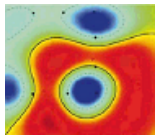
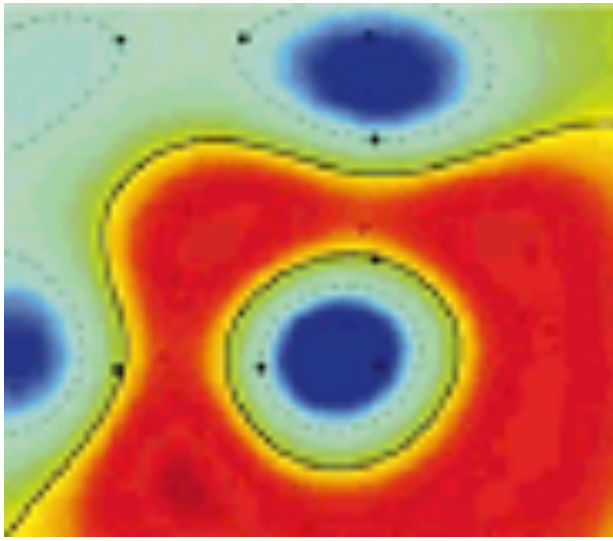


WiSe 2024/25

**Deep Learning 1**

Technische Universität Berlin



Lecture 12

# Explainable AI

# Outline

**Intro to Explainable AI**

- Types of explanations
- Uses of explanations

**Explainable AI Techniques**

- Activation maximization
- Attribution via Shapley Values
- Attribution via LRP

**Application to a Data Science Problem**

- Finding influencial proteins from proteomics data.

# What is an Explanation?

**Example 1:** Synthesize an input pattern that most strongly activates the output of the ML model (e.g. associated to a particular class).


Image source: Nguyen et al. (2016) Multifaceted Feature Visualization: Uncovering the Different Types of Features Learned By Each Neuron in Deep Neural Networks

# What is an Explanation?

**Example 2:** Highlight features that have contributed for a given data point to the ML prediction.

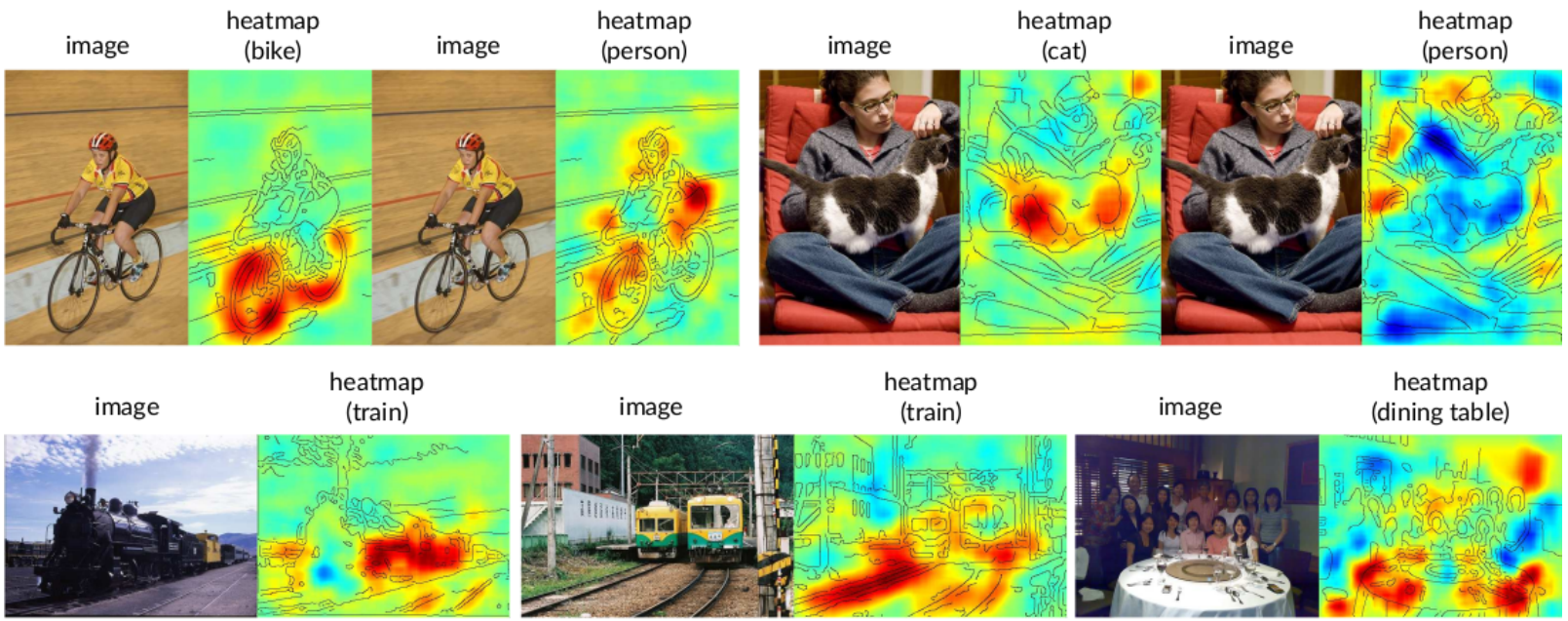
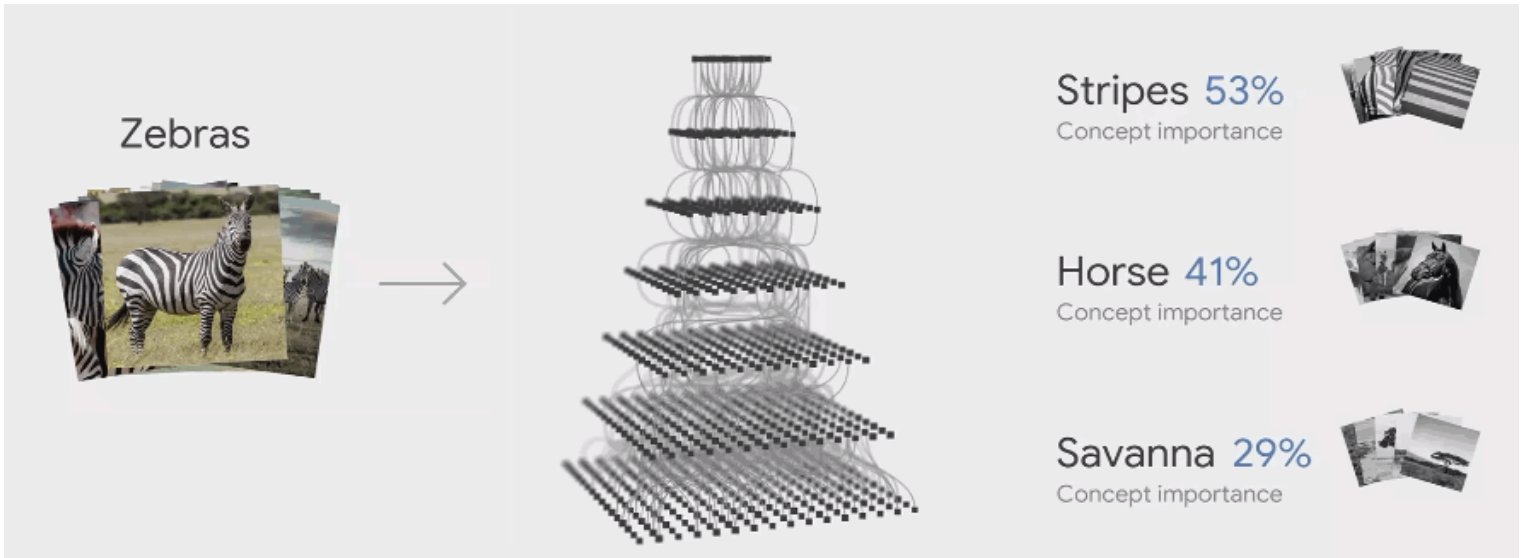



Image source: Lapuschkin et al. (2016) Analyzing Classifiers: Fisher Vectors and Deep Neural Networks

# What is an Explanation?

**Example 3:** Concept activation vectors (TCAV). Highlight the mid-level concepts that explain, for a given data point, the ML prediction.




Source: Google Keynote'19 (URL: `https://www.youtube.com/watch?v=lyRPyRKHO8M&t=2279s`)

# Why Explainable AI: Practical Motivations

**Assistant for Model Validation / Improvement**

- XAI is used to validate a learned ML model, and to identify how to improve it.

**Assistant for Decision Making**

- XAI and ML are used to help users to improve/accelerate their decision making (e.g. highlight relevant regions in large histolopathological slices).
- XAI and ML enable to characterize the input-output behavior of a complex system to meaningfully action it (e.g. calibration/control of a power systems).

**Scientific Assistant**

- XAI + ML are used to identify possible relations between different variables in a complex system of scientific interest (e.g. cell regulatory network).

**Legal Compliance**

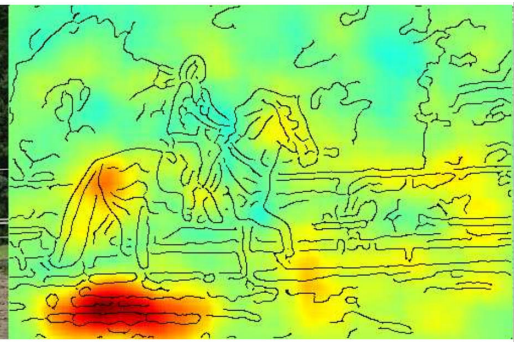
- Explanation is required (e.g. by law) to deploy an AI system and let the AI system take decisions.

# XAI for Model Verification / Improvement

**Example:** The classifier is right for the wrong reasons

image


heatmap (horse)



average precision of the Fisher Vector model on the PascalVOC dataset

| | | | | |
|---|---|---|---|---|
| aer | bic | bir | boa | bot |
| 79.08 | 66.44 | 45.90 | 70.88 | 27.64 |
| bus | car | cat | cha | cow |
| 69.67 | 80.96 | 59.92 | 51.92 | 47.60 |
| din | dog | hor | mot | per |
| 58.06 | 42.28 | 80.45 | 69.34 | 85.10 |
| pot | she | sof | tra | tvm |
| 28.62 | 49.58 | 49.31 | 82.71 | 54.33 |

- In this example, the classifier accurately predicts the horse class, but based on the wrong features (some copyright tag in the corner).
- This incorrect decision strategy cannot be detected by just looking at the test error.

cf. Lapuschkin et al. (2019) Unmasking Clever Hans Predictors and Assessing What Machines Really Learn. Nature Communications

# XAI for Generating Scientific Hypotheses

**Learn something about the data**
*(or about the system that produced the data)*

- **Step 1:** Train a ML model that predicts well the data.
- **Step 2:** Apply XAI to the trained ML model to produce explanations of the ML decision strategy.
- **Step 3:** Based on the XAI explanations, the users can compare their reasoning with that of the ML model, and can potentially refine their own domain knowledge.

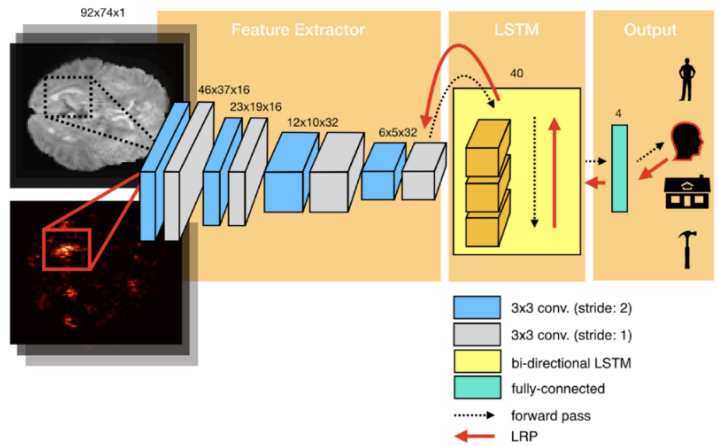



Image source: Thomas et al. (2019) Analyzing Neuroimaging Data Through Recurrent Deep Learning Models

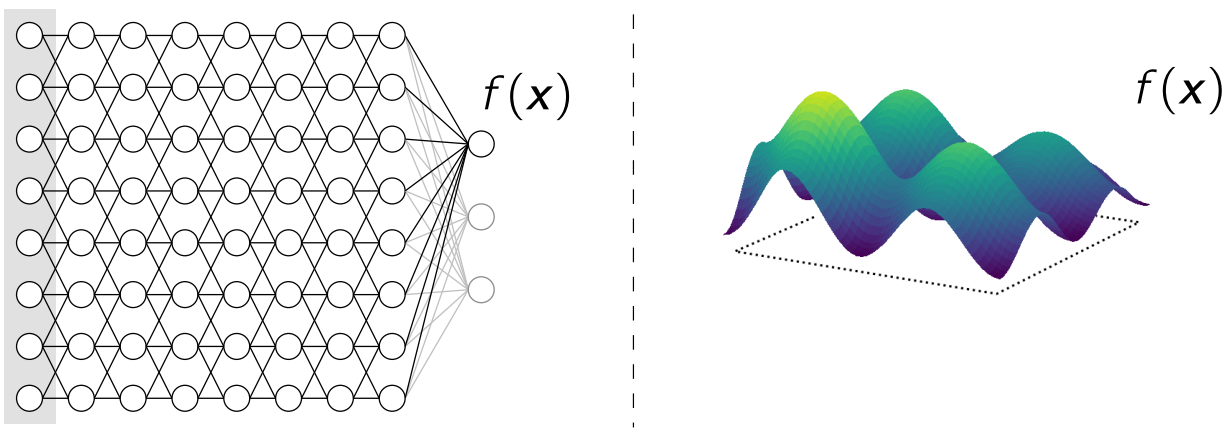
Part 1

# Activation Maximization

# Activation Maximization

Assume a trained a ML model (e.g. a neural network), and we would like to understand what concept is associated to some particular output neuron of the ML model, e.g. the output neuron that codes for the class 'cat'. Activation maximization proceeds in two steps:

- **Step 1:** Think of the ML model as a function of the input




- **Step 2:** Explain the function $f$ by generating a maximally activating input pattern:

$$\boldsymbol{x}^\star = \arg\max_{\boldsymbol{x}} f(\boldsymbol{x})$$

# Activation Maximization

**Problem:**

- In most cases $f(\boldsymbol{x})$ does not have single point corresponding to the maximum. E.g. in linear models, $f(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} + b$, we can keep moving the point $\boldsymbol{x}$ further along the direction $\boldsymbol{w}$, and the output continues to grow).

**Solution:**

- Apply a preference for 'regular' regions of the input domain, i.e.

$$\boldsymbol{x}^\star = \arg\max_{\boldsymbol{x}} f(\boldsymbol{x}) - \Omega(\boldsymbol{x})$$

  In practice, the preference can be for data points with small norm (i.e. we set $\Omega(\boldsymbol{x}) = \lambda \|\boldsymbol{x}\|^2$ so that points with large norm are penalized.)

# Activation Maximization: Probability View

Assume the model produces a log-probability for class $\omega_c$:

$$f(\boldsymbol{x}) = \log p(\omega_c|\boldsymbol{x})$$

The input $\boldsymbol{x}^\star$ that maximizes this function can be interpreted as the point where the classifier is the most *sure* about class $\omega_c$.

Choose the regularizer $-\Omega(\boldsymbol{x}) = \log p(\boldsymbol{x})$, i.e. favor points that are *likely*.

The optimization problem becomes:

$$\begin{aligned}\boldsymbol{x}^\star &= \arg\max_{\boldsymbol{x}} \ \log p(\omega_c|\boldsymbol{x}) + \log p(\boldsymbol{x}) \\ &= \arg\max_{\boldsymbol{x}} \ \log p(\boldsymbol{x}|\omega_c)\end{aligned}$$

where $\boldsymbol{x}^\star$ can now be interpreted as the most *typical* input for class $\omega_c$.

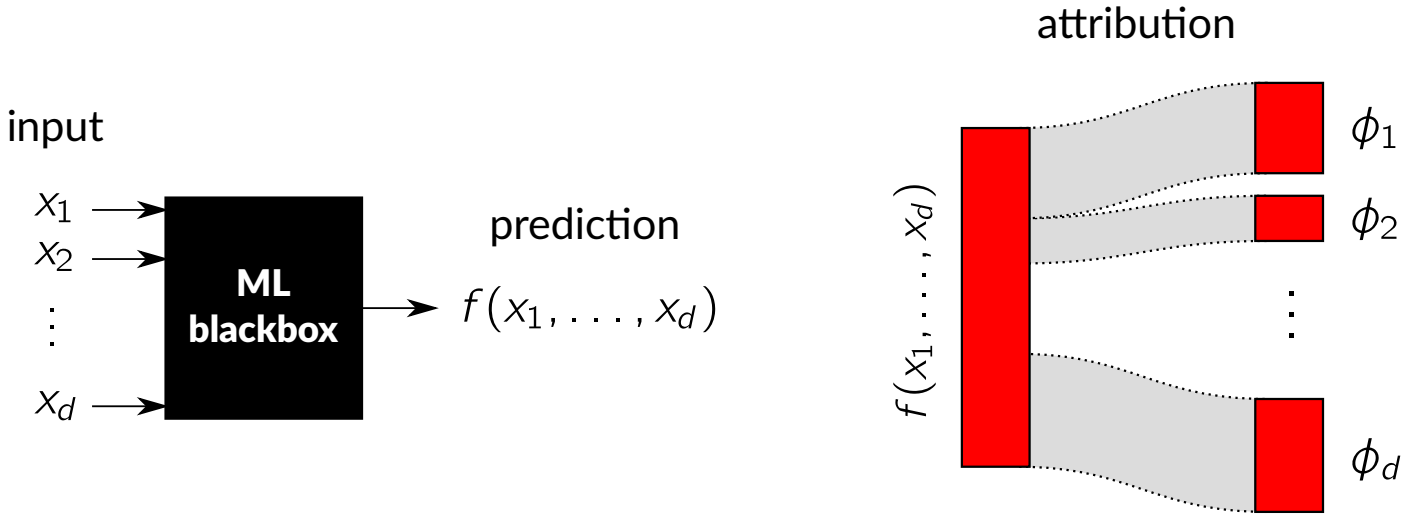
# Activation Maximization with Different Regularizers


Image source: Nguyen et al. Synthesizing the preferred inputs for neurons in neural networks via deep generator networks (2016)

Part 2

# Attribution

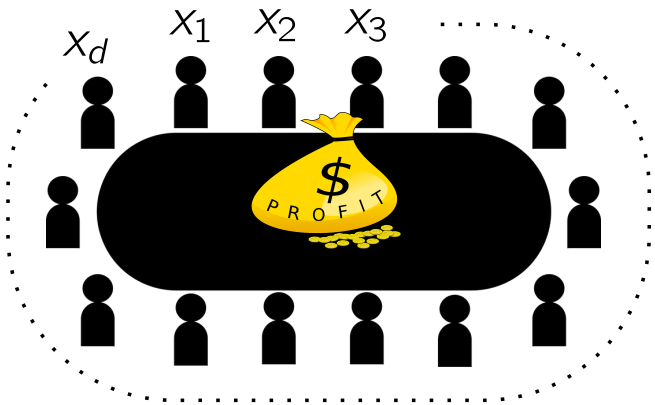
# Attribution of a Prediction to Input Features




1. The data point $\boldsymbol{x} \in \mathbb{R}^d$ is fed to the ML model and we get a prediction $f(\boldsymbol{x}) \in \mathbb{R}$.
2. We explain the prediction by identifying the additive contribution of each input feature.
3. Important property of attribution: **conservation** ($\sum_{i=1}^{d} \phi_i = f(\boldsymbol{x})$).

# Attribution: Shapley Values [5, 6, 3]

- Framework originally proposed in the context of game theory (Shapley 1951) for assigning payoffs in a cooperative game, and recently applied to ML models.
- Each input variable is viewed as a player, and the function output as the profit realized by the cooperating players.




The Shapley values $\phi_1, \ldots, \phi_d$ measuring the contribution of each feature are:

$$\phi_i = \sum_{\mathcal{S}\colon\, i \notin \mathcal{S}} \frac{|\mathcal{S}|!(d-|\mathcal{S}|-1)!}{d!} \left[ f(\boldsymbol{x}_{\mathcal{S}\cup\{i\}}) - f(\boldsymbol{x}_{\mathcal{S}}) \right]$$

where $(\boldsymbol{x}_{\mathcal{S}})_{\mathcal{S}}$ are all possible subsets of features contained in the input $\boldsymbol{x}$.

# Attribution: Shapley Values

*Recall:* $$\phi_i = \sum_{\mathcal{S}\,:\, i \notin \mathcal{S}} \underbrace{\frac{|\mathcal{S}|!(d-|\mathcal{S}|-1)!}{d!}}_{\alpha_{\mathcal{S}}} \underbrace{\left[f(\boldsymbol{x}_{\mathcal{S}\cup\{i\}}) - f(\boldsymbol{x}_{\mathcal{S}})\right]}_{\Delta_{\mathcal{S}}}$$

**Worked-through example:** Consider the function $f(\boldsymbol{x}) = x_1 \cdot (x_2 + x_3)$. Calculate the contribution of each feature to the prediction $f(\mathbf{1})$.

# Attribution: Shapley Values

**Problem:**

- Shapley values require an exponentially large number of evaluations of the function $f$ ($\rightarrow$ practically infeasible).

**Observation:**

- It has been shown that the Shapley value can also be written as:

$$\phi_i = \frac{1}{d!} \sum_{S \in \mathcal{P}} \left[ f(\boldsymbol{x}_{\text{preceq}(S,i)}) - f(\boldsymbol{x}_{\text{prec}(S,i)}) \right]$$

where $\mathcal{P}$ denotes the set of all possible permutations of input features, e.g. for $d = 4$, we have

$$\mathcal{P} = \{(1,2,3,4), (1,2,4,3), (1,3,2,4), \dots\},$$

and where $\text{prec}(S,i)$ is the set of features that precede feature $i$ in the order of $S$, and $\text{preceq}(S,i)$ is the same features plus feature $i$, e.g.

$$\text{prec}((3,1,2,4),2) = (3,1)$$
$$\text{preceq}((3,1,2,4),2) = (3,1,2)$$

# Attribution: Shapley Values

**Shapley Value Sampling:**

- Approximate the Shapley value by replacing the exact form:

$$\phi_i = \frac{1}{d!} \sum_{S \in \mathcal{P}} \left[ f(\boldsymbol{x}_{\text{preceq}(S,i)}) - f(\boldsymbol{x}_{\text{prec}(S,i)}) \right]$$

  by the sampling approximation:

$$\phi_i = \frac{1}{T} \sum_{S \in \{S^{(1)}, \ldots, S^{(T)}\}} \left[ f(\boldsymbol{x}_{\text{preceq}(S,i)}) - f(\boldsymbol{x}_{\text{prec}(S,i)}) \right]$$

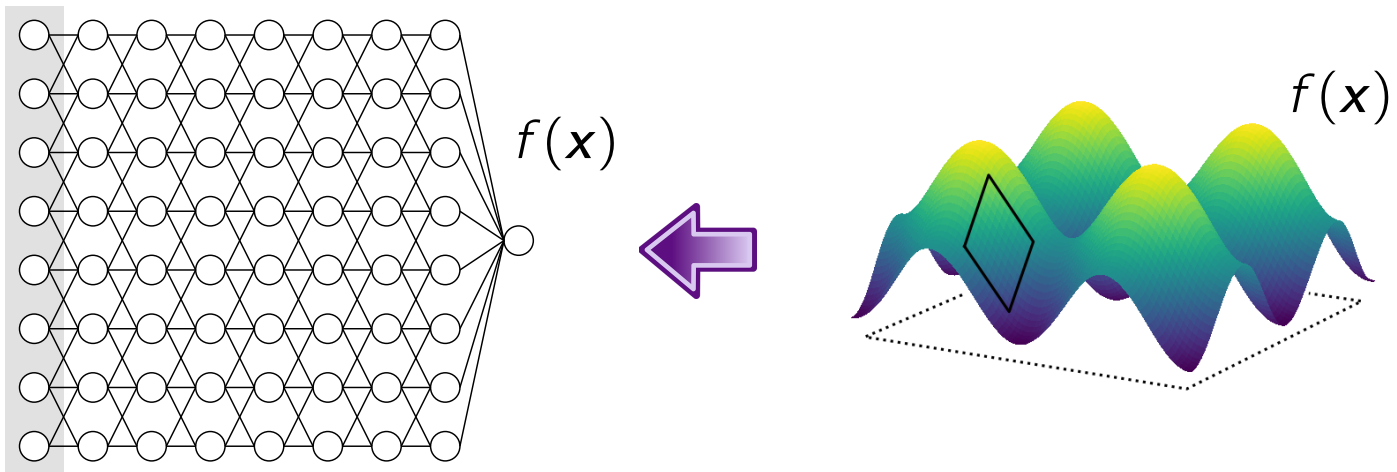
  where $S^{(1)}, \ldots, S^{(T)} \sim \text{uniform}(\mathcal{P})$.

- Converge to the true Shapley Value in the limit of $T \to \infty$.
- The larger $T$, the more precise the evaluation but also the more computationally expensive.

**Example:**

- Applying $T = 10$ on a function with $d = 25$ input dimensions, we need to evaluate $500$ times the function $f$.
- No longer exponential, but still computationally expensive for large $d$.

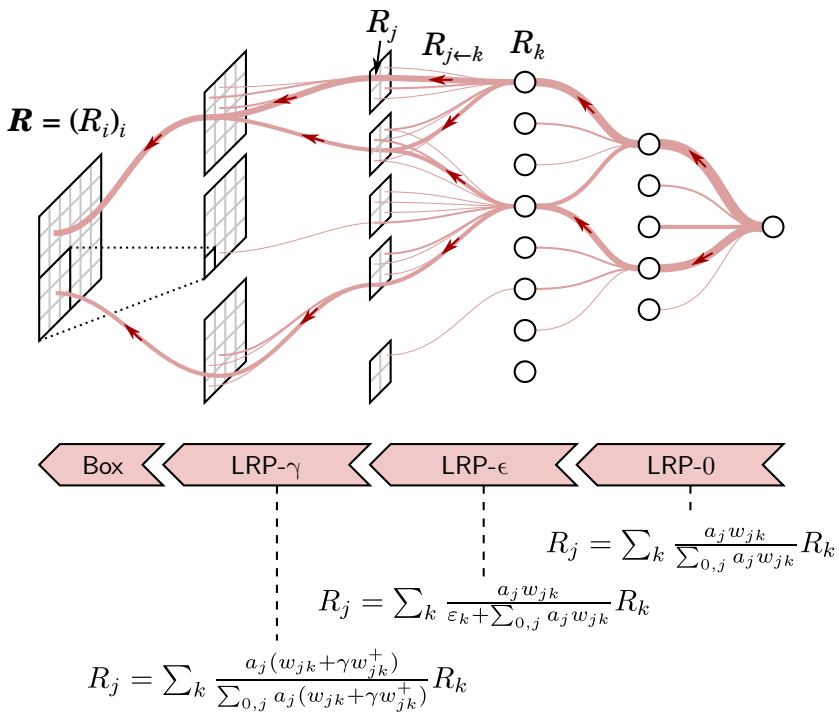
# From Function-Based to Propagation-Based




**Questions:**

- Can we speedup the process of explanation by using the structure of the network (e.g. by running a special backpropagation pass)?

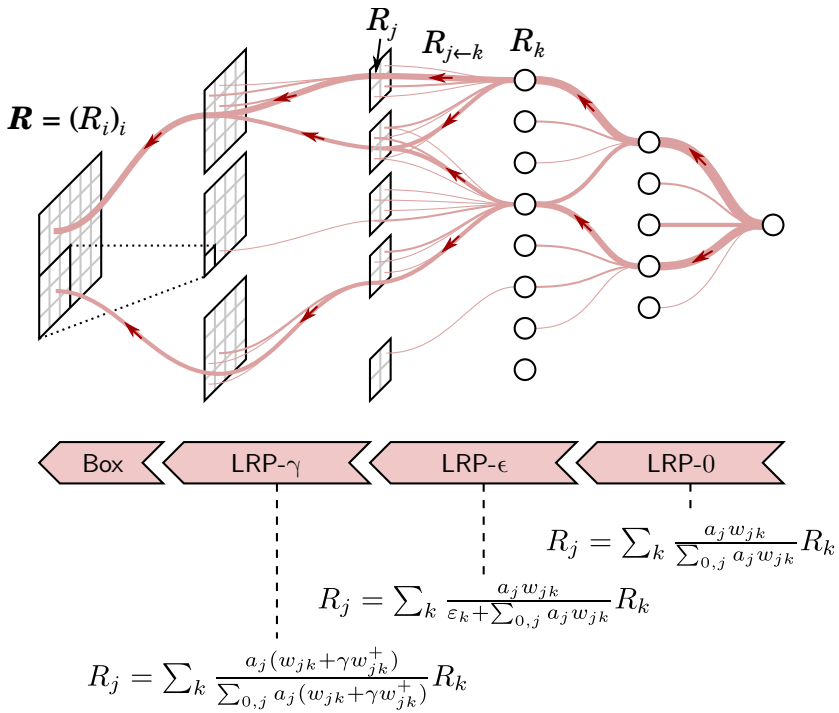
# Layer-wise Relevance Propagation (LRP) [1, 4]




**Ideas:**

- Use the structure of the neural network to robustly compute relevance scores for the input features.
- Propagate the output of the network backwards by means of propagation rules.
- Propagation rules can be tuned for explanation quality. E.g. sensitive in top-layers, robust in lower layers.

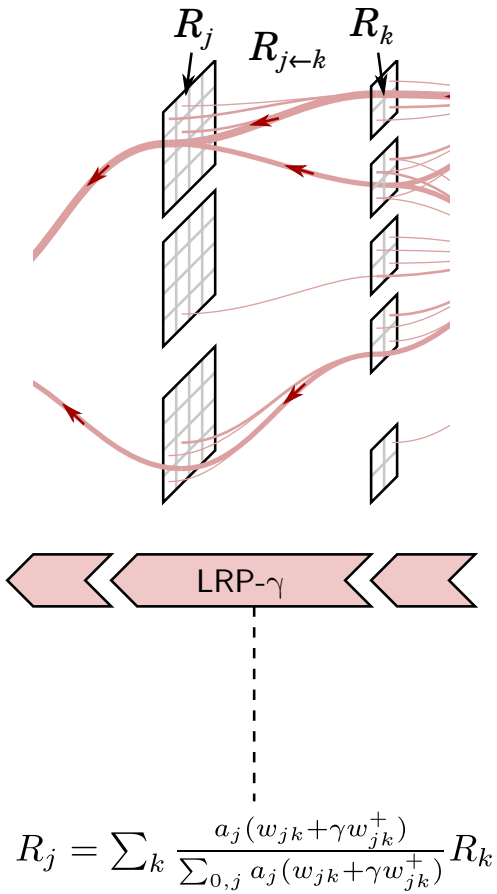
# Layer-wise Relevance Propagation (LRP) [1, 4]




**Some notation:**

- $j$ and $k$: neurons from successive layers
- $w_{jk}$: weight connecting neuron $j$ to neuron $k$
- $w_{0k}$: bias for neuron $k$.
- $\sum_{0,j}$ sum over all input neurons $j$ of neuron $k$ and the bias.
- ReLU neuron: $a_k = \max\left(0, \sum_{0,j} a_j w_{jk}\right)$.

# Dissecting an LRP Propagation Rule

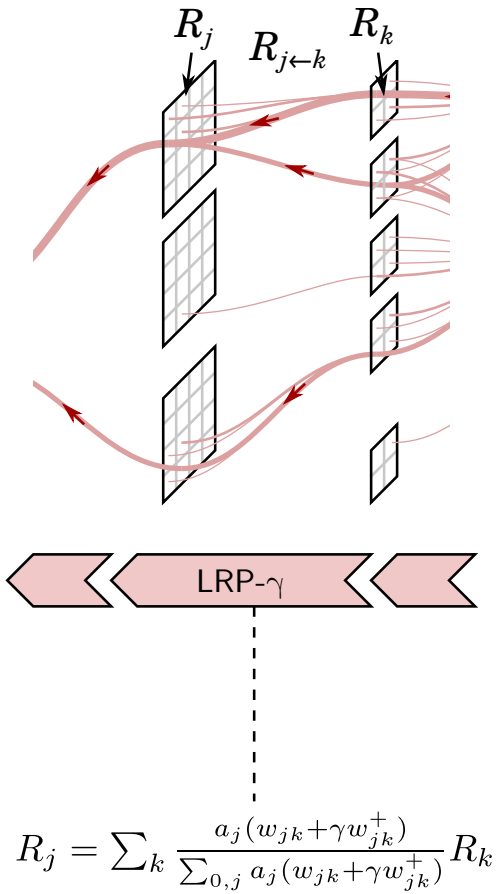



**Example:** LRP-$\gamma$ [4]

$$R_j = \sum_k \frac{a_j(w_{jk} + \gamma w_{jk}^+)}{\sum_{0,j} a_j(w_{jk} + \gamma w_{jk}^+)} R_k$$

- $a_j(w_{jk} + \gamma w_{jk}^+)$: Contribution of neuron $a_j$ to the activation $a_k$.
- $R_k$ 'Relevance' of neuron $k$ available for redistribution.
- $\sum_{0,j} a_j(w_{jk} + \gamma w_{jk}^+)$ Normalization term that implements conservation.
- $\sum_k$: Pool all 'relevance' received by neuron $j$ from the layer above.

# Dissecting an LRP Propagation Rule (2nd view)

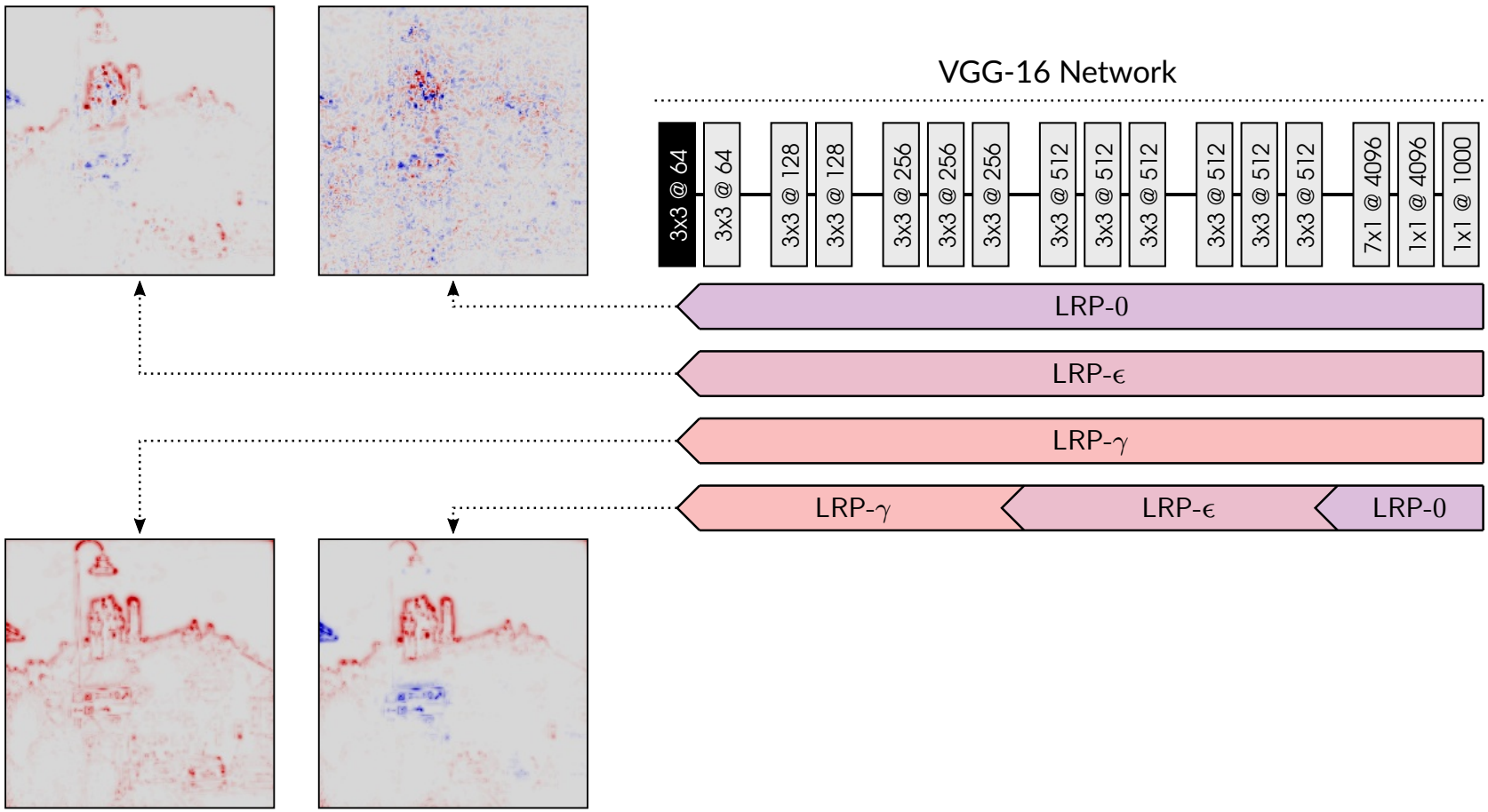



**Example:** LRP-$\gamma$ [4]

$$R_j = a_j \cdot \Big( \sum_k \frac{(w_{jk} + \gamma w_{jk}^+)}{\sum_{0,j} a_j (w_{jk} + \gamma w_{jk}^+)} R_k \Big)$$

- $a_j$ : Activation of neuron $j$.
- $\big(\sum_k \dots\big)$: Sensitivity of neural network output to $a_j$.

# Effect of LRP Rules on Explanation




LRP rules must be chosen carefully to deliver best explanation quality. Generally, LRP rules are set different at each layer (cf. [4] for heuristics).

# Layer-Wise Relevance Propagation

**Advantages**

- *Good explanation quality* on deep networks.
- *Fast* (in the order of a single forward/backward pass).
- *Flexible* (the multiple hyperparameters can be tuned to match the user needs).

**Limitations**

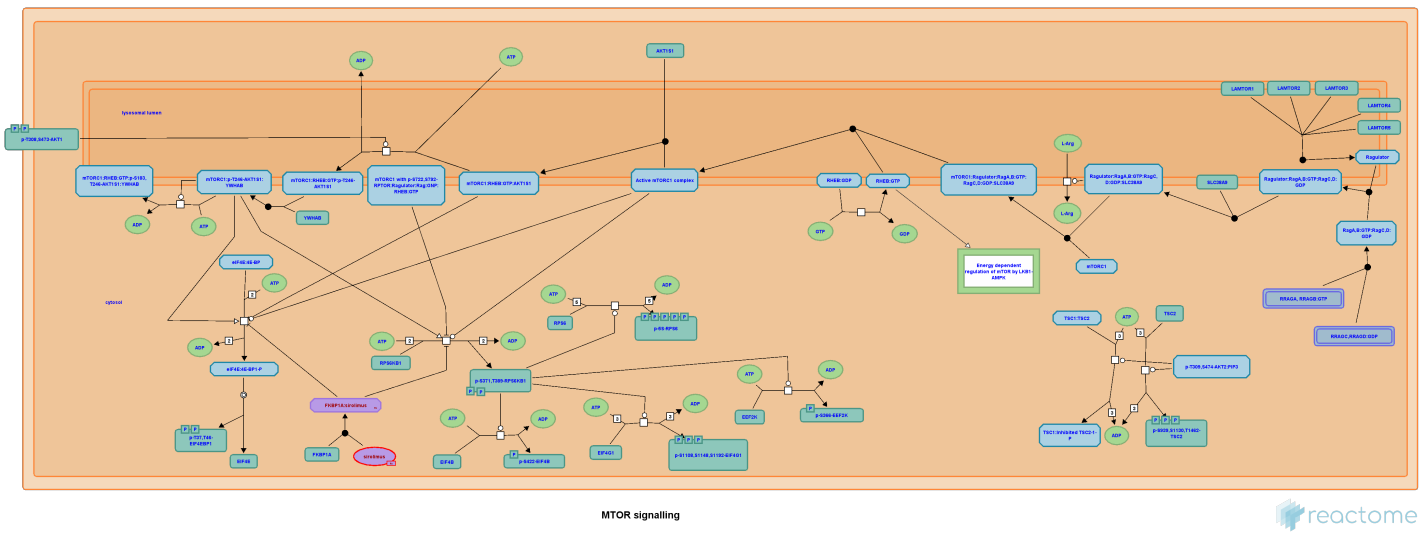
- Need to choose the hyperparameters ($\Rightarrow$ not unique).
- The LRP propagation strategy must be adapted to each new architecture.
- LRP assumes that the model has sufficiently disentangled the function to explain (i.e. it works for many neural networks but not for all models).

Part 3

# Finding Influential Proteins [2]

# Example: Discovering Influencial Proteins

*Example:* MTOR signaling network (from reactome.org)



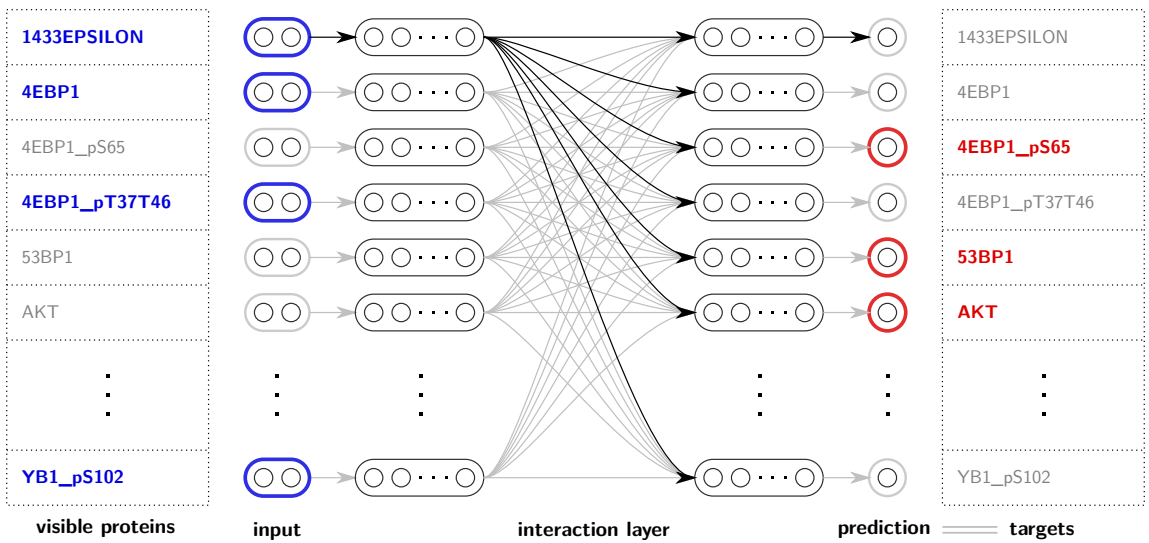

**Question:**

- Can we use ML/XAI to infer these networks (or aspects of them) directly from the data?

# Finding Influential Proteins with ML/XAI

## Step 1: From Data to ML

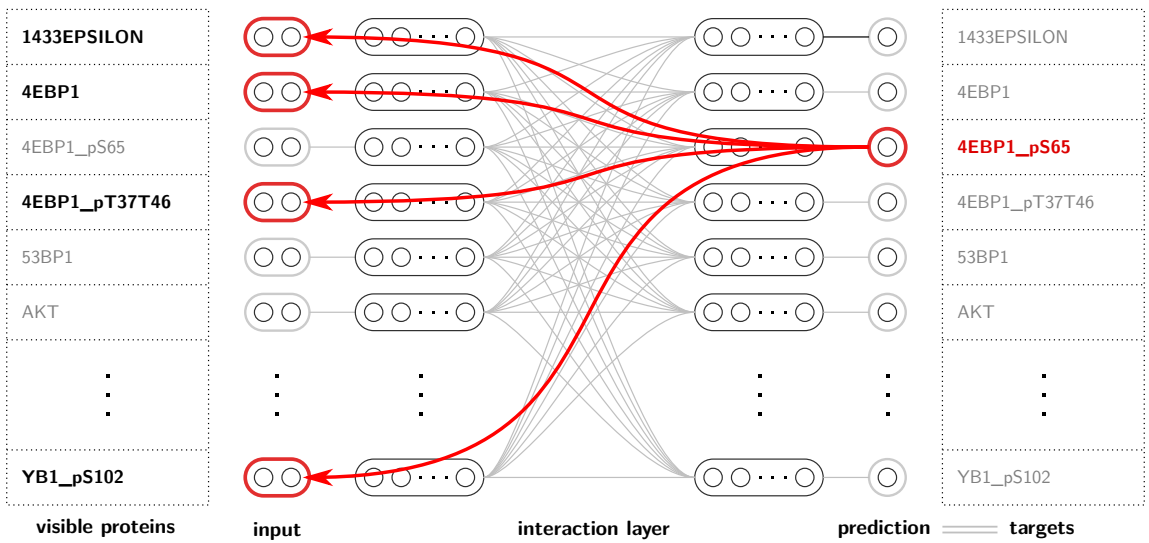
- Assemble a dataset.
- Build a ML model (neural network) that predicts proteins from other proteins with best possible accuracy.



# Finding Influential Proteins with ML/XAI

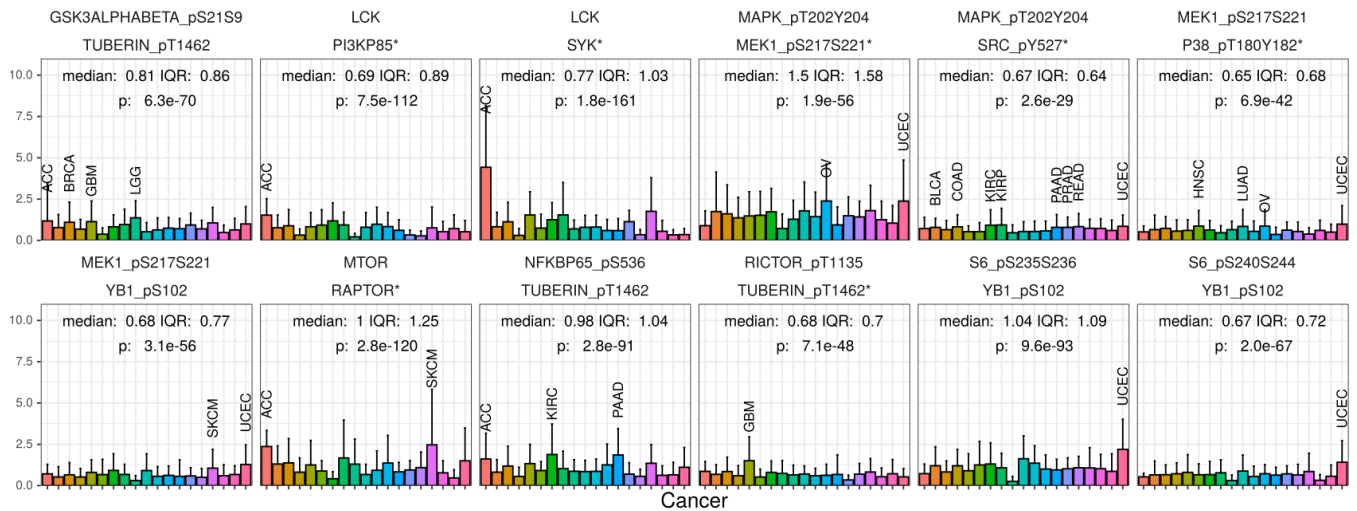
## Step 2: From ML to XAI

- Apply Explainable AI (here the LRP attribution technique) to identify to what extent proteins contribute to the expression of other proteins.

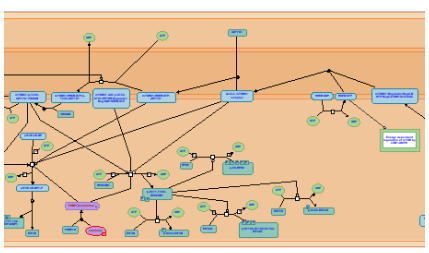


# Finding Influential Proteins with ML/XAI

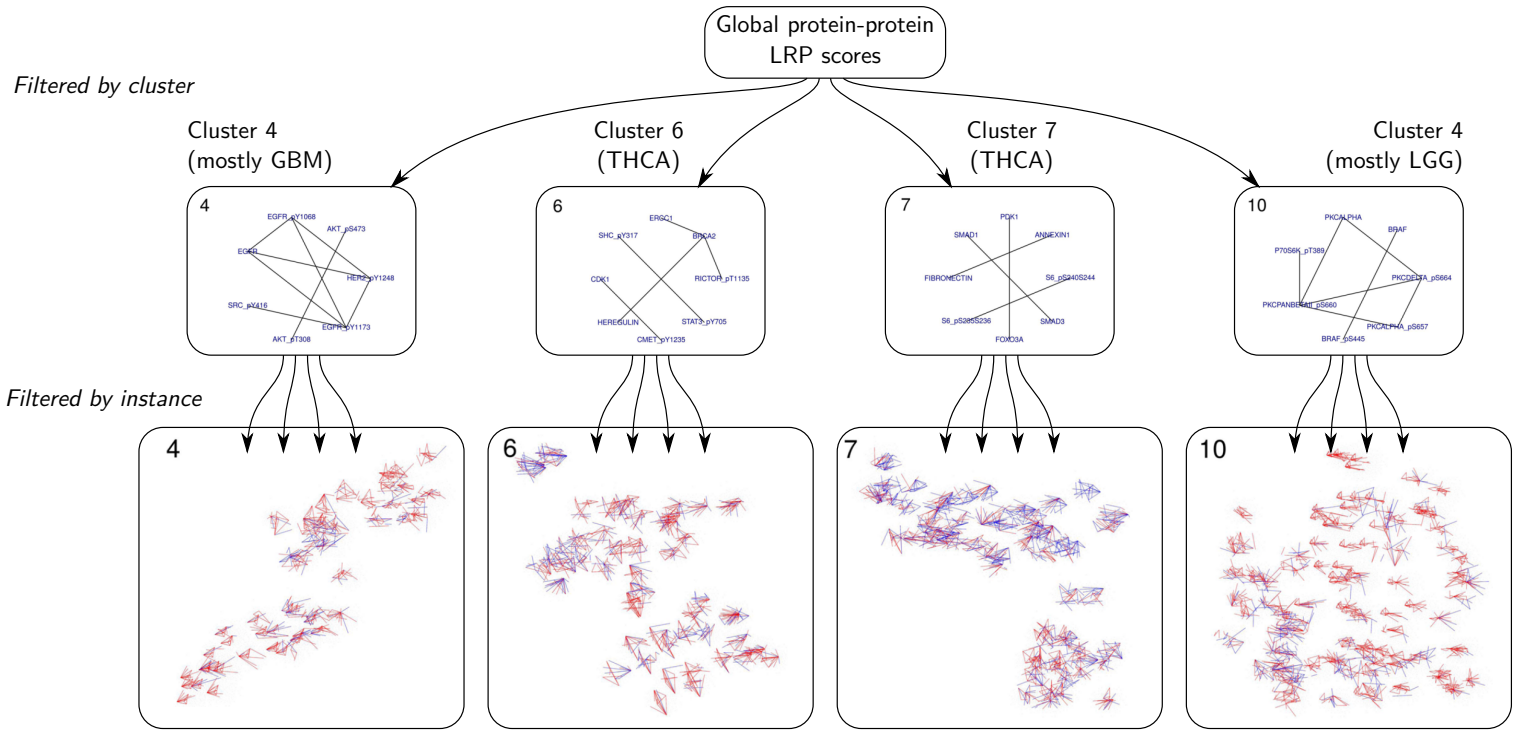
Excerpt of top-$k$ protein influences via XAI (LRP attribution):




- Generally consistent with existing knowledge, e.g. highlights mTOR pathway; correlates with entries in the reactome knowledgebase (`https://reactome.org/`).
- Provides *cancer-specific* (or even *instance-specific*) view of protein influences.



# Finding Influential Proteins with ML/XAI (Keyl et al. 2022)




- Can further enhance existing knowledge with *case-specific* protein influences.

# Summary

# Summary

- Explainable AI is an important addition to classical ML models (e.g. for validating a ML model or extracting knowledge from it).
- Many XAI methods have been developed, each of them, with their strengths and limitations:
  - *Activation maximization* can be used to understand what a ML model has learned, but is unsuitable for explaining an individual prediction $f(\boldsymbol{x})$.
  - *Shapley value sampling* has strong theoretical foundations, but is computationally demanding for high-dimensional input data.
  - *LRP* yields fast explanations of the ML model, but requires to carefully choose the propagation rules.

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