ML Foundations

Iliad Intensive

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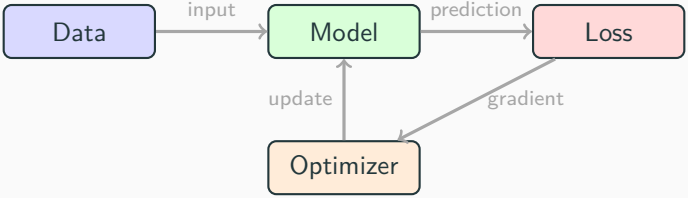
Outline

1. The Training Loop
2. Tensors and PyTorch
3. Loss Functions
4. Optimizers
5. Architectures
6. Hyperparameter Optimization

The Training Loop

Concepts in Machine Learning



Data input to a task we want an AI to do

Model gets data, outputs a prediction

Loss function quantifies how well the model did

Optimizer updates the model to do better

The Training Loop in PyTorch

```
for x, y in dataloader:
    optimizer.zero_grad()
    prediction = model(x)          # forward pass
    loss = loss_fn(prediction, y) # compute loss
    loss.backward()                # backward pass
    optimizer.step()               # update parameters
```

This is *the* loop. Everything else in ML is about making each piece better.

Terminology

Parameters / weights the numbers that represent the model itself, updated by the optimizer (θ)

Activations the numbers created as we feed data through the network

Hyperparameters choices made *before* training: learning rate, batch size, architecture

Stochasticity and Batching

We want to minimize the true loss over the full data distribution:

$$\mathcal{L}(\theta) = \mathbb{E}_{x \sim \mathcal{D}} \left[\ell(f_\theta(x), y) \right]$$

But we only ever see a finite **batch** $\mathcal{B} \subset \mathcal{D}$ at each step:

$$\hat{\mathcal{L}}(\theta) = \frac{1}{|\mathcal{B}|} \sum_{(x,y) \in \mathcal{B}} \ell(f_\theta(x), y)$$

- Every gradient is a noisy estimate of the true gradient
- Batch size controls the noise level

Tensors and PyTorch

Tensors

The central object in PyTorch: multidimensional arrays of numbers.

We use tensors to represent: data, parameters, activations, outputs, losses.

```
x = torch.tensor([1.0, 2.0, 3.0])
M = torch.zeros(3, 4)
```

By convention, everything except parameters has the **batch dimension first**, so we can process many samples at once.

Tensor Operations

```
torch.exp(x)            # elementwise exponential
A @ B                   # matrix multiply
x.unsqueeze(0)          # add a dimension
```

Einstein notation makes index operations explicit:

$$C_{ij} = \sum_k A_{ik} B_{kj}$$

```
torch.einsum('ik,kj->ij', A, B)
```

Einops

Readable notation for tensor reshaping:

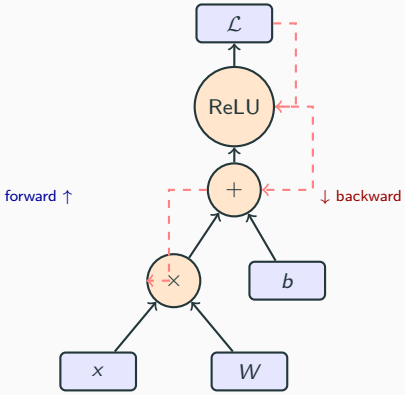
```
# PyTorch (what does this do?)
x.reshape(B, S, n_heads, d_head).permute(0, 2, 1, 3)

# Einops (self-documenting)
rearrange(x, 'b s (h d) -> b h s d', h=n_heads)
```

- `rearrange`: reshape, permute, split, merge
- `reduce`: pool over dimensions
- `repeat`: tile/broadcast

Autograd and the Computation Graph

1. Build expressions from tensors with `requires_grad=True`
2. Call `.backward()` on a scalar
3. Access gradients via `.grad`

You never write derivatives by hand. The graph is rebuilt every forward pass.



Devices

- Tensors live on a **device**: CPU or GPU (`cuda:0`)
- Move with `x.to('cuda')`
- All tensors in an operation must be on the same device
- GPU memory is the main bottleneck for model size and batch size

Exercise 1: PyTorch Basics

25 minutes

Loss Functions

Loss Functions: Supervised Learning

The loss function defines *what* we are optimizing.

When we can directly verify the output:

- Predict something continuous (position of a ball) $\Rightarrow$ MSE
- Predict something discrete (class, next word) $\Rightarrow$ **cross-entropy loss**

$$\mathcal{L} = -\sum_i y_i \log \hat{y}_i$$

Minimizing cross-entropy makes the model **well-calibrated**: its output numbers can be interpreted as probabilities.

Loss Functions: Human Preferences

We do not always have the "correct label." Sometimes we only know a pattern outputs should have.

Example: rating text quality, given only pairwise human preferences ("I prefer A over B").

The preferred text should be rated higher:

$$\mathcal{L} = -\log \sigma(r_\theta(x_w) - r_\theta(x_l))$$

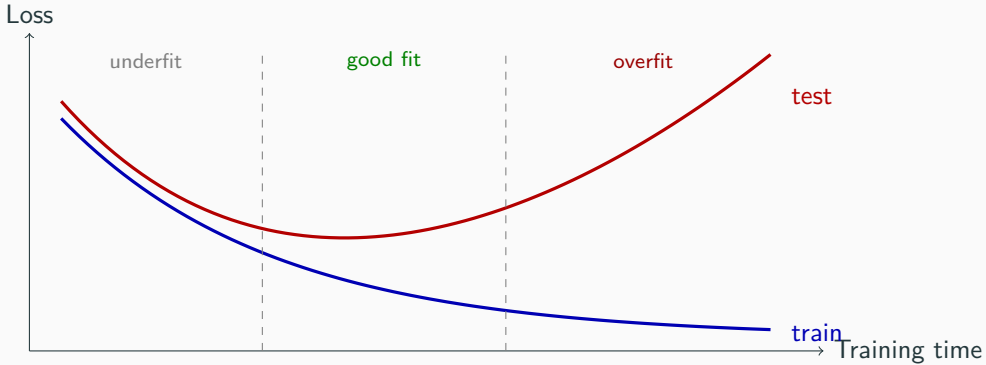
[Christiano et al. 2017]

Loss Functions: Reinforcement Learning

Sometimes we cannot say what the correct output looks like, but we can identify one when we see it (e.g. winning at chess).

- RL loss functions are more complex
- Often involve a learned reward model (from the previous slide) combined with a policy objective

Train Loss vs. Test Loss



- **Underfitting**: both losses high (model too simple or undertrained)
- **Overfitting**: train loss low, test loss rises (model memorizes)
- Regularization (L2, dropout) constrains the model to delay overfitting

Optimizers

Optimizers

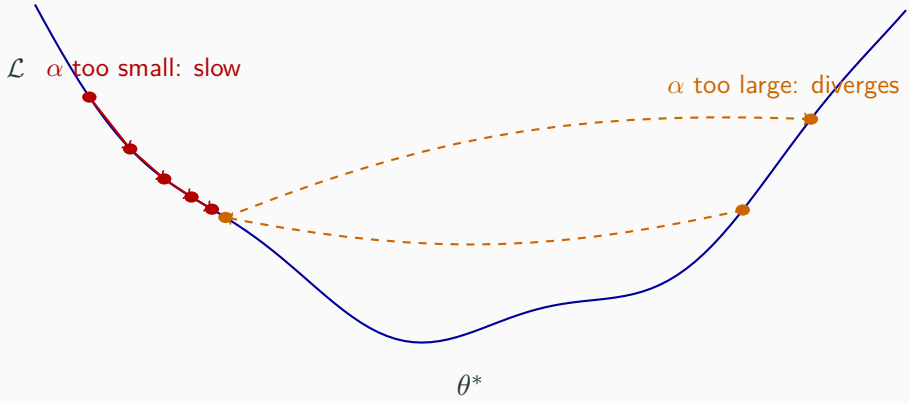
We have a gradient. Which direction do we step?

Stochastic Gradient Descent

$$\theta_{t+1} = \theta_t - \alpha \nabla_\theta \mathcal{L}$$

- α: learning rate (hyperparameter)
- Simple and robust
- Can be slow: oscillates across narrow valleys, crawls along them

Learning Rate



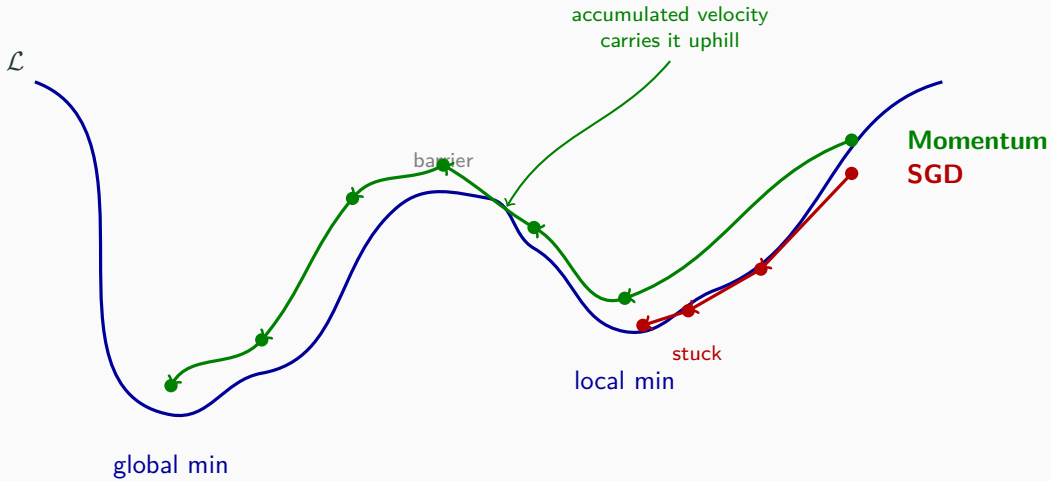
Momentum [Sutskever et al. 2013]

$$v_{t+1} = \beta\, v_t + (1 - \beta)\, \nabla_\theta \mathcal{L}$$

$$\theta_{t+1} = \theta_t - \alpha\, v_{t+1}$$

- Keeps a running velocity, like a ball rolling downhill
- Accelerates through flat regions
- Dampens oscillations in steep directions
- Can roll over small local minima

Momentum Escapes Local Minima



Adam = Momentum + RMSProp [Kingma et al. 2014]

$$m_{t+1} = \beta_1 m_t + (1-\beta_1) g_t \qquad v_{t+1} = \beta_2 v_t + (1-\beta_2) g_t^2$$

$$\hat{m} = \frac{m_{t+1}}{1-\beta_1^{t+1}} \qquad \hat{v} = \frac{v_{t+1}}{1-\beta_2^{t+1}}$$

$$\theta_{t+1} = \theta_t - \alpha \frac{\hat{m}}{\sqrt{\hat{v}} + \epsilon}$$

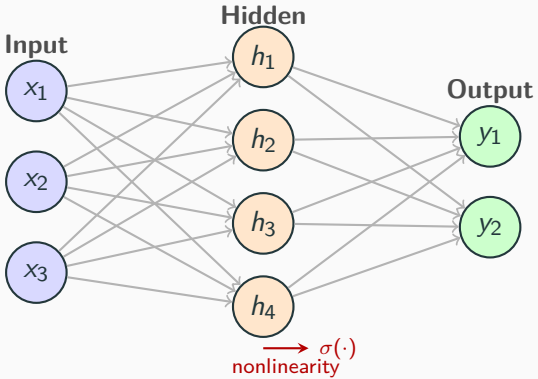
- Adaptive per-parameter learning rates + momentum
- Default choice for most deep learning
- Typical: $\beta_1 = 0.9$, $\beta_2 = 0.999$, $\epsilon = 10^{-8}$

Exercise 2: Implement Optimizers

25 minutes

Architectures

The MLP



- Without a hidden layer, we can only represent linear functions
- The hidden layer with a nonlinearity lets us express richer functions

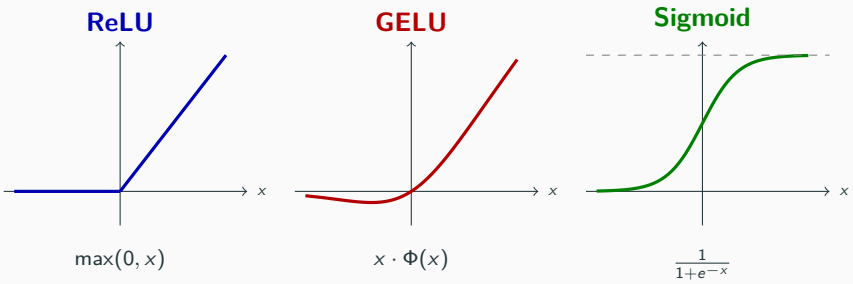
The MLP in PyTorch

```
import torch.nn as nn

mlp = nn.Sequential(
    nn.Linear(3, 128),    # input -> hidden (weights + bias)
    nn.ReLU(),            # nonlinearity
    nn.Linear(128, 2),    # hidden -> output
)

y = mlp(x)  # x: (batch, 3) -> y: (batch, 2)
```

- `nn.Linear`: $y = Wx + b$ (learnable W, b)
- `nn.Sequential`: chain layers into a pipeline

Activation Functions

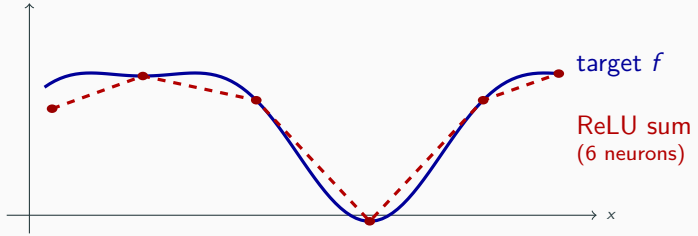
Without nonlinearities, stacking linear layers just gives another linear layer.



- **ReLU**: simple, effective, standard for MLPs
- **GELU**: smooth, used in transformers
- **Sigmoid**: saturates at extremes, mostly historical

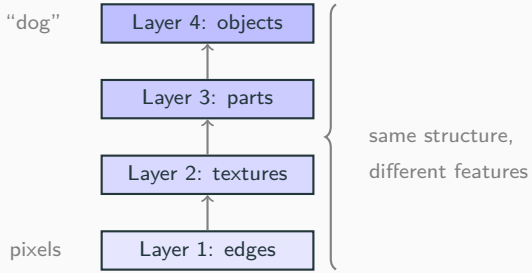
Universal Approximation

Theorem (Cybenko, Hornik et al.): A single hidden layer can approximate any continuous function on a compact set.



- Each ReLU neuron contributes a "hinge"; their weighted sum approximates f
- Existence result, not a recipe: says nothing about how many neurons you need
- In practice, deeper is much more efficient than wider

Depth: Stacking Layers



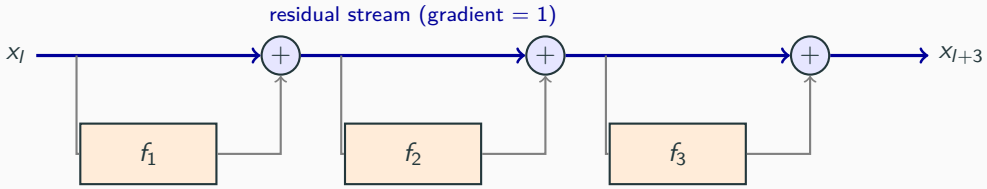
- Each layer builds on the previous one's representations
- The deep learning recipe: repeat a simple block many times

Over/underparameterization:

- Too few parameters $\Rightarrow$ cannot represent the function
- Too many $\Rightarrow$ can memorize, but modern networks often still generalize

Residual Connections

Deep networks suffer from **vanishing gradients**: gradients shrink to zero through many layers.



$$x_{l+1} = x_l + f(x_l)$$

- Gradient flows unimpeded through the skip path (identity)
- Each block only needs to learn the *residual* correction $f(x_l)$

Residual Connections in PyTorch

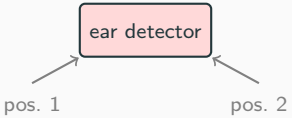
```python
class ResidualBlock(nn.Module):
    def __init__(self, d_model):
        super().__init__()
        self.layers = nn.Sequential(
            nn.Linear(d_model, d_model),
            nn.ReLU(),
            nn.Linear(d_model, d_model),
        )

    def forward(self, x):
        return x + self.layers(x)  # skip connection!
```

- The `x +` is the entire trick
- Stack many of these: `nn.Sequential(*[ResidualBlock(d) for _ in range(n)])`

Architecture Encodes Symmetry

The right architecture exploits structure in the data.

CNN: one detector

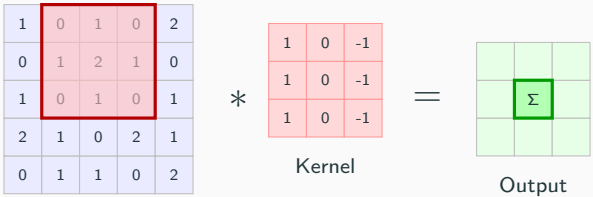


MLP: one detector per position

. . . (one for every pixel)

An architecture that respects a symmetry needs **fewer parameters** and **less data**.

Convolutional Neural Networks



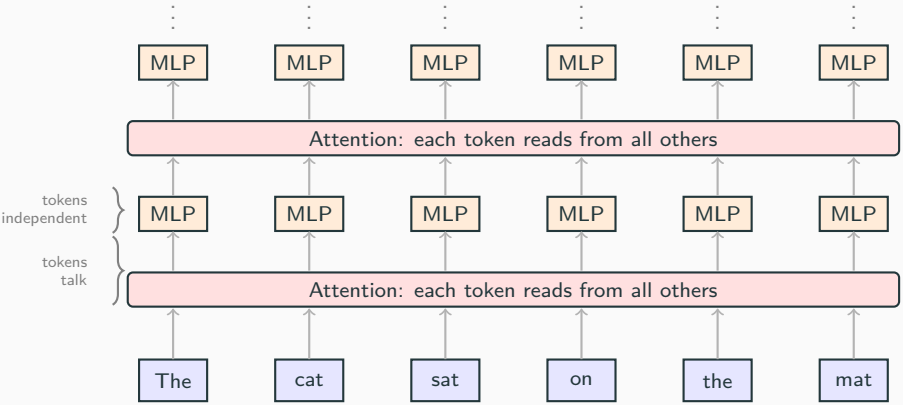
- **Same kernel** slides across every position (weight sharing)
- Same features detected regardless of location $\Rightarrow$ translation invariance
- Hierarchy: edges $\rightarrow$ textures $\rightarrow$ parts $\rightarrow$ objects

CNNs in PyTorch

```
cnn = nn.Sequential(
    nn.Conv2d(1, 16, kernel_size=3, padding=1),  # 1 channel -> 16
    nn.ReLU(),
    nn.MaxPool2d(2),                    # downsample 2x
    nn.Conv2d(16, 32, kernel_size=3, padding=1),
    nn.ReLU(),
    nn.MaxPool2d(2),
    nn.Flatten(),                       # spatial -> vector
    nn.Linear(32 * 7 * 7, 10),          # classify into 10 classes
)
```

- `Conv2d`: the sliding kernel (learnable weights)
- `MaxPool2d`: downsample by taking the max in each region
- Parameters: only the kernel values, shared across all positions

Transformers (Preview)



- **Attention**: tokens mix information (the only place they interact)
- **MLP**: each token processed independently (same weights, different data)
- We will go much deeper in the afternoon session

Exercise 3: Build Simple Architectures

15 minutes

Hyperparameter Optimization

Hyperparameters

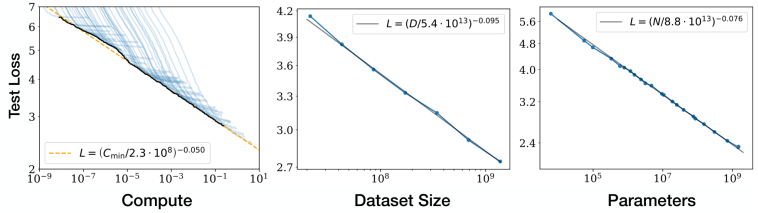
Any property not set by gradient descent is set by the experimenter:

- Model architecture (depth, width, . . .)
- Batch size, number of epochs
- Learning rate, momentum, and other optimizer settings

Finding Good Hyperparameters

- Some we have figured out once and reuse (e.g. $\beta_1 = 0.9$)
- Some we sweep over: run many times, pick the best (typically learning rate)
- Some follow **scaling laws**: cheap small experiments predict large-scale performance

Scaling Laws [Kaplan et al. 2020]



Performance follows smooth power laws across > 6 orders of magnitude in compute, data, and parameters. Cheap small experiments predict large-scale performance.

Exercise 4: Hyperparameter Tuning

Until lunch

`https://playground.tensorflow.org/`

References i

- Christiano, Paul, Jan Leike, Tom B. Brown, Miljan Martic, Shane Legg, and Dario Amodei [June 2017]. *Deep Reinforcement Learning from Human Preferences*. URL: https://arxiv.org/abs/1706.03741.
- Kaplan, Jared, Sam McCandlish, Tom Henighan, Tom B. Brown, Benjamin Chess, Rewon Child, Scott Gray, Alec Radford, Jeffrey Wu, and Dario Amodei [Jan. 2020]. *Scaling Laws for Neural Language Models*. URL: https://arxiv.org/abs/2001.08361.
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- Sutskever, Ilya, James Martens, George Dahl, and Geoffrey Hinton [2013]. "On the Importance of Initialization and Momentum in Deep Learning". In: ICML. URL: https://proceedings.mlr.press/v28/sutskever13.html.