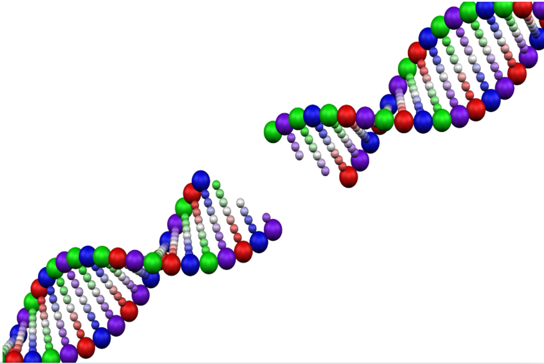
AI-AUGMENTED NANOSCIENCE

Seminar

June 5th, 2025



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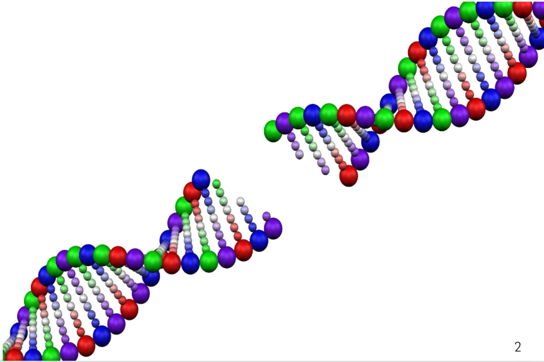
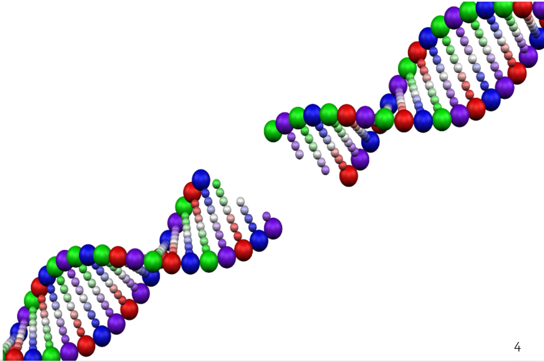


WHY AI IS CRUCIAL FOR NANOSCIENCE TODAY?

- Data Explosion (Big Data): Techniques like TEM, AFM, advanced spectroscopies, and molecular dynamics simulations generate terabytes of data. AI is essential for processing, analyzing, and extracting knowledge.
- Unlimited Design Space: The combination of nanoscale elements offers an almost infinite number of possibilities. AI allows efficient exploration, identifying promising candidates.
- Process Optimization: Precision in nanofabrication and synthesis demands unprecedented control. AI can optimize experimental parameters in real-time.
- Accelerated Discovery (Materialomics): Drastically reduce design-synthesis-characterization-test cycles from years to months or weeks.
- Complex Quantum Phenomena: At nanoscale, quantum effects dominate. AI helps model and understand these computationally intensive phenomena.

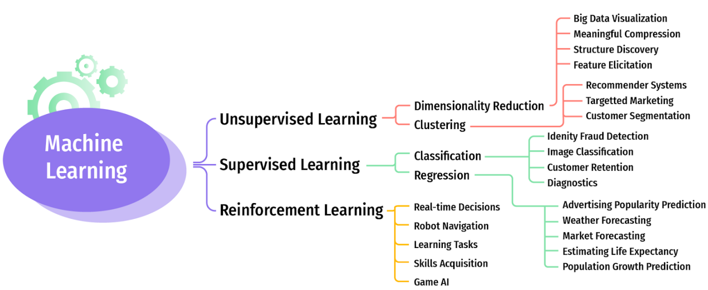


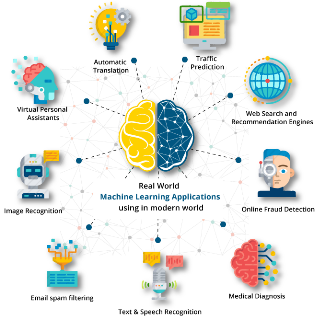
MACHINE LEARNING

Definition

Machine Learning deals with algorithms and models that enable machines to learn and improve automatically from data without being explicitly programmed.

- Importance: Great capacity to process large volumes of data and extract valuable information.
- Applications: Medicine and healthcare, industrial automation, intelligent transportation, logistics, finance, and potentially any human activity.





MACHINE LEARNING

Definition

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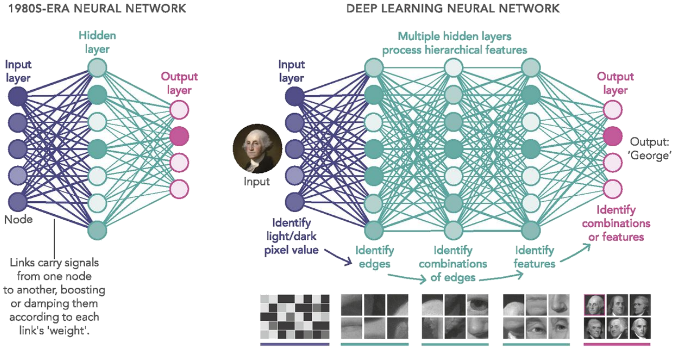
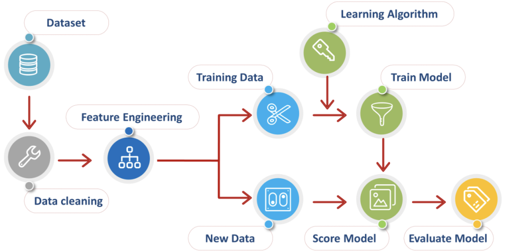


SUPERVISED LEARNING: PREDICTING NANOMATERIAL PROPERTIES

Supervised Learning uses labeled data (input-output pairs) to learn a mapping function. The model tries to find patterns in the data to make accurate predictions on new, unseen data.

Regression: Predicting a continuous numerical value.

- Nanoscience example: Predicting the bandgap (energy gap), Young's modulus (stiffness), or thermal conductivity of a novel nanomaterial based on its atomic structure, composition, and processing parameters.
- Why it's useful: Accelerates the discovery of materials with desired properties, reducing costly and time-consuming experimental trials.



Classification: Assigning data points to discrete categories or classes.

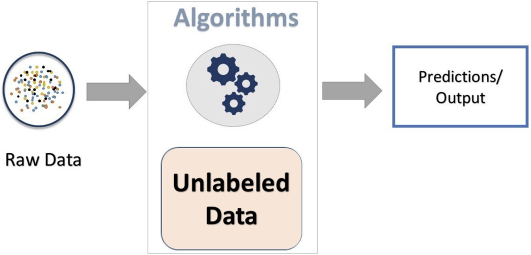
- Nanoscience Example: Classifying nanoparticles by shape (e.g., spherical, cubic, rod-like) directly from electron microscopy images, or identifying if a newly synthesized material is a semiconductor, insulator, or metal.
- Why it's useful: Automates quality control, material identification, and characterization analysis, leading to faster research cycles.

UNSUPERVISED LEARNING: DISCOVERING HIDDEN STRUCTURES

Algorithms work with unlabeled data to discover hidden structures, patterns, or relationships without prior knowledge of the output. It's about finding inherent order in the data.

Clustering: Grouping similar data points into distinct clusters.

- Nanoscience example: Automatically grouping nanomaterials based on similar spectroscopic signatures (e.g., Raman, FTIR spectra) to identify different phases or chemical compositions without manual peak assignment. Also, identifying distinct defects or growth patterns in a large set of microscopy images.
- Why it's useful: Reveals unknown relationships, simplifies data exploration, and helps categorize complex datasets from high-throughput experiments.



Dimensionality Reduction: Simplifying high-dimensional data while preserving essential information.

- Nanoscience example: Analysing massive datasets from molecular dynamics simulations to identify the most relevant atomic coordinates or collective variables that describe a material's behavior or phase transition. Also, extracting key features from complex image datasets for more efficient processing.
- Why it's useful: Makes complex data more manageable, reduces computational load for downstream analysis, and helps visualize high-dimensional information.

REINFORCEMENT LEARNING: AUTONOMOUS NANOSCIENCE EXPERIMENTS

An agent learns to make sequential decisions in an environment to maximize a cumulative reward. It operates through trial and error, getting feedback from its actions to optimize its strategy.

Autonomous experimentation:

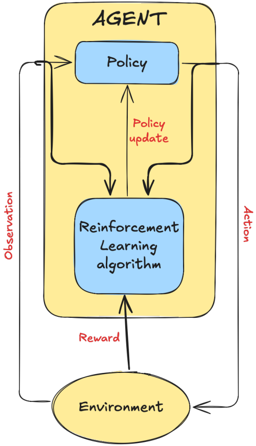
- Nanoscience example: An RL agent controlling an atomic force microscope (AFM) or a scanning tunneling microscope (STM) to autonomously manipulate individual atoms or molecules on a surface, learning the optimal manipulation path to achieve a desired nanostructure.
- Why it's useful: Enables robotic precision at the nanoscale, accelerates the assembly of complex nanostructures, and pushes the boundaries of nanofabrication.

Automated synthesis optimisation:

- Nanoscience example: Optimising reaction parameters (temperature, pressure, precursor concentration, mixing rates) in automated material synthesis setups to achieve specific nanomaterial properties (e.g., precise size, morphology, or defect density), with the RL agent receiving rewards for successful synthesis outcomes.
- Why it's useful: Reduces human intervention, accelerates the discovery of optimal synthesis routes, and improves the reproducibility and scalability of nanomaterial production.

Adaptive sensing and characterisation:

- Nanoscience example: An RL agent controlling a nanosensor network to adaptively adjust sensing parameters or probe locations based on real-time data, optimising for anomaly detection or efficient mapping of a nanoscale environment.
- Why it's useful: Enhances the efficiency and intelligence of sensing platforms for diagnostics, environmental monitoring, or in-situ material characterization.



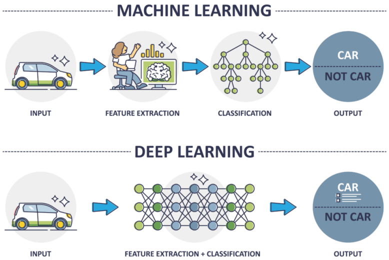
DEEP LEARNING: ADVANCED NEURAL NETWORK LEARNING

What is Deep Learning?

A subfield of Machine Learning that uses artificial neural networks with multiple layers (hence deep) to analyse data of superior complexity. These networks learn hierarchical representations of data.
Advantages: Excellent for handling complex, high-dimensional data like images, spectra, time series, and structural data.

Importance in Nanoscience

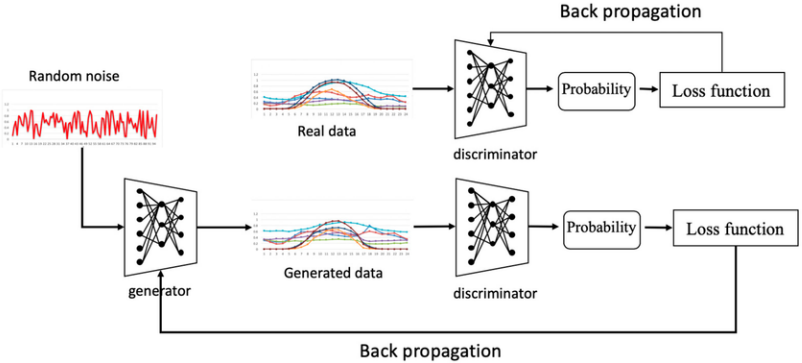
- Nanoscopic image analysis: Deep Learning excels at processing and analysing large sets of complex images obtained from electron microscopy, atomic force microscopy (AFM), etc., enabling automatic identification and classification of nanostructures, defects, and patterns.
- Materials discovery: It can model complex relationships between a nanomaterial's atomic/molecular structure, its composition, and its properties (optical, electronic, mechanical), accelerating the design of new materials with specific functionalities.
- Atomic-scale simulations: Deep Learning can learn from data generated by computational simulations (e.g., molecular dynamics) to predict the behaviour of nanosystems, reducing the need for costly calculations.
- Control and optimisation of nanoscopic processes: It can be used to optimise synthesis parameters for nanomaterials or to control nanoscopic devices with high precision.



DEEP LEARNING (GANS)

Autoencoders and GANs (Generative Adversarial Networks): Generative neural networks that can create new data resembling training data.

- Generation of new molecular or crystalline structures with desired properties.
- Creation of synthetic microscopy data to augment training datasets.

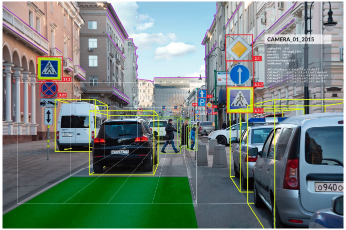


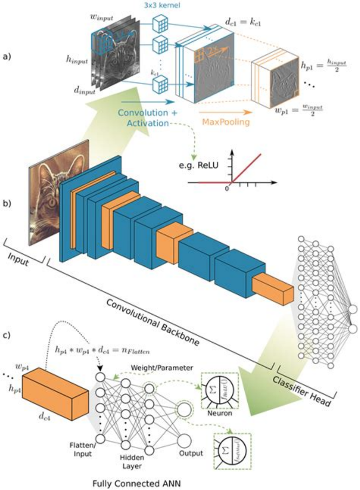
DEEP LEARNING (COMPUTER VISION)

Definition

Computer Vision is a branch of AI focused on developing algorithms and techniques that enable machines to understand and analyse images and videos.

- Importance: Allows machines to perceive and understand the visual world similarly to humans.
- Applications: Object detection, motion tracking, facial recognition, autonomous vehicles, among others.

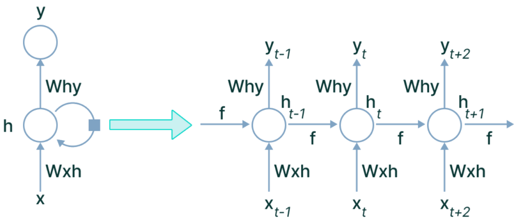


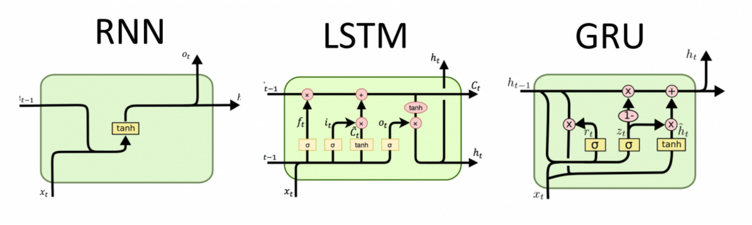


DEEP LEARNING (CNNS AND RNNS)

Relevant Architectures in Nanoscience:

- Convolutional Neural Networks (CNNs): Designed for grid-topology data, like images.
  - Analysis of microscopy images (TEM, SEM, AFM) for defect detection, nanoparticle segmentation, or morphology classification.
  - Pattern identification in X-ray diffraction or electron microscopy patterns.
- Recurrent Neural Networks (RNNs/LSTMs): Suitable for sequential data or time series.
  - Real-time analysis of nanoparticle growth sequences.
  - Modeling the evolution of material properties under stress or temperature.

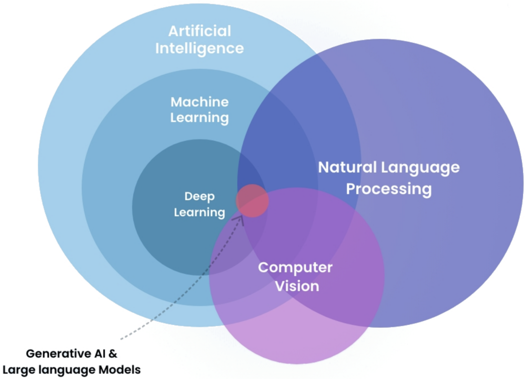




NATURAL LANGUAGE PROCESSING

Application of AI techniques to understand, interpret, and generate human language.
Essential for:

- Information extraction: Analysing vast scientific literature (articles, patents) to discover hidden relationships between nanomaterials, properties, synthesis methods, and applications.
- Database construction: Automating the creation of structured databases from unstructured text, accelerating data curation for ML.
- Hypothesis generation: Identifying emerging trends or promising material/property combinations for future research.
- Summarisation and classification: Automatically summarising scientific articles or classifying documents by nanoscience topics.



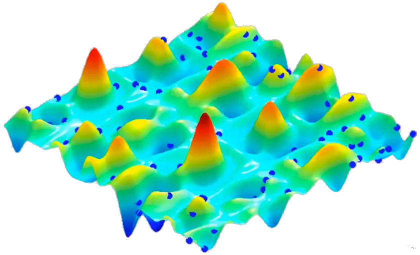
SWARM INTELLIGENCE: GUIDING NANOMATERIAL DESIGN

- Swarm Intelligence: A computational paradigm inspired by the collective behaviour of decentralised, self-organised systems (e.g., bird flocks, ant colonies). SI algorithms are well-suited for complex optimisation problems.
- Particle Swarm Optimisation (PSO): A specific Swarm Intelligence technique where a swarm of particles explores a search space, adjusting their trajectories based on their own best-found position and the best position found by the entire swarm.

PSO in Nanoscience: Applications

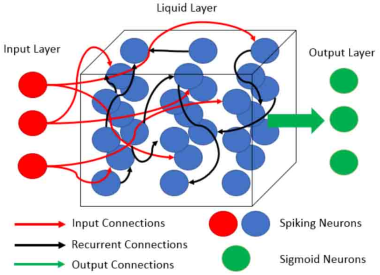
- Nanomaterial Synthesis Optimisation: PSO can optimise the parameters involved in the synthesis of nanomaterials (e.g., temperature, reactant concentrations, reaction time) to achieve desired properties like size, shape, and crystallinity.
- Nanostructure design: PSO can be used to find the optimal arrangement of atoms or molecules in a nanostructure to achieve specific functionalities (e.g., maximising optical absorption, enhancing catalytic activity).
- Spectroscopic data Analysis: PSO can help in the analysis of complex spectroscopic data (e.g., Raman, XPS) to identify and quantify different components or phases in nanomaterials.
- Control of nanodevices: PSO can be employed to optimise the control parameters of nanodevices (e.g., adjusting voltages on an array of nanoelectrodes) to achieve specific operational characteristics.

- Rapid convergence
- Derivative-Free optimisation
- Escaping local optima



RESERVOIR COMPUTING: A SHALLOW LEARNING APPROACH

- Definition: Reservoir Computing (RC) is a neural network paradigm characterised by a randomly connected recurrent neural network (the reservoir) that remains fixed during training. Only the output layer is trained.
- Shallow Learning Core: RC inherently leverages shallow learning because the complex, non-linear feature extraction happens automatically and implicitly within the fixed reservoir. The actual learning (weight optimisation) occurs solely at the single, linear readout layer.
- Efficiency and simplicity: This approach dramatically simplifies the training process compared to traditional recurrent neural networks (RNNs), as only the output weights need to be adjusted. It avoids the vanishing/exploding gradient problems common in deep RNN training.



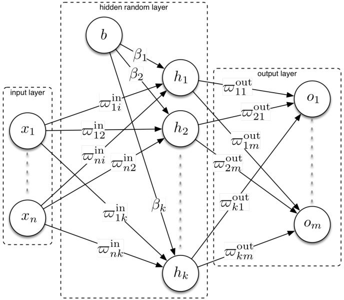
Why Reservoir Computing is considered Shallow Learning:

- Fixed feature space: The reservoir, once initialised, projects the input data into a high-dimensional, non-linear feature space. This feature engineering is done by the fixed, random connections.
- Single trainable layer: The subsequent learning algorithm (e.g., linear regression, SVM) operates on these pre-computed reservoir states, essentially performing a shallow classification or regression task on the transformed features.
- No backpropagation through hidden layers: Unlike deep learning, RC doesn't require backpropagating errors through multiple hidden layers of the reservoir, reinforcing its shallow learning nature.

EXTREME LEARNING MACHINES (ELMS)

What are ELMs? Extreme Learning Machines are a type of feedforward neural network for classification, regression, clustering, sparse approximation, and feature learning. They're a simplified version of single-hidden layer feedforward networks.

- Random hidden layer: Unlike traditional neural networks where all weights are tuned, ELMs randomly assign the input weights and biases of the hidden layer. These parameters remain fixed.
- Analytical output layer solution: The only part that needs to be learned is the output layer's weights. This is done analytically, usually through a single step of generalized inverse (Moore-Penrose pseudoinverse), rather than iterative gradient descent.
- Speed and efficiency: This learn-it-all-at-once approach makes ELMs incredibly fast to train, often orders of magnitude quicker than backpropagation-based algorithms, while still achieving competitive generalization performance.



Advantages of ELMs:

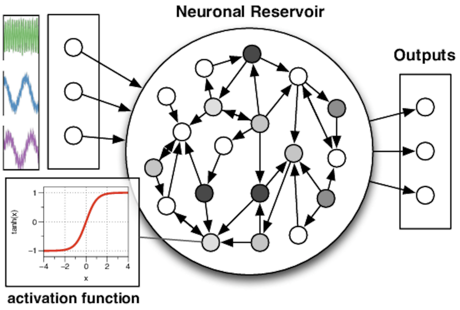
- Extremely fast training: Due to the analytical solution for output weights.
- Good generalization performance: Often comparable to more complex deep learning models, especially on certain tasks.
- No iterative tuning: Eliminates issues like local minima, learning rate selection, and stopping criteria common in gradient descent.

Disadvantages:

- Random initialization sensitivity: Performance can sometimes vary depending on the random initialization of the hidden layer.
- Scaling with large hidden layers: Computing the pseudoinverse can become computationally intensive for very large numbers of hidden nodes.

ECHO STATE NETWORKS

- Echo State Networks (ESN) are a specific type of Recurrent Neural Network that fall under the broader Reservoir Computing (RC) paradigm. They are designed for processing sequential data.
- Fixed recurrent layer (Reservoir): The core is a randomly initialized, sparsely connected recurrent neural network (the reservoir). The connections within this reservoir are fixed after initialization.
- The Echo State property: A crucial requirement for an ESN to function effectively is the echo state property. This property ensures that the internal state of the reservoir is a fading memory of the input history, meaning the influence of past inputs decays over time.
- Output layer training: Only the weights connecting the reservoir's states to the output layer are trained. This training is typically a simple linear regression (e.g., using pseudoinverse), making ESNs incredibly fast and efficient to train compared to traditional RNNs.



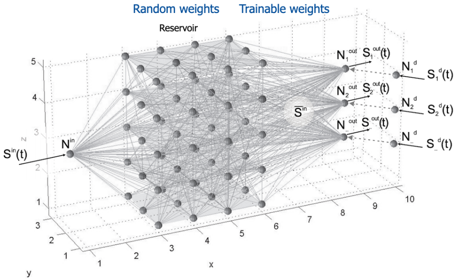
Key characteristics and advantages:

- Handles temporal dependencies: Excellent for time-series prediction, signal processing, and other tasks involving sequential data due to their recurrent nature.
- Fast training: The linear training of the output layer drastically reduces training time.
- Simplicity of implementation: Avoids the complexities of backpropagation through time.
- Avoids vanishing/exploding gradients: By fixing the reservoir weights, ESNs inherently mitigate these common RNN training problems.

LIQUID STATE MACHINES

Liquid State Machines (LSMs) are a specific type of recurrent neural network (RNN). They are particularly well-suited for processing temporal (time-varying) data.

- Bio-inspired reservoir: The liquid in LSM refers to a complex, randomly connected recurrent neural network (often spiking neurons) that acts as a dynamic reservoir. This reservoir processes incoming signals and transforms them into a high-dimensional, time-varying representation, similar to how a biological brain processes information.
- Echo State property (implicit): While not explicitly named for ESNs, LSMs also rely on the concept that the reservoir's internal states should exhibit a fading memory of past inputs. This ensures that the current state provides a rich, informative history of the input signal.
- Linear readout layer: As with other RC models, the connections within the liquid reservoir are fixed. Only a simple, linear output layer (the readout) is trained to map the high-dimensional reservoir states to the desired output.



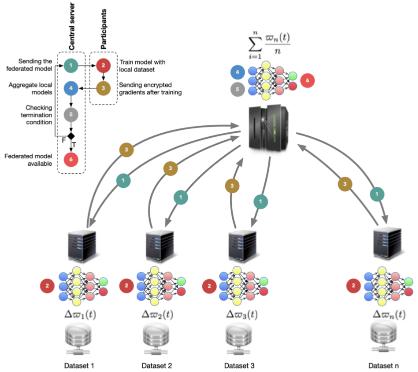
Key features & advantages:

- Excellent for time-series tasks: Naturally handles complex temporal patterns and dependencies in data.
- Fast training: The fixed reservoir means only the output weights are trained, often using efficient linear regression techniques.
- Computational efficiency: Avoids the computational expense and stability issues (like vanishing/exploding gradients) associated with training deep RNNs.

DISTRIBUTED ARTIFICIAL INTELLIGENCE WITH FEDERATED LEARNING

Federated Learning (FL) is a distributed machine learning paradigm. Originally proposed by Google in 2016 for privacy-preserving ML on mobile devices.

- A shared global model is trained via federated computation. The goal is to train state of the art machine learning systems without centralizing data and with privacy by default.
- It enables training models across multiple devices or servers holding local data samples, without exchanging them.
- Key motivation: Privacy, bandwidth efficiency, and regulatory compliance.
- Features:
  - → Massively Distributed. Training data is stored across a very large number of devices
  - → Limited Communication. Only a handful of rounds of unreliable communication with each devices
  - → Unbalanced Data. Some devices have few examples, some have orders of magnitude more
  - → Highly Non-IID Data. Data on each device reflects one individual's usage pattern
  - → Unreliable Compute Nodes. Devices go offline unexpectedly; expect faults and adversaries
  - → Dynamic Data Availability. The subset of data available is non-constant, e.g. time-of-day vs. country



DISTRIBUTED ARTIFICIAL INTELLIGENCE WITH FEDERATED LEARNING

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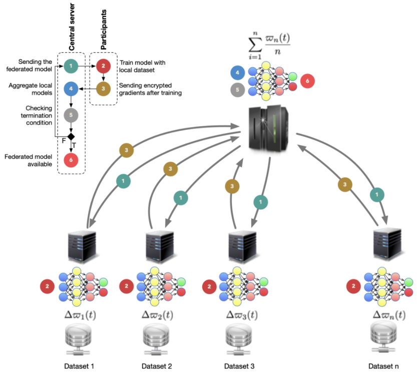
1. Central server orchestrates training rounds.
2. Local clients compute gradient updates using local data.
3. Model updates are sent to the central server and aggregated (e.g., via FedAvg).

$$\text{Global Model} \leftarrow \sum_{k=1}^{K} \frac{n_k}{n} \cdot \text{LocalUpdate}_k$$

4. No raw data leaves the client devices.



ADVANTAGES AND CHALLENGES

Advantages

- Data privacy and security.
- Reduced communication costs.
- Reduced computational costs.
- Real-time personalization on edge devices.

Challenges

- Statistical heterogeneity (non-IID data).
- System heterogeneity (e.g., device failure, varying compute).
- Communication bottlenecks and privacy leakage from updates.

Privacy-Preserving Techniques in FL

- Differential Privacy (DP): Adds noise to updates to obscure individual data points.
- Secure Multiparty Computation (SMC): Enables computations on encrypted data without decryption.
- Homomorphic Encryption: Allows arithmetic operations on encrypted values.

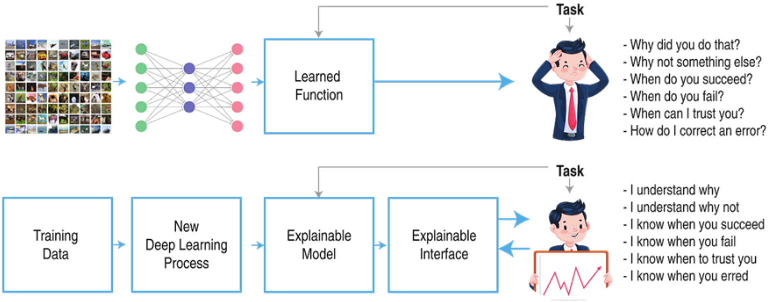
Applications

- Healthcare: Collaborative training across hospitals without sharing patient records.
- Finance: Joint fraud detection models across banks.
- Mobile devices: Keyboard prediction (e.g., Gboard), personalization of voice assistants.
- Industrial IoT: Cross-factory equipment failure prediction models.

WHAT IS EXPLAINABLE AI (XAI)?

XAI refers to methods and techniques that make AI model behavior understandable to humans.

- Goal: Increase trust, transparency, and accountability in AI systems.
- Especially crucial in high-stakes domains: healthcare, law, finance.
- Differentiates between model performance and interpretability.



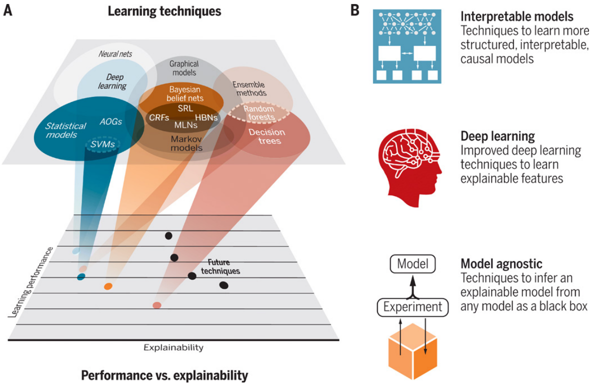
BLACK-BOX VS. WHITE-BOX MODELS

White-Box Models

- Interpretable by design (e.g., decision trees, linear regression).
- Transparency comes at the cost of performance in complex tasks.

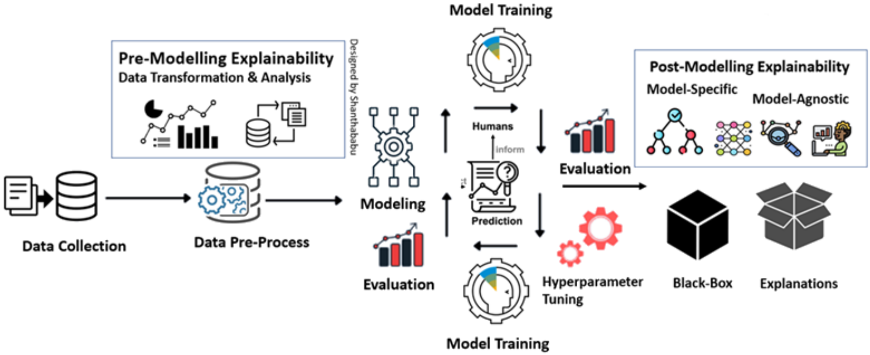
Black-Box Models

- Complex models (e.g., deep neural networks, ensembles).
- High performance but opaque decision-making process.



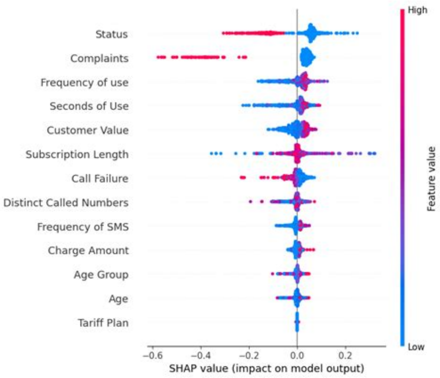
CATEGORIES OF XAI METHODS

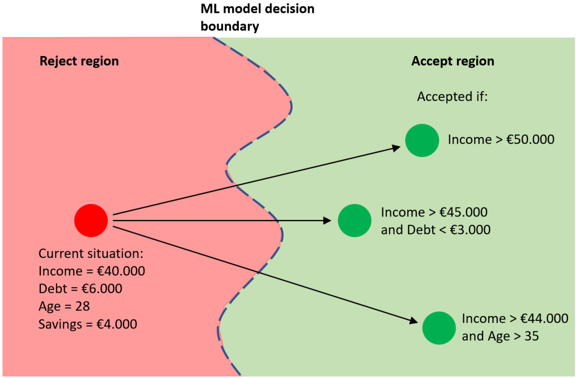
- Intrinsic: Interpretability built into the model (e.g., shallow trees).
- Post-hoc: Explanations extracted after model training.
- Global: Explain the model's overall behavior.
- Local: Explain individual predictions.

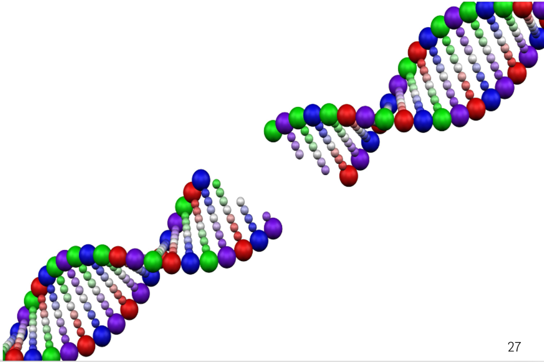


POPULAR XAI TECHNIQUES

- LIME: Local Interpretable Model-agnostic Explanations.
- SHAP: SHapley Additive exPlanations, grounded in cooperative game theory.
- Saliency Maps: Visualize important input regions (CNNs).
- Counterfactual Explanations: “What if” scenarios for alternative outcomes.







GENERATIVE DESIGN

Material design:

- Create entirely new nanomaterial structures or compositions with target properties.
- Uses generative models (e.g., GANs, VAEs) that learn underlying data distributions.
- Explores the vast chemical/structural space beyond human intuition.
- Example: Designing a novel porous carbon structure for enhanced gas storage, or an antimicrobial peptide with specific binding sites.

Assisted synthesis:

- Optimize experimental parameters and synthesis protocols for desired nanomaterial characteristics.
- Utilizes ML and RL to guide automated synthesis platforms.
- Reduces trial-and-error cycles, improves yield and quality.
- Example: Optimizing reaction conditions (temperature, pressure, precursor concentration) for controlled growth of quantum dots, or guiding self-assembly processes of supramolecular structures.

AI IN NANOMATERIAL CHARACTERIZATION

The Artificial Intelligence technologies have a critical role in enhancing the characterization of nanomaterials. Accurate and efficient characterization is paramount for understanding properties and validating synthesis. We will explore how AI improves image quality, enables autonomous microscopy, and streamlines the analysis of complex spectroscopic data.

Image Enhancement and analysis:

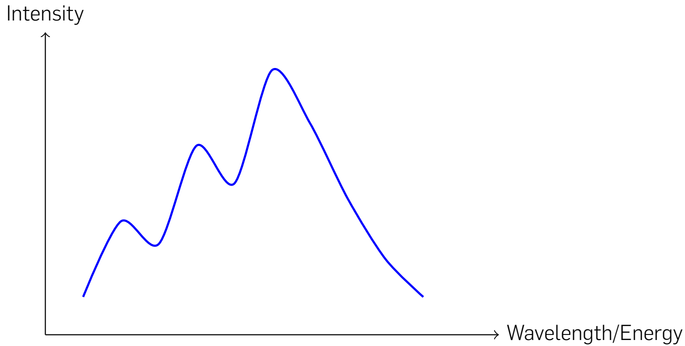
- Denoising and Super-resolution: Improves quality of microscopy images (TEM, SEM, AFM) by removing noise and enhancing resolution.
- Automated Feature Extraction: Identifies and quantifies features like particle size, shape, distribution, defects, and crystalline structures from images.
- Example: Denoising high-resolution TEM images to reveal atomic positions, or automatically counting and sizing nanoparticles in a batch sample.

Autonomous microscopy:

- Enables automated navigation, focusing, and data acquisition in advanced microscopes (e.g., STEM, AFM).
- AI algorithms learn optimal scanning paths and identify regions of interest.
- Increases throughput and reduces human intervention.
- Example: An AI-controlled STEM automatically locating and imaging specific defects in a 2D material, or an AFM robotically mapping surface topography over large areas.

SPECTROSCOPIC DATA ANALYSIS

- Automated Peak Identification and Deconvolution: Analyzes complex spectra (e.g., XPS, FTIR, Raman, NMR) to identify chemical states, functional groups, or molecular structures.
- Quantitative Analysis: Extracts quantitative information (e.g., elemental composition, bond ratios) from spectroscopic data.
- Correlation with Properties: Links spectroscopic signatures to macroscopic properties.
- Example: Rapidly identifying contaminants in a nanomaterial sample from its Raman spectrum, or deconvoluting overlapping peaks in an XPS spectrum to determine precise oxidation states.



Complex Spectroscopic Data

AI IN NANOMEDICINE

This section explores the groundbreaking impact of Artificial Intelligence on the rapidly evolving field of nanomedicine. AI is accelerating the development of next-generation diagnostics and therapeutics by enabling smarter drug delivery, more precise disease detection, and advanced bio-sensing capabilities.

Smart drug delivery systems

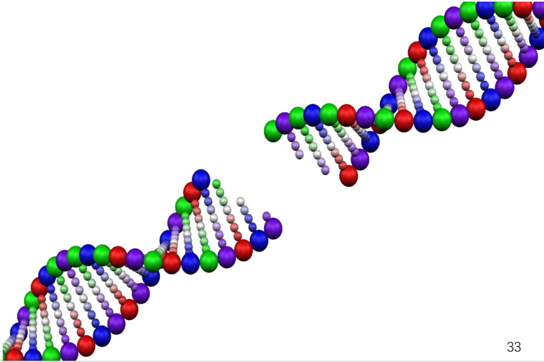
- Design and optimize nanoparticles for targeted drug delivery, controlled release, and improved biocompatibility.
- AI can predict nanoparticle-cell interactions, drug encapsulation efficiency, and release kinetics.
- Example: Developing AI-driven nanoparticles that release chemotherapy drugs only when sensing specific biomarkers in tumor cells, minimizing side effects.

Early disease detection and diagnostics

- Enhance the sensitivity and specificity of nanosensors for detecting disease biomarkers at ultra-low concentrations.
- AI algorithms analyze complex sensor data to identify disease signatures earlier and more accurately.
- Example: Using AI to interpret signals from nanowire-based biosensors for early detection of cancer or viral infections from a blood sample, or developing smart diagnostic patches.

ADVANCED BIOSENSING AND IMAGING

- Optimize the design of nanoscale biosensors for high-throughput screening and personalized medicine.
- AI can interpret complex signals from various biosensing platforms, including those used for genomics and proteomics.
- Integrate AI with advanced nanoscopic imaging techniques (e.g., super-resolution microscopy) for better visualization of biological processes at the nanoscale.
- Example: AI-powered analysis of single-molecule interactions on a plasmonic biosensor, or real-time tracking of drug delivery nanoparticles within living cells.



CHALLENGES AND OPPORTUNITIES

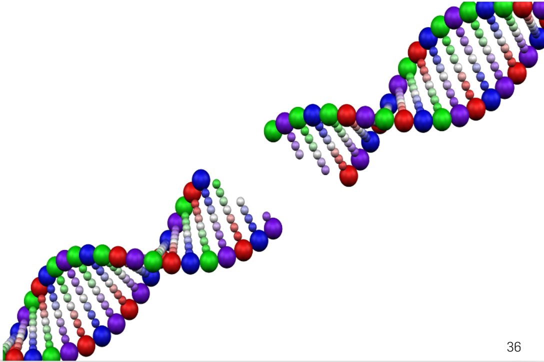
This section addresses the practical challenges and exciting opportunities presented by the integration of Artificial Intelligence in nanoscience. Overcoming these hurdles will unlock the full potential of AI to accelerate scientific discovery, foster innovation, and translate fundamental research into real-world applications.

Current challenges:

- Data quality and quantity: Nanoscience data can be scarce, noisy, or lack standardization. High-quality, labeled datasets are crucial for effective AI training.
- Interpretability of AI models: Black-box nature of some advanced AI models makes it difficult to understand the underlying scientific insights.
- Bridging scales: Connecting atomic-level phenomena to macroscopic properties requires multiscale modeling, which is complex for AI.
- Experimental validation: AI predictions need rigorous experimental validation, which can be time-consuming and expensive at the nanoscale.
- Interdisciplinary expertise: Requires collaboration between AI experts, materials scientists, chemists, physicists, and biologists.
- Computational resources: Training complex DL models requires significant computational power.

FUTURE OPPORTUNITIES

- Autonomous scientific discovery: Fully automated labs where AI designs experiments, conducts them, analyzes data, and iterates, accelerating discovery by orders of magnitude.
- Materials genome initiative: AI will be central to mapping the entire landscape of possible materials and their properties.
- Personalized nanomedicine: Tailoring nanomedicines and diagnostics to individual patient needs based on their unique biological profiles.
- Sustainable nanoscience: AI can optimize green synthesis routes, minimize waste, and identify environmentally friendly nanomaterials.
- New AI srchitectures: Development of AI models specifically designed for sparse, noisy, or complex spatiotemporal nanoscience data.
- Enhanced human-AI collaboration: AI as an intelligent assistant, augmenting human creativity and intuition, rather than replacing it.



THE FUTURE IS NANO-AI

We have explored the profound impact of Artificial Intelligence on the field of Nanoscience, demonstrating its transformative power across discovery, characterization, and nanomedicine. The synergy between AI's analytical capabilities and the unique challenges and opportunities of the nanoscale realm promises an unprecedented era of innovation.

Key Takeaways:

- AI is not just a tool; it's a paradigm shift for nanoscience research.
- It enables us to overcome the limitations of data complexity, vast design spaces, and experimental throughput.
- From predicting new materials to revolutionizing diagnostics, AI is making the impossible, possible.
- Embracing AI is essential for staying at the forefront of nanoscientific discovery and technological advancement.

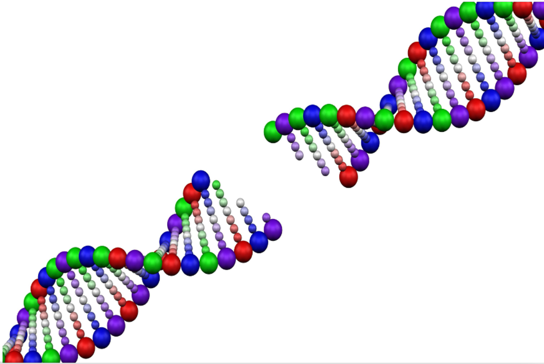
Thank you for your attention!

Questions?

AI-AUGMENTED NANOSCIENCE

Seminar

June 5th, 2025



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