SESSION // 03
TRAINING NEURAL NETWORKS

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SCIENCE AND ENGINEERING
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AGENDA

PyTorch Workflow Overview

Case Study: ARKOMA Robot Dataset

Data Preparation and Model Design

- Preprocessing and normalizing data
- Designing network architecture

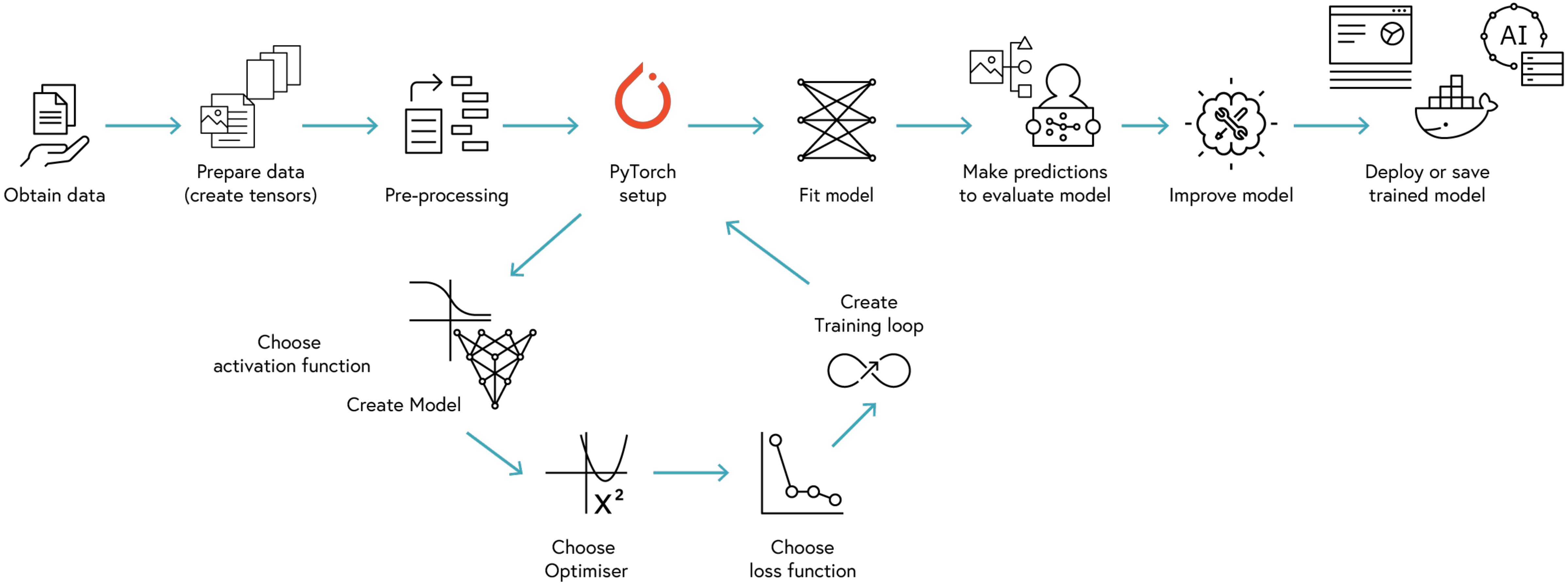
Training and Evaluation

- Implementing loss functions and optimizers
- Monitoring model performance

Results Analysis and Visualization

Challenges & Next Steps

PYTORCH WORKFLOW



ARKOMA ROBOT DATASET

Critical problem in robotics:

"How should joints move to place end-effector at desired position?"

Why Inverse Kinematics Matter:

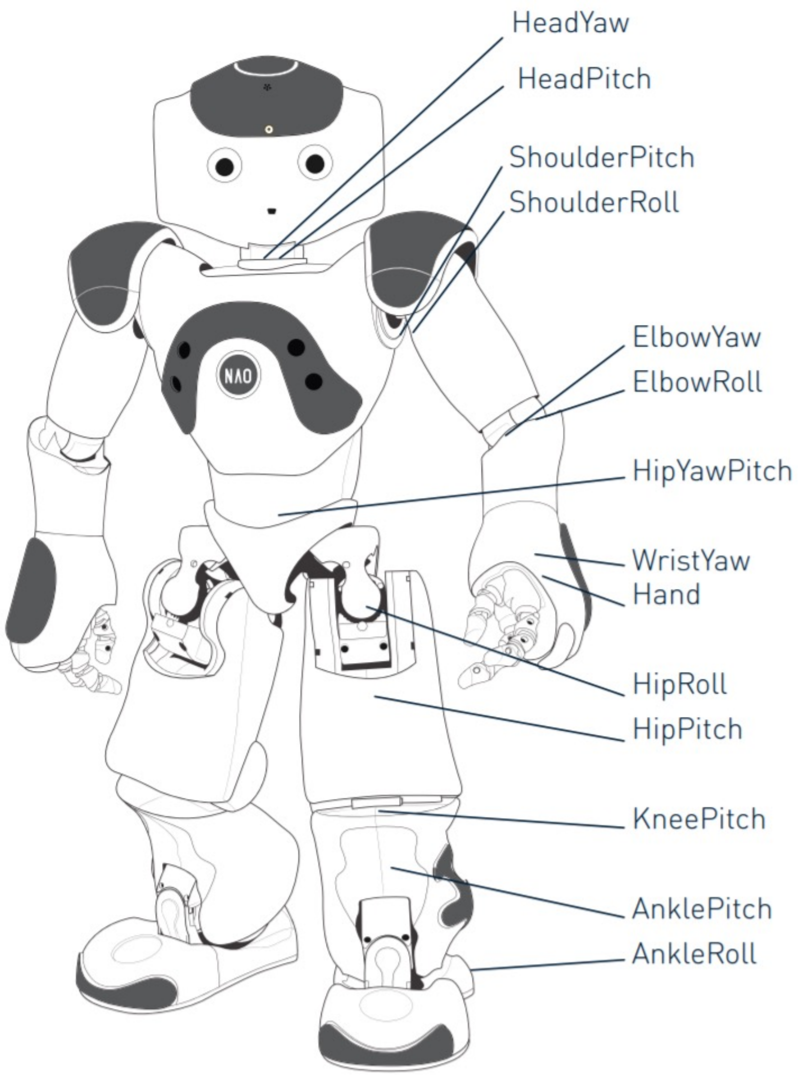
- Forward kinematics: Easy to calculate (joint angles → position)
- Inverse kinematics: Challenging mathematical problem (position → joint angles)

Real-world applications:

- Robot manipulation tasks (grasping objects)
- Manufacturing automation
- Surgical robotics

NAO robot inverse kinematics dataset

- 10,000 input-output pairs
- Inputs: End-effector positions (Px, Py, Pz, Rx, Ry, Rz)
- Outputs: Joint angles (θ1, θ2, θ3, θ4, θ5)
- We'll focus on the right arm



DATA PREPARATION AND PRE-PROCESSING

```python
from sklearn.model_selection import train_test_split

# Load the complete dataset
X = pd.read_csv("dataset_features.csv")
y = pd.read_csv("dataset_targets.csv")

# First split: separate test set (80% train+val, 20% test)
X_temp, X_test, y_temp, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42
)

# Second split: separate validation set (75% train, 25% val from the temp set)
X_train, X_val, y_train, y_val = train_test_split(
    X_temp, y_temp, test_size=0.25, random_state=42
)  # 0.25 * 0.8 = 0.2 of original data

print(f"Training set: {X_train.shape[0]} samples")
print(f"Validation set: {X_val.shape[0]} samples")
print(f"Test set: {X_test.shape[0]} samples")
```

Purpose of each dataset:

- Training (60-80%):
  - Training the model
- Validation (10-20%):
  - Tuning hyperparameters
- Test (10-20%):
  - Final evaluation

DATA NORMALISATION

Why normalise?

- Faster convergence
- Numerical stability
- Equal feature contribution
- Better generalization

Min-Max scaling:

$$X_{norm} = (X - X_{min})/(X_{max} - X_{min})$$

```python
from sklearn.preprocessing import MinMaxScaler

# Create and apply MinMaxScaler
x_scaler = MinMaxScaler()
y_scaler = MinMaxScaler()

x_scaler.fit(X_train_tensor)
y_scaler.fit(y_train_tensor)

X_train_scaled = torch.tensor(x_scaler.transform(X_train_tensor), dtype=torch.float32)
```

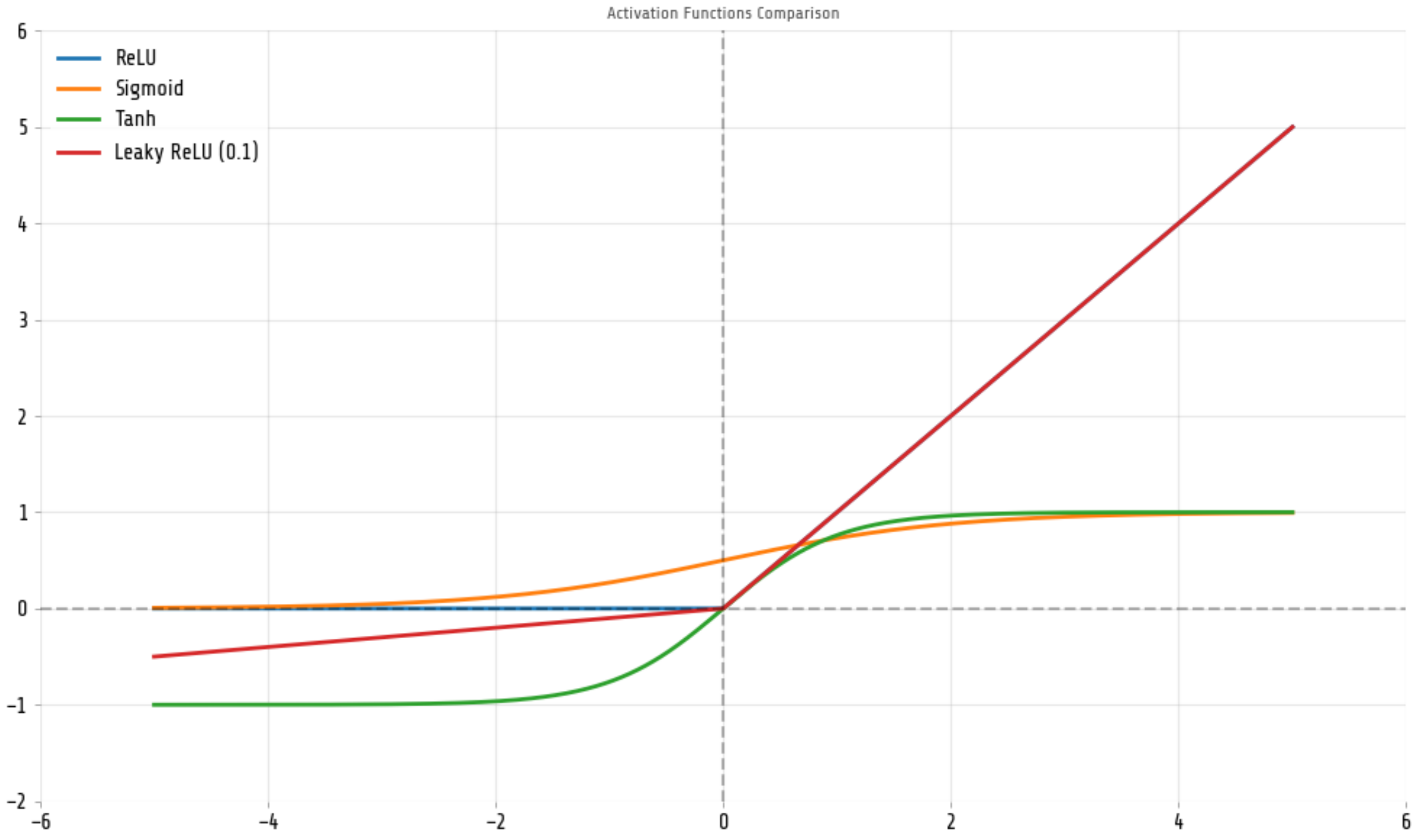
ACTIVATION FUNCTIONS

Purpose:

- Transform linear input to non-linear output
- Enable networks to learn complex patterns and relationships

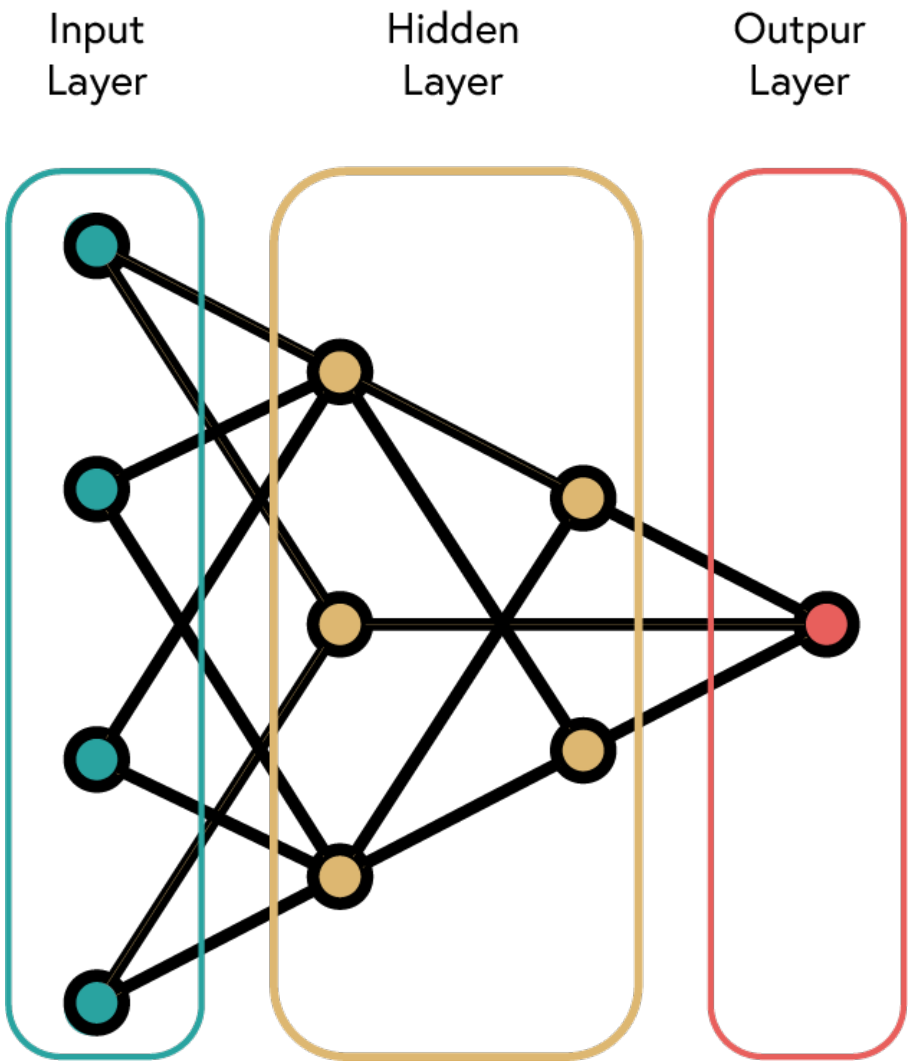
Key properties:

- Differentiable
- Non-linear
- Computationally efficient

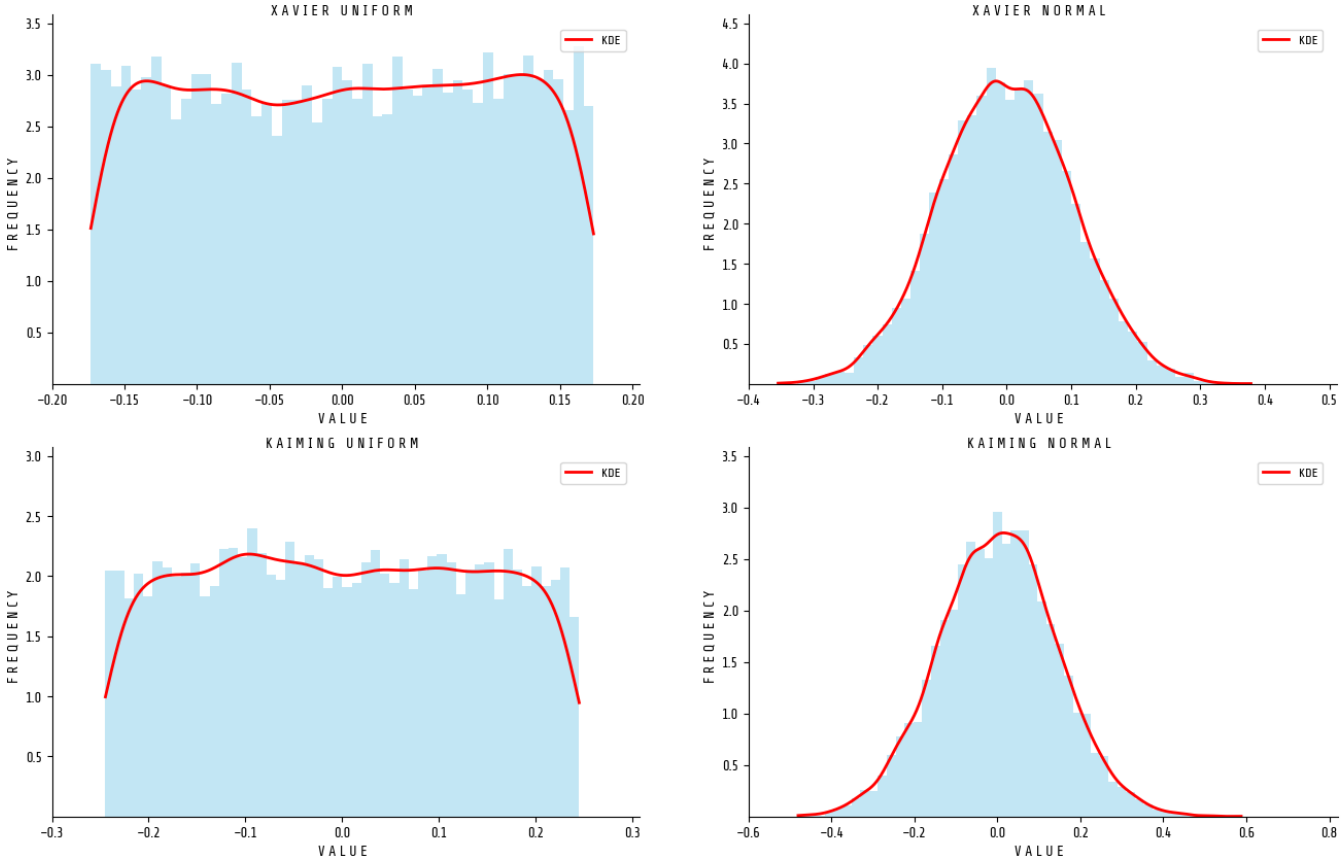


BUILDING NEURAL NETWORKS

- Input Layer: Receives input features
- Hidden Layers: Process information
- Output Layer: Produces predictions
- Width (neurons per layer) vs Depth (number of layers)



WEIGHT INITIALISATION



Importance of proper initialization:

1. **Convergence Speed**: Good initialization leads to faster training
2. **Symmetry Breaking:** Prevents neurons from learning the same features
3. **Vanishing/Exploding Gradients**: Proper scaling helps maintain gradient flow
4. **Training Stability:** Reduces the chance of getting stuck in poor local minima
5. **Reproducibility:** Sets a consistent starting point for experiments

```
# Initialize weights with appropriate methods
torch.nn.init.kaiming_uniform_(self.fc1.weight, nonlinearity='relu')
torch.nn.init.zeros_(self.fc1.bias)
```

ANN IMPLEMENTATION

- PyTorch model implementation for robotic arm
- Simple architecture to avoid overfitting

```
class RobotArmNetwork(torch.nn.Module):
    def __init__(self, input_size, hidden_size, output_size):
        super().__init__()
        self.fc1 = torch.nn.Linear(input_size, hidden_size)
        self.hidden_activation = torch.nn.ReLU()
        self.fc2 = torch.nn.Linear(hidden_size, output_size)

    def forward(self, x):
        x = self.hidden_activation(self.fc1(x))
        x = self.fc2(x)
        return x
```

OPTIMISATION

Popular optimisers:

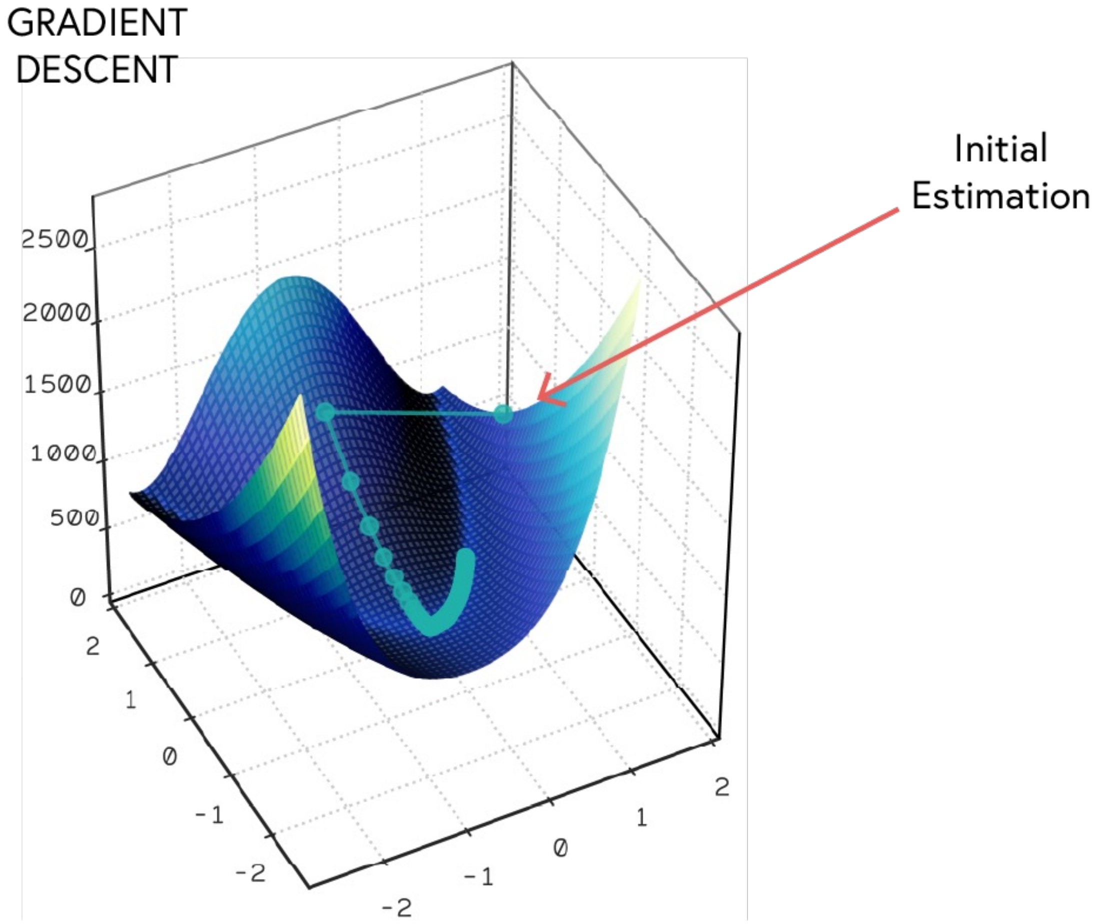
- **SGD**: Simple, works well with momentum
- **Adam**: Adaptive learning rates, widely used
- **RMSProp**: Good for recurrent networks
- **AdamW**: Adam with proper weight decay

Learning rate importance:

- **Too large**: Causes unstable training, overshooting minima
- **Too small**: Results in slow convergence or getting stuck in local minima
- **"Just right"**: Efficient convergence to good solutions

Learning Rate Strategies:

- **Fixed**: Simple but rarely optimal for entire training
- **Decay/Scheduling**: Reduce rate over time (e.g., step, exponential, cosine)
- **Adaptive**: Adjusts automatically based on gradient history



PYTORCH OPTIM

```python
# Fixed learning rate
optimizer = torch.optim.Adam(model.parameters(), lr=0.001)

# Learning rate scheduler
scheduler = torch.optim.lr_scheduler.StepLR(
    optimizer, step_size=30, gamma=0.1)  # Reduce by 10x every 30 epochs

# After each epoch
scheduler.step()
```

LOSS FUNCTION

- Loss functions quantify prediction errors
- We use Mean Squared Error (MSE):

$$MSE = 1/n\,\Sigma(y - \hat{y})^2$$

- Provides direction for optimization

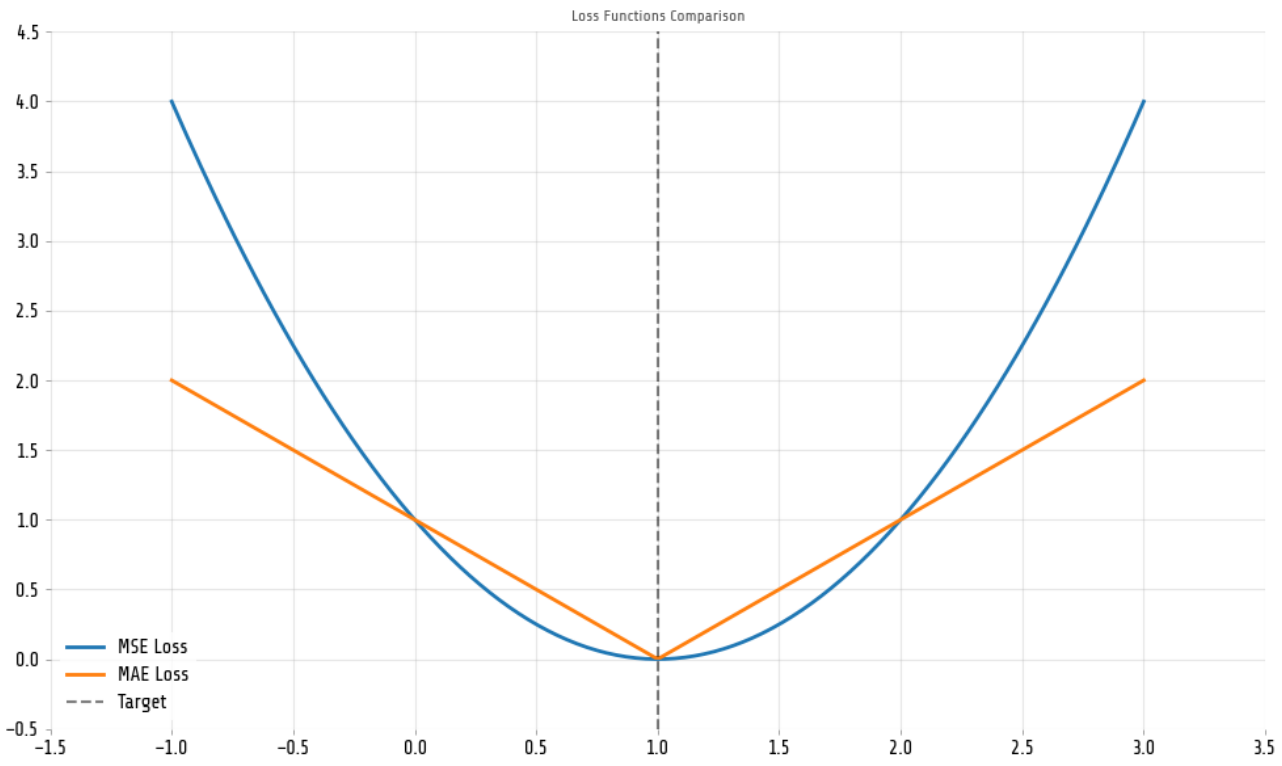
```python
def mse_loss(predictions: torch.Tensor,
             targets: torch.Tensor) -> torch.Tensor:

    squared_diff = (predictions - targets) ** 2
    return squared_diff.mean()
```

LOSS FUNCTIONS

Types of loss functions:

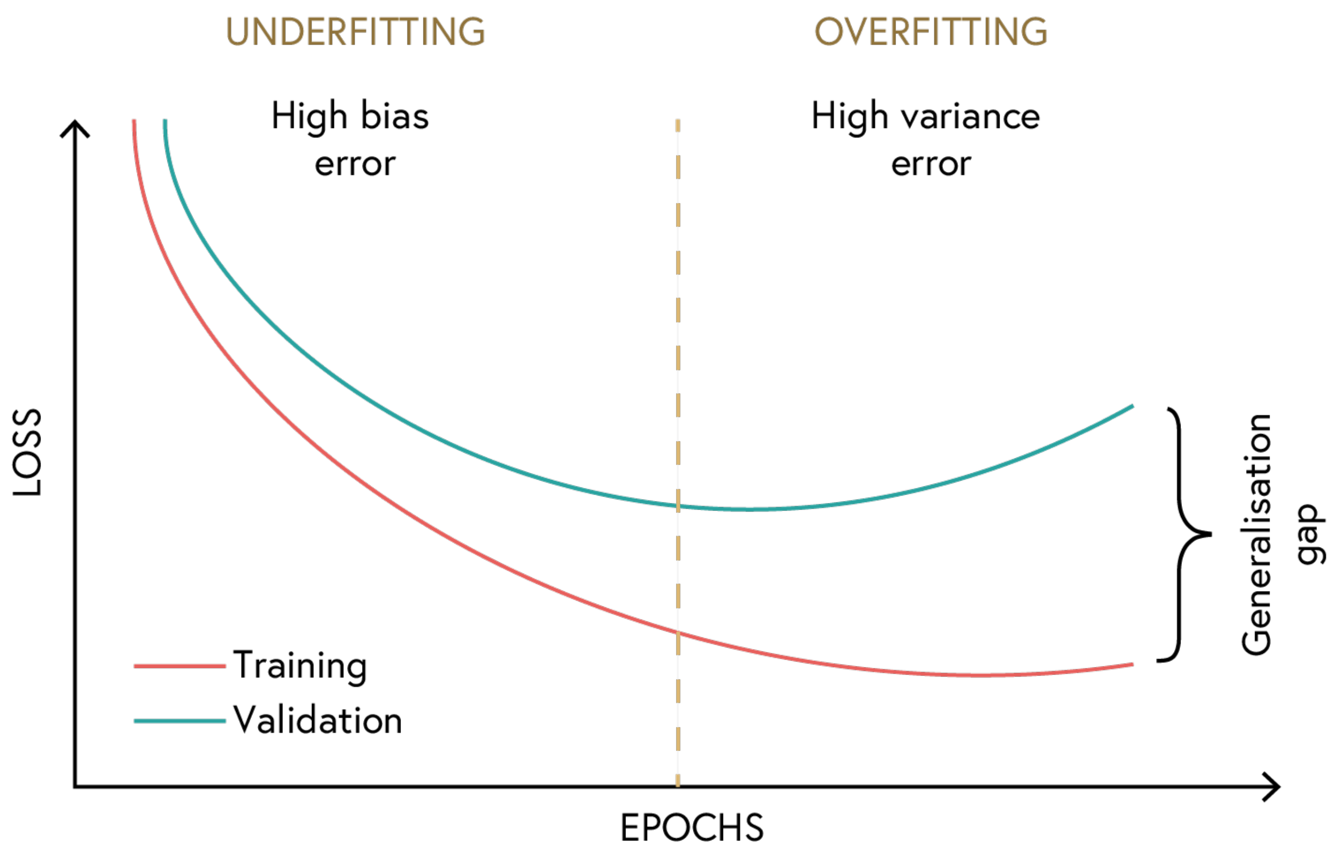
- **MSE**: Regression tasks
- **MAE**: Regression with less sensitivity to outliers
- **Binary Cross-Entropy**: Binary classification
- **Categorical Cross-Entropy**: Multi-class classification
- **For our regression task**: Mean Squared Error

```
loss_function = torch.nn.MSELoss()
```



OVERFITTING AND UNDERFITTING

- **Underfitting:** Model too simple, high bias
- **Overfitting:** Model too complex, high variance
- **Finding the right balance**



MODEL EVALUATION

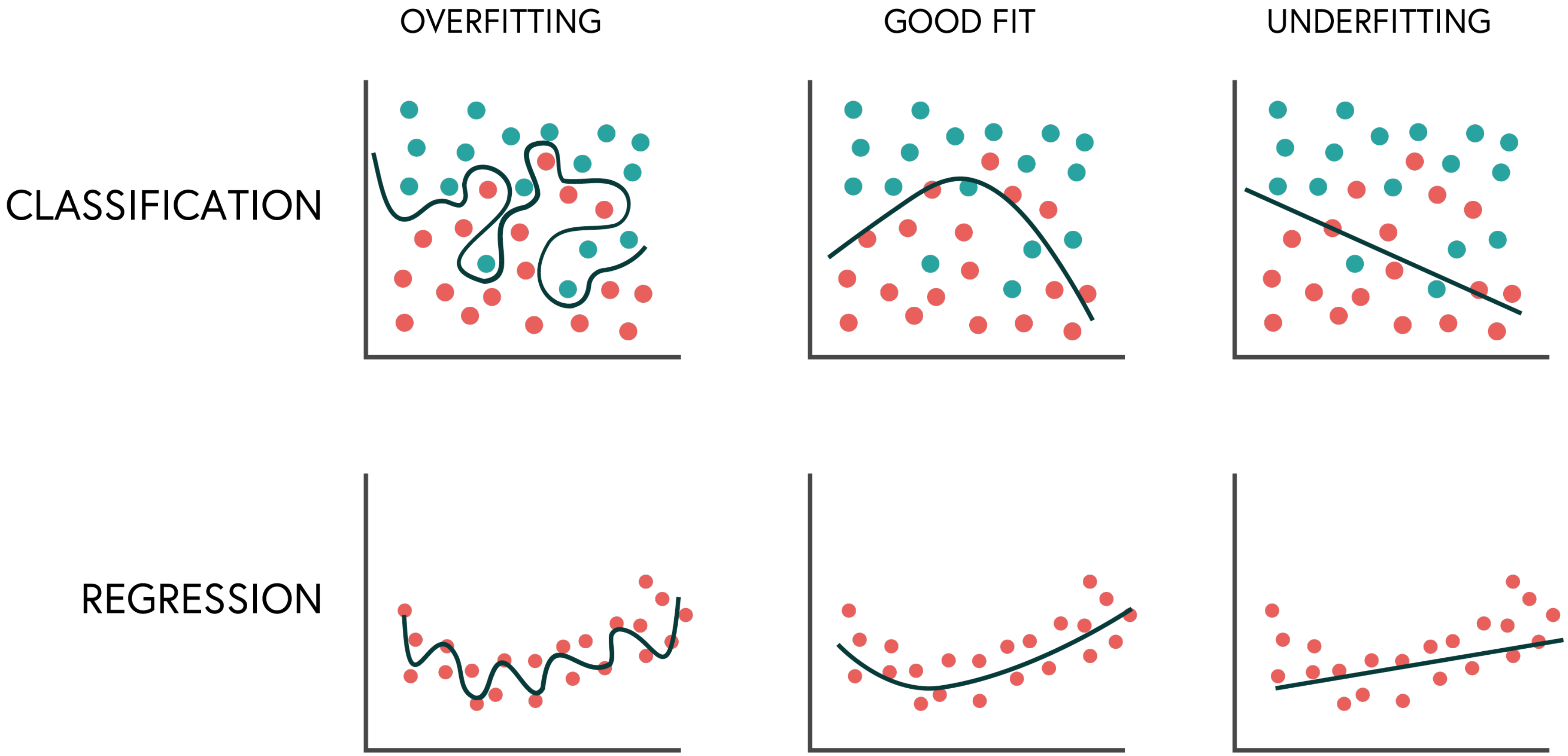
Testing on unseen data

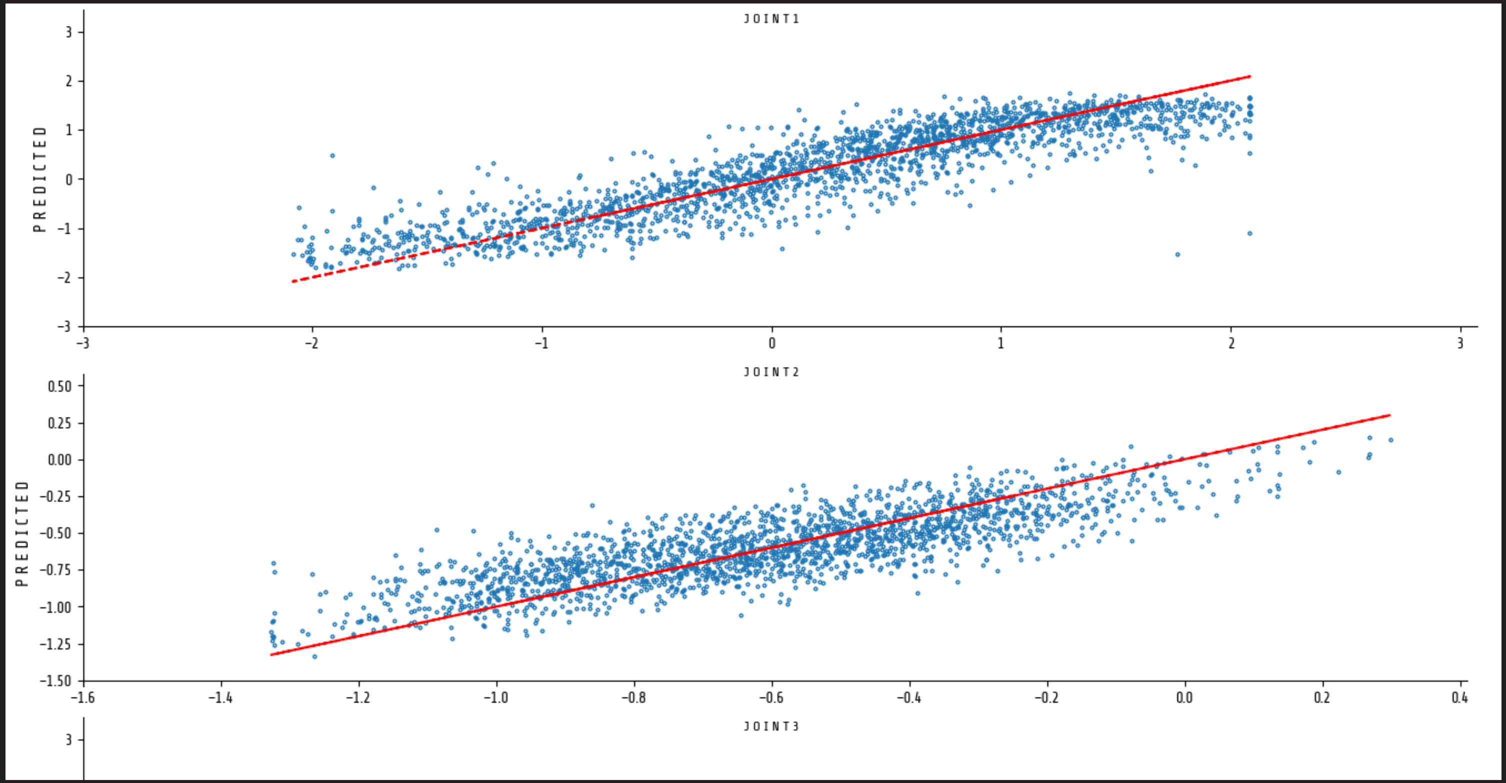
Metrics for regression:

- **Mean Squared Error**
- **R-squared score**

```
model.eval()
with torch.no_grad():
    test_predictions = model(X_test_scaled)
    test_loss = loss_function(test_predictions, y_test_scaled)
```

MODEL EVALUATION





IMPROVING THE MODEL

- Hyperparameter tuning
- Deeper/wider networks
- Regularisation techniques
- Advanced architectures