Parameter Calibration with Neural Network-Based Emulation of a Land Model

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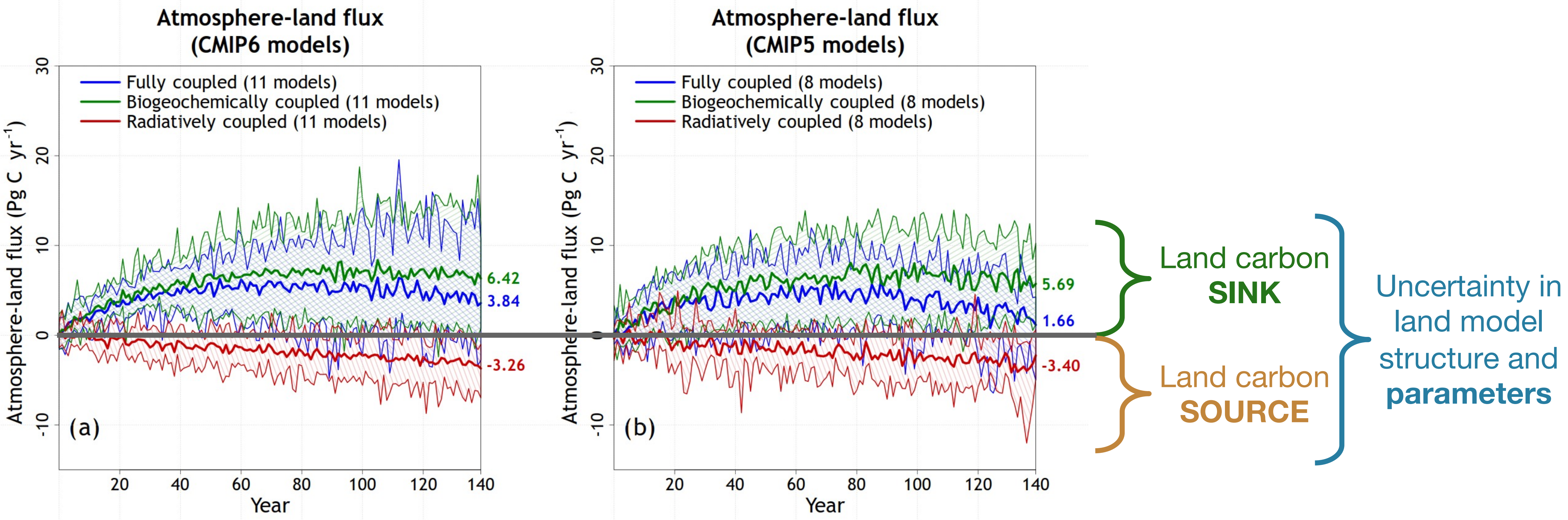
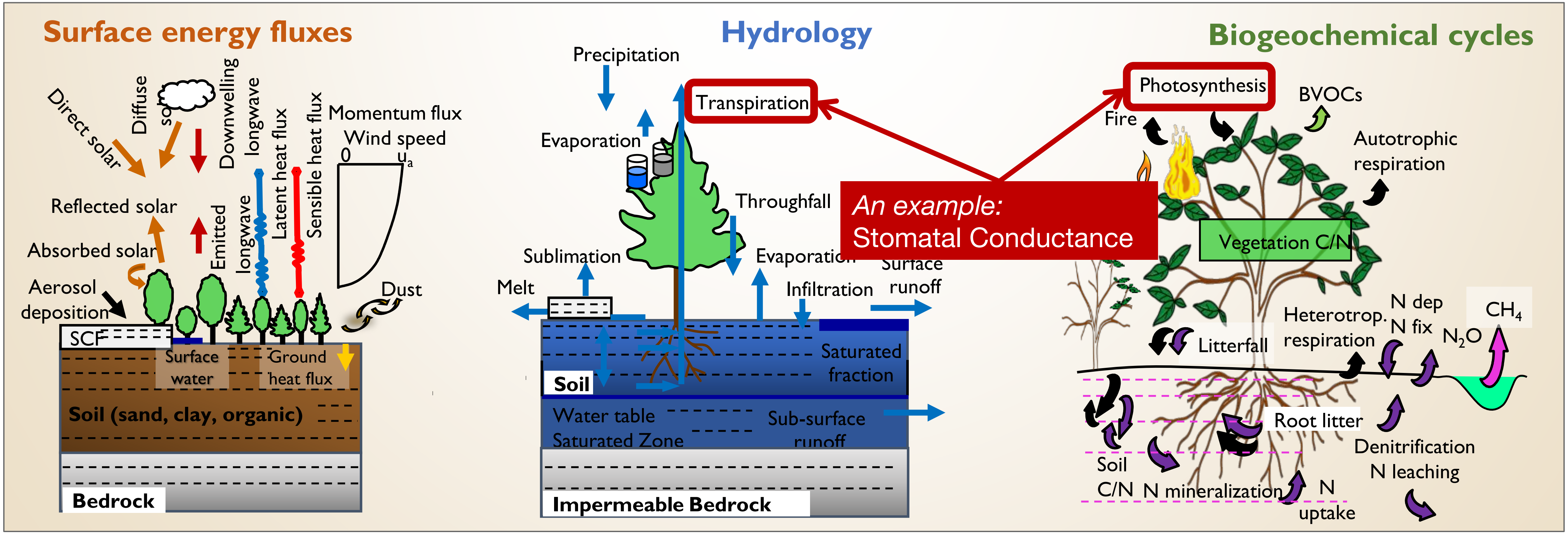
Uncertainty in Land Model Projections



Lovenduski & Bonan (2017)

Arora et al. (2020)

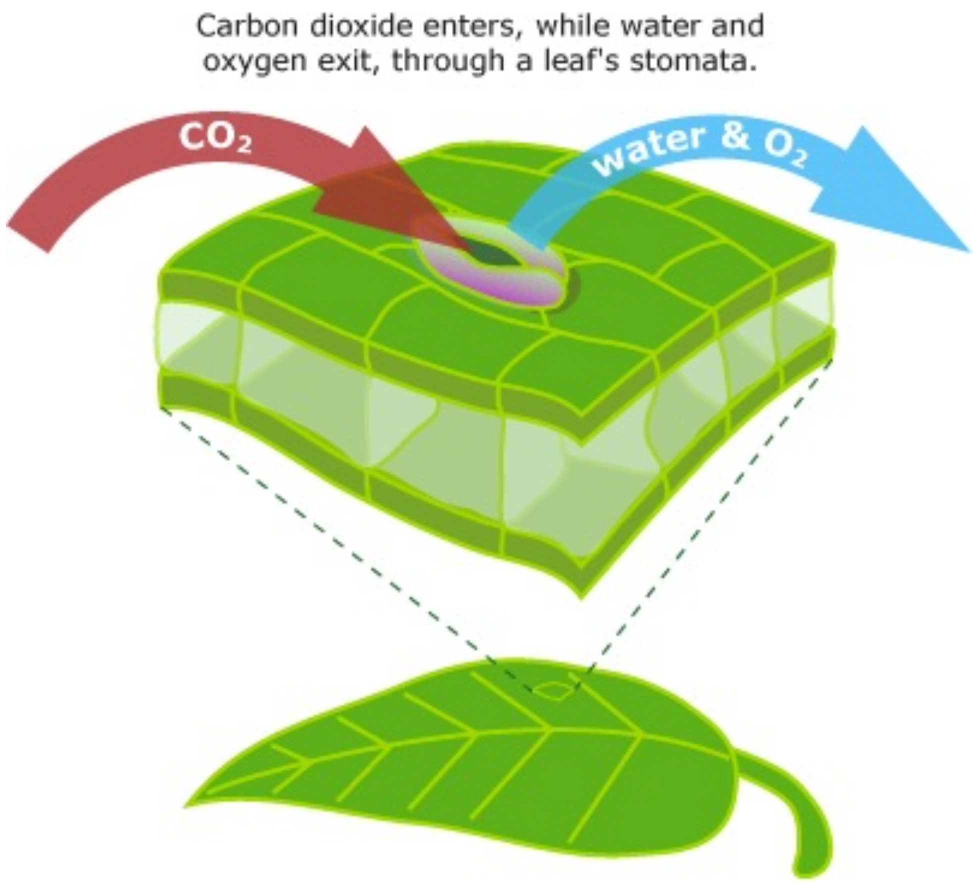
Uncertainty in Land Model Parameters



Schematic of NCAR's Community Land Model (CLM), version 5

Lawrence et al. (2019)

Example of Parameter Uncertainty: Stomatal Conductance



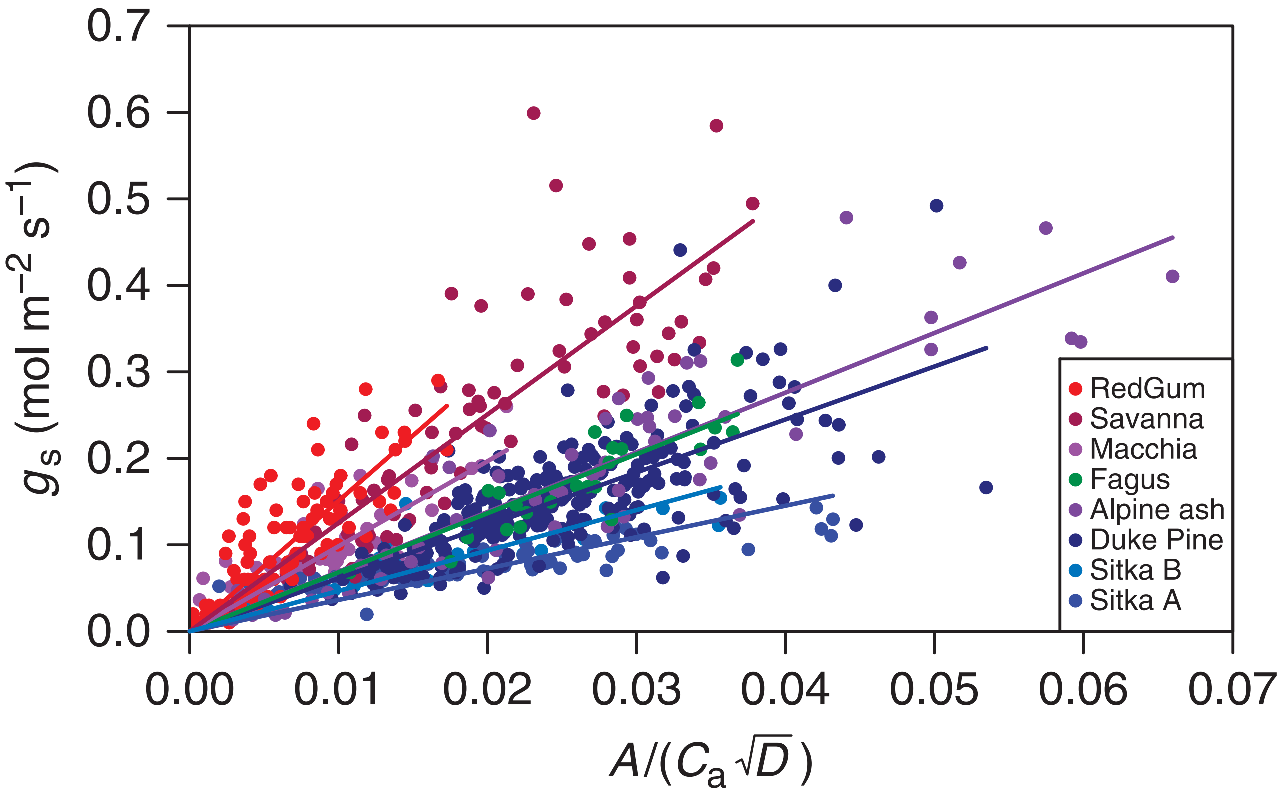


Image: evolution.berkeley.edu

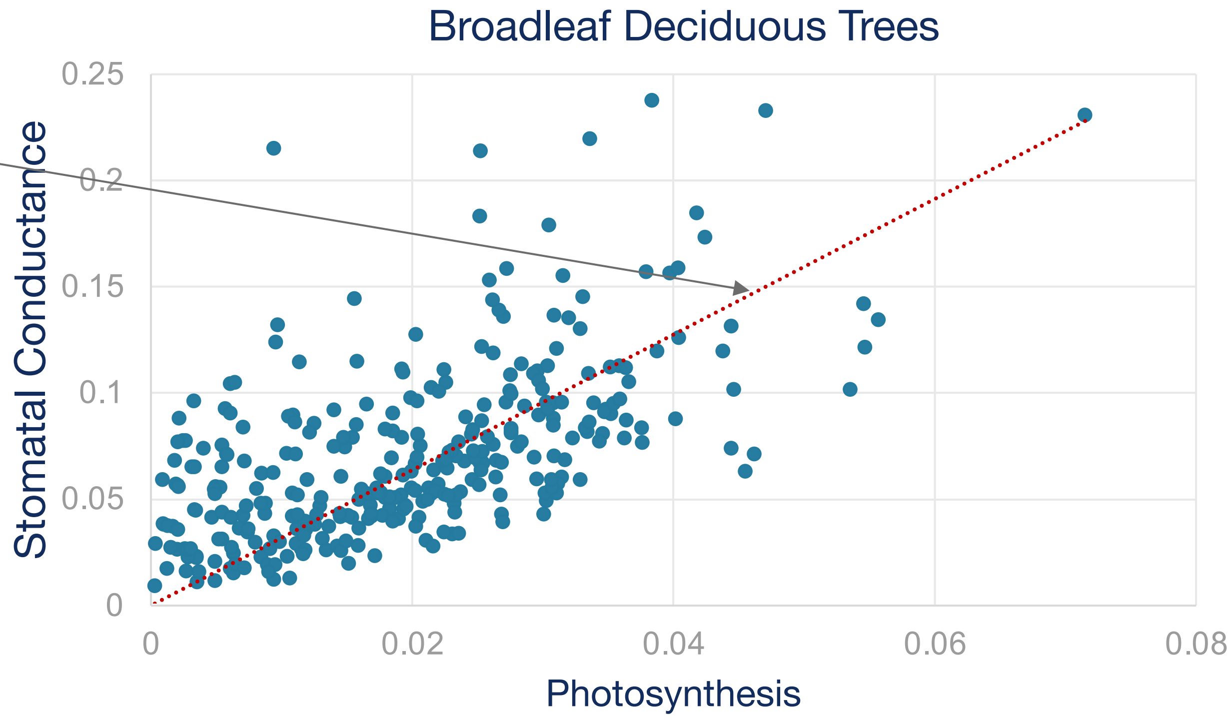
Medlyn et al. (2011)

Example of Parameter Uncertainty: Stomatal Conductance

Slope parameter represents **marginal water cost of carbon gain** and is an important model parameter.

$$g_s = g_o + 1.6\left(1 + \frac{g_1}{\sqrt{D}}\right)\frac{A_n}{c_s/P_{atm}}$$

g_1 = slope parameter (mol H_2O/mol CO_2)

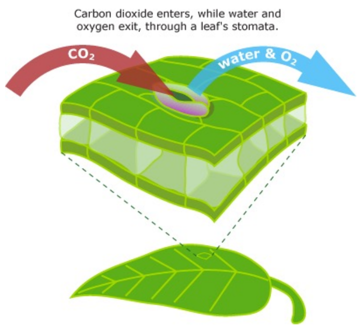


Medlyn et al. (2011)

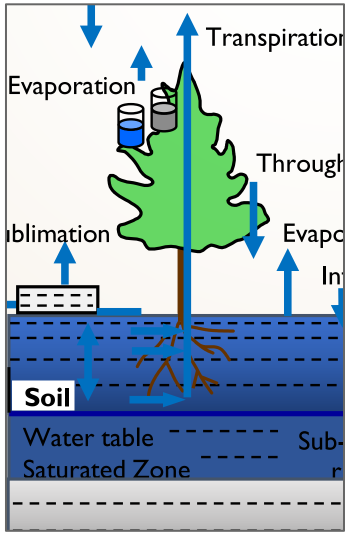
Data from Lin et al. (2015)

Community Land Model Parameters

- Biophysical features (e.g., surface energy balance, hydrology, carbon uptake)
- Individual parameter uncertainty ranges determined by literature review, updated observations
- Parameter selection based on a series of sensitivity tests with objective metrics



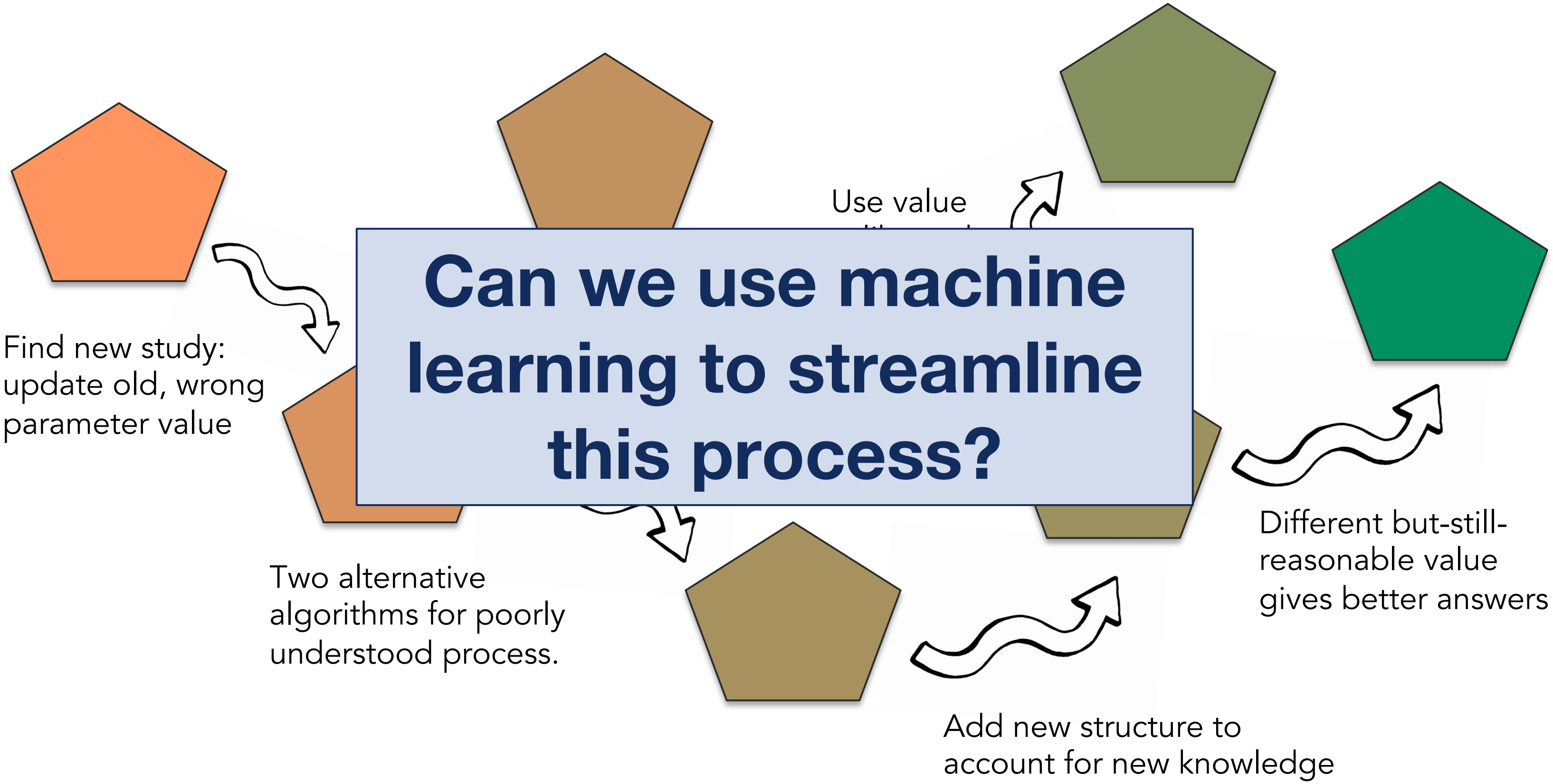
Name	Parameter Description	Biophysical Process
medlynslope	Slope of stomatal conductance-photosynthesis relationship	Stomatal conductance and photosynthesis
dleaf	Characteristic dimension of leaves in the direction of wind flow	Leaf boundary layer resistance
kmax	Plant segment maximum conductance	Plant hydraulic stress
fff	Decay factor for fractional saturated area	Surface runoff
dint	Fraction of saturated soil for moisture value at which dry surface layer initiates	Soil evaporation
baseflow_scalar	Scalar multiplier for base flow rate	Sub-surface runoff



Dagon et al. (2020)

Can we use machine learning to calibrate model parameters?

Hand-tuning parameter values takes a long time (many model runs, trial and error).



Can we use machine learning to streamline this process?

Figure from Rosie Fisher

Machine Learning for Climate Science

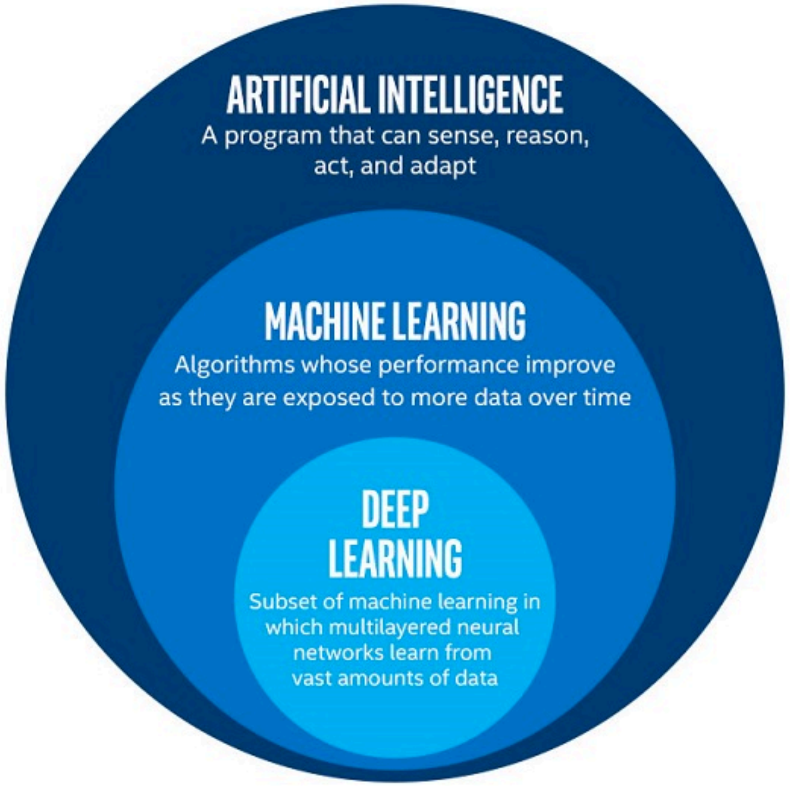
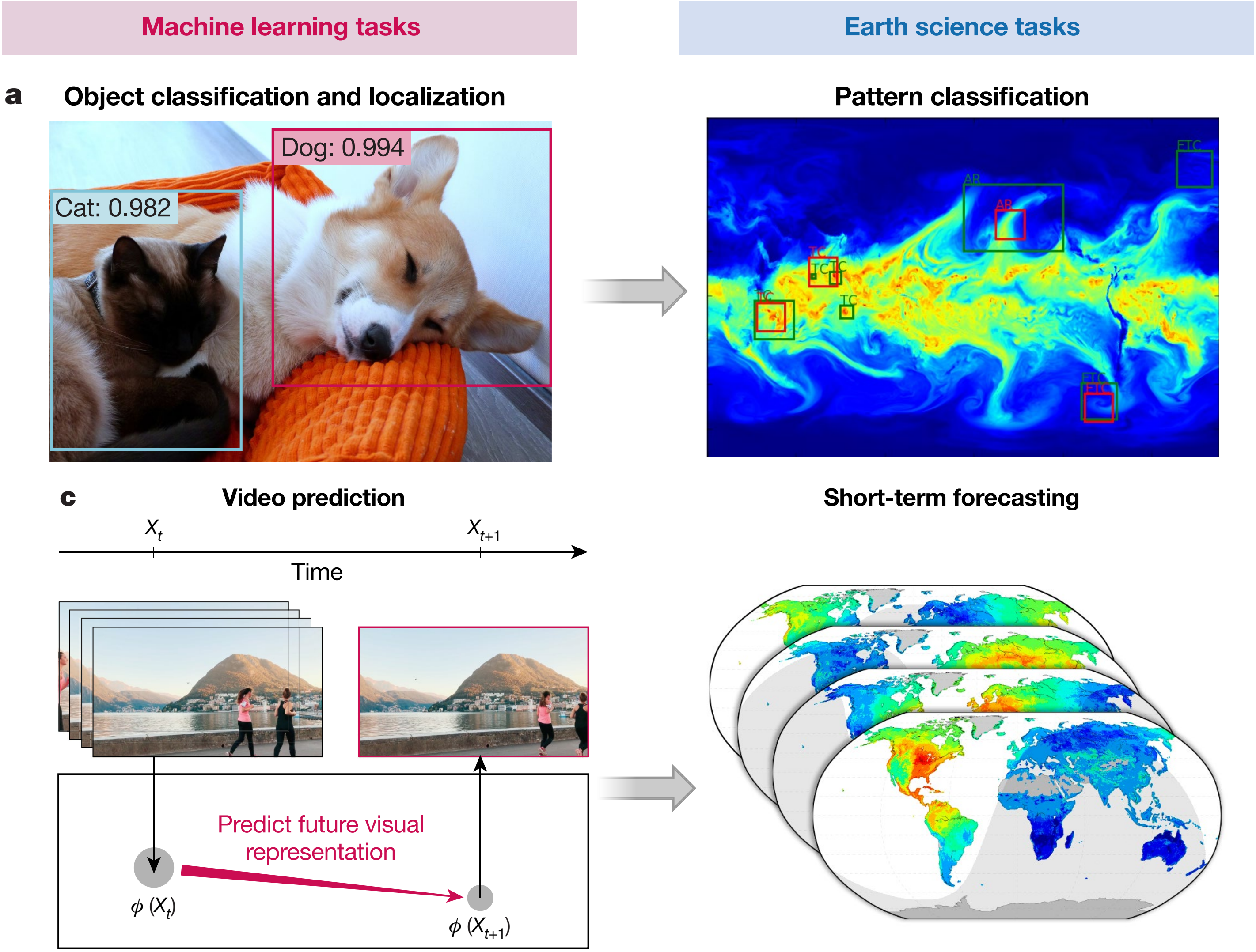


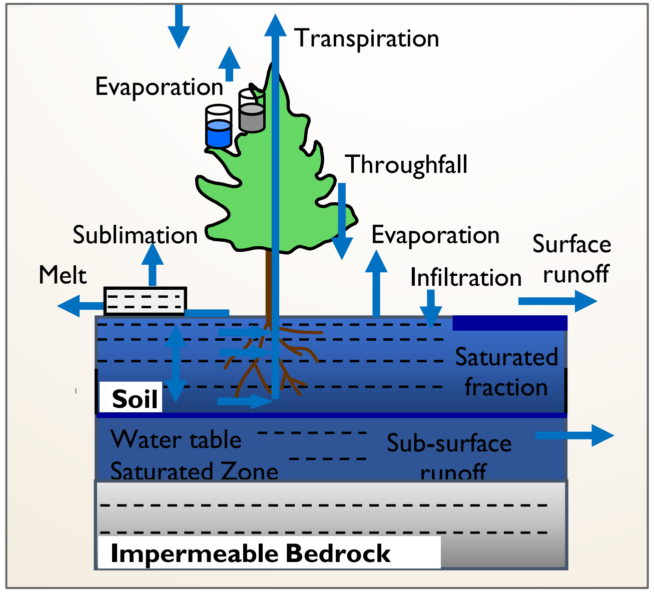
Image: https://becominghuman.ai/an-introduction-to-machine-learning-33a1b5d3a560



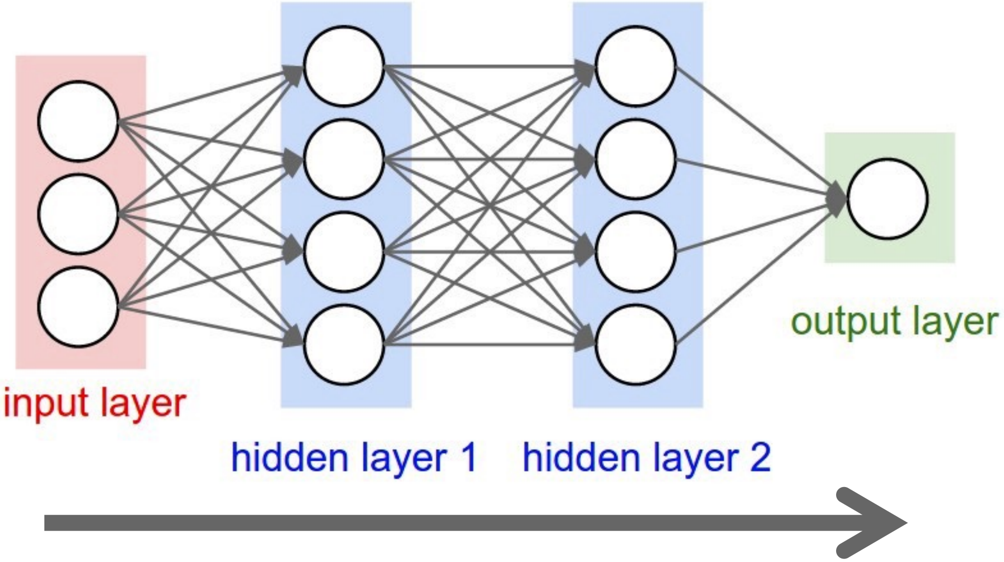
Reichstein et al. (2019)

Neural Networks as Land Model Emulators

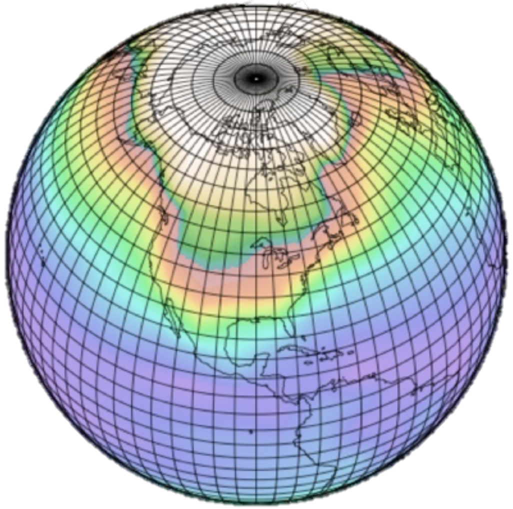
Input: land model parameter values



Neural network emulator



Output: land model predictions

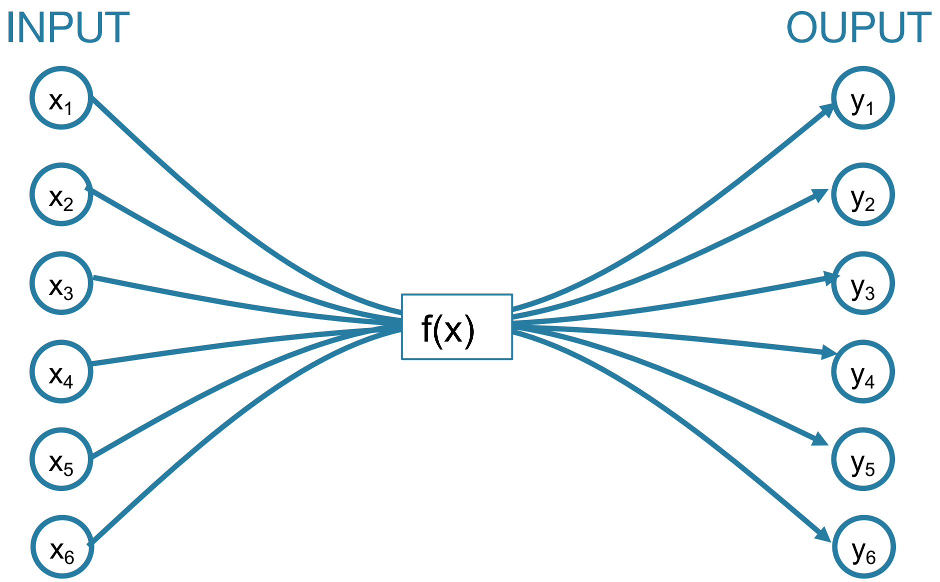


A machine learning algorithm is trained to predict land model output, given parameter values as input.

Network image: http://cs231n.github.io/neural-networks-1/

Neural Network Basics

Supervised Machine Learning: learn functional relationships given data



Given a set of input **x** and output **y** (training data), use an optimizer to search for a function **f(x)** that fits the data well but also generalizes to new values (validation data).

Schematic from David Hall

Machine Learning Roadmap

1. *Train:* Build and train a series of **neural networks (NNs)** to predict land model output, given parameter values as input.

2. *Emulate:* Use trained NNs as **land model emulators** to make predictions with increased computational efficiency.

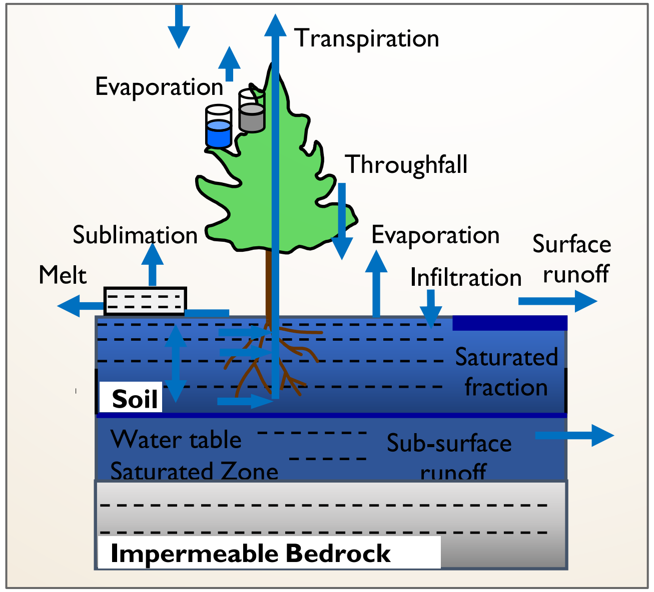
3. *Calibrate:* **Minimize error in predictions** relative to observations; generate optimal parameter values and distributions.

4. *Test:* Use optimal parameter values to **investigate changes in model predictive skill**.

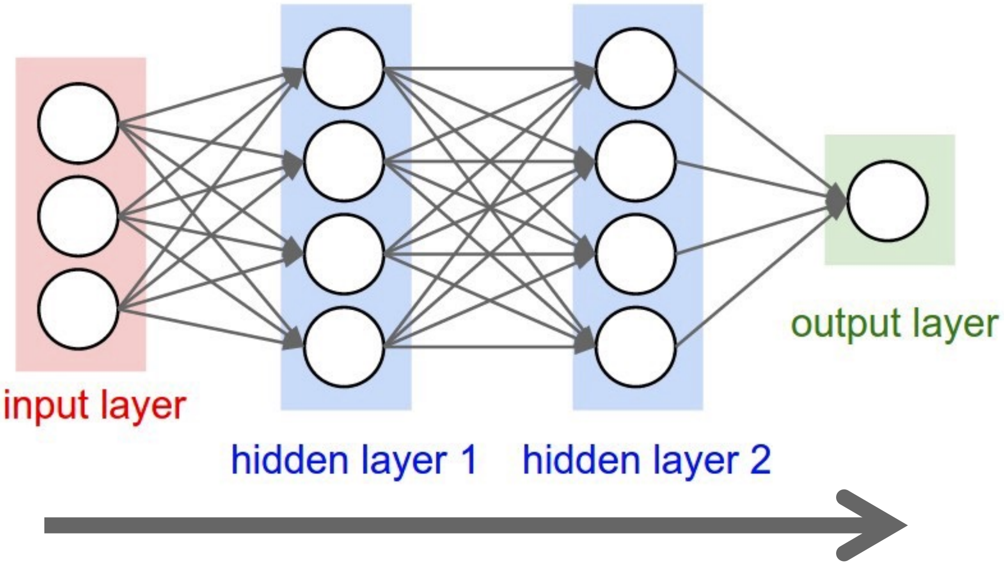
Neural Networks as Land Model Emulators

Step 1: Train

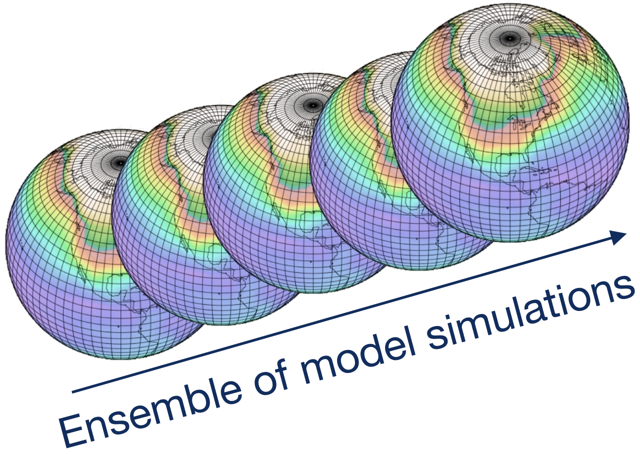
Input: land model parameter values



Neural network emulator

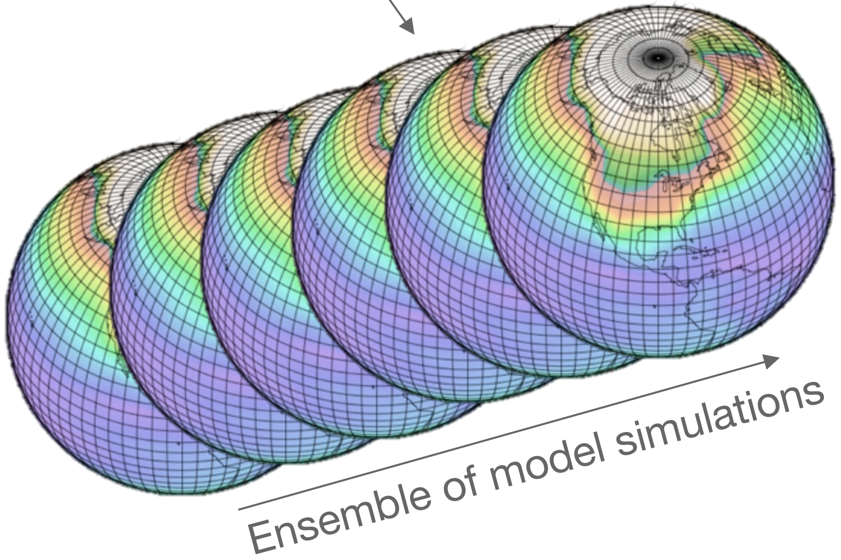


Output: land model perturbed parameter ensemble

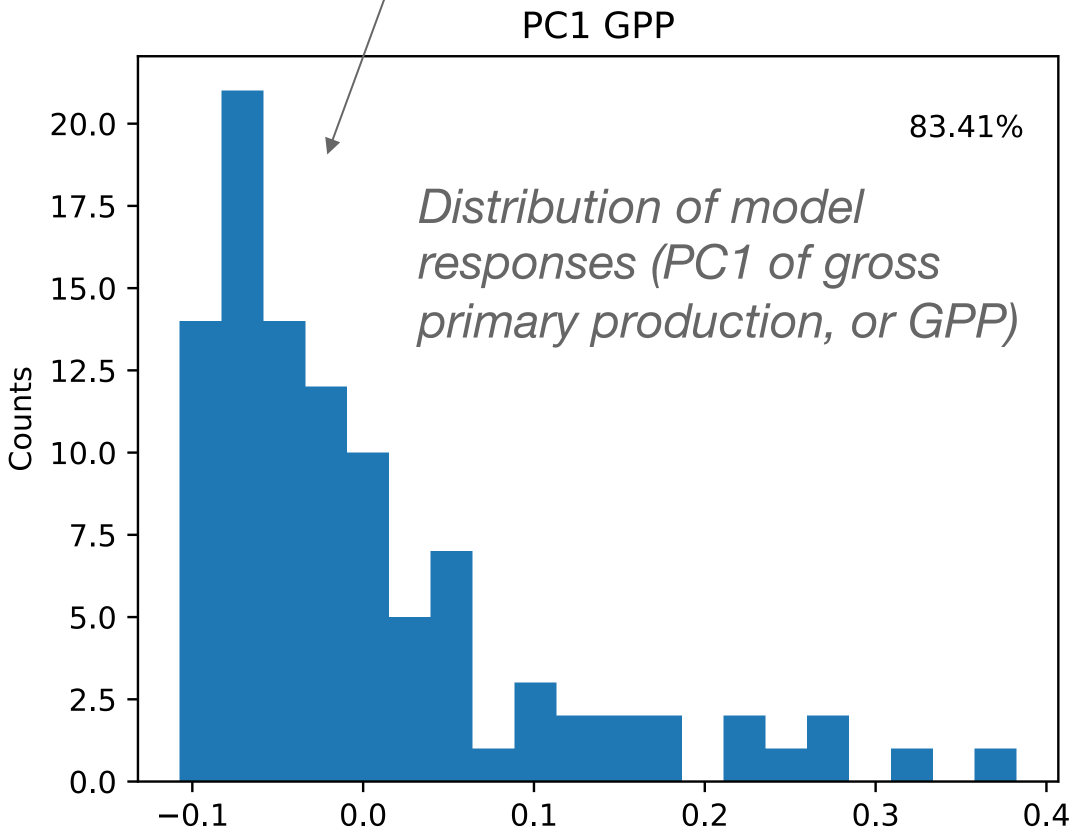


Generating the Training Data

Land model* perturbed parameter ensemble (PPE) using 100 parameter combinations generated with Latin Hypercube sampling

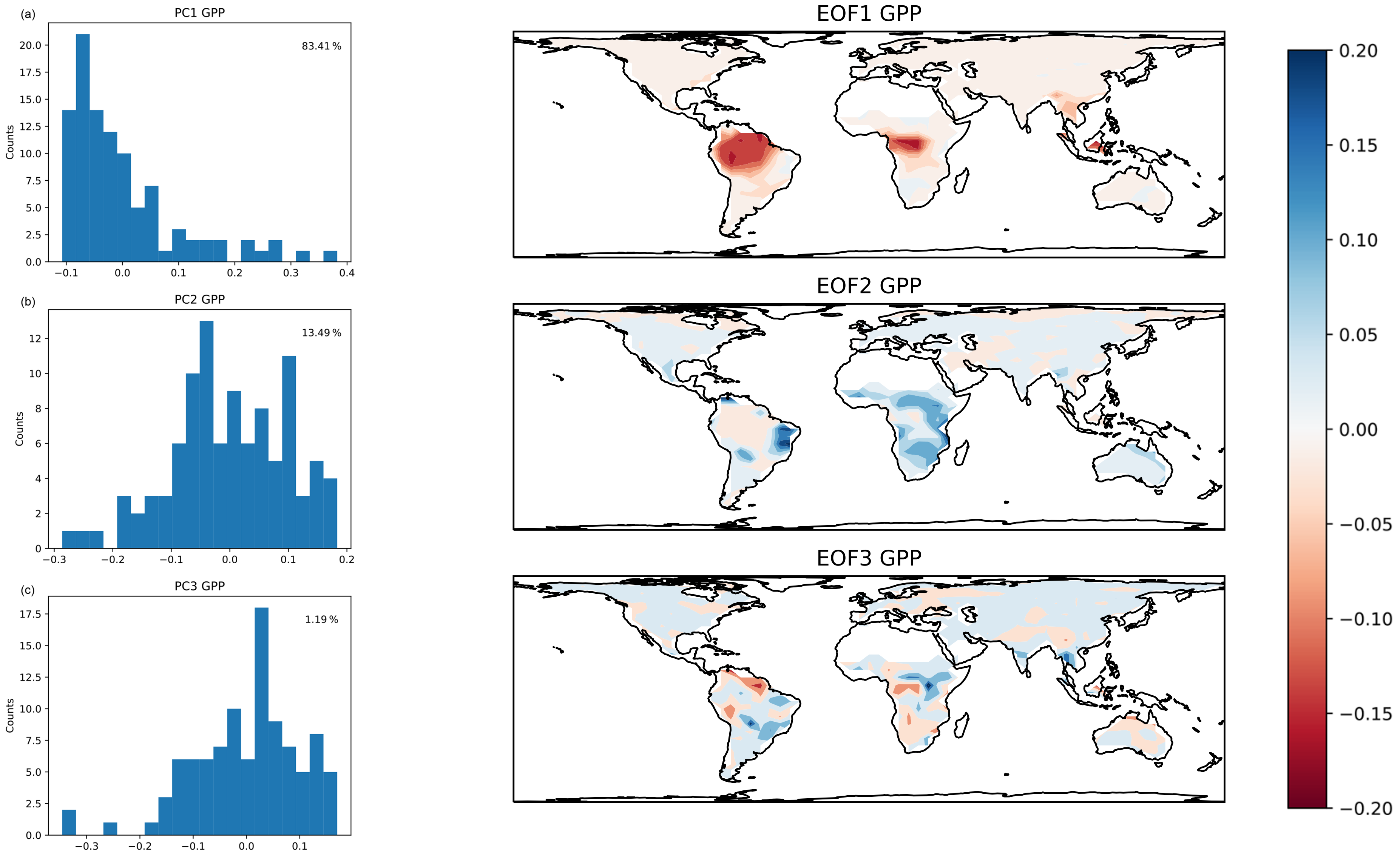


Use principal component analysis (PCA) to predict modes of variability of carbon and water fluxes



**Offline global land-only simulations forced by atmospheric reanalysis data*

Spatial patterns from Empirical Orthogonal Function (EOF) analysis



Dagon et al. (2020)

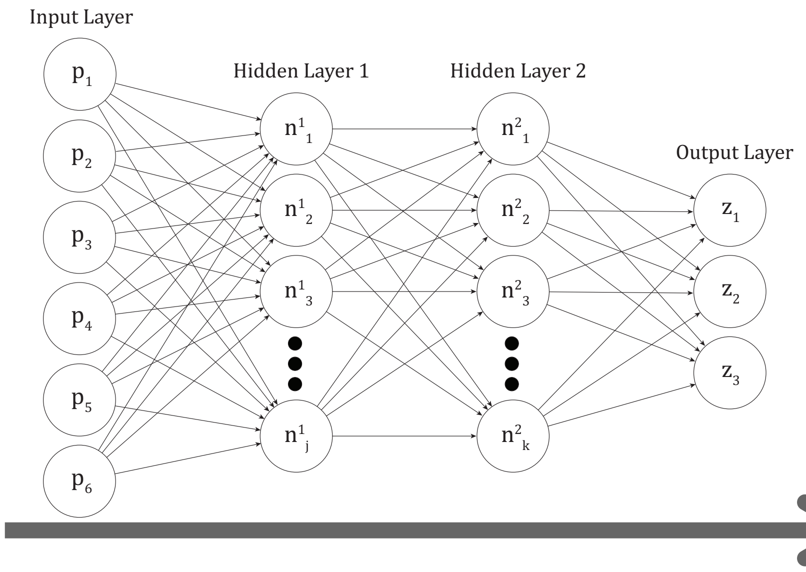
Neural Networks as Land Model Emulators

Step 1: Train

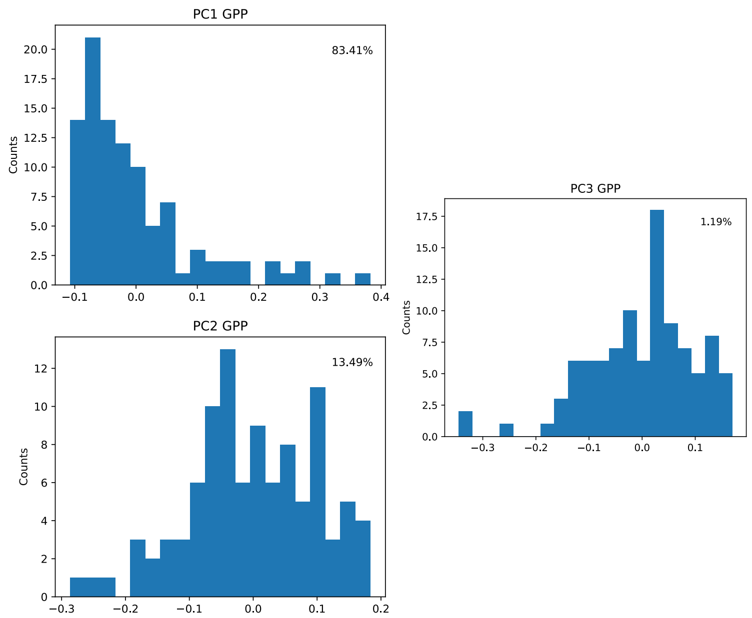
Input: land model parameter values

	P1	P2	P3	P4	P5	P6
S1	x1,1	x1,2	x1,3	x1,4	x1,5	x1,6
S2	x2,1	x2,2	x2,3	x2,4	x2,5	x2,6
S3	x3,1	x3,2	x3,3	x3,4	x3,5	x3,6
…	…	…	…	…	…	…
S100	x100,1	x100,2	x100,3	x100,4	x100,5	x100,6

2-layer feed-forward artificial neural network (ANN)



Output: land model perturbed parameter ensemble

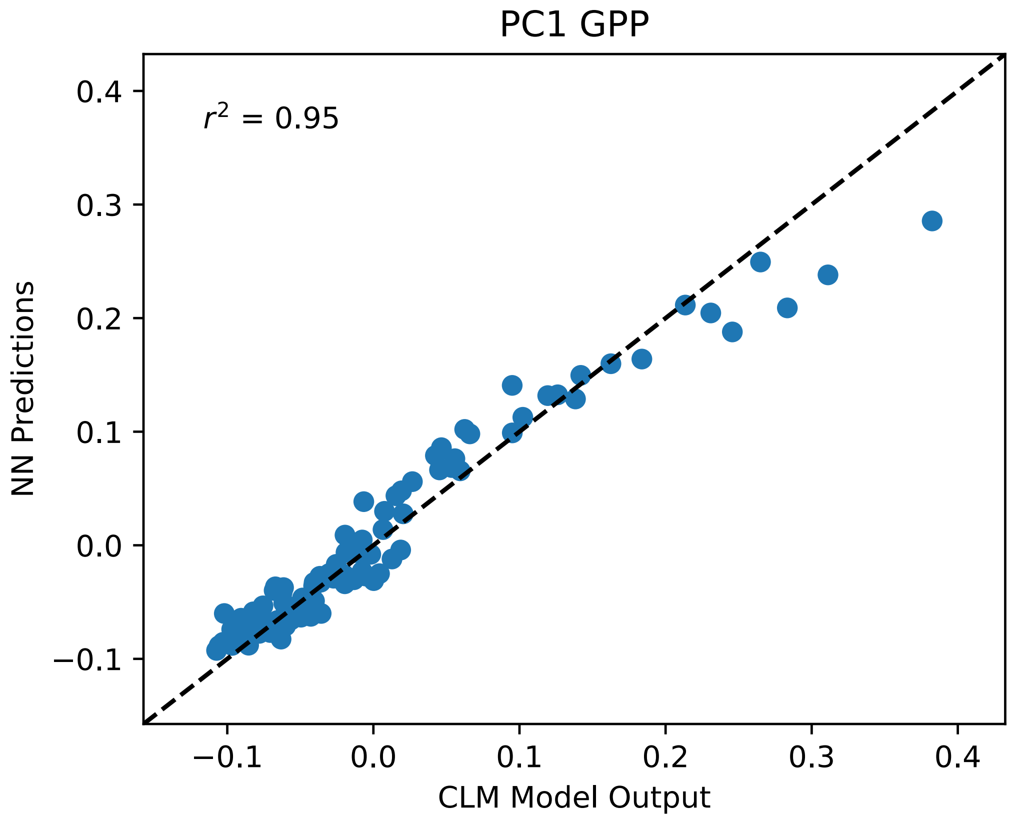


Train to predict spatial variability (first 3 PCs) of gross primary production (GPP).

Separate emulator built for first 3 PCs of latent heat flux (LHF).

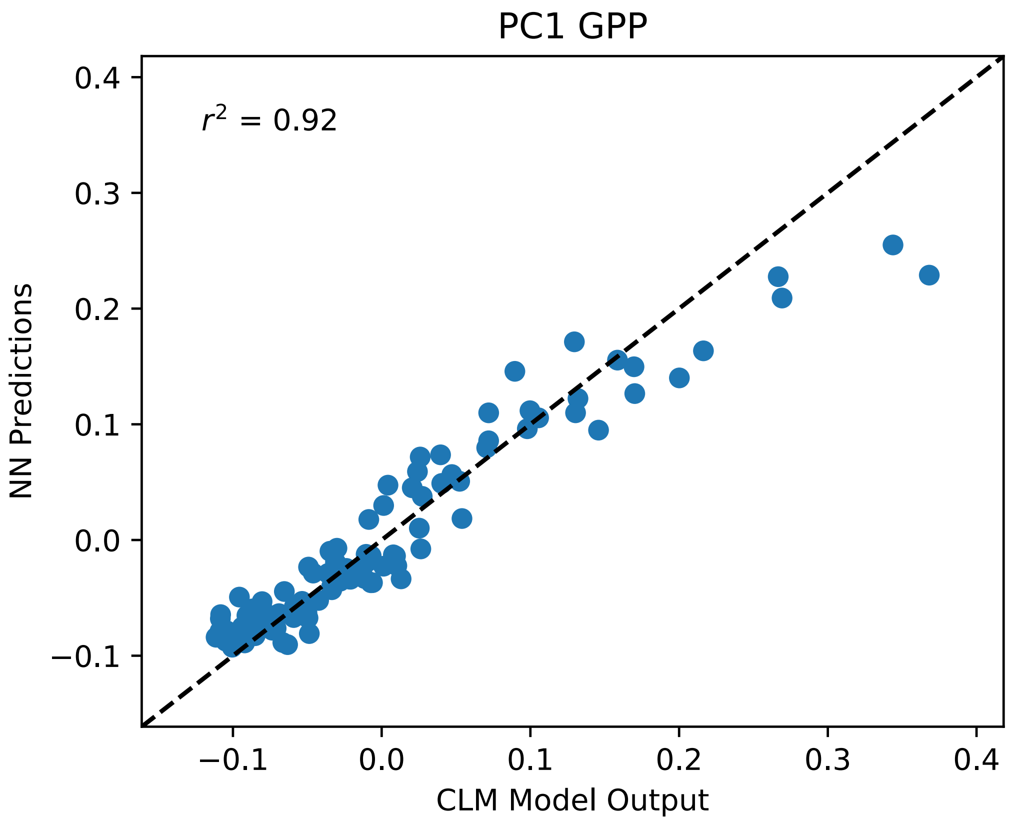
Assessing Emulator Performance

Original ensemble



"Best" emulator trained on original parameter values and model output.

Second ensemble



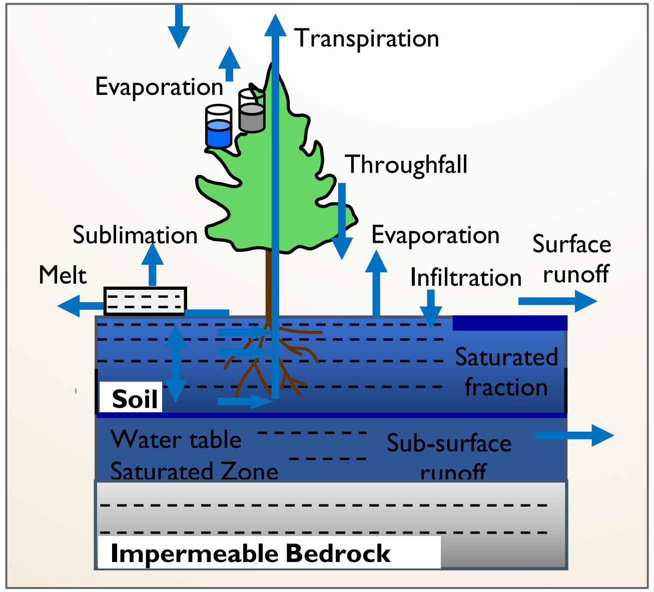
Same emulator; **different** parameter values and resulting model output. **Predictive skill is comparable.**

Dagon et al. (2020)

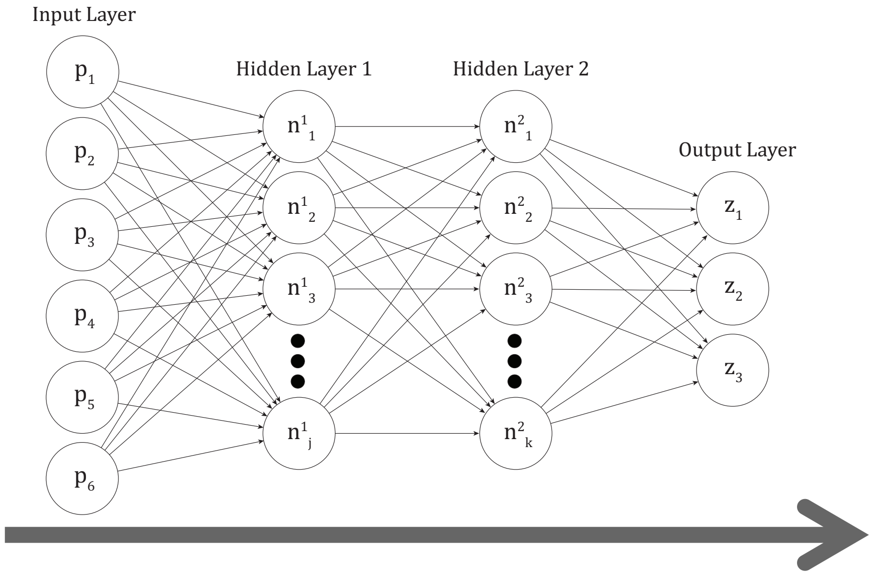
Neural Networks as Land Model Emulators

Step 2: Emulate

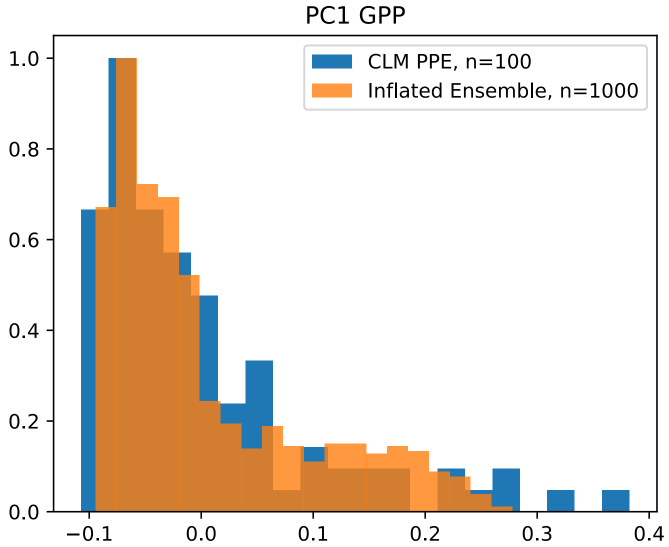
Input: **NEW** land model parameter values



Trained neural network emulator



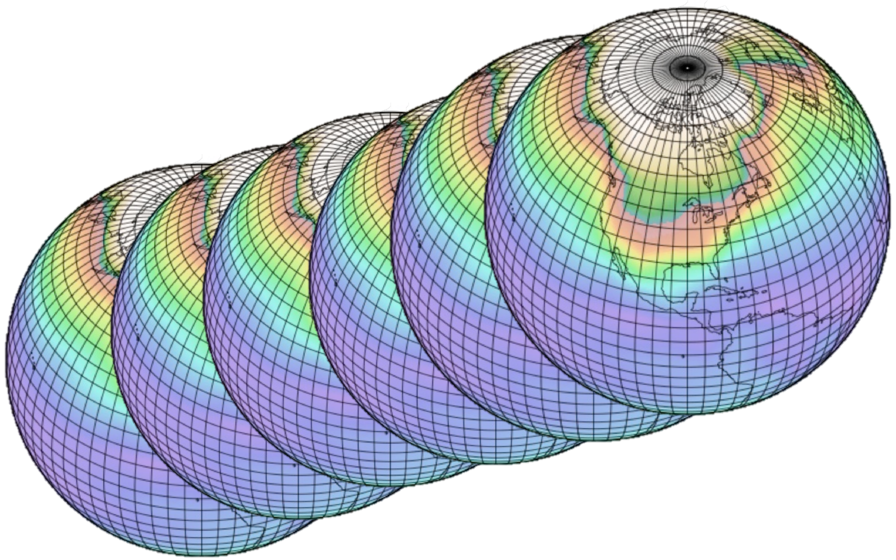
Output: land model **PREDICTIONS**



The trained neural network can be applied to test new parameter values and combinations, much more quickly and efficiently than running the climate model.

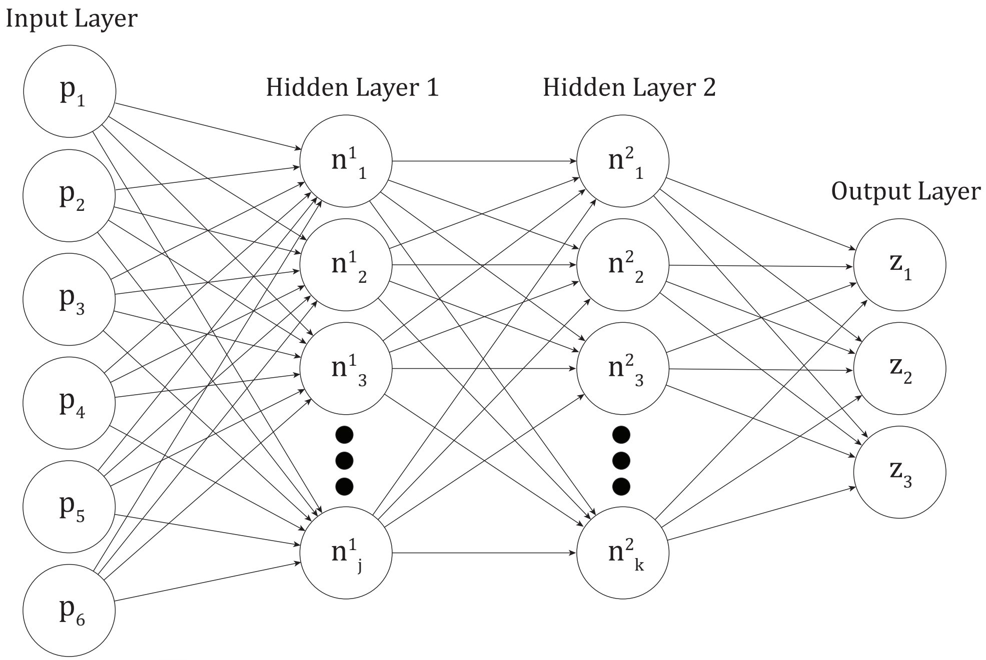
Increase in Computational Efficiency

Land model perturbed parameter ensemble



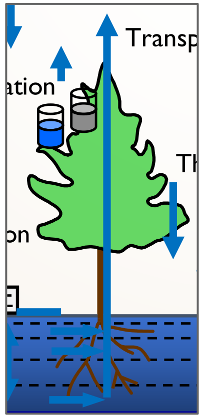
~2 hours per simulation

Machine learning emulator

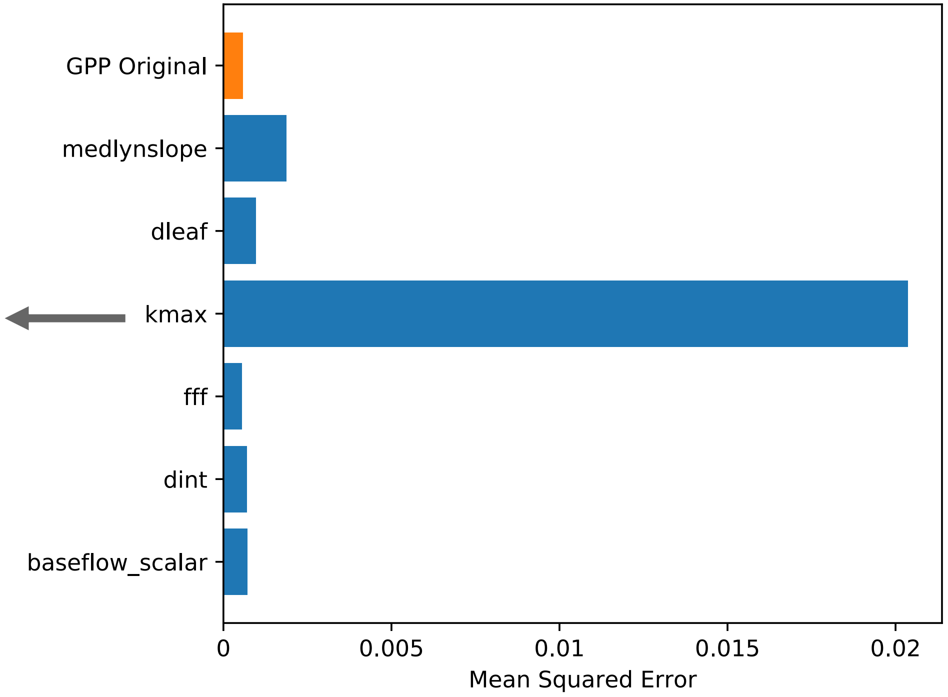


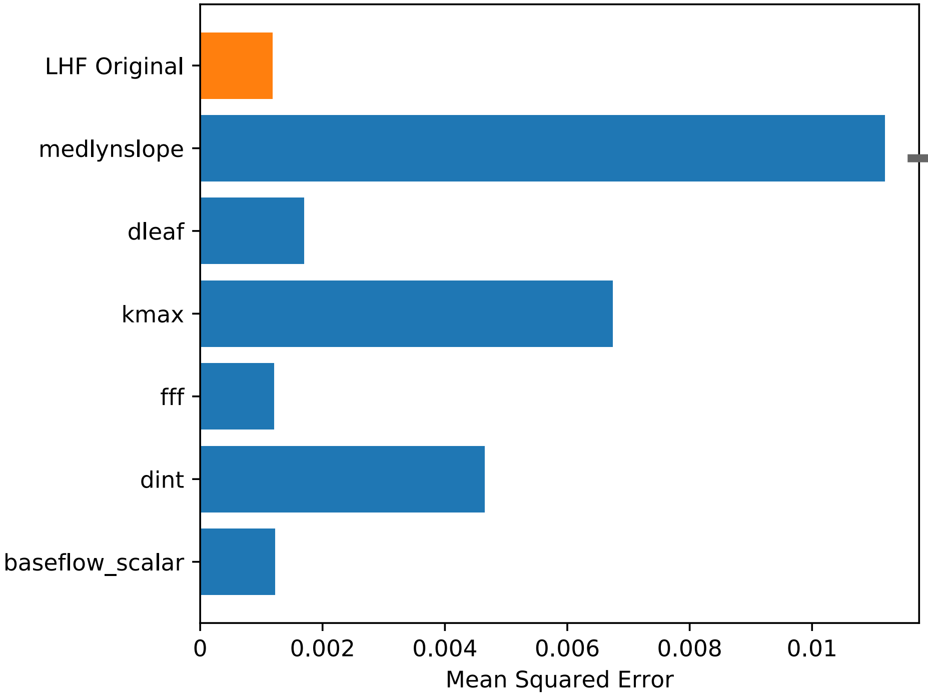
2.6 seconds to generate predictions!

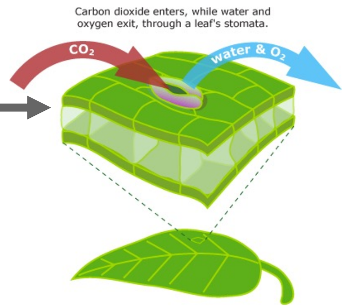
Machine Learning Interpretation: Variable/Feature Importance



Kennedy et al. (2019)







Medlyn et al. (2011)

<u>Variable/Feature Importance</u>

- Randomly shuffle values of one parameter (preserving others) and test performance of emulator.
- Skill metric is mean squared error between predictions and actual values.
- Larger bar means the parameter is **more important to the predictive skill** of the emulator.

Dagon et al. (2020)

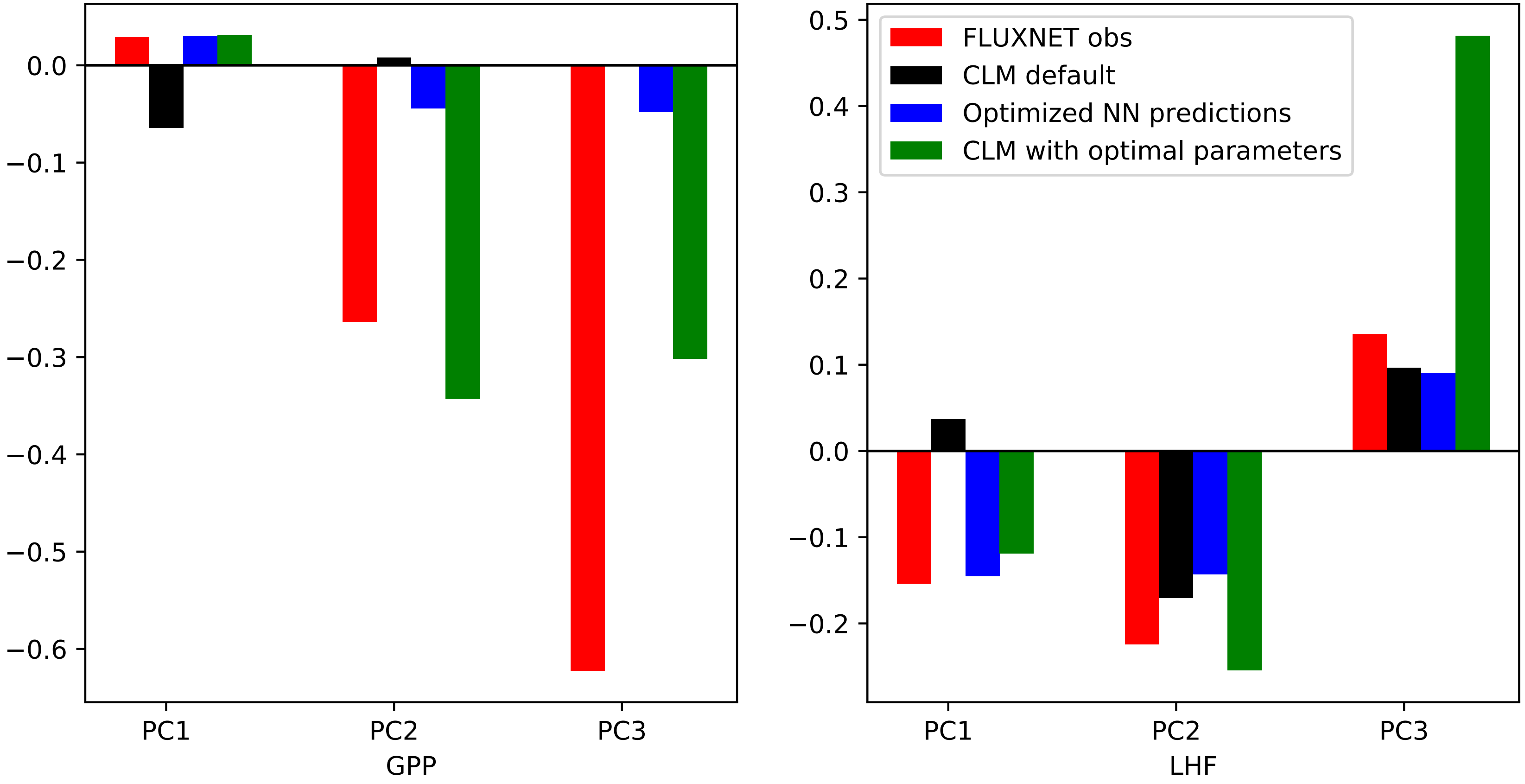
Optimize Emulator Predictions to Reduce Model Biases

Step 3: Calibrate

- Minimize error in emulator (NN) predictions relative to observations.
- How well do optimized NN predictions match observations (compare blue and red bars)?

Step 4: Test (PCs)

- Test land model (CLM) with optimized parameter values; compare default model performance.
- How well do optimized emulator predictions match model tested with optimal parameters (compare blue and green bars)?
- Does the calibration process improve model biases (compare green bars with red and black bars)?



Dagon et al. (2020)

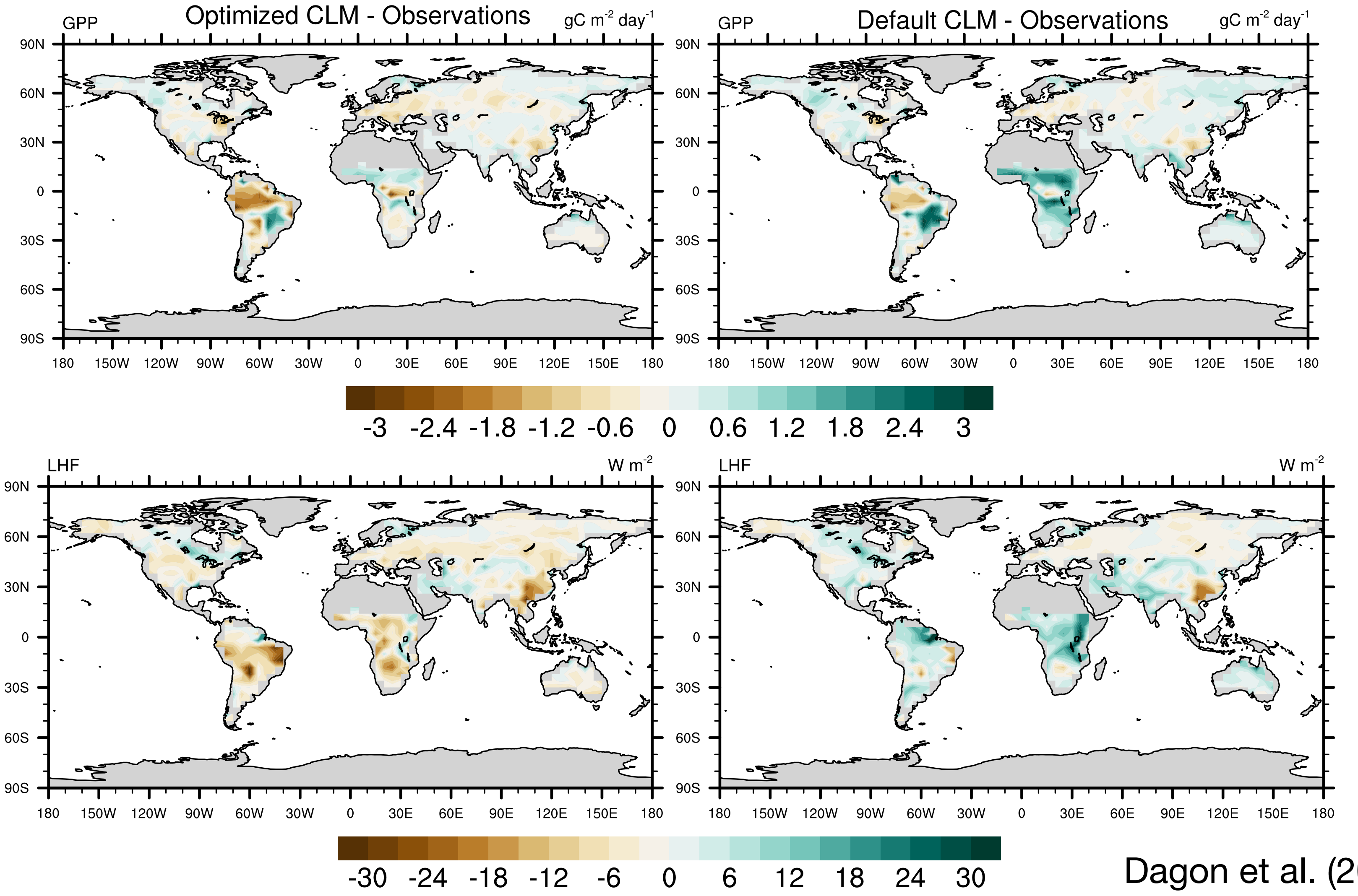
Optimize Emulator Predictions to Reduce Model Biases

Step 4: Test (Global)

- Improvement in global, annual mean biases; regional/seasonal results mixed

Additional Considerations

- Additional sources of uncertainty (e.g., forcing, observations, structural)
- Choice of output variables (GPP and LHF)
- Choice of metrics (**annual mean** spatial variability as determined by PCA)

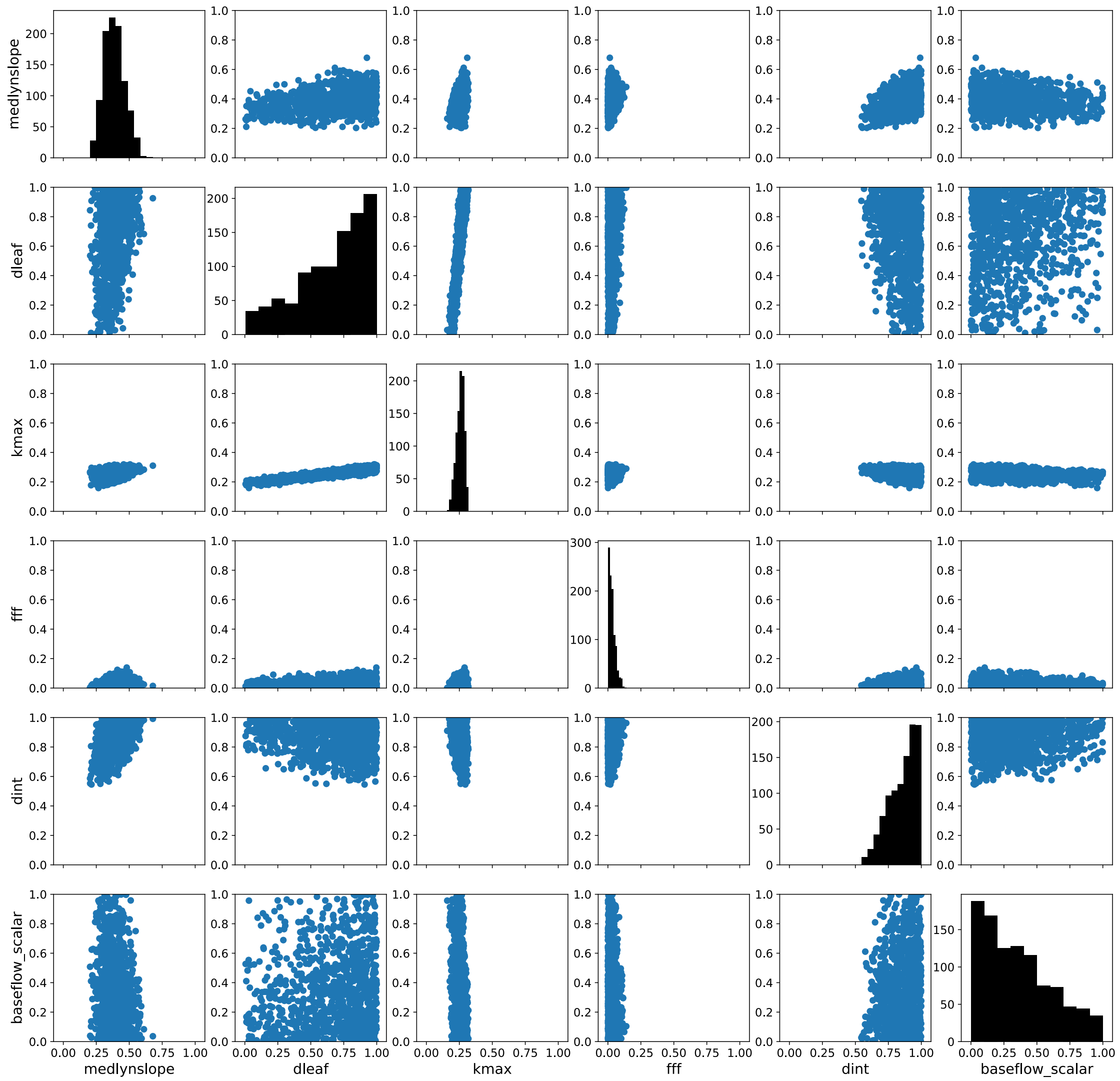


Dagon et al. (2020)

Optimal Parameter Relationships

Step 5: Infer

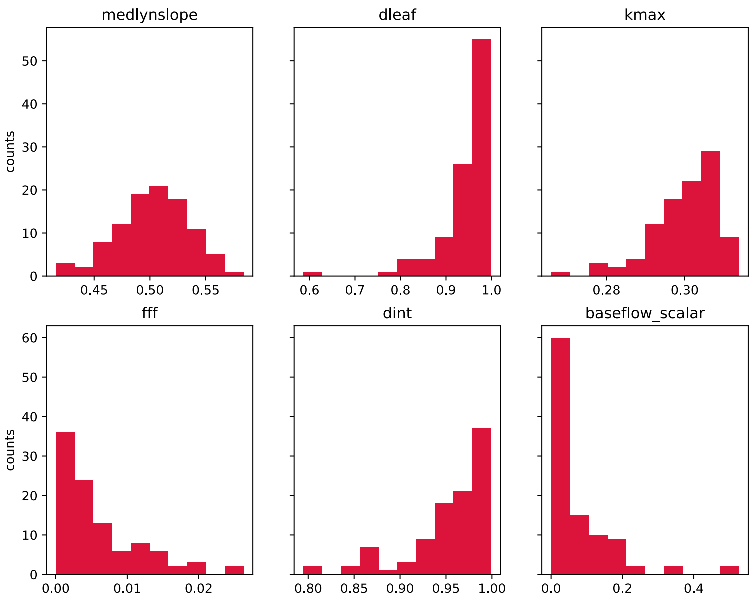
- Generate an additional large parameter sampling (~10^7 members)
- Subset 1000 members with the smallest predicted normalized error
- Explore parameter relationships and resulting distributions
- Also generating posterior parameter distributions via Markov Chain Monte Carlo (MCMC)



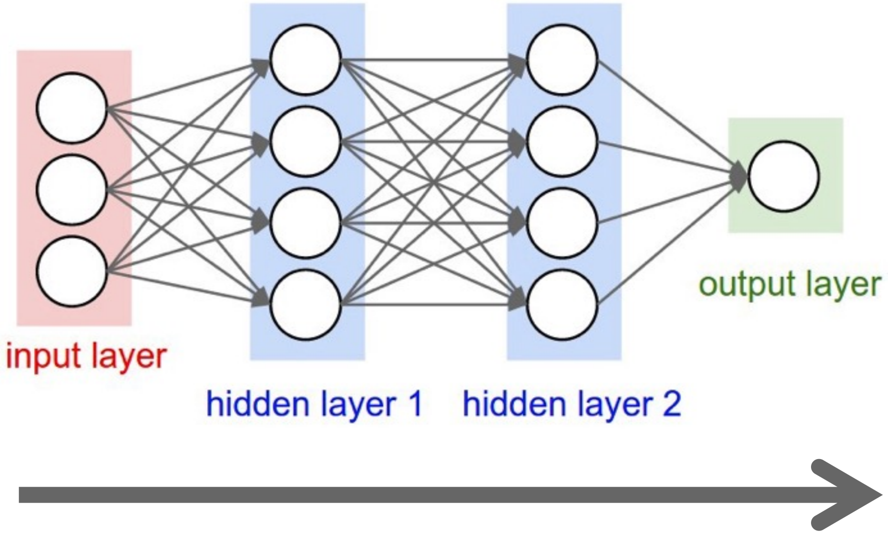
Dagon et al. (2020)

Results in the Context of Climate Predictions

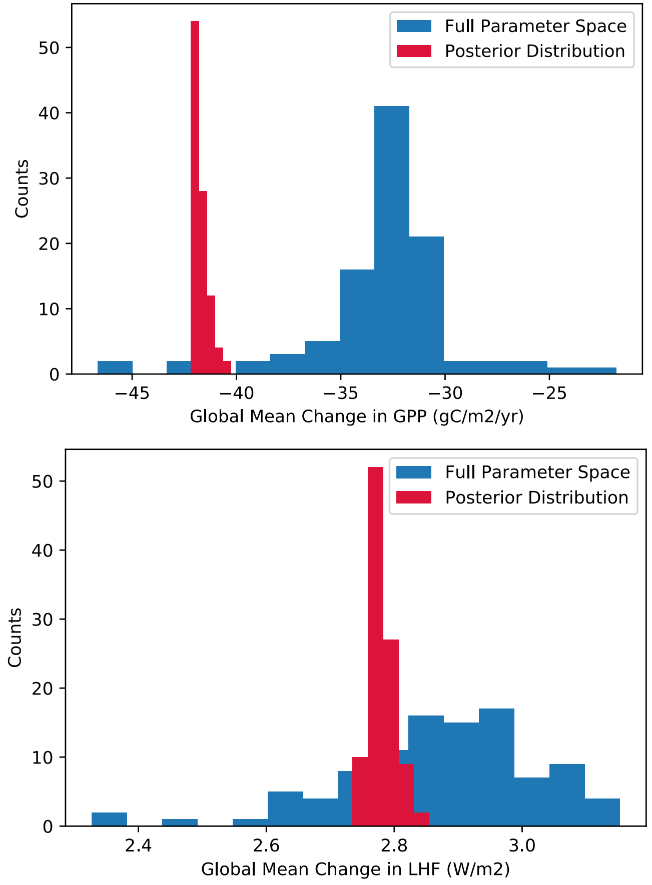
Input: Parameter posterior distributions



DIFFERENT *neural network to emulate future climate response of land surface model*



Output: Predicted change in GPP/LHF accounting for parameter uncertainty



Summary

- Parameter choices are a **major contributor** to uncertainty in land model predictions.
- **Neural network emulators** can be trained to reproduce land model output with greater computational efficiency.
- Emulator predictions are **optimized to minimize error** between model and observations.
- Currently extending this work to a **large CLM perturbed parameter ensemble** (PPE) experiment.

Thanks!
Questions?

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Dagon, K., B.M. Sanderson, R.A. Fisher, D.M. Lawrence (2020), *Adv. Stat. Clim. Meteorol. Oceanogr.*, 6, 223-244, doi:10.5194/ascmo-6-223-2020.