Task: 8/6/2025

## 1. Graph Neural Networks (GNNs) for Molecular Property Prediction

• **Description**: Represent molecules as graphs (atoms = nodes, bonds = edges) and predict properties like solubility or toxicity.

### • Key Techniques:

- Message Passing Neural Networks (MPNN)
- Graph Convolutional Networks (GCN) / Graph Attention Networks (GAT)
- Benchmark with MoleculeNet (e.g., ESOL, FreeSolv datasets)
- What You'll Learn: graph data preprocessing, custom GNN layers in PyTorch Geometric or DGL, transfer learning on small datasets.

## 2. Generative Adversarial Networks (GANs) for Image-to-Image Translation

- **Description**: Train a GAN to convert images from one domain to another—e.g., turning sketches into photos, day to night scenes, or summer to winter landscapes.
- Key Techniques:
  - Conditional GANs (cGAN), Pix2Pix, CycleGAN
  - Adversarial loss + cycle consistency loss
  - Image augmentation & training stability tricks (label smoothing, spectral normalization)
- **Datasets**: CMP Facades, Cityscapes, Horse2Zebra.
- What You'll Learn: advanced generator/discriminator architectures, balancing multi-term loss functions, high-resolution training.

### 3. Transformer-Based Time Series Forecasting

 Description: Use Transformer architectures (originally for NLP) to model long-range dependencies in time series—e.g., stock prices, energy consumption, multivariate weather data.

### • Key Techniques:

- Self-attention over temporal windows
- Positional encodings for time steps
- Encoder–decoder forecasting setup
- **Datasets**: ElectricityLoadDiagrams, M4 Forecasting Competition data.
- What You'll Learn: adapting Transformers beyond text, efficient attention for long sequences, multi-horizon forecasting.

# 4. Deep Reinforcement Learning (DRL) for Continuous Control

- **Description**: Train agents to perform tasks in continuous action spaces—e.g., robotic arm manipulation, autonomous driving simulators.
- Key Techniques:
  - Actor-Critic methods (DDPG, TD3, SAC)
  - Reward shaping and exploration strategies
  - o Sim2Real considerations if you move to physical robots
- Environments: OpenAl Gym's "Pendulum-v0", "MuJoCo" tasks (HalfCheetah, Ant).
- What You'll Learn: stability of policy gradient methods, continuous action discretization, environment interfacing.

# 5. Self-Supervised Learning on Vision Transformers (ViT)

• **Description**: Pre-train a Vision Transformer on unlabeled images using contrastive or masked-patch objectives, then fine-tune on classification tasks.

### • Key Techniques:

- o DINO, MAE (Masked Autoencoders), SimCLR-style losses
- Patch embedding and positional encoding for images
- Large-scale pretraining pipelines
- Datasets: ImageNet-1k for fine-tuning; use a large unlabelled set (e.g. uncurated Flickr images) for pretraining.
- What You'll Learn: transformer internals on vision data, designing pretext tasks, scaling compute.

## 6. Neural Architecture Search (NAS) for Custom Model Design

- **Description**: Automate discovery of high-performance model architectures for a given task/dataset rather than hand-crafting layers.
- Key Techniques:
  - Reinforcement Learning or Evolutionary Algorithms to propose architectures
  - Weight-sharing one-shot NAS (e.g., DARTS) for efficiency
  - Search space definition and constraints
- **Use Case**: CIFAR-10 or CIFAR-100 architecture search; then transfer to your own image or signal domain.
- What You'll Learn: meta-optimization loops, resource-aware search, trade-offs between search cost and accuracy.

# 7. Federated Learning with Differential Privacy

- **Description**: Train a global model across multiple client devices (e.g., phones) without sharing raw data, and guarantee user privacy.
- Key Techniques:
  - Federated Averaging (FedAvg)
  - o Per-client gradient clipping and noise addition for DP
  - Communication efficiency (quantization, sparsification)
- **Simulated Dataset**: Split MNIST or CIFAR into non-IID shards to mimic client heterogeneity.
- What You'll Learn: privacy-preserving ML, cross-device coordination, handling non-IID data distributions.

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