Data assimilation and machine learning

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Thanks to: Matthew Chantry, Marcin Chrust, Massimo Bonavita, Sam Hatfield, Patricia de Rosnay, Peter Dueben

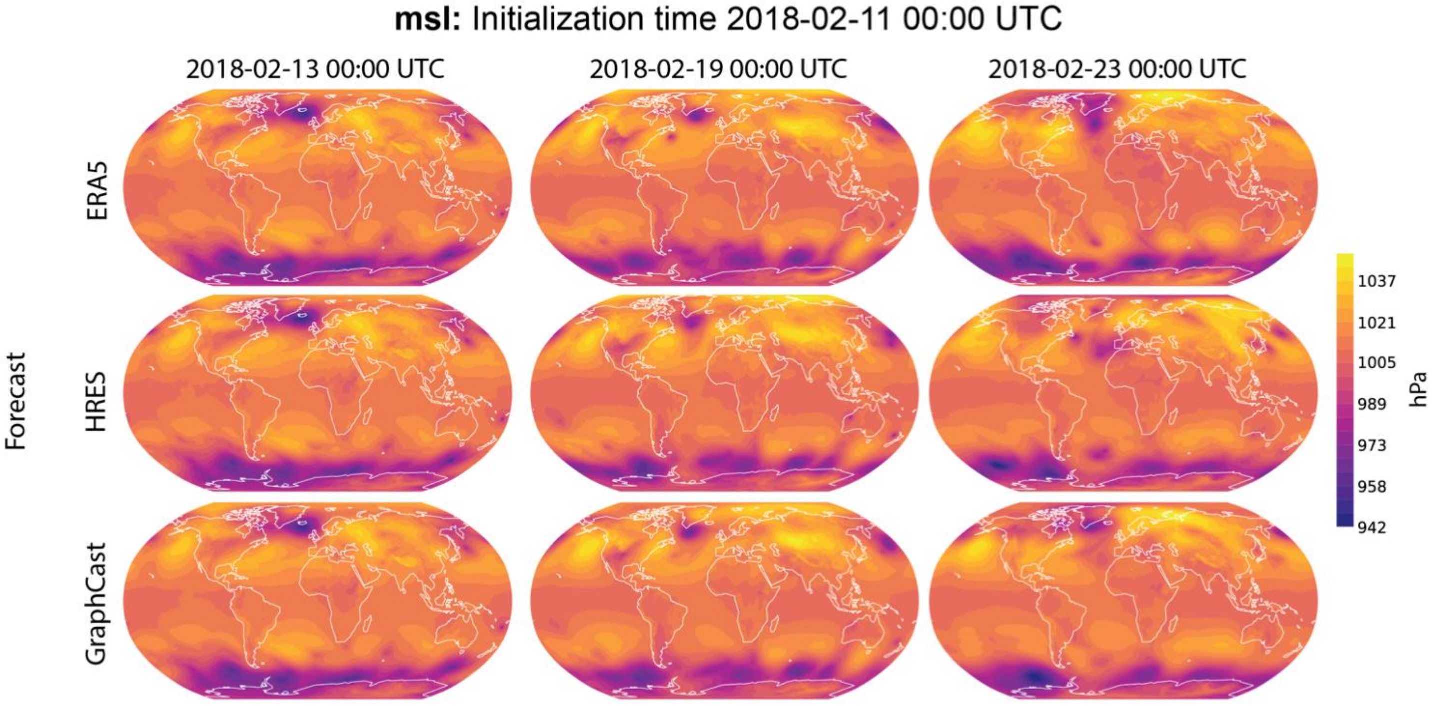
Forecast models based on machine learning are here and they're good!

- Huawei's Pangu-Weather (Bi et al., 2022, *arXiv preprint arXiv:2211.02556*)
- Google DeepMind's GraphCast (Lam et al., 2022, *arXiv preprint arXiv:2212.12794*)

ERA5: reanalysis as **training data (1979-2017)** and validation data (2018)

HRES: ECMWF T1279Co (9 km) 10 day forecast

GraphCast: 10 day forecast at 0.25 degrees (25 km)



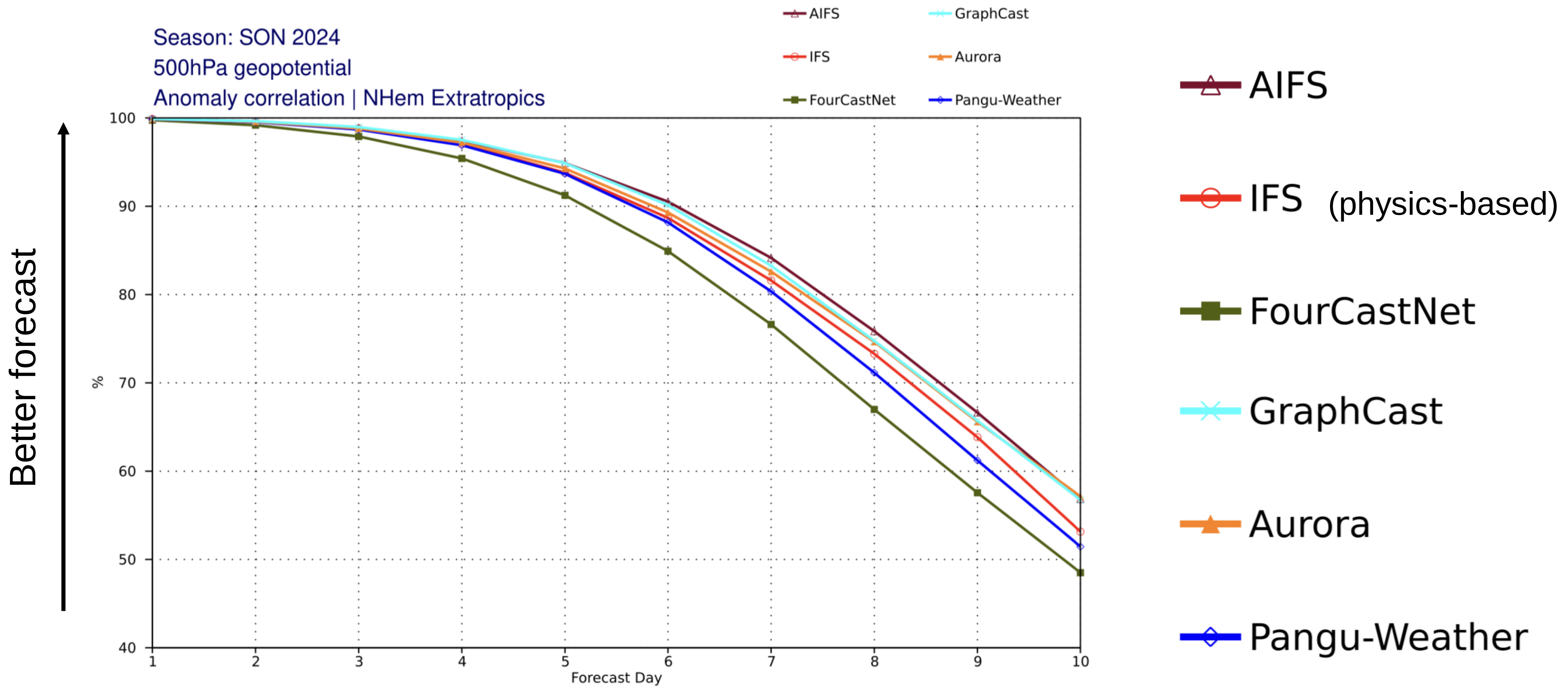
<u>Run time</u>

30 minutes (128 nodes of HPC)

1 minute (1 TPU)

https://arxiv.org/pdf/2212.12794.pdf

Machine learning weather forecasts out-perform* physics-based models



https://charts.ecmwf.int/catalogue/packages/opencharts/products/plwww_3m_fc_aimodels_wp_mean

Ben-Bouallegue et al. (2023) The rise of data-driven weather forecasting - https://doi.org/10.48550/arXiv.2307.10128

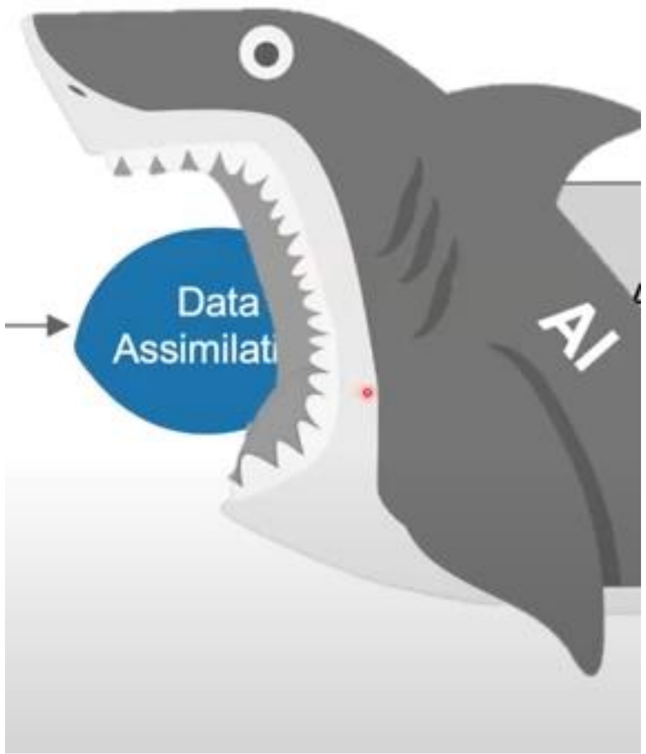
Bi et al. (2023) Accurate medium-range global weather forecasting with 3D neural networks - https://doi.org/10.1038/s41586-023-06185-3

Lam et al. (2023) Learning skilful medium-range global weather forecasting - https://doi.org/10.1126/science.adi2336

* see Massimo's lecture for some big caveats...

Is machine learning going to replace data assimilation?

- Stephan Rasp’s “big shark” at ISDA online - https://www.youtube.com/watch?v=CoiVfwJU4TY



See also e.g:
Vaughan et al., 2024: Aardvark Weather: end-to-end data-driven weather forecasting, https://doi.org/10.48550/arXiv.2404.00411
Cintra et al., 2016: Tracking the mode: Data assimilation by artificial neural network, https://doi.org/10.1109/IJCNN.2016.7727227

An ML example: microwave land surface observation operator

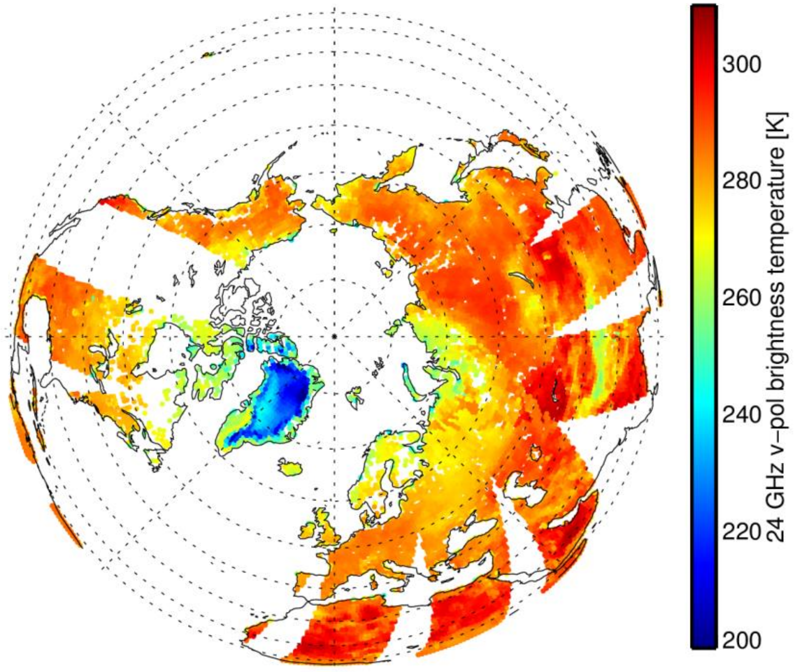
Python, Keras, Tensorflow, Numpy, Matplotlib, Xarray

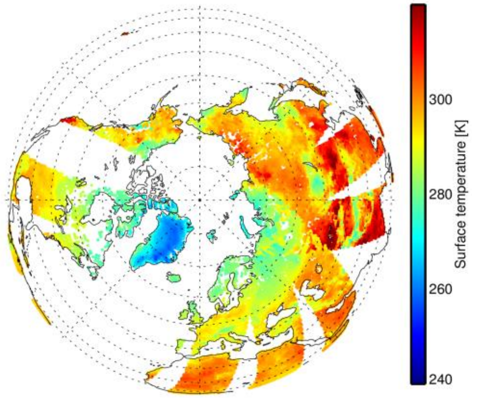
Datasets

10 possible predictors for the brightness temperature from the IFS 12h forecast

AMSR2 24GHz v-pol observations

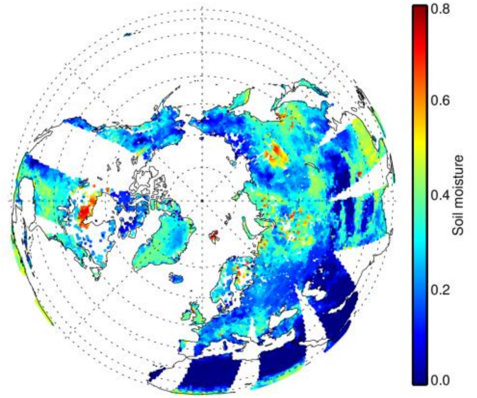
y = labels



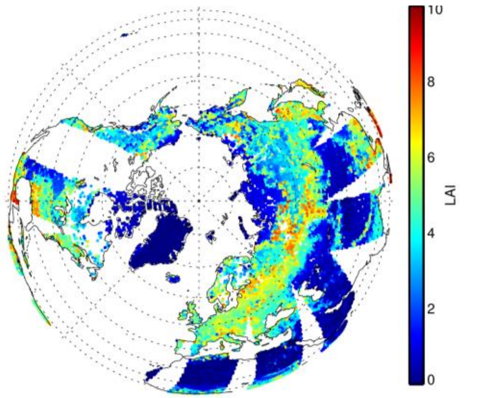


Skin temperature

x = features



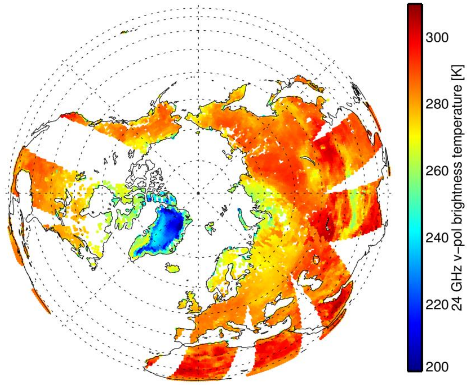
Soil moisture



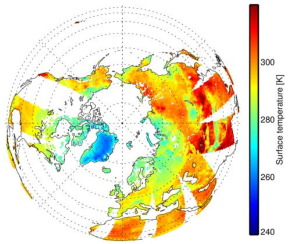
Leaf area index

+ orography, snow depth, snow density, integrated water vapour, cloud, rain and snow water contents

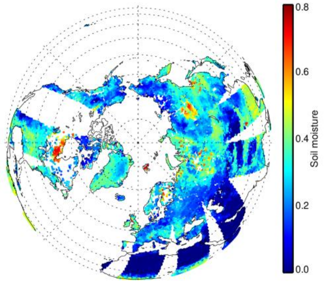
y =
labels



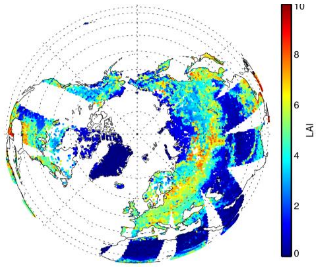
Task of ML:
find y=h(x,w)



x =
features



w =
neural network
weights



Data preparation

Dataset of 470,000 observations and colocated model data

```
obdata = xr.open_dataset('/perm/rd/stg/odb/hkhg/ml_amsr2_chan9.nc')

x0 = np.column_stack([obdata.TSFC,          obdata.SOIL_MOISTURE, obdata.SNOW_DEPTH, \
                      obdata.SNOW_DENSITY, obdata.LAI,           obdata.OROGRAPHY, \
                      obdata.FG_TCWV,      obdata.FG_CWP,        obdata.FG_RWP,       obdata.FG_IWP])
y0 = np.column_stack([obdata.OBSVALUE])

def x_normalise (x_orig):
    x_min = [200.0, 0,    0,   0,   0,  0,    0,  0, 0, 0]
    x_max = [350.0, 0.75, 0.5, 300, 10, 5000, 70, 1, 2, 8]
    x_min = np.outer(np.ones(x_orig.shape[0]),np.array(x_min))
    x_max = np.outer(np.ones(x_orig.shape[0]),np.array(x_max))
    return (x_orig - (x_max+x_min)/2.0) / (x_max-x_min)*2.0

x1 = x_normalise(x0)
```

Prepare numpy arrays of correct shape for Keras

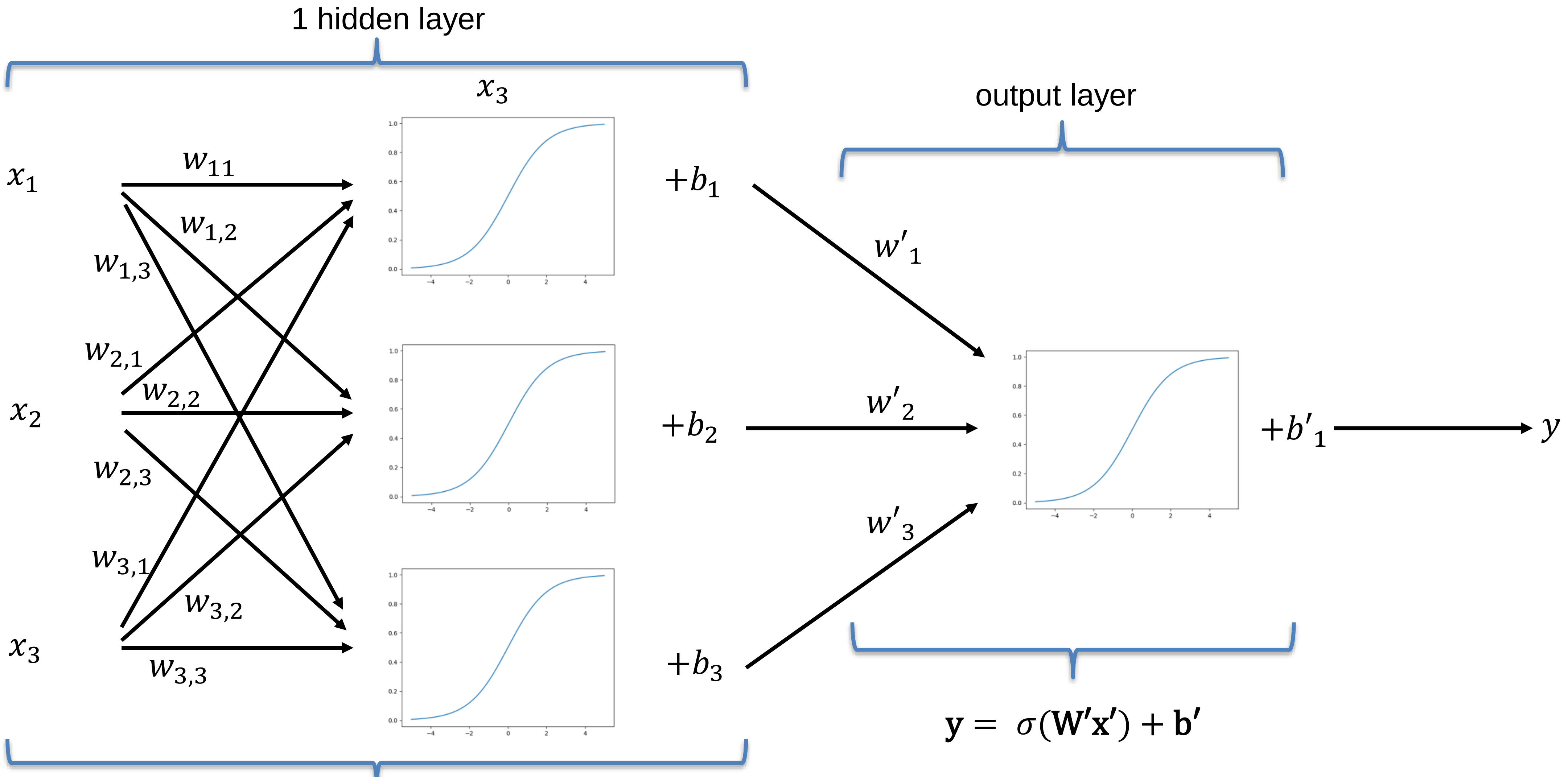
Normalise ‘features’ x to roughly -1 to +1

And... (not shown) normalise labels y to within 0 to 1

Set up a neural network for the land surface observation operator

```
In [21]: model = Sequential()
    ...: model.add(Dense(units=10, activation='sigmoid',input_dim=10))
    ...: model.add(Dense(units=6, activation='sigmoid'))
    ...: model.add(Dense(units=1, activation='sigmoid'))
    ...: model.summary()
    ...:
    ...: model.compile(loss='mean_squared_error', optimizer='adam')
    ...:
Model: "sequential_2"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense_4 (Dense)              (None, 10)                110
_________________________________________________________________
dense_5 (Dense)              (None, 6)                 66
_________________________________________________________________
dense_6 (Dense)              (None, 1)                 7
=================================================================
Total params: 183
Trainable params: 183
Non-trainable params: 0
_________________________________________________________________
```

Feedforward neural network - example



$$\mathbf{y} = \sigma(\mathbf{W}'\mathbf{x}') + \mathbf{b}'$$

$$\mathbf{x}' = \sigma(\mathbf{W}\mathbf{x}) + \mathbf{b}$$

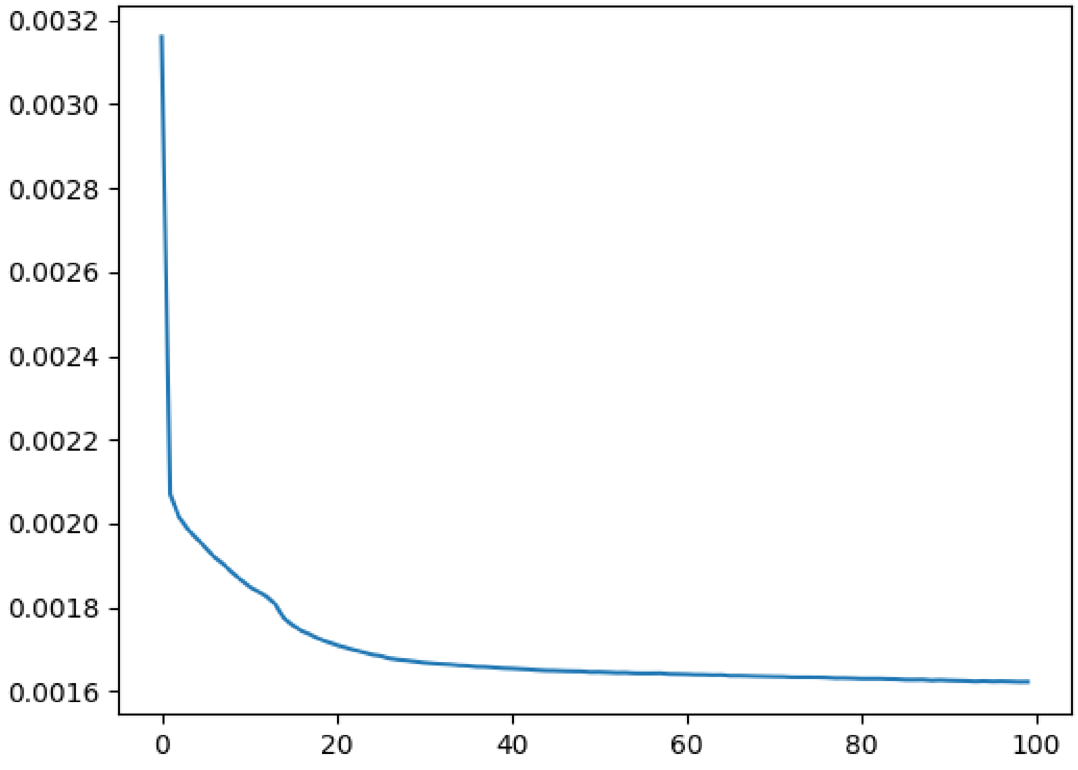
Train it (about 25 minutes on a linux workstation)

```
history = model.fit(x1, y1, epochs=100)
```

Loss function

$$J_{\text{obs}} = \frac{1}{n}\sum_{i=1}^{n}(y_{\text{obs},i} - y_{\text{sim},i})^2$$

Default “loss function” is just the 4D-Var Jo without representation of observation error.



epoch

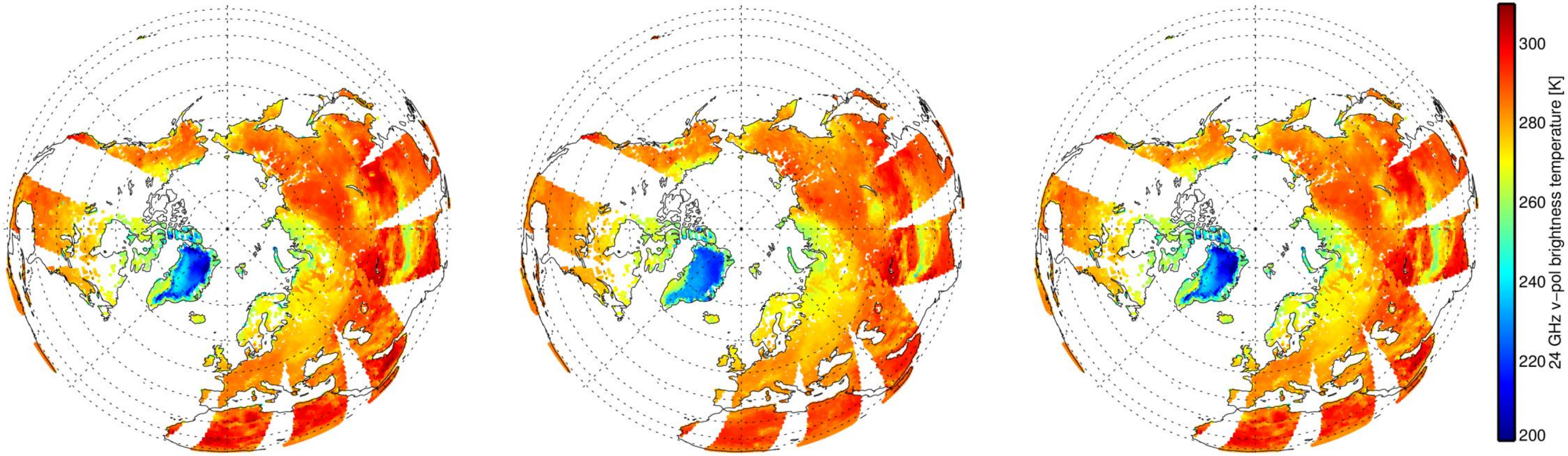
Adam – a sophisticated stochastic gradient descent (SGD) minimiser

Results (ability to fit training dataset)

Observations

ML predicted

Physically-based simulation produced by IFS (RTTOV for atmosphere, dynamical emissivity retrieval for surface emissivity)




```
predict = y_unnormalise(model.predict(x1))
```

Hand-written function to recover TB

Problems with this toy NN model for 24 GHz radiances

- It's not as good as the current physical methods
- The input variables are not sufficient to drive the outputs
  - Missing variables – e.g. over Greenland, detailed knowledge of snow and ice microstructure
- Some of the fundamental problems for machine learning in the earth system domain:
  - Neither the models nor the input state are fully known
  - Chicken and egg problem: can't train the model if you don't know the necessary inputs well enough

Function fitting - under the hood of ML

Apologies for the maths, which in reality is done behind the scenes, automatically

Backpropagation for inputs (compare to earlier TL and adjoint lecture)

- Consider one layer, ignoring the bias weights for simplicity

$$\mathbf{x}' = \mathbf{W}\mathbf{x}$$
$$\mathbf{y} = \sigma(\mathbf{x}')$$

- Differentiate using the chain rule at a given x

$$\left.\frac{d\mathbf{y}}{d\mathbf{x}}\right|_{\mathbf{x}} = \left.\frac{d\sigma}{d\mathbf{x}'}\right|_{\mathbf{W}\mathbf{x}} \left.\frac{d\mathbf{x}'}{d\mathbf{x}}\right|_{\mathbf{x}}$$

- These "Jacobians" can be represented as matrices

$$\left.\frac{d\mathbf{y}}{d\mathbf{x}}\right|_{\mathbf{x}} = \mathbf{G}_{\mathbf{W}\mathbf{x}}\mathbf{W}$$

- The magic of adjoints allows us to compute the gradient of the cost function J with respect to a change in its inputs

$$\left.\frac{dJ}{d\mathbf{x}}\right|_{\mathbf{x}} = \mathbf{W}^T\mathbf{G}^T_{\mathbf{W}\mathbf{x}} \left.\frac{dJ}{d\mathbf{y}}\right|_{\mathbf{x}}$$

Backpropagation for updating weights

For simplicity, differentiate with respect to one weight, w_ij

$$\mathbf{x}' = \mathbf{W}\mathbf{x} \quad \Rightarrow \quad x'_i = \sum_j w_{ij} x_j \quad \Rightarrow \quad \left.\frac{dx'_i}{dw_{ij}}\right|_{x_j} = x_j$$

One output y_i is sensitive to all inputs x_j

$$\mathbf{y} = \sigma(\mathbf{x}') \quad \Rightarrow \quad y_i = \sigma(x'_i) \quad \Rightarrow \quad \left.\frac{dy_i}{dx'_i}\right|_{x'_i} = \left.\frac{d\sigma}{dx'_i}\right|_{x'_i}$$

Gradient of cost function with respect to one weight

$$\left.\frac{dJ}{dw_{ij}}\right|_{x_j} = x_j \left.\frac{d\sigma}{dx'_i}\right|_{x'_i} \left.\frac{dJ}{dy_i}\right|_{x_j}$$

Gradient of cost function with respect to the relevant simulated observation y_i

Gradient depends on x_j (and $x'_i = \sum_j w_{ij} x_j$)

Mini-batch stochastic gradient descent

For a randomly selected batch of paired inputs and outputs update all weights (typical batch size: 32)

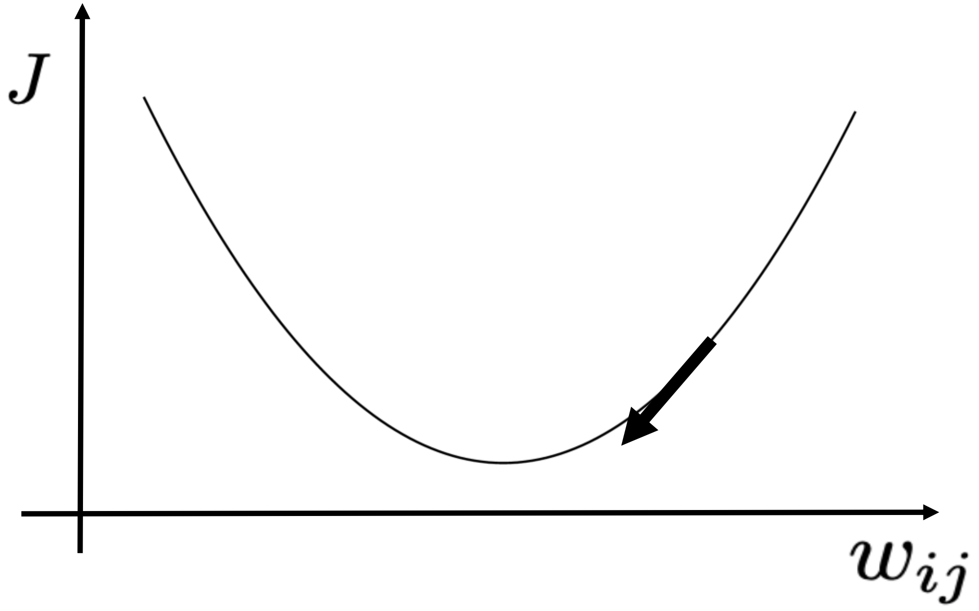
$$w_{ij} = w_{ij} - \eta \frac{dJ}{dw_{ij}}\bigg|_{x_j}$$

New weight setting

Old weight setting

Learning rate

Gradient of loss function with respect to the weight for this x



SGD versus standard gradient descent in DA

- Stochastic gradient descent:
  - Each minimisation is done on one randomly selected mini-batch of data, requiring:
    - One call to the forward model to compute the linearisation state for the gradients
    - One call the the adjoint (backpropagation model)
    - All weights are updated
  - One epoch = one pass through the entire dataset

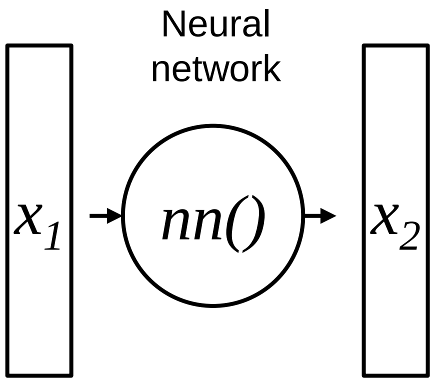
100 epochs * 15,000 mini batches ->
1,500,000 model runs (forward/adjoint)

- Gradient descent in incremental 4D-Var:
  - Each outer loop needs one call of the nonlinear model to update linearisation state
  - Each minimisation needs 30 – 50 "inner loop" iterations, each needing
    - One call the the TL model
    - One call to the adjoint model

4 outer loops * 40 inner loops ->
approx 160 model runs (forward/adjoint)

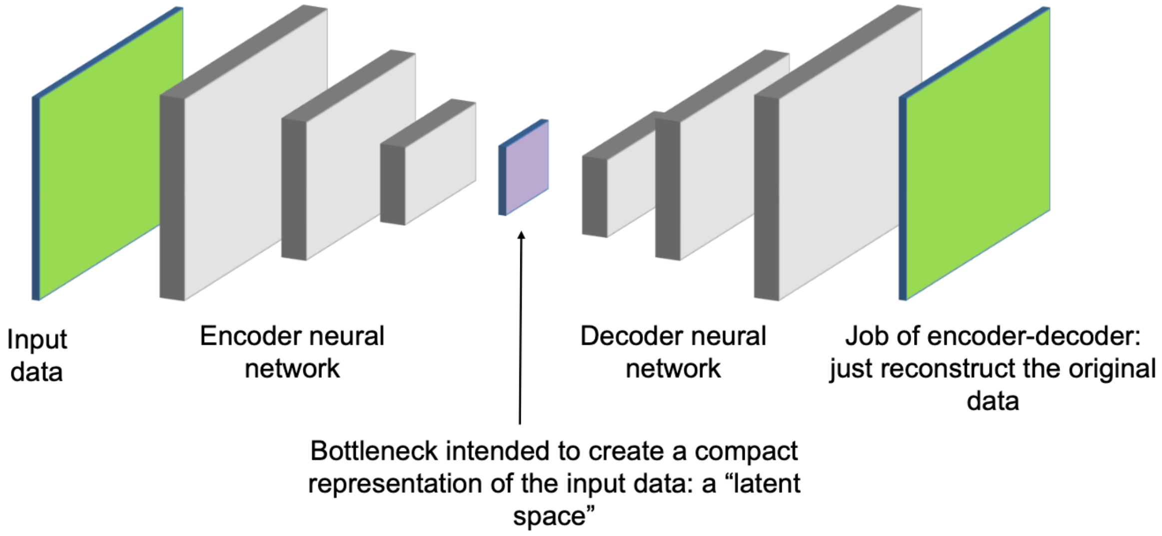
Types of ML

Types of ML – supervised learning



Supervised learning:

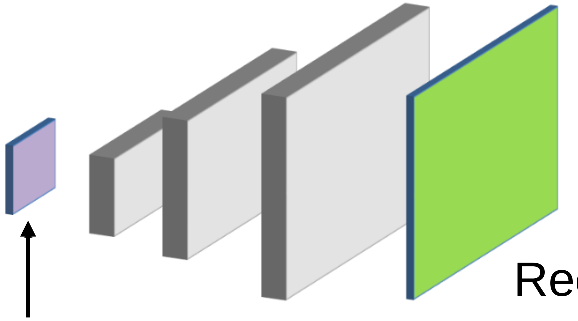
- ML as a "universal function approximator" (Hornik, 1991)
- Both inputs x1 and outputs x2 need to be provided as training data
- An "emulator" / "surrogate" / "empirical model"



Encoder-decoder:

- Data compression
- Data assimilation in the space of an autoencoder (Peyron et al., 2021)
- Still needs both inputs and outputs to train the model

Types of ML – unsupervised learning – generative ML



Reconstruction

Latent space: a reduced statistical description of a phenomemon

A bit like a set of eigenvalues in a principal component decomposition

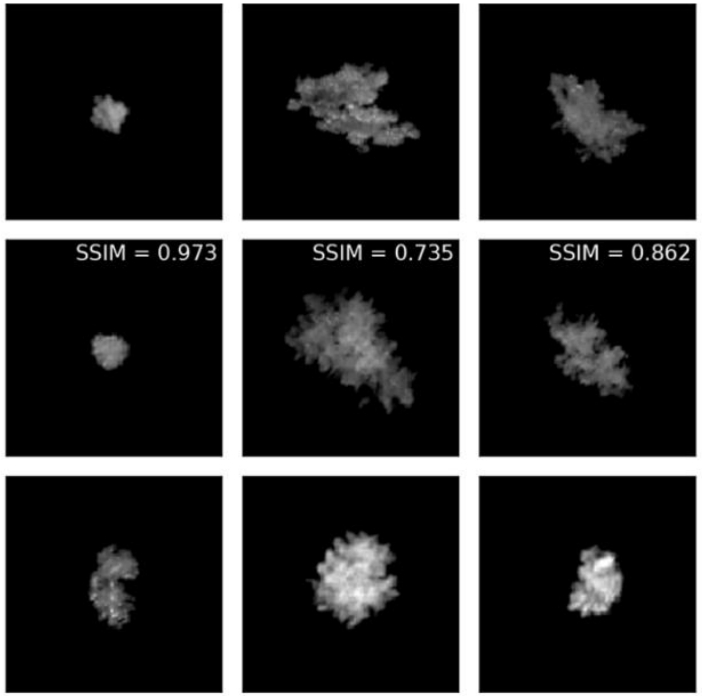
What if we could just have the decoder?

- How do we train it?
  - We could train an encoder-decoder on something, and then throw away the encoder.
  - Or find some more clever way...

Real

Reconstructed

Random vector in latent space



Snowflake images from Leinonen and Berne (2021, https://doi.org/10.5194/amt-13-2949-2020)

Generative Adversarial Network (GAN):

- Generator (~decoder): make an image
- Discriminator (~encoder): given an image, tell if it is real or fake -> drives the loss function

Why has machine learning been so successful?

- Many packages can do all this with just a few Python commands
  - Keras, Pytorch, Tensorflow etc.
- Huge amounts of learning material available – it's easy to get started
  - Open source ML models to extend, copy, give inspiration
- Availability of GPUs to perform extremely fast matrix/tensor multiplications
  - Faster, simpler nonlinear activation functions (e.g. relu)
- Vast pools of data to train on
  - No data-driven forecasting without ERA5 reanalyses to train on
- Modern implementations of stochastic gradient descent (e.g. Adam) are incredibly good
- We are surrounded by ever more successful examples of what a "universal approximator" can be applied to...
  - How much can ML achieve?

Theoretical links between ML and DA

The forward and inverse problem

Forward model

Observations

$$y = h(x, w)$$

Geophysical state

Model parameters

The inverse problem solved by Bayes theorem

with state AND parameters

Observations

Geophysical state

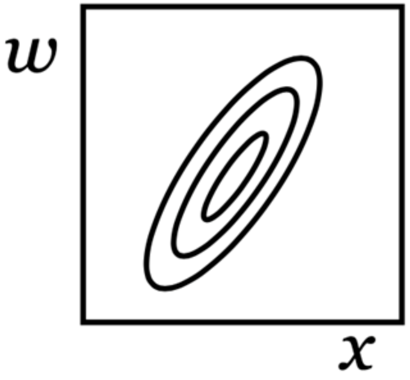
Model parameters

Bayes theorem

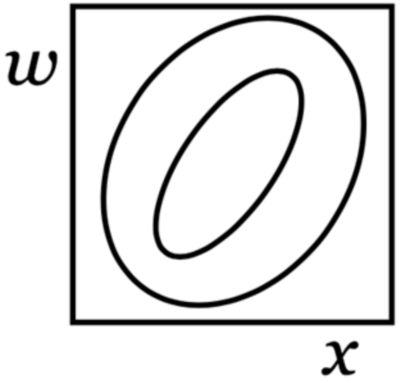
$$P(x,w|y) = K\,(y, P(y|x,w), P(x,w))$$

Probabilistic equivalent of the forward model h()

$P(x,w\,|\,y)$



$P(x,w)$



(Posterior) Probability of x and w given y

Prior probability of x and w

Cost function for variational DA

Assume Gaussian errors (error standard deviation σ)
and for clarity here simplify to scalar variables
and ignore any covariance between observation, model or state error

Prior (background)

$$J(x,w) = \underbrace{\frac{(y-h(x,w))^2}{(\sigma^y)^2}}_{J^y} + \underbrace{\frac{(x^b-x)^2}{(\sigma^x)^2}}_{J^x} + \underbrace{\frac{(w^b-w)^2}{(\sigma^w)^2}}_{J^w}$$

DA

Cost function	Observation term	Prior knowledge of state	Prior knowledge of model

Cost / loss function equivalence of ML and variational DA

Assume Gaussian errors (error standard deviation σ)
and for clarity here simplify to scalar variables
and ignore any covariance between observation, model or state error

ML	Loss function	Basic loss function	Feature error?	Weights regularisation

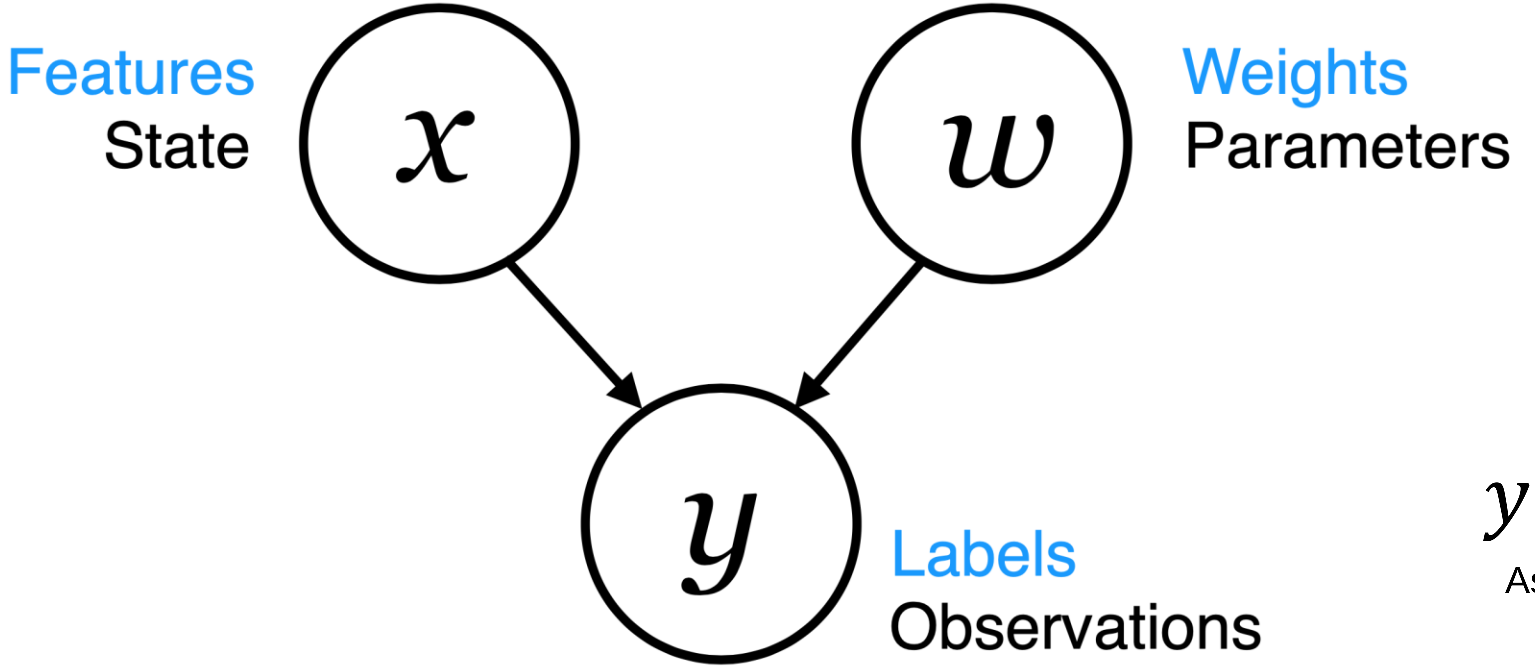
$$J(x,w) = \underbrace{\frac{(y-h(x,w))^2}{(\cancel{\sigma^y})^2}}_{J^y} + \underbrace{\cancel{\frac{(x^b-x)^2}{(\sigma^x)^2}}}_{J^x} + \underbrace{\frac{(\cancel{w^b}-w)^2}{(\cancel{\sigma^w})^2}}_{J^w}$$

DA	Cost function	Observation term	Prior knowledge of state	Prior knowledge of model

Machine learning (e.g. NN)		Variational data assimilation	
Labels	y	Observations	$\mathrm{y^o}$
Features	x	State	x
Neural network or other learned models	$\mathrm{y}' = W(\mathrm{x})$	Physical forward model	$\mathrm{y} = H(\mathrm{x})$
Objective or loss function	$(\mathrm{y} - \mathrm{y}')^2$	Cost function	$J = J^b + \left(\mathrm{y^o} - H(\mathrm{x})\right)^T \mathrm{R}^{-1}\left(\mathrm{y^o} - H(\mathrm{x})\right)$
Regularisation	$\lVert\mathrm{w}\rVert$	Background term	$J^b = \left(\mathrm{x} - \mathrm{x^b}\right)^T \mathrm{B}^{-1}\left(\mathrm{x} - \mathrm{x^b}\right)$
Stochastic gradient descent		Conjugate gradient method (e.g.)	
Back propagation		Adjoint model	$\dfrac{\partial J}{\partial \mathrm{x}} = \mathrm{H}^T \dfrac{\partial J}{\partial \mathrm{y}}$
Train model and then apply it		Optimise state in an update-forecast cycle	

Boukabara et al. (2021) https://doi.org/10.1175/BAMS-D-20-0031.1

Bayesian equivalence of ML and DA



$$y = h(x, w)$$

As a Bayesian network

Geer (2021) https://doi.org/10.1098/rsta.2020.0089

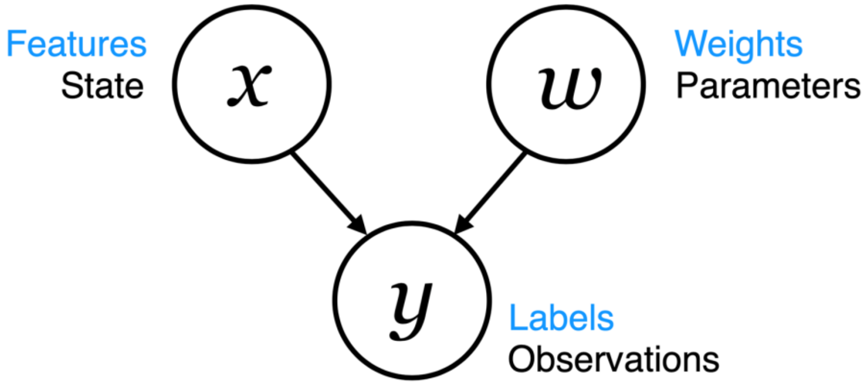
Bocquet et al. (2020) https://arxiv.org/abs/2001.06270

Abarbanel et al. (2018) https://doi.org/10.1162/neco_a_01094

Hsieh and Tang (1998) https://doi.org/10.1175/1520-0477(1998)079%3C1855:ANNMTP%3E2.0.CO;2

Goodfellow et al. (2016) https://www.deeplearningbook.org

Bayesian networks: representing the factorisation of joint probability distributions



$$P(y,x,w)$$

1. Factorise in two different ways using the chain rule of probability

$$P(y,x,w) = P(x|w,y)P(w|y)P(y)$$

$$P(y,x,w) = P(y|x,w)P(x|w)P(w)$$

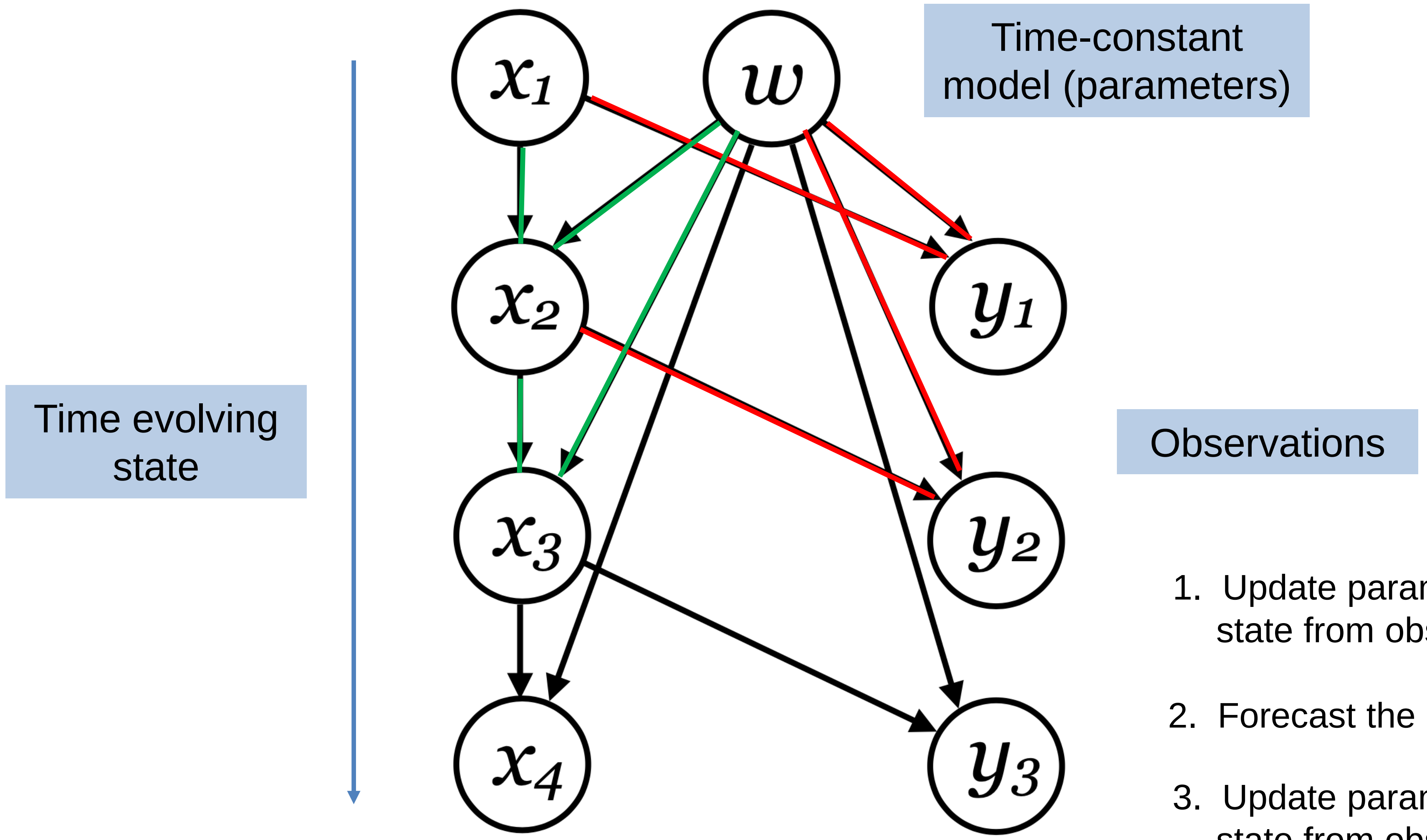
2. Equate the two right hand sides and rewrite

$$P(x|w,y)P(w|y) = \frac{P(y|x,w)P(x|w)P(w)}{P(y)}$$

3. Rewrite by putting back the joint distributions of x,w: Bayes' rule

$$P(x,w|y) = \frac{P(y|x,w)P(x,w)}{P(y)}$$

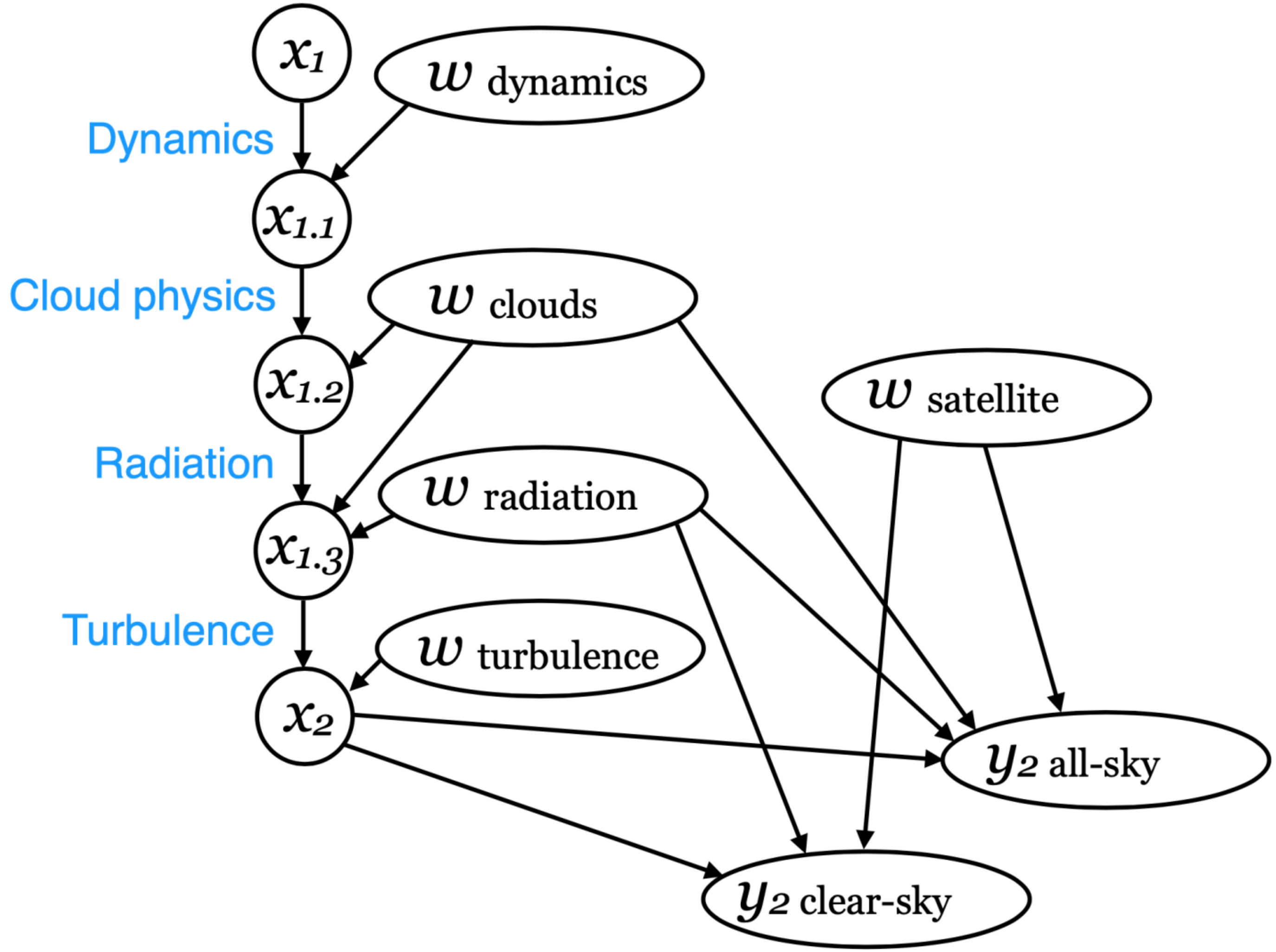
Time evolution of state – cycled data asimilation



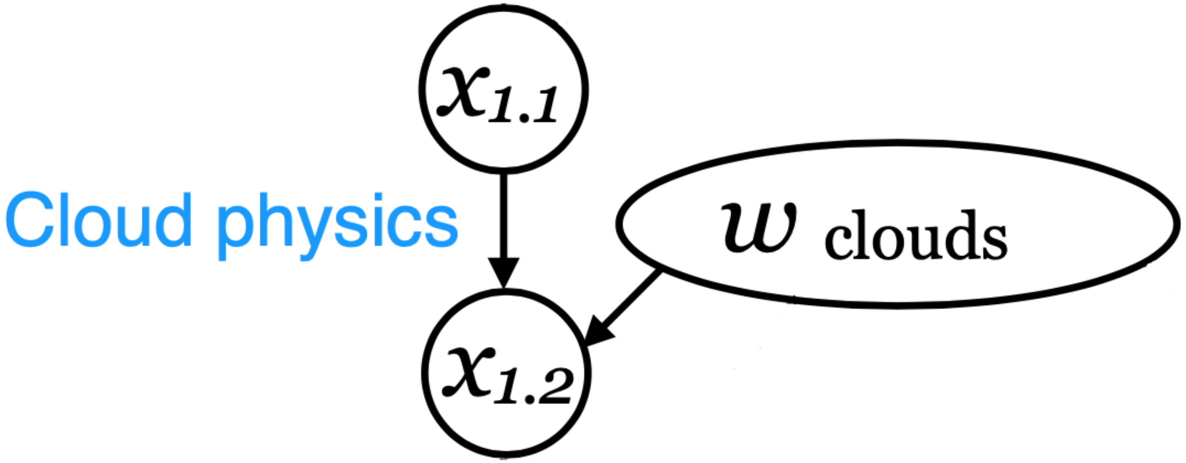
1. Update parameters and state from observations
2. Forecast the next state
3. Update parameters and state from observations
4. Forecast ...

Inside an atmospheric model & data assimilation timestep

One model time-step

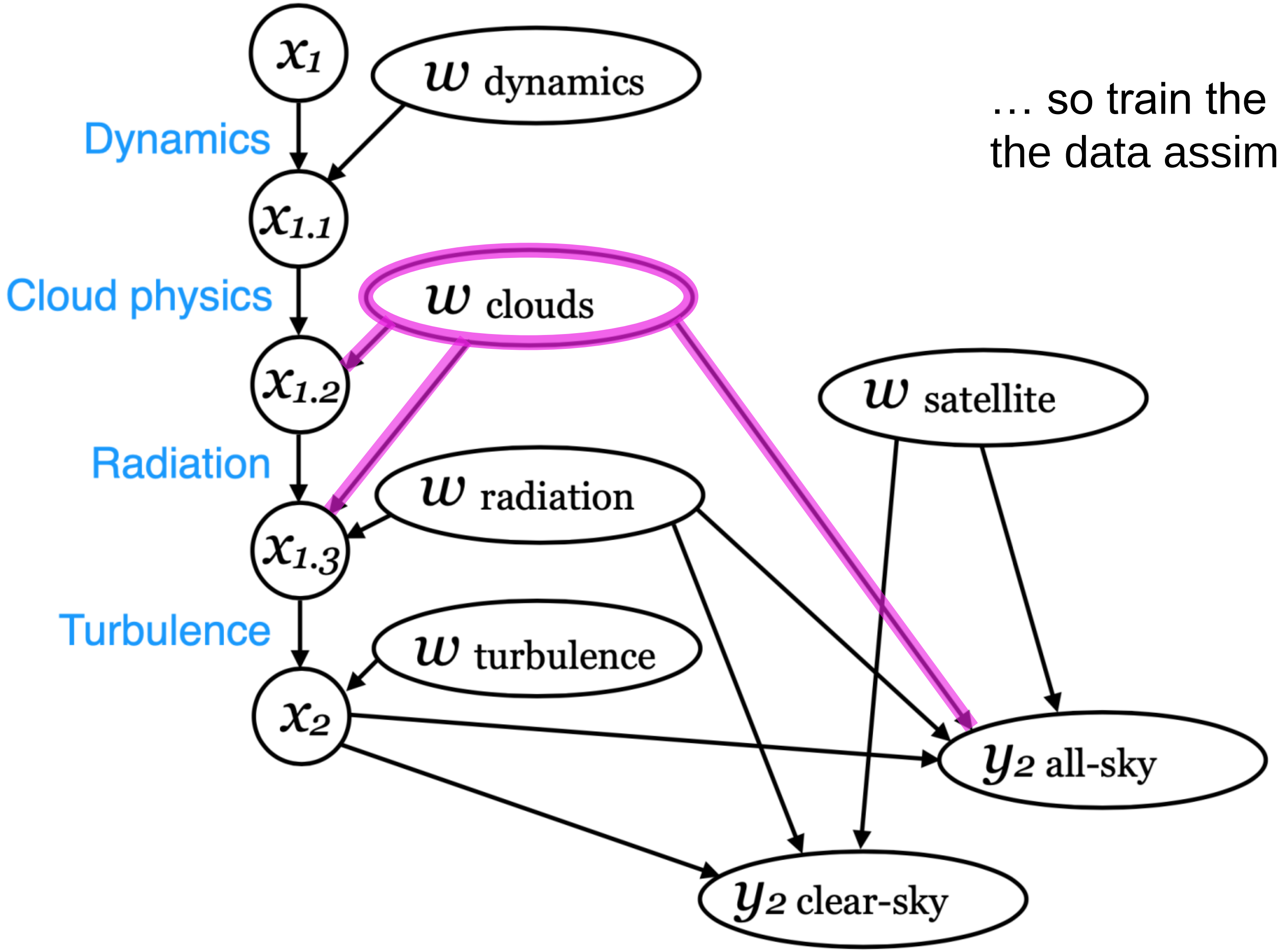


Learning an improved model of cloud physics (ML or DA)



We want to train a model against observations, but we cannot directly observe gridded intermediate states $x_{1.1}$ and $x_{1.2}$ … or more precisely model tendencies …

Inside an atmospheric model

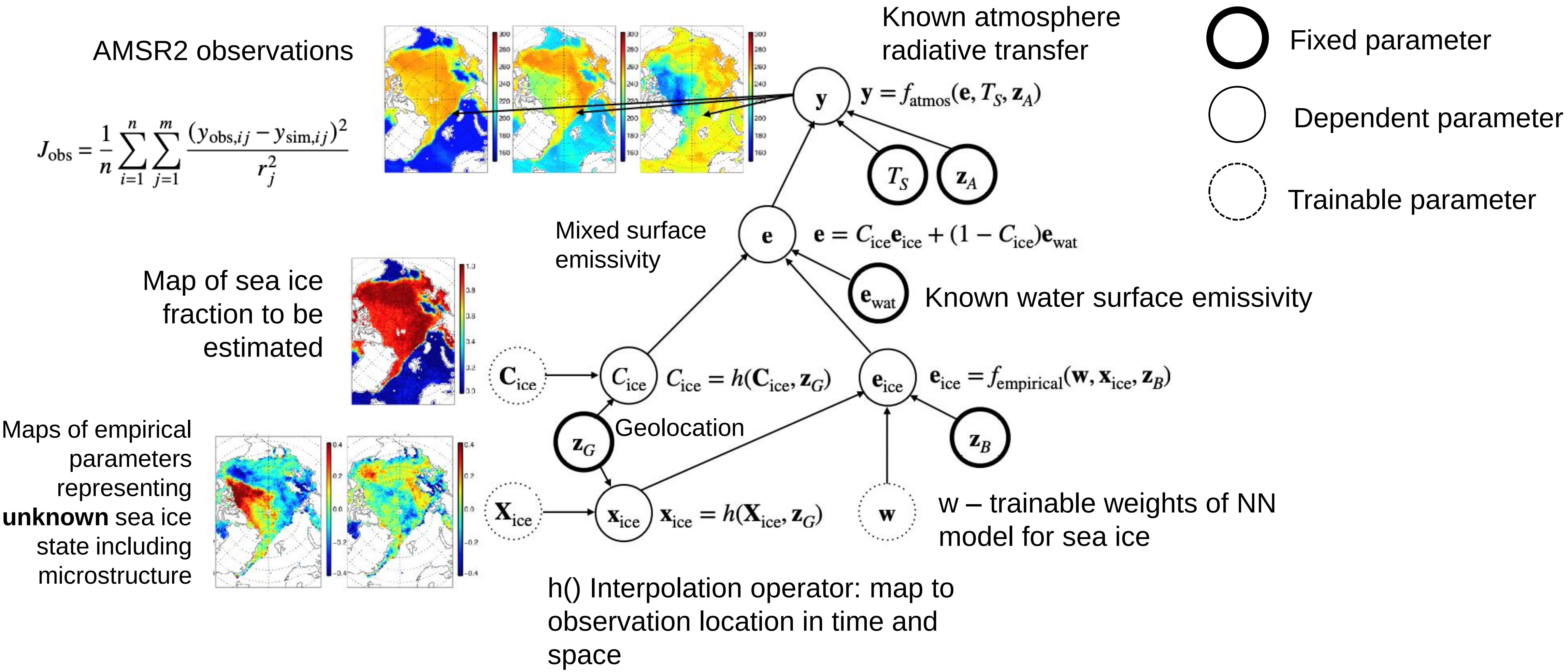


… so train the model inside the data assimilation system

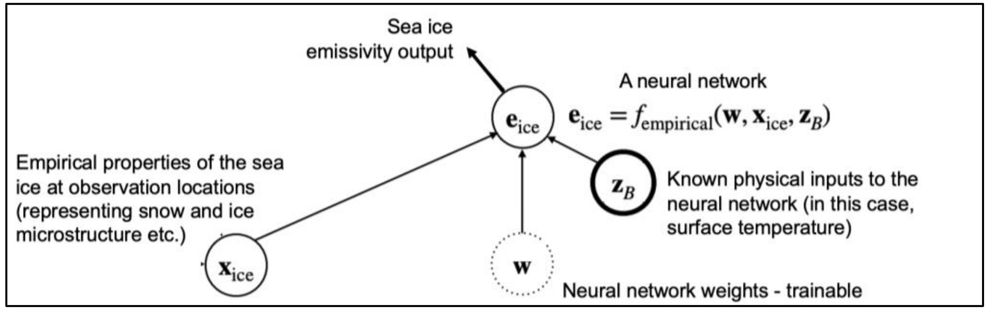
Hybrid data assimilation and machine learning

Sea ice observation operator example

A trainable empirical-physical network for sea ice assimilation



Built in Python and Tensorflow




```
class SeaiceEmis(tf.keras.layers.Layer):
    """
    Linear dense layer representing the sea ice emissivity empirical model.

    The sea ice loss applies to just the first mean emissivity (e.g. channel 10v); it's a single number as required.
    """
    def __init__(self, channels=10, bg_error=0.1, nobs=1, background=0.93):
        super(SeaiceEmis, self).__init__()
        self.dense_1 = tf.keras.layers.Dense(channels,activation='linear',bias_initializer=tf.keras.initializers.Constant(background))
        self.bg_error = bg_error
        self.background = background
        self.nobs = nobs
    def call(self, tsfc, ice_properties):
        inputs = tf.concat([tf.reshape(tsfc,(-1,1)),ice_properties],1)
        ice_emis = self.dense_1(inputs)
        emis_loss = tf.math.squared_difference((self.weights[1])[0],self.background)/tf.square(self.bg_error)/self.nobs
        self.add_loss(emis_loss)
        self.add_metric(emis_loss,name='emis_loss',aggregation='mean')
        return ice_emis
```

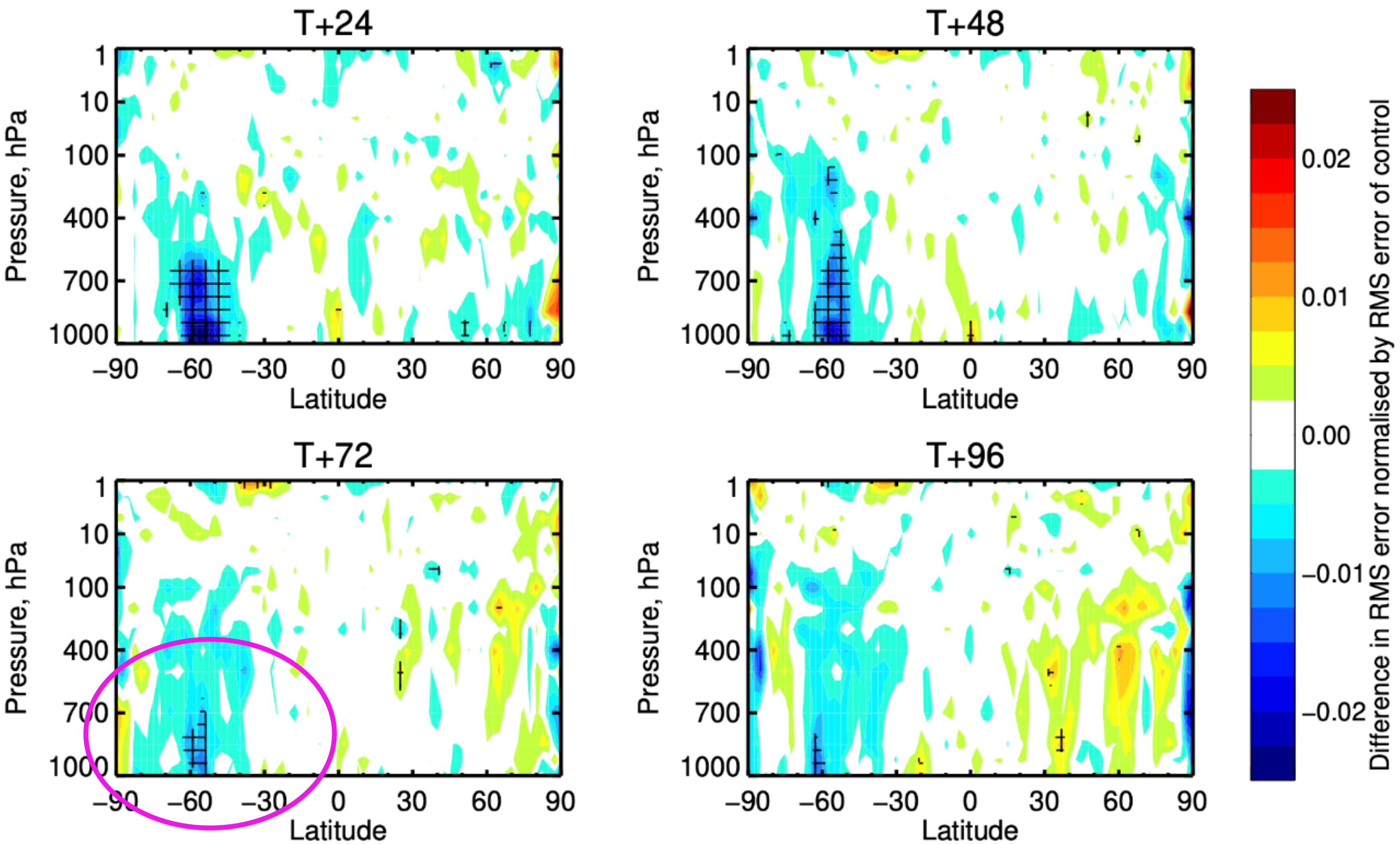
A standard dense neural network layer with linear activations

Custom loss functions to regularise / constrain the solution

https://github.com/ecmwf-projects/empirical-state-learning-seaice-emissivity-model/blob/master/seaice_layers.py

Forecast impact on temperature from adding observations obs over sea ice regions to 4D-Var
(blue = reduced error; +++ = statistical significance)

Improved temperature forecasts out to 72 hours in the Southern Ocean



Hybrid physical-empirical networks - sea ice example

- Sea ice concentration and empirical state estimation is included in cycle 49r1 of the IFS
  - Model for sea ice emissivity is the simple neural network trained within the hybrid-empirical physical network (and held fixed for now)
  - Operational implementation autumn 2024 – one of the first machine-learned components of the operational IFS
    - Maintainability? Retraining?
  - Sea ice concentration retrievals from this system will be assimilated in the ocean data assimilation component from cycle 50r1 (autumn 2025)

- Preprints

Geer (2023) Simultaneous inference of sea ice state and surface emissivity model using machine learning and data assimilation https://doi.org/10.22541/essoar.169945325.51725282/v1

Geer (2024) Joint estimation of sea ice and atmospheric state from microwave imagers in operational weather forecasting https://doi.org/10.22541/essoar.170431213.35796940/v1

Summary: generating new empirical models using ML and DA

Machine learning with physical constraints

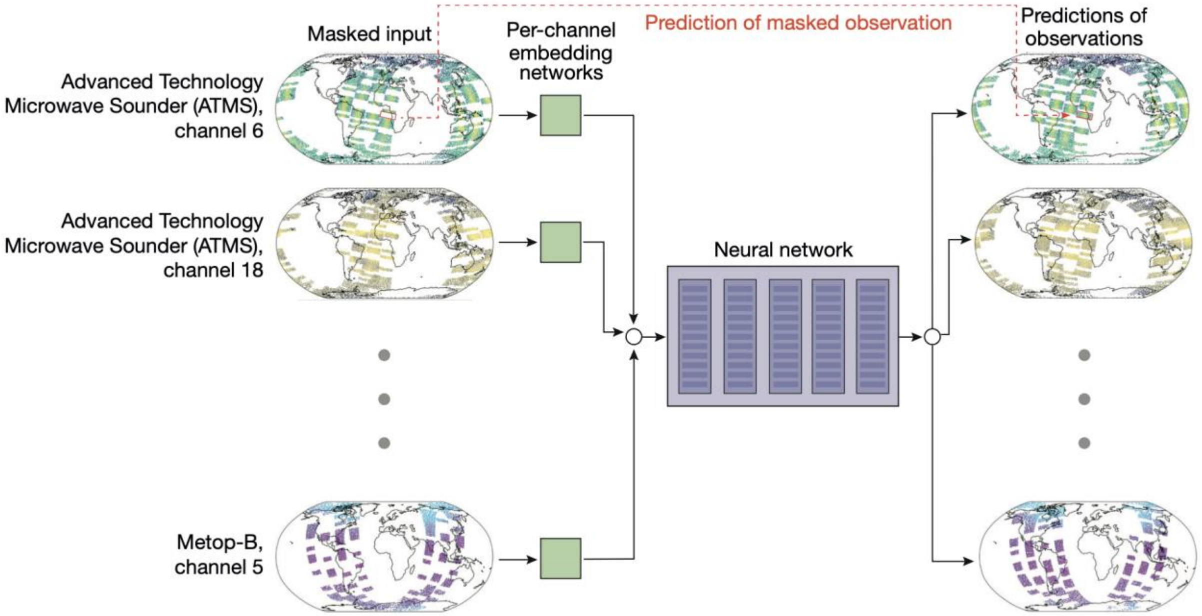
Machine learning and data assimilation: hybrid physical-empirical networks

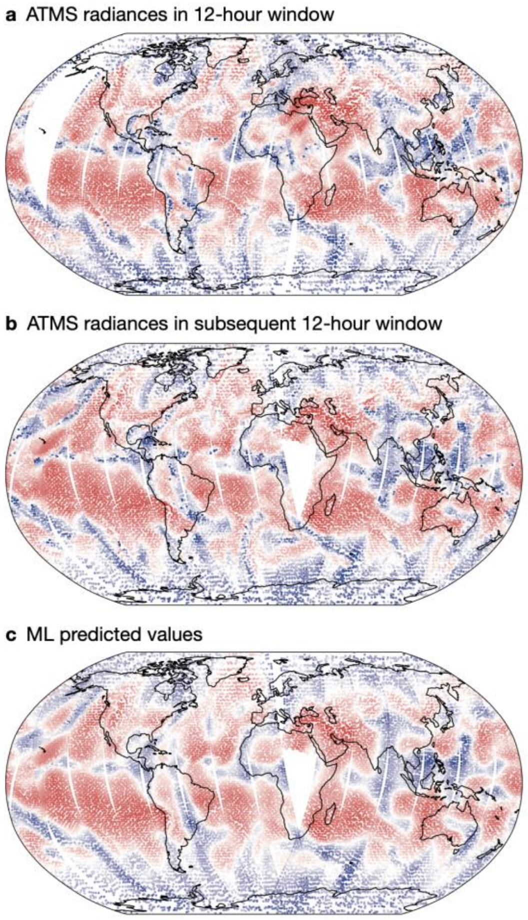
Data assimilation with parameter estimation

- Typical machine learning and variational data assimilation are similar implementations of Bayes' theorem
- Including known physics into a trainable network is a way of adding prior information in a Bayesian sense
- Existing data assimilation approaches can be very helpful in machine learning:
  - Physically-based loss functions
  - Physically-based observation (label) and background (feature) errors
  - Observation operators to map from grid to irregular and transformed observation space (e.g. satellite radiances)
- Data assimilation frameworks (e.g. weather forecasting) are evolving to be able to train and update empirical models (e.g. neural networks) as part of routine data assimilation activities

Don't throw away the physical model – improve it!

Direct observation prediction – a new project at ECMWF





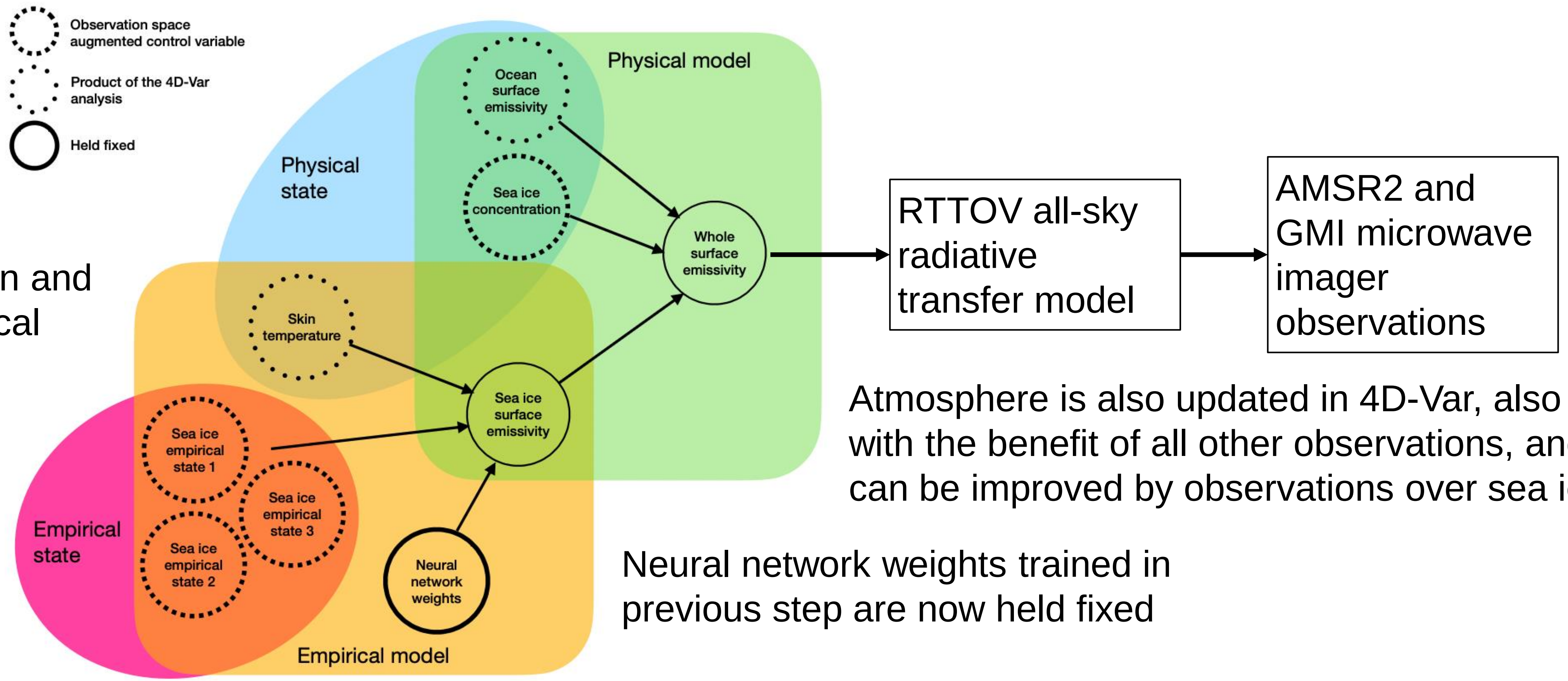
12 UTC 22nd Mar 2024 00 UTC 23rd Mar 2024

Tony McNally et al. (2024, ECMWF newsletter) - https://www.ecmwf.int/en/newsletter/178/earth-system-science/red-sky-night-producing-weather-forecasts-directly

Arxiv paper: https://arxiv.org/pdf/2412.15687v1

Empirical sea ice emissivity model used to retrieve sea ice concentration in atmospheric 4D-Var and to allow radiance assimilation over sea ice

Sea ice concentration and three empirical parameters retrieved at observation locations



Atmosphere is also updated in 4D-Var, also with the benefit of all other observations, and can be improved by observations over sea ice

Neural network weights trained in previous step are now held fixed