Uncertainty Quantification in (Residual) Neural Networks

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Thanks to: Oscar Diaz-Ibarra, Javier Murgoitio-Esandi, Joshua Hudson, Marta D'Elia, Habib Najm

Outline

A mix and extension of my talks at
UNCECOMP, FASTMath All Hands, and LDRD review.

- UQ for NNs: review and state of the art
  - Loss landscape perspective, challenges, metrics
- UQPANN: concept exploratory project between FASTMath and RAPIDS
- Weight parametrization in Residual NNs (ResNets)
  - Reduces generalization gap
  - Enables easier UQ
- QUiNN: ongoing work and software plug

Probabilistic NN == Bayesian NN

Ghahramani, “Probabilistic Machine Learning and Artificial Intelligence”. Nature, 2015

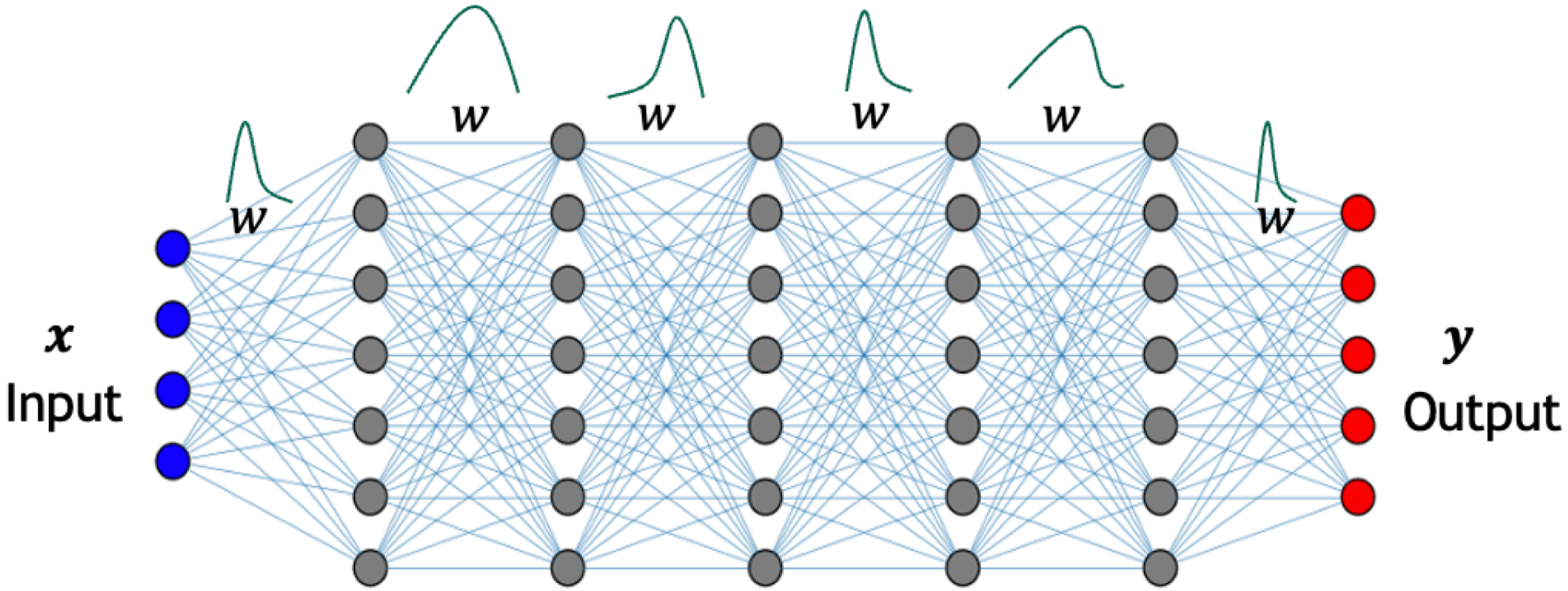
> *“Nearly all approaches to probabilistic programming are* ***Bayesian*** *since it is hard to create other coherent frameworks for automated reasoning about uncertainty”*

- Bayesian NN methods have been around since 90s *[MacKay, 1992; Neal, 1996]*

- Full Bayesian treatment was infeasible back then….
    - … and still is, generally, not industry-standard by any means.

UQ-for-NN: Bayesian perspective

Training for NN weights reformulated as a Bayesian inference problem



Posterior, Likelihood, Prior:

$$p(w\,|\,y) \propto p(y\,|\,w)\,p(w)$$

$$\propto \exp\left(-\frac{||y-f_w(x)||^2}{2\sigma^2}\right)\exp\left(-\frac{||w||^2}{2\lambda^2}\right)$$

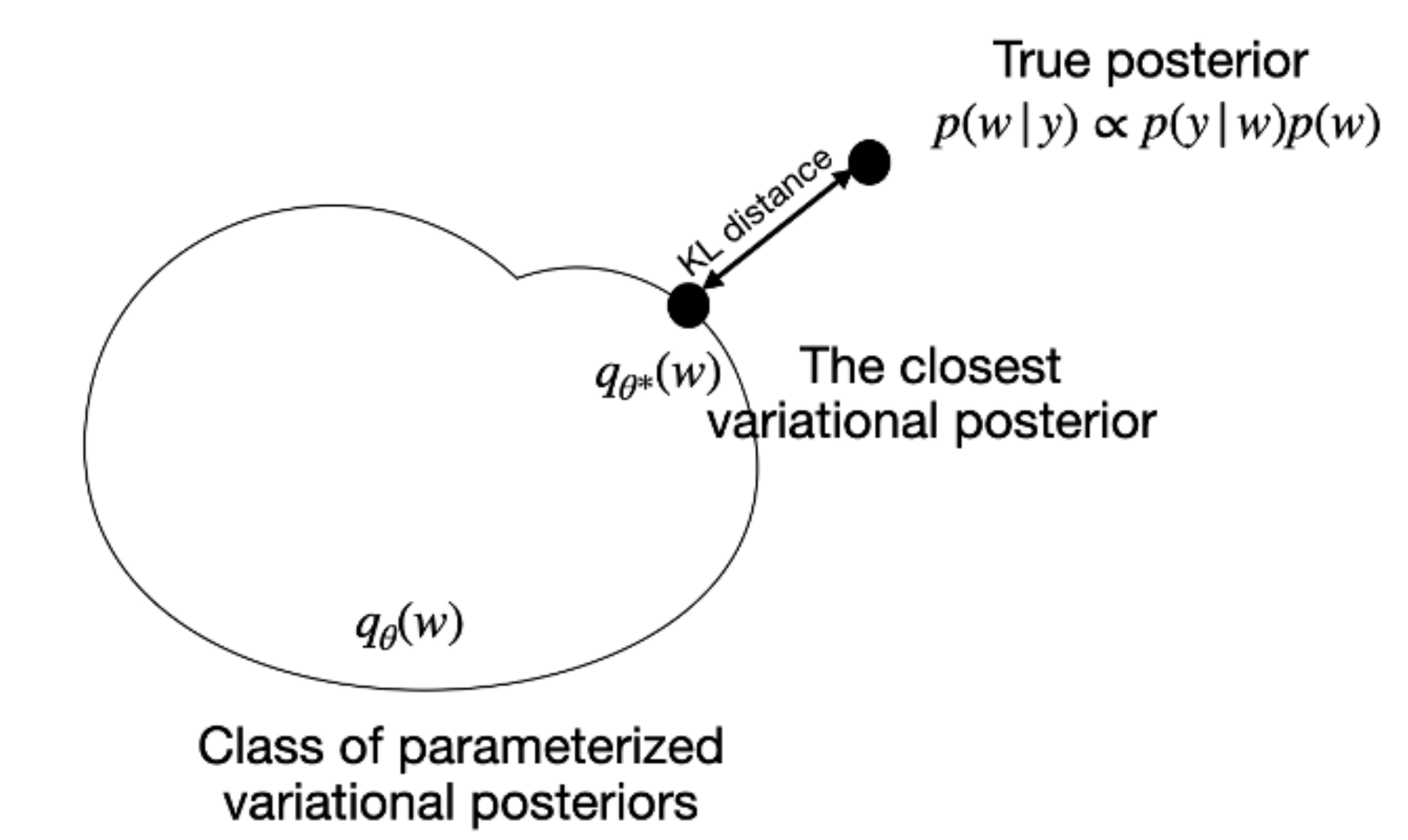
Negative Log-Posterior $\simeq a\,||y-f_w(x)||^2 + b\,||w||^2 \simeq$ Training Loss Function

- ✓ Markov chain Monte Carlo (MCMC) sampling; Hamiltonian MC *[Levy, 2018]*
- ◉ Tuning is an art: essentially infeasible outside academic examples

UQ-for-NN: variational methods

- Bayes by Backprop *[Blundell, 2015]*
  - has become mainstream in ML literature
  - also called BNN

  - Mean-field VI (i.e. i.i.d. normal variational class)
  - Reparameterization trick
  - Gaussian mixture prior: wide and narrow
  - Variational st.dev. $\sigma = ln(1 + e^{\rho})$



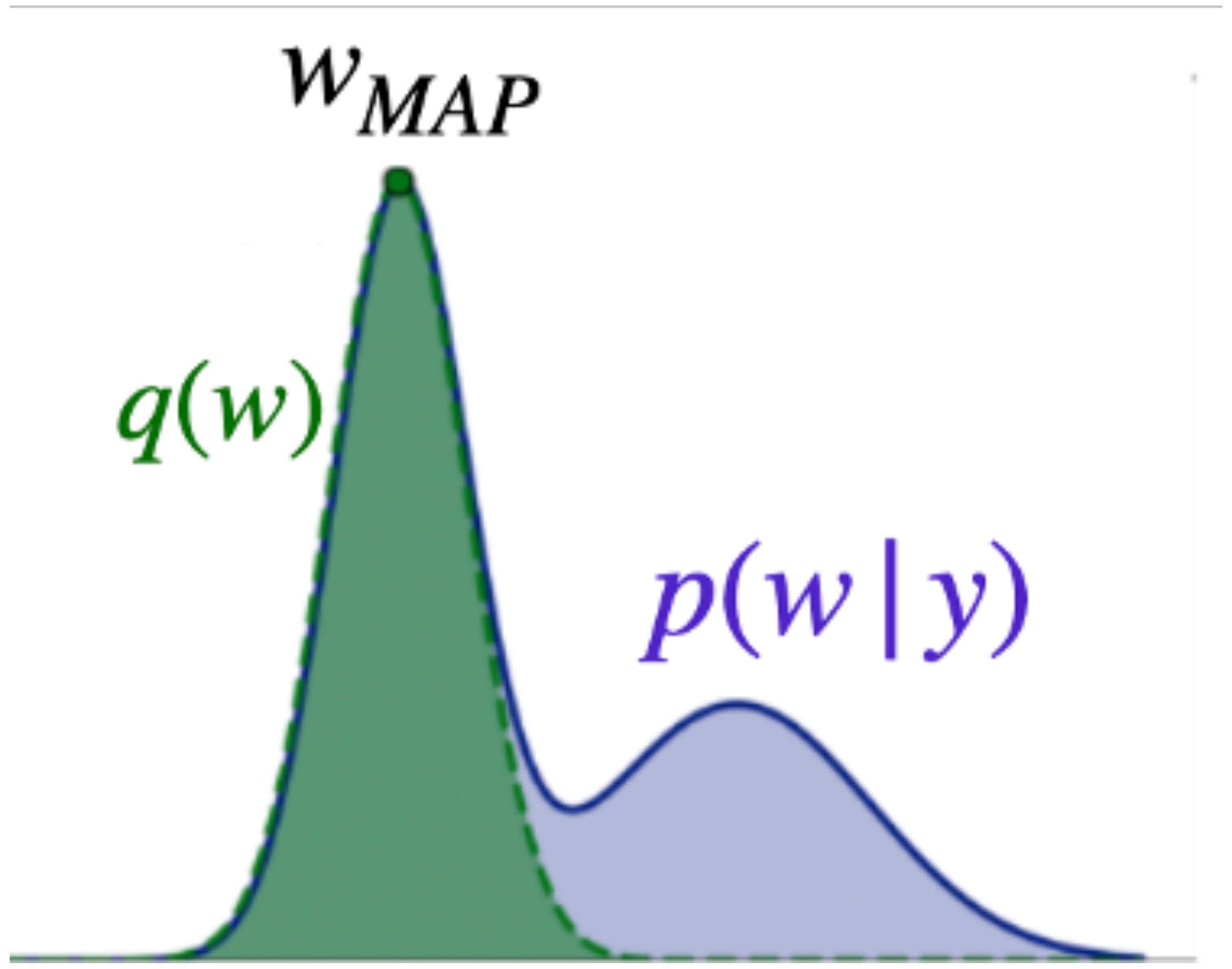
- SVI, ADVI, BBVI, BBBVI, CCVI, CATVI, ….

◉ Typically underestimates predictive uncertainty
◉ Restricted to variational class
◉ Hard to train

UQ-for-NN: approximate methods

- **Probabilistic backprop, or PBP** *[Hernandez-Lobato, 2015]*
  - Layer-to-layer updates from $\mathcal{N}(\mu, \sigma^2)$ to $\mathcal{N}(\mu_{new}, \sigma^2_{new})$
  - Deriving back propagation formulas for this update
  - $\mu, \sigma^2 \rightarrow \mu_{new}, \sigma^2_{new}$ updates similar to PC propagation (first order HG-PC)
  - ◉ Did not really lift off
  - ◉ Original implementation in Theano:)

- **Laplace methods**: *[Ritter, 2018]*
  - ✓ Relies on Gaussian apprx near maximum;
  - ✓ Can be generalized to GMM
  - ◉ Good only locally
  - ◉ Hessian computation challenging
  - ◉ Fails to explore the full posterior



UQ-for-NN: other (more empirical) methods

- **Ensembling methods:** work surprisingly well!
  - ✓ Deep Ensembles *[Lakshminarayanan, 2017];*
  - ✓ Interpreting ensembles from Bayesian perspective *[Garipov, 2018; Fort, 2019]*
  - ✓ Randomized MAP Sampling *[Pearce, 2020]*
  - ✓ MC-Dropout *[Gal, 2015]*
  - ✓ Stochastic Weight Averaging – Gaussian (SWAG) *[Maddox, 2019]*:shipped w PyTorch1.6
  - ✓ Delta-UQ *[Anirudh, 2021]*,
  - ◉ Little theoretical backing
  - ◉ Too expensive, albeit parallelizable

- **Direct learning of predictive RV**
  - ✓ Distance-based methods *[Postels, 2022],*
  - ✓ DEUP *[Lahlou, 2023]*
  - ✓ AVUC *[Krishnan, 2020]*.

- **Other**
  - ✓ Information-bottleneck UQ *[Guo, 2023]*,
  - ✓ Conformal UQ *[Hu, 2022]*,
  - ✓ Bayesian Last Layer *[Watson, 2021]*.

Randomized MAP Sampling (RMS)

[Pearce, 2020]

- Consider log-posterior: $-\log P(w|y) = ||y - NN_w(x)||^2 + R(w)$

- Consider regularized training problem $\min \left(\alpha ||y - NN_w(x)||^2 + \beta ||w - w^*||^2 \right)$

- If one samples w^* from prior $\sim e^{-R(w)}$, the set of deterministic solutions <u>approximately</u> forms the posterior $P(w|y)$

- It is exact for gaussian priors, linear models:

but the authors show that it extends well to larger class, including NNs

- What is missing: proper attribution of uncertainty: is it really RMS or the initialization that drives the good results?

Challenges of UQ-for-NN

✓ Complicated posterior distribution (loss surface):
- invariances and symmetries: permuting some weights leads to the same loss,
- multimodality: multiple local minima in the weight space,
- “ridges”: low-d manifolds with same or similar loss.

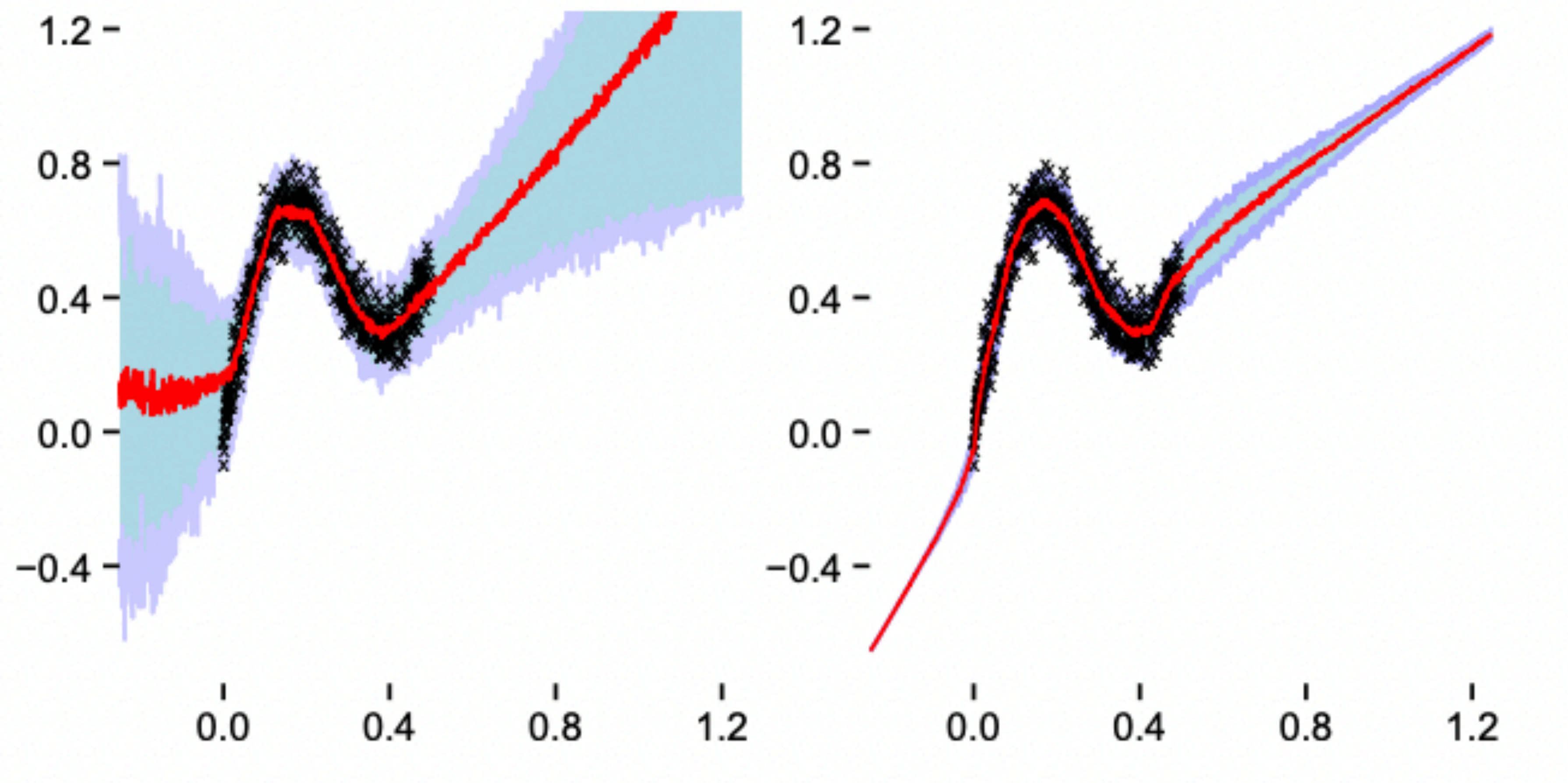
✓ Prior on weights hard to elicit/interpret/defend
- what does a uniform/gaussian prior on weight matrix elements mean?
- perhaps a prior is needed in the ‘matrix’-space, or…
- driven by outputs, or physics-constraints.

✓ Large number of weights:
- scales linearly with depth and quadratically with width,
- hard to visualize the high-d surface.

How to measure if uncertainty estimate is correct?

✓ Still a lot of eyeballing and 1d fit examples,

✓ Striving to match a GP

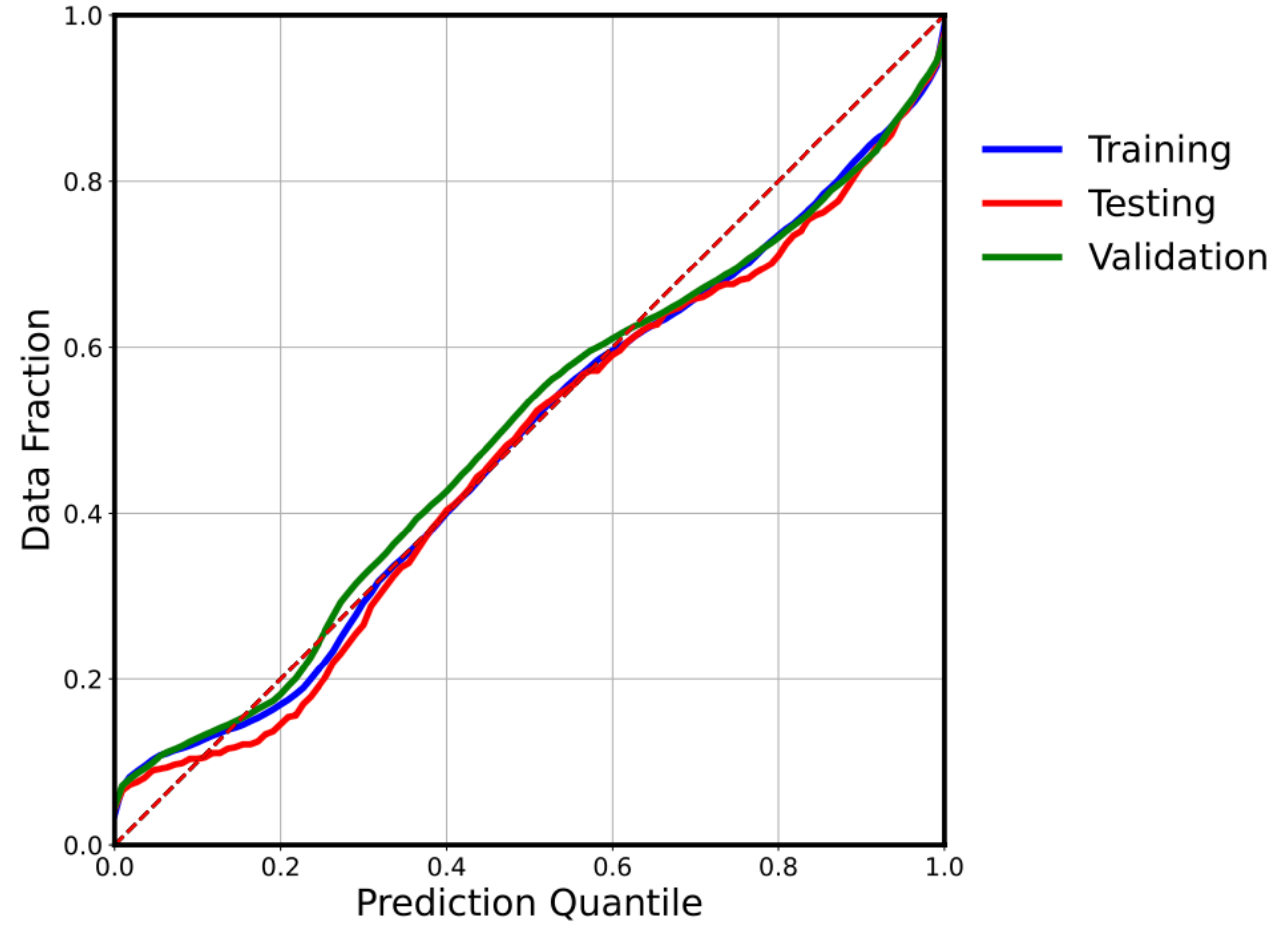


✓ Benchmarking efforts are picking up:

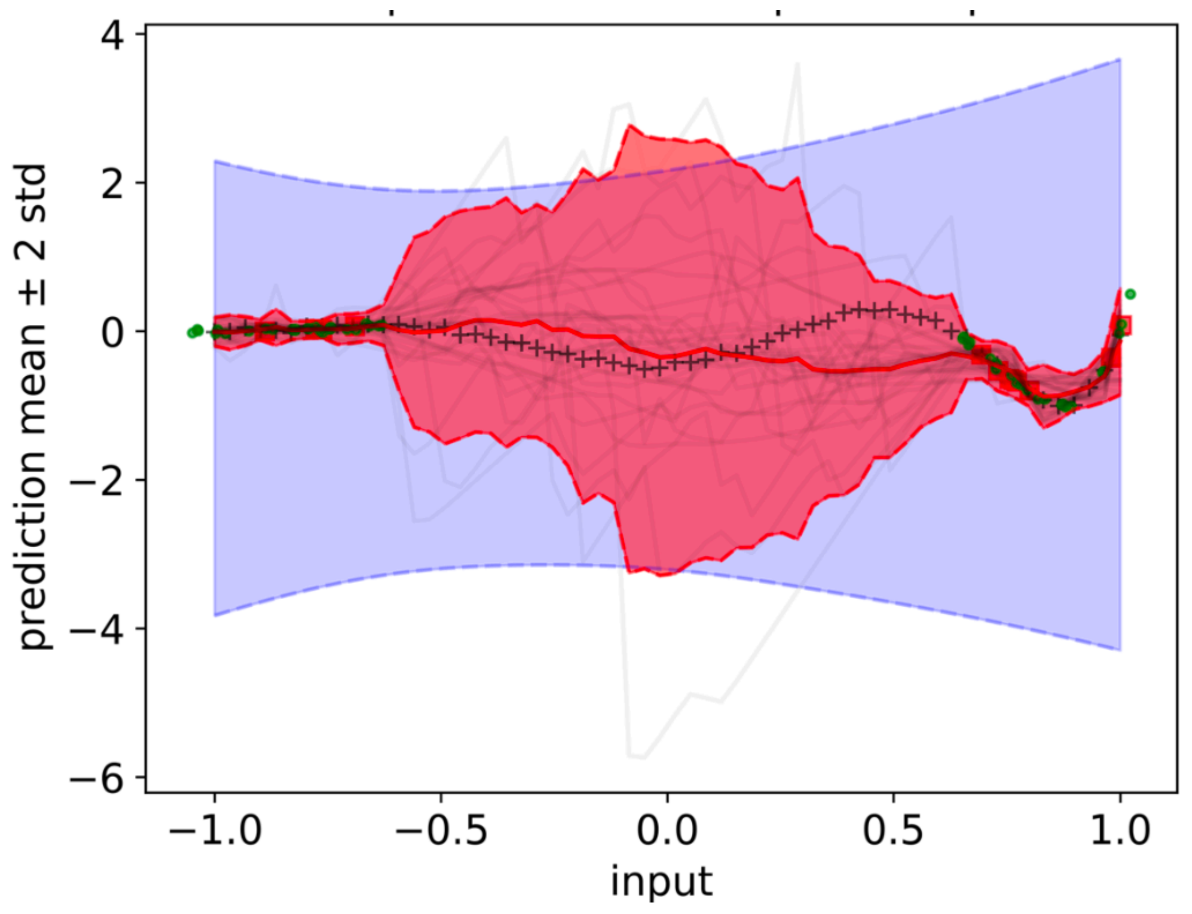
- UCI Dataset, both regression and classification
- Recent work specific to Bayesian NN

[Yao, 2019; Navratil, 2021; Nado, 2021; Staber, 2022; Basora, 2023]

Uncertainty-Accuracy Plot



Posterior predictive with no data —> Prior predictive



UQPANN: visualizing and quantifying uncertainties in physics-aware NNs

FASTMath+RAPIDS Exploratory 1yr Project: FY24, $250k

Benjamin Erichson (LBL), Khachik Sargsyan (SNL)

RAPIDS

FASTMATH

Accurate UQ for Neural Networks (NNs)
hinges on the loss surface's behavior

Physics-driven regularization
will improve loss surface and
enable more accurate and efficient UQ

Physics-driven regularization should help

- We hypothesize that incorporating prior knowledge of physics will regularize the loss/log-posterior landscapes, making them more amenable to sampling and analysis.

- This means both:
  - *soft* regularization (like PINN) and
  - *hard* architectural changes
    - physics-driven rewiring (invariance, symmetries, positivity, feature extraction),
    - numerical convenience (ResNet/NODE, weight reparameterization, layer/batch normalization).

- This regularization process should enable the derivation of well-calibrated, generalizable, and scalable predictive uncertainties.

Our Plan: Visualization + (Physics) + Laplace

- Visualization of loss surface is key to help understand and characterize NN performance *[Li, 2018; Garipov, 2018; Fort, 2019; Yang, 2021]*,
- We will develop special slicing schemes, anchored at points of interest, such as local minima and saddle points found with conventional SGD methods,
- We will try to develop metrics of regularity, generalizability and "sample-ability" of the loss surface (a.k.a. log-posterior), incl. both local and global features.

- We will establish a systematic approach to categorize and interrogate the loss surface and measure the impact of physics-driven regularization on them,
- We will leverage the idea of Laplace approximation to obtain uncertainty estimates for NNs *[Ritter, 2018; Daxberger, 2021]*,
- Motivated and informed by the loss surface analysis, we will develop scalable mixture-of-Laplace approximations to model posterior distributions of varying shapes.

Gear switch: ResNet/NODE ideas that helped UQ

ResNet (discrete)

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

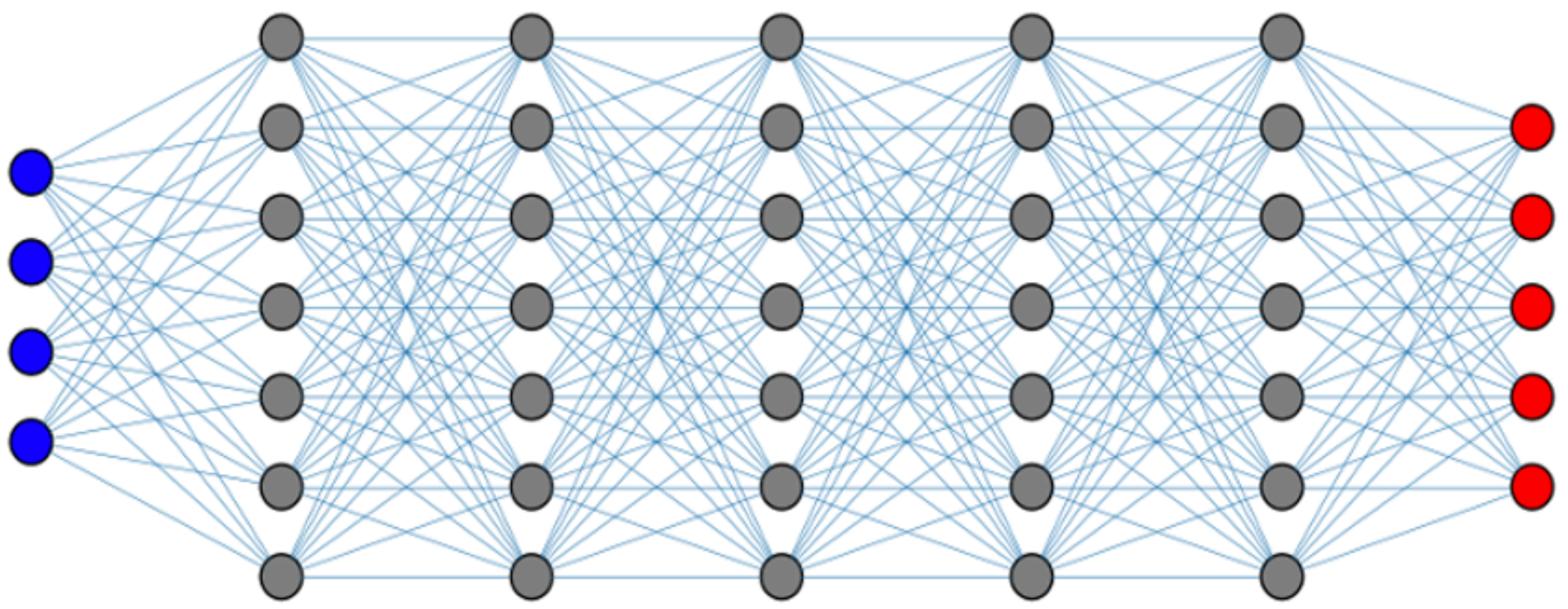
Neural ODE (continuous)

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

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

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

Input



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

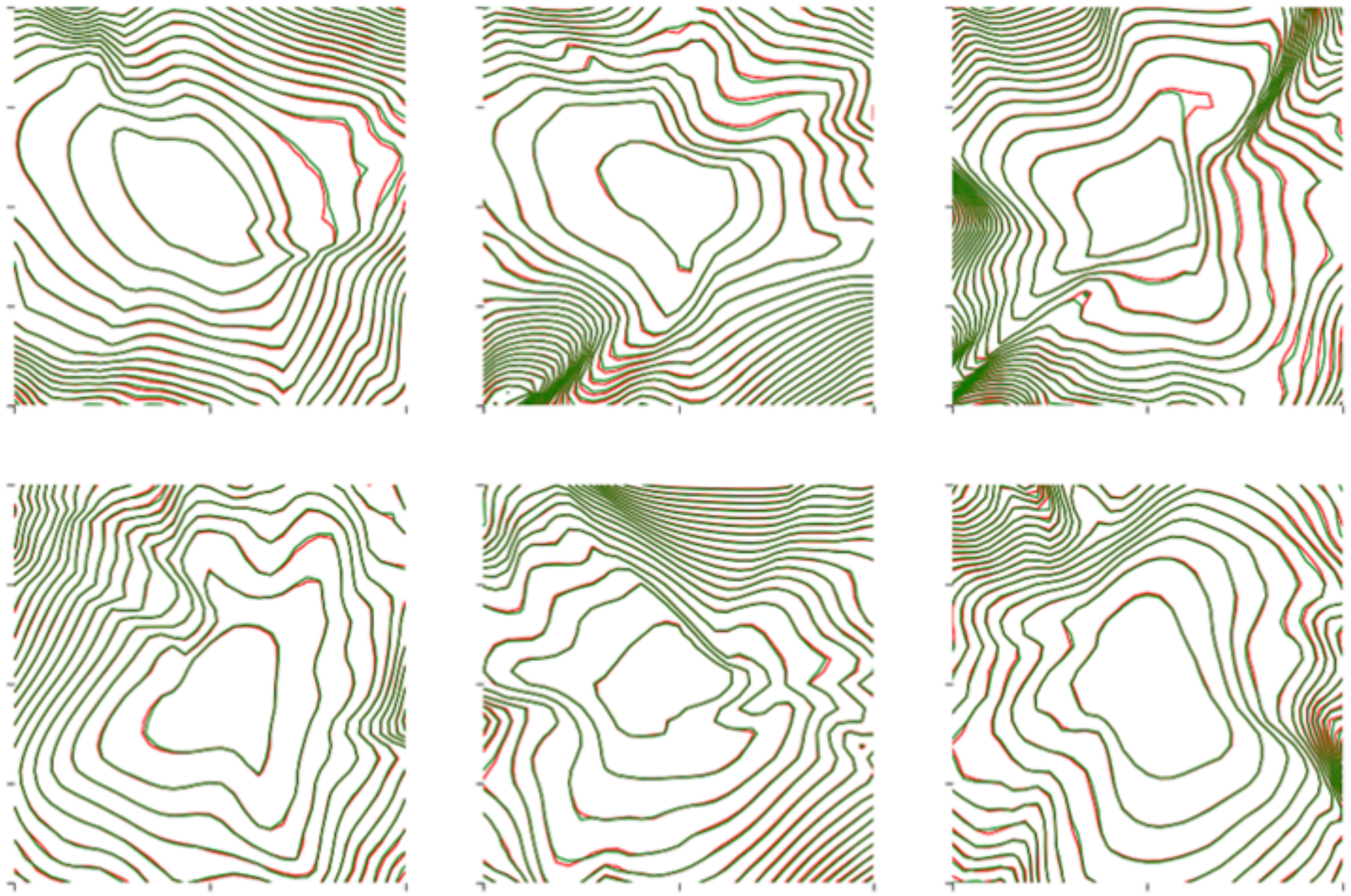
Output

[E, 2017; Chen, 2018; Ruthotto, 2018]

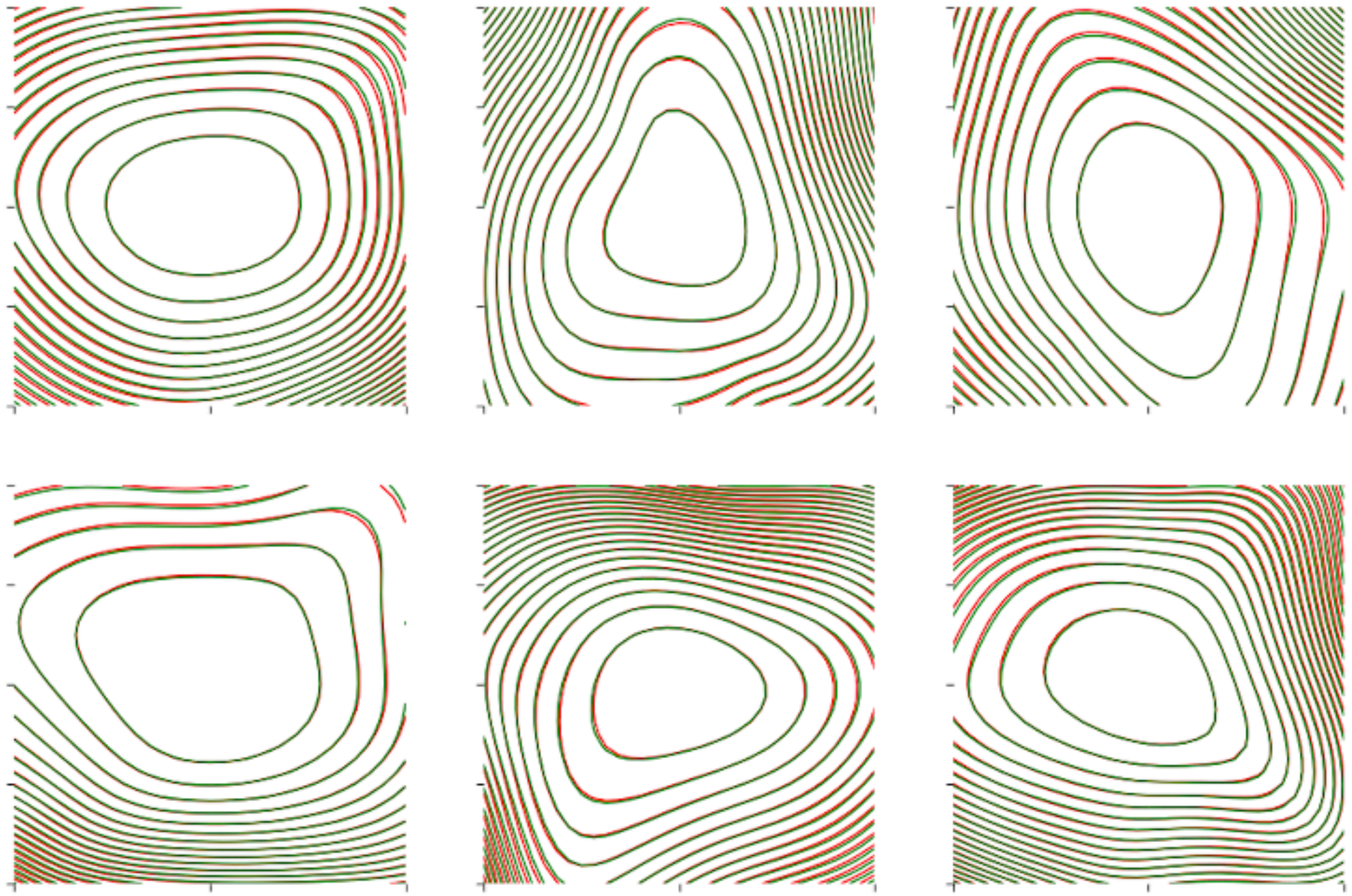
ResNet example

ResNets regularize loss landscape compared to MLPs

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



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

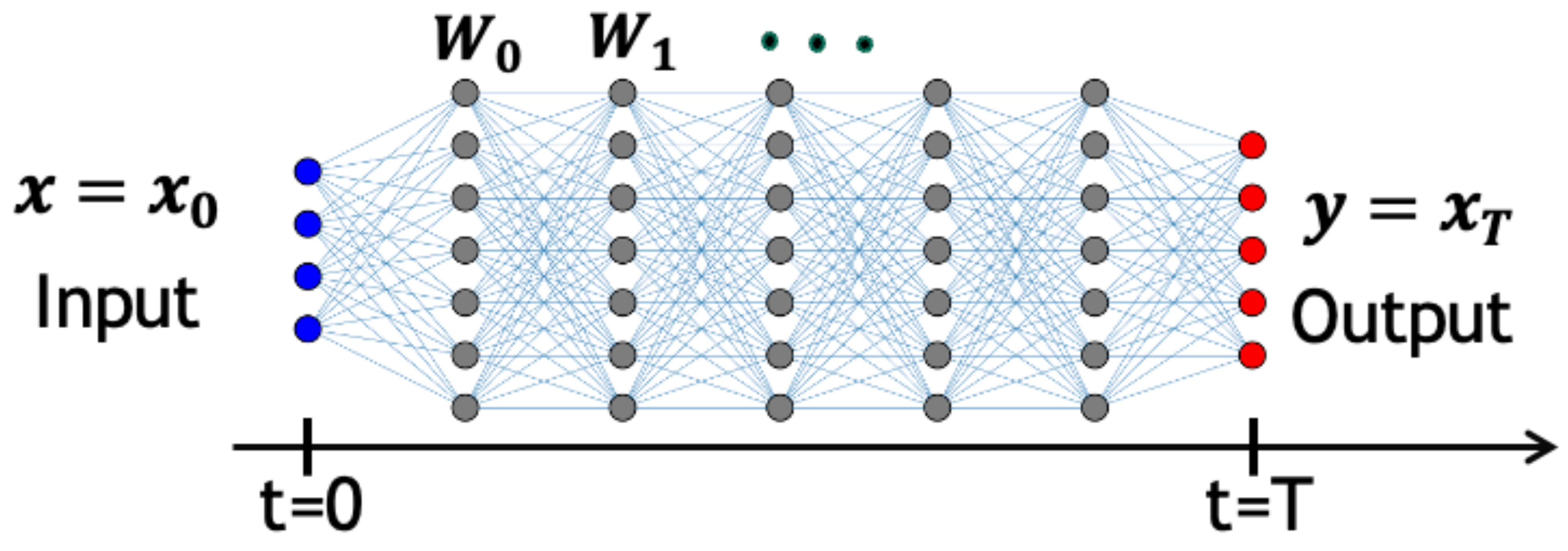


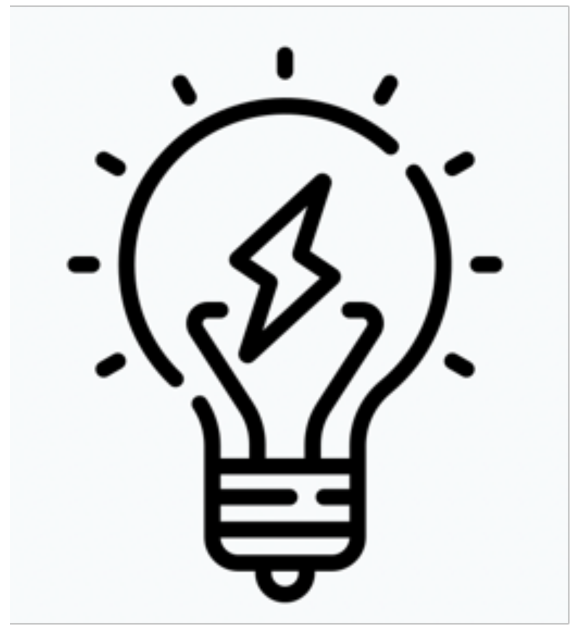
See *[Lee, 2017]* for a more comprehensive study.

Weight Parameterization inspired by NODE analogy

Neural ODE: $$\frac{dx}{dt} = \sigma(W(t)x + b(t))$$

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



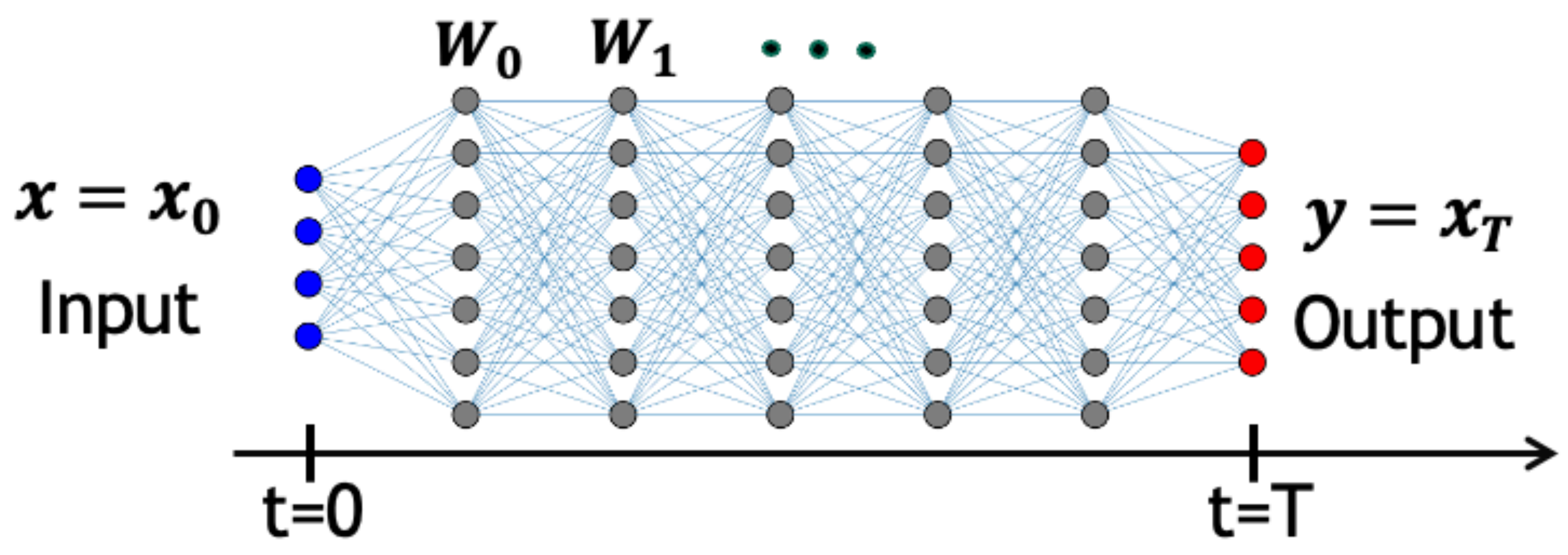


Parameterize weight matrices with respect to time (aka depth)

$W(t;\theta)$ and train for θ's.

Weight Parameterization as a regularization tool

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

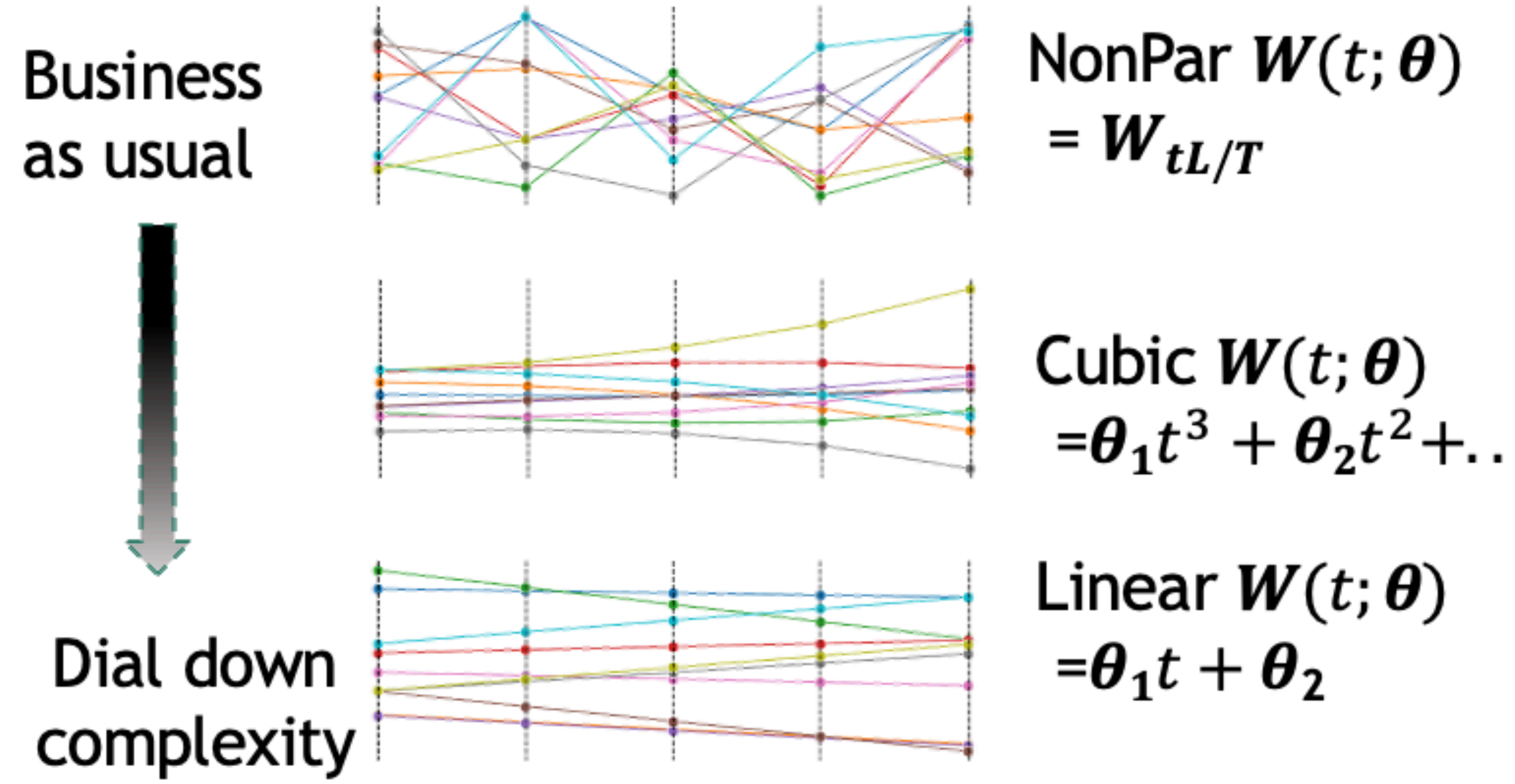


Training for weight matrices $W_0, W_1, \ldots$

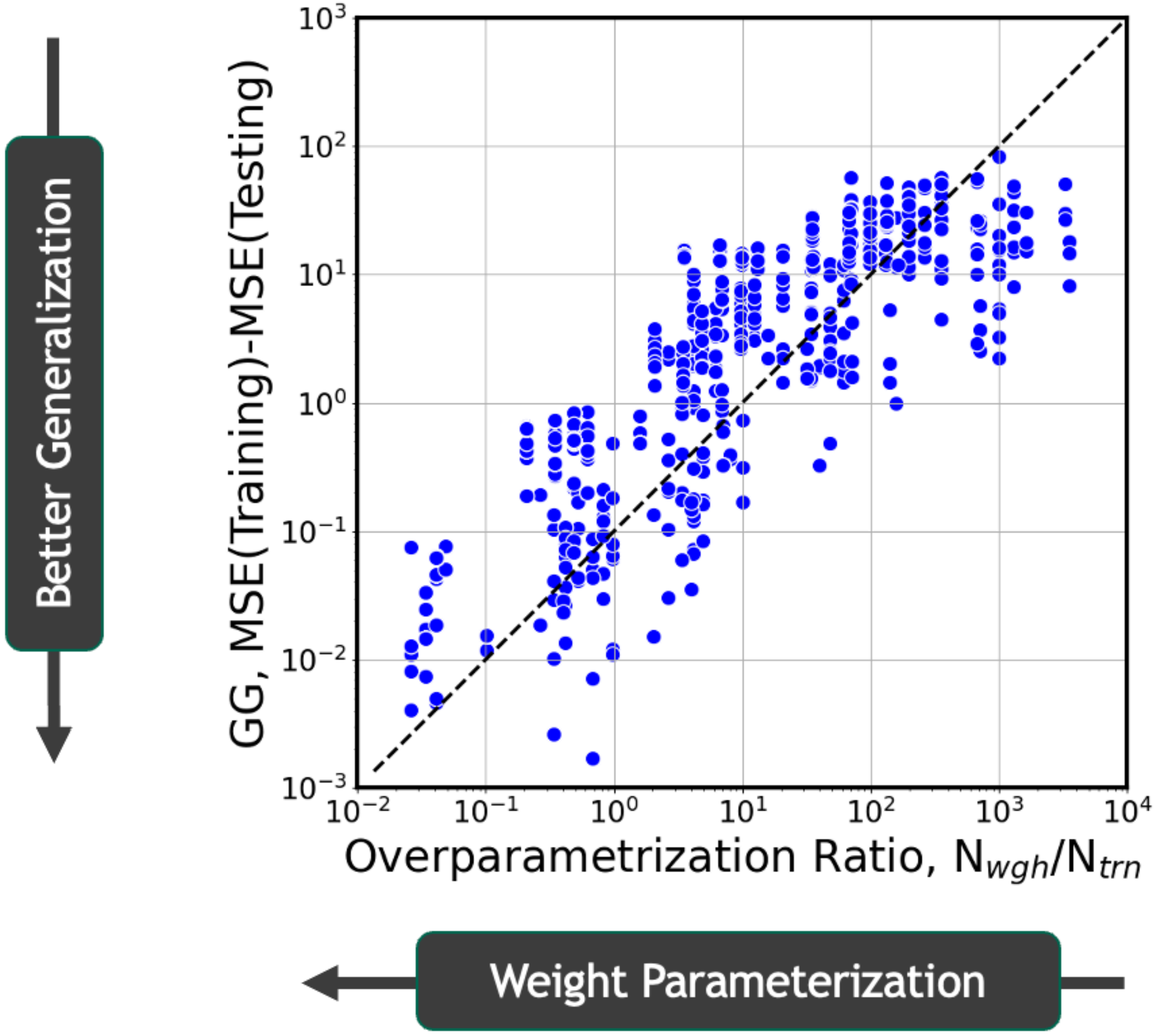
Heavily overparameterized, does not generalize well

Parameterize $W(t;\theta)$ and train for θ's.

Parameterization of weight functions reduces capacity and improves generalization



Weight Parameterization improves generalization

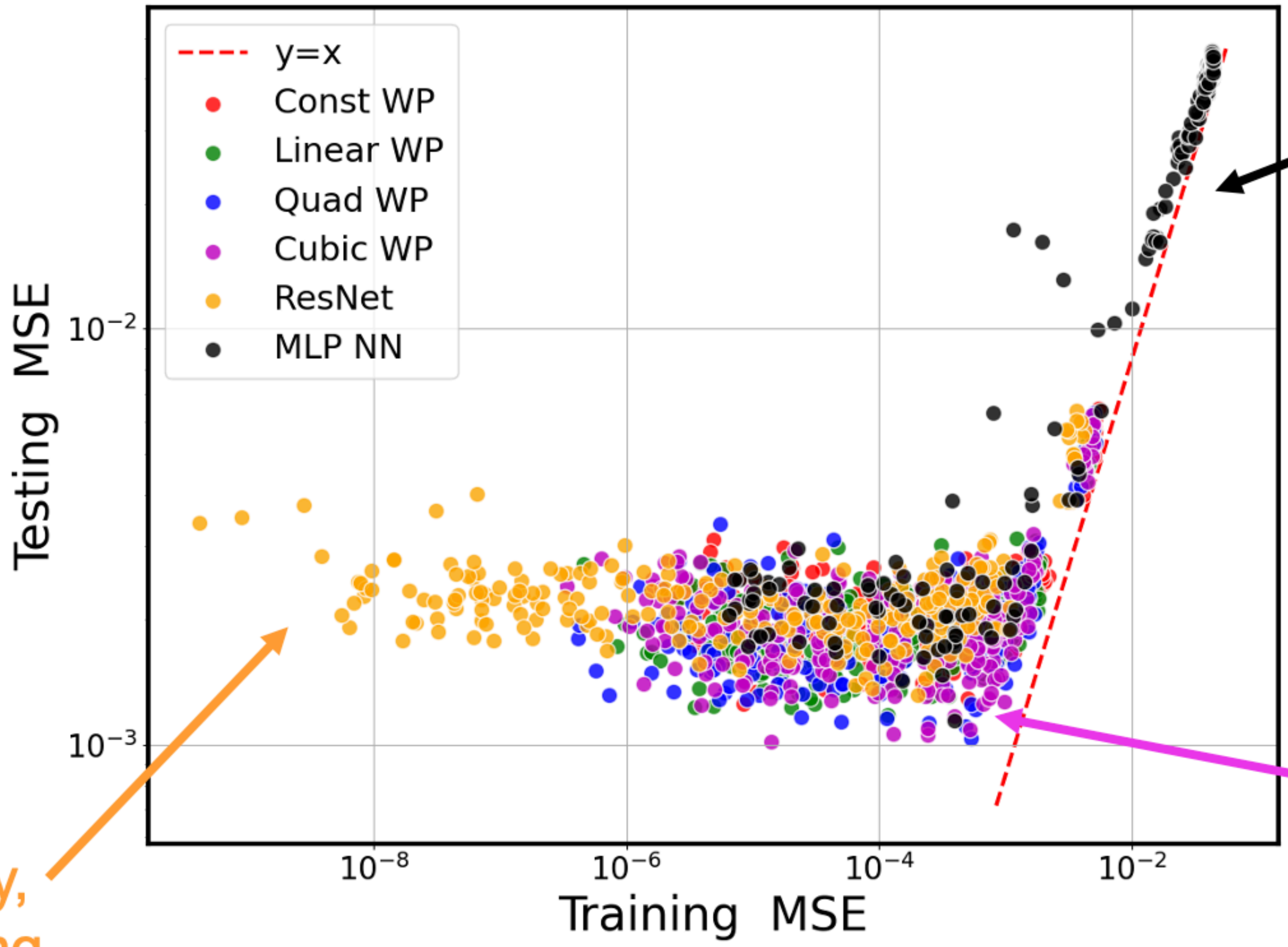


- Generalization Gap correlates with overparameterization

- Weight-parameterized ResNets reduce Generalization Gap

Each dot is a training run with varying weight parameterization functions

Weight Parameterization improves accuracy



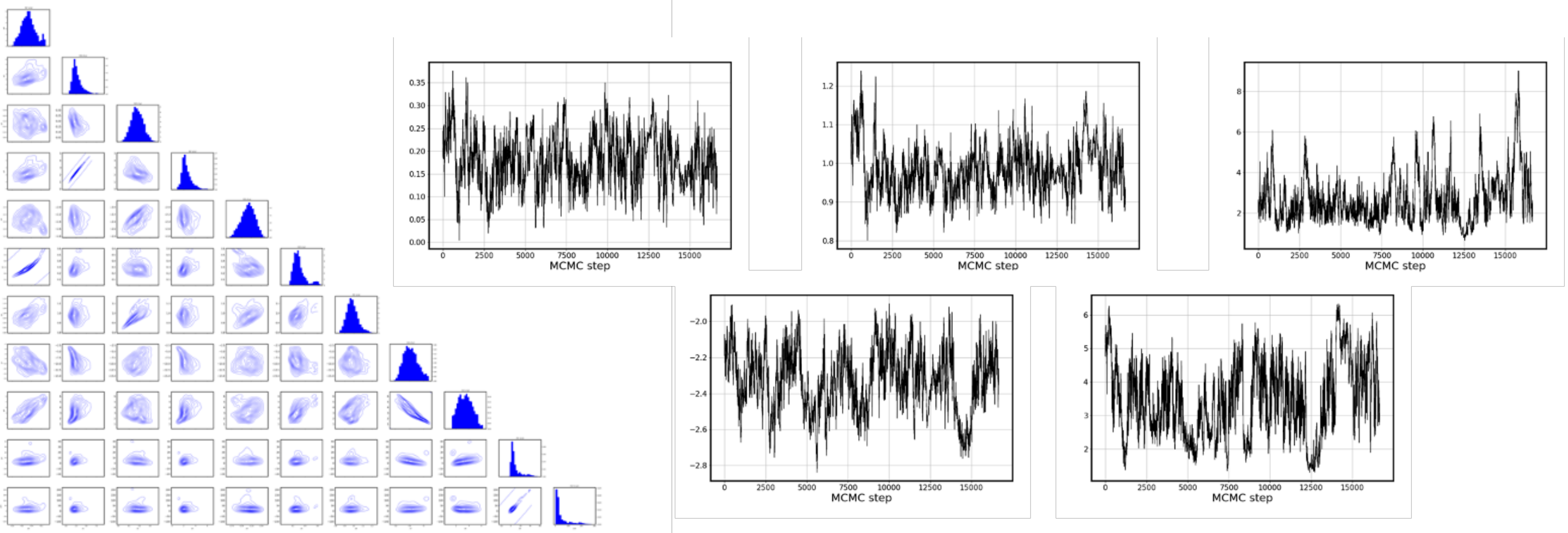
MLP:
bad accuracy

ResNet:
ok accuracy,
but overfitting

WP:
perfect tradeoff

WP ResNet enables UQ

- Number of parameters in ResNets, as well as MLPs, **grows with linearly depth**.
- Number of parameters in weight-parameterized ResNets is **independent of depth**.
- We can easily achieve regimes with manageable MCMC dimensionality and posterior PDFs that out-of-box MCMC methods can easily sample.



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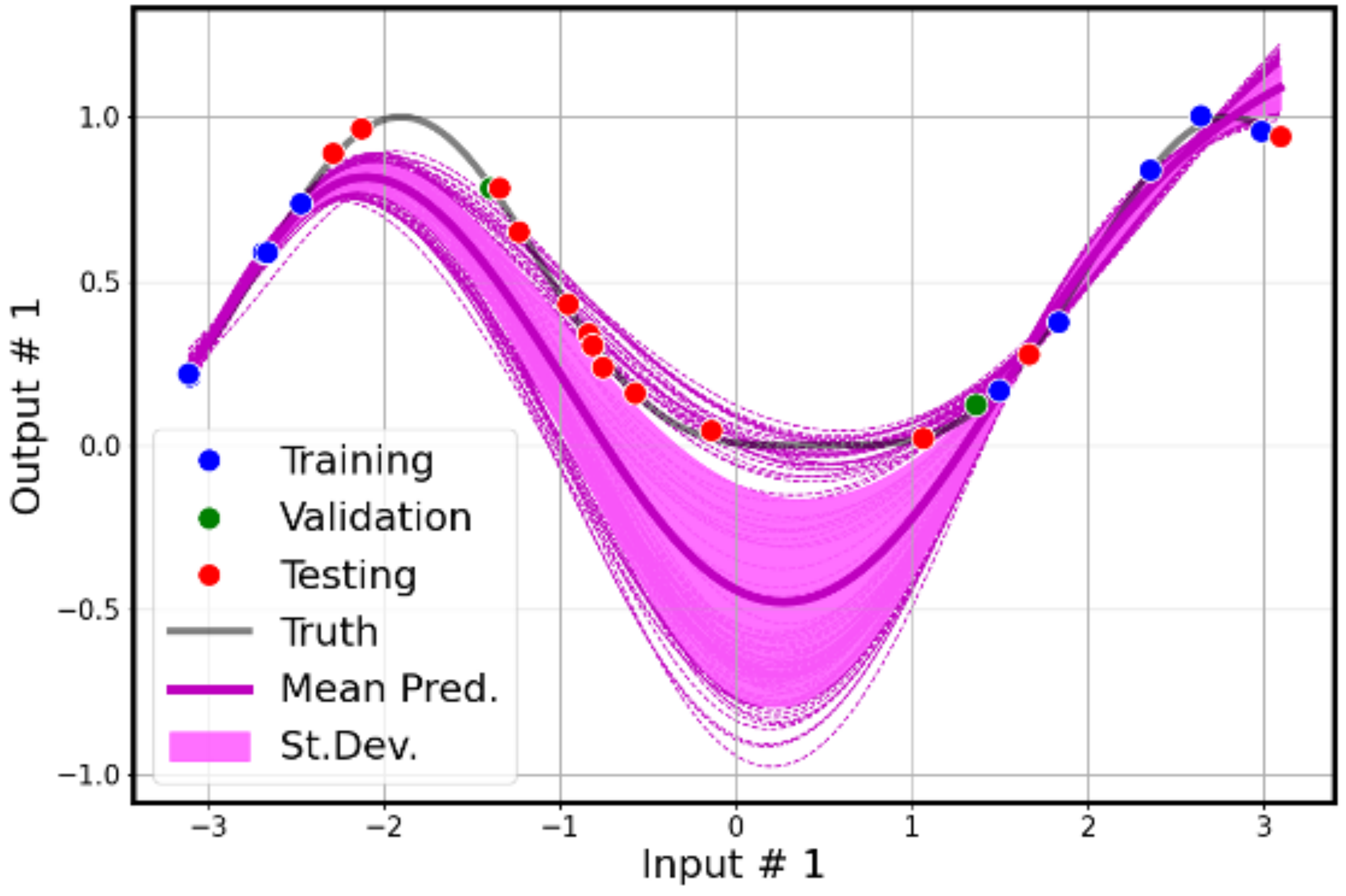
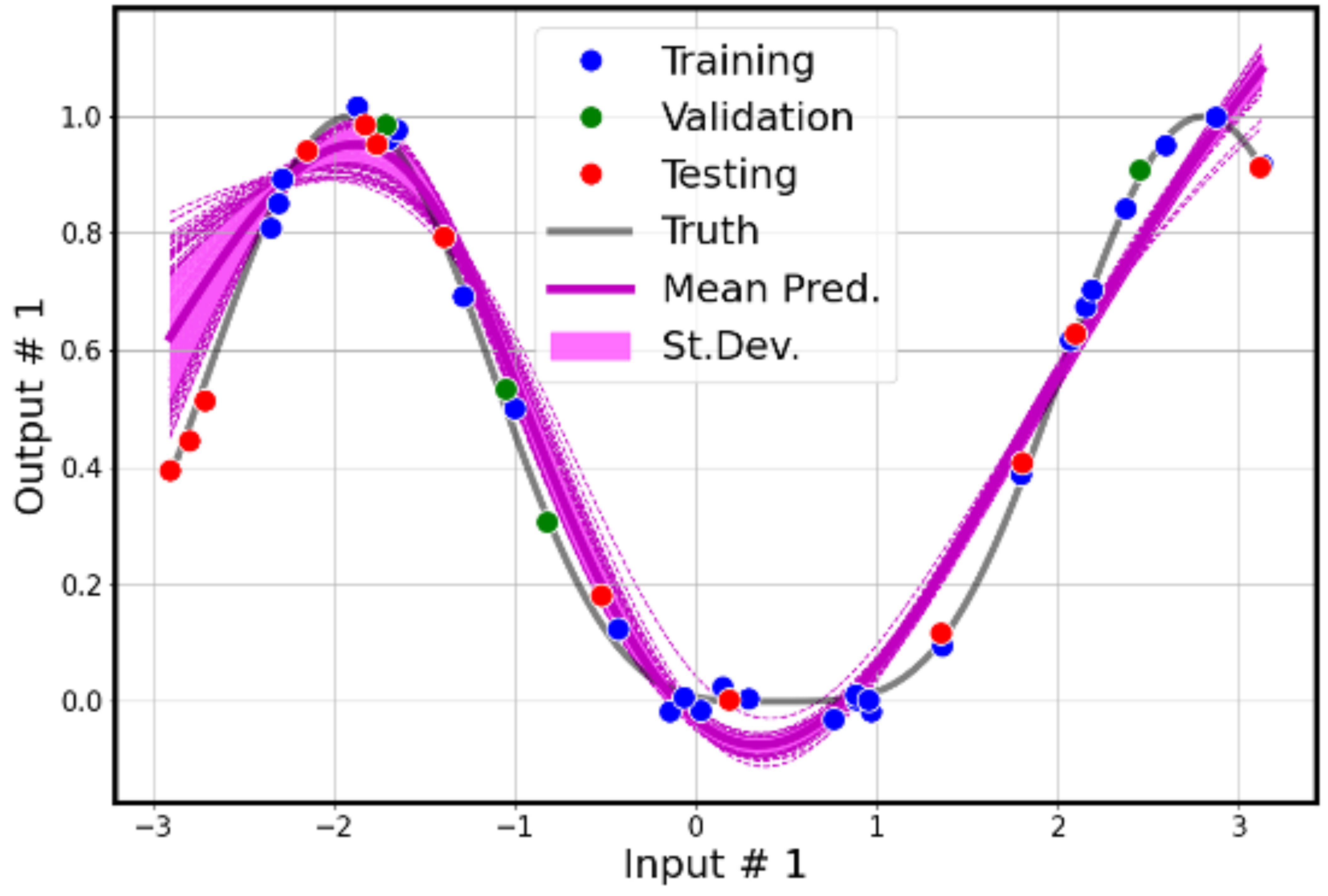




QUiNN: github.com/sandialabs/quinn

Deterministic → **Probabilistic**

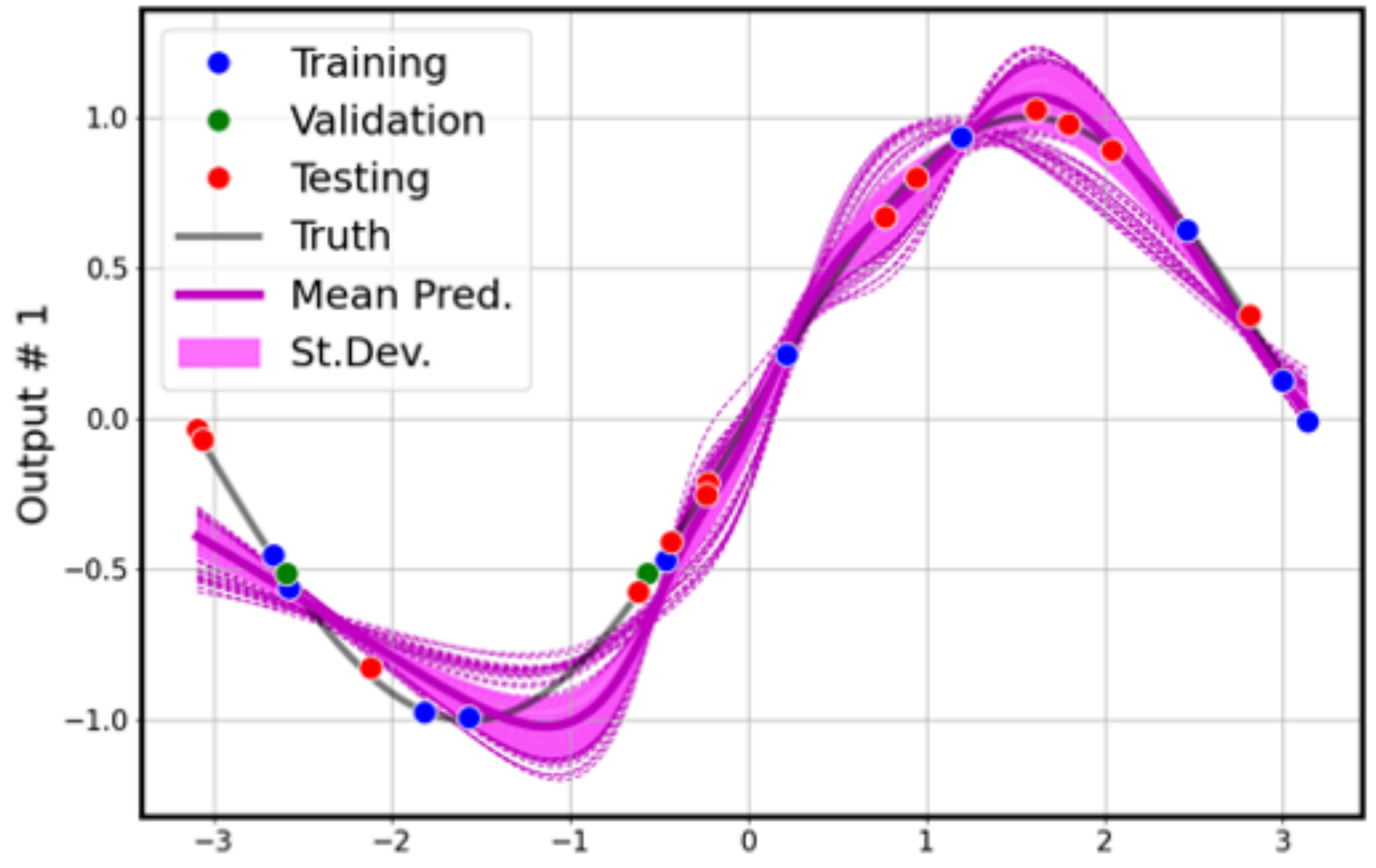
torch.nn.module → wrapper(torch.nn.module)

Usage: →

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

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

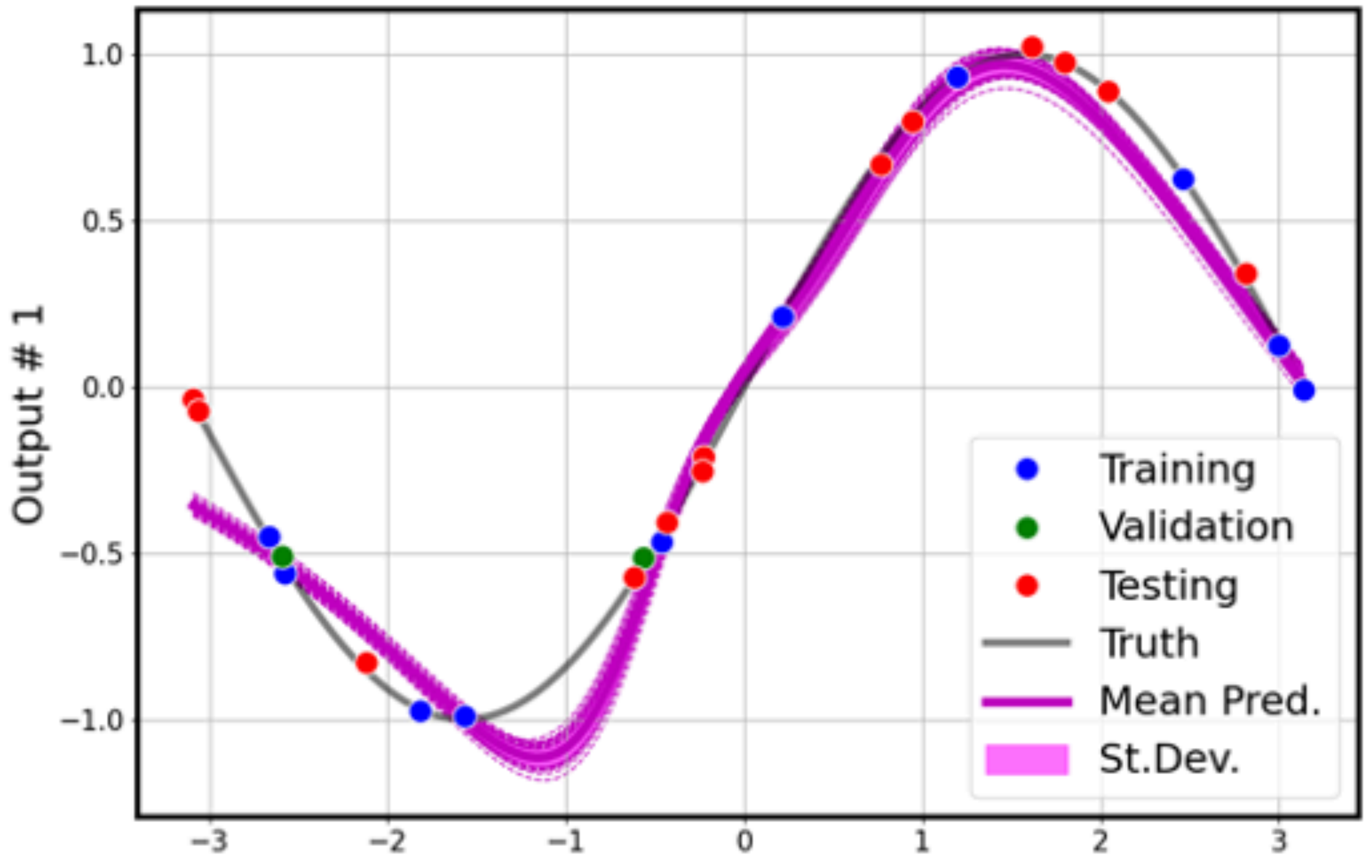
Option 1: MCMC




```
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
```

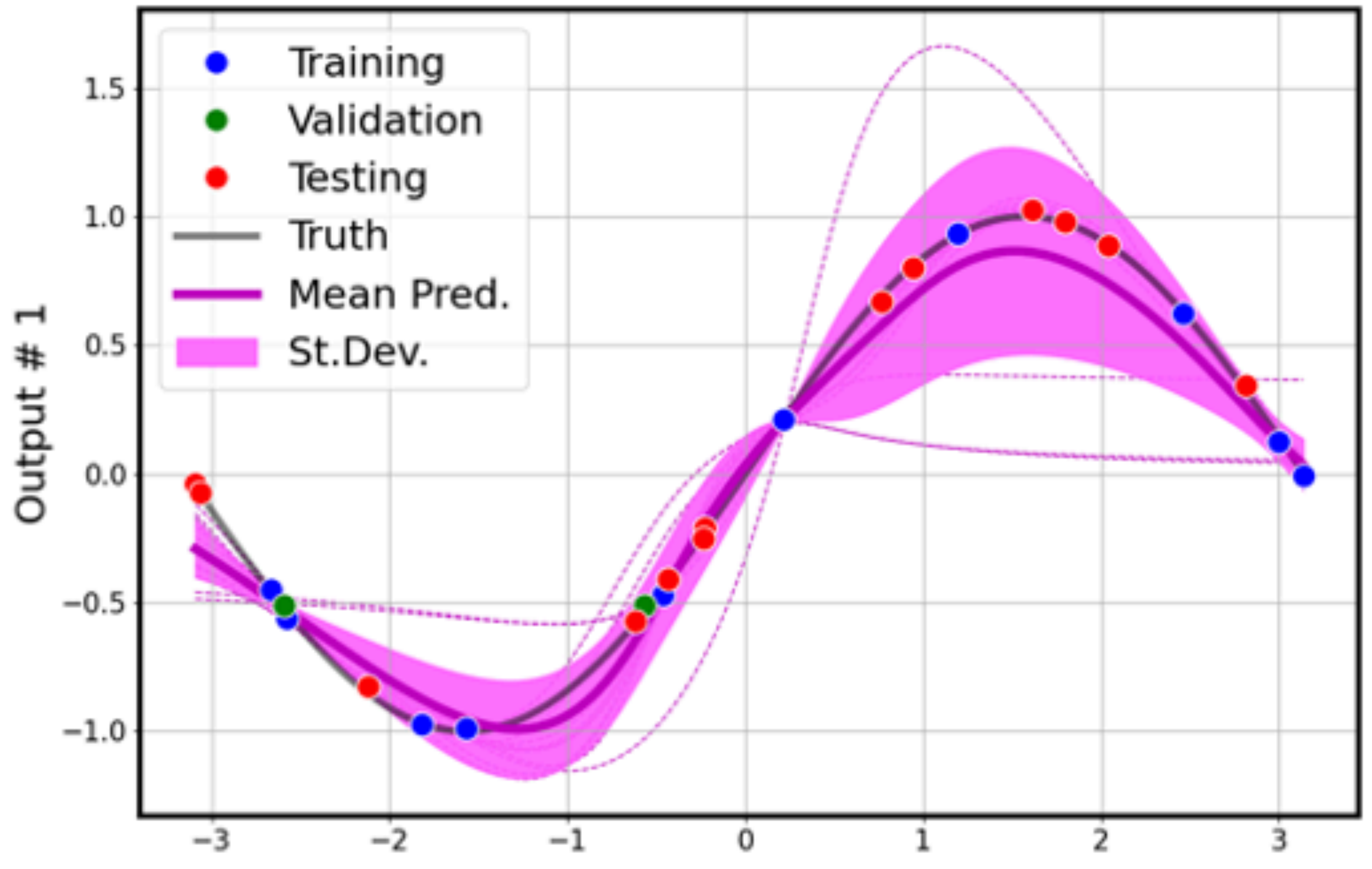
Option 2: Variational Inference




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

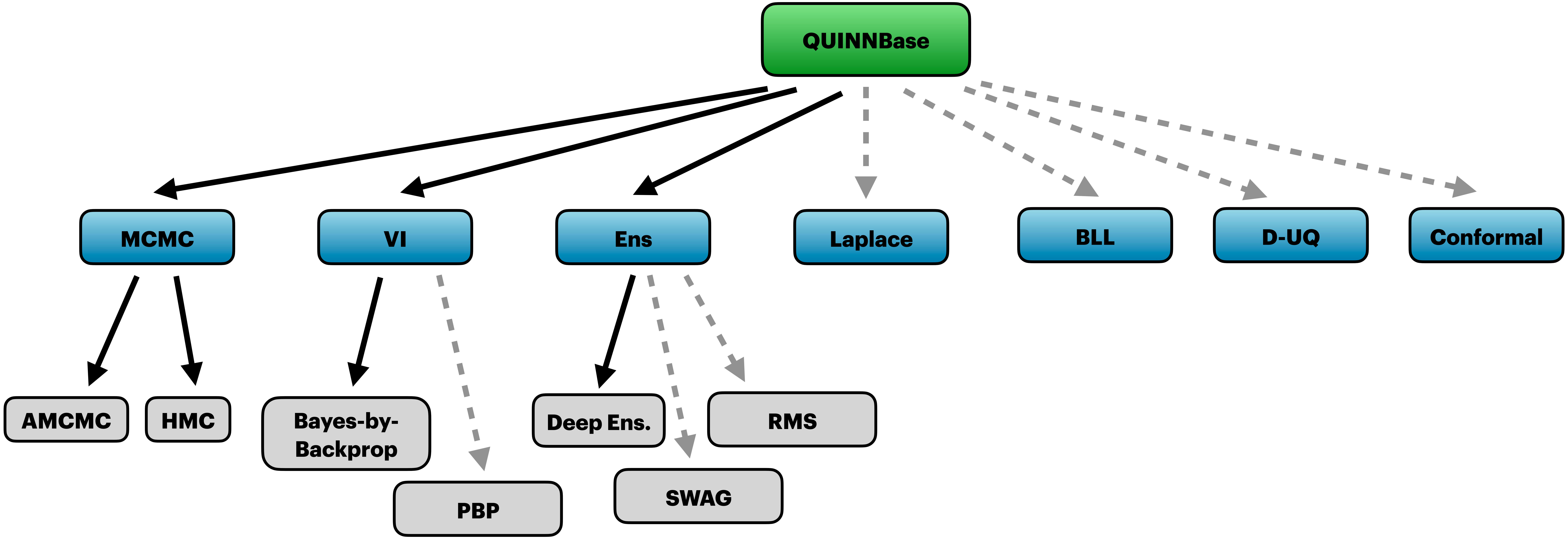
```
class Ens_NN(QUiNNBase):
    def __init__(self, nnmodule, nens=1, verbose=False):
        super(Ens_NN, self).__init__(nnmodule)
        self.verbose = verbose
        self.nens = nens
```

Option 3: Ensembling



QUiNN: github.com/sandialabs/quinn

```
uqnet = QUINNBase(torch.nn.module)
```



Summary

- UQ for NN
  - An attempt to categorize the methods
  - Most methods rely on loss landscape
  - Metrics/diagnostics of accuracy
  - Major challenges

- New FASTMath/RAPIDS concept project: visualize and study loss landscapes, add physics.

- ResNet/ODE:
  - Draw inspiration from ODE and infinite depth limit
  - ResNets regularize the learning problem, smoother loss/log-posterior surface
  - Weight parameterization (WP) allows regularization without losing much expressivity
  - Full Bayesian UQ treatment made more feasible with WP ResNets

- Implemented in QUiNN: github.com/sandialabs/quinn modular code as a wrapper to categories of methods (MCMC/HMC, VI, Ens)

Literature

General probabilistic NN:

- Z. Ghahramani, "Probabilistic machine learning and artificial intelligence". Nature 521, 452–459 (2015)
- D. J. C. MacKay, "A practical Bayesian framework for backpropagation networks". Neural Computation 4 448–472 (1992)
- R. M. Neal, "Bayesian Learning for Neural Networks". Springer, New York (1996)

UQ for NN methods:

- D. Lévy, M. D. Hoffman, and J. Sohl-Dickstein, "Generalizing Hamiltonian Monte Carlo with Neural Networks". ICLR (2018)
- C. Blundell, J. Cornebise, K. Kavukcuoglu, D. Wierstra, "Weight uncertainty in neural networks". arXiv:1505.05424 (2015)
- J.M. Hernández-Lobato, R. Adams, "Probabilistic backpropagation for scalable learning of Bayesian neural networks". ICML (2015)
- H. Ritter, A. Botev, D. Barber, "A Scalable Laplace Approximation for Neural Networks", ICLR (2018)
- E. Daxberger, A. Kristiadi, A. Immer, R. Eschenhagen, M. Bauer, P. Hennig, "Laplace Redux-Effortless Bayesian Deep Learning" Advances in neural inf. proc. systems 34 (2021)
- Y. Gal, Z. Ghahramani, "Dropout as a Bayesian approximation: representing model uncertainty in deep learning". ICML (2016)
- B. Lakshminarayanan, A. Pritzel, and C. Blundell, "Simple and scalable predictive uncertainty estimation using deep ensembles". NIPS'17. 6405–6416 (2017)
- T. Pearce, F. Leibfried, A. Brintrup, "Uncertainty in Neural Networks: Approximately Bayesian Ensembling". Artificial Intelligence and Statistics, 108:234-244 (2020)s" Machine Learning: Science and Technology, 3-4 (2022)
- Y. Yang , L. Hodgkinson, R. Theisen, J. Zou, J. E. Gonzalez , K. Ramchandran, M. Mahoney. "Taxonomizing local versus global structure in neural network loss landscapes", NIPS (2021)
- R. Anirudh, J. J. Thiagarajan. "Delta-UQ: Accurate Uncertainty Quantification via Anchor Marginalization", arxiv.org/abs/2110.02197 (2021)
- R. Krishnan, O. Tickoo, "Improving model calibration with accuracy versus uncertainty optimization". arXiv:2012.07923 (2020)

Literature

UQ for NN methods, cont.:

- W.J. Maddox, P Izmailov, T. Garipov, D.P. Vetrov, A. G. Wilson, "A simple baseline for Bayesian uncertainty in deep learning". NIPS (2019)
- T Garipov, P. Izmailov, D. Podoprikhin, D. Vetrov, A. G-Wilson, “Loss Surfaces, Mode Connectivity, and Fast Ensembling of DNNs”. NIPS (2018)
- S. Fort, H. Hu, B. Lakshminarayanan , Deep Ensembles: A Loss Landscape Perspective”, arxiv.org/abs/1912.02757, (2019)
- H. Li, Z. Xu, G. Taylor, C. Studer, T. Goldstein, "Visualizing the Loss Landscape of Neural Nets, NIPS (2018)
- Y. Hu, J. Musielewicz, Z. W. Ulissi and A. J. Medford, "Robust and scalable uncertainty estimation with conformal prediction for machine-learned interatomic potentials" Machine Learning: Science and Technology, 3-4 (2022)
- L. Guo, H. Wu, W. Zhou, Y. Wang, T. Zhou, "IB-UQ: Information bottleneck based uncertainty quantification for neural function regression and neural operator learning", https://arxiv.org/abs/2302.03271 (2023)
- J. Postels, M. Segu, T. Sun, L. Sieber, L. Van Gool, F. Yu , F. Tombari, “On the Practicality of Deterministic Epistemic Uncertainty”, ICLR (2022)
- J. Watson, J. A Lin, P. Klink, J. Pajarinen, J. Peters, “Latent Derivative Bayesian Last Layer Networks”, AISTATS (2021)
- S. Lahlou, M. Jain, H. Nekoei, V. Butoi, P. Bertin, J. Rector-Brooks, M. Korablyov, Y. Bengio “DEUP: Direct Epistemic Uncertainty Prediction”, TMLR (2023)

Neural ODE:

- R. T. Q. Chen, Y. Rubanova, J. Bettencourt, D. Duvenaud, "Neural ordinary differential equations". NIPS'18 (2018).
- L. Ruthotto, E. Haber, "Deep neural networks motivated by partial differential equations". arXiv preprint arXiv:1804.04272 (2018)
- W. E, "A Proposal on Machine Learning via Dynamical Systems". Commun. Math. Stat. 5, 1–11 (2017)

Literature

Benchmarks:

- UCI Dataset, https://archive.ics.uci.edu/datasets
- J. Yao, W. Pan, S. Ghosh, F. Doshi-Velez, "Quality of Uncertainty Quantification for Bayesian Neural Network Inference", https://arxiv.org/abs/1906.09686 (2019)
- J. Navratil, B. Elder, M. Arnold, S. Ghosh, P. Sattigeri, "Uncertainty Characteristics Curves: A Systematic Assessment of Prediction Intervals", https://arxiv.org/abs/2106.00858 (2021)
- Z. Nado et al. "Uncertainty Baselines: Benchmarks for Uncertainty & Robustness in Deep Learning", https://arxiv.org/abs/2106.04015 (2021), https://github.com/google/uncertainty-baselines
- B. Staber, S. Da Veiga, "Benchmarking Bayesian neural networks and evaluation metrics for regression tasks", https://arxiv.org/abs/2206.06779 (2022)
- L. Basora, A. Viens, M. Arias Chao, X. Olive, "A Benchmark on Uncertainty Quantification for Deep Learning Prognostics", https://arxiv.org/abs/2302.04730 (2023)