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System 2 Applied Mathematics: Machine Learning for Power Market Clearing

Misha Chertkov Applied Math @ UArizona

May 23, 2022 - DANniversary, MIP2022, Rutgers





 "Uncertainty"2010 (theory+experiment)

SIAM REVEN

Chance-Constrained Optimal Power Flow: Risk-Aware Network Control under Uncertainty*

> Daniel Bienstock[†] Michael Chertkov[‡] Sean Harnett[§]

 "System 1 Learning"/2018 (experiment)

> Learning from power system data stream: phasor-detective approach

Mauro Escober, Daniel Bienstock? & Michael Chertkov† "Columbia University, NY, USA [Los Alamos National Laboratory, NM, USA & Skoltech, Moseow, Russin

 "System 2 Learning"/2022 (experiment+ opportunity for theory)

> ACCEPTED FOR PRESENTATION IN 11TH BULK POWER SYSTEMS DYNAMICS AND CONTROL SYMPOSIUM (IREP 2022), JULY 25-30, 2022, BANFF, CANADA

Machine Learning for Electricity Market Clearing

Laurent Pagnier *, Rebert Fernande *, Yung Drevini *, Daniel Biensteck + and Michael Cardow * Neurona Neurophie Matematics. Utivenity & Artonas. Theore. At USA Cardow * [harrentpagnier/firmanda.cardowley]@math.aitematics * Eachtrisia and Compate Engineering. New York (Nrivenity, New York, NY, USA diversitier Brucher * Indentral Engineering and Queenties Research, Calambia Utiversity, New York, NY

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System 2 Applied Mathematics

Modern Applied Mathematics as System 2 Physics Informed AI/ML



System 1 & 2 in DL and AI

- "From System 1 Deep Learning to System 2 Deep Learning" – Yoshua Bengio, NeurIPS 2019
- "Combining Fast and Slow Thinking for Human-like and Efficient Navigation in Constrained Environments" – M. Ganappini, et al, arXiv:2201.07050

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Modern ('21) Applied Mathematics as System 2 ... Harvesting 20's Applied Math + (System 1.8) Data & Model Revolution (System 1)

- System 1 operates automatically & quickly [Deep Learning, empowered by Automatic Differentiation]
- System 2 allocates attention to effortfull mental activities [Building **Explainable Heuristics in Quantitative Sciences**]

Modern Applied Mathematics as System 2 Physics Informed AI/ML

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Applied Math '21 = Harvesting Data and Model Revolution

- Applied Math '21 = Traditional AM + Contemporary AM
- Traditional Applied Math
 - Natural Science Based (motivated by Physics, later Biology, Enviromental Sciences, etc ...)
 - Originally largely ODE, PDE, Dynamical Systems, Chaos, Turbulence, ...
- Contemporary AM
 - More applications, e.g. Engineering, Social sciences, Networks
 - Al disciplines: Statistics, Data Science, Computer Science, Machine Learning, Optimization, Control
 - Deep Learning most prominent recent addition (automatic differentiation, very efficient large scale optimization) ... based a lot on "old" stuff (stochastic gradient descent, sensitivity analysis)

Modern Applied Mathematics as System 2 Physics Informed AI/ML

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Physics Informed Machine Learning: Principal Ideas (active discussions)

- A-Priori: run a (physics-blind) ML scheme, check physics
 - Diagnostics: hierarchy of tests
- A-Posteriori: embed physics in ML
 - Loss Function
 - Graphical Model (structure=explainable) Learning
 - What we know (structure) vs what we do NOT know (NN)
- Model Reduction
 - Check Hypotheses, Phenomenologies (e.g. forgotten)
- Derive New/Old Physical Laws

Outline

Introduction: Scientific AI & ML ⊂ Applied Math

- Modern Applied Mathematics as System 2
- Physics Informed AI/ML
- System 1 & System 2 ML for Power Systems
 - Machine Learning for Power Systems

- PIML for State & Parameter Estimation
- Learning Locational Marginal Prices & Dispatch
 - Formulation and System 2 Idea
 - Validation: Configurations vs Noise vs # Samples
 - Future Work. Theory help is needed.

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Machine Learning for Power Systems PIML for State & Parameter Estimation

Machine Learning for Power Systems PIML for State & Parameter Estimation

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Physics Informed Machine Learning for Power Systems

Machine Learning (e.g. Neural Network, Graph Models, etc)

- will make Power System Computations
 - faster (efficient)
 - possible even when data/measurements incomplete
- requires ground-truth data
 - actual measurements (Phasor Measurement Units, etc)
 - power flow <u>solvers</u> (microscopic simulations) reliable, possibly heavy
- can be power-system <u>"informed"</u> (System 2) vs "agnostic" (System 1)
 - What is System 1 today may become System 2 tomorrow (with proper theory & enough of experiments)
- methods/options are many
 - should be gauged to available data, level of uncertainty, etc

Incomplete Review: Brief, Recent, Biased AI/ML in Power Systems (System 1, System 2 & juxtaposition)

- <u>Structure Learning</u>, <u>Sparse Measurements</u>, <u>Graphical Models</u>, Focus on Power Distribution: Deka, et al [2016-2019]
- <u>Learning ODE</u>: Power Transmission, Dynamic Coefficients in Swing Equations, Deterministic and Stochastic, Lokhov, et al [2017]
- Real-time Faulted Line Localization and PMU Placement in Power Transmission through CNN: Li, et al [2018]
- <u>Collocation Point Neural ODE</u> for Power Systems: Misuris, et al [2018]
- Learning a Generator Model from Terminal Bus Data: many ML schemes, tradeoffs, ranking models according to regimes, Stulov et al [2019]
- Learning from power system <u>data stream</u>, <u>phasor-detective</u> approach, Escobar et al [2019]

Machine Learning for Power Systems PIML for State & Parameter Estimation

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Incomplete Review: Brief, Recent, Biased

AI/ML in Power Systems (System 1, System 2 & juxtaposition)

- Physics-Informed Graphical Neural Network for Parameter & State Estimations in Power Systems https://arxiv.org/abs/2102.06349 (Pagnier & MC))
- Embedding Power Flow into Machine Learning for Parameter and State Estimation https://arxiv.org/abs/2103.14251 (Pagnier & MC)
- Which Neural Network to Choose for Post-Fault Localization, Dynamic State Estimation and Optimal Measurement Placement in Power Systems? https://arxiv.org/abs/2104.03115 (Afonin & MC))

Machine Learning for Power Systems PIML for State & Parameter Estimation

Machine Learning (Neural Networks) Setting

NN models: General	NN models: Loss Functions						
• $NN_{\vec{o}}(\vec{x}) = \vec{y}$	● L2 norm ∥····∥						
• Vector, $\vec{\phi}$, of Not-Interpretable Parameters	 Probabilistic (Cross Entropy or Kullback-Leibler) 						
 Input vector: x Output vector: y Regularizations, e.g. L1 (spars physical, etc) 							
NN models: Architectures							
• Convolutional NN (LeCun 1989	-)						
• Graph NN (Scarcelli. et al 2009	• Graph NN (Scarcelli. et al 2009 –)						
• Neural ODE (Chen et al 2008 –)							
• Collocation Point NN (Lagaris	• Collocation Point NN (Lagaris et al 1998, Raissi et al 2019 –)						
• Hamiltonian NN (Greydanus et	• Hamiltonian NN (Greydanus et al 2018 –)						

Machine Learning for Power Systems PIML for State & Parameter Estimation

Power Flow Equations

- grid-graph, $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
- complex-valued powers: $\forall a \in \mathcal{V}$: $S_a \equiv p_a + iq_a$
- complex-valued (electric) potentials, $\forall a \in \mathcal{V} : V_a \equiv v_a \exp(i\theta_a)$,
- Power Flow (PF) equations:

$$p_{a} = \sum_{b; \{a,b\} \in \mathcal{E}} v_{a}v_{b} \Big[g_{ab} \cos \left(\theta_{a} - \theta_{b}\right) + \beta_{ab} \sin \left(\theta_{a} - \theta_{b}\right) \Big],$$
$$q_{a} = \sum_{b; \{a,b\} \in \mathcal{E}} v_{a}v_{b} \Big[g_{ab} \sin \left(\theta_{a} - \theta_{b}\right) - \beta_{ab} \cos \left(\theta_{a} - \theta_{b}\right) \Big],$$

 Direct PF Map: Π_Y: S ≡ (S_a|a ∈ V) → V ≡ (V_a|a ∈ V) - implicit (need to solve eqs. - System 1 & System 2 ML may be useful https://arxiv.org/abs/2103.14251 L. Pagnier & MC)

Machine Learning for Power Systems PIML for State & Parameter Estimation

Task: State & Parameter Estimation

- Inverse PF Map: $S = \Pi_{Y}^{-1}(V)$ explicit (do not need to solve eqs. System 1 and System 2 ML may be useful https://arxiv.org/abs/2102.06349 L. Pagnier and MC)
- State Estimation
 - Full Observability: given ${\cal G}$ and ${\bm Y}$ to estimate injected/consumed active and reactive powers = application of the inverse PF map, Π^{-1}
 - Limited Observability:
 - Complement Missing power injections/consumptions at the nodes where voltages and phases are measured
 - <u>Challenging Version</u>: to reconstruct injected/consumed powers and also voltages and phases at all nodes of the system. (super-resolution – will not discuss)
- Parameter Estimation
 - Reconstruct Graph, $\mathcal{G}=(\mathcal{V},\mathcal{E}),$ and line characteristics, \boldsymbol{Y}

Machine Learning for Power Systems PIML for State & Parameter Estimation

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Task SE & PE. Reduced Modeling.

- Setting of Partial Observability
- Find Equivalent (Reduced) Model of Power System
- "Inspired" by Kron Reduction

•
$$I^{(o)} = Y^{(r)} V^{(o)}$$

• "o" - observed; "r" - reduced

•
$$\mathcal{G}^{(r)}\equiv(\mathcal{V}^{(o)},\mathcal{E}^{(r)})$$

- Y^(r) = ({a, b}|Y^(r)_{ab} ≠ 0) associated with the effective (not necessarily real) power lines, {a, b} ∈ E^(r). Y^(r)
- Reduced Model

•
$$\pmb{S}^{(o)} = \Pi^{-1}_{\pmb{Y}^{(r)}}(\pmb{V}^{(o)})$$

• Learn it !?

Machine Learning for Power Systems PIML for State & Parameter Estimation

Task: SE & PE. PIML of Reduced Model

• Power Graphical NN (System 2):

$$\begin{split} & \min_{\varphi, \mathbf{Y}^{(r)}} L_{\mathsf{Power-GNN}}\left(\varphi, \mathbf{Y}^{(r)}\right), \\ & L_{\mathsf{Power-GNN}}\left(\varphi, \mathbf{Y}^{(r)}\right) \equiv \frac{1}{N|\mathcal{V}^{(o)}|} \sum_{n=1}^{N} \left\| \mathbf{S}_{n}^{(o)} - \underbrace{\prod_{\mathbf{Y}^{(r)}}^{-1}\left(\mathbf{V}_{n}^{(o)}\right)}_{\mathsf{physics = interpretable}} - \underbrace{\sum_{\mathbf{V}^{\varphi}\left(\mathcal{V}_{n}^{(o)}, S_{n}^{(o)}\right)}_{\mathsf{NN} = \text{"sub-scale"}} \right) \right\|^{2} + \underbrace{\mathcal{R}(\varphi)}_{\mathsf{regularization}} \end{split}$$

- SIMULTANEOUSLY physics-informed and physics-blind parts
- Compare with Vanilla-NN (System 1)

$$L_{\text{NN}} \doteq \frac{1}{N|\mathcal{V}^{(0)}|} \sum_{n=1}^{N} \left\| \boldsymbol{S}_{n}^{(o)} - \text{NN}_{\varphi}(\boldsymbol{V}_{n}^{(o)}) \right\|^{2}$$

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Machine Learning for Power Systems PIML for State & Parameter Estimation

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Task: SE & PE. Power GNN vs Vanilla NN. Experiments.

IEEE 14-bus [panel (a)], IEEE 118-bus [panel (b)] and PanTaGruEI [panel (c)] models



<u>State Estimation Test:</u> Six set of samples were generated for each network. Average mismatch of predicted power injections (on the training set in parentesis)

	case #1	case #2	case #3	case #4	case #5	case #6
Vanilla NN	4.9E-6	7.2E-5	6.3E-3	5.2E-2	6.3E-2	1.4E0
	(4.2E-6)	(6.6E-5)	(5.0E-5)	(3.7E-5)	(1.2E-4)	(4.2E-6)
Power-GNN	3.0E-6	5.8E-7	6.9E-7	1.3E-6	2.9E-7	3.0E-6

Machine Learning for Power Systems PIML for State & Parameter Estimation

Task: SE & PE. Power GNN vs Vanilla NN. Experiments.



Full Observability. Parameter Estimation.

- Reconstruction of the admittance matrix
 Y for IEEE 14-bus (a), IEEE 118-bus (b) and PanTaGruEl (c) models
- The min, mean and max values are displayed as circles, crosses and squares respectively (for 10 realizations.)

Notice !!

 Quality of the reconstruction by Power-GNN – especially for large network

(a)

Machine Learning for Power Systems PIML for State & Parameter Estimation

(a)

Task: SE & PE. Power GNN vs Vanilla NN. Experiments.



Partial Observability. Parameter Estimation. PanTaGruEl model

- Initial (pre-training) values in green.
- Trained values and their Kron-reduction counterparts red and blue respectively.
- (c) shows alternative visualization of the reference-vs-predicted values of the line conductances (purple) and susceptances (black)

Notice !!

• Quality of the reconstruction by Power-GNN – especially for large network

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Outline

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

- Introduction: Scientific AI & ML ⊂ Applied Math
 - Modern Applied Mathematics as System 2
 - Physics Informed AI/ML
- 2 System 1 & System 2 ML for Power Systems
 - Machine Learning for Power Systems

- PIML for State & Parameter Estimation
- 3 Learning Locational Marginal Prices & Dispatch
 - Formulation and System 2 Idea
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(a)

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Learning LMP & Dispatch

$$\begin{array}{ll} \min_{p_g,\theta} & \sum_g (q_g p_g^2 + c_g p_g) \\ \text{s.t.} \\ \forall g: p_g \in \text{Range} \\ \hline \forall i: p_i - l_i = \sum_{j \in i} b_{ij}(\theta_i - \theta_j) \\ \theta_{\text{slack bus}} = 0 \\ \hline \text{Line Constraints} \\ \forall \{i,j\}: b_{ij}(\theta_i - \theta_j) \in \text{Range} \end{array}$$

- Linear Programming (in DC-approximation)
- Locational Marginal Prices are part of the solution

Observation:

• Very few lines are saturated

The Challenge:

- To run the dispatch for MANY /-load configurations under given network conditions
- Do it faster than your good LP (plus) solvers can do

(a)

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Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Learning LMP & Dispatch

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- Systems 2 [Physics, i.e. Power System, Informed] Machine Learning ?

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Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Efficient Learning of LMPs & Dispatch

Handy to get rid of PF eqs. (and θ – phase angles)

$$\begin{array}{ll} \min_{D_g} & \sum_g (q_g p_g^2 + c_g p_g) \\ \text{s.t.} & \\ \forall g: p_g \in \mathsf{Range} \\ & \sum_g p_g = \sum_i l_i \\ & \\ & \\ \hline & \underline{\mathsf{Line \ Constraints}} \\ & \\ \forall k = \mathsf{line}: & \sum_{i \in k} \Phi_{ki} (p_i - l_i) \in \mathsf{Range} \end{array}$$

- Power Transfer Distribution Factor (PTDF) Matrix Φ
- Generalizable to AC-OPF (linearization around an operational point)

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

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Efficient Learning of LMPs & Dispatch

Lagrangian Formulation & Locational Marginal Prices (LMP)

•
$$\mathcal{L}(p_g, \lambda, \mu_k, \nu_k) = \sum_g (q_g p_g^2 + c_g p_g) + \lambda \left(\sum_g p_g - \sum_i l_i \right) + \sum_k \mu_k \left(\sum_i \Phi_{ki}(p_i - l_i) - f_k^{max} \right) - \sum_k \nu_k \left(\sum_i \Phi_{ki}(p_i - l_i) + f_k^{min} \right)$$

• $\forall i : LMP_i = \frac{\partial \mathcal{L}}{\partial l_i} = -\lambda + \sum_k \Phi_{ki}(\nu_k - \mu_k)$

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Efficient Learning of LMPs & Dispatch

Financial Coherency Conditions = Consequences of KKT:

- Revenue Adequacy (RA): $\sum_{g} LMP_{g}p_{g} \leq \sum_{i} LMP_{i}l_{i}$
- Cost Recovery (CR): $q_g p_g^2 + c_g p_g \leq LMP_g p_g$
- Engineer Desiderata: Reduced Model (faster, possibly approximate evaluation of OPF) guarantees RA & CR

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Efficient Learning of LMPs & Dispatch

System 2 Idea:

 Take Advantage of Strong Duality (Complementary Slackness + Dual Feasibility)

•
$$\forall k : \mu_k \left(\sum_i \Phi_{ki}(p_i - l_i) - f_k^{max} \right) =$$

- $\sum_k \nu_k \left(\sum_i \Phi_{ki}(p_i - l_i) + f_k^{min} \right) = 0, \quad \mu_k, \nu_k \ge 0$

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

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Suppose we know the saturated lines $(\mu_k^* \neq 0 \text{ or } \nu_k^* \neq 0)$

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Suppose we know the saturated lines $(\mu_k^* \neq 0 \text{ or } \nu_k^* \neq 0)$

Then the task is much easier than solving OPF !!

• Solving the System of Linear Equations (for $p_g, \mu_k, \nu_k, \lambda$):

$$\forall \mu_k^* \neq 0 : \qquad \sum_i \Phi_{ki}(p_i - l_i) = f_k^{max}$$

$$\forall \nu_k^* \neq 0 : \qquad \sum_i \Phi_{ki}(p_i - l_i) = f_k^{min}$$

$$\forall g : \qquad 2q_g p_g + c_g + \lambda + \sum_k \Phi_{ki} \mu_k^* + \sum_k \Phi_{ki} \nu_k^* = 0$$

$$\sum_g p_g = \sum_i l_i$$

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Suppose we know the saturated lines
$$(\mu_k^* \neq 0 \text{ or } \nu_k^* \neq 0)$$

Then the task is much easier than solving OPF !!

• Solving the System of Linear Equations (for $p_g, \mu_k, \nu_k, \lambda$):

$$\begin{aligned} \forall \mu_k^* \neq \mathbf{0} : & \sum_i \Phi_{ki}(p_i - l_i) = f_k^{max} \\ \forall \nu_k^* \neq \mathbf{0} : & \sum_i \Phi_{ki}(p_i - l_i) = f_k^{min} \\ \forall g : & 2q_g p_g + c_g + \lambda + \sum_k \Phi_{ki} \mu_k^* + \sum_k \Phi_{ki} \nu_k^* = \\ & \sum_g p_g = \sum_i l_i \end{aligned}$$

System 2 (PIML) learning:

- Train a model (System 1, NN) to find saturated lines
- Then solve the Linear System of Eqs.

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Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Classification of Saturated/Binding Lines

Neural Network

•
$$NN_{\psi}: I \rightarrow \begin{pmatrix} B(\mu) \\ B(\nu) \end{pmatrix}$$
, $B(x) = (1: \text{ if } x \neq 0, \text{ 0otherwise})$

• simple ... 4 CNN layers, 500 neurons/layer, last layer sigmoid activation f.

Loss Function (logistic regression)

•
$$L_{\psi} = \sum_{s} \sum_{k} \left(L_{reg}(y_{k}^{\mu(s)}, B(\mu_{k}^{(s)})) + L_{reg}(y_{k}^{\nu(s)}, B(\nu_{k}^{(s)})) \right)$$

 $L_{reg}(x, y) = \begin{cases} -log(x), & \text{if } y = 1\\ -log(1-x), & \text{if } y = 0 \end{cases}$

Supervise Learning (classification): I -input data; y - output data

Training = Supervised Learning (classification):

• Minimize the loss function over the NN parameters, ψ

• Given: *I* -input data; *y* - output data (saturated lines)

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Test: IEEE 118-bus system

	Free generators
Config. #1	$\{3, 5, 11, 12, 18, 30, 34, 40, 42, 43\}$
Config. #2	$\{2, 5, 12, 26, 30, 39\}$
Config. #3	$\{5, 12, 14, 20, 30, 37, 39\}$

- Generate many samples of Noise for given configuration of the Generator Commitments (minutes to an hour). Consider Different Unit Commitments (Configurations).
- The intra-hour re-dispatch only on "free" generators

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

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	Free generators
Config. #1	$\{3, 5, 11, 12, 18, 30, 34, 40, 42, 43\}$
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- Generate many samples of Noise for given configuration of the Generator Commitments (minutes to an hour). Consider Different Unit Commitments (Configurations).
- The intra-hour re-dispatch only on "free" generators

		Config. #1		Con	fig. #2	Config. #3		
σ	size	training	testing	training	testing	training	testing	
1%	50	0(0.00)	0(0.00)	0(0.00)	34(0.02)	1(0.01)	66(0.05)	
1%	100	0(0.00)	0(0.00)	0(0.00)	48(0.03)	0(0.00)	273(0.20)	
1%	200	0(0.00)	6(0.00)	0(0.00)	104(0.06)	0(0.00)	342(0.25)	
5%	50	0(0.00)	0(0.00)	0(0.00)	16(0.01)	9(0.03)	50(0.05)	
5%	100	0(0.00)	0(0.00)	0(0.00)	43(0.03)	0(0.00)	165(0.14)	
5%	200	0(0.00)	6(0.00)	0(0.00)	79(0.05)	0(0.00)	232(0.19)	
10%	50	0(0.00)	0(0.00)	4(0.00)	19(0.02)	26(0.05)	36(0.04)	
10%	100	0(0.00)	0(0.00)	0(0.00)	24(0.02)	6(0.01)	103(0.01)	
10%	200	0(0.00)	2(0.00)	0(0.00)	35(0.03)	1(0.00)	133(0.15)	

Table I: Number of misidentifications, i.e. $y_k^{\nu|\mu(s)} = 1$ and $\mathcal{B}(\nu|\mu_k^{(s)}) = 0$ or vice versa, over the training and testing sets. The ratio of misidentifications to number of binding line constraints is given in parenthesis.

 Quality of Training depends on Configuration and Noise (Uncertainty)

(a)

Decays with Noise

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Test: IEEE 118-bus system

σ	#4	#5	#6	#7	#8	#9	#10	#11	#12	#13	#14	#15
1%	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.00
5%	0.04	0.01	0.02	0.00	0.03	0.07	0.02	0.00	0.02	0.06	0.05	0.01
10%	0.05	0.03	0.04	0.02	0.06	0.08	0.06	0.02	0.06	0.09	0.05	0.05

Table II: Fraction of misidentifications over testing set for the 13 unit commitment configurations not presented in Table I.

• Testing is on different samples than training (to make sure we do not overfit)

		Config. #1		Con	fig. #2	Config. #3		
σ	size	training	testing	training	testing	training	testing	
1%	50	0(0.00)	0(0.00)	0(0.00)	34(0.02)	1(0.01)	66(0.05)	
1%	100	0(0.00)	0(0.00)	0(0.00)	48(0.03)	0(0.00)	273(0.20)	
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10%	100	0(0.00)	0(0.00)	0(0.00)	24(0.02)	6(0.01)	103(0.01)	
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 Quality of Training depends on Configuration and Noise (Uncertainty)

(a)

• Decays with Noise

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Test: IEEE 118-bus system

σ	#4	#5	#6	#7	#8	#9	#10	#11	#12	#13	#14	#15
1%	0.00	0.00	0.00	0.00	0.00	0.02	0.01	0.00	0.00	0.01	0.01	0.00
5%	0.04	0.01	0.02	0.00	0.03	0.07	0.02	0.00	0.02	0.06	0.05	0.01
10%	0.05	0.03	0.04	0.02	0.06	0.08	0.06	0.02	0.06	0.09	0.05	0.05

Table II: Fraction of misidentifications over testing set for the 13 unit commitment configurations not presented in Table I.

• Testing is on different samples than training (to make sure we do not overfit)

σ	Revenue Adequacy	Strong Duality	Cost Recovery
1%	1.000	1.000	0.808
5%	0.999	0.997	0.352
10%	0.999	0.992	0.060

Table III: Fraction of the testing samples (over all 15 unit commitment configurations) that satisfy the key (in)equalities as stated in Eq. (16)-(18).

• Checking for other criteria than used in training

(a)

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Test: IEEE 118-bus system



Figure 1: Mismatch between obtained LMPs (top) and generator outputs (bottom) for different load volatility standard deviations: 1% (blue), 5% (orange) and 10% (green) of their nominal values, and the training set consists of: 50 (solid), 100 (dashed) are 200 (dotted) samples. Each panel shows the fraction of the testing set that get maximal mismatches smaller than the ordinate.

- Success depends on the Unit Commitment Configuration, Level of the Noise and Number of Samples
- \Rightarrow Phase Transition Type of Behavior = Sharp Changes

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Test: IEEE 118-bus system



Figure 1: Mismatch between obtained LMPs (top) and generator outputs (bottom) for different load volatily standard deviations: 1% (blue), 5% (orange) and 10% (green) of their nominal values, and the training set consists of: 50 (solid), 100 (dashed) are 200 (dotted) samples. Each panel shows the fraction of the testing set that get maximal mismatches smaller than the ordinate.

- Success depends on the Unit Commitment Configuration, Level of the Noise and Number of Samples
- \Rightarrow Phase Transition Type of Behavior = Sharp Changes
- Larger System ? More realistic Noise (longer correlations)?

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

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Test: New-York ISO Model (designed by Dan-The-Man)

THE MODEL (ARPA-E project led by Dan)

- Based on carefully curated real data for New York ISO
- 1814 buses, 395 generators, 2203 lines
- Time: August 28, 2018, 5 pm hour
- From Security Constrained Unit Commitment (SCUC): get unit commitment; factor in committed generators as negative load
- Noise
 - (a) Re-scaled white noise to wind farms. Ignore short time scales (10-20 min) between consecutive unit commitments
 - (b) From base load: add noise using factor stressing methodology developed by Dan
- Major Tool Real-Time Simulator (SCUC + Security Control Energy Dispatch/OPF) – developed by Dan

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Test: New-York ISO Model (designed by Dan-The-Man)



- Preliminary Results (more in two three weeks next ARPA-E review)
- Under low noise, NN correctly identifies 90% of the line dual variables as zero or nonzero pretty good
- ... but can be improved, perhaps with alternative ML schemes (may be even simpler than NN, e.g. Support Vector Machine)

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

(a)

Take Home Message



• Reduced Modeling = faster, less data, accurate (enough)

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Take Home Message



- Seems Like a General Approach
- Open Challenge (for theorists):
 - Given recent NN theories (for System 1 = quality of estimations faster/less data/accurate) ⇒ How does the quality/error propagate to the overall output (of the reduced model)?

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Trustworthy Scientific AI

Facets of Expert (e.g. scientist/engineer) Trust in AI

- Autonomy (distributed agents)
- Beneficence (useful for all)
- Nonmaleficence (no harm)
- Justice (fairness)

- Explainability "system 2 level", i.e. in use-inspired expert (physicist, power engineer, epidemiologist) terms
- **Prepardness** (for rare but possibly devastating events)
- **Reproducability** (at least two principally different models agree)

(a)

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

Theory is Needed for (Scientists & Engineers) Trust

Desiderata:

- Explain with Asymptotics: Explain SIMPLE System 1 ML/AI system (one layer & many neurons, many layers & neurons, ReLU or whatever ..., phase transitions = asymptotic theory, finite size effects = e.g. finite system # of samples) to enable System 2
- Explain with Structure: Inject more structure in your theory (e.g. optimization, inference & learning) — Graphical Models
 System 2 (structure) enabler
- Prepare with Better Extrapolation: especially of extreme events, System 2 is needed to generalize into unseen regimes
- Reproduce with Alternatives: Many more and complementary (System 2 and System 1, evolving) Models (and thus Theories) are NEEDED

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.



Laurent Pagnier



Yury Dvorkin



Dan Bienstock



Robert Ferrando

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Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.



Support is Appreciated !!

• Energy Systems: UArizona start up + DOE/ARPA-E

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Thanks for your attention !

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System 2 Applied Mathematics

Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

- Research focused, since 1976, one of the US first [dynamical systems, integrability, turbulence ...]
- Interdisciplinary: 100+ professors/ 26 departments/ 8 colleges across UA campus (CoS & CoE & Optics – top 3)
- Mixing traditional @ contemporary Applied Math
- Graduate, Ph.D. focused, no terminal M.Sc.
- 60 Ph.D students (15/13/16/10 enrolled in 2022/21/20/19)
- <u>3 Core Courses</u> (1st year -- Methods, Analysis, Algorithms) <u>https://appliedmath.arizona.edu/students/new-core-courses</u>
- Strong collaborations with Industry (e.g. Raytheon, Uber, Intel, Critical Path, etc) and National Labs (e.g. LANL, LLNL, NREL, NNSS, BNL, SNL etc)
- 5 seminar/colloquium series recorded and posted online
- · Participation in many UA & National Edu Projects



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Formulation and System 2 Idea Validation: Configurations vs Noise vs # Samples Future Work. Theory help is needed.

How does Mathematics work with Applications @ UArizona?



Core courses provide hands on teaching of the AM-cycle methodology

- Training in methods (Math/APPL 581), theory (Math/APPL 584), algorithms (Math/APPL 589)
- Math (quantitative) and Application-specific (qualitative) intuition