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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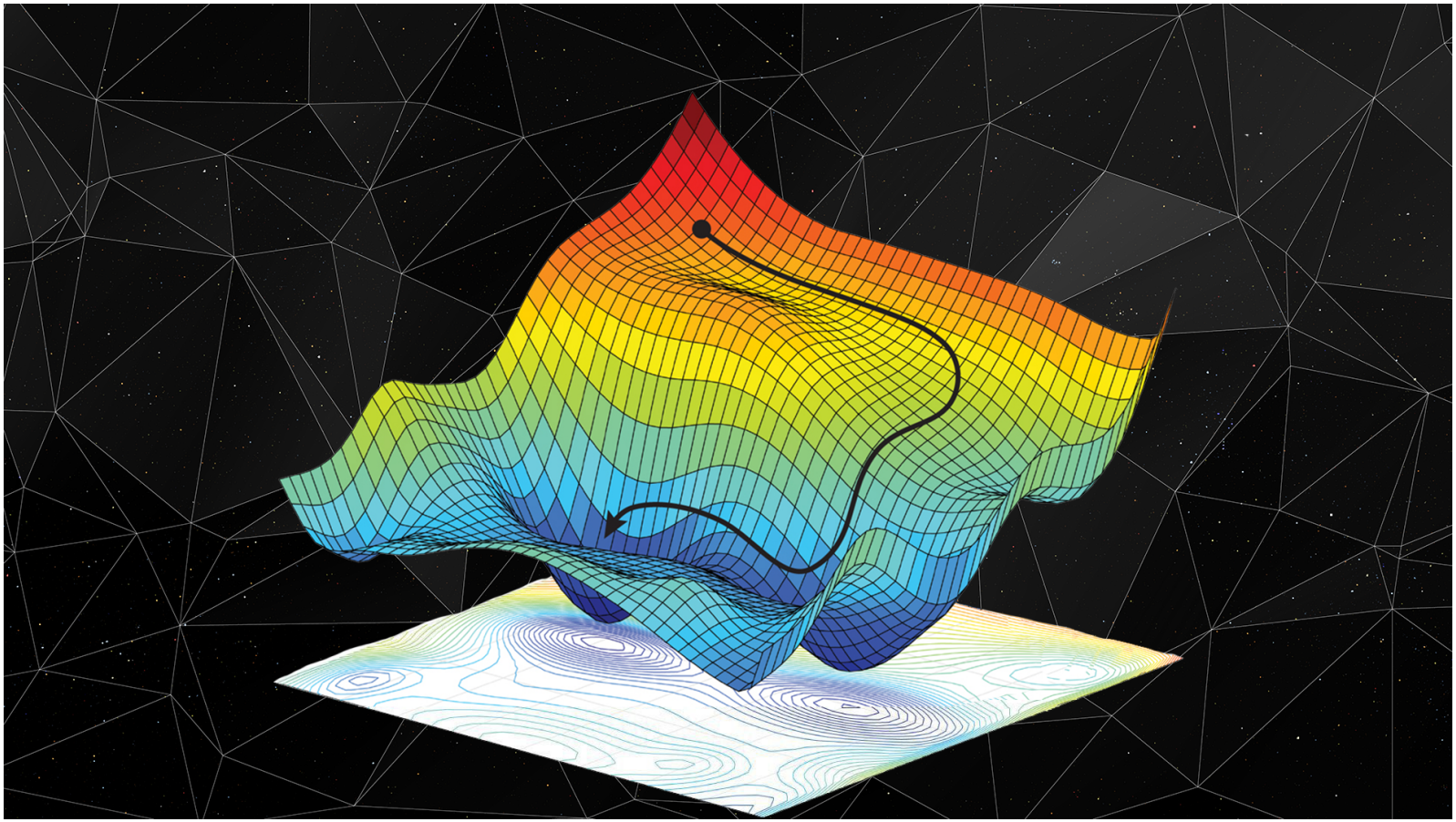
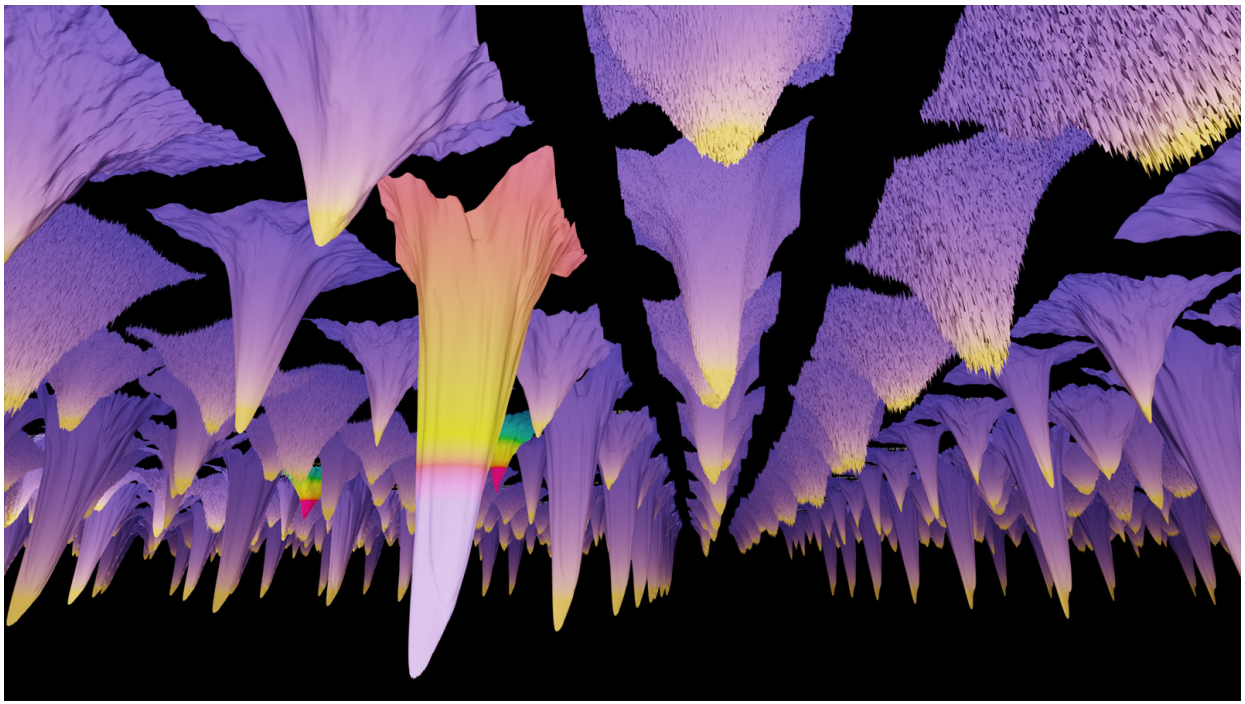
Minimizing a smooth loss functions – what algorithm?



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

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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:

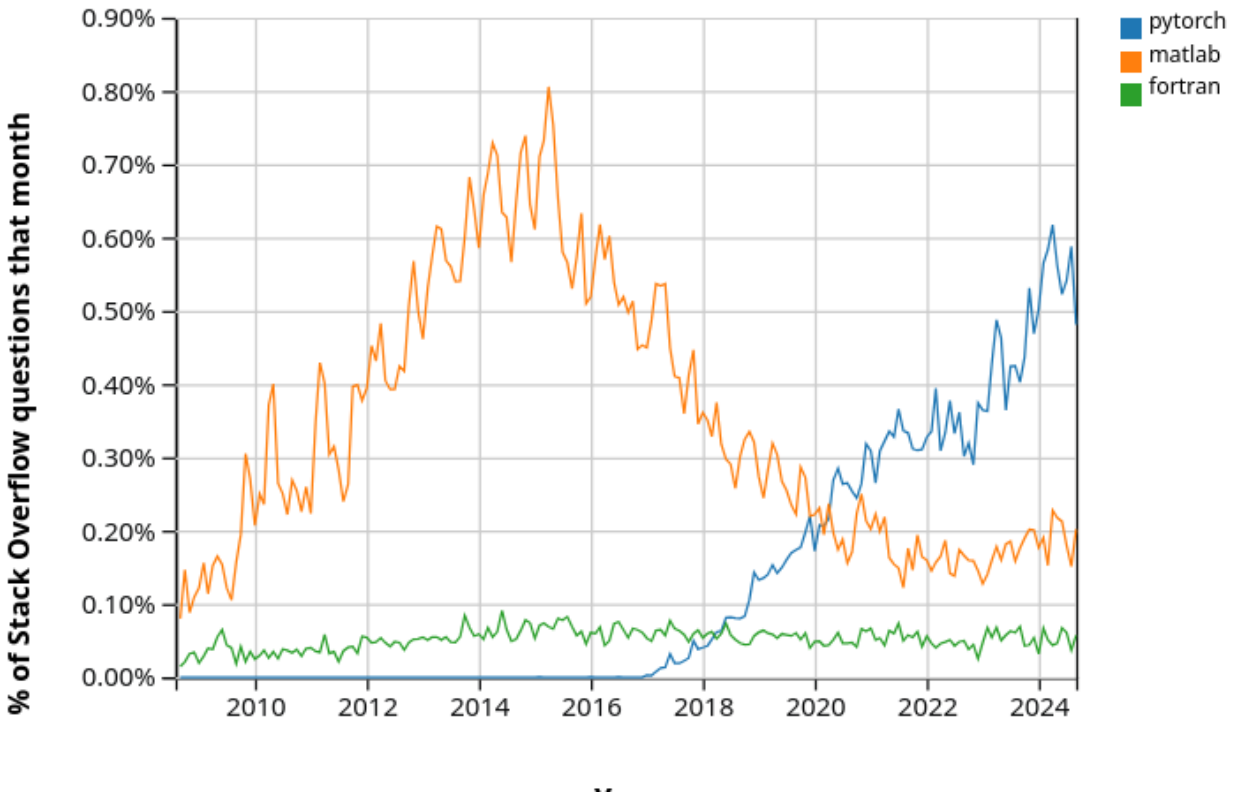
- compiler needs less type information
- can specialize based on parameter types / shapes
- can automatically specialize to CPUs / GPU / TPU

Platforms

Platforms that support AI / deep learning:

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

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
- automatic parallelization

```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

Let's say that you want to do computational macro rather than deep learning per se

Can these new AI tools be applied?

Answer: Yes!

- fast matrix algebra
- fast solutions to linear systems
- fast nonlinear system solvers
- fast optimization, etc.

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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 \$10,000 mainframe with 356 CPUs and 1TB RAM
- runtime $=$ 12 hours

Rewrite in Python $+$ Google JAX

- runs on \$400 gaming GPU with 10GB RAM
- runtime $=$ 4.17 seconds