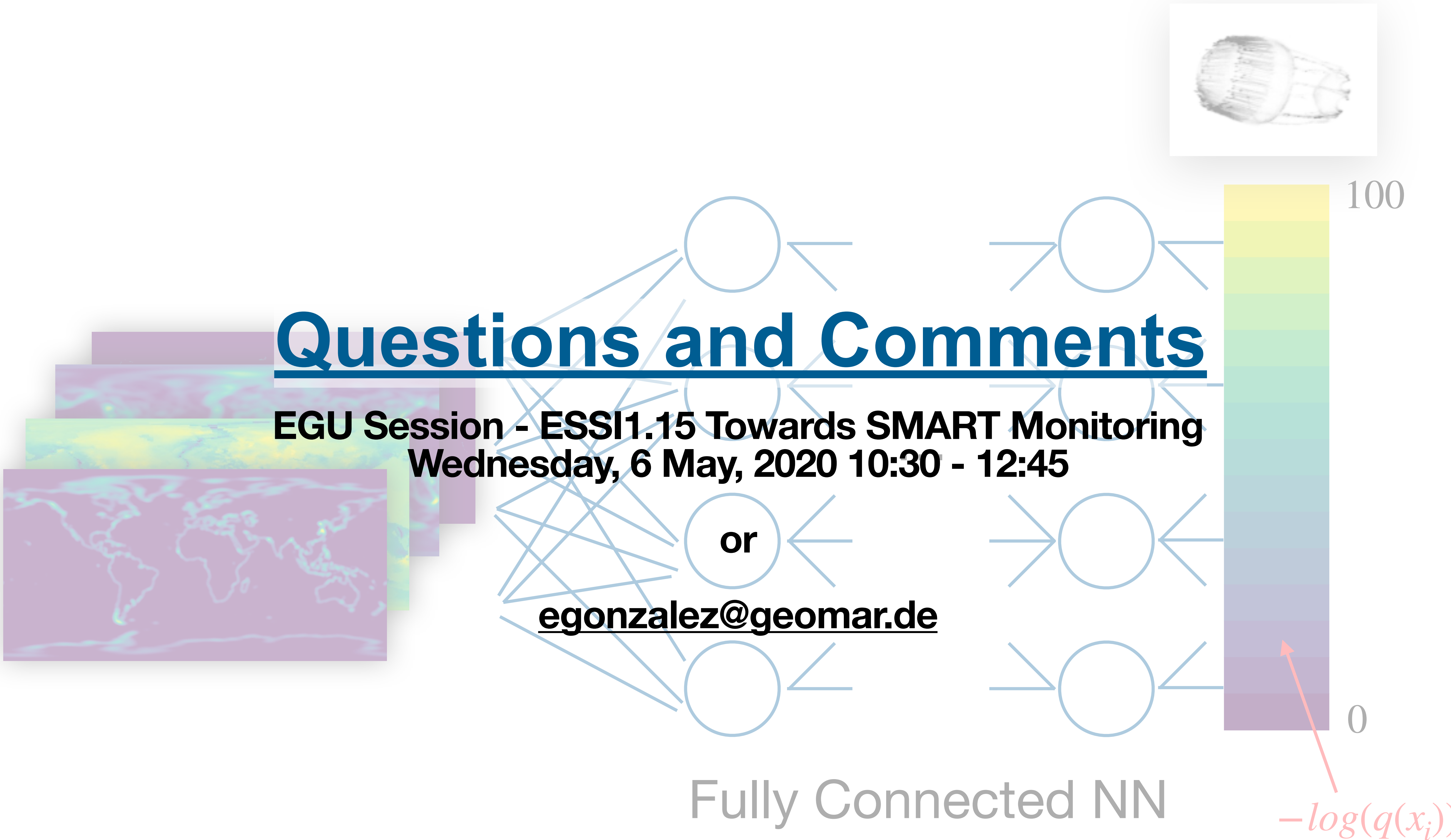

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