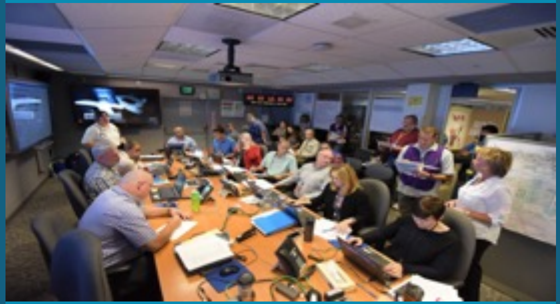
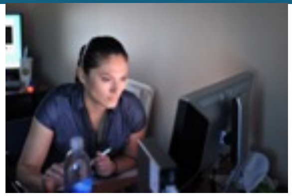
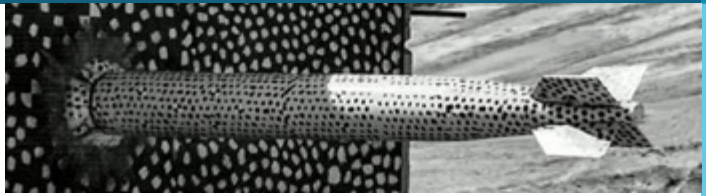
SAND2022-9064 C

Training and Generalization of Residual Neural Networks as Discrete Analogues of Neural ODEs







Khachik Sargsyan (SNL-CA)

SNL-CA : Joshua Hudson, Oscar Diaz-Ibarra, Marta D'Elia, Habib Najm
Emory U : Lars Ruthotto, Haley Rosso

July 26, 2022

MLDL Workshop

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

SNL LDRD Project:
Analysis of Neural Networks as Random Dynamical Systems

Despite all the success, there are many
recognized challenges and unknowns in neural network behavior

Generalization / predictability

Confidence assessment

Physical insight / interpretation

Robustness to adversarial attacks

Take advantage of 'continuous' limit
of residual neural networks.

Probabilistic viewpoint opens even
more opportunities

Neural ODEs

Probabilistic NN

Road to Trusted AI

Arguably, the two most important hurdles along the way

Goals: Generalization / predictability | Confidence assessment

Tools: Neural ODEs / ResNets — Probabilistic NN

Take advantage of legacy knowledge in ODEs and UQ to achieve

- Improved architectures
- Generalizable models
- Confidence assessment
- Robustness to noise

Main building block: ResNets

Neural Networks (NNs) layer-to-layer function

$$h_{t+1} = F(\underbrace{h_t}_{\text{state}}, \underbrace{\theta}_{\text{weights}})$$

Main building block: ResNets

Neural Networks (NNs) layer-to-layer function

$$h_{t+1} = F(\underbrace{h_t}_{\text{state}}, \underbrace{\theta}_{\text{weights}})$$

Residual NN: learn the residual, not the state

$$\boxed{h_{t+1} = h_t + F(h_t, \theta)}$$

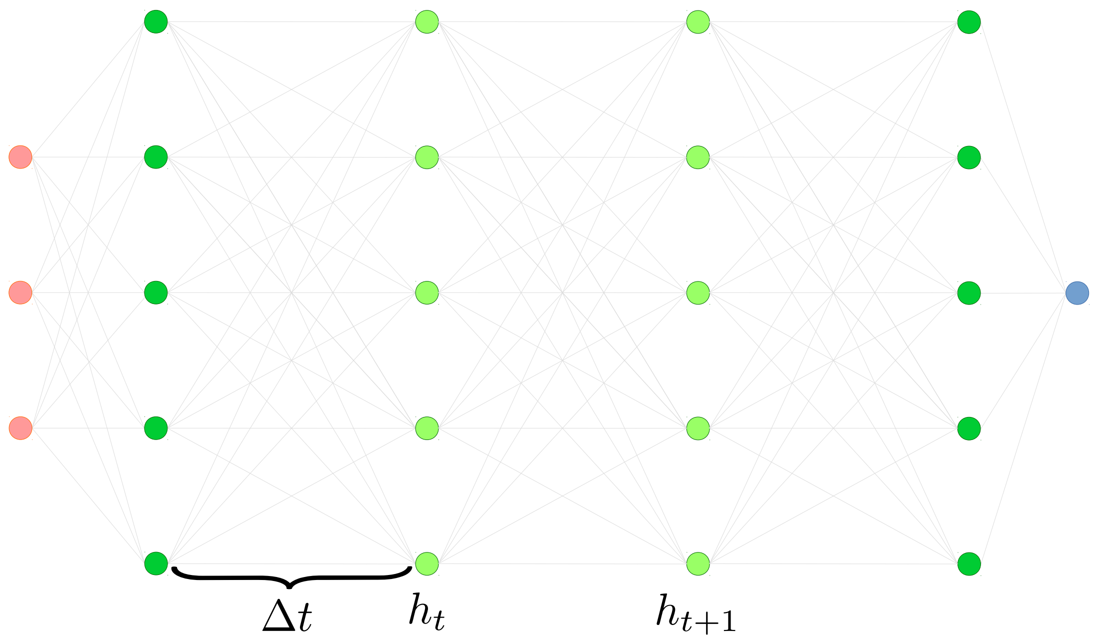
Main building block: ResNets

Neural Networks (NNs) layer-to-layer function $$h_{t+1} = F(\overset{\text{state}}{h_t}, \overset{\text{weights}}{\theta})$$

Residual NN: learn the residual, not the state $$h_{t+1} = h_t + F(h_t, \theta)$$

Now, take the limit of infinite layers

$$\frac{dh(t)}{dt} = F(h(t), \theta)$$



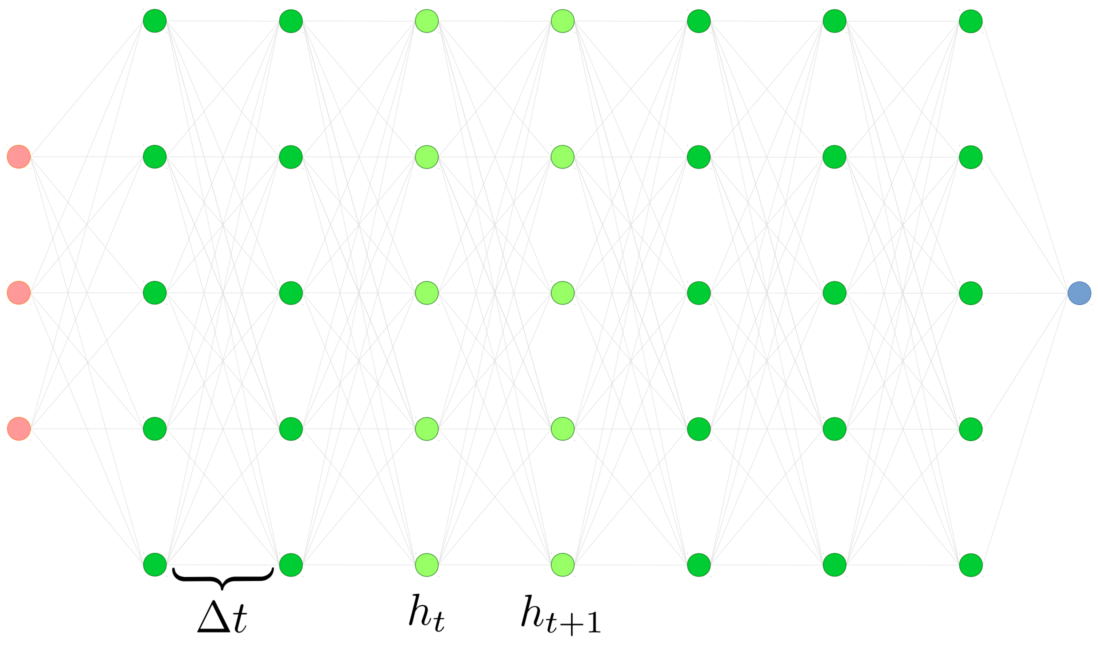
Main building block: ResNets

Neural Networks (NNs) layer-to-layer function $$h_{t+1} = F(\overset{\text{state}}{h_t}, \overset{\text{weights}}{\theta})$$

Residual NN: learn the residual, not the state $$\boxed{h_{t+1} = h_t + F(h_t, \theta)}$$

Now, take the limit of infinite layers

$$\frac{dh(t)}{dt} = F(h(t), \theta)$$



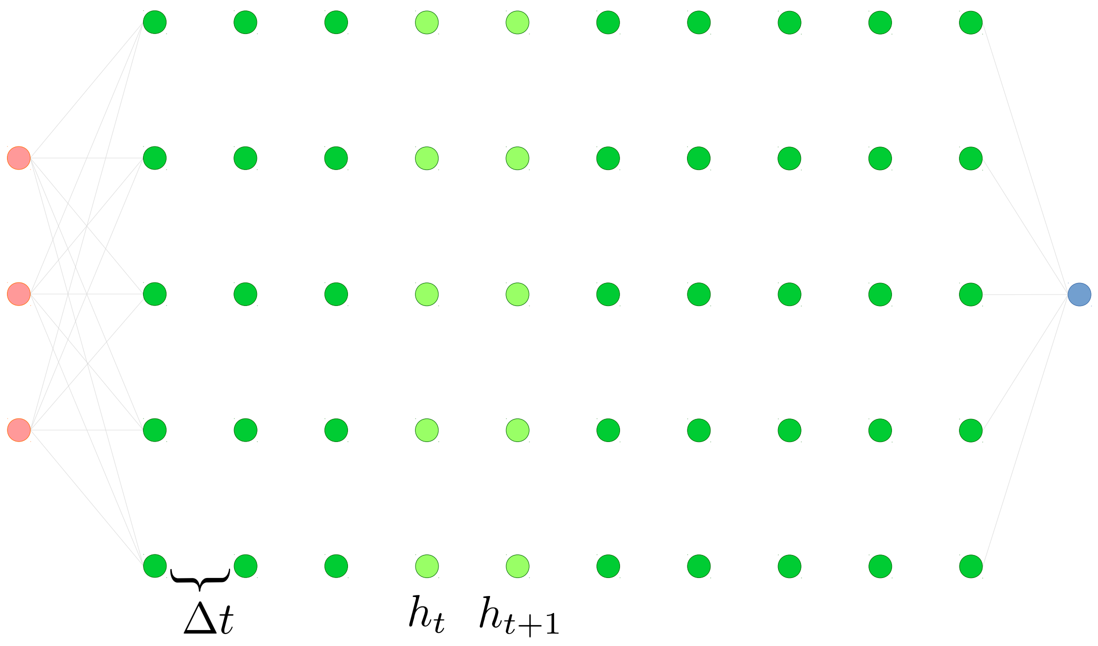
Main building block: ResNets

Neural Networks (NNs) layer-to-layer function $$h_{t+1} = F(\underset{\text{state}}{h_t}, \underset{\text{weights}}{\theta})$$

Residual NN: learn the residual, not the state $$h_{t+1} = h_t + F(h_t, \theta)$$

Now, take the limit of infinite layers

$$\frac{dh(t)}{dt} = F(h(t), \theta)$$



Main building block: ResNets

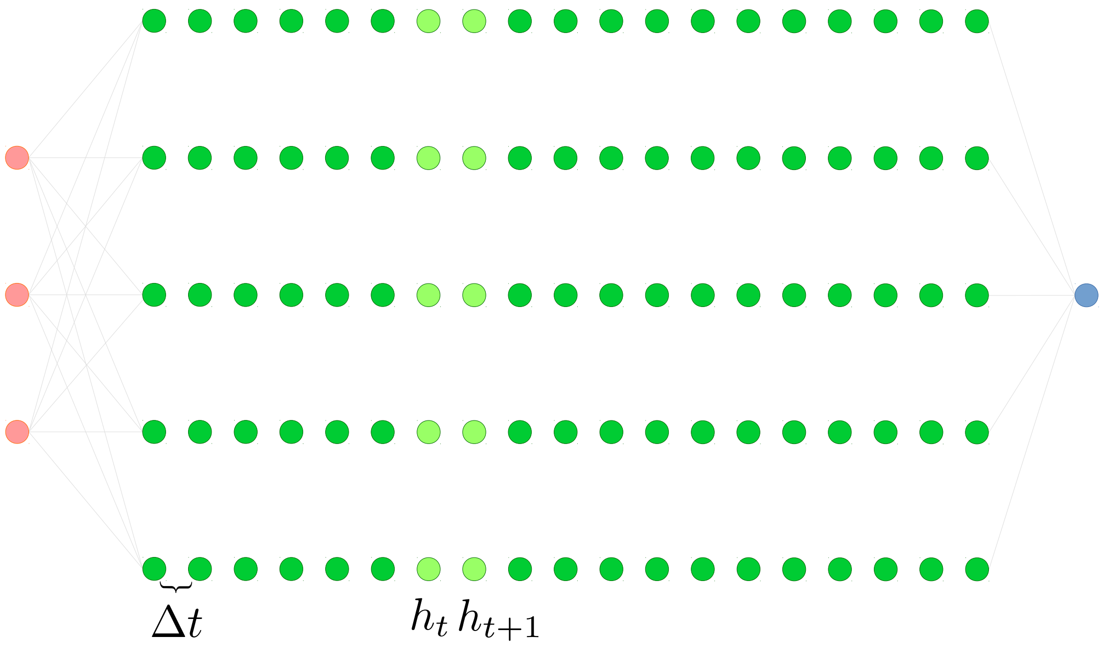
Neural Networks (NNs) layer-to-layer function

$$h_{t+1} = F(\underbrace{h_t}_{\text{state}}, \underbrace{\theta}_{\text{weights}})$$

$$\boxed{\textit{Residual}\text{ NN: learn the residual, not the state} \qquad h_{t+1} = h_t + F(h_t, \theta)}$$

Now, take the limit of infinite layers

$$\frac{dh(t)}{dt} = F(h(t), \theta)$$



Main building block: ResNets

Neural Networks (NNs) layer-to-layer function

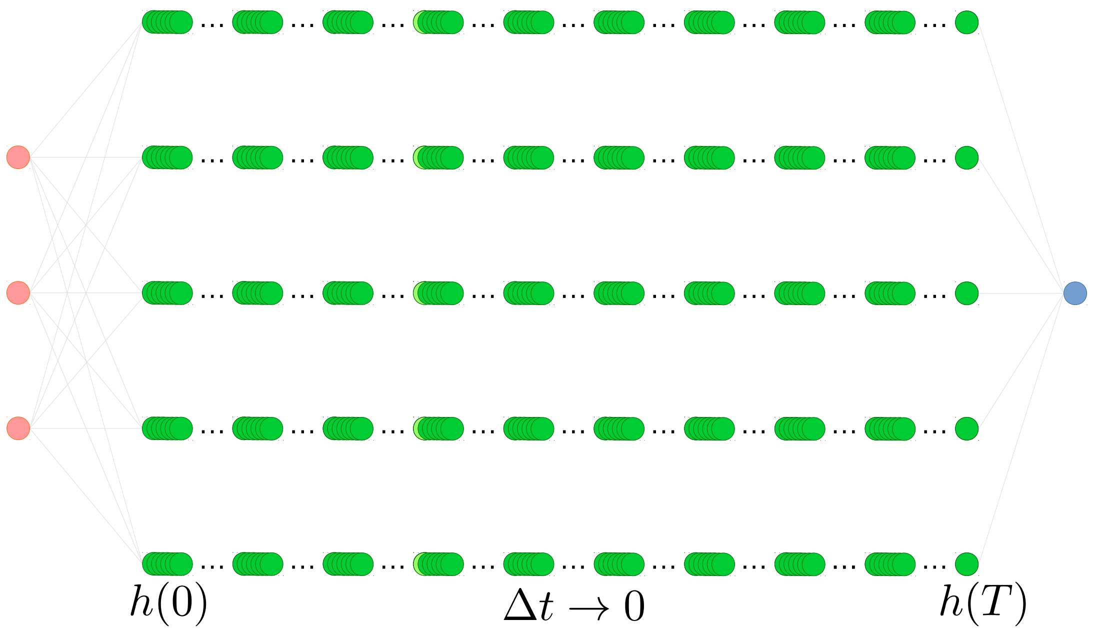
$$\overset{\text{state}}{h_{t+1} = F(h_t,} \overset{\text{weights}}{\theta)}$$

Residual NN: learn the residual, not the state

$$\boxed{h_{t+1} = h_t + F(h_t, \theta)}$$

Now, take the limit of infinite layers

$$\frac{dh(t)}{dt} = F(h(t), \theta)$$



Focus on: ResNet and NODE in a regression setting (supervised ML)

ResNet (discrete)

$$\begin{cases} \boldsymbol{x}_1 = \boldsymbol{x} + \alpha_0 \boldsymbol{\sigma}(\boldsymbol{W}_0 \boldsymbol{x}_0 + \boldsymbol{b}_0) \\ \vdots \\ \boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \alpha_n \boldsymbol{\sigma}(\boldsymbol{W}_n \boldsymbol{x}_n + \boldsymbol{b}_n) \\ \vdots \\ \boldsymbol{y} = \boldsymbol{x}_{L-1} + \alpha_{L-1} \boldsymbol{\sigma}(\boldsymbol{W}_{L-1} \boldsymbol{x}_{L-1} + \boldsymbol{b}_{L-1}) \end{cases}$$

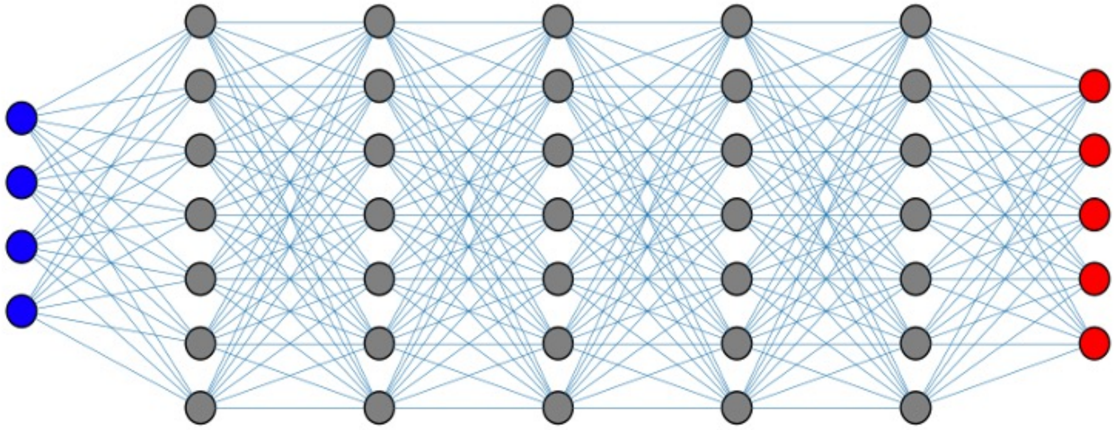
Neural ODE (continuous)

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{\sigma}(\boldsymbol{W}(t)\boldsymbol{x} + \boldsymbol{b}(t))$$

$$\boldsymbol{x}(0) = \boldsymbol{x} \qquad \boldsymbol{x}(T) = \boldsymbol{y}$$

$\boldsymbol{x} = \boldsymbol{x}_0$

Input



$\boldsymbol{y} = \boldsymbol{x}_T$

Output

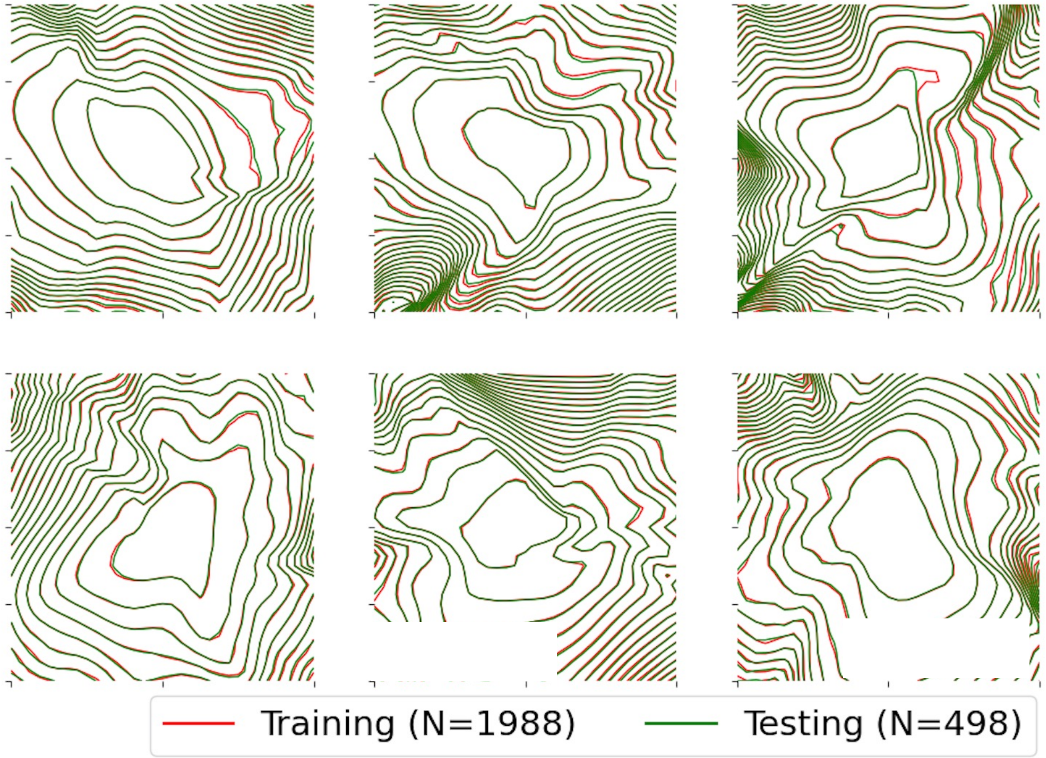
ResNets regularize loss landscape compared to MLPs

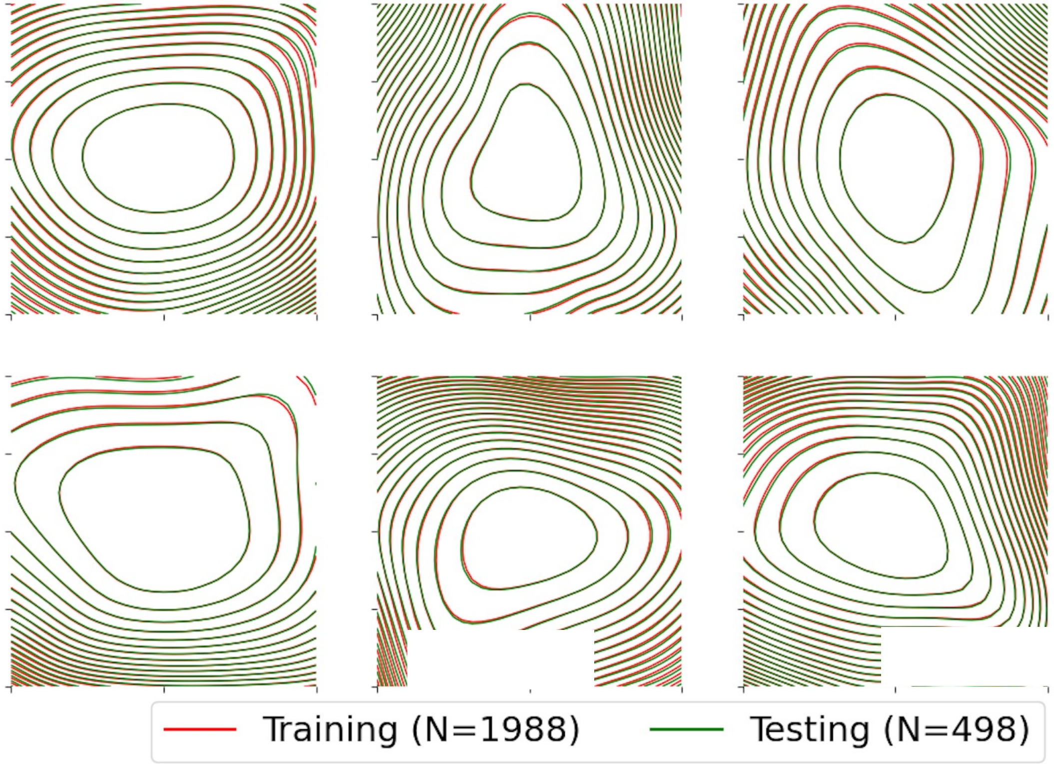
MLP NN: $x_{n+1} = \sigma(W_n x_n + b_n)$

Multilayer Perceptron (learning the layer)

ResNet: $x_{n+1} = x_n + \alpha_n \sigma(W_n x_n + b_n)$

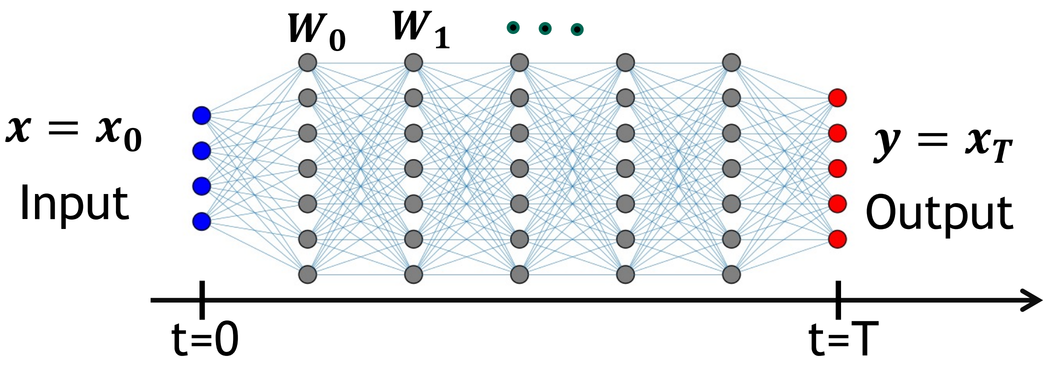
ResNets (learning the layer diff.)





Weight parameterization as a regularization tool, inspired by ODEs

ResNet: $x_{n+1} = x_n + \alpha_n \sigma(W_n x_n + b_n)$

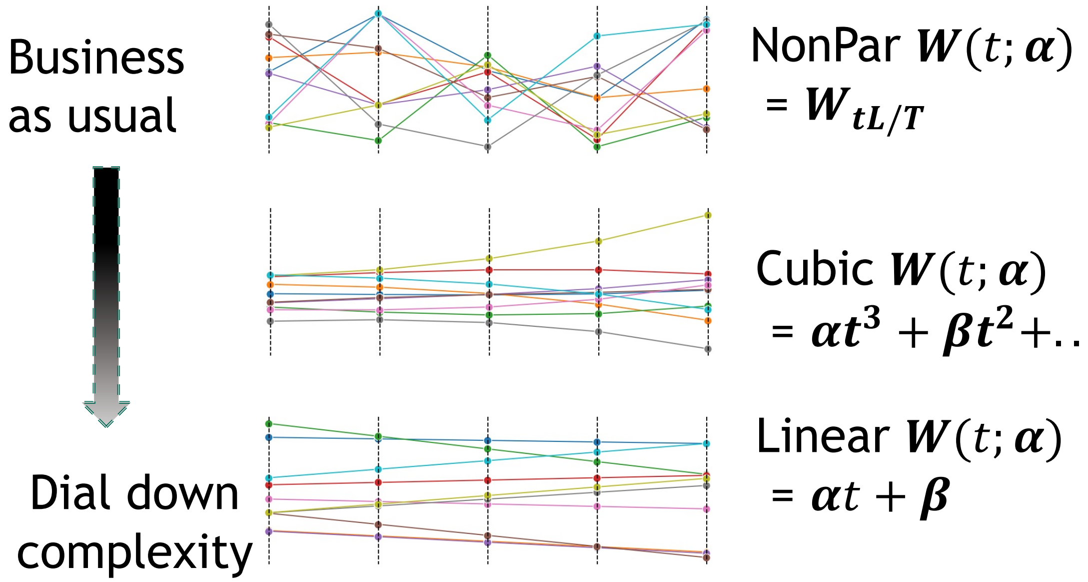


Training for weight matrices $W_0, W_1, \ldots$

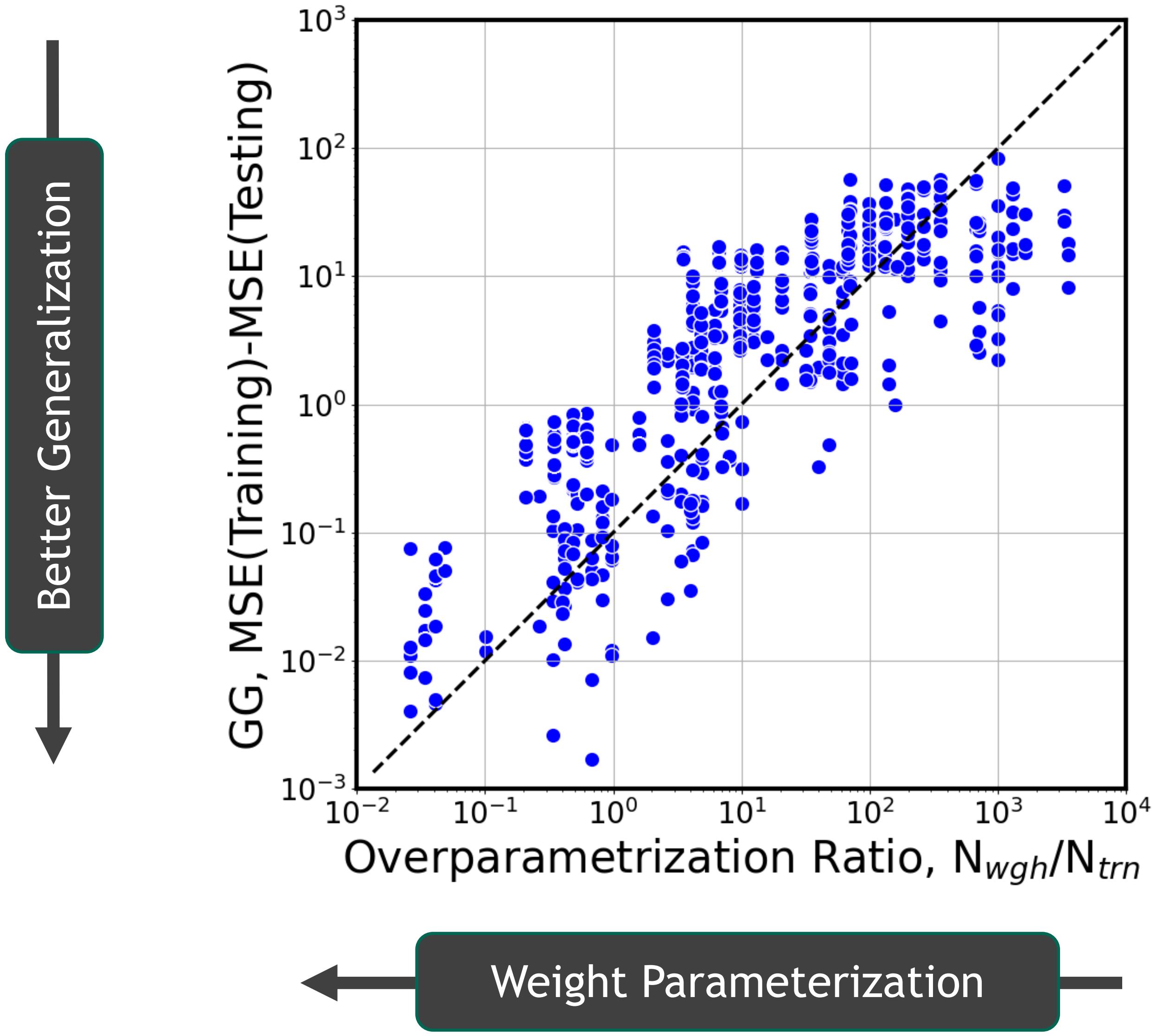
Heavily overparameterized, does not generalize well

Parameterize $W(t; \alpha)$ and train for α's.

Parameterization of weight functions reduces capacity and improves generalization



Weight parameterization (WP) improves generalization

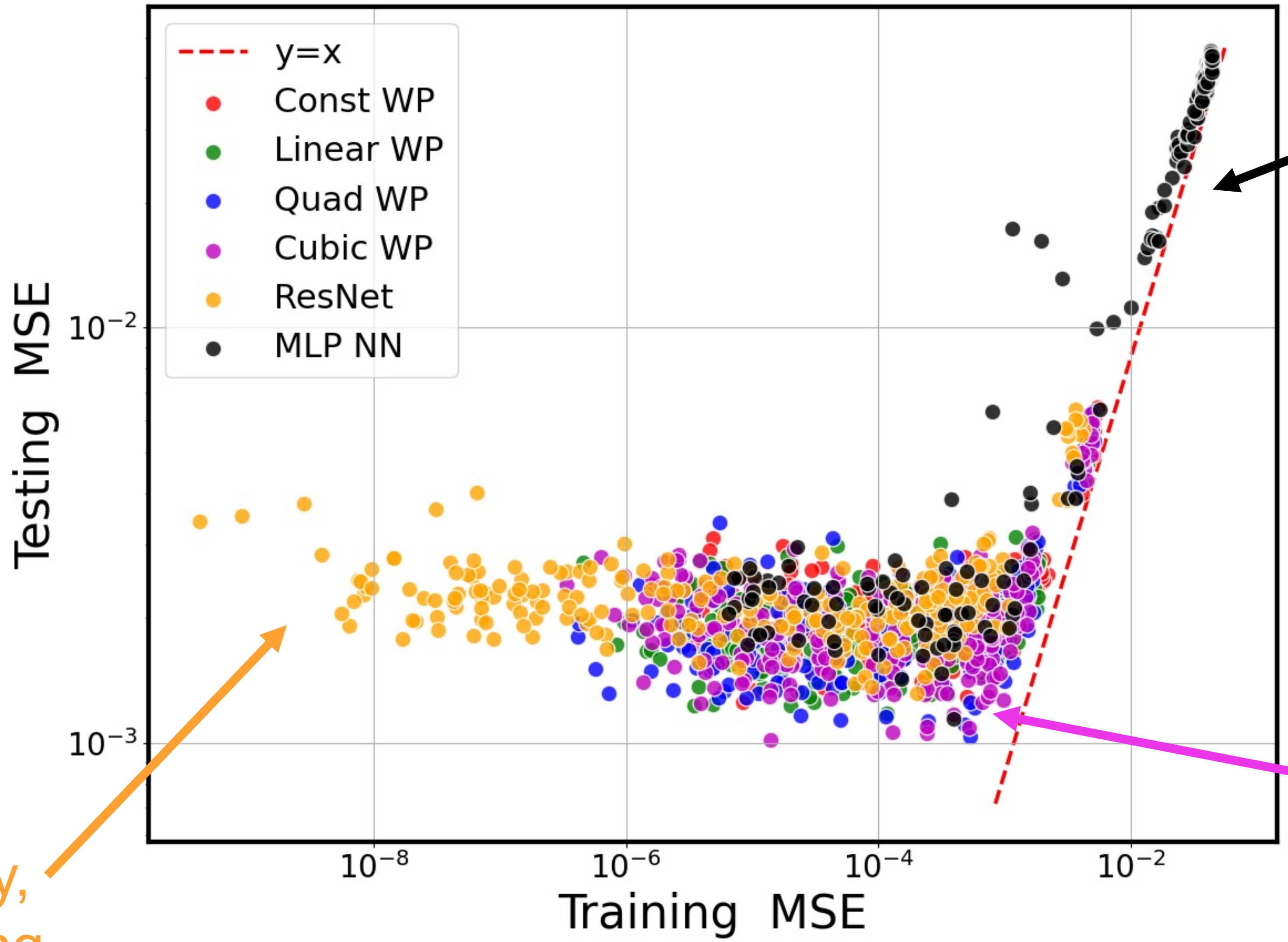


- Generalization Gap correlates with overparameterization

- Weight-parameterized ResNets reduce Generalization Gap

Each dot is a training run with varying weight parameterization functions

ResNet + WP improves accuracy

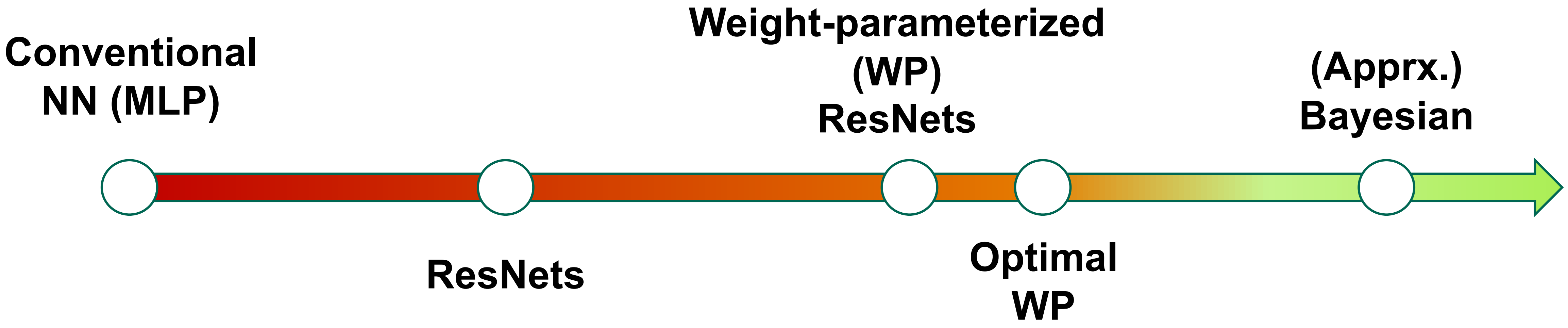


MLP:
bad accuracy

ResNet:
ok accuracy,
but overfitting

WP:
perfect tradeoff

Progressive improvements:
path toward generalization and confidence assessment



Probabilistic Learning: Bayesian NN

- Conventional NN: training for *deterministic* weight matrices $\boldsymbol{W_0}, \boldsymbol{W_1}, \ldots$
- *Probabilistic* approach: training for probability distributions $\boldsymbol{p}(\boldsymbol{W_0}), \boldsymbol{p}(\boldsymbol{W_1}), \ldots$
- Three classes of options:

Full Bayesian → Approximate Bayesian → Ensemble methods

Full Bayesian

- ➢ Markov chain Monte Carlo (MCMC)
- Typically, infeasible for overparameterized NNs
- With weight parameterization loss functions are better behaved (lower-dimensional, fewer symmetries), hence MCMC path more feasible

Approximate Bayesian

- ➢ Variational methods
- Practically feasible, but many hyperparameters to tune
- Typically underestimates extrapolative predictions

Ensemble methods

- ➢ Heuristic, but
- … works best for complex models
- Deep ensembles, committee of models
- Many recent papers connecting as a Bayesian approximation

QUiNN: Quantifying Uncertainties in NN
software soon-to-be-released on github

Deterministic → **Probabilistic**

torch.nn.module → wrapper(torch.nn.module)

Usage:

```
uqnet = MCMC_NN(nnet)
```

```
class MCMC_NN(QUiNNBase):
    def __init__(self, nnmodule, verbose=True):
        super(MCMC_NN, self).__init__(nnmodule)
        self.verbose = verbose
```

Option 1: MCMC

```
uqnet = VI_NN(nnet)
```

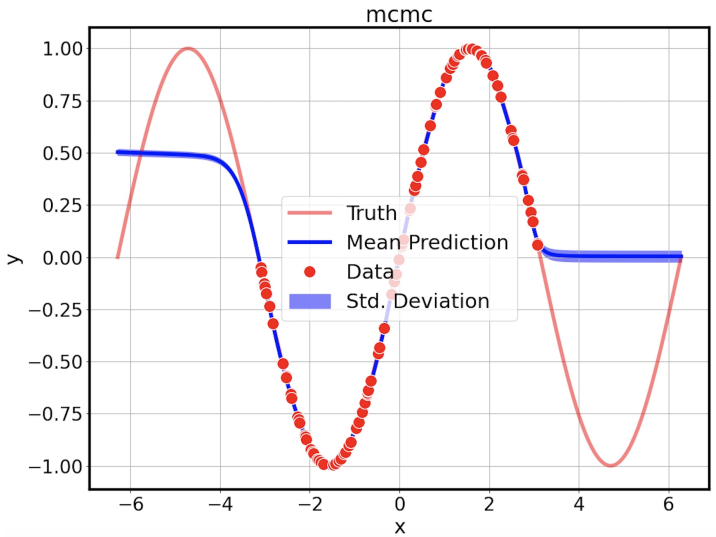
```
class VI_NN(QUiNNBase):
    def __init__(self, nnmodule, verbose=False):
        super(VI_NN, self).__init__(nnmodule)
        self.bmodel = BNet(nnmodule)
        self.verbose = verbose
```

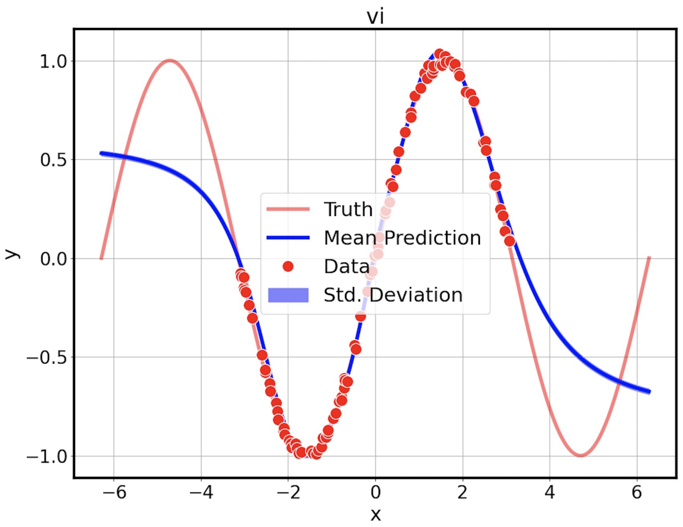
Option 2: Variational Inference

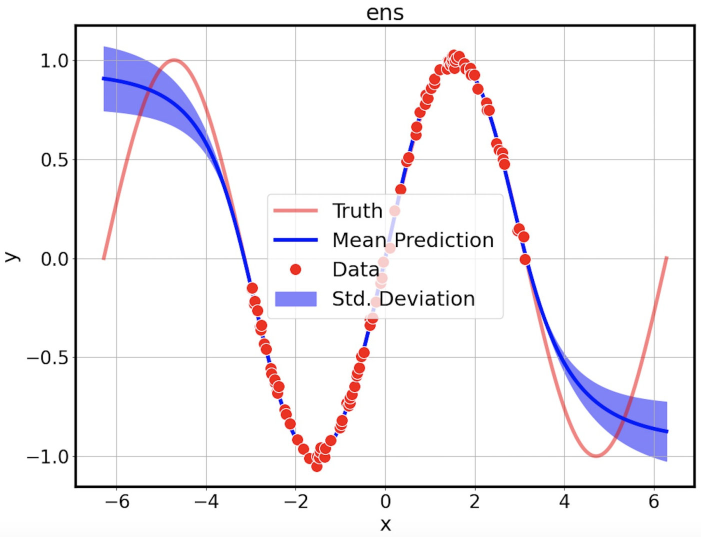
```
uqnet = Ens_NN(nnet, nens=nmc)
```

```
class Ens_NN(QUiNNBase):
    def __init__(self, nnmodule, nens=1, verbose=False):
        super(Ens_NN, self).__init__(nnmodule)
        self.verbose = verbose
        self.nens = nens
```

Option 3: Ensembling







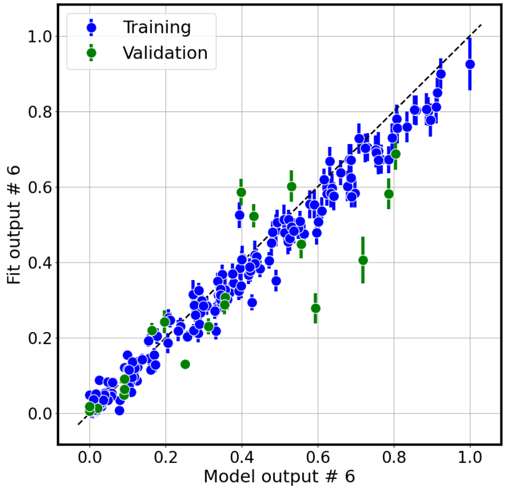
Apps:

- Multiple applications are informing the development of foundational research
- None of these applications have been previously exposed to NN prediction uncertainties, particularly in the context of ResNets and weight parameterization

E3SM Vegetation Dynamics

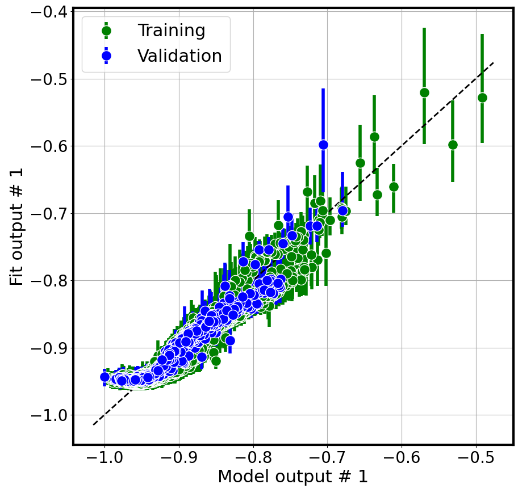
- 15 input parameters
- 10 static output QoIs
- 2K training simulations

Energy Exascale Earth System Model



FitSNAP Entropy Dataset

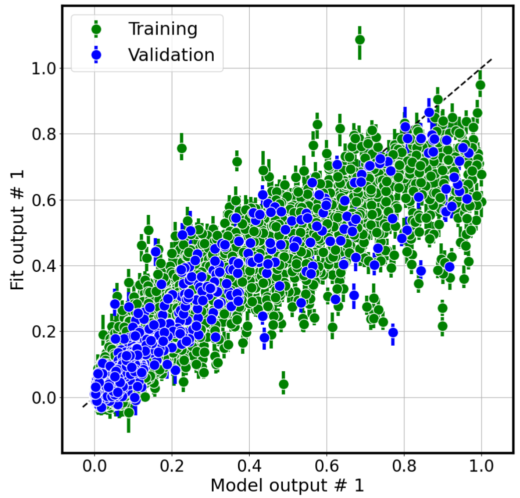
- 30 input bases
- 1 output (Energy/Force/Stress)
- 20K training DFT simulations



CO-on-Pt(111) Adsorbate

- 6 input d.o.f.
- 1 output (Energy)
- 10K training DFT simulations

Exascale Catalytic Chemistry



Summary

- Focus on ResNets and draw inspiration from ODEs
- ResNets regularize the learning problem, smoother loss surface
- **Weight parameterization (WP)** allows further regularization
- Optimal (e.g., ortho basis) WP for better training and more accuracy

- **Probabilistic approaches** more feasible with weight-parameterized ResNets
- Need to find sweet spot between empirical to fully Bayesian

Extra Materials

Analysis of Neural Networks as Random Dynamical Systems

Neural ODEs

Probabilistic NN

PNODEs

Dynamical Analysis

- Singular perturbation
- Stiffness
- Model reduction
- Non-local interactions

Regularization

- Random field parameterization of weights
- Enforce structure: smoothness, sparsity, low-rank

Stability

- Robustness with noise
- Eigenvalue structure under uncertainty

Generalizable model; improved architecture; confidence assessment; robustness to noise

Foundational capabilities impacting multiple applications

Predictive capability of Neural Networks (NNs) hinges on **generalization** (ability to predict well outside training data).

Regularization of NNs as a way to achieve generalization.

- ✓ Stiffness Penalization
- ✓ Weight Parameterization
- ✓ Probabilistic Weights

Methods

- ✓ Climate Land Modeling
- ✓ Catalytic Chemistry
- ✓ Materials Science

Applications

DTO vs OTD

ResNet

$$\boldsymbol{x}_{\boldsymbol{n}+\mathbf{1}} = \boldsymbol{x}_{\boldsymbol{n}} + \boldsymbol{\alpha}_{\boldsymbol{n}} \boldsymbol{\sigma}(\boldsymbol{W}_{\boldsymbol{n}} \boldsymbol{x}_{\boldsymbol{n}} + \boldsymbol{b}_{\boldsymbol{n}})$$

NODE

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{\sigma}(\boldsymbol{W}(t)\boldsymbol{x} + \boldsymbol{b}(t))$$

Forward equivalence:

Neural ODE discretized using explicit Euler and ResNet produce identical outputs choosing time step: $\Delta t = \frac{T}{L}$, $\alpha_n := \Delta t$, $\boldsymbol{W}_{\boldsymbol{n}} := \boldsymbol{W}(n\Delta t)$ and $\boldsymbol{b}_{\boldsymbol{n}} := \boldsymbol{b}(n\Delta t)$ for all n.

Backward not so much:

Gradient computations differ!

Consider $W(t) \equiv W$ and $b \equiv 0$:

Discretized Neural ODE with adjoint method:

$$\nabla loss = 2\big((1 + \delta t\, W)^L x - y\big)(1 + \delta t\, W)^{\boxed{L}} x$$

ResNet with backpropagation:

$$\nabla loss = 2\big((1 + \delta t\, W)^L x - y\big)(1 + \delta t\, W)^{\boxed{L-1}} x$$

- Gradients converge as $L \to \infty$ but differences can be large for small L,
- Optimize then discretize (adjoint method) $\neq$ discretize then optimize (backpropagation).

Prior Work on Probabilistic NN

- **Probabilistic NN** have been around since 90s [*MacKay, 1992; Neal, 1997*]
  - Full probabilistic treatment was infeasible back then (and still is, generally)
  - Recent work showed avenues via variational methods with clever tricks:

    Bayes by Backprop [*Blundell, 2015*]; Probabilistic backprop [*Hernandez-Lobato 2015*]
  - *Ghahramani, "Probabilistic Machine Learning and Artificial Intelligence". Nature, 2015*
    - *"Nearly all approaches to probabilistic programming are Bayesian since*

      it is hard to create other coherent frameworks for automated reasoning about uncertainty"
  - Industry ***is*** catching up: Bayesflow at Google, infer.NET at Microsoft, Uber has shown interest
  - Still not industry-standard: expensive, not well understood.