The AI-driven Revolution in Scientific Computing

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Topics

Part 1: Workshop

- AI-driven scientific computing
- Applications

Part 2: Hands on coding

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

Quick poll:

- Python programmers?
    - NumPy? Numba? PyTorch? JAX?
- Julia?
- R?
- MATLAB?
- C?
- Fortran?

Regular GPU users?

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: find an approximation to 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 $y_{n+1} \approx f(x_{n+1})$

Training: minimize the empirical loss

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

But what is $\{f_\theta\}_{\theta \in \Theta}$?

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
- σ is a nonlinear “activation” function

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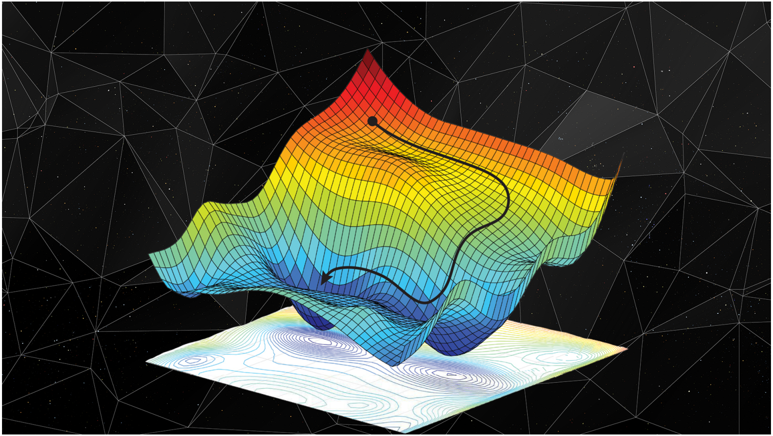
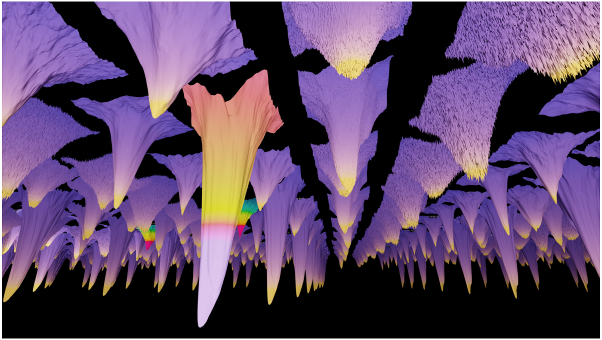
Minimizing a smooth loss functions – what algorithm?



Source: https://danielkhv.com/

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



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

Hardware

“NVIDIA supercomputers are the factories of the AI industrial revolution.” – Jensen Huang

Software

Core elements

- automatic differentiation (for gradient descent)
- parallelization (GPUs! — how many?)
- Compilers / JIT-compilers

These components must be well integrated

Platforms with these features

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

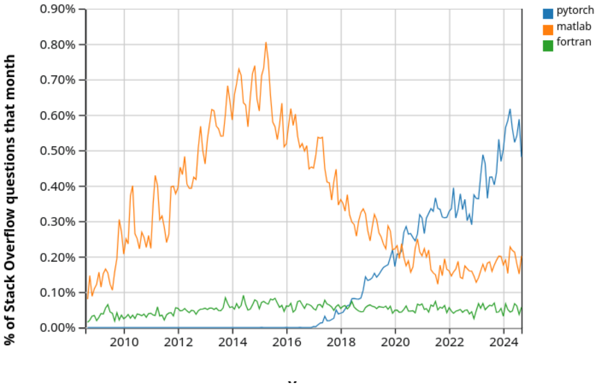
```python
import jax.numpy as jnp
from jax import grad, jit

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
```

Popularity



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

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 $=$ 30K
- 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 or 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 → 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