Machine learning for power systems

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Energy in DTU

DTU Wind Energy
DTU Electrical Engineering
DTU Energy Conversion
DTU Management Engineering

DTU Photonicns
Solar PV systems

Dynamic systems and smart cities

Building energy, Solar thermal and District heating

Thermal systems

Energy system analysis and policy
Center for Electric Power and Energy (CEE)

- **Established 15 August 2012** by merging two existing units (Lynbgy + Risø)
  - Among the strongest university centers in Europe with approx. 110 employees and 12 faculty members

- **Bachelor and Master programs**: Sustainable Energy Design, Electrical Engineering, Wind Energy, Sustainable Energy

- **Direct support from**: ENERGINET, Ørsted, Siemens, Danfoss

*DTU consistently ranks among the top 10 universities of the world in Energy Science and Engineering (Shanghai ranking, 2016, 2017, 2018)*
Strong National and International Collaboration
Selected collaboration partners

**Academic partners:**
- ETH Zürich (CH)
- EPFL (CH)
- Nanyang Technological University (SG)
- University of Delaware (US)
- University of Strathclyde Glasgow (UK)
- Berkeley University of California (US)
- DTU (DK)

**Commercial and industrial partners:**
- Energinet (DK)
- Ørsted (DK)
- Siemens (DE+DK)
- Børnehåbs Energii & Forsyning (DK)
- National Grid (UK)
- IBM (CH)
- Vestas (DK)
- Energinet (DK)

>100 formal partners

>80 formal partners
Our (my) research topics – 11 researchers – 8 nationalities

- Zero-inertia systems
- Market integration of HVDC
- North Sea Wind Power Hub
- Data-driven control and markets in distribution grids
- Machine learning for power systems

10 February 2020

DTU Center for Electric Power and Energy – Spyros Chatzivasileiadis
North Sea Wind Power Hub
• Will probably be the first true zero-inertia AC system in the world

• A range of challenges:
  – How do you ensure N-1 between grid-forming converters?
  – What kind of controls are necessary to maintain stability against much faster transients?
  – Need for new simulation tools (RMS-based tools, e.g. Powerfactory, insufficient to capture stability)

More on www.multi-dc.eu!
Our (my) research topics – 11 researchers – 8 nationalities

- Zero-inertia systems
- Market integration of HVDC
- North Sea Wind Power Hub
- Data-driven control and markets in distribution grids
- Machine learning for power systems
- North Sea Wind Power Hub
Machine learning: Why shall we apply it in power systems?
Machine learning: Why shall we apply it in power systems? (1/3)

1. **ML methods can handle well extremely complex systems**
   - Sometimes impossible or very difficult to develop models based on first principles, e.g. weather forecasting, image processing, etc.

2. **ML methods can infer from incomplete data**
   - Given a limited set of training data, ML methods are known to generalize well, e.g. written text recognition

3. **ML methods can be extremely fast**
   - Milliseconds instead of seconds, minutes, or hours: Require a limited set of linear and simple non-linear computations instead of e.g. computationally intensive numerical integration methods
# Machine learning: Why shall we apply it in power systems? (2/3)

<table>
<thead>
<tr>
<th>Machine Learning</th>
<th>Power Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. ML methods can handle well extremely complex systems</td>
<td>1. Real-life power systems are described by thousands of variables, parameters, and differential-algebraic equations</td>
</tr>
<tr>
<td>2. ML methods can infer from incomplete data</td>
<td>2. It is computationally impossible (intractable) to check for all possible operating conditions</td>
</tr>
<tr>
<td>3. ML methods can be extremely fast</td>
<td>3. Modern power systems have high variability and uncertainty in generation and demand: Need to assess and decide fast</td>
</tr>
</tbody>
</table>
Machine learning: Why shall we apply it in power systems? (3/3)

BUT:

1. Power Systems are safety-critical systems
   - An operator would never trust a neural network if it cannot interpret or anticipate its behavior

2. Researchers and Engineers have spent the last 100 years developing high-quality models to describe power systems
   - Why neglect all this and use black-box techniques only based on data?
Takeaway #1

**Solid motivation is key:** If you wish to apply machine learning (including deep learning) methods on any problem, develop **solid arguments** why this is the only or the best way to do it.
BUT:

1. Power Systems are safety-critical systems
   – An operator would never trust a neural network if it cannot interpret or anticipate its behavior

2. Researchers and Engineers have spent the last 100 years developing high-quality models to describe power systems
   – Why neglect all this and use black-box techniques only based on data?

Neural network verification: neural networks are no longer a black-box

Physics-informed neural networks: exploit the underlying physical models
Goals of this lecture

1. Basic principles of neural network training

2. Unifying framework for power system security assessment and optimization
   - Capture constraints impossible to capture before through ML and exact transformations

3. The importance of high quality data: sampling beyond statistics

4. Neural network verification

5. Physics-informed neural networks
Let’s talk about power systems!

Why are they safety-critical?
Why are they complex?
Spot the difference!
North East Blackout 2003

- North East Blackout 2003
- Affected 55 million people in the US and Canada
- Estimated cost of 7-10 billion USD
- Took 2 days (!) for full restoration!
Blackouts are rare but costly!

- Frequency of power interruptions
  - 1 hour per year

- Economic damage from power interruptions
  - about 80 billion USD/year (US only, 2005)

- Total electric energy cost in the US:
  - 370 billion USD/year

India Blackout 2012 → affected 700 million people (!)
Operators run every day a security assessment

- Security = ability to withstand disturbances

- Security Assessment:
  - Screen contingency list every 15 mins
  - Prepare contingency plans for critical scenarios

- Run both:
  - Steady-state, i.e. power flows to check N-1 and violation of limits
  - Dynamic simulations
Challenges

- Dynamic simulations are hard
  - System of differential-algebraic equations with 10k degrees of freedom

- Checking for N-k contingencies is a hard combinatorial problem
  - Usually computationally impossible to check even for all N-2 in a realistic systems with thousands of buses

- The safe operating region is a non-linear non-convex region
  - Impossible to use analytical tricks to determine it

So.... what do we do?
So... what do we do?

Identifying the power system security region

- Run a lot of simulations assessing each operating point
  - Several approaches for efficient approximations to boost computation speed

- Stability certificates
  - Extract sufficient conditions for sub-areas of the security region

- Machine learning approaches
  - Train for a given dataset and infer for all new points
Power System Security Assessment
The safe operating region of power system operations

Feasible region:
Operating points that satisfy the AC power flow equations

- Non-linear and non-convex AC power flow equations
- Component limits
The feasible space of power system operations

- Non-linear and non-convex AC power flow equations
- Component limits
- N-1 security criterion
The feasible space of power system operations

- Non-linear and non-convex AC power flow equations
- Component limits
  + N-1 security criterion
  + Stability Limits
The feasible space of power system operations

- Non-linear and non-convex AC power flow equations
- Component limits
  - N-1 security criterion
  - Stability Limits

Intersection of all security/stability criteria:
Non-linear and non-convex security region
Operators have to check for all instability types

Power System Stability

- Rotor Angle Stability
  - Small-Disturbance Angle Stability
    - Short Term
  - Transient Stability
    - Short Term

- Frequency Stability
  - Transient Stability
    - Short Term
  - Long Term

- Voltage Stability
  - Large-Disturbance Voltage Stability
    - Short Term
  - Small-Disturbance Voltage Stability
    - Long Term

AND steady-state security!

N-1 contingency analysis through power flows

Kundur et al., IEEE TPWRS, 2004
Guiding example for this lecture:
Machine Learning for Power System Security Assessment

Possible Machine Learning Tools

- Decision Trees
  - First proposed by Louis Wehenkel (Univ of Liege) in the ‘90s
  - Very successful
  - Applications in the industry
  - Research is still ongoing; latest focus is on interpretability

- Neural networks (several papers)

- Deep Neural Networks (same as neural networks but deep 😊)
  - One paper on feature extraction (Sun, Konstantelos, Strbac, 2018)
  - One paper inspired by image processing (Hidalgo, Hancharou, Thams, Chatzivasileiadis, 2019)
  - Few additional papers over the past 6 months
Machine learning applications
(for power system security assessment)
A very short overview
The ingredients

What do we need?

If we want to apply machine learning approaches for power system security
The ingredients

- A training database
- A training algorithm
- A test database
  - To test accuracy of the approach
Test Database
Test Database

Traditionally:
- Split training database to e.g. 80% training samples and 20% test samples
- Train with the 80%
- Test with the 20%

Modern toolboxes have this integrated and automatized → only need to provide a training database

Point to remember:

The test database determines the performance of your method. If the test data come from the same simulations as your training data, the accuracy can be deceivingly high. Would it be equally high in reality?

Ideally → use a different real-life dataset

(Unfortunately, not always possible)
Takeaway #2

The quality of your test database is crucial: the test database determines the performance of your method; for a valid assessment, it needs to include a wide range of operating conditions with the same frequency of occurrence as in real-life.
Training a neural network
Decision Trees

• Decision rules
  – If line_flow>FF then …. else…

Neural Networks

• Linear weights
• On every node: a non-linear activation function
  – e.g. RELU: \( u_j = \max(0, w_{ij}x_i + b_i) \)
  – Many other possibilities, e.g. sigmoid function and others

Training a neural network

- Batch size vs Iterations vs Epochs

- Loss function

- Evaluation of performance
  - Confusion matrix
  - Performance metrics
Batch size vs Iterations vs Epochs

Example from linear regression; neural network works similarly

Goal: *estimate* $w_1, w_2$ *to fit* $\hat{y} = w_1 + w_2 x$
Batch size vs Iterations vs Epochs

Example from linear regression; neural network works similarly

Goal: estimate $w_1, w_2$ to fit $\hat{y} = w_1 + w_2 x$

- Ideally we want to enter all our data in our linear regression algorithm to estimate $w_1, w_2$
- But, the size of data can be immense!
- That’s why we need to split our dataset in batches
Batch size vs Iterations vs Epochs

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- But, the size of data can be immense!
- That’s why we need to split our dataset in batches
- Total #data = batch_size * iterations
e.g. if 1000 datapoints and batch_size=200, then 1000=200*5 iterations
Batch size vs Iterations vs Epochs

Example from linear regression; neural network works similarly

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- Ideally we want to enter all our data in our linear regression algorithm to estimate $w_1, w_2$
- But, the size of data can be immense!
- That’s why we need to split our dataset in batches
- Total #data = `batch_size` * `iterations`
e.g. if 1000 datapoints and `batch_size`=200, then 1000=200*5 iterations
- **Epochs:** passing the whole dataset only once is not enough!
  - 1 Epoch = passing the dataset through the neural network ONCE

More info: https://towardsdatascience.com/epoch-vs-iterations-vs-batch-size-4dfb9c7ce9c9
Loss function:
To find the best estimates for $w_1, w_2$ we need to run an optimization!

$$\min_{w_1, w_2} \| y_i - \hat{y}_i \|$$

s.t.
$$\hat{y}_i = w_1 + w_2 x_i \quad \forall i$$

$y_i$: actual/correct value
$\hat{y}_i$: estimated value
Loss function:
To find the best estimates for \( w_1, w_2 \) we need to run an optimization!

\[
\hat{y}_i = w_1 + w_2 x_i
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Rewrite:
\[
\min_{w_1, w_2} \| y_i - \hat{y}_i \|
\]

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\( y_i \): actual/correct value
\( \hat{y}_i \): estimated value
Loss function:
To find the best estimates for $w_1, w_2$ we need to run an optimization!

What cost function shall we use?

Rewrite:
$$\min_{w_1, w_2} \|y_i - \hat{y}_i\|$$

s.t.
$$\hat{y}_i = w_1 + w_2 x_i \quad \forall i$$

Where:
- $y_i$: actual/correct value
- $\hat{y}_i$: estimated value

$\hat{y}_i = w_1 + w_2 x_i$
Cost function (often called “Loss function”)

• A series of different options:
  https://isaacchanghau.github.io/post/loss_functions/

• Often used for classification problems: cross-entropy

• For 2 classes, i.e. $y_i = \{0,1\}$ and $\hat{y}_i = [0,1]$:

\[
L = -\frac{1}{n} \sum_{i=1}^{n} y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)
\]
Cross-entropy: the insights

• Insight #1: you minimize over the estimation errors of all points in the batch

\[
\mathcal{L} = -\frac{1}{n} \sum_{i=1}^{n} y_i \log \hat{y}_i + (1 - y_i) \log (1 - \hat{y}_i)
\]

• Insight #2:
  – Actual values: either 0 or 1
  – Estimated values: between 0 and 1

\[y_i = \{0,1\} \quad \text{but} \quad \hat{y}_i = [0,1]\]
Cross-entropy: the insights

• Insight #1: you minimize over the estimation errors of all points in the batch

\[ L = -\frac{1}{n} \sum_{i=1}^{n} y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i) \]

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• Insight #3: Why the minus?

Hint: explain it for one point

\[ L = -(y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)) \]
Cross-entropy: the insights

- **Insight #1:** you minimize over the estimation errors of all points in the batch

\[ \mathcal{L} = -\frac{1}{n} \sum_{i=1}^{n} y_i \log \hat{y}_i + (1 - y_i) \log (1 - \hat{y}_i) \]

- **Insight #2:**
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- **Insight #3:** Why the minus?
  Hint: explain it for one point

\[ \mathcal{L} = -(y_i \log \hat{y}_i + (1 - y_i) \log (1 - \hat{y}_i)) \]

- **Insight #4:** \(y_i=1, \mathcal{L}\) when \(\hat{y}_i = [0,1]\)
Evaluating the performance: Confusion matrix

<table>
<thead>
<tr>
<th>Target class (actual values)</th>
<th>1</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Output class (predicted values)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>True positive (TP)</td>
<td>False positive (FP)</td>
</tr>
<tr>
<td>0</td>
<td>False negative (FN)</td>
<td>True Negative (TN)</td>
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Evaluating the performance: Confusion matrix

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**Classification for power system security**

<table>
<thead>
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<th>Actually Safe</th>
<th>Actually Unsafe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Predicted safe</td>
<td>True positive (TP)</td>
</tr>
<tr>
<td>Predicted Unsafe</td>
<td>False negative (FN)</td>
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</tbody>
</table>
Performance Metrics: Accuracy

- **Accuracy**: The proportion of correct classifications in the whole dataset

\[
\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}
\]

- **Example**: Assume 1000 datapoints
  - Actually safe: 500  TP=480  FP=30
  - Actually unsafe: 500  FN=20  TN=470

Accuracy = ?
Performance Metrics: Accuracy

- **Accuracy**: The proportion of correct classifications in the whole dataset

\[
\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}
\]

- **Example**: Assume 1000 datapoints
  - Actually safe: 500  TP=480  FP=30
  - Actually unsafe: 500  FN=20  TN=470

\[
\text{Accuracy} = \frac{480 + 470}{480 + 20 + 470 + 30} = 95\%
\]

Evaluating performance by measuring only accuracy is often not enough

**Why?**
Performance Metrics: Accuracy

• Accuracy: The proportion of correct classifications in the whole dataset

$$\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}$$

• Example: Assume 1000 datapoints
  – Actually safe: 500 TP=480 FP=30
  – Actually unsafe: 500 FN=20 TN=470

$$\text{Accuracy} = \frac{480+470}{480+20+470+30} = 95\%$$

Evaluating performance by measuring only accuracy is often not enough

Why?

• Example: Assume 1000 datapoints
  – Actually safe: 20 TP=480 FP=30
  – Actually unsafe: 980 FN=19 TN=950

$$\text{Accuracy} = ?$$
Performance Metrics: Accuracy

- **Accuracy**: The proportion of correct classifications in the whole dataset

\[
\text{Accuracy} = \frac{TP + TN}{TP + FP + TN + FN}
\]

- **Example**: Assume 1000 datapoints
  - Actually safe: 500  \(TP=480\)  \(FP=30\)
  - Actually unsafe: 500  \(FN=20\)  \(TN=470\)

\[
\text{Accuracy} = \frac{480+470}{480+20+470+30} = 95\%
\]

Evaluating performance by measuring only accuracy is often not enough

**Why?**

- **Example**: Assume 1000 datapoints
  - Actually safe: 20  \(TP=1\)  \(FP=30\)
  - Actually unsafe: 980  \(FN=19\)  \(TN=950\)

\[
\text{Accuracy} = \frac{1+950}{1+19+950+30} = 95\%
\]

- 95% accurate but we have misclassified almost all truly safe points!
- For heavily unbalanced data, accuracy is not sufficient!
Performance metrics

- **Accuracy**
- **Recall**: True Positive Rate \( \frac{TP}{TP+FN} \)
- **Specificity**: True Negative Rate \( \frac{TN}{TN+FP} \)
- **Precision**: Positive Predictive Value \( \frac{TP}{TP+FP} \)
- **F1**: harmonic mean of Precision and Recall \( F1 = \frac{Precision \cdot Recall}{Precision+Recall} \)
- **MCC (Matthews correlation coefficient)** (only for binary classification – 2 classes only)
  - MCC=1 → perfect prediction
  - MCC=0 → random (like flipping a coin)
  - MCC=−1 → Completely mistaken

\[
MCC = \frac{(TP \cdot TN) - (FP \cdot FN)}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}
\]
Key hints for your implementation

• Regularization: Training of neural networks work better if you normalize your inputs
  – Try to normalize your active power setpoints (e.g. if PG1 = 30 MW and PG1max = 100 MW, then PG1=0.3)

• 1-hot encoding: Neural networks work better if you use one vector for each class

Instead of:

<table>
<thead>
<tr>
<th></th>
<th>Safe=1</th>
<th>Unsafe=0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_1$</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>$x_2$</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>$x_3$</td>
<td>0</td>
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Instead of:

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</tr>
<tr>
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</table>
Takeaway #3: 
Neural networks (or Decision Trees) for classification: you need a balanced training database → similar number of safe and unsafe points

Takeaway #4: 
Accuracy is not sufficient to assess the NN/DT performance. We need additional metrics

Takeaway #5: 
Neural Network training requires additional “tricks” to boost its performance (e.g. 1-hot encoding/regularization)
Training database
We need data!

• Data that accurately capture the whole security region
  – so that we can successfully use machine learning
    approaches for classification

• Historical data are insufficient
  – Contain very limited number of abnormal situations

• Need to generate simulation data

• Assessing the stability of 100’000s of operating points is
  an extremely demanding task
  – Immense search space
Sampling beyond Statistics: Efficient Database Generation

• Modular and highly efficient algorithm

• Can accommodate numerous definitions of power system security (e.g. N-1, N-k, small-signal stability, voltage stability, transient stability, or a combination of them)

• 10-20 times faster than existing state-of-the-art approaches

• Our use case: N-1 security + small-signal stability

• Generated Database for NESTA 162-bus system online available!
  
  https://github.com/johnnyDEDK/OPs_Nesta162Bus (>500,000 points)

Sampling beyond Statistics: Efficient Database Generation

• The goal
  – Focus on the **boundary between stability and instability**
  – We call it: “high information content” region

• How?
  1. Using convex relaxations
  2. And “Directed Walks”

Real data for the IEEE 14-bus system
N-1 security and small-signal stability
Convex relaxations to discard infeasible regions

Non-convex stable region
Convex relaxations to discard infeasible regions

- **Certificate**: if point infeasible for semidefinite relaxation $\rightarrow$ infeasible for the original problem.
Convex relaxations to discard infeasible regions

- Certificate: if point infeasible for semidefinite relaxation → infeasible for the original problem
- If infeasible point: find minimum radius to feasibility
Convex relaxations to discard infeasible regions

- **Certificate**: if point infeasible for semidefinite relaxation → infeasible for the original problem
- If infeasible point: find minimum radius to feasibility
- Discard all points inside the (hyper)sphere
- 3D projection of hyperspheres
- IEEE 14-bus system
- Rapidly discarding (=classifying) large chunks of the search space as infeasible to focus on the boundary

Convex relaxations to discard infeasible regions

- Extension of this work to hyperplanes

Directed Walks

• “Directed walks”: steepest-descent based algorithm to explore the remaining search space, focusing on the area around the security boundary

1. Variable step-size
2. Parallel computation
3. Full N-1 contingency check
Results

<table>
<thead>
<tr>
<th>Points close to the security boundary (within distance $\gamma$)</th>
<th>IEEE 14-bus</th>
<th>NESTA 162-bus</th>
</tr>
</thead>
<tbody>
<tr>
<td>Brute Force</td>
<td>100% of points in 556.0 min</td>
<td>intractable</td>
</tr>
<tr>
<td>Importance Sampling</td>
<td>100% of points in 37.0 min</td>
<td>901 points in 35.7 hours</td>
</tr>
<tr>
<td>Proposed Method</td>
<td>100% of points in 3.8 min</td>
<td>183’295 points in 37.1 hours</td>
</tr>
</tbody>
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- We tested these databases with decision trees. Further benefits for the decision trees:
  - Higher accuracy
  - Better classification quality (Matthews correlation coefficient)

Generated Database for NESTA 162-bus system online available!
https://github.com/johnnyDEDK/OPs_Nesta162Bus
Takeaway #6

Creating high-quality training databases is extremely complex and an open research topic. We need to go beyond purely statistical methods and exploit the underlying physics during sampling.
From decision trees to mixed integer linear programming
The feasible space of power system operations

Intersection of all security/stability criteria:
Non-linear and non-convex security region

Electricity markets should determine setpoints that are only within this area

Optimization constraints should represent this area

Impossible → differential and non-linear algebraic equations
What do TSOs and market operators do?

**Linear approximations**

Net Transfer Capacity

- Inaccurate
- Too conservative

Flow-based market coupling

Single convex region
Our proposal: Data-driven Security Constrained OPF

How does it work?

Database of secure and insecure operating points
\{P, Q, V, \theta, \zeta\}

Operating points provided by the TSOs through simulated and real data

Train a decision tree to classify secure and insecure regions

Exact formulation to MILP

\[
\text{PTDF} \cdot (P_G - P_D) \leq F_{\text{L},p} y_p + F_{\text{L}} \max (1 - y_p)
\]

\[
\text{PTDF} \cdot (P_G - P_D) \geq F_{\text{L},p} y_p - F_{\text{L}} \min (1 - y_p)
\]

Thams et al IREP 2017,
Halilbasic et al PSCC 2018
Data-driven security-constrained OPF

Offline security assessment

Database of stable and unstable OPs

\{P,Q,V,\theta,\zeta\}

Decision Tree

Thams et al IREP 2017, Halilbasic et al PSCC 2018
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Decision Tree

Partitioning the secure operating region

Thams et al IREP 2017, Halilbasic et al PSCC 2018
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Partitioning the secure operating region

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Data-driven security-constrained OPF

**Offline security assessment**

- Database of stable and unstable OPs \( \{P,Q,V,\theta,\zeta\} \)

**Optimization**

Integer Programming to incorporate partitions (DT)
- DC-OPF (MILP)
- AC-OPF (MINLP)
- Relaxation (MIQCP, MISOCP)

- Each leaf is a convex region
- FBMC corresponds to the leaf that maps the largest convex region

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Thams et al IREP 2017, Halilbasic et al PSCC 2018
We gain ~22% of the feasible space using data and Mixed Integer Programming

Largest convex region covers ~78%

Thams et al IREP 2017, Halilbasic et al PSCC 2018
MIP + convex AC-OPF approximation finds better solutions than nonconvex problem!

Optimum located at boundary of considered security region

Thams et al IREP 2017, Halilb et al PSCC 2018
Takeaway #7

Decision Trees can convert to a MILP and help capture optimization constraints that were impossible to capture before. E.g. small-signal stability constraints can now be accurately captured in an OPF.
Neural Network Verification
Why is neural network verification important?

• Neural networks have been shown to be extremely fast
  – Assess if an operating point is safe or unsafe 100x-300x faster (combination of different security criteria)
  – Application in optimization: find the optimal point >100x faster

• However, neural networks will never be applied in critical (power system) operations, if there are no guarantees about how they behave

• Until recently, the only way to assess the output of the neural networks was to **individually test** each input of interest and pass it through the neural network
  – Accuracy was assessed on discrete samples
  – **Challenge #1:** No way to guarantee what the output is for a **continuous** range of inputs
Evaluating Accuracy: Test Database

Challenge #2:

The test database determines the performance of the neural network.

Neural network verification does not depend on a test database:

a. Performance metrics are not based on statistics!

b. Rigorous performance guarantees = certificates
Adversarial examples

- Adversarial example: small perturbations lead to a false prediction

“panda” + .007 × noise = “gibbon”
Adversarial examples

- Adversarial example: small perturbations lead to a false prediction

- Challenge #3: No way to systematically identify adversarial examples
Neural Network Verification: HOW?

1. Convert the neural network to a set of linear equations with binaries
   • The Neural Network can be included in mixed-integer linear program

2. Formulate an optimization problem (MILP)

3. Solve the MILP to zero duality gap (find the global optimal) → certificate for the behavior for neural network

4. Assess if the neural network output complies with the ground truth
   • Two types of optimization problem:
     a. Certify that in a region around a given input $x_{ref}$ the neural network maintains the same classification → guarantee that all input points (continuous range) in the neighborhood will be classified the same
     b. Find the minimum distance from $x_{ref}$ that the classification changes (possibility of adversarial examples)
From Neural Networks to Mixed-Integer Linear Programming

- Most usual activation function: ReLU
- ReLU: Rectifier Linear Unit
From Neural Networks to Mixed-Integer Linear Programming

- Linear weights
- On every node: a non-linear activation function
  - ReLU: $u_j = \max(0, w_{ij}x_i + b_i)$
- But ReLU can be transformed to a piecewise linear function with binaries

![Diagram of a neural network with linear weights and ReLU activation function]
From Neural Networks to Mixed-Integer Linear Programming

- Output
  - For now: binary classification
  - Security assessment for power systems
  - Output vector $\mathbf{y}$ with two elements:
    - $y_1 \geq y_2$: safe
    - $y_2 \geq y_1$: unsafe
Certify the output for a continuous range of inputs

- We assume a given input $x_{\text{ref}}$ with classification $y$: $y_1 > y_2$

1. For distance $\epsilon$ evaluate if input $x$ exists with different classification $y_2$

\[
\begin{align*}
\max_{x,y} & \quad y_2 - y_1 \\
\text{s.t.} & \quad y = NN(x) \\
& \quad \|x - x_{\text{ref}}\|_\infty \leq \epsilon
\end{align*}
\]
Adversarial examples in safety-critical systems

- Adversarial examples exist in many (deep) learning applications
- Major barrier for adoption of machine learning techniques in safety-critical systems!

Systematically identify adversarial examples

- We assume a given input \( x_{\text{ref}} \) with classification \( y : y_1 > y_2 \)

2. Minimize distance \( \epsilon \) from \( x_{\text{ref}} \) to input \( x \) with classification \( y_2 \)

\[
\begin{align*}
\min_{x,y,\epsilon} & \quad \epsilon \\
\text{s.t.} & \quad y = NN(x) \\
& \quad |x - x_{\text{ref}}|_{\infty} \leq \epsilon \\
& \quad y_2 \geq y_1
\end{align*}
\]
Challenges

• **Tractability** for large neural networks
  – Up to now, we have verified NNs with 5 layers and 50 nodes at each layer (NN used for the 162-bus system)
  – We require weight sparsification, bound tightening, and ReLU pruning (remove binary variables) to maintain tractability

• **Connect verification with ground truth assessment**
  – Currently, we can first certify the neural network output, and we should then assess if this output is correct (i.e. that the NN can be trusted in real operation)
  – Currently working on a verification procedure that will be integrated in the training of the neural network \( \rightarrow \) training results in a certificate of performance (no more statistics!)

• **Retraining** is necessary to avoid adversarial examples
  – The **quality of the training database is crucial** for good performance!
Takeaway #8

Neural network verification removes the barrier for neural network applications in safety-critical operations. High potential for power system applications.
Physics-Informed Neural Networks for Power Systems
Loss function: Estimate best $w_1, w_2$ to fit the training data

\[ \min_{w_1, w_2} \| y_i - \hat{y}_i \| \]
\[ \text{s.t.} \quad \hat{y}_i = w_1 + w_2 x_i \quad \forall i \]

Rewrite:

\[ \min_{w_1, w_2} \| y_i - (w_1 + w_2 x_i) \| \quad \forall i \]

$y_i$: actual/correct value
$
\hat{y}_i$: estimated value

Traditional training of neural networks required no information about the underlying physical model. Just data!
Physics Informed Neural Networks

• Automatic differentiation: derivatives of the neural network output can be computed during the training procedure

• A differential-algebraic model of a physical system can be included in the neural network training*

• Neural networks can now exploit knowledge of the actual physical system

• Machine learning platforms such as Tensorflow enable these capabilities

Physics-Informed Neural Networks for Power Systems

Loss function

\[
\min_{W, b} \frac{1}{|N_\delta|} \sum_{i \in N_\delta} |\hat{\delta} - \delta^i|^2 + \frac{1}{|N_f|} \sum_{i \in N_f} |f(\hat{\delta})|^2
\]

\[\text{s.t.} \quad \hat{\delta} = NN(t, P_m, W, b) \quad (6a)\]

\[
\dot{\delta} = \frac{\partial \hat{\delta}}{\partial t}, \quad \ddot{\delta} = \frac{\partial \dot{\hat{\delta}}}{\partial t}
\]

\[
f(\hat{\delta}) = M\ddot{\delta} + D\dot{\hat{\delta}} + A\sin \hat{\delta} - P_m \quad (6c)
\]

Swing equation

Code is available on GitHub: https://github.com/gmisy/Physics-Informed-Neural-Networks-for-Power-Systems/

Physics-Informed Neural Networks for Power Systems

- Physics-Informed Neural Networks can potentially replace solvers for systems of differential-algebraic equations

- In our example: PINN 87 times faster than ODE solver

- Can directly estimate the rotor angle at any time instant

Code is available on GitHub: [https://github.com/gmisy/Physics-Informed-Neural-Networks-for-Power-Systems/](https://github.com/gmisy/Physics-Informed-Neural-Networks-for-Power-Systems/)

Takeaway #9

Physics-informed neural networks exploit the underlying physics in the training procedure. They are still at a very initial development stage; they have the potential to accelerate by 100-1000 times functions of conventional solvers.
Takeaway wrap-up

1. Before applying machine learning, develop a solid motivation about *why* ML would work better.
2. The quality of your test database is crucial.
3. Neural network and Decision Trees for classification: you need a *balanced* training database.
4. Accuracy is not a sufficient performance metric.
5. Get familiar with the tips and tricks to improve neural network training (e.g. 1-hot encoding).
6. Sampling beyond statistics: creating high-quality training databases is extremely complex; exploit the physical laws. **Open research topic**
7. Decision trees can convert to a MILP and help capture optimization constraints that were impossible to capture before. **Open research topic**
8. Neural network verification removes the barrier for neural network applications in safety-critical operations. **Open research topic**
9. Physics-informed neural networks exploit the underlying physical laws during training. **Open research topic**
Highlights

- Decision Trees can be converted to a MILP through an exact transformation
  - Capture constraints impossible to capture before (e.g. based on differential equations)

- Sampling beyond statistics
  - Need to exploit physics for creating the training databases -- an open research topic

- Neural network verification
  - A world of new opportunities for practical applications in power systems
  - Certify the behavior of neural networks
  - Systematically identify adversarial examples

- Physics-Informed Neural Networks
  - Exploit the underlying physical model in the neural network training
  - Extremely fast computing times: no need to integrate $t_0 \rightarrow t_1$, can directly estimate $x(t_1)$
  - Potential to replace differential-algebraic solvers for real-time applications?
Thank you!

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Deep learning, NIPS Tutorial 2017: https://www.youtube.com/watch?v=YJnddoa8sHk

Sampling beyond Statistics: Efficient Database Creation

Neural Network Verification

Physics-Informed Neural Networks

Physics-Informed Neural Networks