

AI, Transformers, and the Acceleration of Science

From Core Technology to Scientific Discovery and Economic Impact

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AI in Science: From Analysis to Generation

- AI is a field that has been revitalized by advancements in computational technologies and data availability (Cardon et al., 2018)
- AI techniques are affecting the entire scientific pipeline, from hypothesis formulation to knowledge sharing and public engagement (Galindo et al., 2020)
- AI is making a big impact on scientific discovery, increasing productivity for scientists and spreading rapidly across all domains (Cockburn et al., 2019; Furman et al., 2020; Bianchini et al., 2022)
- More recently, AI has reached an "inflection point" (The Royal Society, 2024), with Generative AI enabling *de novo* design (Das, 2025) and acting as a "metacognitive partner" for researchers (Tan & Li, 2025).

AI as a General Purpose Technology (GPT)

The Paradigm Shift in Technological Innovation

Artificial Intelligence manifests the defining attributes that characterize transformative general purpose technologies (like electricity or the steam engine):

- **Pervasiveness:** Diffusion across virtually all economic sectors—from healthcare diagnostics to financial modeling and scientific research.
- **Continuous Improvement:** Exponential performance gains following predictable "scaling laws".
- **Complementary Innovation Spawning:** Catalyzing secondary innovations in data infrastructure, software, and new scientific methods.

The Fundamental Economic Function: Prediction

Specifying AI's Precise Economic Role

To understand AI's economic impact, we must specify its **precise function**:

AI fundamentally reduces the cost of prediction

Where **Prediction** is the process of using available information to generate missing information.

Application Domains

- Predicting protein structures from a gene sequence.
- Predicting material properties from molecular formations.
- Predicting paper classification from an abstract.

The Bottlenecks of Pre-Transformer Architectures

Sequential Processing Constraints

Problem 1: The Memory Constraint

Recurrent Neural Networks (RNNs) process text sequentially:

$$h_t = f(h_{t-1}, x_t)$$

Critical Limitations:

- Effective context window: $\approx 10\text{--}20$ tokens.
- Information degradation (Vanishing Gradient): By the end of a long sentence, the model "forgets" the beginning.

Problem 2: The Parallelization

Constraint The sequential nature was a computational bottleneck:

- Token t cannot be processed until $t - 1$ is complete.
- Fundamentally **non-parallelizable**.
- Inefficient use of modern GPUs.
- Training was slow and expensive.

"Attention Is All You Need" (Vaswani et al., 2017)

The Architectural Innovation

The Transformer architecture abandoned sequential processing, introducing **parallel processing** of all tokens simultaneously.

Core Innovation: Self-Attention

For each token, the model computes an "attention score" with every other token, creating a rich map of contextual relationships.

$$\text{Attention}(Q, K, V) = \text{softmax} \left(\frac{QK^T}{\sqrt{d_k}} \right) V$$

Example: Contextual Understanding

"The robot picked up the apple because it was red." Self-attention dynamically computes:

- High attention score: **it** \leftrightarrow **apple**
- Low attention score: **it** \leftrightarrow **robot**

This allows the model to learn which relationships matter, regardless of distance.

Architectural Variants: BERT vs. GPT

Task-Specific Adaptations

1. Encoder-Only (e.g., BERT)

- **Bidirectional** attention: each token attends to all others (past and future).
- **Training:** Predicts masked-out words.
- **Optimized for: Understanding and analysis.**
- **Use Case:** Text classification, semantic search, sentiment analysis.

2. Decoder-Only (e.g., GPT series)

- **Causal (unidirectional)** attention: token t attends only to tokens $\leq t$.
- **Training:** Predicts the next word.
- **Optimized for: Text generation.**
- **Use Case:** Summarization, writing assistance, programming, chatbots.

The Accessibility Paradox

Democratizing Access via Open-Source and Transfer Learning

High Development Costs Supply-Side

Concentration:

- Pre-training: \$10M–\$200M
- Data requirements: 10^9 – 10^{12} tokens
- Computational infrastructure: thousands of GPUs

Market Structure:

- Dominated by: OpenAI, Google, Anthropic, Meta, Microsoft

Low Deployment Costs Demand-Side

Democratization:

- Fine-tuning: \$1K–\$100K
- Data requirements: 10^3 – 10^5 examples
- Consumer hardware sufficient (single GPU)

The Key: Transfer Learning

- A 100 – $10,000\times$ cost reduction.
- This makes AI accessible to individual researchers and smaller labs.

Infrastructure for Accessible AI: Hugging Face

The "GitHub" of Machine Learning

URL: <https://huggingface.co/> This ecosystem provides the essential components for researchers:

① Model Hub:

- 500,000+ pre-trained models.
- Includes domain-specific models (e.g., SciBERT, Legal-BERT, FinBERT).

② Datasets Library:

- 100,000+ datasets with a unified API.

③ Transformers Library:

- A unified, simple API ('pipeline') to use any model.
- Makes fine-tuning and inference accessible with a few lines of code.

The Power of Fine-Tuning and PEFT

Adapting Foundation Models for Specific Research

1. Transfer Learning (Fine-Tuning):

- **Paradigm Shift:** Don't train from scratch.
- **Process:** 1. Start with a pre-trained model (e.g., BERT). 2. Freeze the lower layers (general linguistic knowledge). 3. Train only the upper layers on your small, domain-specific dataset (e.g., your JEL-coded abstracts).

2. Parameter-Efficient Fine-Tuning (PEFT / LoRA):

- **Problem:** Fine-tuning large models (7B, 70B) is still expensive.
- **Solution (LoRA):** Freeze all pre-trained weights. Train only tiny "adapter" matrices (0.1–1% of parameters).
- **Result:** Comparable performance to full fine-tuning, but possible on a single consumer GPU. This is a game-changer for academic research budgets.

Retrieval-Augmented Generation (RAG)

Grounding LLMs in Factual Data

This is a critical technique for scientific and enterprise use. It solves "hallucination".

- ① **Retrieve (Search):** When a user asks a query, the system first searches a private knowledge base (e.g., your research archive, a database of papers).
- ② **Augment (Context):** The system takes the relevant documents it found and "pastes" them into the LLM's prompt.
- ③ **Generate (Answer):** The LLM is instructed: *"Answer the user's query using only the context provided."*

Advantages for Researchers:

- Access to up-to-date information (beyond the model's training cutoff).
- Reduced hallucination; answers are "grounded" in real data.
- **Citations and Sources:** The model can cite which document it used to generate the answer.

AI in "Rugged" Knowledge Landscapes

Solving Problems Where Human Intuition Fails

Rugged Landscapes: Complex, Non-Linear Problem Spaces Characteristics:

- High-dimensional search spaces (10^{100+} possibilities)
- Non-linear relationships between variables
- Multiple local optima (misleading signals)
- Human intuition provides limited guidance

AI (and Transformers in particular) excels through **exhaustive exploration** and **pattern recognition** at scales impossible for humans.

Example 1: Protein Structure Prediction (AlphaFold)

A Grand Challenge in Biology Solved by AI

The Challenge: Predicting the 3D shape of a protein from its 1D amino acid sequence. A problem that was unsolved for 50 years.

Traditional Method:

- X-ray crystallography or cryo-EM
- Timeline: 6–12 months per protein
- Cost: \$100K–\$1M+ per structure

AlphaFold (DeepMind, 2020):

- Deep learning (a type of Transformer)
- Timeline: **Minutes per protein**
- Accuracy: 95%+ match with experimental structures
- Impact: Predicted and open-sourced 200+ million protein structures, accelerating drug discovery and biology research.

Example 2: Antibiotic and Material Discovery

Hypothesis Generation Beyond Human Chemical Spaces

Novel Antibiotic Discovery (MIT, 2020) Challenge: Antibiotic resistance crisis, declining drug discovery pipeline.

AI Approach:

- A deep learning model was trained on molecular properties.
- Screened 6,000+ compounds *in silico* (in simulation).
- Identified **Halicin**: a novel antibiotic with a new mechanism, active against drug-resistant bacteria.

Significance: This demonstrates AI's capability for **hypothesis generation** beyond human-designed chemical spaces, accelerating the discovery process from years to days.

A (Personal) Case Study: AI to Solve a Bottleneck in Economic Science

The Interdisciplinarity Paradox

- 1. The Research Problem:** Is interdisciplinarity (IDR) in economics a **reward** (higher impact) or a **penalty** (evaluative hurdles, citation lag)?
- 2. The Bottleneck (Why it was unsolved):**

- Researchers could not empirically *separate* two different types of diversity:
 - **Topic Diversity** (WHAT you study, e.g., "Health" + "Finance")
 - **Methodological Diversity** (HOW you study it, e.g., "Econometrics" + "Field Experiment")
- Past methods (keywords, citation analysis) failed. Fontana et al. (2020) found their measures were "essentially the same property ($r > 0.9$)".
- We couldn't distinguish a paper *developing* a new method from one just *using* it.

Case Study: AI-Enabled Findings

Decomposing "Risk" vs. "Reward"

3. The AI Solution (Unlocking the Bottleneck):

- We used a **Llama-3-70B** model as a "JEL expert".
- The AI was prompted to read $\approx 245,000$ abstracts and classify the function of each JEL code (Topic vs. Method).
- This semantic classification was impossible at scale for humans but is a perfect task for an LLM.

4. The Model (With AI-Classified Data):

- We used a **Hurdle Model** on 5-year citations.
- This model separates two distinct processes:
 - **The Risk (Logit)**: What is the probability of getting zero citations?
 - **The Reward (Count)**: Given it's cited, how many citations does it get?

Case Study: The paradox is Solved

5. The Finding (The Paradox is Solved):

- Topic Diversity (RS_T) is a High-Risk, High-Reward strategy.
 - It *increases* the risk of getting 0 citations (the "penalty").
 - But *if* it crosses the hurdle, it gets *significantly more* citations (the "reward").
- Methodological Diversity (RS_M) is a Risk-Reducing strategy.
 - It *helps* a paper get seen and cross the 0-citation hurdle.

Conclusion: The "paradox" was a measurement error. AI-driven semantic analysis is a possible way to disentangle these two effects.

The Broader Framework: Prediction and Complementarity

Understanding AI's Economic Impact

Our case study is one example of a broader economic principle.

The Core Function: AI makes "prediction" cheap.

The Economic Principle: When the price of a good (X) declines, demand for its complements (Z) increases.

What are the complements to cheap AI prediction?

1. Data

- The input for prediction.
- Its value increases, which is why data infrastructure, collection, and curation are now critical competitive assets.

2. Human Judgment

- The *output* of prediction.
- AI provides a prediction, but a human provides judgment on what to *do* with it.

The Value of Human Judgment

Why Humans Become More Valuable, Not Less

AI automates **prediction**; humans provide **judgment**.

The economic value of judgment increases precisely because prediction is commodified.

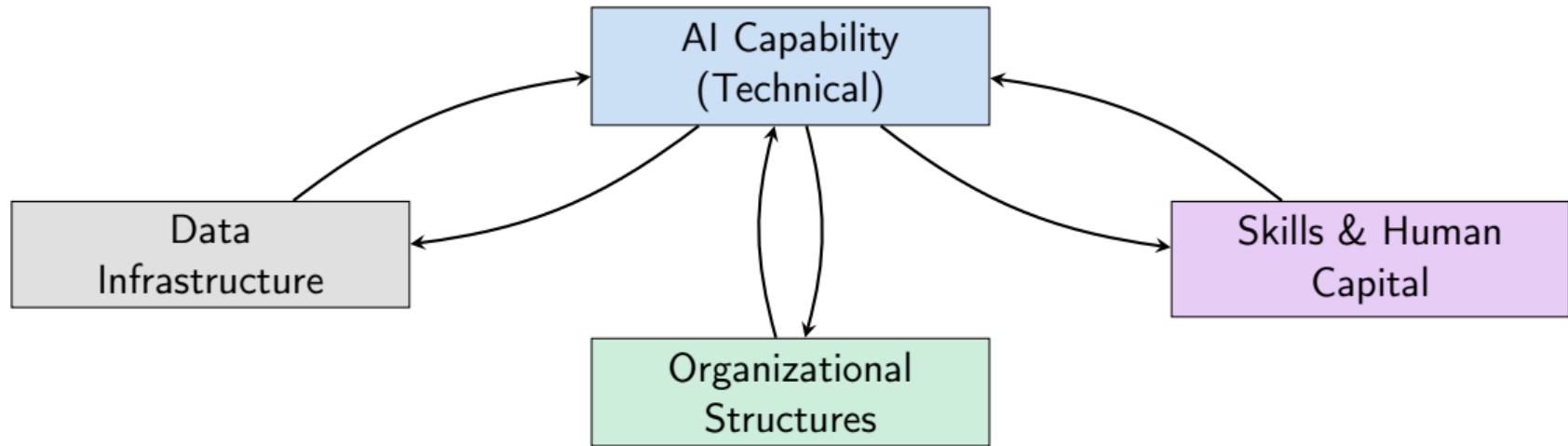
Judgment is a multi-dimensional capability:

- **Contextual Reasoning:** Recognizing when the AI's prediction, though statistically valid, is wrong in a specific, novel context.
- **Trade-off Evaluation:** Weighing competing, non-quantifiable objectives (e.g., scientific rigor vs. research cost).
- **Novelty Handling:** Extrapolating principles to new problems the AI has never seen (i.e., framing new research questions).
- **Ethical Reasoning:** Identifying hidden biases or stakeholder impacts in a prediction.

The Co-Evolutionary Process

Why Societal Impact Lags Behind Technical Capability

AI's societal value depends on **co-evolution** with complementary systems:



The Co-Evolution Lag: Technical capability advances rapidly (months); but institutions, organizational structures, and human skills adapt slowly (years/decades).

The Productivity Paradox: Explained

Why Don't We See AI in the Productivity Statistics?

The Paradox:

- We see spectacular AI breakthroughs (AlphaFold, GPT-4).
- Yet: **Aggregate productivity growth remains modest.**
- This mirrors the "Solow Paradox" for computers (1987).

The Co-Evolutionary Explanation: Productivity realization requires massive, slow, and costly **complementary investments**:

- ① **Organizational Restructuring** (Workflow redesign, role redefinition)
- ② **Complementary Investment** (Data infrastructure, new software)
- ③ **Institutional Adaptation** (Human capital, training, new standards)

These adaptations occur over **decades**, not months.

The Labor Market Transformation

Automation of Prediction, Augmentation of Judgment

The Skill Premium Divergence Economic Prediction:

$$\text{As Cost(Prediction)} \downarrow \Rightarrow \begin{cases} \text{Wage}(S_{\text{prediction}}) \downarrow & (\text{substitution effect}) \\ \text{Wage}(S_{\text{judgment}}) \uparrow & (\text{complementarity effect}) \end{cases}$$

where $S_{\text{prediction}}$ = prediction-substitutable skills, S_{judgment} = judgment-complementary skills

Occupational Impact Taxonomy

- **High Substitution Risk:** Tasks that are purely prediction (e.g., routine data analysis, standardized report writing).
- **Low Substitution Risk:** Tasks that are judgment-intensive (e.g., strategic management, creative problem-solving, empathetic counseling).

Income Inequality: Mechanisms and Projections

Why AI May Increase Inequality

Skill-Biased Technological Change:

- AI automates routine cognitive tasks disproportionately performed by middle-skill workers.
- High-skill workers (judgment-intensive roles) experience productivity gains.
- Result: **Hollowing of the middle**, and polarization.

Capital vs. Labor:

- AI as capital investment that substitutes for labor.
- Returns accrue to capital owners (shareholders, investors).
- Labor share of income may decline in automated sectors.

Winner-Take-Most Markets:

- Superstars with AI augmentation can capture disproportionate value.
- Scale economies: The best AI-augmented professionals can serve global markets, concentrating wealth.

Synthesis: The Co-Evolutionary Framework

Integrating Technical, Economic, and Institutional Dimensions

Multi-Level Integration Level 1: Technical Innovation

- **Transformer architecture** (2017) solved computational bottlenecks, enabling massive scale.
- Result: AI capabilities (like in our case study) that accelerate scientific discovery.

Level 2: Economic Transformation

- Core economic function: **Reduction in prediction costs**.
- Complementarity principle: Increased value of **Data** and **Human Judgment**.

Level 3: Institutional Adaptation

- **Human capital**: Educational reform toward judgment capabilities.
- **Co-evolution lag**: Technical capability advances rapidly; institutional adaptation (skills, organizations) proceeds slowly.

Final Synthesis: The Transformer's Legacy

From Technical Innovation to Societal Transformation The Transformer architecture represents far more than a technical achievement:

- ① **Technical Level:** Solved computational constraints, enabling unprecedented scale for pattern recognition and generation.
- ② **Scientific Level:** Accelerates discovery by solving complex search problems (AlphaFold) and automating large-scale analysis (our case study).
- ③ **Economic Level:** Commodified prediction, fundamentally altering the economics of information work.
- ④ **Social Level:** Creates a "co-evolution lag," forcing our labor markets and educational systems to adapt.

The Central Insight: AI's societal impact is not deterministic. It depends on the quality and speed of our **institutional co-evolution**.

Thank You

Questions?

Appendix: Llama-3 Prompt

As a JEL (Journal of Economic Literature) classification expert, analyze the following academic paper details to provide a comprehensive JEL code classification that captures both methodological and topic aspects...

TITLE: [title] ABSTRACT: [abstract]

JEL CODE CATEGORIES: A: General Economics... [full list]... Z: Other Special Topics

Your task is to:

1. First identify the key METHODOLOGICAL approaches used...
2. Then identify the main TOPIC or SUBJECT MATTER areas...
3. Map both aspects to appropriate JEL codes

When classifying codes:

- Classify a code as METHODOLOGICAL when the paper is developing new methods, extending existing methods, or when the methodological approach is a significant focus of the paper's contribution.
- Classify a code as TOPIC when the paper is applying methods to study a particular economic phenomenon, theory, or subject matter.

Consider the paper's primary contribution when determining classification (method development vs. application to a subject area)...

For each identified JEL code:

- A. Provide the code
- C. Explain why this classification fits...
- D. Indicate if it's primarily METHODOLOGICAL or TOPIC in nature

Format your response as a pipe-separated list...

JEL CODE | JUSTIFICATION | TYPE (METHODOLOGICAL or TOPIC)

Return ONLY the formatted list with no additional text.

Discussion: The "Black Box" vs. The Scientific Method

Context: We have just demonstrated that tools like Cerebras can answer in milliseconds and Ollama can run locally on a laptop. *But how do we establish trust?*

Key Questions

- **Speed vs. Validation:** You saw the model classify an abstract in one second. In traditional science (e.g., Protein Structure, Slide 14), we spend months validating a method.
- **The Origin of Hypotheses:** If we use AI to generate hypotheses (like Halicin, Slide 15) rather than just testing them...
- **The Scientist's Role:** ...how does our identity change? Are we evolving from *creators* of knowledge into mere "*verifiers*" of machine outputs?