$\mathcal{P}^2$ LAB
@EE, IIT Roorkee

Optimization Proxies for Power Systems

The Idea, Data Efficiency, Feasibility & Confidence

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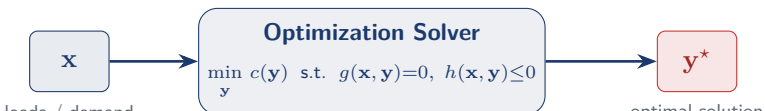
What is an Optimization Proxy?



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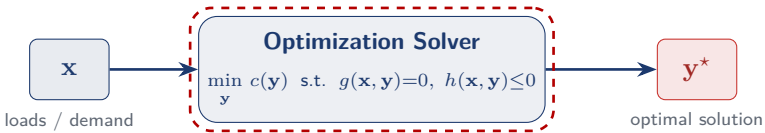

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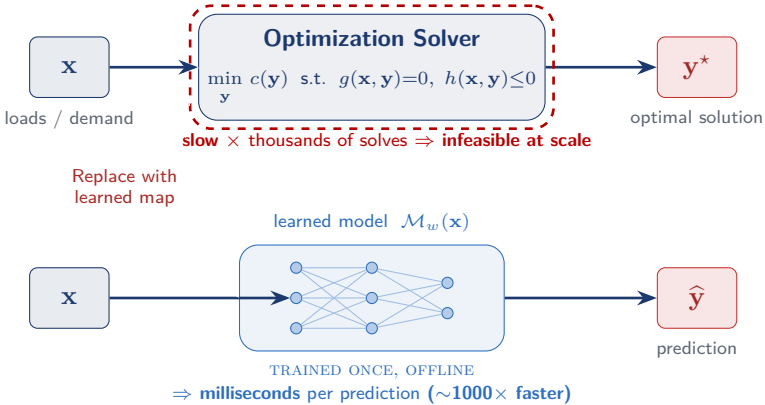

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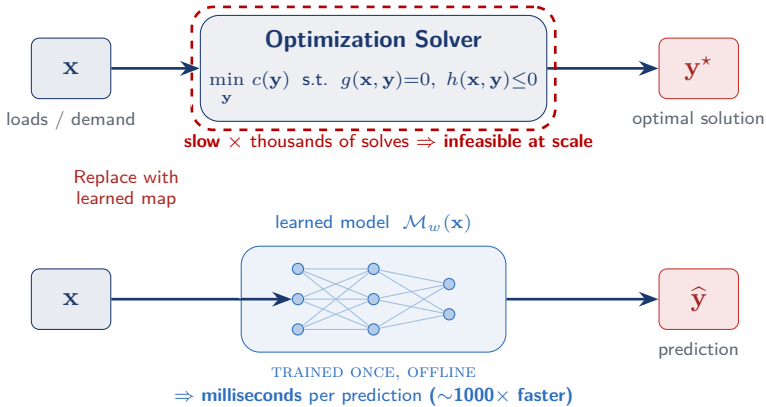

Fast — but is $\widehat{\mathbf{y}}$ **feasible**? **optimal**? **trustworthy**? ⇒

Data Efficiency · **Feasibility** · **Confidence**

Before We Walk Further:

There are Two Ways ML Meets Optimization!

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Optimization problem

$\min_{\mathbf{y}} c(\mathbf{y})$ s.t. $g(\mathbf{x}, \mathbf{y}) = 0,\ h(\mathbf{x}, \mathbf{y}) \leq 0$

THIS TALK

1. Learn the solution

end-to-end optimization proxy

Replace the solver entirely:

$\mathbf{x} \to \mathcal{M}_w(\mathbf{x}) \to \widehat{\mathbf{y}} \approx \mathbf{y}^\star$

Fast, but approximate — must check feasibility & optimality.

2. Learn inside the solver

ML-accelerated exact solving

Keep the solver; learn its choices:

- learn to branch [Gasse '19]
- cut selection [Tang '20]
- node / variable ordering
- warm-starts & primal heuristics

Still **exact** — only **faster**.

Loss Functions Across Proxies: Who Uses What

- Proxy losses range from pure label-matching to fully objective-driven

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Loss Family	Schematic Training Loss	Representative Work	Venue
MSE/MAE + PF recovery	$\left\|\hat{\mathbf{y}} - \mathbf{y}^\star\right\|^2$	Pan et al. (2021)	IEEE TPS'21
Supervised + Lagrangian penalty	$\left\|\hat{\mathbf{y}} - \mathbf{y}^\star\right\|^2 + \boldsymbol{\lambda}^\top \nu(\hat{\mathbf{y}})$	Fioretto et al. (2020b)	AAAI'20
Completion + correction (soft loss)	$c(\hat{\mathbf{y}}) + \lambda \left\|\text{ReLU}[h]\right\|^2$	Donti et al. (2021)	ICLR'21
Self-supervised primal–dual	$c(\hat{\mathbf{y}}) + \hat{\boldsymbol{\lambda}}^\top g + \hat{\boldsymbol{\mu}}^\top h + \frac{\rho}{2}\nu(\cdot)$	Park and Van Hentenryck (2023b)	AAAI'23
Unsupervised (objective + penalty)	$c(\hat{\mathbf{y}}) + \lambda\, \mathcal{V}(\hat{\mathbf{y}})$	Huang et al. (2024)	IEEE TPS'24
Physics-informed (KKT)	$\left\|\hat{\mathbf{y}} - \mathbf{y}^\star\right\|^2 + \lambda \left\|\text{KKT res.}\right\|$	Nellikkath and Chatzivasileiadis (2022a)	EPSR'22

Trend

Move from **label-hungry** MSE → **label-free** objective+penalty;

How Proxies Enforce Feasibility: An Architecture Spectrum

(a) Vanilla

✗ no guarantee ≈ partial / approximate ✓ guaranteed feasible ⇒ **(e)** repairs feasibility *by construction*, at scale.

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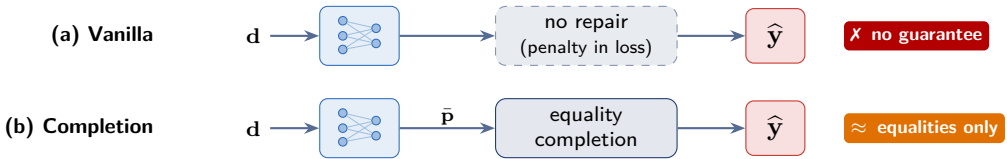

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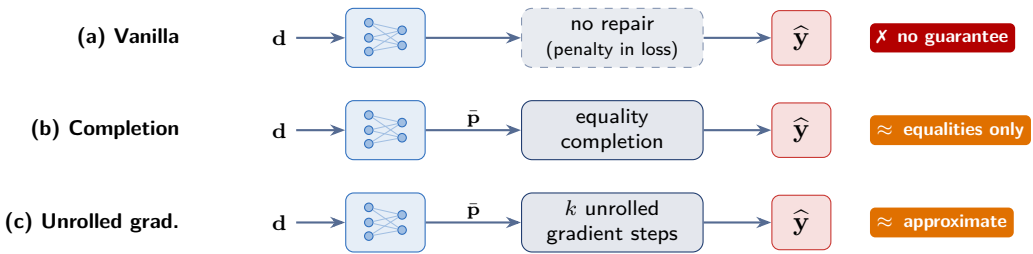

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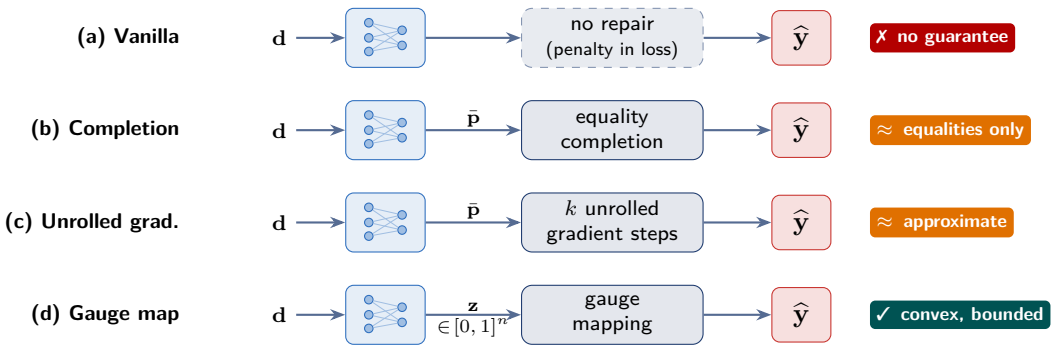

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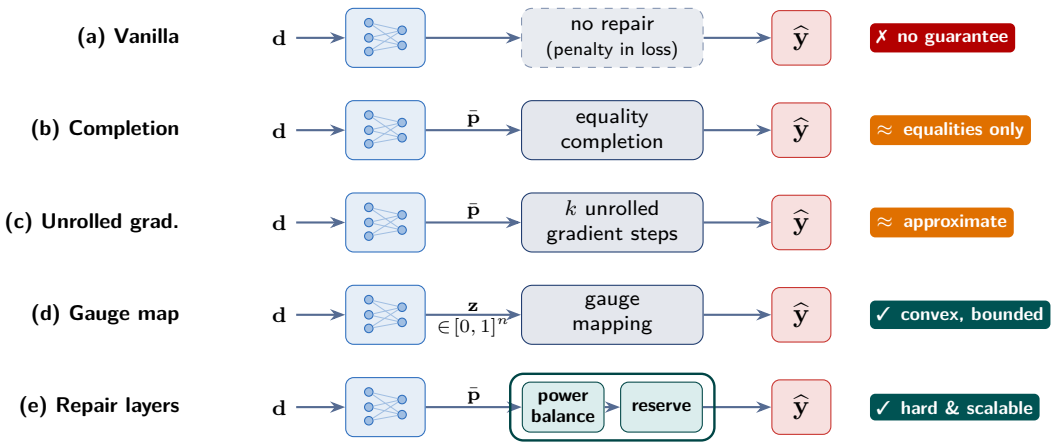

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The ML's Time Equation

$$T_{Total} = T_{Data} + T_{Training} + T_{Prediction}$$

T_{Data}	$T_{Training}$	$T_{Prediction}$
Training Data Generation Validation Data Generation	Hyperparameter Optimization Variational Inference	Prediction Time Validation Time

The Problem

How to Overcome Constraints on Training Time and Data?

Time and Data Constraints

- **Optimization proxies must be trained efficiently within strict time constraints**
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- **Physical systems require 'some' guarantees on learning quality**
  - Vanilla statistical validation demands a large validation dataset

    `Hoeffding's Inequality:` $\varepsilon \propto 1/\sqrt{N}$

Bayesian for Rescue under Low Data

- **What are Bayesian Neural Networks (BNNs)?**
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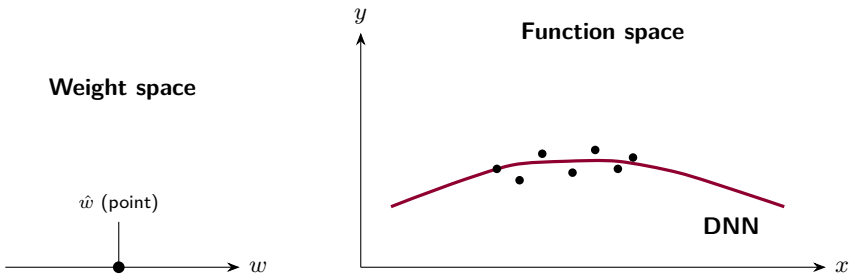
  - Prevent overfitting: **Weight Distribution**, **Regularization via Priors**, **Posterior Averaging**
- **Advantages over DNNs:**
  - Separates two types of uncertainty:
    - **Epistemic uncertainty**: Uncertainty in model parameters $p(w|D)$.
    - **Aleatoric uncertainty**: Noise inherent in data $p(y|x, w)$.
  - Assigns high uncertainty to points far from the training set, avoiding overconfident predictions.

From DNN to BNN: One Picture



DNN: fixed weights $\Rightarrow$ *one* function — confident even where there is no data.

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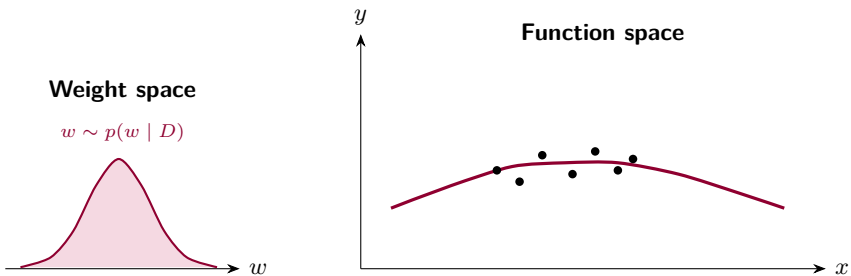

BNN: each weight is a distribution, $w \sim p(w \mid D)$ — not a single value.

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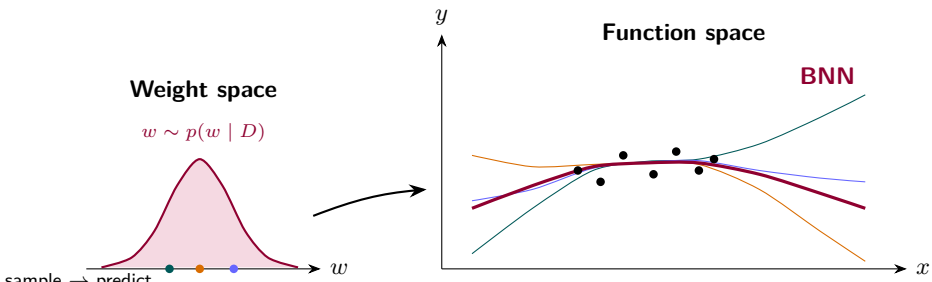

Sampling weights ⇒ an **ensemble** of functions: they agree on data, disagree away from it.

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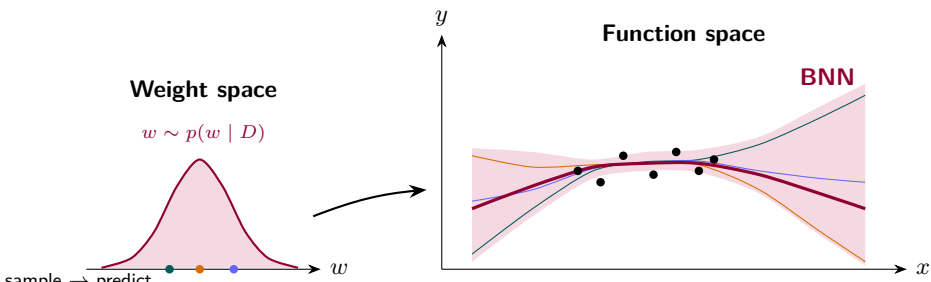

Posterior averaging ⇒ mean ± uncertainty. The band **widens far from data**.

Our Problem, Target, Motivation and Idea

Standard Constrained Optimization Problem

$$\min_{\mathbf{y}} \quad c(\mathbf{y}) \tag{1a}$$

$$\text{s.t.} \quad g(\mathbf{x}, \mathbf{y}) = 0 \tag{1b}$$

$$h(\mathbf{x}, \mathbf{y}) \leqslant 0 \tag{1c}$$

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- **Idea:**
  Using large unlabeled dataset to enforce **Feasibility** & limited supervised dataset for **Optimality + Feasibility**

The TL;DR: An Optimal Solution Has To Be Feasible

Feasibility Condition

$$\mathcal{F}(\mathbf{y}, \mathbf{x}) = \lambda_e \underbrace{\left\| g(\mathbf{x}, \mathbf{y}) \right\|^2}_{\texttt{Equality Gap}} + \lambda_i \underbrace{\left\| \mathsf{ReLU}[h(\mathbf{x}, \mathbf{y})] \right\|^2}_{\texttt{Inequality Gap}}. \tag{2}$$

Feasibility Condition on Network Weights

Network weights should be such that, for any input, predicted output provides $\mathcal{F}(\mathbf{y}, \mathbf{x}) = 0$

If input sampling is cheap, we can create an **Augmented Labeled Dataset** for **Free**

$$\mathcal{D}^f = \{(\mathbf{x}_j, \mathcal{F}(\cdot, \mathbf{x}) = 0)\}_{j=1}^{M}$$

Sandwich Model

Alternating Training Phases for BNNs in Time-Constrained Bursts

$$p_W^1 \equiv p(w \mid \mathbf{y}, \mathbf{x}) \propto p(\mathbf{y} \mid \mathbf{x}, w)\, p_w^0$$

$$\xrightarrow[\mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})]{p_W^0} \underbrace{\text{Sup}}_{T_s}$$

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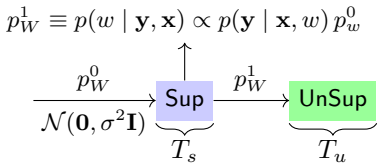

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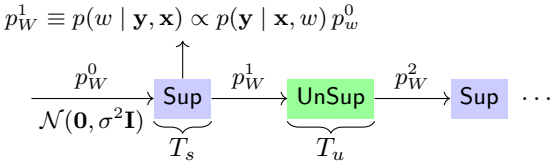

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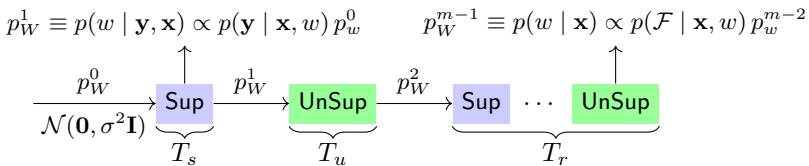

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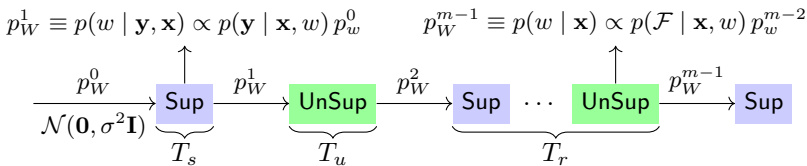

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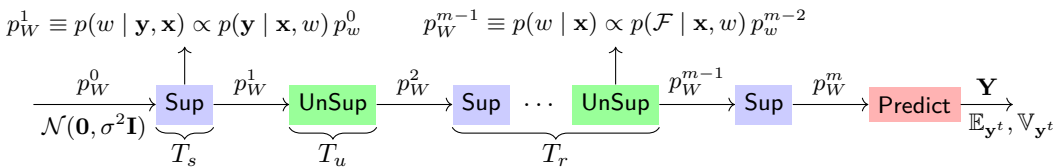

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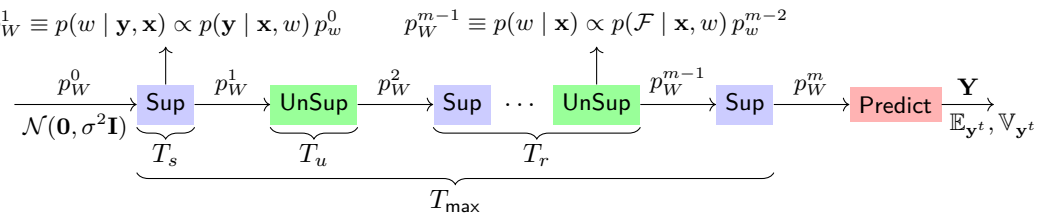

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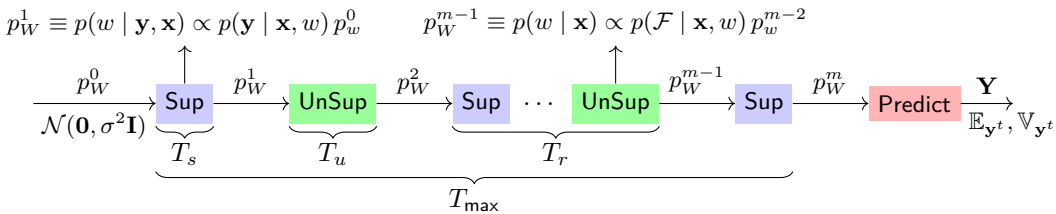


➠ `Selection via Posterior`: Among BNN weights, select the one providing **'Best'** results for the selected criteria

$$W^\star = \arg\min_j \left[\max_i \left| g_i(\mathbf{x}^t, \mathbf{Y}_{\cdot j}) \right| \right] : \quad \text{Minimizes the maximum equality gap}$$

Bounding the Error

- We want to know, how far expected error can be compared to the error we calculated!

$$\mathbb{P}\left\{\left|\mathbb{E}[|e|] - \frac{1}{M}\sum_{i=1}^{M}|e_i|\right| \leqslant \varepsilon\right\} \geqslant 1-\delta$$

- Error bound ε in PCBs, provided by different concentration inequalities.

Hoeffding's	Empirical Bernstein	Theoretical Bernstein
$R\sqrt{\frac{\log(2/\delta)}{2M}}$	$\sqrt{\frac{2\widehat{\mathbb{V}}_e \log(3/\delta)}{M}} + \frac{3R\log(3/\delta)}{M}$	$\sqrt{\frac{2\mathbb{V}_e \log(1/\delta)}{M}} + \frac{2R\log(1/\delta)}{3M}$

- `Hypothesis:` $\alpha\,\mathsf{MPV} \geqslant \mathbb{V}_e = \underbrace{\mathbb{E}_M\left[\mathbb{V}_W[e]\right] + \mathbb{E}_W\left[\mathbb{V}_M[e]\right]}_{\texttt{Total Variance in Error}} \geqslant \mathbb{V}_{|e|}$
- `Proposed Bound:`

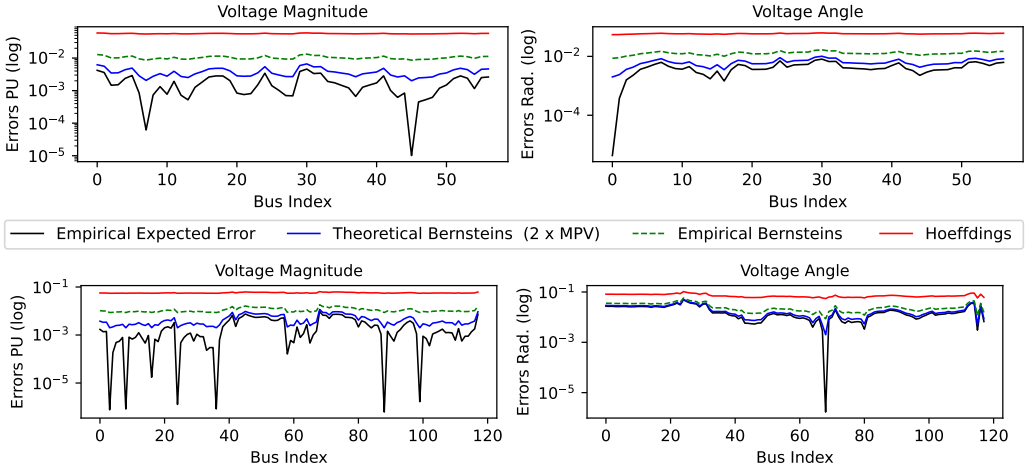
$$\sqrt{\frac{2(2\times \mathsf{MPV})\log(1/\delta)}{M}} + \frac{2R\log(1/\delta)}{3M}$$

Matchup: Sandwich, BNN & DNN

Table: Comparative performance results for the ACOPF Problem for **'case118'** with 512 labeled training samples, 2048 unlabeled samples, and $T_{\text{max}} = 600$ sec.

Method	Gap%	Max Eq.	Mean Eq.	Max Ineq.	Mean Ineq.
Sandwich BNN SvP (Ours)	**1.484**	**0.089**	0.018	0.008	**0.000**
Sandwich BNN (Ours)	1.485	0.100	**0.016**	0.008	0.000
Supervised BNN SvP (Ours)	1.568	0.147	0.022	0.013	0.000
Supervised BNN (Ours)	1.567	0.205	0.020	0.013	0.000
Naïve MAE	1.638	2.166	0.187	**0.000**	0.000
Naïve MSE	1.622	3.780	0.242	0.000	0.000
MAE + Penalty	1.577	1.463	0.102	0.000	0.000
MSE + Penalty	1.563	2.637	0.125	0.000	0.000
LD + MAE	1.565	1.284	0.083	0.000	0.000

Probabilistic Bounds



➧ Theoretical Bernstein bounds with 2 $\times$MPV are tightest.

We consider $\delta = 0.95$ and 1000 *out-of-sample* testing data points i.e. $M = 1000$

Conclusions

- **The Idea:** learned proxies replace slow solvers with millisecond predictions ($\sim$1000$\times$ faster) — for probabilistic OPF, $N-1$ screening and planning at scale.
- **Data Efficiency:** Bayesian NNs with the *Sandwich* schedule reach solver-quality solutions under tight label and training-time budgets; cheap unlabeled inputs enforce feasibility for free.
- **Feasibility:** an optimal solution *must* be feasible — feasibility-by-construction layers turn 'no guarantee' into 'guaranteed feasible'.
- **Confidence:** distribution-free concentration bounds — Theoretical Bernstein with $2\times$MPV — give the tightest probabilistic error guarantees.

Learning to Solve, Learning to Trust

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