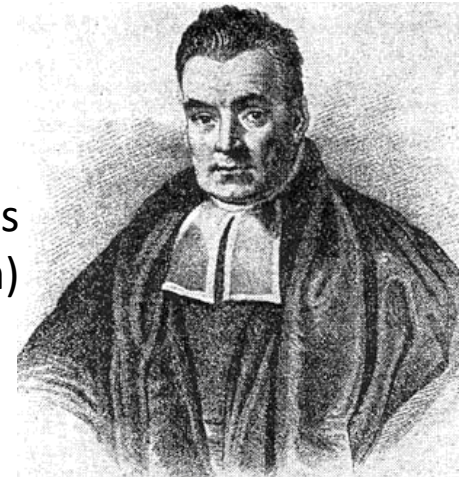


Data-Driven Optimization using **Limited Data**: the power of

Thomas Bayes
(with high probability, this is him)



Parikshit Pareek



Sidhant Misra



Kaarthik Sundar

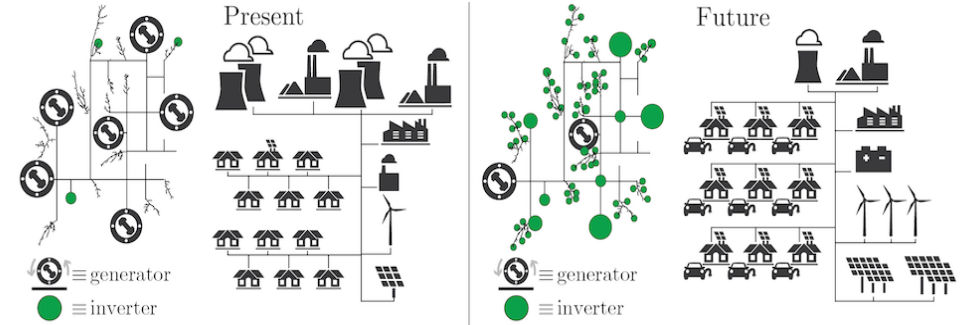


Deep Deka
Research Scientist,

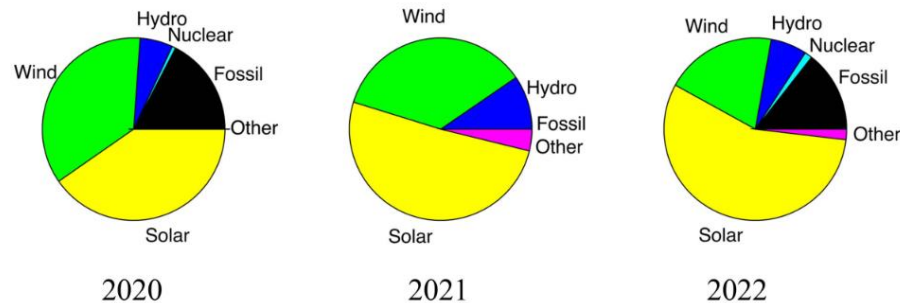


Energy Infrastructure of the future: the case for **resilience**

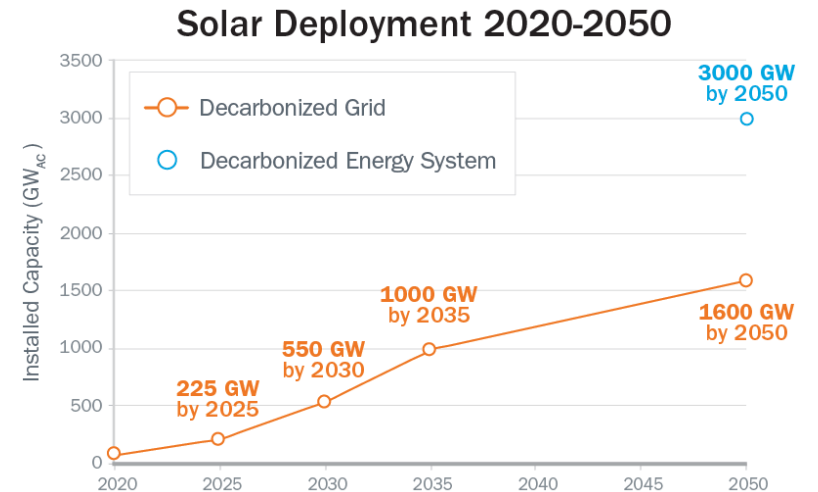
- Renewables and smart devices are leading to a paradigm shift in grid operations.
 - Greater **Variability**/intermittent
 - Lesser **inertia**/stability
 - More measurements and data-driven capabilities
- Need: faster but **risk-aware** data-driven decision making



Smart but *stochastic*



Global new generation



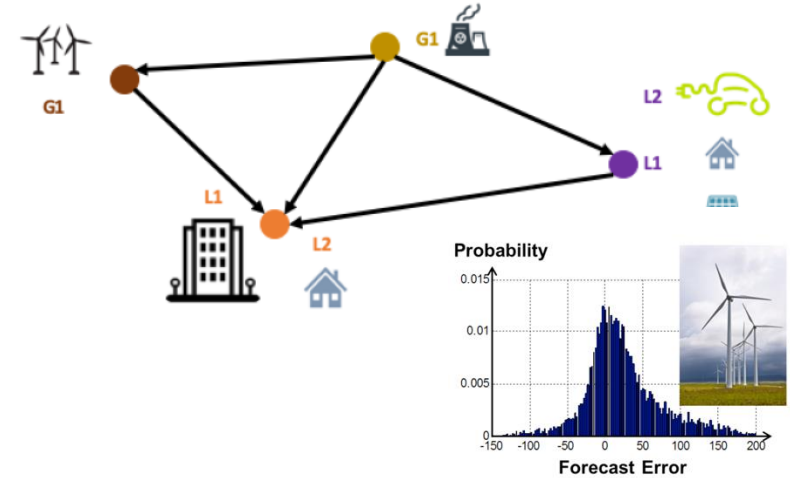
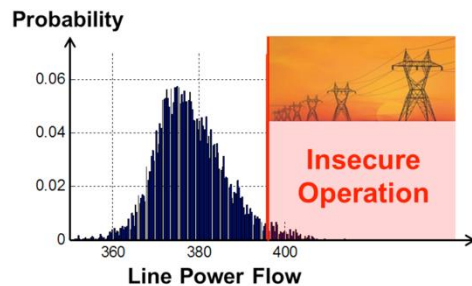
Transmission Grid Optimization under uncertainty

Optimal Power Flow: minimize generation costs while satisfying injection/demand, technical constraints

Problem:

$$\begin{aligned} \min \quad & \sum_{g \in \mathcal{G}} c(p_g) && \text{Cost} \\ \text{s.t.} \quad & \sum_{g \in \mathcal{G}_i} p_g - P_i = \sum_{j \in \mathcal{B}} v_i v_j (G_{ij} \cos(\theta_i - \theta_j) + B_{ij} \sin(\theta_i - \theta_j)) && \forall i \in \mathcal{B} \\ & \sum_{g \in \mathcal{G}_i} q_g - Q_i = \sum_{j \in \mathcal{B}} v_i v_j (G_{ij} \sin(\theta_i - \theta_j) - B_{ij} \cos(\theta_i - \theta_j)) && \forall i \in \mathcal{B} \\ & (p, q, v, \theta) \in \mathcal{T} \end{aligned}$$

↓
Safety Constraint



Non-linear power flow physics

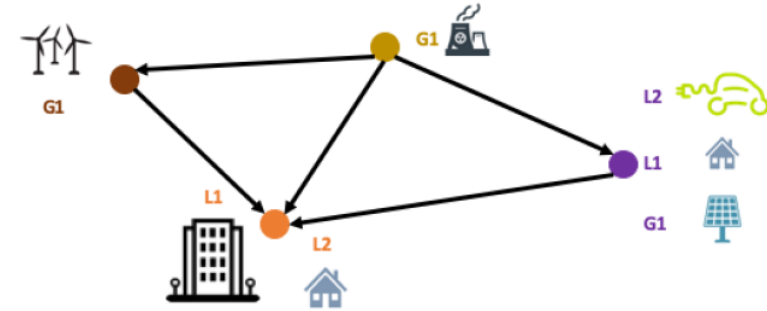
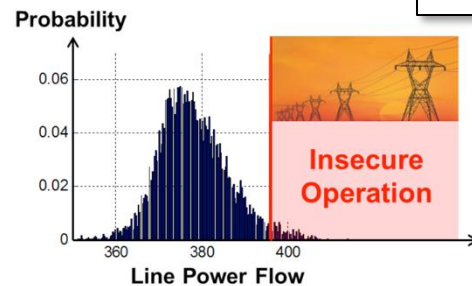
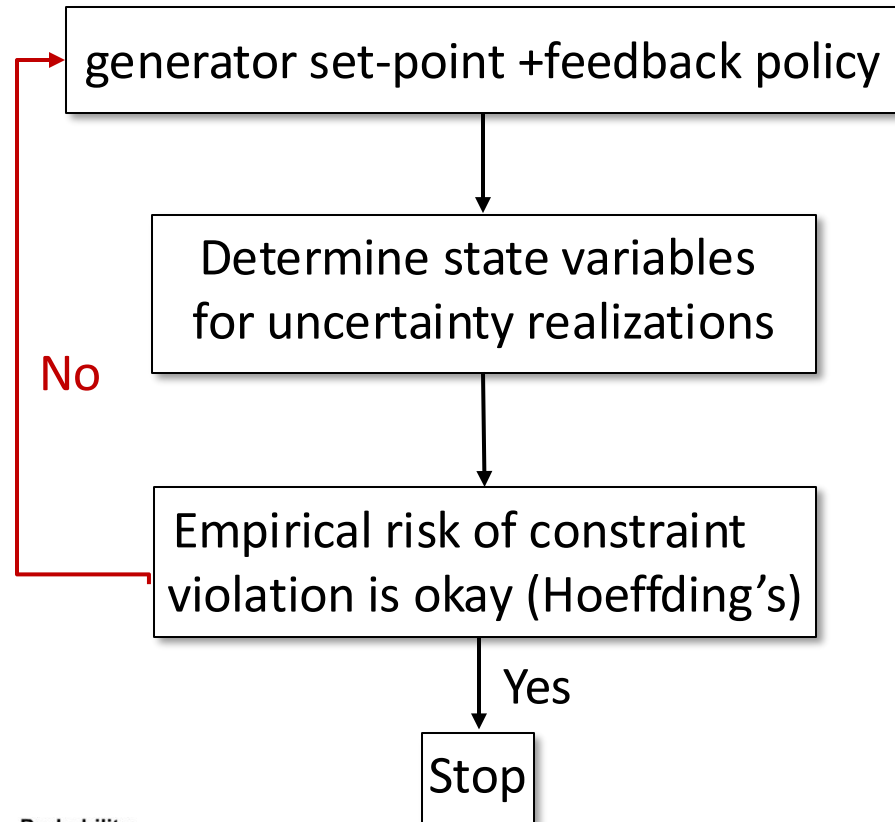
Hard to Solve generally:

- ✓ *Approximate analytical optimization (linear models, Gaussian uncertainty)*
- ✓ *ML surrogates + validation*

ML based: Jalali, Pareek, Velloso, Zamzam, Singh, Kekatos, Baker, Bernstein, van- Hentenryck, Fioretto, Donti, Chatzivasileiadis, Misra, Nagarajan, Zhu, Qiu(incomplete)

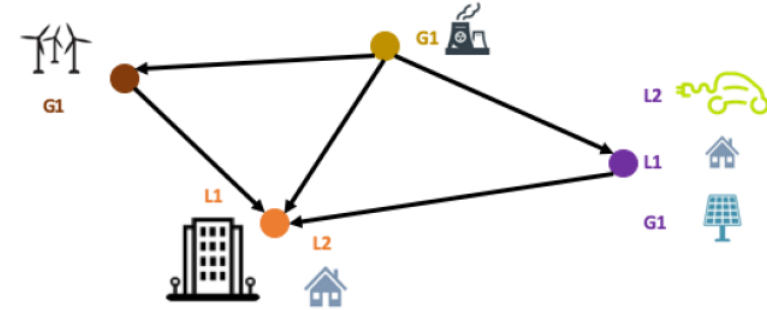
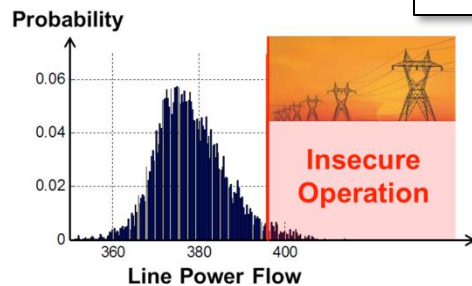
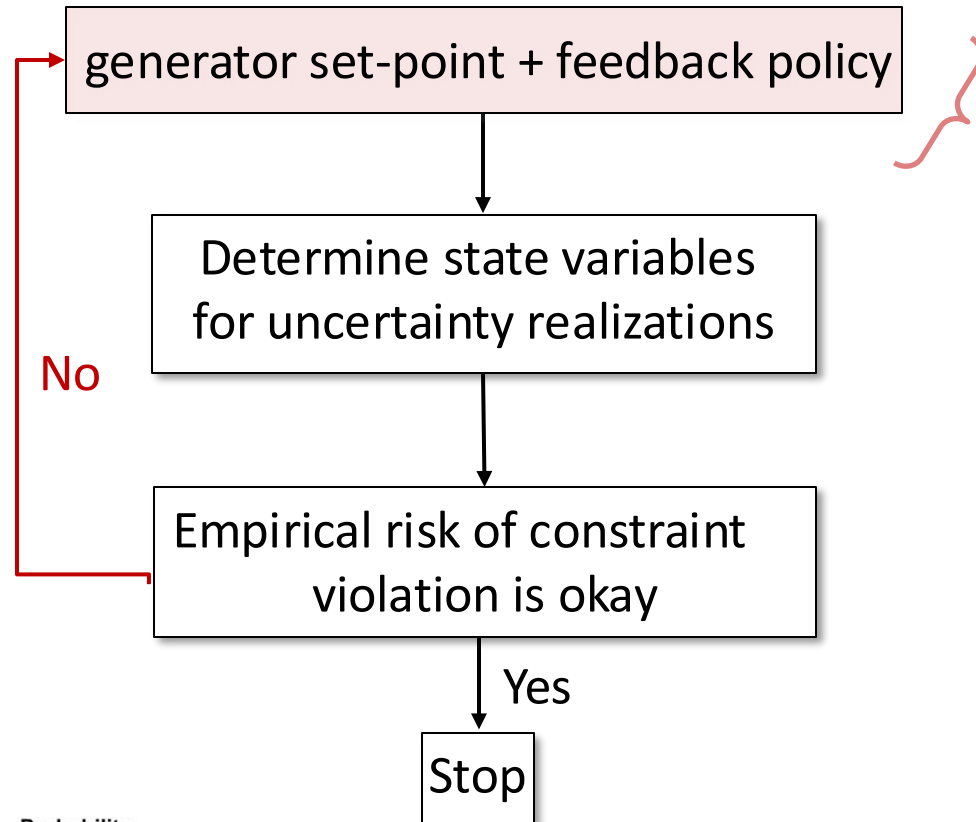
Work-Flow for reliable grid decisions

Every 5- 15 mins:



Improvements in the Work-Flow

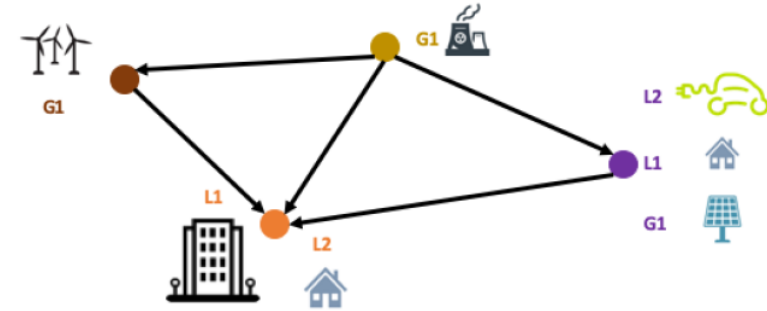
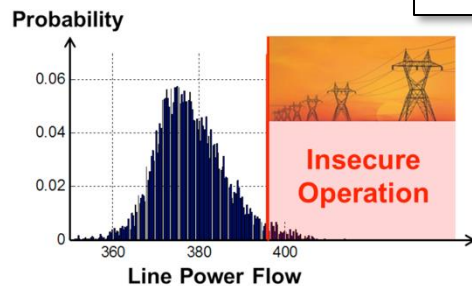
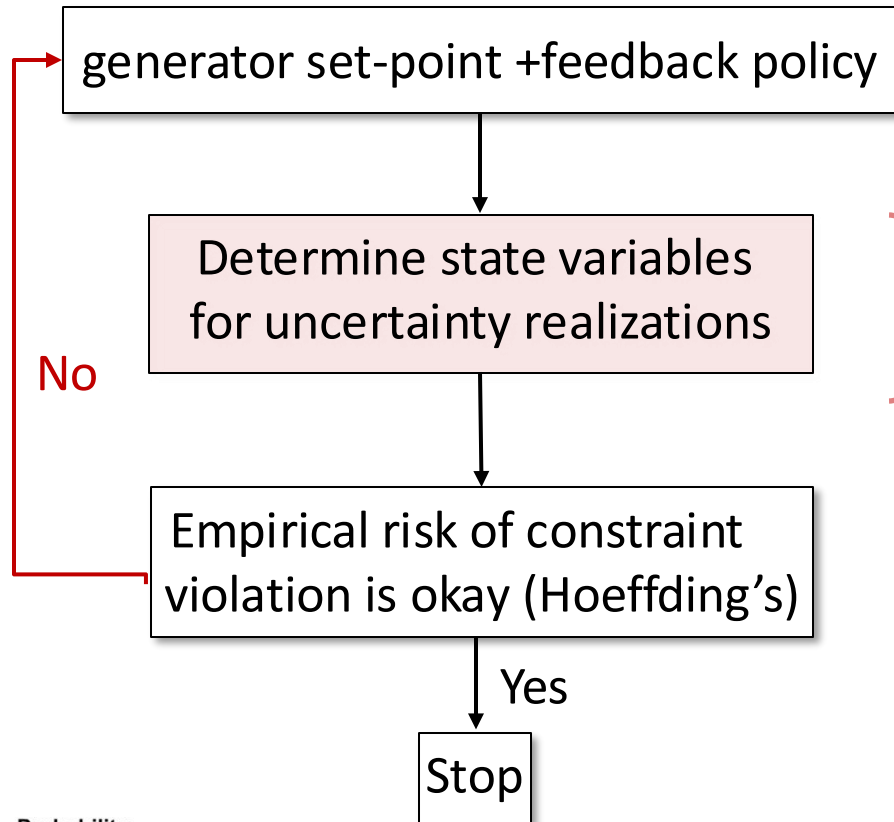
Every 5- 15 mins:



- Optimization with Hard non-convex/ non-linear constraints
- Needs to be solved fast
- Limited training data if system changes

Improvements in the Work-Flow

Every 5- 15 mins:



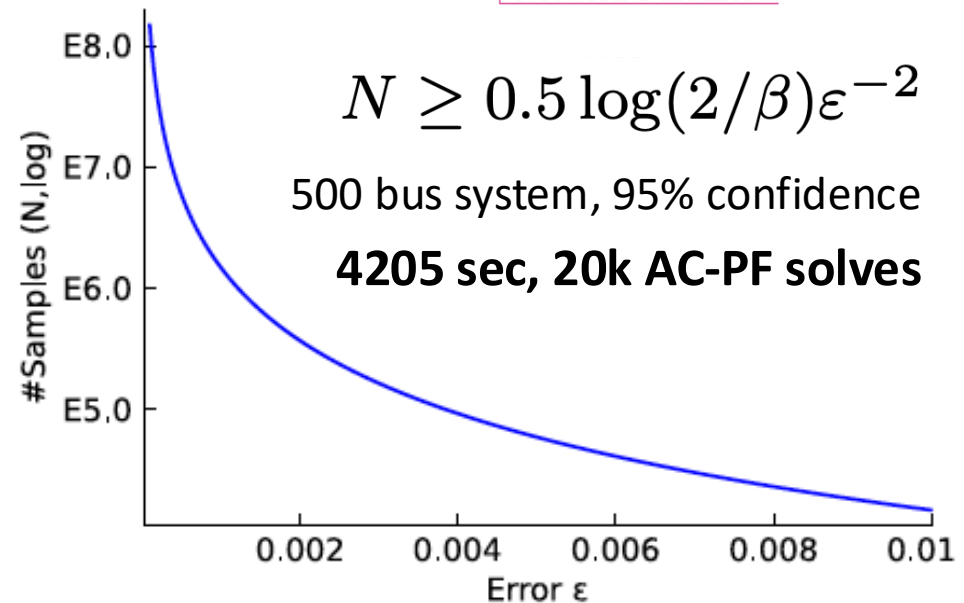
- VOLTAGE is **implicit, non-linear** function of Injection

$$S_i = \sum_{j \in \mathcal{N}} Y_{ij}^{\dagger} (v_i v_i^{\dagger} - v_i v_j^{\dagger})$$

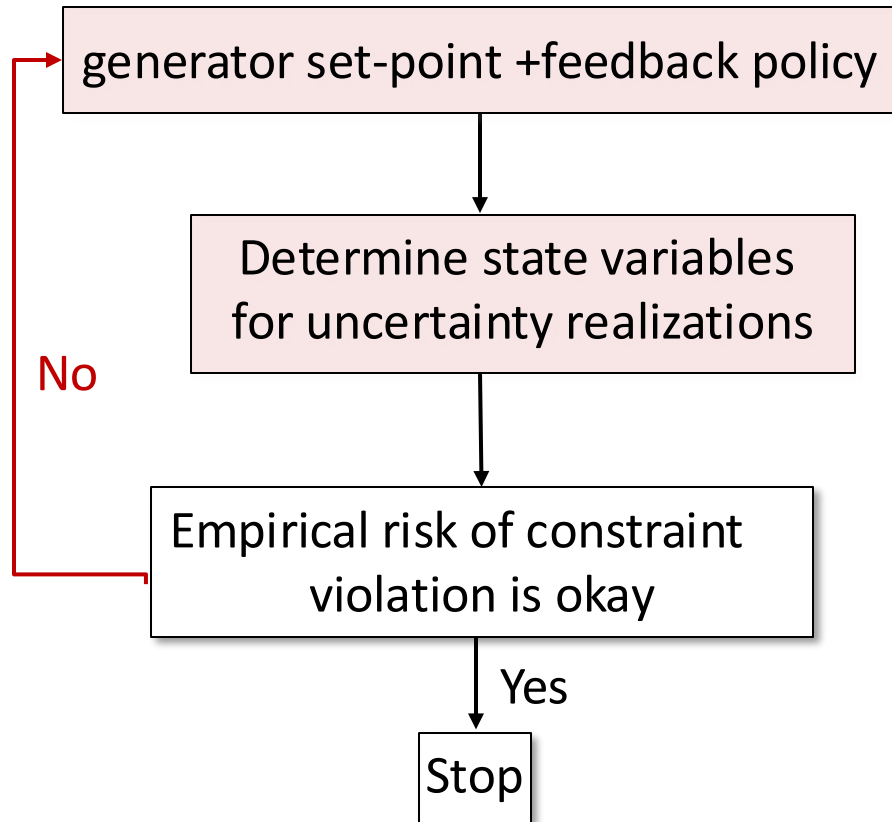
Net Power Injection (red arrow pointing to S_i)

Complex Voltage (blue arrow pointing to $v_i v_i^{\dagger}$)

Network Parameter (pink arrow pointing to Y_{ij}^{\dagger})



Every 5- 15 mins:



Research Question:

a. Can we design ML optimization models that use limited data for solutions with confidence?

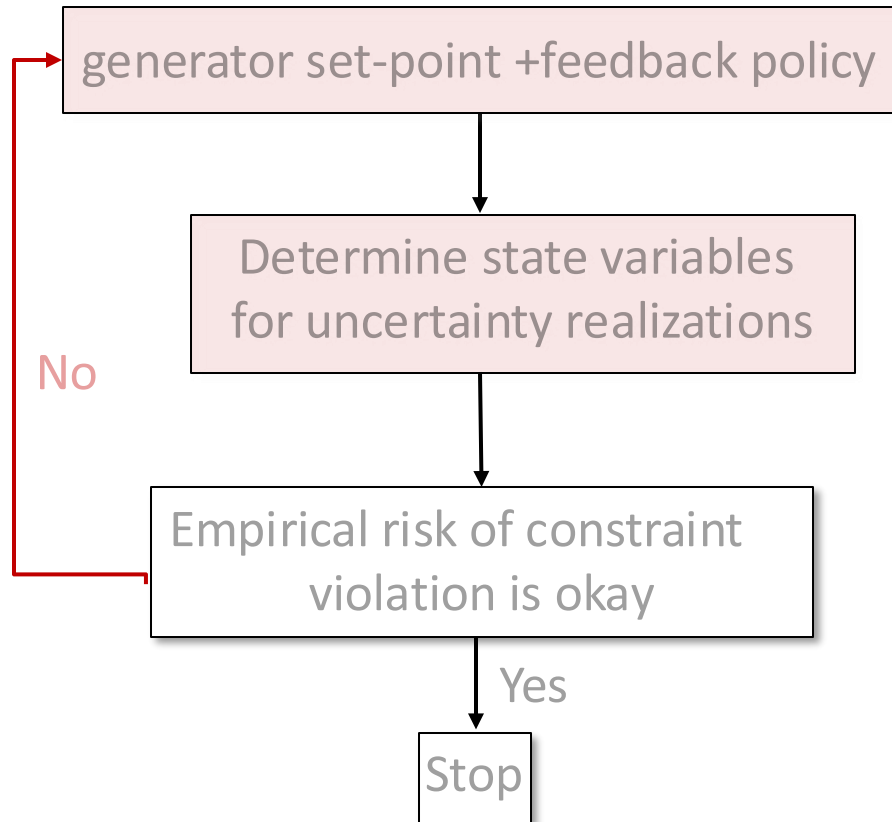
b. Can we design injection $S \rightarrow$ voltage V map for faster risk assessment using limited data?

Solution: **Bayesian** machine learning

a. Semi-supervised Bayesian Neural network for OPF

b. Network-aware Gaussian Process for voltage maps

Every 5- 15 mins:



Parameters: w , input: x , output: y

Research Question:

a. Can we design ML optimization models that use limited data for solutions with confidence?

b. Can we design injection $S \rightarrow$ voltage V map for faster risk assessment using limited data?

Solution: **Bayesian** machine learning

a. Semi-supervised Bayesian Neural network for OPF

b. Network-aware Gaussian Process for voltage

maps Evaluate Posterior of parameters given prior and data

$$p(w|\mathbf{x}, \mathbf{y}) \propto p(\mathbf{y}|\mathbf{x}, w) p(w)$$

- Estimate Posterior prediction of output for new input

$$p(\mathbf{y}^t|\mathbf{x}^t, \mathcal{D}) = \mathbb{E}_{p(w|\mathcal{D})}[p(f_w(\mathbf{x}^t))]$$

b. Can we design a data-driven input-output (injection $S \rightarrow$ voltage V) map?

$$S_i = \sum_{j \in \mathcal{N}} Y_{ij}^\dagger (v_i v_i^\dagger - v_i v_j^\dagger)$$

Diagram illustrating the equation with annotations:

- Net Power Injection** (red text) points to S_i .
- Complex Voltage** (teal text) points to $v_i v_j^\dagger$.
- Network Parameter** (pink text) points to Y_{ij}^\dagger .

Properties of a **'good'** approximator:

- Explicit $S \rightarrow V$
- Easy to Evaluate, Differentiable
- Interpretable in terms of network structure
- Re-trainable/ transferable

Gaussian Process Regression for injection $S \rightarrow$ voltage V

$$S_i = \sum_{j \in \mathcal{N}} Y_{ij}^\dagger (v_i v_i^\dagger - v_i v_j^\dagger)$$

Net Power Injection (red arrow pointing to S_i)
Complex Voltage (blue arrow pointing to $v_i v_j^\dagger$)
Network Parameter (pink arrow pointing to Y_{ij}^\dagger)

Properties of a 'good' approximator:

- Explicit $S \rightarrow V$
- Easy to Evaluate, Differentiable
- Interpretable in terms of network structure
- Re-trainable/ transferable

- Non-parametric model for V as function of injection s

$$\hat{V} = f(s) + \epsilon$$
$$f(s^i) \sim \mathcal{GP}(0, k(s^i, s^j))$$

Zero Mean (red arrow pointing to 0)
Kernel Function (blue arrow pointing to $k(s^i, s^j)$)

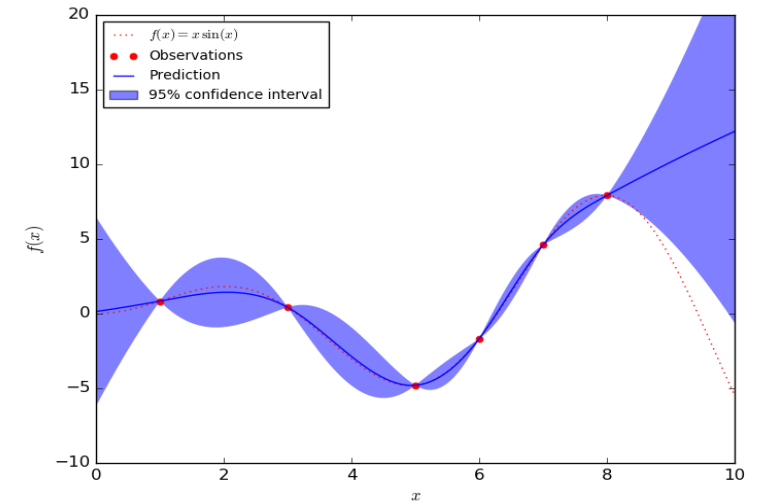
$$k(s^i, s^j) = \tau^2 \exp \left\{ \frac{-\|s^i - s^j\|^2}{2\ell^2} \right\}$$

Squared Exponential Kernel

Gaussian Process Regression for injection $S \rightarrow$ voltage V

$$S_i = \sum_{j \in \mathcal{N}} Y_{ij}^\dagger (v_i v_i^\dagger - v_i v_j^\dagger)$$

Net Power Injection \rightarrow S_i
Complex Voltage \rightarrow $v_i v_i^\dagger$
Network Parameter \rightarrow Y_{ij}^\dagger



- Non-parametric model for V as function of S

$$\hat{V} = f(\mathbf{s}) + \epsilon$$

$$f(\mathbf{s}^i) \sim \mathcal{GP}(0, k(\mathbf{s}^i, \mathbf{s}^j))$$

Zero Mean \rightarrow 0
Kernel Function \rightarrow $k(\mathbf{s}^i, \mathbf{s}^j)$

$$k(\mathbf{s}^i, \mathbf{s}^j) = \tau^2 \exp \left\{ \frac{-\|\mathbf{s}^i - \mathbf{s}^j\|^2}{2\ell^2} \right\}$$

Squared Exponential Kernel

- Learn the Kernel parameters using Maximum Likelihood on training data

$$S = [\mathbf{s}^1 \dots \mathbf{s}^i \dots \mathbf{s}^N] \quad \hat{\mathbf{V}}_j = [V_j^1 \dots V_j^N]$$

- Prediction for new injection sample

Mean : $\mathbb{E}[f(\mathbf{s})] = V_j(\mathbf{s}) = \mathbf{k}^T [K + \sigma_\epsilon^2 I]^{-1} \hat{\mathbf{V}}_j$
Variance : $\sigma^2[f(\mathbf{s})] = k(\mathbf{s}, \mathbf{s}) - \mathbf{k}^T [K + \sigma_\epsilon^2 I]^{-1} \mathbf{k}$

Network scale (Full) Gaussian Process is slow

- Prediction

$$\hat{V} = f(\mathbf{s}) + \epsilon$$

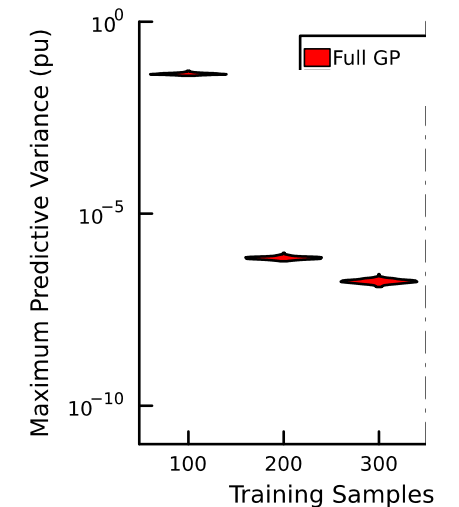
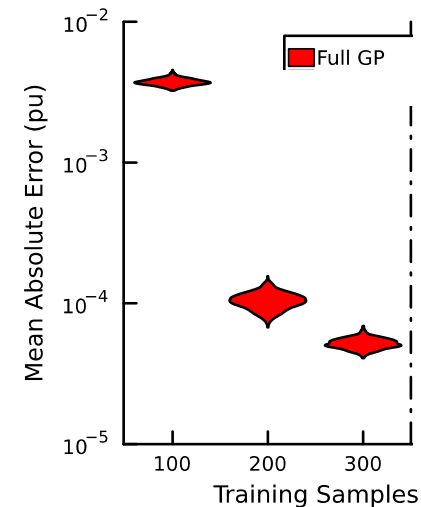
$$\text{Mean : } \mathbb{E}[f(\mathbf{s})] = V_j(\mathbf{s}) = \mathbf{k}^T [K + \sigma_\epsilon^2 I]^{-1} \hat{V}_j$$

$$\text{Variance : } \sigma^2[f(\mathbf{s})] = k(\mathbf{s}, \mathbf{s}) - \mathbf{k}^T [K + \sigma_\epsilon^2 I]^{-1} \mathbf{k}$$

- No network dependence
- Scales as $O(N^3)$ with samples
- **Can we improve further?**

Squared Exponential Kernel

$$k(\mathbf{s}^i, \mathbf{s}^j) = \tau^2 \exp \left\{ \frac{-\|\mathbf{s}^i - \mathbf{s}^j\|^2}{2\ell^2} \right\}$$



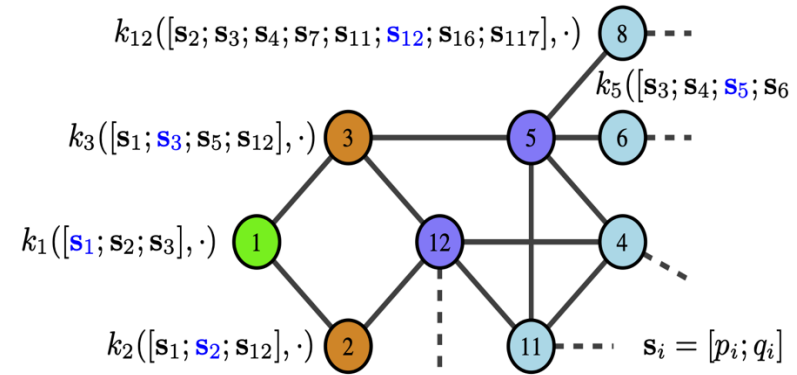
500 random trials for 500-node network
Testing 1000 out-of-sample data points.

Vertex-Degree Kernel (VDK) GP

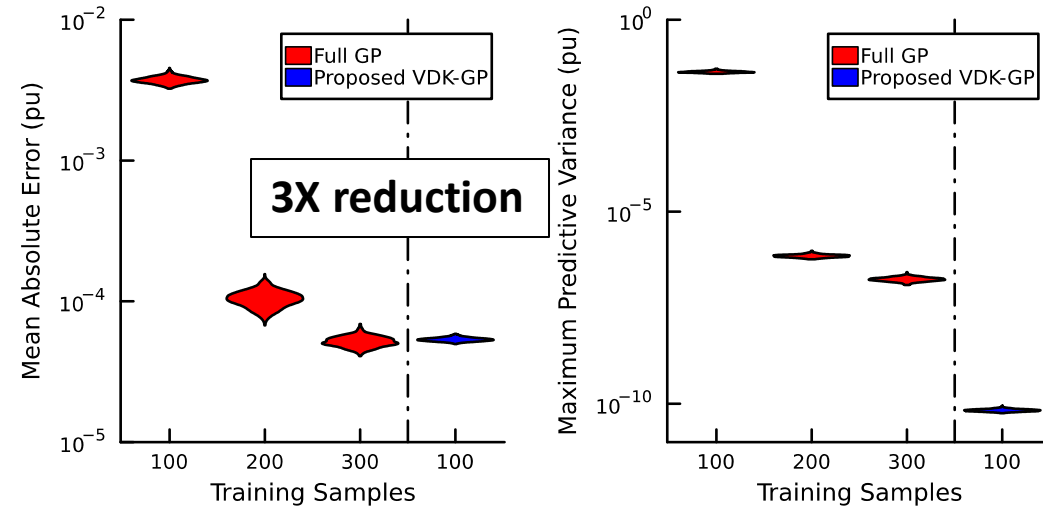
- Additive Kernels over node-neighborhoods

$$k_v(\mathbf{s}^i, \mathbf{s}^j) = \sum_{b=1}^{|\mathcal{B}|} k_b(\mathbf{x}_b^i, \mathbf{x}_b^j)$$

- Why?
 - Neighboring injections have correlated effect on voltage
 - Effect of far away injections is approximately independent
- Dimension Reduction
 - Effective input dimension is max. vertex degree



Idea of Vertex Degree Kernel (VDK)



500 random trials for 500-node network
Testing 1000 out-of-sample data points.

VDK-GP with Active Learning (AL) for further gains!

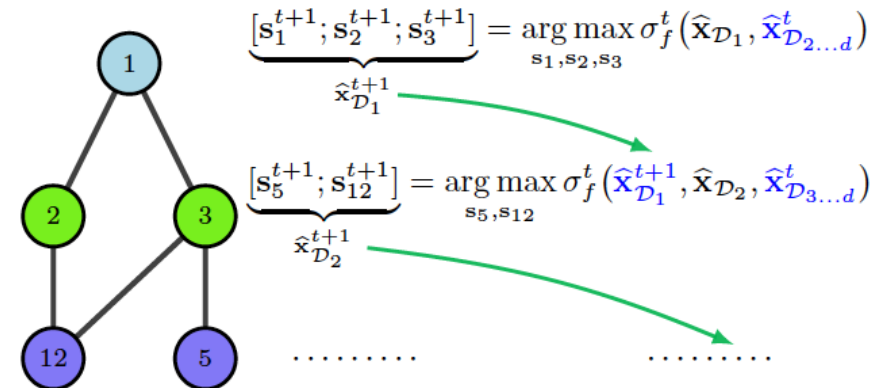
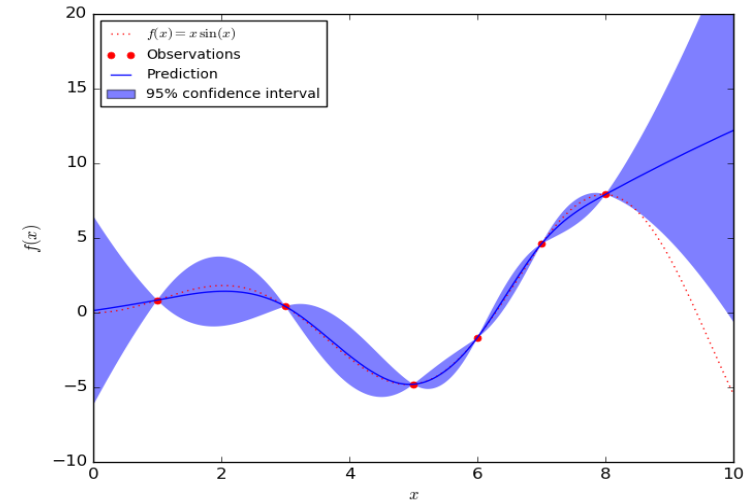
- Select training samples iteratively to maximize information gain/variance

$$s^{t+1} = \arg \max_{s \in \mathcal{L}} [\sigma_f^t(s)]^2$$

- Hard:
 - Finding maximum variance point for large-dimensional input, non-trivial

- Network-swipe Active Learning (soln)

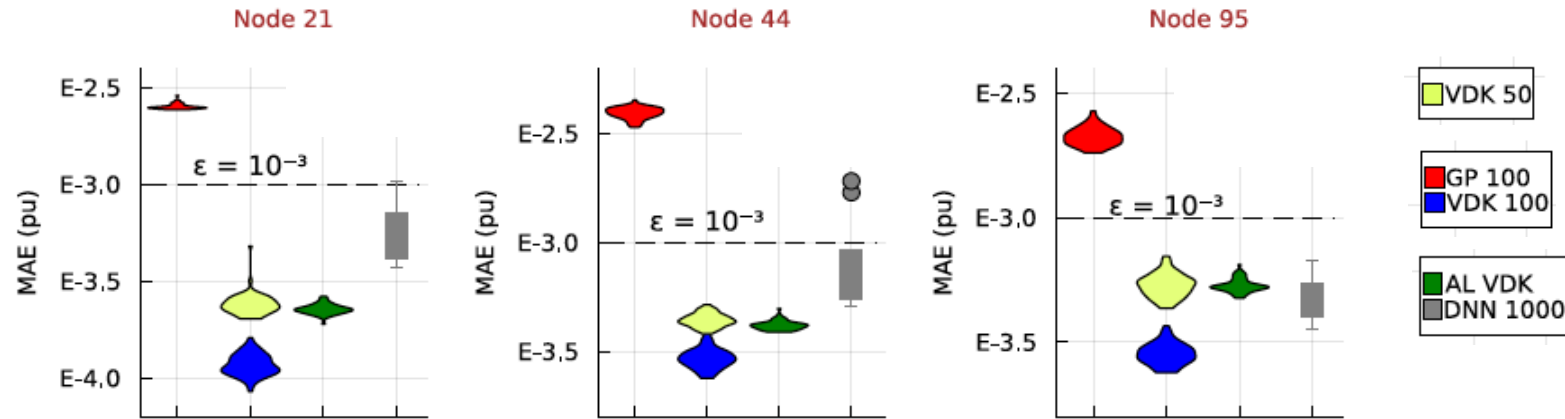
- Leverage VDK-GP's structure for maximizing iteratively over graph hops
- After a few hops, no Kernel overlap between nodes (can be parallelized)
- Low-dimensional sub-kernels: numerical optimization works fine



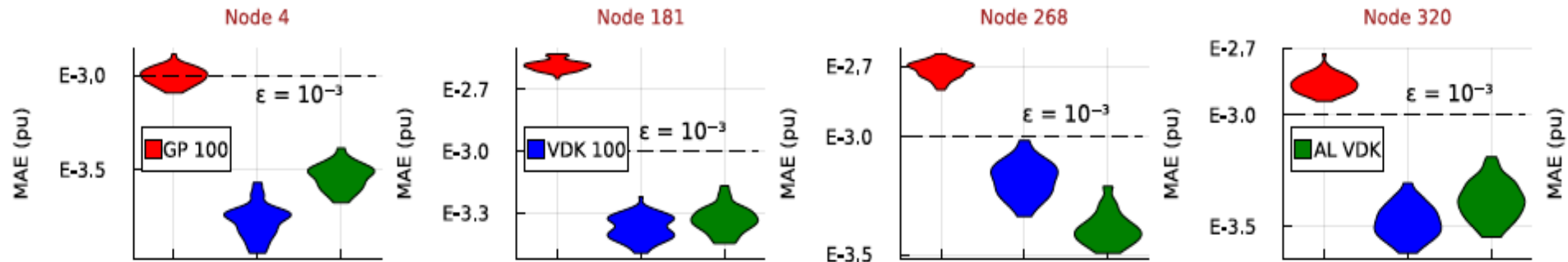
Idea of Network-Swipe Active Learning

Performance in estimating voltage in test networks

- Sample needed: GP >> VDK-GP >> AL VDK-GP (GP much better than DNN)

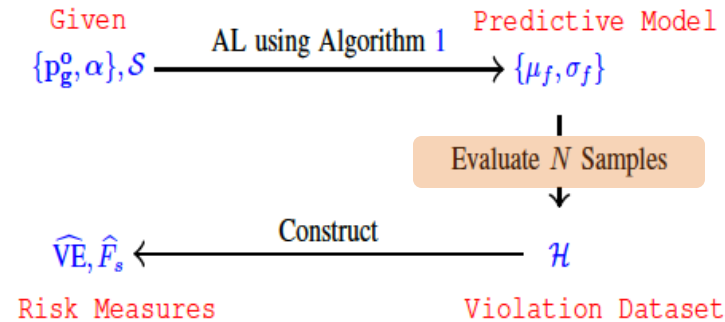


118-Bus system with 1000 out of sample data points. AL requires ~45 samples



500-Bus system with 1000 out of sample data points. AL requires ~70 samples

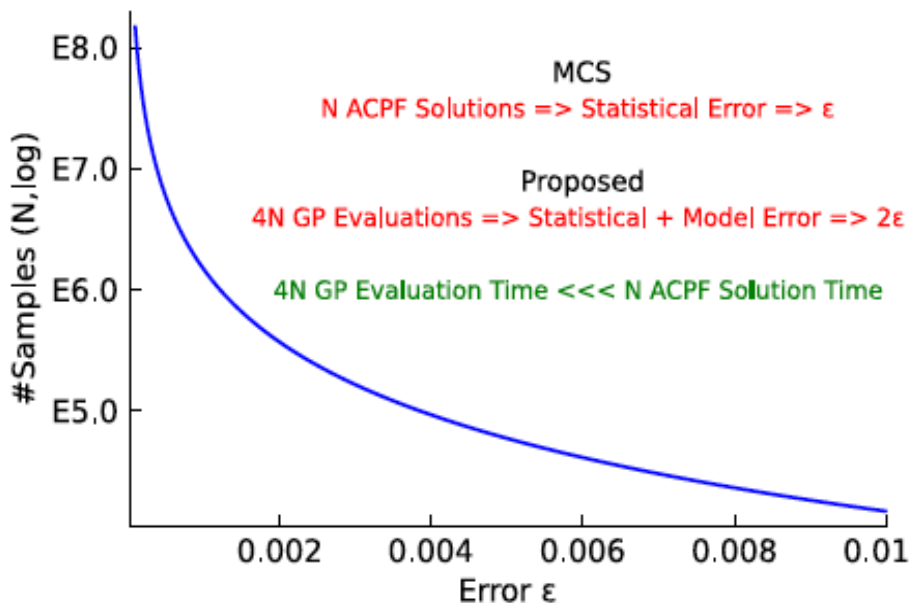
Violation Estimate (VE) using VDK-GP samples:



Theorem 1. Expected Value Estimation Error Bound: Given that voltage values, for any two arbitrary load vectors, are jointly Gaussian. Then, $\mathbb{P}\{|V(\mathbf{s}) - \widehat{V}(\mathbf{s})| \geq \varepsilon_m\} \leq \delta(\kappa)$ where $\widehat{V}(\mathbf{s}) = \mu_f(\mathbf{s}^i) \pm \kappa\sigma_f(\mathbf{s})$ for any $\varepsilon_m > 0$. And with $h(\cdot)$ being Sigmoid function, error in VE using GP is probabilistically bounded as

$$\mathbb{P}\left\{|VE - \widehat{VE}| < \varepsilon_m(1 - \delta(\kappa)) + M\delta(\kappa) + \varepsilon_h\right\} \geq 1 - \beta$$

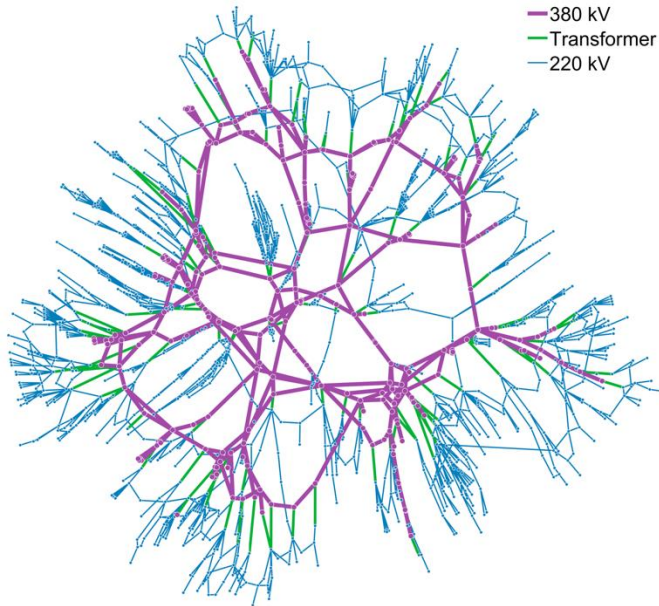
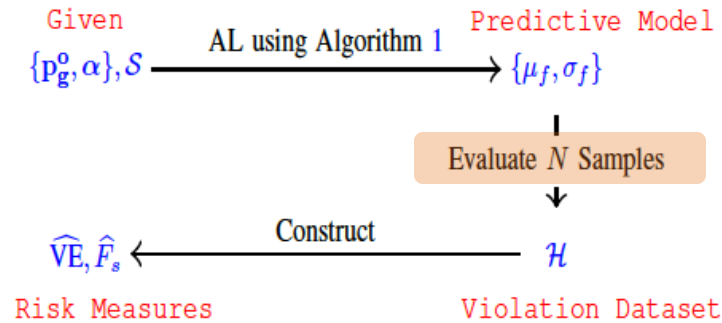
where, $\beta \in (0, 1)$, $\varepsilon_h = \sqrt{\frac{\log(2/\beta)}{2N}}$, M is a large value such that $M > |h_p(\mathbf{s}) - h_m(\mathbf{s})|$, and N is number of samples.



500 bus system, 95% confidence
 20k AC-PF solves == 4205 sec
 80k GP evaluations == 33.2 sec

(120x speedup), easily within grid operator limits

Violation Estimate (VE) using VDK-GP samples:



	Samples	Time(s)	\widehat{VE}	$\Delta VE \times 10^{-4}$
4	67 - 70	28 - 30	-0.0018	7.8 ± 0.5
181	71 - 76	30 - 33	-0.0032	8.0 ± 0.2
268	102 - 109	53 - 58	+0.0008	7.9 ± 0.2
320	72 - 76	30 - 33	+0.0013	7.8 ± 0.4
321	70 - 77	30 - 33	+0.0021	6.8 ± 0.5
-	Mean evaluation time for 80100 samples is ≈ 33.2 sec			
-	NRLF running time for 20025 samples is ≈ 4205 sec			

ΔVE : Difference in risk estimation using NRLF and AL-VDK
 \widehat{VE} is the mean across the 50 AL-VDK trials

500 node grid: 90 sec v/s 4200 sec (**45x speedup**)

	Samples	Time(s)	\widehat{VE}	$\Delta VE \times 10^{-4}$
183	77 - 81	159 - 168	+0.0010	8.0 ± 0.5
287	77 - 81	154 - 164	+0.0009	8.2 ± 0.2
-	Mean evaluation time for 8010 samples is ≈ 29.8 sec			
-	NRLF running time for 2025 samples is ≈ 3879 sec			

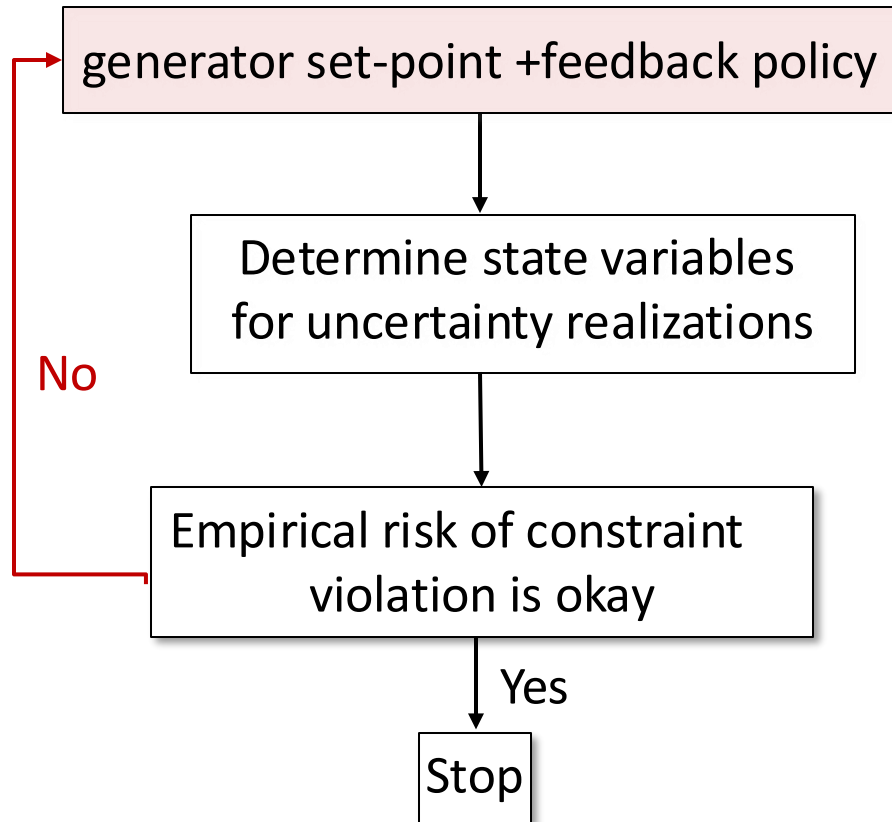
ΔVE : Difference in risk estimation using NRLF and AL-VDK
 \widehat{VE} is the mean across the 10 AL-VDK trials

1354 node grid: 200 sec v/s 3870 sec (**20x speedup**)

[1] P Pareek, D Deka, S Misra, Fast Risk Assessment in Power Grids through Novel Gaussian Process and Active Learning, arXiv preprint arXiv:2308.07867.

[2] P. Pareek, D. Deka, S. Misra, Data-Efficient Power Flow Learning for Network Contingencies. arXiv preprint arXiv:2310.00763.

Every 5- 15 mins:



Research Question:

a. Can we design ML optimization models that use limited data for solutions with confidence?

b. Can we design injection $S \rightarrow$ voltage V map for faster risk assessment using limited data?

Solution: **Bayesian** machine learning

a. Semi-supervised Bayesian Neural network for OPF

b. Network-aware Gaussian Process for voltage maps

ML proxy for OPF with *limited* training data

- Need optimal solution and constraint feasibility
- Standard ML proxies give point estimates for an input

$$\begin{aligned} \min \quad & \sum_{g \in \mathcal{G}} c(p_g) \\ \text{s.t.} \quad & \sum_{g \in \mathcal{G}_i} p_g - P_i = \sum_{j \in \mathcal{B}} v_i v_j (G_{ij} \cos(\theta_i - \theta_j) + B_{ij} \sin(\theta_i - \theta_j)) \quad \forall i \in \mathcal{B} \\ & \sum_{g \in \mathcal{G}_i} q_g - Q_i = \sum_{j \in \mathcal{B}} v_i v_j (G_{ij} \sin(\theta_i - \theta_j) - B_{ij} \cos(\theta_i - \theta_j)) \quad \forall i \in \mathcal{B} \\ & (p, q, v, \theta) \in \mathcal{T} \end{aligned}$$

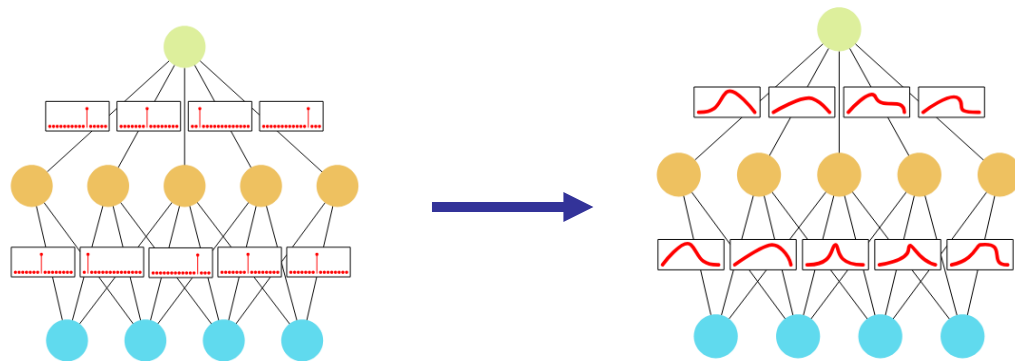
ML proxy for OPF with *limited* training data

- Need optimal solution and constraint feasibility
- Standard ML proxies give point estimates for an input

$$\begin{aligned} & \min_{\mathbf{y}} c(\mathbf{y}) \\ \text{s.t. } & g(\mathbf{x}, \mathbf{y}) = 0; h(\mathbf{x}, \mathbf{y}) \leq 0 \end{aligned}$$

- Goals:
 - ✓ **Probabilistic solution with estimated confidence/variance**
 - Overcome limited labeled data (for feasibility)

- Bayesian Neural Network (BNN) for OPF Proxy:



- Static weights
- Maximum Likelihood (MLE)
- Random weights (prior/posterior)
- Maximum A posteriori (MAP)

Labeled training data

$$p(\mathbf{y}|\mathbf{x}, w) = \prod_i \mathcal{N}(\mathbf{y}_i | f_w(\mathbf{x}_i), \sigma_s^2)$$
$$p(w|\mathbf{x}, \mathbf{y}) \propto p(\mathbf{y}|\mathbf{x}, w) p(w)$$

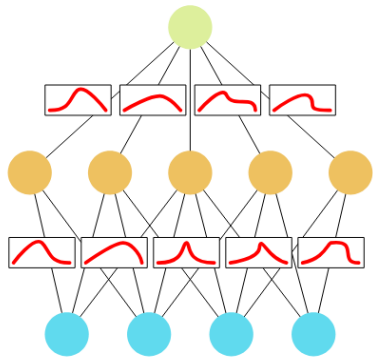
Solved using variational inference (VI)

ML proxy for OPF with *limited* training data

- Need optimal solution and constraint feasibility
- Standard ML proxies give point estimates for an input
- Goals:
 - ✓ Probabilistic solution with estimated confidence/variance
 - ✓ **Overcome limited labeled data (for feasibility)**

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- Bayesian Neural Network (BNN) for OPF Proxy:



Labeled training data

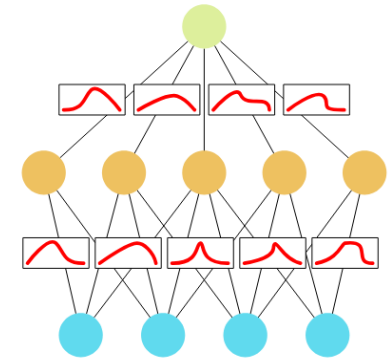
$$\begin{aligned} p(w|\mathbf{x}, \mathbf{y}) & \propto p(\mathbf{y}|\mathbf{x}, w) p(w) \\ p(\mathbf{y}|\mathbf{x}, w) & = \prod_i \mathcal{N}(\mathbf{y}_i | f_w(\mathbf{x}_i), \sigma_s^2) \end{aligned}$$

- Random weights (prior/posterior)
- Maximum A posteriori (MAP)

Feasibility Enhancement
(unlabeled data, true value is 0)

$$\begin{aligned} \mathcal{L}(\mathbf{y}, \mathbf{x}) & = \underbrace{\|g(\mathbf{x}, \mathbf{y})\|^2}_{\text{Equality Gap}} + \underbrace{\|\text{ReLU}[h(\mathbf{x}, \mathbf{y})]\|^2}_{\text{Inequality Gap}} \\ p(\mathcal{L}|\mathbf{x}, w) & = \prod_j \mathcal{N}(0 | \mathcal{L}(f_w(\mathbf{x}_j), \mathbf{x}_j), \sigma_u^2) \end{aligned}$$

Bayesian Neural Network (BNN) for OPF Proxy



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

Labeled loss \swarrow

\swarrow Unlabeled loss

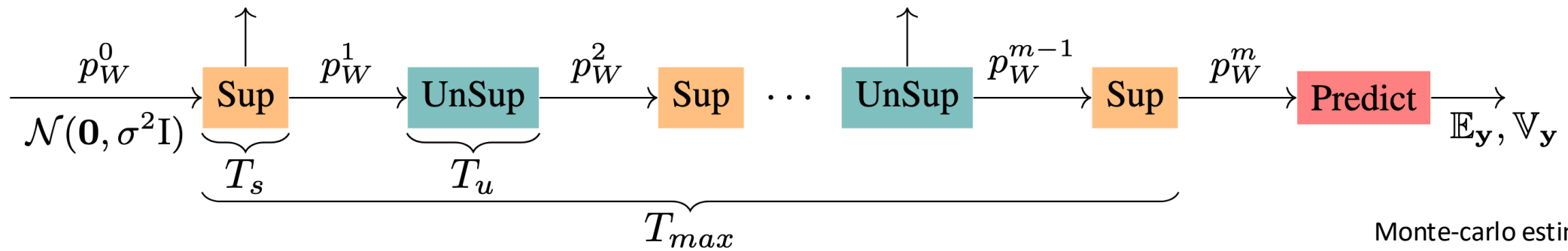
$$p(\mathbf{y}|\mathbf{x}, w) = \prod_i \mathcal{N}(\mathbf{y}_i | f_w(\mathbf{x}_i), \sigma_s^2)$$

$$p(\mathcal{L}|\mathbf{x}, w) = \prod_j \mathcal{N}(0 | \mathcal{L}(f_w(\mathbf{x}_j), \mathbf{x}_j), \sigma_u^2)$$

- Semi-supervised Sandwiched training (optimality and feasibility):

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

$$p_W^{m-1} \equiv p(w | \mathbf{x}) \propto p(\mathcal{L} | \mathbf{x}, w) p_w^{m-2}$$

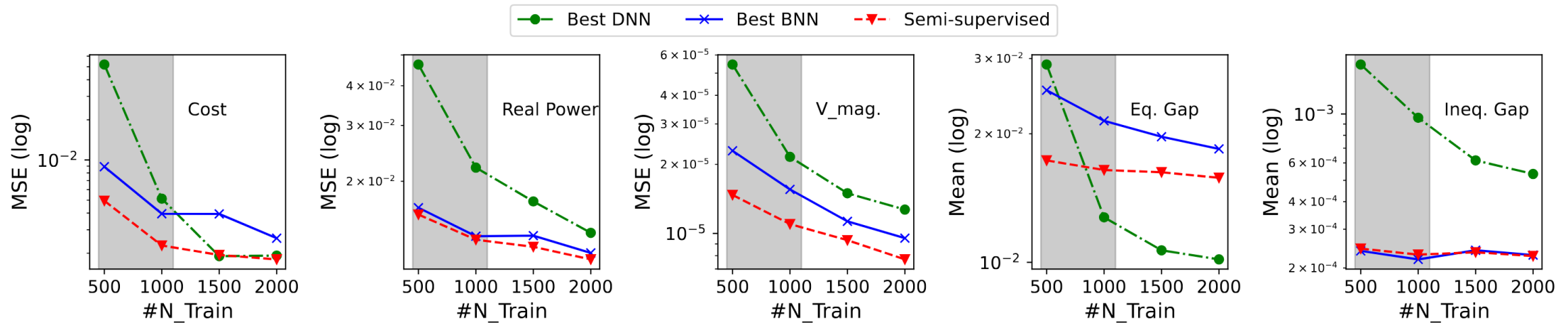
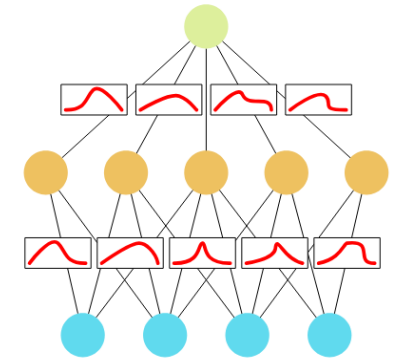


Monte-carlo estimator via sampling

Bayesian Neural Network (BNN) for OPF Proxy

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

- Preliminary results for 57 bus system:
 - Outperforms DNN at low labelled samples and low training time

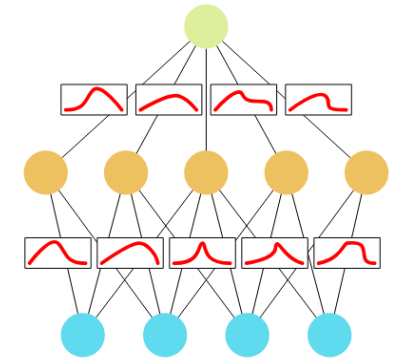


1000 sec total training, 20k unsupervised samples, BNN on Numpyro, DNN on Pytorch

Bayesian Neural Network (BNN) for OPF Proxy

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

- Preliminary results for 57 bus system:
 - Outperforms DNN at low labelled samples and low training time



Method	Correction	Obj. Gap	Mean Eq.	Mean Ineq.	Testing Time (s)
Proposed	No	0.02 (0.00)	0.01 (0.00)	0.00(0.00)	0.003 (0.000)
BNN	No	0.04 (0.00)	0.02 (0.00)	0.00 (0.00)	0.003 (0.000)
DC3 [3]	Yes	0.01 (0.00)	0.00 (0.00)	0.00 (0.00)	0.089 (0.000)
DC3, no soft loss [3]	Yes	0.70 (0.05)	0.07 (0.00)	0.03 (0.01)	0.088 (0.000)
Eq. NN [21]	Yes	0.00 (0.00)	0.00 (0.00)	0.00 (0.00)	0.039 (0.000)

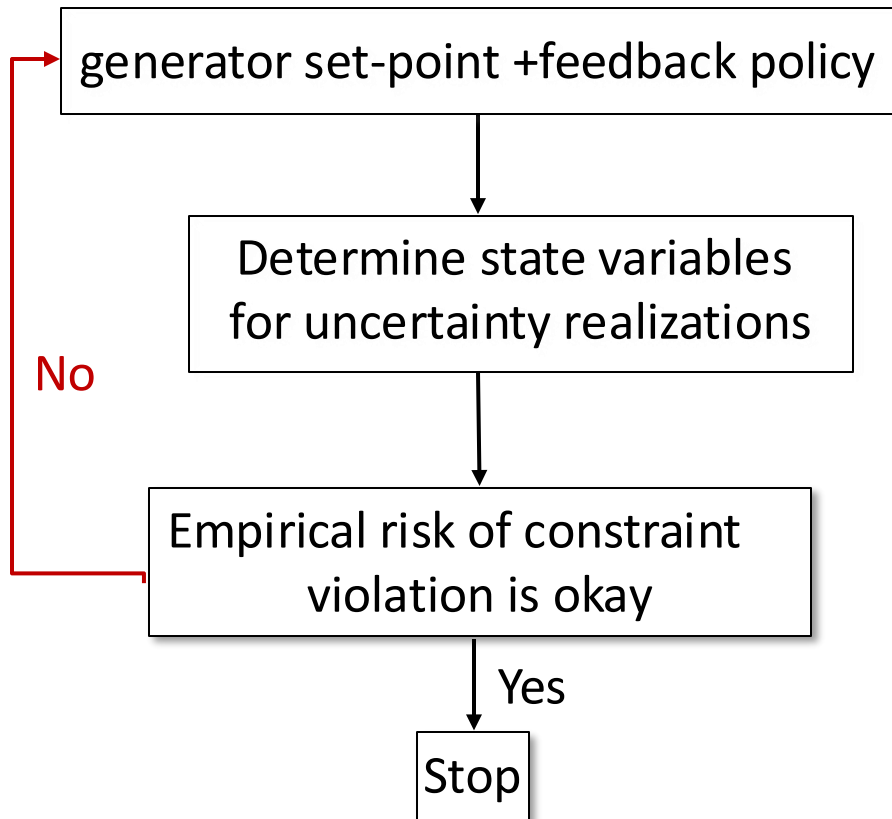
100 test instances for 57-Bus, 1000 labeled samples, 1000 sec for training, no projection in BNN

[3] P. Donti, D. Rolnick, and J. Z. Kolter. Dc3: A learning method for optimization with hard constraints. In International Conference on Learning Representations, 2021.

[21] A. S. Zamzam and K. Baker. Learning optimal solutions for extremely fast ac optimal power flow. In *2020 IEEE international conference on communications, control, and computing technologies for smart grids (SmartGridComm)*, pages 1–6. IEEE, 2020.

Next Steps:

Every 5- 15 mins:



- a. Bayesian Neural networks for OPF
 - More testing
 - Use of confidence in follow up applications

- b. Network-aware GP for voltage modeling
 - Use in distribution grids (limited data)
 - N-k applications

❖ Use BNN OPF confidence values to guide Monte Carlo or GP based validation of bounds (better than Hoeffding)

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[1] P Pareek, D Deka, S Misra, Graph-Structured Kernel Design for Power Flow Learning using Gaussian Processes, arXiv preprint arXiv:2308.07867.

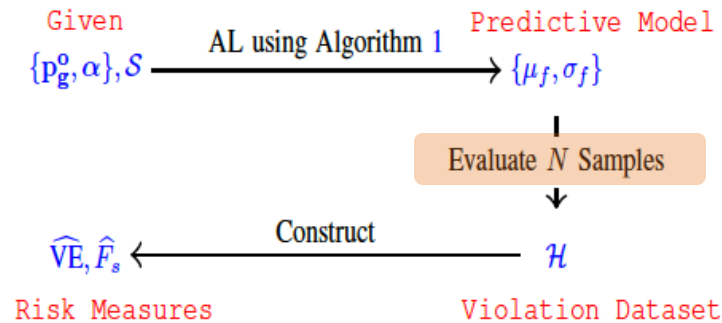
[2] P. Pareek, D. Deka, S. Misra, Data-Efficient Power Flow Learning for Network Contingencies. arXiv preprint arXiv:2310.00763.

Support from:



Thank You. *Questions!*

Violation Estimate (VE) using VDK-GP samples:



	Samples	Time(s)	\widehat{VE}	$\Delta VE \times 10^{-4}$
4	67 - 70	28 - 30	-0.0018	7.8 ± 0.5
181	71 - 76	30 - 33	-0.0032	8.0 ± 0.2
268	102 - 109	53 - 58	+0.0008	7.9 ± 0.2
320	72 - 76	30 - 33	+0.0013	7.8 ± 0.4
321	70 - 77	30 - 33	+0.0021	6.8 ± 0.5
-	Mean evaluation time for 80100 samples is ≈ 33.2 sec			
-	NRLF running time for 20025 samples is ≈ 4205 sec			

ΔVE : Difference in risk estimation using NRLF and AL-VDK
 \widehat{VE} is the mean across the 50 AL-VDK trials

Theorem 2. *The GP-based predictive model overestimates probability of voltage violation i.e.*

$$\mathbb{P}\{h(\mathbf{s}) > 0\} \geq \widehat{\mathbb{P}}\{h_m(\mathbf{s}) > 0\} \text{ for } \mathbf{s} \in S.$$

