This symposium involves audio/video recording of all presentations, discussions, and comments. The recording for this symposium will be made available to the public. By receiving this notification, your participation consents to recording your interactions with the symposium and public release.

Your audio and video is muted by default.

Use the “Chat” feature to ask questions. All questions will be addressed at the end of each presentation (time permitting).

Use the “Chat” feature to let us know if you have technical difficulties.

For low-quality connections, switch off video and do not use VPN, if possible. A separate audio PIN will be provided when you sign in for the phone-in audio option.
Welcome

Ronald Boring, PhD, FHFES
Manager, Human Factors and Reliability Department
INL
Craig Primer, Light Water Reactor Sustainability
Nuclear Safety and Regulatory Research Division
Idaho National Laboratory

Machine Learning & Artificial Intelligence Symposium 5.0

Tuesday, June 8, 2021
Moving from 2020 to 2021 - Symposium 5.0

- Last year INL sponsored quarterly symposiums on Artificial Intelligence (AI) and Machine Learning (ML) approaches and activities related to science and engineering
  - The “1.0 Symposium” focused on internal-to-INL activities and capabilities
  - Symposium 2.0 we broadened the focus and highlighted activities and capabilities around the nuclear industry and universities
  - Symposium 3.0, we invited researchers provide updates on nuclear-related applications using AI/ML
  - Symposium 4.0, introduced the concept of "Trustworthy" as it relates to AI/ML
- We continue our discussion today on the importance of Trustworthy AI/ML development and hear from researchers about their work in these areas
<table>
<thead>
<tr>
<th>Time</th>
<th>Topic</th>
<th>Presenter(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11:00 (MDT)</td>
<td>Welcome, Introduction, and Agenda</td>
<td>Craig Primer, INL</td>
</tr>
<tr>
<td>11:05</td>
<td>Machine Learning Pillars to Avoid Embarrassment for Trustworthy and Explainable ML</td>
<td>Rita Foster, INL</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Andrea Mack, INL</td>
</tr>
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<td></td>
<td></td>
<td>Shaya Wolf, UofWY</td>
</tr>
<tr>
<td>11:35</td>
<td>Large-scale Optimization of Boiling Water Reactor Bundles with Hybrid Reinforcement Learning and Evolutionary Intelligence</td>
<td>Majdi Radaideh, MIT</td>
</tr>
<tr>
<td>11:45</td>
<td>Robust data-driven sensor placement</td>
<td>Krithika Manohar, UW</td>
</tr>
<tr>
<td>11:55</td>
<td>Cyber-Physical State Awareness, Automated Response and Confirmed Resilience</td>
<td>Craig Rieger, INL</td>
</tr>
<tr>
<td>12:05</td>
<td>Human-Centered Artificial Intelligence</td>
<td>Ben Shneiderman, UMD</td>
</tr>
<tr>
<td>12:35</td>
<td>Designing Explainable AI</td>
<td>Torrey Mortenson, INL</td>
</tr>
<tr>
<td>12:45</td>
<td>Explainable Dimensionality Reduction Using Scientific Constraints</td>
<td>Ramakrishnan (Ramki) Kannan, ORNL</td>
</tr>
<tr>
<td>12:55</td>
<td>Closing Remarks</td>
<td>Craig Primer, INL</td>
</tr>
</tbody>
</table>
Agenda

• Background
• ML/Graph Pillars
  – Purpose
  – Relevance
  – Data Types
  – Data Sources
  – Data Management and more data
  – Data Validation
  – Explainable
  – Trustworthy
Why it is relevant to ML/AI Future

• Why ML Pillars?
  – Layers of validated assumptions for purpose, relevance, data and ML concepts
  – Provide improvement, feedback to challenge all concepts
  – Assist in explaining ML concepts to potential sponsors
    • Enable refinement to match sponsor’s needs
    • Gain critical partnerships based on problem, data and ML relevance

• Our experience with test corpora concepts enable multi-faceted analysis
  – Benefits of rapid prototyping of new ML/AI methods
  – Actionable ML results from Agile data sets
  – Higher fidelity analysis with ability to challenge assumptions and results

Good research yields more questions enabling future research questions
Machine Learning for Cyber Protection Critical Infrastructure

Historical Journey

Reverse Engineered Binaries

- **2017 - 2021**
  - DOE-CESER Firmware Indicator Translation (FIT) – implemented 2 LDRD methods from RE@Scale

- **2020 - 2023**
  - Grid Modernization Laboratory Call – Firmware Command and Control (FC2)

Structured Threat

- **2019 - 2022**
  - DOE-CESER Competitive Laboratory Call Geo Threat Observable (GTO)

Malware

- **2020 - 2023**
  - Grid Modernization Laboratory Call – Deep Learning Malware (DLM)
Case Study 1 – Structure Threat - Explainable

ML Pillars | Structured Threat
---|---
Explainable | STIG

Russians in the Grid Example – Bryan Beckman
Essential Abilities for Intelligence

- Flexibility - Respond to situations. Take advantage of fortuitous circumstances;
- Make sense out of ambiguous or contradictory messages;
- Recognize the relative importance of different elements of a situation;
- Find similarities between situations despite differences which may separate;
- Draw distinctions between situations despite similarities which may link;
- Synthesize new concepts by taking old concepts and putting together in new ways;
- Generate novel concepts and ideas.
ML Concept Pillars

- Adversarial AI Protections
- Trustworthy
- Explainable
- Data Validation
- Data Management
- Data Sources
- Data Type
- Relevance
- Purpose
### Case Study 1 – Structure Threat - Purpose

<table>
<thead>
<tr>
<th>ML Pillars</th>
<th>Structured Threat</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purpose</td>
<td>GTO will connect missing cyber threat links and provide prediction, mapping to situational awareness for impact, threat analysis and ad-hoc scenarios enabling better use of limited cyber defense resources.</td>
</tr>
</tbody>
</table>

#### Goal and Objectives
- **Goal**: Provide common operational picture for cyber defenders to stage limited resources
- Leverage visualization mechanisms for GIS
- Define structured threat to GIS layers for visualization

#### Capabilities/Gap Analysis

#### Potential Outcomes
- Interactive GIS display of current and evolving threat
- Test corpora …machine learning of similarities to past and predict evolving
- Ad-hoc scenario capability…for Machine Learning threat behavior

#### Scope definition
- ML/Al Appropriateness
- origin and accounting for uncertainty
Case Study 1 – Structure Threat - Relevance

Structured Threat Information Expression
- International Standard Open Source
- OASIS Standard
- Hundreds of Users
- Active Standard being Enriched
- Large use enables technology adoption
- STIX has proven to be **Sharable, Actionable** and **Implementable**
- Relevance for Critical Cost Share Partners: Splunk, Forescout, FortiNet, Eclypsium, Asset Owners, and many original equipment manufacturers
### Case Study 1 – Structure Threat – Data Type & Sources

<table>
<thead>
<tr>
<th>ML Pillars</th>
<th>Structured Threat</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Data Type</strong></td>
<td>Structured Threat in Graph database</td>
</tr>
<tr>
<td><strong>Data Sources</strong></td>
<td>Threat Feeds; Scraped, Enriched</td>
</tr>
</tbody>
</table>

- STIG – Jed Haile
- Ripple20 – Shaya Wolf

![Diagram](image-url)
Case Study 1 – Structure Threat – Managed & Validation

### ML Pillars | Structured Threat
---|---
Data Managed | Graph Database
Data Validation | Nodal Analysis

Node Analysis Andrea Mack

**Graph Databases for Management:**
- Edges, Nodes, Properties
- Graph Traversal – Simple: vertices/edges, Breath or Deep First Search

**Structure - Feature generation using iGraph**
- Communities within graphs;
- Degree of the graph;
- Cliques mean/max clique lengths
- Global Transitivity

**Deeper context rich narratives**
- Descriptions, evidence-based sources

**Nodal Analysis for Validation of Assumptions**
- Validate Test Corpora
- Validate Data Assumptions
  - Subject Matter Expert Review
- Repeatable Embeddings for ML – Graph CNN to Persistent Homology
  i.e., Feature Vector count validated by simple Graph Queries
Nodal Analysis – Validation of Assumptions
What are the Context of All and Two node graphs?

Validation of Graph Context
Challenging the Value of one node graphs
Nodal Analysis
Over 100 Node Graph Analysis

Validation of Graph Context > 100 Nodes
13 static vs 658 Enriched Graphs with more tools, behaviors
Case Study 1 – Structure Threat - Explainable

<table>
<thead>
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<th>ML Pillars</th>
<th>Structured Threat</th>
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<tbody>
<tr>
<td>Explainable</td>
<td>Geo Threat</td>
</tr>
<tr>
<td>Observables</td>
<td></td>
</tr>
</tbody>
</table>

Visualization

- Location of Cyber Attack
  - Kiev, Ukraine December 2016
- Electric Infrastructure Layers
- GIS
- Redrawn impact areas after ad-hoc scenarios; enhanced threat and prediction

Kiev, Ukraine – Ryan Hruska
Case Study 1 – Structure Threat - Trustworthy

<table>
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<tbody>
<tr>
<td>Trustworthy</td>
<td>Sources, Notes, Observables &amp; Scoring</td>
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</table>

Evidence-Based Threat: Sources, Reports, Cyber Observables and Scoring to Trend Threat Value; Provides Feedback

http://sourceforge.net/docman/display_doc.php?docid=19314&group_id=22806

Enrichment Scoring – Bryan Beckman

1.36

>6

4.77
Case Study 1 – Structure Threat - Trustworthy

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</table>

**Process for Trustworthy**
- Baseline Test Corpora
- Baseline Embeddings for ML
- Validate Baselines
- Trend Quality Scores
- Accuracy, repeatability, False Positives, False Negatives (F1)
- Feedback for enhancements and improvements
- Ability to Challenge Results

And Above All …

**Curiosity**

Attack Surface – Bryce McClurg
Looking Ahead

Continued use of ML Pillars
- Refined by external ML experts, research partners and included in strategy
- Focus concepts for future sponsors and stakeholders
- Relevance and actionable results
- Higher fidelity data understanding with visualizations for explainable basis
- Enabling feedback and ability to challenge concepts for improvement

• Test Corpora
  - Easier scope discussions – next iteration tasking
  - Repeatable embeddings with further analysis and validation
  - Two large test corpora Structured Threat and Translated Binaries

Future: critical infrastructure cyber protection issues
Majdi I. Radaideh
MIT Nuclear Science and Engineering

Large-scale Optimisation of BWR Bundles with Hybrid Reinforcement Learning and Evolutionary Intelligence

Machine Learning & Artificial Intelligence Symposium 5.0
June 8, 2021
Reinforcement Learning & Evolutionary Computation

Reinforcement Learning

Genetic Algorithms

Grey wolf Optimization

Particle Swarm Optimization
Game-playing AI

I am almost there 😊
Why AI/ML for Fuel Optimization

- **Expensive** (fuel depletion is included and a bigger assembly is optimized GE14-10x10).
- **Combinatorial** (discrete input space)
- **High-dimensional** (~10^{65} possibilities in the space)
- **Heavily-constrained** (43 constraints)
- **Multi-objective** (maximize burnup, minimize peaking factor)

\[
\min_x f(x) = \left[ \frac{1}{2} \sum_{i=1}^{3} B^{C_i} - 10 \max(PPF_{405}, ..., PPF_{405}, ..., PPF_{405}, ..., PPF_{405}) \right],
\]

subject to the following constraints

\[
g_1(x) = 16 \leq N_{\text{poison}}^{C_1} \leq 18, \quad g_2(x) = 16 \leq N_{\text{poison}}^{C_2} \leq 18, \quad g_3(x) = 13 \leq N_{\text{poison}}^{C_3} \leq 16,
\]

\[
g_4(x) = PPF_{405}^{C_1} \leq 1.45, \quad g_5(x) = PPF_{405}^{C_2} \leq 1.45, \quad g_6(x) = PPF_{405}^{C_3} \leq 1.45,
\]

\[
g_7(x) = PPF_{405}^{C_1} \leq 1.4, \quad g_8(x) = PPF_{405}^{C_2} \leq 1.4, \quad g_9(x) = PPF_{405}^{C_3} \leq 1.4,
\]

and many more!

Divide-and-Conquer

- Step 1: Layout matchup
  - $E, G, N_{gad}, GAD$ Positioning
- Step 2: $PPF$ (40%) met (each CASMO case is 1.5s)
  - For all axial zones (PSZ, DOM, VAN1, VAN2)
- Step 3: ALL $PPF$ are met (each CASMO case is 8s)
  - For all axial zones (PSZ, DOM, VAN1, VAN2)
  - For 0%, 40%, 70% void
  - For Rodded/Unrodded conditions
- Step 4: deplete the bundle and get $k_{cold}/k_{hot}$ (each CASMO case is 2 min)
  - For all axial zones (PSZ, DOM, VAN1, VAN2)
- Step 5: Search for the best burnup & Lowest $PPF$
Large-scale Optimization

Results

Standard RL, not efficient, 14 feasible designs in about 2.5 million iterations!

Highly efficient, 80 feasible designs in only 40000 iterations!

A speedup factor of ~250 for neuroevolution!

Looking Ahead

• With **NO** human intervention, fully optimized bundle by a **neuroevolution algorithms**.
• Fuel engineers at Exelon are getting **reduced design efforts**.
• The results are **very competitive to** the designs used by Exelon/GE.
• The search can be done in **12-24 hrs** using **a modest computing power** of 32 processors!
• When scaled to the full core, **expected savings on fuel costs** are about 3 million dollars
  – Still a preliminary guess, core optimization is on the road for future work.
Robust Data-Driven Sensor Placement

Krithika Manohar
University of Washington

June 8, 2021

Collaborators
Steven L. Brunton, UW
J. Nathan Kutz, UW
Scalable + optimal sensor placement

- Measurements crucial for prediction and control of complex systems
  - Expensive to deploy
  - Spatial constraints on placement
  - Governing models unavailable

- **Our approach**: Robust, data-driven sensor placement
  - Extract low-dimensional structure from data using ML
  - Sparse sensing to determine important locations in state space
Scalable + optimal sensor placement

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- **Our approach**: Robust, data-driven sensor placement
  - Extract low-dimensional structure from data using ML
  - Sparse sensing to determine important locations in state space

Sensors for classification, [Brunton et al]
Overview

Sparse sensors/actuators [Manohar et al., IEEE CSS, 2018]
Sparse sensing for reconstruction

- Reconstruct $\mathbf{x}$ from measurements $\mathbf{y}$ in a basis of descriptive features
  - Recover coefficients $\mathbf{a}$ of $\mathbf{x}$ in basis (gappy POD, Everson & Sirovich 1995)
- Design sensing matrix $\mathbf{C}$ to minimize error covariance of estimate

\[
\mathbf{x} \approx \Phi_r \mathbf{a} \\
\mathbf{y} = \mathbf{C} \mathbf{x} + \eta \\
\approx \mathbf{C} \Phi_r \mathbf{a} + \eta \\
\hat{\mathbf{a}} = (\mathbf{C} \Phi_r)^\dagger \mathbf{y} \\
\hat{\mathbf{x}} = \Phi_r (\mathbf{C} \Phi_r)^\dagger \mathbf{y}
\]
Sparse sensing for reconstruction

- Reconstruct $\mathbf{x}$ from measurements $\mathbf{y}$ in a basis of descriptive features
  - Recover coefficients $\mathbf{a}$ of $\mathbf{x}$ in basis (gappy POD, Everson & Sirovich 1995)
- Design sensing matrix $\mathbf{C}$ to minimize error covariance of estimate

$$\text{Var}[\mathbf{a} - \hat{\mathbf{a}}] = \sigma^2 \left[ (\mathbf{C} \Phi_r)^T \mathbf{C} \Phi_r \right]^{-1}$$

$$\max_{\mathbf{C} \in \mathbb{R}^{q \times n}} \det((\mathbf{C} \Phi_r)^T \mathbf{C} \Phi_r)$$

subject to point sensors $\mathbf{C}$

Recovered signal

$$\hat{\mathbf{a}} = (\mathbf{C} \Phi_r)^\dagger \mathbf{y}$$

$$\hat{\mathbf{x}} = \Phi_r (\mathbf{C} \Phi_r)^\dagger \mathbf{y}$$

Brute-force search is NP-hard, scales combinatorially with $N$
Sparse sensing via QR pivoting

- Factor basis into orthonormal $\mathbf{Q}$, upper-triangular $\mathbf{R}$, and row permutation $\mathbf{C}$
  - Determinant objective = \textit{product of diagonal entries in $\mathbf{R}$}
  - Use pivoting to introduce diagonally dominant structure
  - \textit{Pivot indices correspond to optimal sensor locations (interpolation points in basis)}
  - Origin: empirical interpolation methods for model reduction  

\[
\Phi^T \Phi = \begin{pmatrix}
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\end{pmatrix}
\]

\[
\mathbf{C}^T = \mathbf{QR} = \mathbf{Q}
\]

\[
\mathbf{C}^T = \begin{pmatrix}
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast \\
\end{pmatrix}
\]

Drmac & Gugercin, SIAM, 2016
Robust reconstruction

- Reconstruction with minimal number of optimal sensors (compared to random)

With & Without spatial constraints
[Clark, Askham, Brunton & Kutz 2019]

\[ \gamma = 0 \]

\[ \gamma = 225 \]
Robustness

- Interpretable – each sensor corresponds to a principal component (POD mode)
- Feature basis can be adapted to downstream task
  - POD modes ordered by energy content
  - Robust PCA extracts outliers in data
  - Dynamic mode decomposition into spatial modes and frequencies
  - Balanced POD modes ordered by joint controllability and observability
- Adapt model to changing/failing sensors

POD/PCA
\[ X = \Phi \Sigma V^T \]

Robust PCA
\[ \min_{L,S} \|L\|_* + \|S\|_1 \text{ such that } L + S = X \]

DMD
\[ x(t) = \Psi \text{ diag}(\exp(\omega t))a \]
Joint sensor & actuator placement

- Optimal sensors and actuations for control
  - Leverage observable/controllable features
  - QR adapted method nearly optimal (bottom right) for linearized Ginzburg–Landau discretized model

\[ \dot{x} = Ax + Bu \]
\[ y = Cx \]
Robust sensors: predictive shimming

>99% of all predicted points have error < 0.005”


   doi.org/10.1016/j.jmsy.2018.01.011

“Resilience” is the capacity of a control system to maintain state awareness and an accepted level of operational normalcy in response to disturbances, including threats of an unexpected and malicious nature. (2009)
Resilient Control Systems Evaluation

- Physical Disturbances
  - Time Latency Affecting Stability
  - Data Integrity Affecting Stability
- Cyber Disturbances
  - Time Latency
  - Data Confidentiality, Integrity and Availability
- Cognitive Disturbances
  - Time Latency in Response
  - Data Digression from Desired Response
- Responder
  - Resources
  - Coordination
Distributed Infrastructure Cyber-Physical State Awareness

- **Distributed Physical State-awareness**
  - Capability for optimally integrating, monitoring, and controlling the distributed energy systems to prioritize the emergency response to critical infrastructure despite uncertainties.

- **Distributed Cyber State-awareness**
  - Capability for detecting and evaluating cyber threats to allow threat accommodation and reconfiguration of the proposed resilient system against attacks.
Cyber-Physical Common Operating Visualization

• Integrated Physical and Cyber State Awareness into a Visualization Engine
  − The visible aspect of this solution is the display interfaces on devices that present information to humans to make more efficient and effective emergency response
Anomaly Detection and Automated Response & Recovery

• **Cyber-Physical Detection and Analysis of Anomalies**
  - Ingestion of cyber-physical alerts
  - Tradeoff space analysis to validate mitigation benefit and physical impacts that may result
  - Role based actions at the human machine interface

• **Automated Response and Moving Target Defense**
  - Software defined network response actions to redirect or limit traffic for analysis
  - Moving target defenses to deceive actor
Transformative Research and Deployable Solutions for Inherent Infrastructure Resilience

Intelligent Cyber Detection & Feedback Mechanisms

Functional Infrastructure Dependency Modeling for Data Driven Decision Making

Role-based, Cyber-Physical State and Context Awareness

Adaptive and Agile Resilience Control Architectures

Infrastructure Trustworthiness Assessment & Proactive Control
Annual Symposium
http://www.resilienceweek.com

Join us for the Resilience Week symposium to discuss how private and public partners can work together to ensure a secure and reliable flow of energy across the nation.

• Topical/Track Areas
  − Cognitive Systems
  − Communications Systems
  − Control Systems
  − Cyber Systems
  − Critical Infrastructure
  − Communities
  − Industry

• Participants
  − DOD/DOE National Labs
  − Cyber-Control-Energy Industries
  − Universities

Plenaries for 2020

- Jamey Sample, VP CSO (Xcel Energy)
- Kimberly Denbow, Managing Director, Security & Operations (American Gas Association)
- Laura Schepis, Sr Dir, National Security (Edison Electric Institute)
- David Solan, Deputy Assistant Secretary for Renewable Power (EERE)
- Michael Pesin, Deputy Assistant Secretary for Advanced Grid Research and Development (OE)
- Qinghua Li, Associate Professor, Department of Computer Science and Computer Engineering (University of Arkansas)
- Mikhail Falkovich, Director, Information Security (Consolidated Edison Company of New York, Inc.)
- Niyo Little Thunder Pearson, Sr., CISSP, CCSP, Supervisor, Cybersecurity/Cyber Operations (ONE Gas)
- Edward Chiu, Cybersecurity Strategist (Chevron Corp.)
- Chick Macal (Argonne National Laboratory)
- Serena Reynolds, National Risk Management Center (NRMC), Cybersecurity and Infrastructure Security Agency (CISA)
- Amanda Toman, Director of 5G Initiatives (Office of the Under Secretary of Defense)
- Maria Dillard, Acting Director of Disaster and Failure Studies (Engineering Laboratory) (National Institute of Standards and Technology)
Human-Centered AI: Reliable, Safe & Trustworthy

Ben Shneiderman  @benbendc

Founding Director (1983-2000), Human-Computer Interaction Lab
Professor, Department of Computer Science

Member, National Academy of Engineering

Photo: BK Adams
Interdisciplinary research community
- Computer Science & Info Studies
- Psych, Socio, Educ, Jour & MITH

hcil.umd.edu
vimeo.com/72440805
Designing the User Interface

Design Theories

Direct manipulation
Menus, speech, search
Social Media
Information Visualization

www.cs.umd.edu/hcil/DTUI6

Sixth Edition: 2016
The University of Maryland, College Park (often referred to as the University of Maryland, Maryland, UM, UMD, UMCP, or College Park) is a public research university located in the city of College Park in Prince George's County, Maryland, approximately 4 miles (6.4 km) from the northeast border of Washington, D.C. Founded in 1856, the university is the flagship institution of the University System of Maryland. With a fall 2010 enrollment of more than 37,000 students, over 100 undergraduate majors, and 120 graduate programs,
Spotfire
Treemaps
FinViz
NodeXL
EventFlow
What is Human-Centered AI?
What is Human-Centered AI?

Amplify, Augment, Empower & Enhance People
Human-Centered AI

Human Values
Rights, Justice & Dignity
Human-Centered AI

- **Human Values**: Rights, Justice & Dignity
- **Individual Goals**: Self-efficacy, Creativity, Responsibility & Social Connections
Human-Centered AI

Human Values
Rights, Justice & Dignity

Individual Goals
Self-efficacy, Creativity, Responsibility & Social Connections

Design Aspirations
Reliable, Safe & Trustworthy
Team, Organization, Industry & Government
Human-Centered AI

- Human Values
  Rights, Justice & Dignity

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  Self-efficacy, Creativity, Responsibility & Social Connections

- Design Aspirations
  Reliable, Safe & Trustworthy
  Team, Organization, Industry & Government

Stakeholders
- Researchers
- Developers
- Business Leaders
- Policy Makers
- Users
Human-Centered AI

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Design Aspirations
Reliable, Safe & Trustworthy
Team, Organization, Industry & Government

Stakeholders
Researchers
Developers
Business Leaders
Policy Makers
Users

Threats
Malicious Actors
Bias
Flawed Software
Human-Centered AI

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Reliable, Safe & Trustworthy
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Stakeholders
Researchers
Developers
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HCAI Framework

Threats
Malicious Actors
Bias
Flawed Software
Human-Centered AI

Stakeholders:
- Researchers
- Developers
- Business Leaders
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- Users

Human Values
- Rights, Justice & Dignity

Individual Goals
- Self-efficacy, Creativity, Responsibility & Social Connections

Design Aspirations
- Reliable, Safe & Trustworthy
- Team, Organization, Industry & Government

HCAI Framework

Design Metaphors

Threats:
- Malicious Actors
- Bias
- Flawed Software
Human-Centered AI

Stakeholders
- Researchers
- Developers
- Business Leaders
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- Users

Threats
- Malicious Actors
- Bias
- Flawed Software

Human Values
Rights, Justice & Dignity

Individual Goals
Self-efficacy, Creativity, Responsibility & Social Connections

Design Aspirations
Reliable, Safe & Trustworthy
Team, Organization, Industry & Government

HCAI Framework

Design Metaphors

Governance Structures

Oxford University Press (Early 2022) https://hcil.umd.edu/human-centered-ai/
Supertools

Digital Camera Controls

Navigation Choices

Texting Autocompletion

Spelling correction
Active Appliances

Coffee maker, Rice cooker, Blender

Dishwasher, Clothes Washer/Dryer

Cuisinart Grind & Brew Coffee Maker

Panasonic Rice Cooker

Nutri Ninja Blender

Miele Dishwasher

General Electric Washer

General Electric Dryer
Implanted Cardiac Pacemakers
NASA Mars Rovers are Tele-Operated
Da Vinci Tele-Operated Surgery

“Robots don’t perform surgery. Your surgeon performs surgery with da Vinci by using instruments that he or she guides via a console.”

https://www.davincisurgery.com/
Bloomberg Terminal
Hospital Control Center
Counter Terrorism Center
Governance Structures for Human-Centered AI

GOVERNMENT REGULATION

INDUSTRY:
Trustworthy Certification: External Reviews

ORGANIZATION:
Safety Culture: Organizational Design

TEAM:
Reliable Systems: Software Engineering
Technical Practices:
- Audit Trails, SE Workflows
- Verification & Bias testing
- Explainable UIs

Management Strategies:
- Leadership Commitment
- Hiring & Training
- Failures & Near Misses
- Internal Reviews
- Industry Standards

Independent Oversight:
- Auditing Firms
- Insurance Companies
- NGOs & Civil Society
- Professional Societies

Governance Structures for Human-Centered AI

**GOVERNMENT REGULATION**

**INDUSTRY:**
Trustworthy Certification: External Reviews

**ORGANIZATION:**
Safety Culture: Organizational Design

**TEAM:**
Reliable Systems: Software Engineering
  Technical Practices:
  - Audit Trails, SE Workflows
  - Verification & Bias testing
  - Explainable UIs

**MANAGEMENT STRATEGIES:**
- Leadership Commitment
- Hiring & Training
- Failures & Near Misses
- Internal Reviews
- Industry Standards

**INDEPENDENT OVERSIGHT:**
- Auditing Firms
- Insurance Companies
- NGOs & Civil Society
- Professional Societies

*ACM TIIS (Oct 2020) [https://dl.acm.org/doi/10.1145/3419764](https://dl.acm.org/doi/10.1145/3419764)*
Reliable systems based on software engineering practices

1) Audit trails and analysis tools
2) Software engineering workflows
3) Verification & validation testing
4) Bias testing to improve fairness
5) Explainable user interfaces
Reliable systems based on software engineering practices

1) Audit trails and analysis tools
2) Software engineering workflows
3) Verification & validation testing
4) Bias testing to improve fairness
5) Explainable user interfaces
Reliable Systems
Software engineering practices for a TEAM

1) Audit trails and analysis tools

“Flight Data Recorder for Every Robot”

- Retrospective analysis of failures
  - Understanding near misses
- Analysis to support preventive maintenance
Reliable Systems
Software engineering practices for a TEAM

5) Explainable user interfaces

- Retrospective explanations (local & global)

New Goal: **Prevent** confusion and surprise -

Prospective user interfaces
- Interactive, visual, exploratory
Mortgage Loan Explanations

Post-hoc Report

<table>
<thead>
<tr>
<th>Enter amounts to request mortgage:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mortgage amount requested</td>
<td>375000</td>
</tr>
<tr>
<td>Household monthly income</td>
<td>7000</td>
</tr>
<tr>
<td>Liquid assets</td>
<td>48000</td>
</tr>
<tr>
<td>Submit</td>
<td></td>
</tr>
</tbody>
</table>
Mortgage Loan Explanations

Post-hoc Report

Enter amounts to request mortgage:

<table>
<thead>
<tr>
<th>Description</th>
<th>Amount</th>
</tr>
</thead>
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Submit

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</tr>
<tr>
<td>Liquid assets</td>
<td>48000</td>
</tr>
</tbody>
</table>

We’re sorry, your mortgage loan was not approved. You might be approved if you reduce the Mortgage amount requested, increase your Household monthly income, or increase your Liquid assets.

Done
Post-hoc Report

Enter amounts to request mortgage:

- Mortgage amount requested: 375000
- Household monthly income: 7000
- Liquid assets: 48000

Submit

Prospective User Interface

Adjust sliders to report your situation:

- Mortgage amount requested: 375000
- Household monthly income: 7000
- Liquid assets: 48000

Score needed for approval

Your score

We’re sorry, your mortgage loan was not approved. You might be approved if you reduce the Mortgage amount requested, increase your Household monthly income, or increase your Liquid assets.

Done
Recommenders: Whichbook.net
Recommender Control Panels

Modify Attributes
- Acousticness: 40
- Instrumentalness: 60
- Danceability: 80
- Valence: 60
- Energy: 40

Recommended Songs
- Oblivion
- Grimes
- My December
- Linkin Park
- I've got that tune
- Chinese Man
- Got the Life
- Korn
- Good Riddance (Time of Y... Green Day
- Burn It To The Ground
- Nickelback

Slider technique

Create Your Better Life Index

Rate the topics according to their importance to you:

- Housing
- Income
- Jobs
- Community
- Education
- Environment
- Civic Engagement
- Health
- Life Satisfaction
- Safety
- Work-Life Balance
Human-Centered AI

- **Human Values**: Rights, Justice & Dignity
- **Individual Goals**: Self-efficacy, Creativity, Responsibility & Social Connections
- **Design Aspirations**: Reliable, Safe & Trustworthy Team, Organization, Industry & Government
- **HCAI Framework**
- **Design Metaphors**
- **Governance Structures**

**Stakeholders**:
- Researchers
- Developers
- Business Leaders
- Policy Makers
- Users

**Threats**:
- Malicious Actors
- Bias
- Flawed Software

Oxford University Press (Early 2022)  https://hcil.umd.edu/human-centered-ai/
Governance Structures for Human-Centered AI

GOVERNMENT REGULATION

INDUSTRY:
Trustworthy Certification:
External Reviews

ORGANIZATION:
Safety Culture:
Organizational Design

TEAM:
Reliable Systems:
Software Engineering
Technical Practices:
Audit Trails, SE Workflows
Verification & Bias testing
Explainable UIs

Management Strategies:
Leadership Commitment
Hiring & Training
Failures & Near Misses
Internal Reviews
Industry Standards

Independent Oversight:
Auditing Firms
Insurance Companies
NGOs & Civil Society
Professional Societies


Human-Centered Artificial Intelligence: Three fresh ideas,  
*AIS Trans. on Human-Computer Interaction* 12, 3 (Oct 2020).  https://aisel.aisnet.org/thci/vol12/iss3/1/


**Summary & resources:** https://hcil.umd.edu/human-centered-ai/
The Future is Human-Centered

Google Group
https://groups.google.com/g/human-centered-ai

Twitter Account
@HumanCenteredAI

Website
https://hcai.site
The Future is Human-Centered
Designing Explainable AI
Why do we need to design explainable ML/AI?

- Because of its application to things that matter.
  - Critical infrastructure instead of cereal selection
- ML/AI is inscrutable at scale
  - We don’t really understand in a fundamental way how these algorithms work. (Mickens, 2018)
- Stochasticity isn’t a good explanation, e.g. gradient descent

Designing for inscrutability – Role of Human Centered design
Human Centered Design from day one

• Involvement of human factors is critical
  - Model implications
  - Measure implications
  - Every aspect of the model needs to be explainable.
    • Impossible to predict what may need to be explained.

• Why human factors?
  - AI/ML is often an inscrutable black box, do you know what else is an inscrutable black box?
Dave!

- Any resemblance to any “Daves” living or dead is purely coincidental.
- Your HF colleagues have spent their career understanding and designing for Daves.
- Designing for inscrutability is human factors at its core.
- Late or no involvement of HF will lead to an AI/ML algorithm that is not transparent, explainable, or trustworthy and therefore unfit for use in critical human infrastructure.
Predictive maintenance project

- Predicting the health of a circulating water pump
  - XAI/HCAI as communication
  - What if we could only talk to the model?

  "How do you know?"
  "What is specifically wrong?"
  "How ‘unhealthy’ – how bad is it doc?"
  "Are you sure?"
  "Which sensors are you seeing?"
  "What should we do?"

Unhealthy

Can the model answer these? Clearly, precisely, and verifiably?
Predictive maintenance project (cont.)

• HF researchers worked closely with the model development team to shape the specific user questions that the model needed to support.
• Your ultimate visualization and display has to support the aspects of explainability.
• By working with modelers, we were able to explore different methods of interpretability like SHAP, feature interaction, and feature importance.
• Currently in the process of testing prototype visualization with users and will have feedback on adjustments to the model moving forward.
Designing for trust, and failure

- AI/ML algorithms will fail and will fall under scrutiny
- Consider how to explain the model to:
  - Regulators
  - Policy makers
  - The courts
  - Operators
  - Lay people
  - Communities
- When it fails, what does it do? How does it communicate?
Explainable Dimensionality Reduction Using Scientific Constraints

Ramakrishnan Kannan
Group Lead, Discrete Algorithms
https://ramkikannan.github.io
https://github.com/ramkikannan
https://ramkikannan.github.io/planc-api
Acknowledgements

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- Students - Srinivas Eswar (GATech), Koby Hayashi(Wake Forest), Jeff Graves (TNTech), Rina Singh(TNTech), Mosharraf Hossain (TNTech), Luna Xu (VATEch), Sekeong Hong (NCSU), Euna Kim(GATech), Seema Chouhan(UMASS), Mark Heimann(Umich), Pravallika Devineni (UCR), Thomas Blum(UCI)
Unmixing

- Understanding terrestrial information in an unknown place from satellite images
- Identifying presence of hidden unknown/foreign bodies in a scanned image - Eg., contamination in food articles, camouflaged explosives etc.
- Biological application - spectral karyotyping, immunofluorescence, live-cell imaging, drug discovery, and tissue pathology – Eg., Unmixing on Spectral imaging of the stained tissues using multiple dyes.
- Physics and Material Sciences – Mapping properties to end-members. Comparing different materials
Matrix Factorization (MF)

$$X \approx UV$$

Input

Features

Representatives

Samples

Samples distribution over representatives

Low Rank Factors

Dimensionality Reduction – ML Community
Inverse Problem – Scientific Community
Low Rank Approximation – Numerical Community
Matrix Factorization – Internet community
Example 1: NMF vs. PCA

Both PCA and NMF are insufficient.
They do not consider the neighbourhood information.
To consider this information, we use regularization.

TOF SIMS Data – Collaboration w/ Anton
Atomic Motion of MoSe2 – (https://smc-datachallenge.ornl.gov)

\[
\min_{L,S} \|A - L - S\|_F^2
\]
subject to
\[\text{rank}(L) \leq r; \quad \text{card}(S) \leq k\]

Symmetric NMF

\[
\min_{H \geq 0} \|A - HH^T\|_F^2.
\]

- ANLS Variant
  \[
  \min_{(W,H) \geq 0} \|A - WH^T\|_F^2 + \gamma \|W - H\|_F^2.
  \]
- Gauss Newton based Conjugate Gradient
  – Computing Gradient
  – Applying Gramian of Jacobian
  \[
  x^{(t+1)} = x^{(t)} + \arg\min_p \left\| J(t) p + r(t) \right\|_2^2.
  \]

Algorithm 2 \([W,H] = \text{SymGNCG}(A,k,s_{\text{max}})\)

Require: \(A \in \mathbb{R}^{n \times n}\) is distributed across a \(\sqrt{p} \times \sqrt{p}\) grid of processors, \(k > 0\) is rank of approximation, \(p\) divides \(n\)

Require: Local matrices: \(H_{ij}, X_{ij}, P_{ij}, R_{ij}, Y_{ij}\) are \(n/p \times k\)

1: Proc \(p_{ij}\) initializes \(H_{ij}\)
2: while stopping criteria not satisfied do
3: \(X = 0\) \% Initialize \(x_0 = 0\)
4: \(R = \text{Compute-Gradient}(A,H)\) \% \(r = b - Jx_0\)
5: \(p_{ij}\) sets \(P_{ij} = R_{ij}\) \% \(P = r\)
6: \(p_{ij}\) computes \(c_{ij} = (R_{ij}, R_{ij})\)
7: compute \(c_i = \sum_j c_{ij}\) using all-reduce across all procs
8: for \(s = 1\) to \(s_{\text{max}}\) do
9: \(Y = \text{Apply-Gramian}(H,P)\) \% \(y = J^T p\)
10: \(p_{ij}\) computes \(\alpha_{ij} = c_{ij}/(R_{ij}, P_{ij})\)
11: compute \(\alpha = \sum_r \alpha_{ij}\) using all-reduce across all procs
12: \(p_{ij}\) computes \(X_{ij} = X_{ij} + \alpha P_{ij}\) \% \(x = x + \alpha p\)
13: \(p_{ij}\) computes \(R_{ij} = R_{ij} - \alpha Y_{ij}\) \% \(r = r - \alpha y\)
14: \(p_{ij}\) computes \(e_i = (R_{ij}, R_{ij})\)
15: compute \(e = \sum_i e_i\) using all-reduce across all procs
16: \(p_{ij}\) computes \(P_{ij} = R_{ij} + (e/\alpha_{ij}) P_{ij}\) \% \(p = r + \beta p\)
17: end for
18: \(p_{ij}\) computes \(H_{ij} = [H_{ij} - X_{ij}]_+\) \% projected GN step
19: end while
Ensure: \(H = \arg\min_{H \geq 0} \|A - HH^T\|_F^2\)
Ensure: \(H\) is \(n \times k\) row-wise distributed across processors

Table I

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>flops (\frac{4n^2k}{p} \pm O\left(\frac{n{k^2}}{p}\right))</th>
<th>words (\frac{n{k^2}}{\sqrt{p}} + k^2)</th>
<th>messages (O(\log p))</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANLS</td>
<td>(\frac{2n^2k}{p} \pm O\left(\frac{s_{\text{max}}n^2}{p}\right))</td>
<td>(\frac{n{k^2}}{\sqrt{p}} + s_{\text{max}}k^2)</td>
<td>(O(s_{\text{max}}\log p))</td>
</tr>
</tbody>
</table>

S. Eswar, K. Hayashi, G. Ballard, R. Kannan, H. Park and R. Vuduc: Distributed-Memory Parallel Symmetric Non-negative Matrix Factorization. Accepted at SC’20
Hierarchical Non-negative Matrix Factorization

L. Manning, G. Ballard, R. Kannan, H. Park: Parallel Hierarchical Clustering using Rank-Two Nonnegative Matrix Factorization. Communicated to HiPC’2020

Recursively solve a Rank-2 NMF

\[
\begin{align*}
\min_{\hat{h}_{i,1}, \hat{h}_{i,2} \geq 0} \| w_1 \begin{bmatrix} \hat{h}_{i,1} \\ \hat{h}_{i,2} \end{bmatrix} - a_i \| \\
= \min_{\hat{h}_{i,1}, \hat{h}_{i,2} \geq 0} \| \hat{h}_{i,1} w_1 + \hat{h}_{i,2} w_2 - a_i \|
\end{align*}
\]

Algorithm 2 Hierarchical Clustering [15]

```
Require: A is m \times n, k is target number of leaf clusters
1: function \( T = \text{HIER-R2-NMF}(A) \)
2: \( \mathcal{R} = \text{node}(A) \) % create root node
3: \( \text{SPLIT}(\mathcal{R}) \)
4: \( \text{inject}(\mathcal{Q}, \mathcal{R} \text{.left}) \) % create priority queue
5: \( \text{inject}(\mathcal{Q}, \mathcal{R} \text{.right}) \) % of frontier nodes
6: while size(\( \mathcal{Q} \)) < k do
7: \( \mathcal{N} = \text{eject}(\mathcal{Q}) \) % frontier node with max score
8: \( \text{SPLIT}(\mathcal{N} \text{.left}) \) % split left child
9: \( \text{inject}(\mathcal{Q}, \mathcal{N} \text{.left}) \) % and add to \( \mathcal{Q} \)
10: \( \text{SPLIT}(\mathcal{N} \text{.right}) \) % split right child
11: \( \text{inject}(\mathcal{Q}, \mathcal{N} \text{.right}) \) % and add to \( \mathcal{Q} \)
12: end while
13: end function
```

Ensure: \( T \) is binary tree rooted at \( \mathcal{R} \) with \( k \) frontier nodes, each node has subset of cols of \( A \) and feature vector \( w \)

Figure 1: Hierarchical Clustering of DC Mall HSI

Figure 2: Hierarchy node classification
Multifrontal NMF (MFNMF)

Piyush Sao, Ramakrishnan Kannan: Multifrontal Non-negative Matrix Factorization. PPAM (1) 2019: 543-554
Dense Tensor Factorization
Dimensionality Reduction in Scientific Data

- Multimodal characterization of materials – comprehensive characterization from chemical composition to functional properties on the nanoscale

Thanks: Anton Ievlev
<table>
<thead>
<tr>
<th>technique</th>
<th>dimensionality</th>
<th>target data set</th>
<th>target data size</th>
</tr>
</thead>
<tbody>
<tr>
<td>band excitation piezoresponse force microscopy (BE-PFM)</td>
<td>3D, space and $\omega$</td>
<td>$(256 \times 256) \times 64$</td>
<td>32 MB</td>
</tr>
<tr>
<td>switching spectroscopy PFM (SS-PFM)</td>
<td>3D, space and $\omega$</td>
<td>$(64 \times 64) \times 128$</td>
<td>4 MB</td>
</tr>
<tr>
<td>time relaxation PFM (TR-PFM)</td>
<td>3D, space and time</td>
<td>$(64 \times 64) \times 128$</td>
<td>4 MB</td>
</tr>
<tr>
<td>AC sweeps</td>
<td>4D, space, $\omega$, voltage</td>
<td>$(64 \times 64) \times 64 \times 256$</td>
<td>512 MB</td>
</tr>
<tr>
<td>BE polarization switching (BEPS)</td>
<td>4D, space, $\omega$, voltage</td>
<td>$(64 \times 64) \times 64 \times 128$</td>
<td>256 MB</td>
</tr>
<tr>
<td>BE thermal</td>
<td>4D, space, $\omega$, temperature</td>
<td>$(64 \times 64) \times 64 \times 256$</td>
<td>512 MB</td>
</tr>
<tr>
<td>time relaxation BE (TR-BE)</td>
<td>4D, space, $\omega$, time</td>
<td>$(64 \times 64) \times 64 \times 64$</td>
<td>64 MB</td>
</tr>
<tr>
<td>FORC BEPS</td>
<td>5D, space, $\omega$, voltage, voltage</td>
<td>$(64 \times 64) \times 64 \times 64 \times 16$</td>
<td>2 GB</td>
</tr>
<tr>
<td>time relaxation on sweep, BE</td>
<td>5D, space, $\omega$, voltage, time</td>
<td>$(64 \times 64) \times 64 \times 64 \times 64$</td>
<td>16 GB</td>
</tr>
<tr>
<td>FORC time BE</td>
<td>6D, space, $\omega$, voltage, voltage, time</td>
<td>$(64 \times 64) \times 64 \times 64 \times 16 \times 64$</td>
<td>128 GB</td>
</tr>
<tr>
<td>FORC IV BEPS</td>
<td>5D, space, $\omega$, voltage, cycle</td>
<td>$(64 \times 64) \times 64 \times 64 \times 16$</td>
<td>4 GB</td>
</tr>
<tr>
<td>FORC IV and FORC IV-Z</td>
<td>4D, space, voltage, cycle</td>
<td>$(64 \times 64) \times 64 \times 20$</td>
<td>200 MB</td>
</tr>
<tr>
<td>time-resolved Kelvin probe force microscopy (KPFM)</td>
<td>3D, space, time</td>
<td>$(60 \times 20) \times 1 \times 10^3$</td>
<td>8 MB</td>
</tr>
<tr>
<td>open loop (OL) BE KPFM</td>
<td>4D, space, $\omega$, voltage</td>
<td>$(256 \times 256) \times 32 \times 16$</td>
<td>256 MB</td>
</tr>
<tr>
<td>general-mode PFM (G-PFM)</td>
<td>3D, space and voltage</td>
<td>$(256 \times 256) \times 1.6 \times 10^4$</td>
<td>4 GB</td>
</tr>
<tr>
<td>G-mode voltage spectroscopy (G-VS)</td>
<td>ND, space, voltage</td>
<td>$(256 \times 256) \times 1.6 \times 10^6$</td>
<td>400 GB</td>
</tr>
</tbody>
</table>
Existing DR for NHOT - Matricization

- Works only when some of the dimensions are independent
- Matricizing NHOT is non-trivial
NTF and Piezoresponse Force Spectroscopy

- 3600 Vectorized Spatial Locations
- 128 Time Steps
- 16 different voltage steps

Fig. 4 NTF analysis on dynamic piezoresponse force microscopy data. Components 1–4 are shown in a–d, respectively, with corresponding relaxation behavior (time tensor factor, red) and voltage dependence (voltage tensor factor, green) plots. Large color maps correspond to normalized abundance maps for individual components. Kelley, K.P., Li, L., Ren, Y. et al. Tensor factorization for elucidating mechanisms of piezoresponse relaxation via dynamic Piezoresponse Force Spectroscopy. npj Comput Mater 6, 113 (2020).
FLOPS vs Parameterization – Spatial Data

Pravi Devineni, Vagelis Papalexakis, Ramakrishnan Kannan
Convolutional Autoencoder

- Encoder:
  - Conv layer \((d \times d)\)
  - Fully connected layer
  - Fully connected layer
  - Conv Transpose layer \((d \times d)\)

- Decoder:

Accuracy

Size of the network

Network size compared to ConvAE

OAK RIDGE
National Laboratory
Thank You
Thank you