AI Tools in Scientific Workflows

Ulrich Degenhardt[1]

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[1]Max-Planck-Institut for Dynamics and Self-Organization
Göttingen

Introduction

Github Repository

`https://github.com/udegenh1/genAI-Talk-January-2026`

- Notes
- Slides
- Prompts
- Transcripts of chats

Why talk about LLMs in science?

- LLMs are widely used in practice, but rarely discussed openly → Emerging taboo?
- The dominant narrative is: “LLMs are just hallucinating stochastic parrots”. Using LLMs is evil, or at least viewed with suspicion.
- But LLMs are here to stay. If we want it or not, there is no going back.
- Goal: Identify *high-value* uses and *high-risk* failure modes.

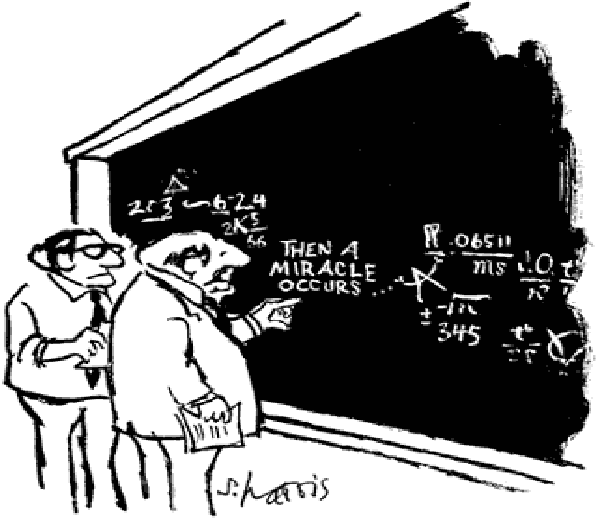
Note

> *”Once a new technology rolls over you, if you’re not part of the steamroller you’re part of the road.”*
>
> *Anonymous*

Intro example 1: When keyword search fails

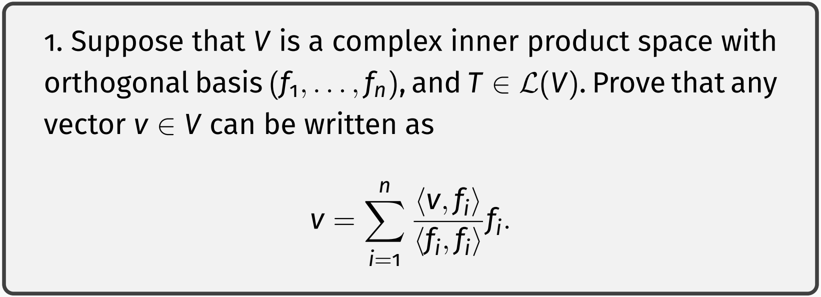
- Vague memory: a cartoon with two guys standing at a blackboard, mathematical equations and maybe the word "magic".
- Google fails because there are no reliable keywords.
- Try this: Give an LLM a verbal description of your vague memories and let it look for an answer
- Repo: https://github.com/udegenh1/genAI-Talk-January-2026

Intro example 1: When keyword search fails



"I think you should be more explicit here in step two."

Intro example 2: Solving undergrad math exercises



1. Suppose that V is a complex inner product space with orthogonal basis $(f_1, \ldots, f_n)$, and $T \in \mathcal{L}(V)$. Prove that any vector $v \in V$ can be written as

$$v = \sum_{i=1}^{n} \frac{\langle v, f_i \rangle}{\langle f_i, f_i \rangle} f_i.$$

- Provide a screenshot of a math exercise and request a solution (Chat transcript in the repo, subdirectory `chats`).
- Repo: https://github.com/udegenh1/genAI-Talk-January-2026
- **Key point:** LLMs seem to simulate understanding of nontrivial math problems and are able to compose a plausible looking answer in LaTeX.

Intro example 3: Help writing slides for a talk

- Upload your notes to the LLM.
- Then ask the LLM to create slides based on the uploaded file.
- Ask the LLM to format the slides in LaTeX for use with the Beamer class, then ask it to save the result as a file and to create a download link (works with ChatGPT).
- Use the result as scaffolding and revise the slides.
- Iterate until you are happy with the solution.
- Repo: https://github.com/udegenh1/genAI-Talk-January-2026

Note

> *”The best way to get the right answer on the internet is not to ask a question; it’s to post the wrong answer.”*
>
> *Cunningham’s law*

Intro: Cognitive Offloading

- Science has always offloaded cognition to tools: calculators, numerical methods, symbolic systems.
- Outputs of pre-LLM tools are constrained by explicit algorithms and models.
- LLMs are not deterministic. Asking the same question twice will result in different answers.

Intro: Cognitive Offloading

- LLMs generate the most probable next statement, not necessarily the correct one.
- LLMs generate plausible statements. In science, that is far more dangerous than obvious nonsense.
- The novelty is not technical, it is the exploitation of the ingrained human tendency to trust.

Intro: Implications for Scientific Use

Note

LLM outputs are not results

- Risk depends on error severity.
- Costs for verification and corroboration of LLM output must be weighed against cognitive savings.

Intro: Brandolini’s law

> *”The amount of energy needed to refute bullshit is an order of magnitude bigger than that needed to produce it.”*
>
> *Alberto Brandolini*

- This is known as **Brandolini’s Law** aka the *Bullshit Asymmetry Principle* on the debunking of misinformation
- LLMs are talkative and generate lots of text. Reading and vetting LLM output may well exceed the cognitive resources of a human.

Intro: Preliminaries before using LLMs

- To be useful in science LLM sessions need documentation. Use a note taking system (e.g. Obsidian) as an “LLM lab book”.
- Export complete chats into your notes.
- Prompts and responses should be numbered.
- Change the overall behavior of the LLM with prompts: E. g. ”No Yes-man mode”, ”advocatus diaboli mode” (Details are in the Github repo).
- Repo: https://github.com/udegenh1/genAI-Talk-January-2026

Trust

Why trust is so important to humans

- Humans are evolutionarily tuned to cooperate with other humans.
- Trust makes cooperation simpler. Simplifying things has always been a major driving force for humans.
- Humans tend to want to trust.

The Turing Test and Trust

Definition: A test of machine intelligence in which a human judge engages in text-only conversations with a hidden human and a hidden machine.

Passing Criterion: The machine passes if the judge cannot distinguish it from the human better than chance.

- LLMs pass the Turing-test
- LLMs show behavior that resembles kindness, empathy or patience
- When we see this our brain defaults to ”There must be a human behind this”. And then we trust

LLMs have no intentions

- LLMs have no consciousness, no intentions and no inner emotional life.
- What appears as kindness, empathy, or patience is the result of statistical pattern generation. These behaviors are simulations, not manifestations of genuine affects.
- LLMs do not want to help, nor can they decide to deceive. Outputs are just statistically plausible continuations of text.

Note

An interaction with an LLM is not a social encounter.

Tool-based trust vs social trust

- The appropriate category of trust is not social trust but tool-based (or technical) trust.
- Some tools in scientific and engineering practice are ”battle tested” and that’s why we trust them.
- Examples include: the Unix stream editor `sed`, Linux and LAPACK.

Software Development

Making expensive things cheap

Some things may require a lot of effort:

- Analyzing error messages
- Looking for answers in bulky manuals
- Analyzing GitHub repositories

LLMs are surprisingly helpful and significantly lower the effort needed to tackle these tasks.

Prototyping: Turning ideas into computational plans

- Ask for a minimal working example for a concrete research task.
- Get an instant draft in Python/Julia/C++/Fortran/...
- You still verify, but the barrier to prototyping collapses.

This is about leverage. It is like having a bright grad student working for you. You certainly have to check his (or her) work, but he is enthusiastic, works 24/7 and never complains.

Case study: Iterative development with an LLM

A more dangerous way of LLM assisted software development:

- Build a Go tool for encrypting a directory tree (example *without* security measures).
- Add features via LLM prompts.
- Iterate by copy-pasting compiler errors back to the LLM.
- Result: a working executable after a few days of tinkering.

Warning: Don’t do this to create production code!

Details can be found in the GitHub repository
https://github.com/udegenh1/genAI-Talk-January-2026

What this teaches (and why it is dangerous)

Lessons learned:

1. Feasible even without prior language knowledge.
2. Having no guardrails is scary (Again: Don’t do this for real!).
3. Strong temptation to stop checking changes over time.

Agents and Automation

What we have now:

- A mixture of genuine AI assistance and manual steps
- A clumsy workflow
- A strong incentive to further automate the process

And here is why new LLM developments are so scary:

- Agent-like tools can execute code, issue system commands and fix errors on their own. Human intervention is no longer necessary.
- Risks explode. Negative consequences range from subtle logical errors to serious system-level problems.
- This is so new that we don’t even know what we don’t know about the risks.

Safeguards

Note

Safeguards become essential, not optional

Some Safeguards are:

- Sandboxed execution, limited permissions.
- Clear audit trails and logging of sessions.
- Mandatory human checkpoints.

Pragmatic workflow

Despite these risks, the idea is extremely appealing.

- General-purpose LLMs like ChatGPT are used to design the computational plan,
- Agentic tools such as Codex CLI handle the concrete tasks of writing and debugging code.
- Depending on your risk appetite modify your usual dev workflow using these tools.

Literature Search

The real bottleneck: search, not access

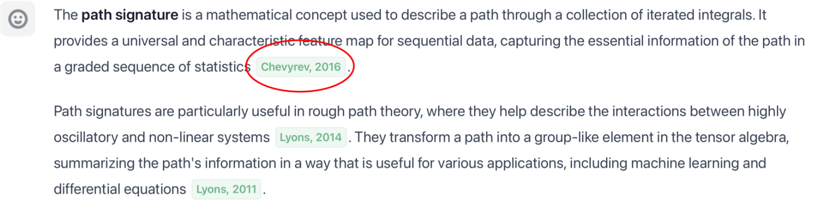
Search for literature and search in literature are common tasks:

- Use specialized LLMs that are able to search huge curated collections of literature abstracts with minimal effort.
- Search in a potentially large collection of documents (scienceOS: up to 4000 documents).
- Ask questions based on a collection of abstracts or documents. No need for keywords.

Searching for papers

Question: What is the path signature?

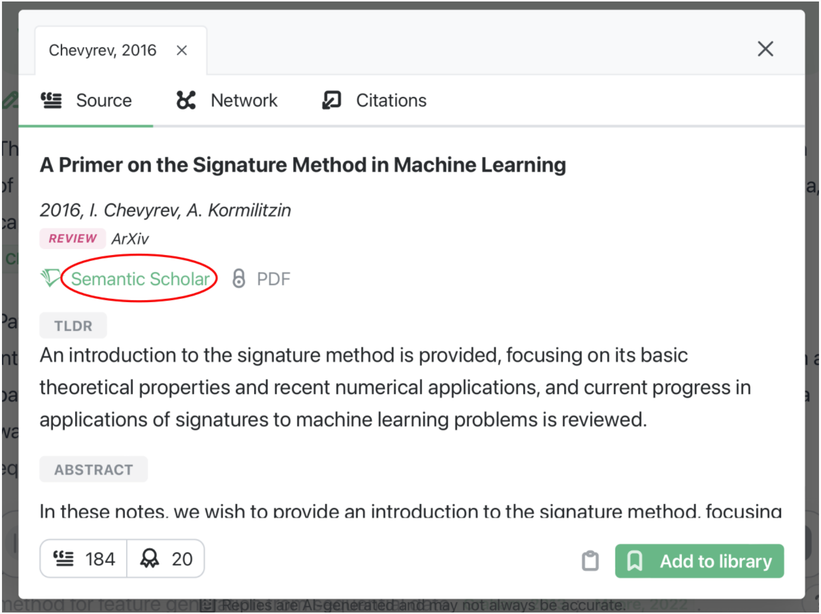
Answer:



The **path signature** is a mathematical concept used to describe a path through a collection of iterated integrals. It provides a universal and characteristic feature map for sequential data, capturing the essential information of the path in a graded sequence of statistics Chevyrev, 2016 .

Path signatures are particularly useful in rough path theory, where they help describe the interactions between highly oscillatory and non-linear systems Lyons, 2014 . They transform a path into a group-like element in the tensor algebra, summarizing the path's information in a way that is useful for various applications, including machine learning and differential equations Lyons, 2011 .

Source: `www.scienceos.ai`



A Primer on the Signature Method in Machine Learning

2016, I. Chevyrev, A. Kormilitzin

REVIEW *ArXiv*

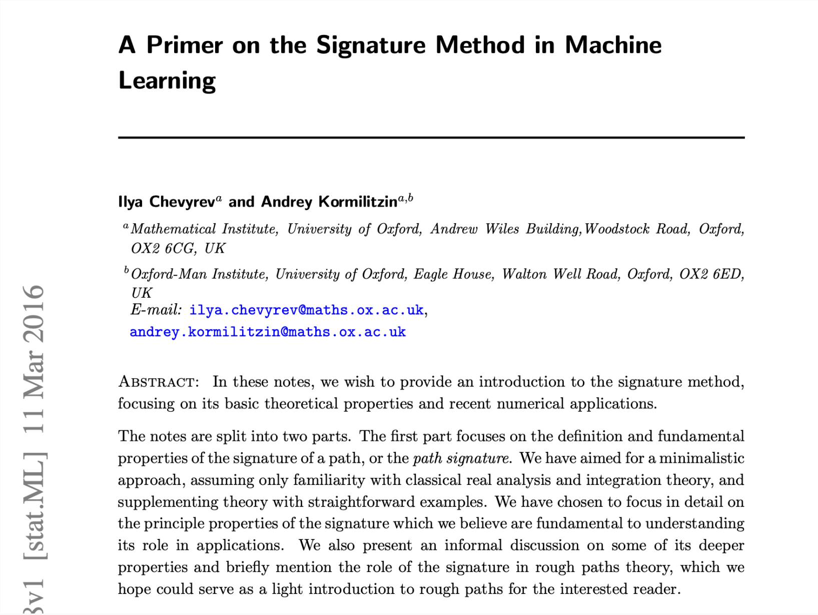
TLDR

An introduction to the signature method is provided, focusing on its basic theoretical properties and recent numerical applications, and current progress in applications of signatures to machine learning problems is reviewed.

ABSTRACT

In these notes, we wish to provide an introduction to the signature method, focusing

Replies are AI-generated and may not always be accurate.



A Primer on the Signature Method in Machine Learning

Ilya Chevyrev[a] **and Andrey Kormilitzin**[a,b]

[a] *Mathematical Institute, University of Oxford, Andrew Wiles Building, Woodstock Road, Oxford, OX2 6CG, UK*

[b] *Oxford-Man Institute, University of Oxford, Eagle House, Walton Well Road, Oxford, OX2 6ED, UK*

E-mail: ilya.chevyrev@maths.ox.ac.uk,
andrey.kormilitzin@maths.ox.ac.uk

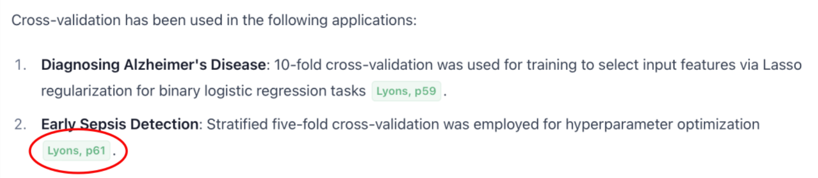
Abstract: In these notes, we wish to provide an introduction to the signature method, focusing on its basic theoretical properties and recent numerical applications.

The notes are split into two parts. The first part focuses on the definition and fundamental properties of the signature of a path, or the *path signature*. We have aimed for a minimalistic approach, assuming only familiarity with classical real analysis and integration theory, and supplementing theory with straightforward examples. We have chosen to focus in detail on the principle properties of the signature which we believe are fundamental to understanding its role in applications. We also present an informal discussion on some of its deeper properties and briefly mention the role of the signature in rough paths theory, which we hope could serve as a light introduction to rough paths for the interested reader.

Example: A long review paper

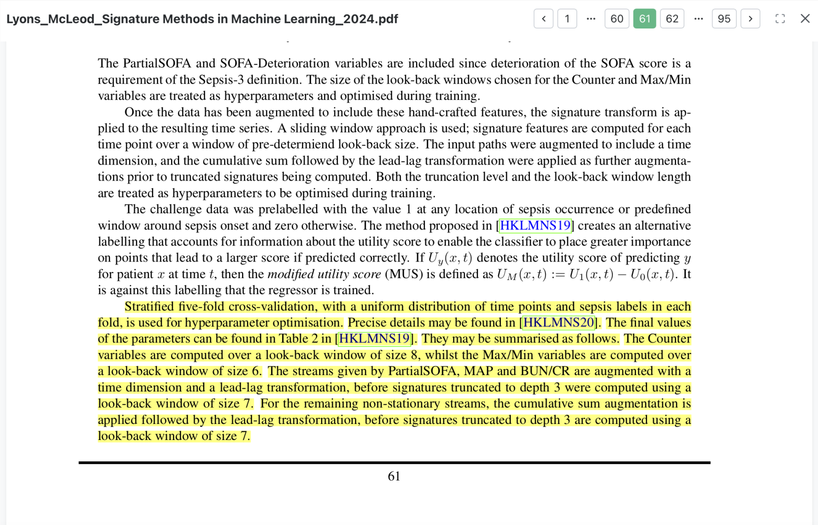
Question: Which of the applications uses cross validation?

Answer:



Cross-validation has been used in the following applications:

1. **Diagnosing Alzheimer's Disease**: 10-fold cross-validation was used for training to select input features via Lasso regularization for binary logistic regression tasks Lyons, p59 .
2. **Early Sepsis Detection**: Stratified five-fold cross-validation was employed for hyperparameter optimization Lyons, p61 .



The PartialSOFA and SOFA-Deterioration variables are included since deterioration of the SOFA score is a requirement of the Sepsis-3 definition. The size of the look-back windows chosen for the Counter and Max/Min variables are treated as hyperparameters and optimised during training.

Once the data has been augmented to include these hand-crafted features, the signature transform is applied to the resulting time series. A sliding window approach is used; signature features are computed for each time point over a window of pre-determiend look-back size. The input paths were augmented to include a time dimension, and the cumulative sum followed by the lead-lag transformation were applied as further augmentations prior to truncated signatures being computed. Both the truncation level and the look-back window length are treated as hyperparameters to be optimised during training.

The challenge data was prelabelled with the value 1 at any location of sepsis occurrence or predefined window around sepsis onset and zero otherwise. The method proposed in [HKLMNS19] creates an alternative labelling that accounts for information about the utility score to enable the classifier to place greater importance on points that lead to a larger score if predicted correctly. If $U_y(x,t)$ denotes the utility score of predicting y for patient x at time t, then the *modified utility score* (MUS) is defined as $U_M(x,t) := U_1(x,t) - U_0(x,t)$. It is against this labelling that the regressor is trained.

Stratified five-fold cross-validation, with a uniform distribution of time points and sepsis labels in each fold, is used for hyperparameter optimisation. Precise details may be found in [HKLMNS20]. The final values of the parameters can be found in Table 2 in [HKLMNS19]. They may be summarised as follows. The Counter variables are computed over a look-back window of size 8, whilst the Max/Min variables are computed over a look-back window of size 6. The streams given by PartialSOFA, MAP and BUN/CR are augmented with a time dimension and a lead-lag transformation, before signatures truncated to depth 3 were computed using a look-back window of size 7. For the remaining non-stationary streams, the cumulative sum augmentation is applied followed by the lead-lag transformation, before signatures truncated to depth 3 are computed using a look-back window of size 7.

The Expertise Paradox

- Beginners benefit: orientation, terminology, scaffolding.
- Experts suffer: oversimplifications, missing assumptions, edge cases.
- “Almost correct” outputs can be the most dangerous for an expert.

RAG helps — but does not provide real expertise

- Resource Augmented Generation (RAG) reduces hallucinations and improves traceability.
- But models tend to summarize rather than critically evaluate sources.
- Uncertainty and methodological weaknesses are often omitted or glossed over unless prompted.

Discussion

Four Categories of LLM Outputs

High-level distinction

LLM outputs are heterogeneous and fall into four distinct categories.

- **Epistemic claims** — truth-apt statements about the world
- **Conceptual proposals** — definitions, distinctions, framings
- **Technical artifacts** — objects intended for use
- **Creative constructs** — rhetorical or fictional content

Examples: Epistemic Claims

- Gravitational waves propagate at the speed of light
- Neutrinos have non-zero rest mass
- Time dilation has been experimentally confirmed with atomic clocks

Evaluation

Truth-apt statements, assessed by empirical evidence and reasoning.

Examples: Conceptual Proposals

- Spacetime geometry as a dynamical entity
- Symmetry principles as organizing foundations
- Emergence as a legitimate explanatory framework

Evaluation

Judged by clarity, coherence, and explanatory usefulness.

Examples: Technical Artifacts

- Numerical simulations of the Navier–Stokes equations
- Variational derivations of the Schrödinger equation
- Gravitational lensing ray-tracing algorithms

Evaluation

Verified for correctness and validated for fitness for purpose.

Examples: Creative Constructs

- Spacetime as a stretched rubber sheet
- Particles surfing on quantum fields
- The universe as a cosmic symphony

Evaluation

Assessed for intuition and communicative effectiveness, not truth.

Checklist I: Decomposition of Output & SeparateEvaluation

Step 1 — Decompose the output

- Epistemic claims (truth-apt statements)
- Conceptual proposals (definitions, framings)
- Technical artifacts (code, workflows, formulas)
- Creative constructs (metaphors, narratives)

Step 2 — Evaluate each type of output separately

- **Epistemic claims:** What evidence would falsify this?
- **Conceptual proposals:** Does this clarify or solve a problem?
- **Technical artifacts:** Does it work as specified?
- **Creative constructs:** Is this illustrative, not evidential?

Checklist II: Propagation Risks & Decision Rule

Step 3 — Check for cross-category contamination

- Are epistemic claims trusted because artifacts look correct?
- Are metaphors mistaken for mechanisms?
- Are conceptual distinctions treated as discoveries?
- Is rhetorical polish replacing evidence?

Common red flags

- Unqualified claims (“always”, “guaranteed”)
- “Studies show …” without sources
- Anthropomorphic or intentional language

Takeaway

LLMs do not produce knowledge; they produce candidates for knowledge and use.

Questions?

Backup Slides

Github Repository

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An unsuccessful attempt to write an aphorism (it falls flat...)

*LLMs can produce results
without knowing why they are right
and without noticing when they are wrong.*

*If this were acceptable in physics,
derivations would be optional.*

Invitation to the Journal Club in the style of Shakespeare

Good friends and colleagues all, give ear,
For mark ye well what fortune brings this week:
A Journal Club of special note and cheer,
Where learned discourse shall richly have its speak.
Dr. Ulrich Degenhardt, wise and well-esteemed,
Shall take the floor and with keen wit unfold
How arts of thinking wrought by cunning schemes
May serve our labours and our works of old—
Those tools of AI, bent to scholars' ways,
In workflows fit for science' noble ends.
This meet shall come, as custom hath its stays,
Upon this Friday, when the clock strikes eleven, friends,
Within the Riemann Room, our chosen place.

If thou by Zoom must join our gathered throng,
Pray tell me ere Thursday’s evening pace,
That I may grant thee passage, sure and strong.
The order of the weeks that yet shall be
Is writ herein for all who wish to see:
`https://pad.gwdg.de/NAVFQ7TvQw-7qWI1aY6STw?both`

With kindest thoughts and greetings fair,
I rest, thy servant,
Giulia