AI is Driving a Revolution in Scientific Computing

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Topics

Part 1: Slides

- AI-driven scientific computing
- Applications

Part 2: Hands on coding

`https://github.com/QuantEcon/rba_workshop_2024`

AI-driven scientific computing

AI is changing the world

- image processing / computer vision
- speech recognition, translation
- scientific knowledge discovery
- forecasting and prediction
- generative AI

Plus killer drones, skynet, etc....

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Projected spending on AI in 2024:

- Google: \$50 billion
- Microsoft: \$60 billion
- Meta: \$40 billion
- etc.

What kinds of problems are they solving?

Deep learning in two slides

Aim: approximate an unknown functional relationship

$$y = f(x) \qquad (x \in \mathbb{R}^d,\ y \in \mathbb{R})$$

Examples.

- $x =$ cross section of returns, $y =$ return on oil futures tomorrow
- $x =$ weather sensor data, $y =$ max temp tomorrow

Problem:

- observe $(x_i, y_i)_{i=1}^n$ and seek f such that $y_{n+1} \approx f(x_{n+1})$

Nonlinear regression: choose model $\{f_\theta\}_{\theta\in\Theta}$ and minimize the empirical loss

$$\ell(\theta) := \sum_{i=1}^{n}(y_i - f_\theta(x_i))^2 \quad \text{s.t.} \quad \theta \in \Theta$$

In the case of ANNs, we consider all f_θ having the form

$$f_\theta = \sigma \circ A_1 \circ \cdots \circ \sigma \circ A_{k-1} \circ \sigma \circ A_k$$

where

- $A_i x = W_i x + b_i$ is an affine map
  - `output = dot(kernel, input) + bias`
- σ is a nonlinear "activation" function

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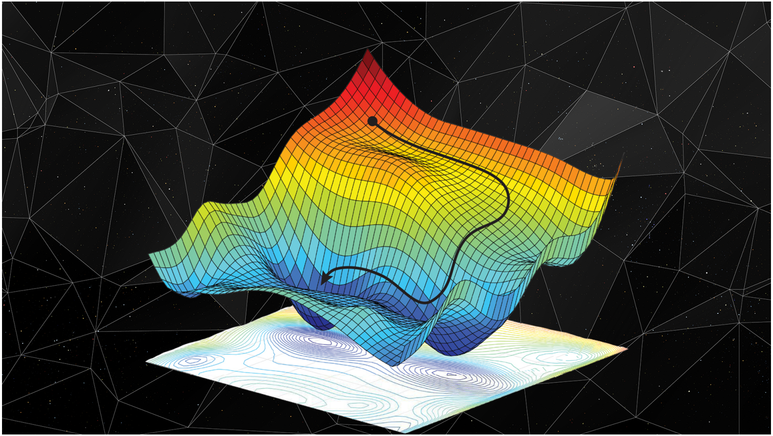
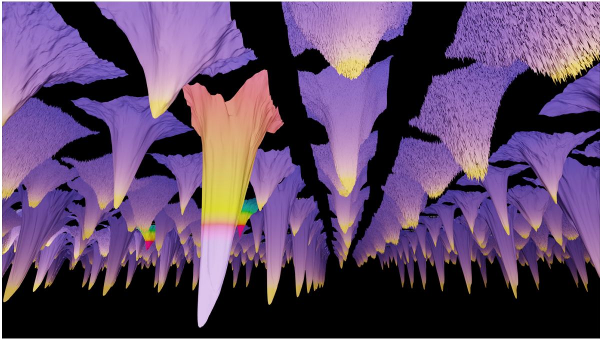
Minimizing a smooth loss functions – what algorithm?



Source: https://danielkhv.com/

Deep learning: $\theta \in \mathbb{R}^d$ where $d = ?$



Source: https://losslandscape.com/gallery/

How does it work?

Why is it possible to minimize over $\theta \in \mathbb{R}^d$ when $d = 10^{12}$?!?

Core elements

- automatic differentiation (for gradient descent)
- parallelization (GPUs or TPUs)
- Compilers / JIT-compilers

How does it work?

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Automatic differentiation

"Exact numerical" differentiation

```
def loss(θ, x, y):
  return jnp.sum((y - f(θ, x))**2)

loss_gradient = grad(loss))
```

Now use gradient descent...

Parallelization

```
outputs = pmap(f, data)
```

- multithreading over GPU cores (how many?)
- multiprocessing over accelerators in a GPU farm (how many?)

Just-in-time compilers

```
@jit
def f(x):
    return jnp.sin(x) - jnp.cos(x**2)
```

Advantages:

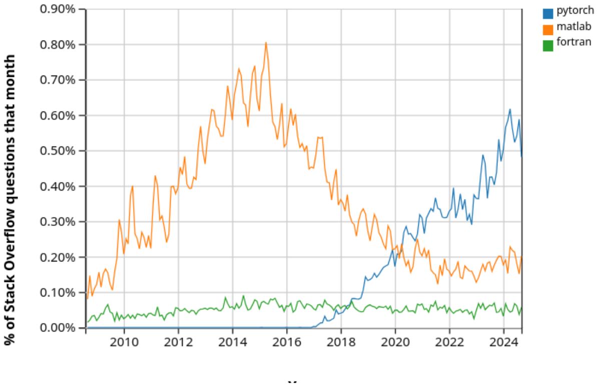
- compiler needs less type information
- can specialize based on parameter types / shapes
- can automatically specialize to CPU / GPU / TPU

Platforms

Platforms that support AI / deep learning:

- PyTorch (Llama, ChatGPT)
- Google JAX (Gemini, DeepMind)
- Keras (backends = JAX, PyTorch)
- Mojo? (Modular (Python))

Popularity


% of Stack Overflow questions that month
0.90%
0.80%
0.70%
0.60%
0.50%
0.40%
0.30%
0.20%
0.10%
0.00%
2010
2012
2014
2016
2018
2020
2022
2024
pytorch
matlab
fortran

Focus on JAX

- Just-in-time compilation
- Automatic differentiation
- Xccelerated linear algebra

Advantages for economists:

- exposes low level functions
- elegant functional programming style – close to maths

```python
import jax.numpy as jnp
from jax import grad, jit

def f(θ, x):
  for W, b in θ:
    w = W @ x + b
    x = jnp.tanh(w)
  return x

def loss(θ, x, y):
  return jnp.sum((y - f(θ, x))**2)

grad_loss = jit(grad(loss))  # Now use gradient descent
```

Example. AlphaFold3 (Google JAX)

Highly accurate protein structure prediction with AlphaFold

John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool,...

Nature Vol. 596 (2021)

- Citation count $=\ 30$K
- Nobel Prize in Chemistry 2024

AI tools for economic modeling

AI-driven scientific computing provides many powerful new tools

And most of the relevent code is open source

Can be used for deep learning <u>or</u> mathematical modeling

In particular, can be used to accelerate macro models

Case Study

The CBC uses the "overborrowing" model of Bianchi (2011)

- credit constraint loosens during booms
- bad shocks $\rightarrow$ sudden stops

CBC implementation in MATLAB

- runs on $10K mainframe with 356 CPUs and 1TB RAM
- runtime $=$ 12 hours

Rewrite in Python JAX

- runs on $400 gaming GPU
- runtime $=$ 4.17 seconds