



Explainable AI for LLMs

Wojciech Samek TU Berlin & Fraunhofer HHI



Today's LLMs: Impress

Please tell me how to cut bread.





(source: https://www.shutterstock.com)

Today's LLMs: Impress

Please tell me how to cut bread



Cutting bread might seem simple, but there's an art to doing it well! Here's a step-by-step guide to get clean, even slices without squishing the loaf:

- 1. Choose the Right Knife
- 2. Place the Bread on a Cutting Board
- 3. Position Your Hand Correctly
- 4. Start Slicing
- 5. Slice Thickness
- **Extra Tips**

Today's LLMs: Hallucinate

Have there been any reports of implantation of a subcutaneous defibrillator immediately after cardiac surgery and please provide references



Today's LLMs: Hallucinate

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Yes, there have been reports of implantation of subcutaneous defibrillators (S-ICDs) immediately after cardiac surgery. Here are some references:

1. 'Immediate postoperative implantation of a subcutaneous defibrillator in a patient undergoing cardiac surgery.' J Interv Card Electrophysiol. 2016 Feb;45(2):203–5. doi: 10.1007/s10840-015-0087-6. Epub 2015 Dec 17. PMID: 26676620.

2. 'Immediate postoperative subcutaneous implantable cardioverter-defibrillator implantation in patients undergoing cardiac surgery: feasibility, safety and outcomes.' Europace. 2017 Jul 1;19(7):1150–1156. doi: 10.1093/europace/euw235. PMID: 27614059.

3. 'Immediate postoperative implantation of a subcutaneous defibrillator in a patient undergoing cardiac surgery.' J Arrhythm. 2017 Dec;33(6):639–641. doi: 10.1016/j.joa.2017.06.008. Epub 2017 Jul 5. PMID: 29276432.

Today's LLMs: Hallucinate

Have there been any reports of implantation of a subcutaneous defibrillator immediately after cardiac surgery and please provide references



ChatGPT hallucinating: can it get any more humanlike?

Konstantinos C. Siontis 0 , Zachi I. Attia, Samuel J. Asirvatham, and Paul A. Friedman 0*

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Construction of the constr

To trust or not to trust AI; that is the question

We need to solve the "Black Box" problem!



First Wave of Explainable AI



Debug models (Lapuschkin et al. Nat Comm, 2019)





Debug models (Lapuschkin et al. Nat Comm, 2019)





New insights (Wong et al. Nature, 2023)





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"BLUE XAI" (Biecek & Samek, ICML, 2024)

Human-values oriented

- Responsible models
- Legal issues
- Trust in predictions
- Ethical issues

Debug models (Lapuschkin et al. Nat Comm, 2019)





New insights (Wong et al. Nature, 2023)





"BLUE XAI" (Biecek & Samek, ICML, 2024)

Human-values oriented

- Responsible models
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Provide citations in LLMs

What is the capital of Germany? **ChatGPT**: The capital of Germany is Berlin.

= WIKIPEDIA	List of national capitals			
Beirut	Lebanon	Asia		
Belgrade	Serbia	Europe		
Belmopan	Belize	North America		
Berlin	Germany	Europe		

LRP: Faithful + Comput. Efficient + Latent Attribution



Theoretical Interpretation:

Deep Taylor Decomposition

zjk measures how much has j contributed to activation of k

(Bach et al. 2015)

<u>LRP</u>: Faithful + Comput. Efficient + Latent Attribution



Theoretical Interp



(Montavon et al. 2017)

LRP: Faithful + Comput. Efficient + Latent Attribution



(Arras et al. 2019)

LRP: Faithful + Comput. Efficient + Latent Attribution



AttnLRP: Attention-Aware Layer-wise Relevance Propagation for Transformers

Reduan Achtibat¹ Sayed Mohammad Vakilzadeh Hatefi¹ Maximilian Dreyer¹

Thomas Wiegand^{1,2,3} Wojciech Samek^{1,2,3,†} Aakriti Jain¹ Sebastian Lapuschkin^{1,†}

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³ BIFOLD – Berlin Institute for the Foundations of Learning and Data, 10587 Berlin, Germany

Proposition 3.1 Decomposing the softmax function by a Taylor decomposition (4) at reference point x yields the following relevance propagation rule:

$$R_{i}^{l} = x_{i}(R_{i}^{l+1} - s_{i}\sum_{j}R_{j}^{l+1})$$
(13)

where s_j denotes the *j*-th output of the softmax function.

The hidden bias term **Proposition 3.2** Decomposing element-wise multiplication error, consequently a with N input variables of the form

$$f_j(\mathbf{x}) = \prod_i^N x_i$$

by Shapley (with baseline zero) or Taylor decomposition (4) at reference point \mathbf{x} (without bias or distributing the bias uniformely) yields the following uniform relevance propagation rule:

$$R_{i\leftarrow j}(x_i) = \frac{1}{N} R_j \,. \tag{14}$$

https://proceedings.mlr.press/v235/achtibat24a.html

https://github.com/rachtibat/LRP-eXplains-Transforme

Proposition 3.4 Decomposing LayerNorm or RMSNorm by a Taylor decomposition (4) with reference point $\boldsymbol{0}$ (without bias or distributing the bias uniformly) yields the identity relevance propagation rule:

$$P_i^{l-1} = R_i^l \tag{19}$$

Proposition 3.3 Decomposing matrix multiplication with a sequential application of the uniform rule (14) and the ε -rule (8) yields the following relevance propagation rule:

$$R_{ji}^{l-1}(\mathbf{A}_{ji}) = \sum_{p} \mathbf{A}_{ji} \mathbf{V}_{ip} \frac{R_{jp}^{l}}{2 \mathbf{O}_{jp} + \varepsilon}$$
(15)

Comparison

explanation for "dog"



Faithfulness

Table 1. Faithfulness scores as area between the least and most relevant order perturbation curves (Blücher et al., 2024) on different models and datasets. To assess plausibility, the (top-1) accuracy along with the IoU in parentheses are depicted for SQuAD v2. Methods marked with (*) have been proposed here. Additional results for ViT-L-16 and ViT-L-32 are in Appendix Table B.6.

Methods	ViT-B-16	LLaN	la 2-7b	Mixtral 8x7b	Flan-T5-XL	
	ImageNet ↑	IMDB ↑	Wikipedia ↑	SQuAD v2 \uparrow	SQuAD v2 \uparrow	
Random	0.01 ± 0.01	-0.01 ± 0.05	-0.07 ± 0.13	$0.03\ (0.09)$	$0.03 \ (0.08)$	
Input×Grad (Simonyan et al., 2014)	0.80 ± 0.03	0.12 ± 0.05	0.18 ± 0.13	$0.56\ (0.35)$	0.60 (0.39)	
IG (Sundararajan et al., 2017)	1.54 ± 0.03	1.23 ± 0.05	4.05 ± 0.13	0.68(0.44)	$0.10 \ (0.16)$	
SmoothGrad (Smilkov et al., 2017)	-0.04 ± 0.03	0.25 ± 0.05	-2.22 ± 0.14	0.47~(0.24)	0.05~(0.09)	
GradCAM (Chefer et al., 2021b)	0.27 ± 0.04	-0.82 ± 0.05	2.01 ± 0.15	0.82(0.72)	0.81 (0.70)	
AttnRoll (Abnar and Zuidema, 2020)	1.31 ± 0.03	-0.64 ± 0.05	-3.49 ± 0.15	0.05~(0.10)	$0.02 \ (0.08)$	
Grad×AttnRoll (Chefer et al., 2021a)	2.60 ± 0.03	1.61 ± 0.05	9.79 ± 0.14	$0.91 \ (0.40)$	0.94 (0.53)	
AtMan (Deb et al., 2023)	0.70 ± 0.02	-0.20 ± 0.05	3.31 ± 0.15	0.86 (0.83)	0.88(0.80)	
KernelSHAP (Lundberg and Lee, 2017)	4.71 ± 0.03	-	-	-	-	
CP-LRP (ε -rule, Ali et al. (2022))	2.53 ± 0.02	1.72 ± 0.04	7.85 ± 0.12	0.50(0.40)	0.91 (0.83)	
CP-LRP (γ -rule for ViT, as proposed here)*	6.06 ± 0.02	-	-	-	-	
AttnLRP (ours)*	6.19 ± 0.02	2.50 ± 0.05	10.93 ± 0.13	0.96 (0.72)	$0.94 \ (0.84)$	

Results



Results

Question: In what country is Normandy located? Answer: France

AttnLRP

The Normans (Norman: Nourmands; French: Normands; Latin: Normanni) were the people who in the 10th and 11th centuries gave their name to Normandy, a region in France. They were descended from Norse ("Norman" comes from "Norseman") raiders and pirates from Denmark, Iceland and Norway who, under their leader Rollo, agreed to swear fealty to King Charles III of West Francia. Through generations of assimilation and mixing with the native Frankish and Roman-Gaulish populations, their descendants would gradually merge with the Carolingian-based cultures of West Francia. The distinct cultural and ethnic identity of the Normans emerged initially in the first half of the 10th century, and it continued to evolve over the succeeding centuries.

AtMan

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Integrated Gradient

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Input x Gradient

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Grad-CAM

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CP-LRP

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Evaluation on the Mixtral 8x7b model

Comparison with other LRP Rules

	Methods	Softmax	Matrix Multiplication	Layer Normalization
	(Ding et al., 2017)	Identity rule	0-LRP	not available
			(bi-linear)	
		\Rightarrow unstable (Appendix A.2.1)	\Rightarrow violates conservation	
	(Voita et al., 2021)	Taylor decomposition at x	z^+ -LRP	Taylor decomposition at x
		(distributes the bias uniformly)	(bi-linear)	(distributes the bias uniformly)
		\Rightarrow unstable (Appendix A.2.1)	\Rightarrow violates conservation	\Rightarrow unstable (Appendix A.2.1)
	(Chefer et al., 2021b)	Identity rule	0-LRP	Identity rule
			& post-hoc normalization	
			(bi-linear)	
		\Rightarrow unstable (Appendix A.2.1)	\Rightarrow ensures conservation	\Rightarrow ensures conservation
				& faithful
	(Ali et al., 2022)	Regarded as constant	0-LRP	Identity rule
			(linear only)	
		\Rightarrow stable & no attribution	\Rightarrow ensures conservation	\Rightarrow ensures conservation
		inside attention module	100	& faithful
	AttnLRP	Taylor decomposition at x	ε -LRP	Identity rule
fully within Deen	•	(with bias)	& uniform rule	
			(bi-linear)	
Laylor Decomposition		\Rightarrow stable & faithful	\Rightarrow ensures conservation	\Rightarrow ensures conservation
Framework			& faithful	& faithful

Towards Concept-Level XAI

Interpretation Gap

Local XAI functions as marker for important features



Does it help understanding?

Local XAI tells us "where" important features occur.

However, it neither tells us "what" this feature is nor how it is used by the model.

nature	mac	hine	intel	ligen	ce
				\mathbf{u}	

Article

https://doi.org/10.1038/s42256-023-00711-8

From attribution maps to humanunderstandable explanations through Concept Relevance Propagation

Received: 7 June 2022	Reduan Achtibat © ^{1,4} , Maximilian Dreyer ^{1,4} , Ilona Eisenbraun ¹ , Sebastian Bosse ¹ ,				
Accepted: 31 July 2023	i nomas wiegand "~", wojciech Samek 🕲 "~" 🖂 & Sebastian Lapuschkin 🛡 ' 🖂				
Published online: 20 September 2023					
Check for updates					

https://doi.org/10.1038/s42256-023-00711-8

<u>Known</u>: Hidden layers encode semantic concepts.



<u>Goal</u>: Explain in terms of these concepts.

Concept: "animal on branch" Known: Hidden Bee layers encode \bigcirc eater semantic concepts. Heatmap \cap

<u>Goal</u>: Explain in terms of these concepts.





Addressing the "What"-Question

(Chen et al., 2020) data-based activation maximization



Idea: Image which maximally active the neuron contain the "concept" encoded by the neuron.

input input output

What does this channel encode?

We can find out by activation maximization.

From Activation To Relevance Maximization

activation vs relevance flow \longrightarrow result in different example sets



without task-context



AM: Images which maximally "stimulate" channel (unrelated to prediction which we aim to explain)

RM: Images contain the concept encoded by the channel for which the channel is "most useful" to the model.



within task-context

Concept Relevance Propagation (CRP)



Concept Composition



Concept-based Reverse Search

input



input heatmap



most relevant channels in region 15 361 414203486443

<u>Reverse search</u>: Find other images, where these channels are also relevant.

Concept-based Reverse Search



conditional heatmap $R(\mathbf{x}|\theta = \{c_{361}, y\})$



Fixing the Model: Adapt encoding space globally [Anders, Weber, et al. 2022] or rather outcome-dependently?

From Individual Explanations to Understanding Global Behaviour

Prototypical Concept-based Explanation (PCX)





(Dreyer et al. 2024)

https://doi.org/10.1109/CVPRW63382.2024.00353

Prototypical Concept-based Explanation (PCX)

from local explanations to global prototypes training samples $class \ a$ relevance concept 1 $\mathbf{2}$ finding 3 prototypes 4 0 class b(using GMM) ... concept relevance vectors $\boldsymbol{\nu}$





Identifying Bugs in the Model / Data



For the ImageNet class "lacewing" (VGG-16, layer features.28), there are also samples of Leopard Lacewing butterflies in the training data.

Identifying Bugs in the Model / Data





prototypes

Validating AI Predictions



Firstly, we examine the characteristic concepts of each prototype.

Secondly, clusters of training predictions that deviate strongly from prototypes can be studied for spurious behavior.

How much Manual Work does XAI Require?



From Explainable to Trustworthy AI

Reveal and Revise Framework



[Pahde et al. 2023]

https://doi.org/10.1007/978-3-031-43895-0_56

ISIC Dataset Artifacts:

- Skin Marker



--- Reveal Step ----

R2R	corrected	$\downarrow \operatorname{artifact}$	↑ F1 (%)		\downarrow artifact \uparrow F1 (%) \uparrow accuracy (%)			r (%)
iteration	artifacts	relevance $(\%)$	poisoned	original	poisoned	original		
0	-	$18.4 \mid45.5\vert24.2$	$61.3 \mid 59.7 \mid 60.5$	73.9	$71.8 \mid 71.5 \mid 68.7$	80.1		

[Pahde et al. 2023]

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R2R	corrected	\downarrow artifact	↑ F1 (%)		artifact \uparrow F1 (%) \uparrow accuracy			7 (%)
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0	-	$18.4 \mid 45.5 \mid 24.2$	$61.3 \mid 59.7 \mid 60.5$	73.9	71.8 71.5 68.7	80.1		
1	\mathbf{SM}	$13.1 \mid 35.0 \mid 21.3$	$61.6 \mid 61.0 \mid 60.7$	73.8	$72.2 \mid 72.6 \mid 68.4$	80.0		

[[]Pahde et al. 2023]

ISIC Dataset Artifacts:

- Skin Marker
- Band-Aid



--- Reveal Step ----

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[[]Pahde et al. 2023]

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1	\mathbf{SM}	$13.1 \mid 35.0 \mid 21.3$	61.6 61.0 60.7	73.8	72.2 72.6 68.4	80.0
2	SM, BA	12.8 16.8 16.8	61.5 63.6 61.1	73.9	72.3 74.6 68.6	79.7



ISIC Dataset Artifacts:

- Skin Marker
- Band-Aid
- Ruler



--- Reveal Step ----

R2R	corrected	$\downarrow \operatorname{artifact}$	↑ F1 (%)		\uparrow accuracy (%)		
iteration	artifacts	relevance $(\%)$	poisoned	original	poisoned	original	
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- Skin Mai
- Band-Ai
- Ruler

```
--- Revise
```

	skin marker (SM)		band-aid (BA)		ruler (R)			
illa Input	* * * * * * * * * * * * * * * * * * *	+	*	0	(•	1	
(Van		7. 3		18. C. 3	e. C			, r
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O BA		£2	×*	ð. 1	e.	0		6
		\$.**	197 1	ð.1	e : 1	0	\$	
\uparrow F1 (% poisoned or	5) riginal p	↑ accura oisoned	cy (%) origine	al				
61.3 59.7 60.5 61.6 61.0 60.7 61.5 63.6 61.1 62.0 63.4 64.0	73.971.873.872.273.972.3 74.072.4	71.5 68.7 72.6 68.4 74.6 68.6 74.5 71 .4	7 80.1 4 80.0 5 79.7 8 79.9			[Pah	ide et a	al. 2023]
	thdu thdu	skin marker	skin marker (SM) fid_{I} elitter filter $filter$	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	skin marker (SM) band-aid (BA filtred filter fil	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $	skin marker (SM) band-aid (BA) ruler (R H = 1 $H = 1$ $H =$

Back to LLMs

The San Diego Electric Railway (SDERy) was a mass transit system in Southern California, United States, using 600 volt DC streetcars and (in later years) buses.

Maintenance of way (commonly abbreviated to MOW) refers to the maintenance, construction, and improvement of rail infrastructure, including tracks, ballast, grade, and lineside infrastructure such as signals and signs.

France currently operates the second-largest European railway network, with a total of 29,901 kilometres of railway.

The MHR had, in 1846, amalgamated with the "Little" North Western Railway (NWR), which was taken over by the Midland Railway in 1874.Awdry, p.97CThe rival London and North Western Railway (LNWR) built its own branch line to Morecambe in 1864, joining the main LNWR line at Hest Bank.

Some railway companies had a standard signalbox design, such as the London & North Western Railway, whereas others, such as the Great Eastern Railway had many different designs.

AttnLRP attributions on top 10 ActMax sentences collected over the Wikipedia summary dataset for neuron #256, inlayer 18. The knowledge neuron seems to activate for transport systems (railways in particular).

The volume presents six short stories, with the titular story featuring Yahiro, a substitute teacher, who begins having an affair with his student Kago.

In 2018, Derek Michael Boyce, a high school math and science teacher at the school, was arrested for having an inappropriate relationship with one of his students, a fifteen-year-old girl.

The film follows a school teacher as she suspects one of her students is suffering from personal problems in his home life, not knowing that the student is harboring an evil demon in his house.

During his time as a teacher Franco admitted to having sex with several of his students, which led to lawsuits and a \$2 million sexual-misconduct settlement in 2021.

It tells the story of a schoolteacher who falls in love with one of his students, and moves away in order to escape his infatuation. AttnLRP attributions on top 10 ActMax sentences collected over the Wikipedia summary dataset for neuron #2207, inlayer 20.The knowledge neuron is activating for 'teacher', in unusual context such as inappropriate behavior, sexual misconduct etc.

INPUT

Ice bears live in the ...







Pruning By Explaining



https://arxiv.org/pdf/2408.12568

Pruning By Explaining



(Hatefi et al. 2024)

https://arxiv.org/pdf/2408.12568

Pruning By Explaining



Required number of reference samples (per class) is very low.

(Hatefi et al. 2024)

https://arxiv.org/pdf/2408.12568

Future Work



(Longo et al. 2024)

https://doi.org/10.1016/j.inffus.2024.102301

Toolboxes

Benchmarking: QUANTUS

Benchmarking: CLEVR-XAI



https://github.com/ahmedmagdiosman/clevr-xai

https://github.com/understandable-machine-intelligence-lab/Quantus



iNNvestigate

https://github.com/albermax/innvestigate



ExplainableAI.jl



zennit

https://github.com/adrhill/ExplainableAI.jl

https://github.com/rachtibat/zennit-crp

https://github.com/chr5tphr/zennit



https://github.com/dilyabareeva/quanda

