Tutorial on Interpreting and Explaining Deep Models in Computer Vision

Wojciech Samek (Fraunhofer HHI)

Grégoire Montavon (TU Berlin)

Klaus-Robert Müller (TU Berlin)

08:30 - 09:15	Introduction KRM
09:15 - 10:00	Techniques for Interpretability GM
10:00 - 10:30	Coffee Break ALL
10:30 - 11:15	Applications of Interpretability WS
11:15 - 12:00	Further Applications and Wrap-Up KRM

2018 CVPR
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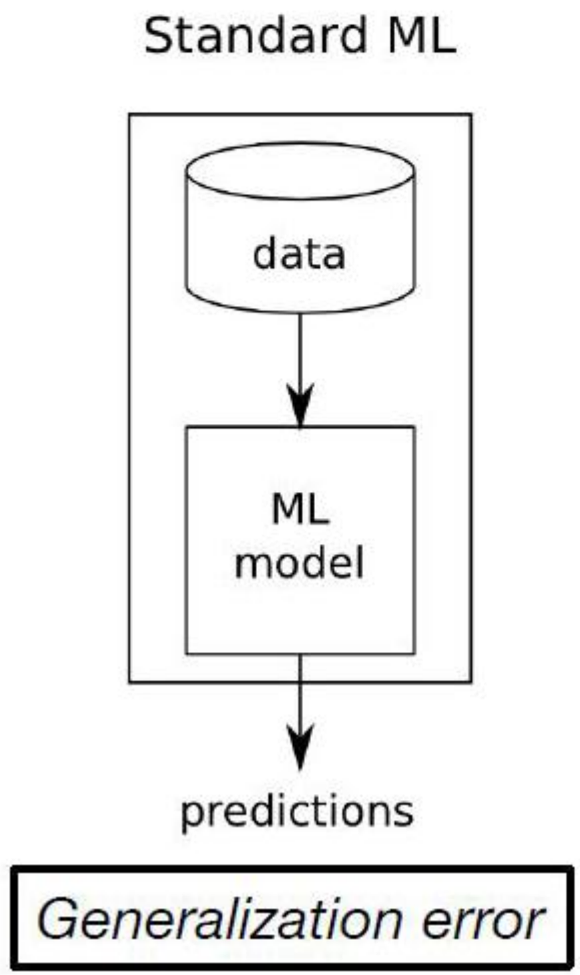
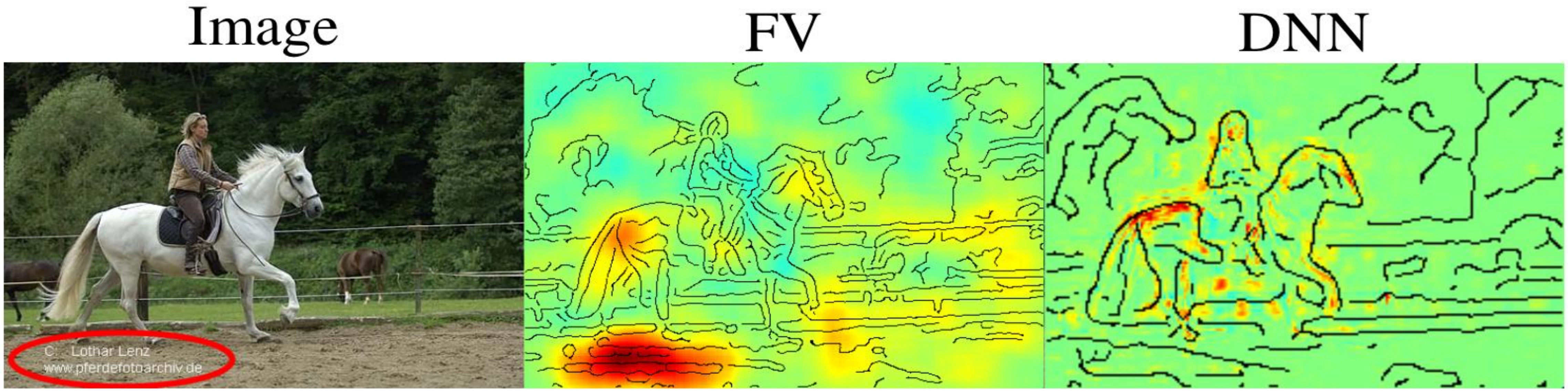
Is the Generalization Error all we need?



Application: Comparing Classifiers

Test error for various classes:

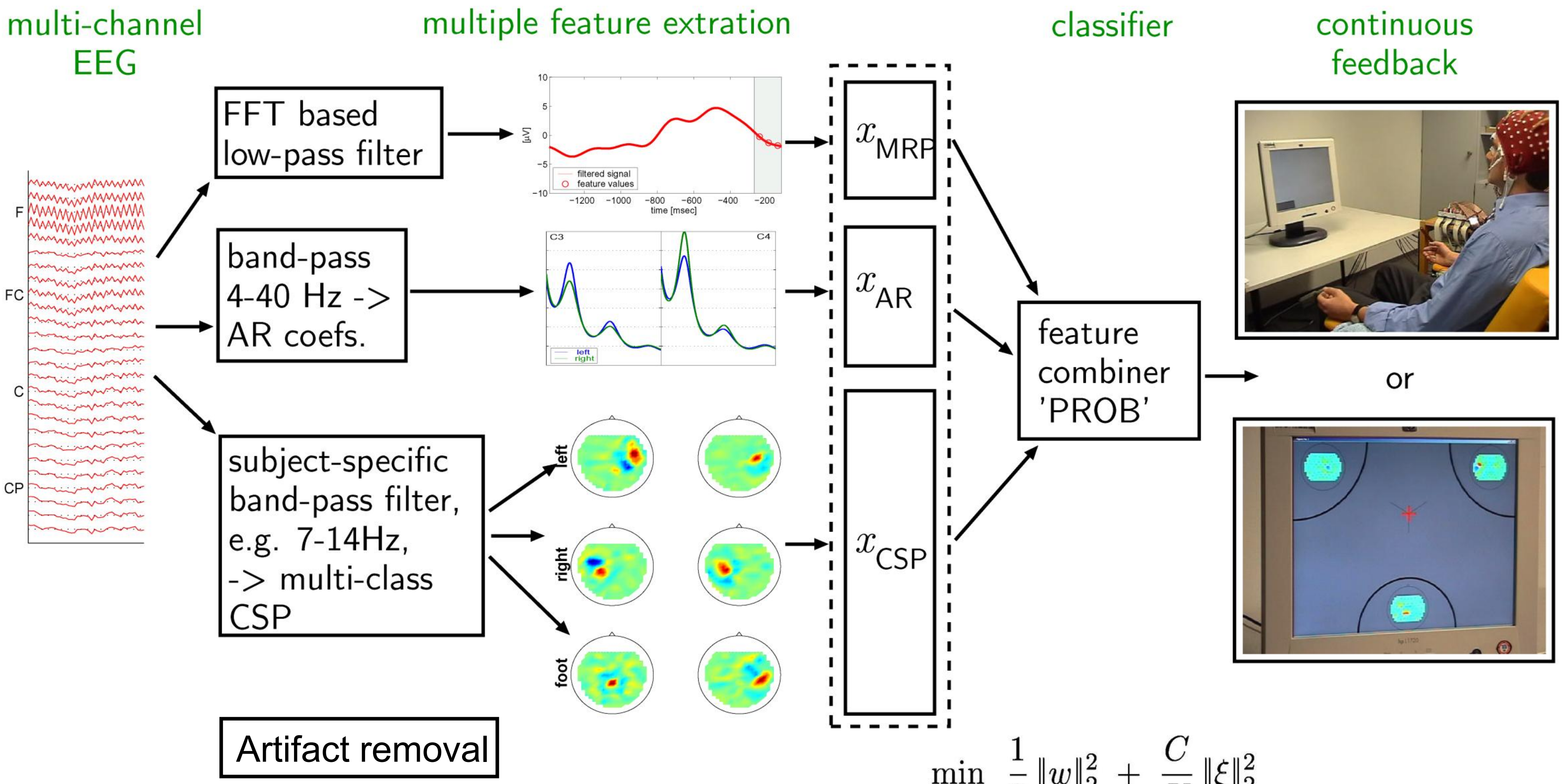
	aeroplane	bicycle	bird	boat	bottle	bus	car
Fisher	79.08%	66.44%	45.90%	70.88%	27.64%	69.67%	80.96%
DeepNet	88.08%	79.69%	80.77%	77.20%	35.48%	72.71%	86.30%
	cat	**chair**	**cow**	**diningtable**	**dog**	**horse**	**motorbike**
Fisher	59.92%	51.92%	47.60%	58.06%	42.28%	80.45%	69.34%
DeepNet	81.10%	51.04%	61.10%	64.62%	76.17%	81.60%	79.33%
	person	**pottedplant**	**sheep**	**sofa**	**train**	**tvmonitor**	**mAP**
Fisher	85.10%	28.62%	49.58%	49.31%	82.71%	54.33%	59.99%
DeepNet	92.43%	49.99%	74.04%	49.48%	87.07%	67.08%	72.12%



Machine Learning in the Sciences

Machine Learning in Neuroscience

BBCI Set-up: *Let the machines learn*



$$\min_{w,b,\xi} \frac{1}{2}\|w\|_2^2 + \frac{C}{K}\|\xi\|_2^2$$

$$\text{subject to} \quad y_k(w^\top x_k + b) = 1 - \xi_k \quad \text{for } k = 1, \ldots, K$$

[cf. Müller et al. 2001, 2007, 2008, Dornhege et al. 2003, 2007, Blankertz et al. 2004, 2005, 2006, 2007, 2008]

Brain Computer Interfacing: ‚Brain Pong'

Berlin Brain Computer Ínterfac

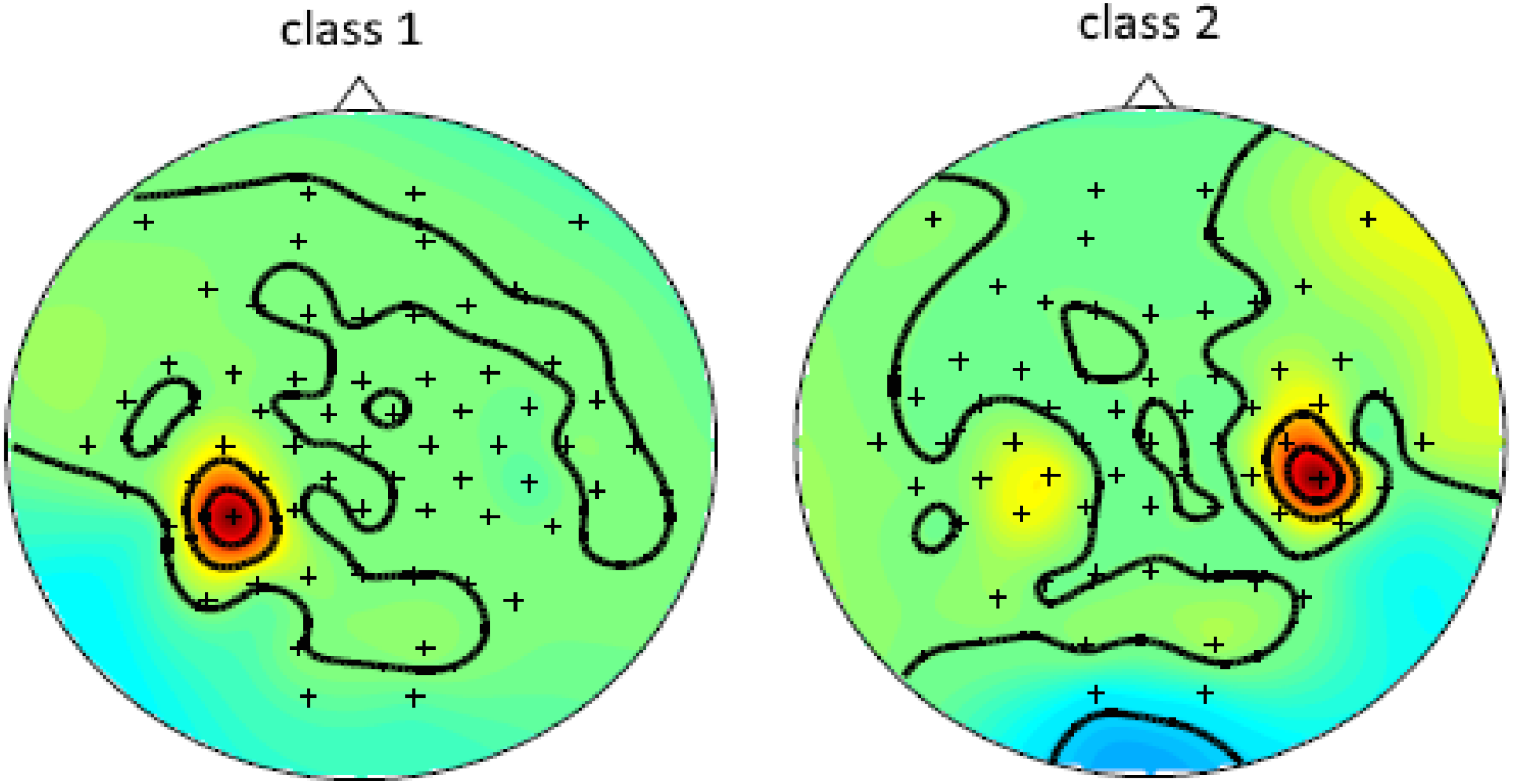
- ML reduces patient training fron 300h -> 5min

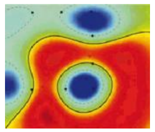
Applications

- help/hope for patients (ALS, stroke…)
- neuroscience
- neurotechnology (video coding, gaming, monitoring driving)

Leitmotiv: *›let the machines learn‹*

DNN Explanation Motor Imagery BCI





Note: Explanation available for single Trial (Sturm et al 2016)

Explaining in Physics

Machine Learning in Chemistry, Physics and Materials

Matthias Rupp, Anatole von Lilienfeld,
Alexandre Tkatchenko, Klaus-Robert Müller

Machine Learning for chemical compound space

Ansatz:

$$\{Z_I, \mathbf{R}_I\} \xmapsto{\text{ML}} E$$

instead of

$$\hat{H}(\{Z_I, \mathbf{R}_I\}) \quad \xmapsto{\Psi} \quad E$$

$$\hat{H}\Psi = E\Psi$$

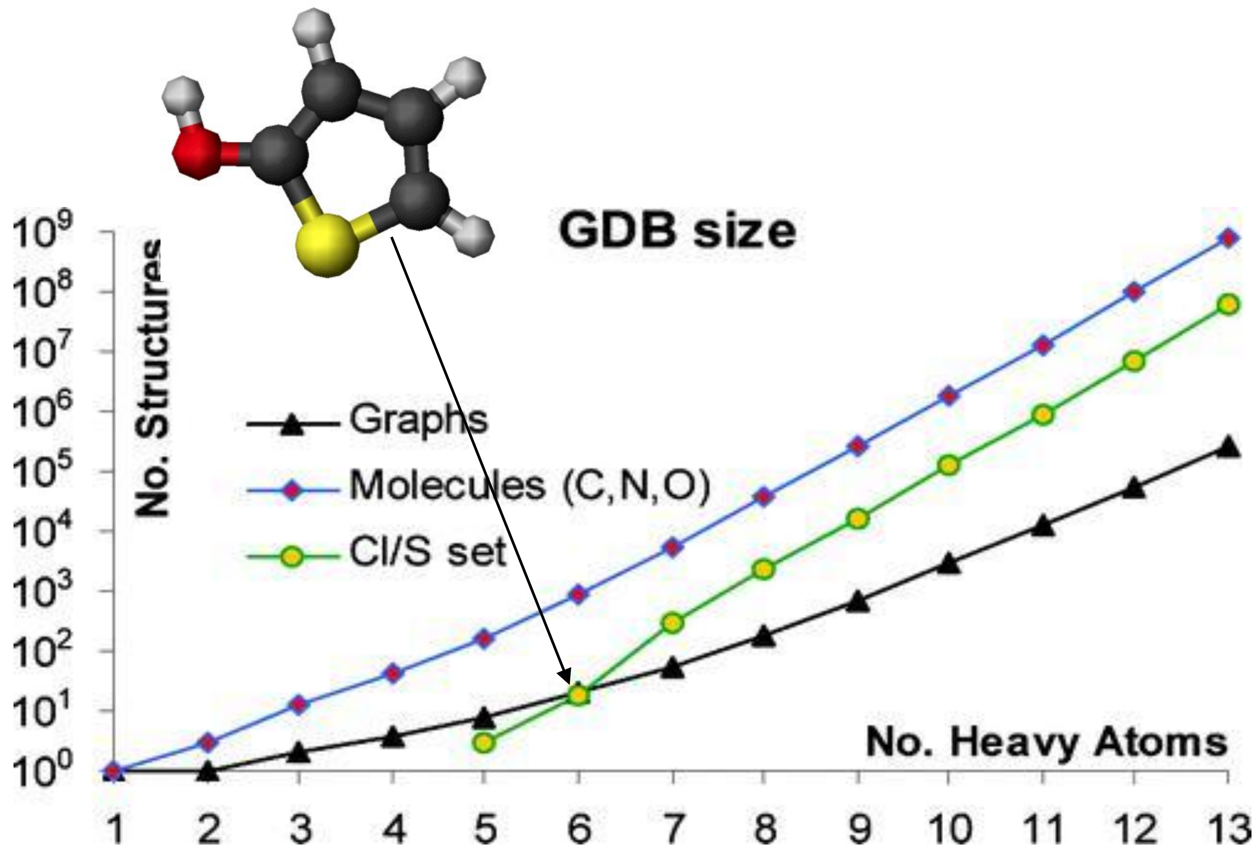
[from von Lilienfeld]

The data

GDB-13 database of all organic molecules (within stability & synthetic constraints) of 13 heavy atoms or less: 0.9B compounds

Table 1. Structure Generation Statistics for GDB-13

nodes[a]	graphs[b]	GDB[c]	Cl/S[d]	CPU time (h)[e]
1	1	1	0	0.00
2	1	3	0	0.00
3	2	12	0	0.00
4	4	43	0	0.00
5	8	155	3	0.01
6	20	934	19	0.02
7	57	5726	315	0.05
8	194	37151	2438	0.33
9	706	255542	17056	2.68
10	2831	1784626	130465	25.26
11	12011	12961686	938704	223.49
12	53789	99821343	7240108	3023.79
13	250268	795244451	59027533	36606.45
Total	**319892**	**910111673**	**67356641**	**39882.08**



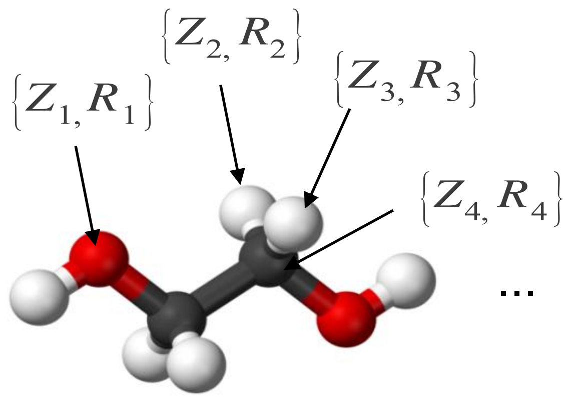
Blum & Reymond, *JACS* (2009)

[from von Lilienfeld]

Coulomb representation of molecules

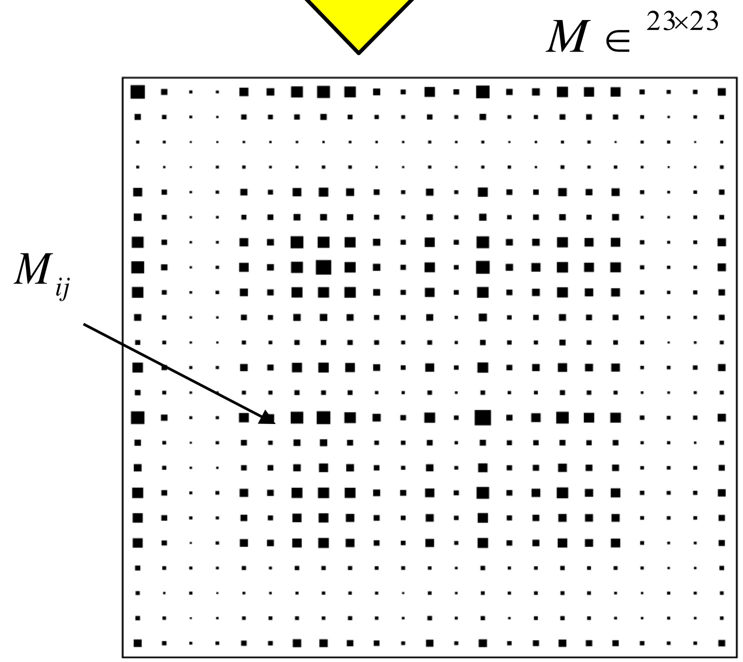
$$M_{ii} = Z_i^{2.4}$$

$$M_{ij} = \frac{Z_i Z_j}{\left\| R_i - R_j \right\|}$$



+ phantom atoms

$\{0, R_{21}\}$ $\{0, R_{22}\}$ $\{0, R_{23}\}$



Coulomb Matrix (Rupp, Müller et al 2012, PRL)

$$d(\mathbf{M}, \mathbf{M}') = \sqrt{\sum_{IJ} |M_{IJ} - M'_{IJ}|^2}$$

Kernel ridge regression

Distances between **M** define Gaussian kernel matrix **K**

$$k(\mathbf{M}, \mathbf{M}') = \exp\left(-\frac{d(\mathbf{M}, \mathbf{M}')^2}{2\sigma^2}\right)$$

Predict energy as sum over weighted Gaussians

$$E^{est}(\mathbf{M}) = \sum_i \alpha_i k(\mathbf{M}, \mathbf{M}_i) + b$$

using weights that minimize error in training set

$$\min_{\alpha} \sum_i \left(E^{est}(\mathbf{M}_i) - E_i^{ref}\right)^2 + \lambda \sum_i \alpha_i^2$$

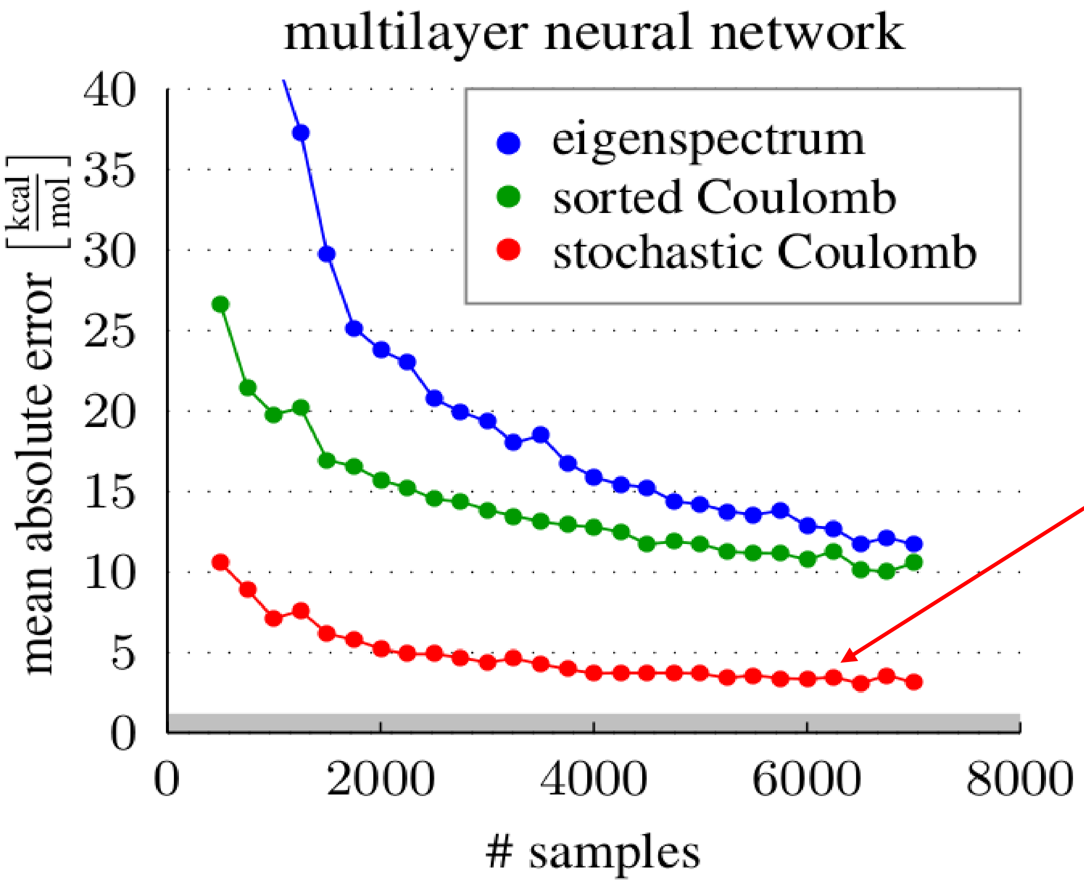
$$\alpha = (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{E}^{ref}$$

Exact solution

As many parameters as molecules + 2 global parameters, characteristic length-scale or kT of system (σ), and noise-level (λ)

[from von Lilienfeld]

Predicting Energy of small molecules: Results



March 2012
Rupp et al., PRL
9.99 kcal/mol
(kernels + eigenspectrum)

December 2012
Montavon et al., NIPS
3.51 kcal/mol
(Neural nets + Coulomb sets)

2015 Hansen et al 1.3kcal/mol at **10 million** times faster than the state of the art

Prediction considered chemically accurate when MAE is below **1 kcal/mol**

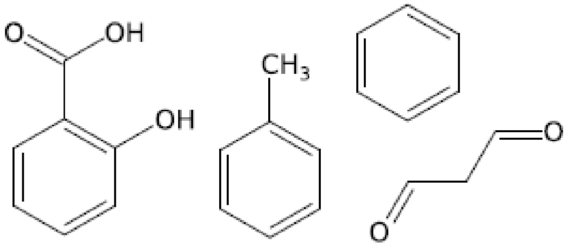
Dataset available at http://quantum-machine.org

Learning Atomistic Representations with Deep Tensor Neural Networks

Kristof Schütt,Farhad Arbabzadah,
Stefan Chmiela, Alexandre Tkatchenko,
Klaus-Robert Müller

Deep Tensor Neural Network (DTNN) for representing molecules

Input: Atomic numbers and interatomic distances



$$Z = [\, Z_1 \quad Z_2 \quad \cdots \quad Z_n \,]$$

$$D = \begin{bmatrix} d_{11} & d_{12} & \cdots & d_{1n} \\ d_{21} & d_{12} & \cdots & d_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{n1} & d_{n2} & \cdots & d_{nn} \end{bmatrix}$$

Embedding of based on atom types

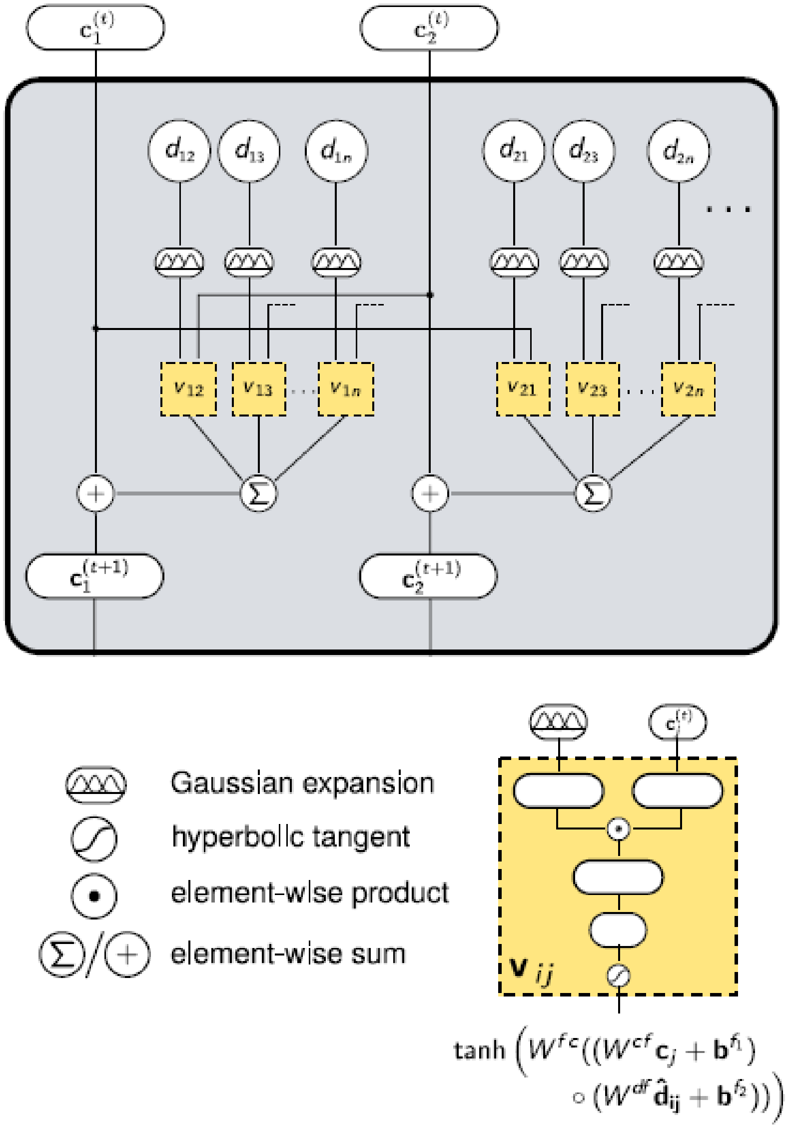
$$\mathbf{x}_i^{(0)} = \mathbf{x}_{Z_i} \in \mathbb{R}^d$$

Add interaction with environment using $t = 1 \ldots T$ sequential refinements $\mathbf{v}_i^{(t)}$

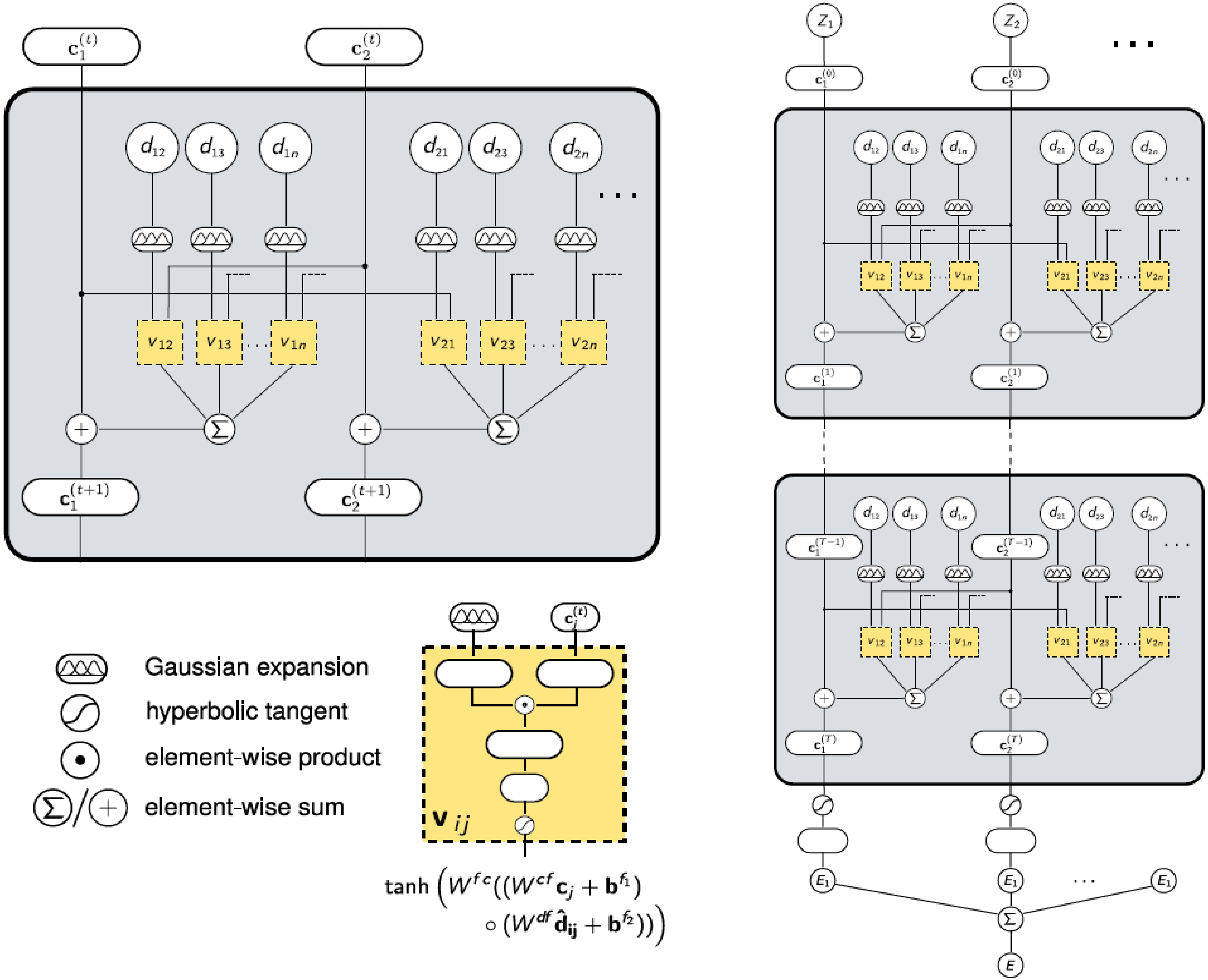
$$\mathbf{x}_i^{(t+1)} = \mathbf{x}_i^{(t)} + \mathbf{v}_i^{(t)} \left(\mathbf{x}_1^{(t)}, \ldots \mathbf{x}_{n_{\text{atoms}}}^{(t)}, d_{i1}, \ldots, d_{in_{\text{atoms}}} \right)$$

Prediction via atom-wise contributions:

$$\hat{E} = \sum_{i=1}^{n_{\text{atoms}}} f_{\text{out}}(\mathbf{x}_i^{(T)})$$



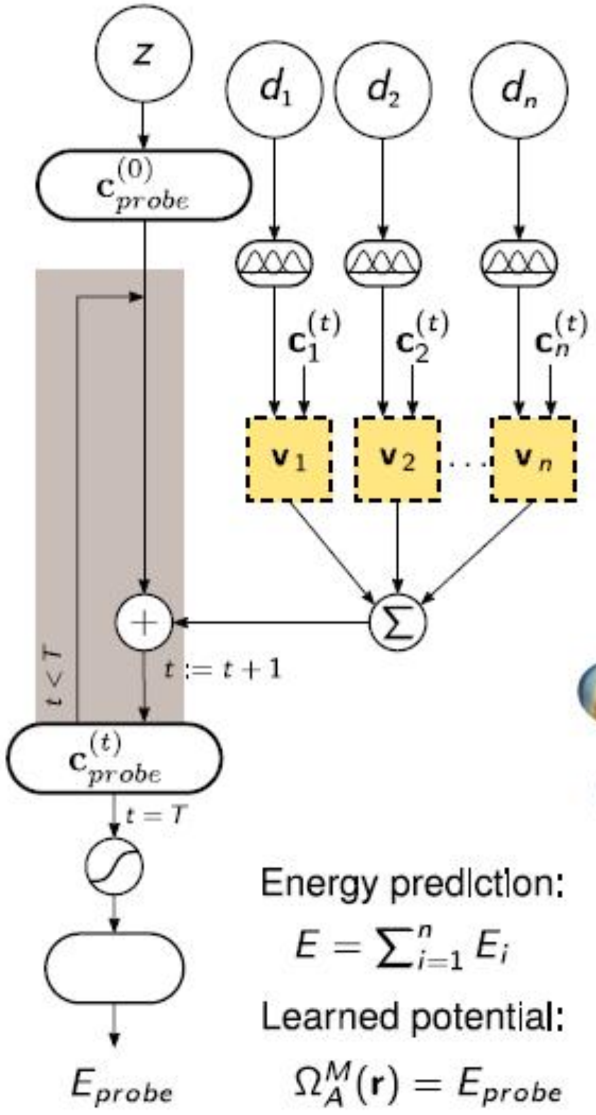
Schütt, Arbabzadah, Chmiela, Müller, Tkatchenko, Nature Communications **8**, *13890 (2017)*



$c_1^{(t)}$
$c_2^{(t)}$
d_{12} d_{13} d_{1n} d_{21} d_{23} d_{2n}
v_{12} v_{13} v_{1n} v_{21} v_{23} v_{2n}
$c_1^{(t+1)}$
$c_2^{(t+1)}$
Gaussian expansion
hyperbolic tangent
element-wise product
element-wise sum
$c_j^{(t)}$
$\mathbf{v}_{ij}$
$\tanh\left(W^{fc}((W^{cf}\mathbf{c}_j + \mathbf{b}^{f_1}) \circ (W^{df}\hat{\mathbf{d}}_{\mathbf{ij}} + \mathbf{b}^{f_2}))\right)$
Z_1 Z_2
$c_1^{(0)}$ $c_2^{(0)}$
$c_1^{(1)}$ $c_2^{(1)}$
$c_1^{(T-1)}$ $c_2^{(T-1)}$
$c_1^{(T)}$ $c_2^{(T)}$
E_1 E_1 E_1
E

Gaining insights for Physics

Toward Quantum Chemical Insights: supervised

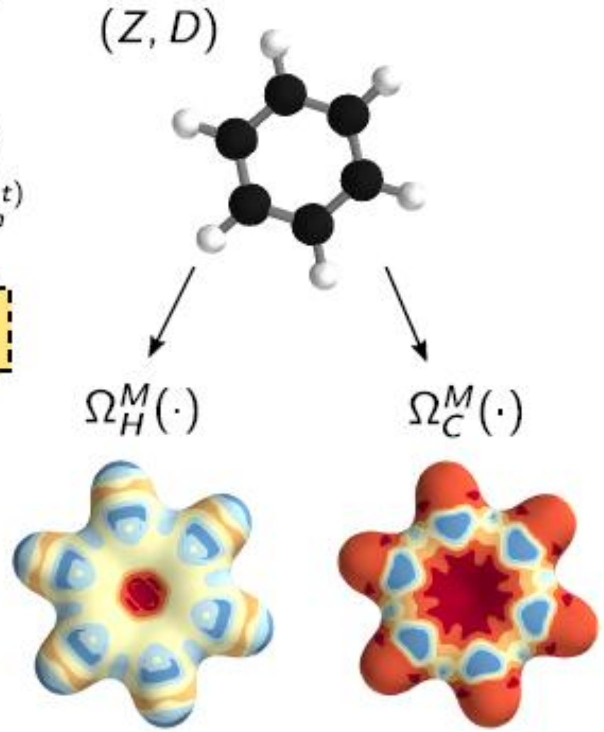


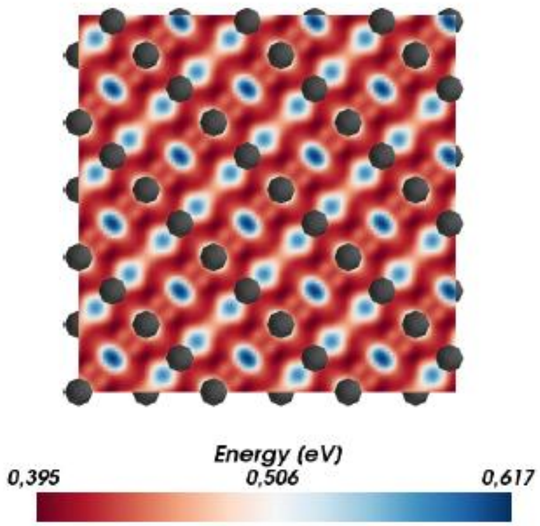
Energy prediction:

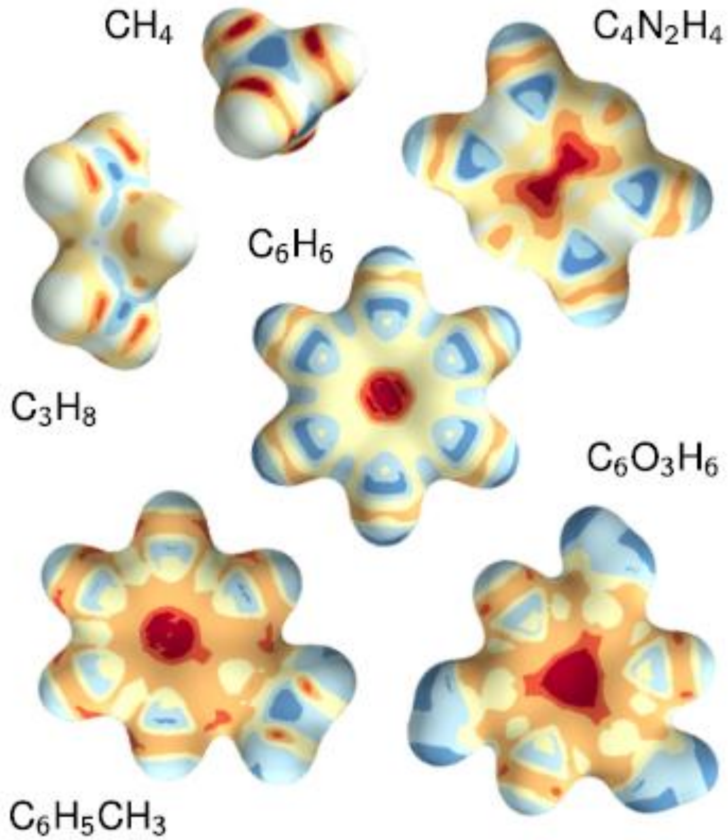
$$E = \sum_{i=1}^{n} E_i$$

Learned potential:

$$\Omega^M_A(\mathbf{r}) = E_{probe}$$

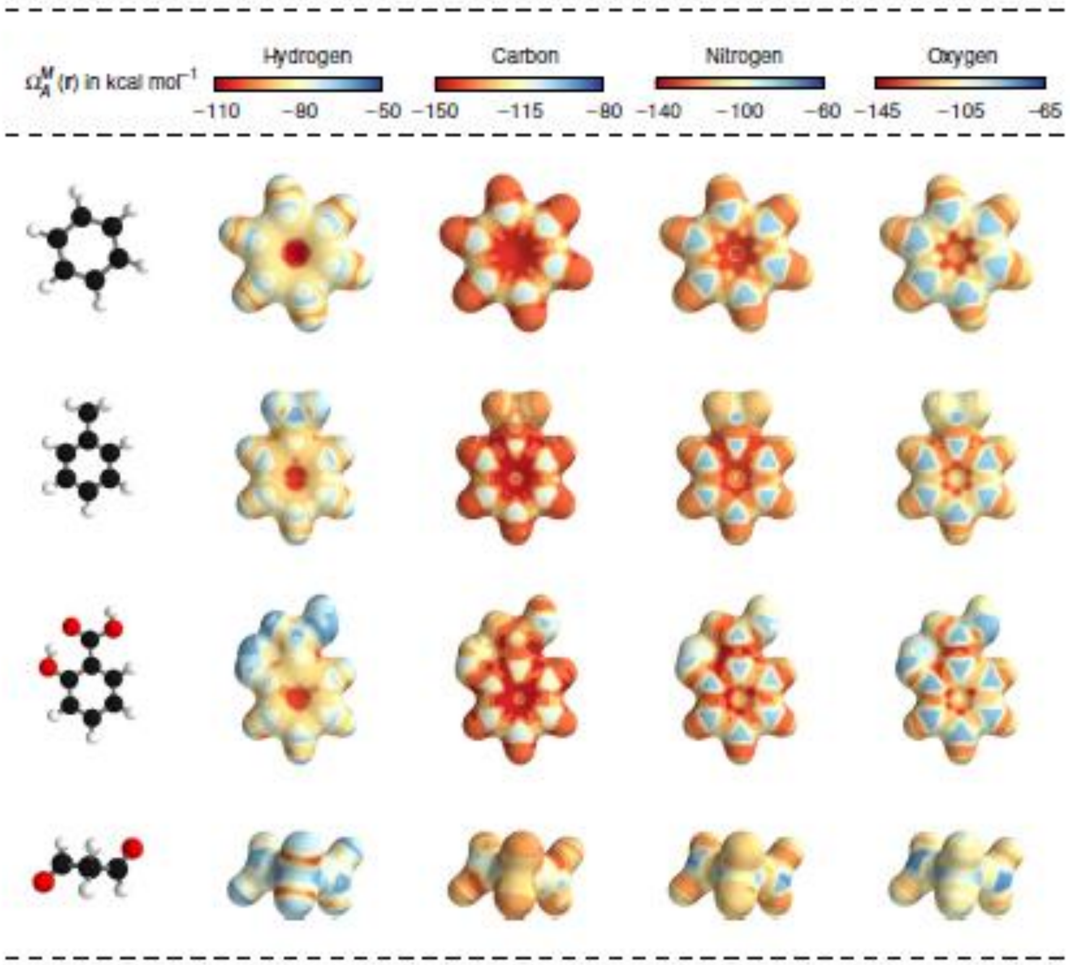




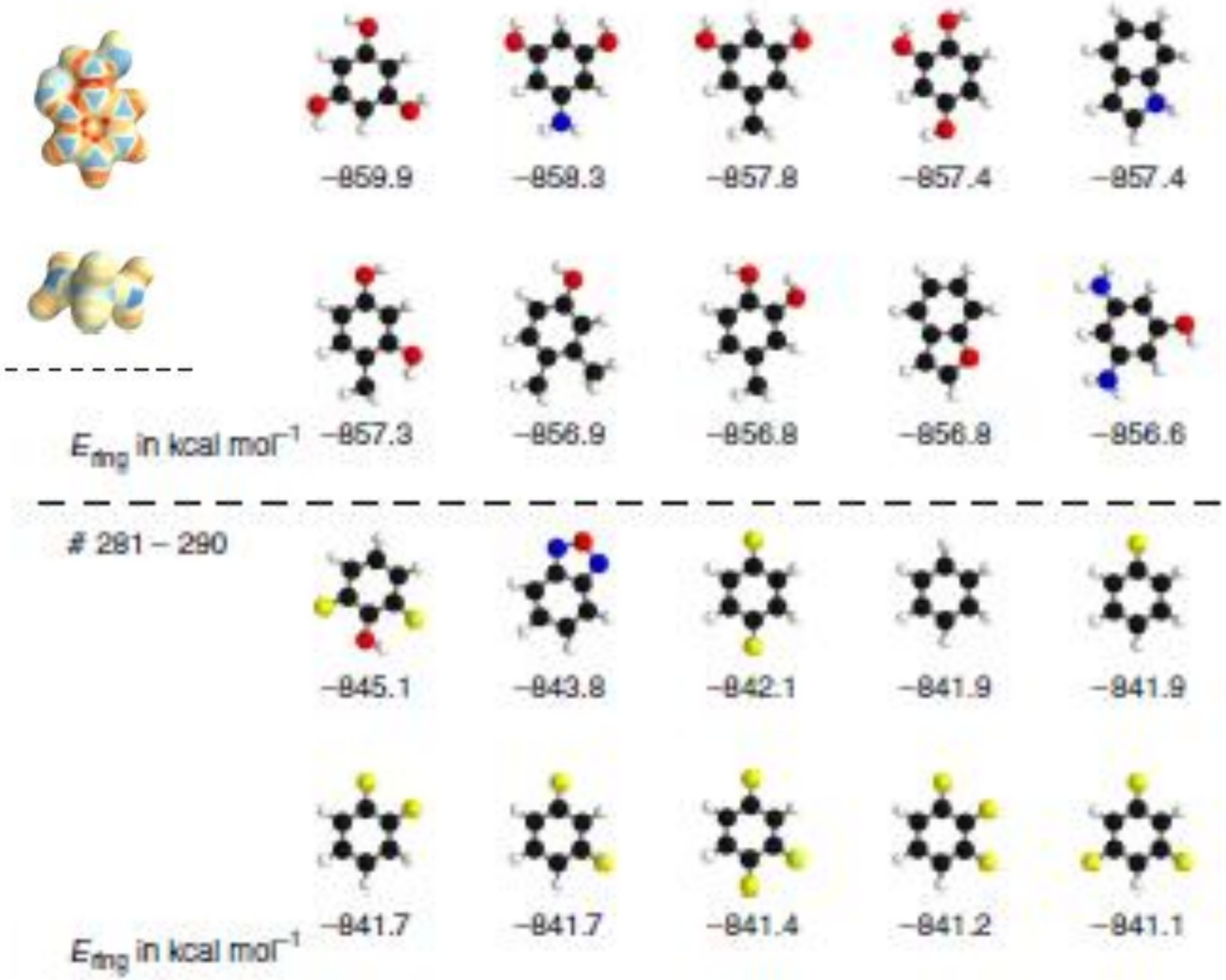


[Schütt et al. Nat Comm. 2017,
Schütt et al JCP 2018]

Quantum chemical insights



Inferred chemical potentials

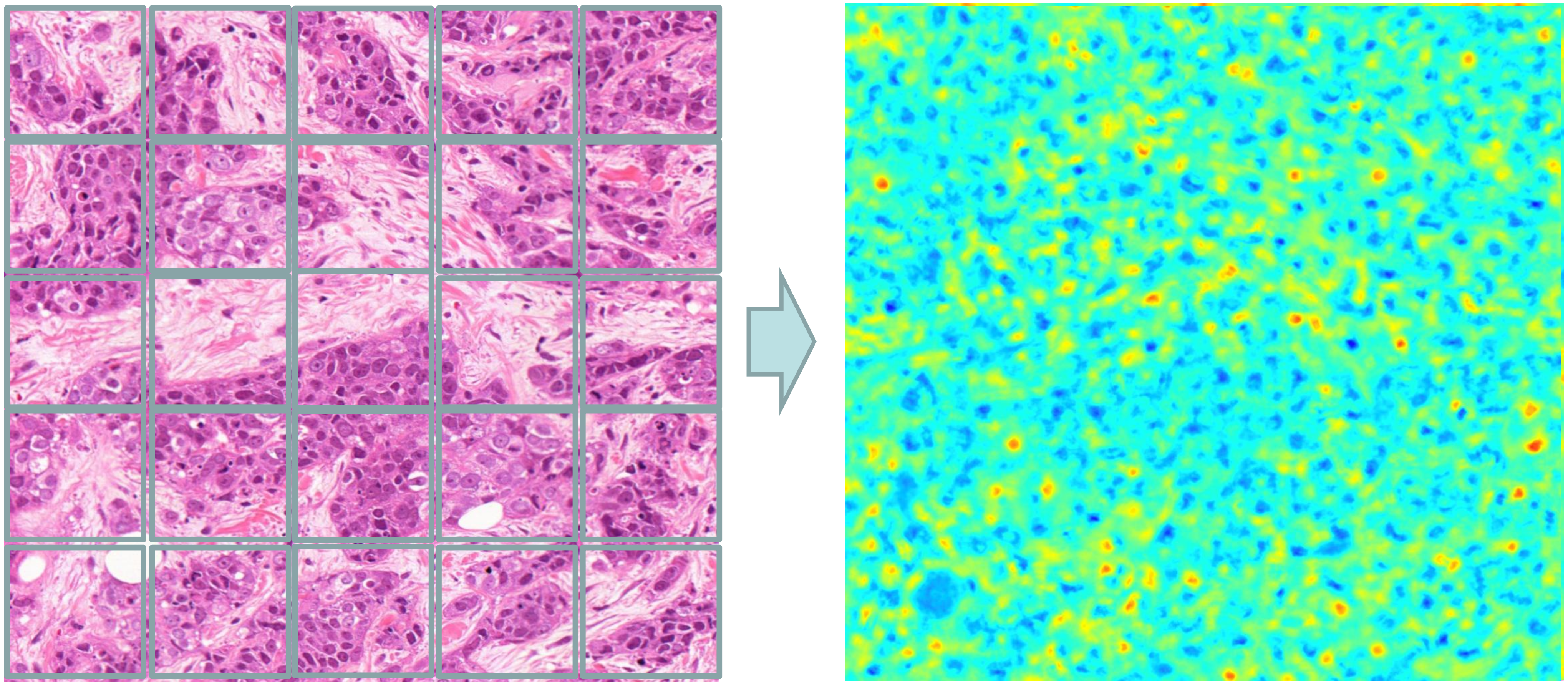


Inferred stable and unstable carbon ring classification ‚aromaticity‘

Machine Learning for morpho-molecular Integration

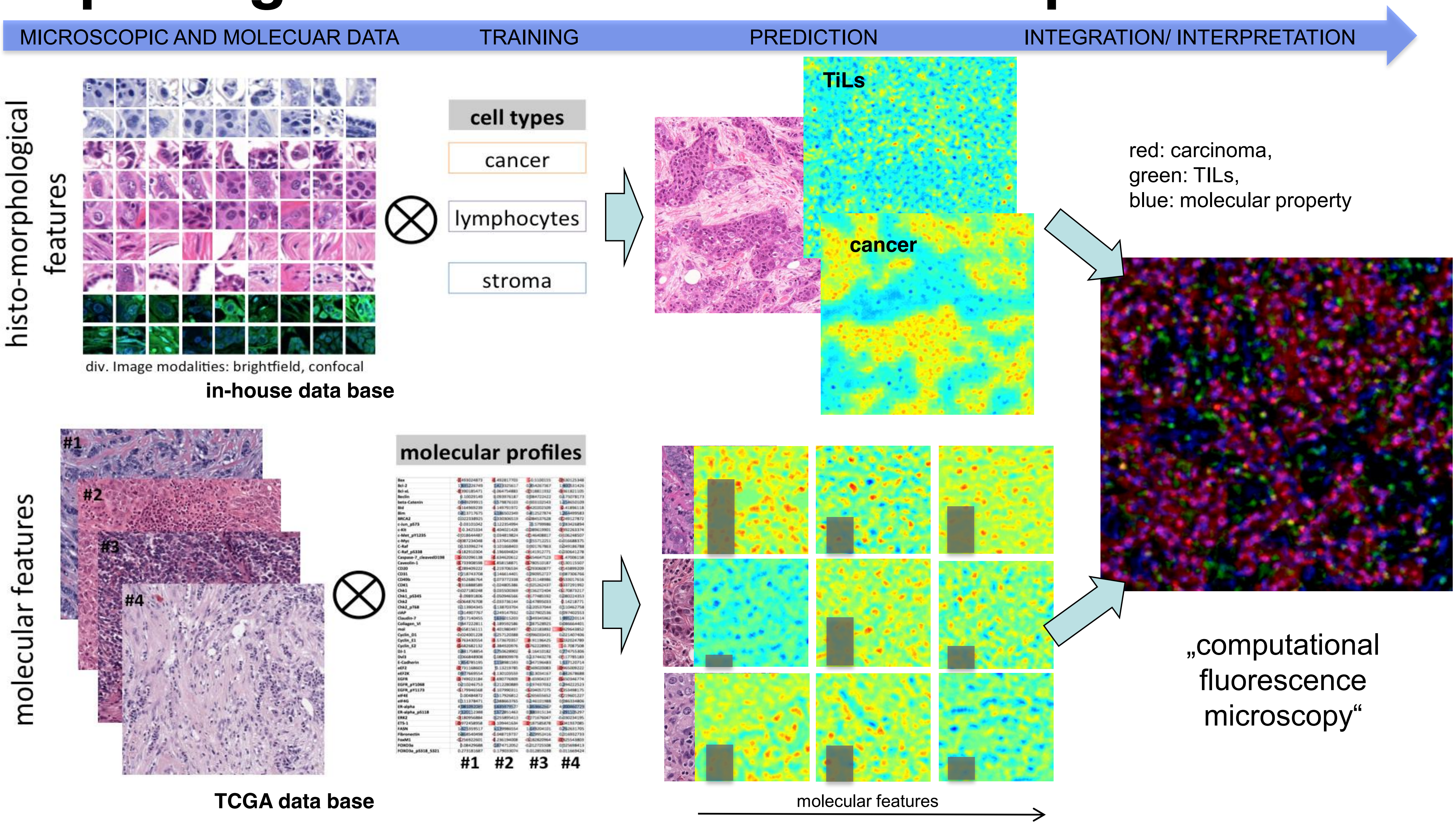
Alexander Binder[1,6], Michael Bockmayr[2,10], Miriam Hägele[1], Stephan Wienert[2], Daniel Heim[2], Katharina Hellweg[3], Albrecht Stenzinger[4], Laura Parlow[2], Jan Budczies[2], Benjamin Goeppert[4], Denise Treue[2], Manato Kotani[5], Masaru Ishii[5], Manfred Dietel[2], Andreas Hocke[3], Carsten Denkert[2,7], Klaus-Robert Müller[1,8,9,*] and Frederick Klauschen[2,7,*]

Interpretable ML



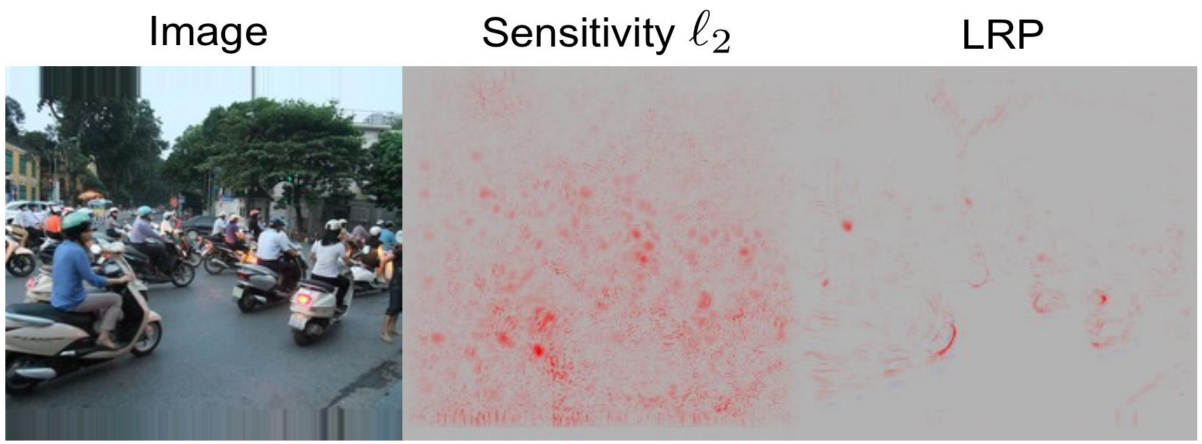
Bach et al., PLoS1 2015
Klauschen et al., US Patent #9558550
Binder et al., *in revision*

Machine learning based integration of morphological and molecular tumor profiles



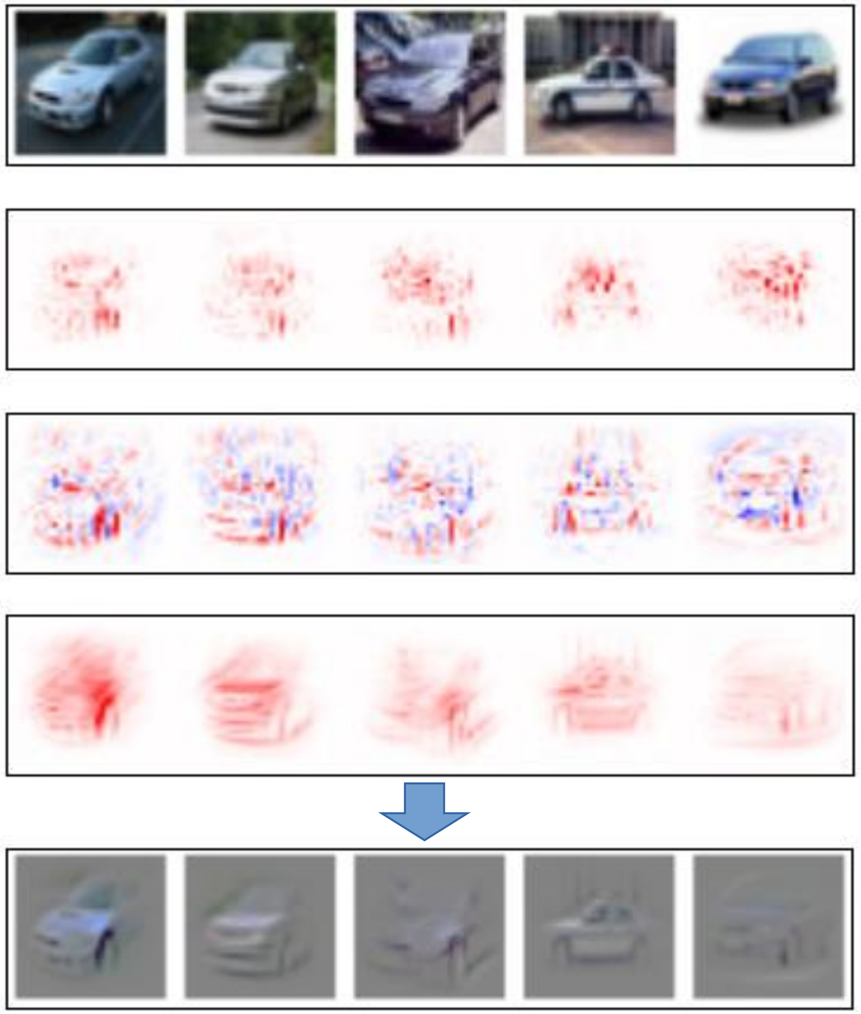
Take Home messages

Sensitivity analysis is not the question that you would like to ask!

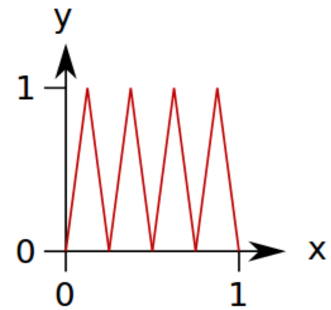


Explanation for simple models does not necessary work for deep models

What works for simple models doesn't work for deep models.



gradient-based methods } vulnerable to shattered gradients



Our LRP method is robust to this.

Layer-Wise Relevance Propagation

Desirable properties of an explanation

positivity
conservation
selectivity
continuity

“Tricks of the trade”

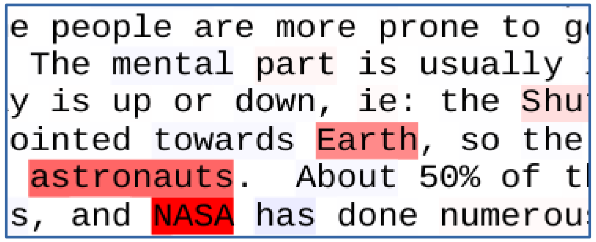
Underlying theory for consistency

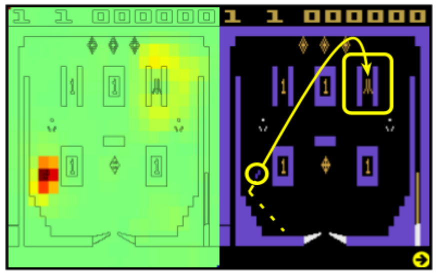
$$R_i = \sum_j \frac{\partial R_j}{\partial a_i} \cdot (a_i - \tilde{a}_i^{(j)})$$

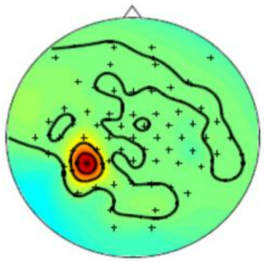
Deep Taylor Decomposition

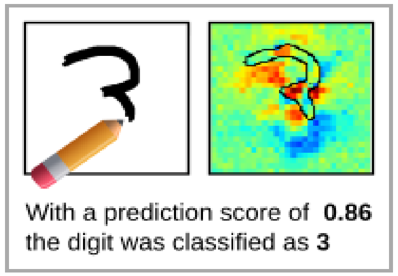
LRP Explanation Framework

(software, tutorials, demos, insights, applications)

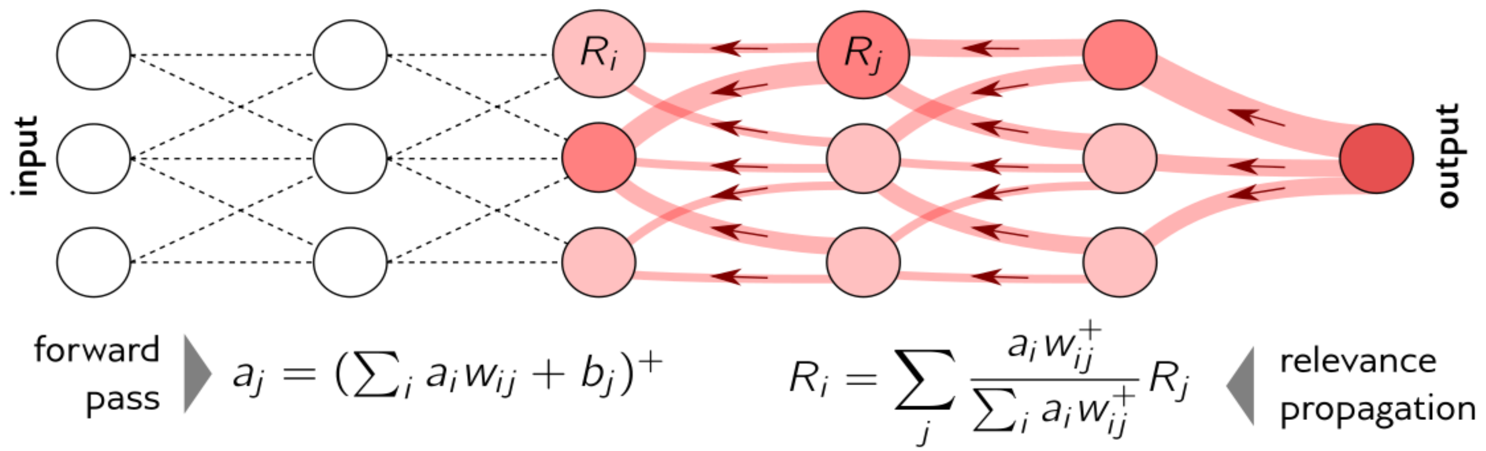








LRP works 4 all: deep models, LSTMs, kernel methods …



A Clarification on LRP

$$\text{LRP} \neq \text{Gradient} \times \text{Input}$$

… except for special cases. LRP was developed among others because gradient-based methods aren't satisfying.

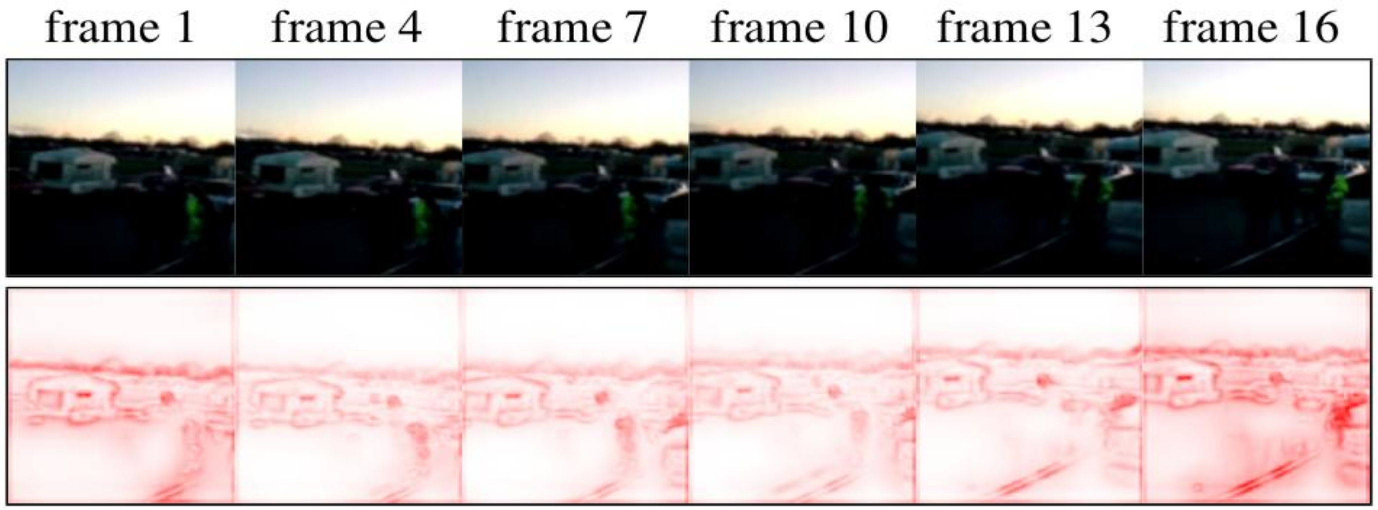
When comparing with LRP, please use appropriate LRP parameters (Like when comparing different ML techniques).

Good news: No need to reimplement LRP, check our software at www.heatmapping.org.

Explanations can be evaluated:
Pixel flipping (model agnostic)
And beyond LRP and DTD

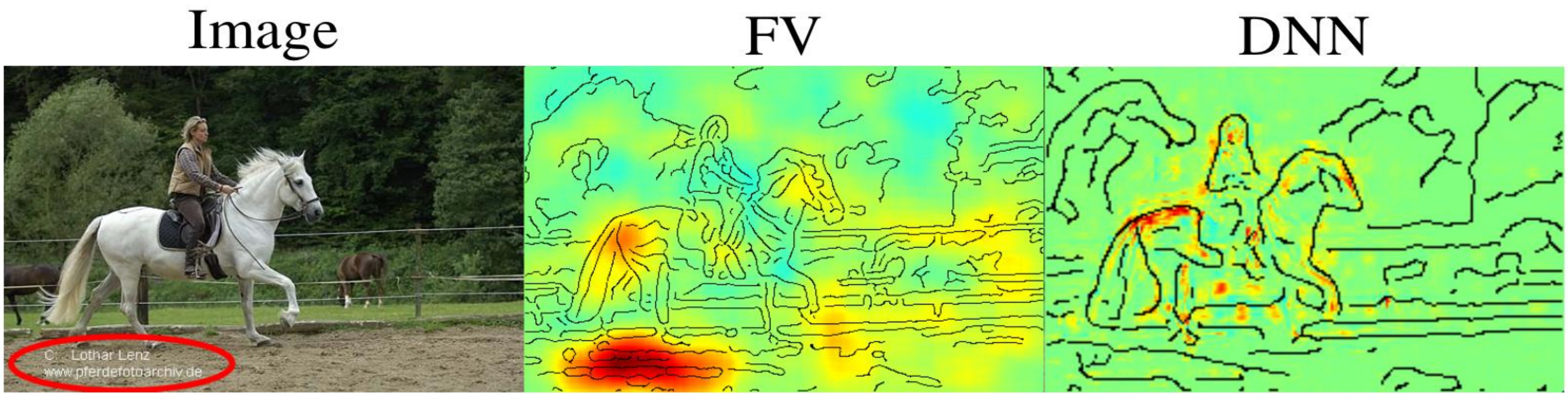
[Samek et al. IEEE TNNLS 2017]

Explanation helps to improve models



Explaining ML, Now What?

Explanation helps to find flaws in models



[Lapuschkin et al CVPR 2016]

Getting new Insights in the Sciences

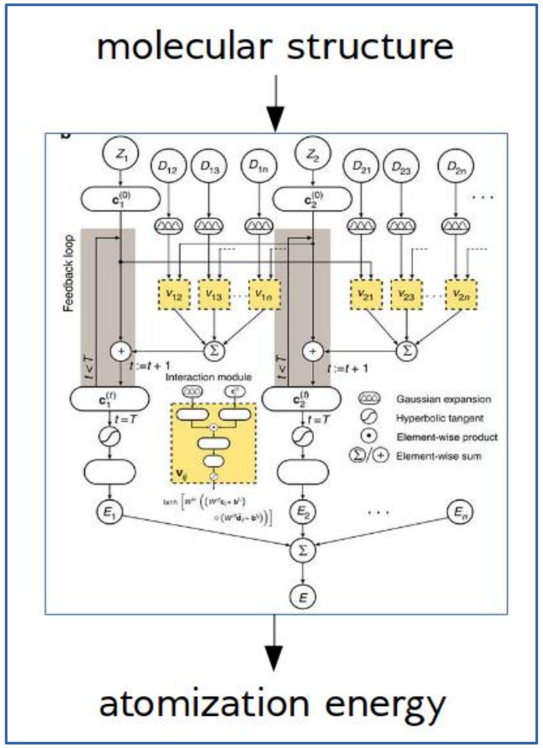
Example: Understanding physical systems at the quantum level.

time-independent
Schrödinger Equation

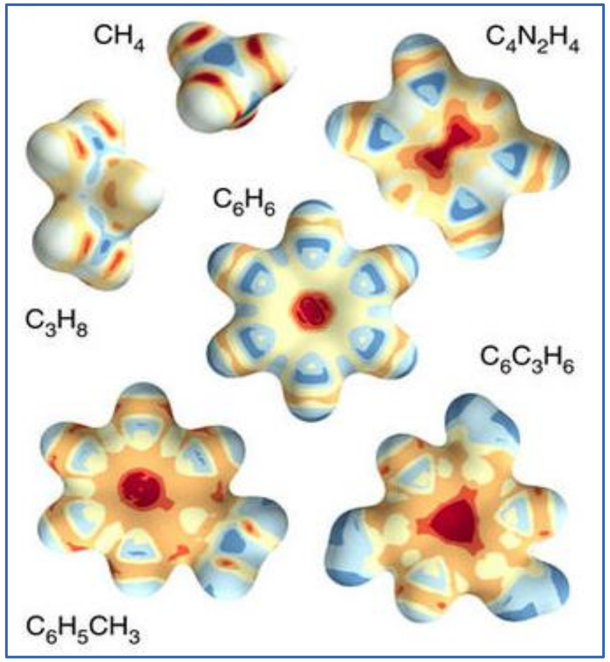
$$\hat{H}\Psi = E\Psi$$

Hamiltonian energy

equation describing
general physical systems



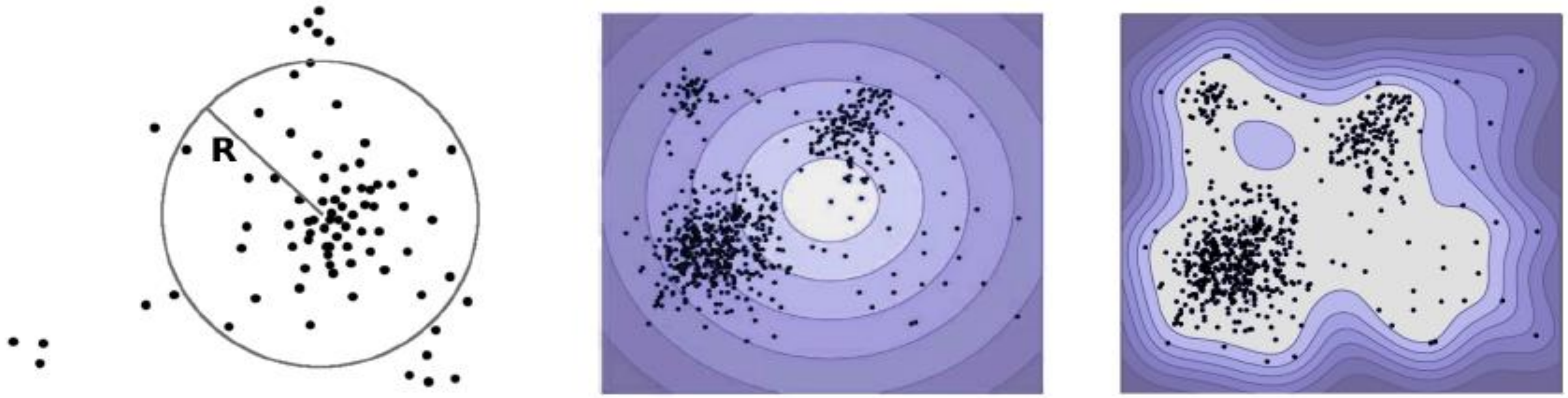
DNN approximation
for organic molecules



Interpretation of the trained
DNN model

[Schütt et al. Nat Comm. 2017, Schütt et al JCP 2018, Chmiela et al. Sci. Adv. 2017,…]

Support Vector Data description



Support Vector Data Description (SVDD)

- Compute minimal enclosing sphere with center $\mathbf{c}$ and radius R
- Anomaly score as the distance to center $\mathbf{c}$, that is $f(\mathbf{x}) = \|\phi(\mathbf{x}) - \mathbf{c}\|$
- Accept data point $\mathbf{x}$ if $f(\mathbf{x}) \leq R$ and ...

  ... reject $\mathbf{x}$ if $f(\mathbf{x}) > R$

Explaining one-class

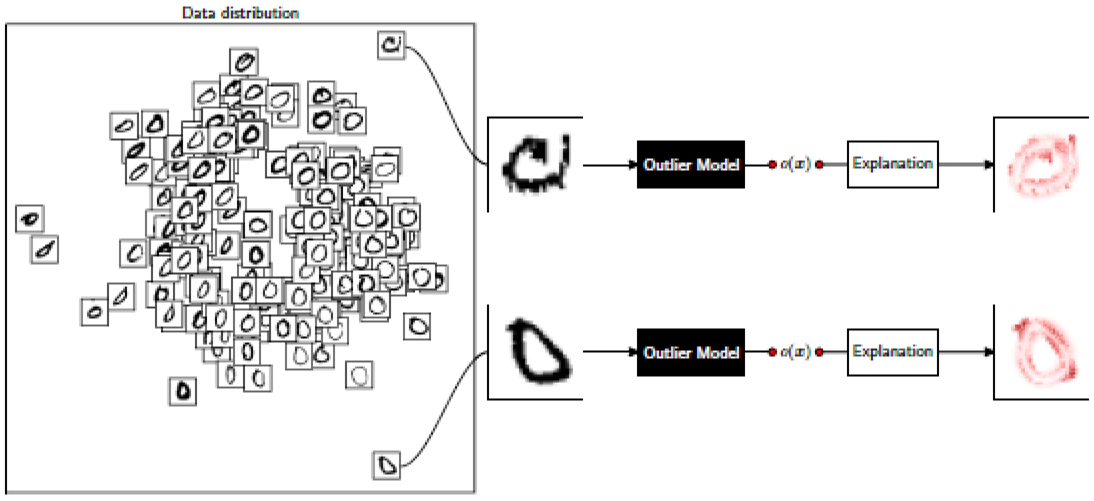


Figure 1: Illustration of the outlier detection and explanation setting. *Left:* Data is generated from an unknown distribution, we are for example interested in potential outliers; *Middle:* Unsupervised machine learning techniques estimate the data generating distribution and assign an outlier score $o(x)$ to unlikely data points; *Right:* Our explanation method assigns a relevance score to every input variable that reflects the contribution of input variable x_i to the model decision. We apply dithering to all heatmaps for printing reliability.

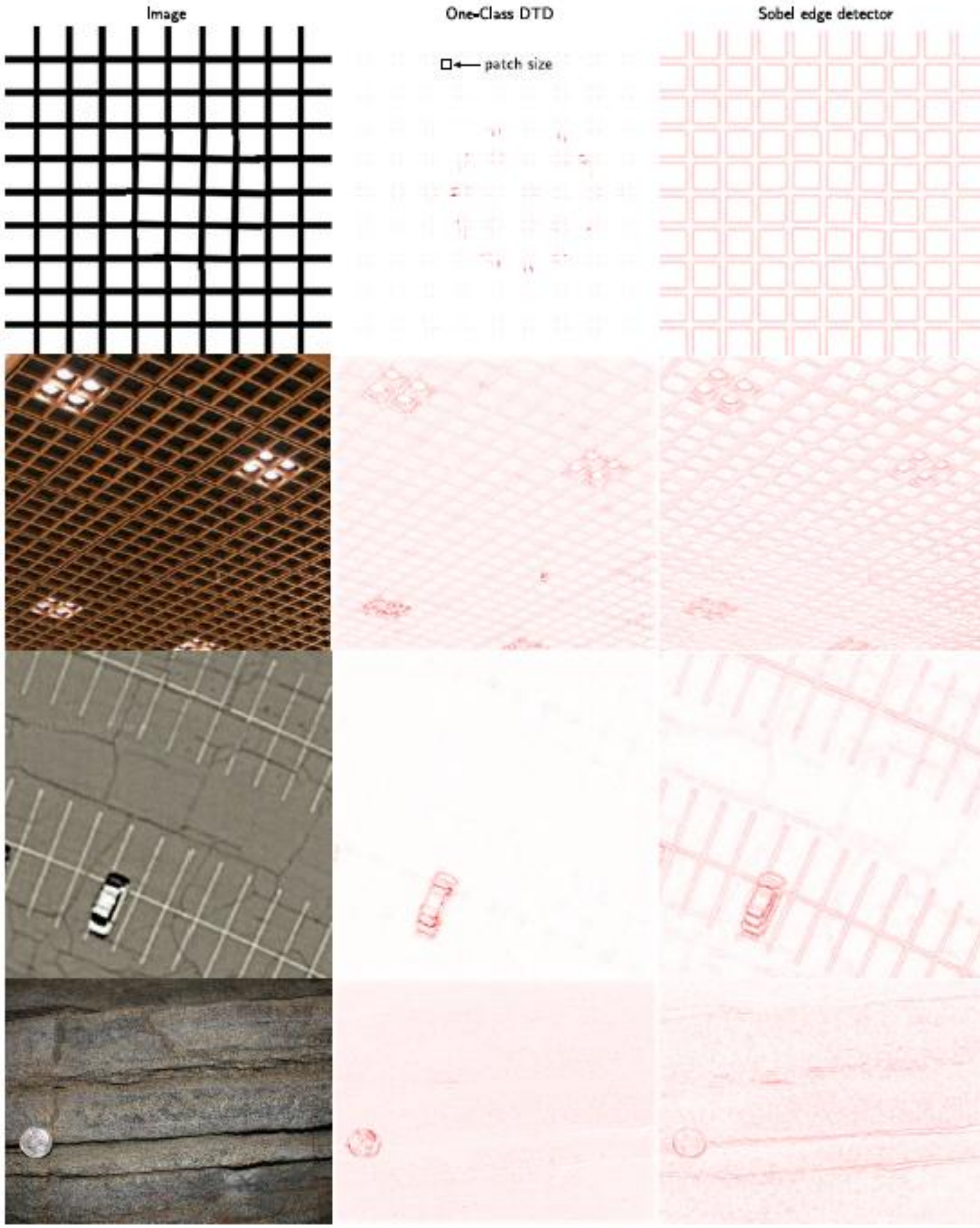


Figure 5: A One-Class SVM is trained on small 7×7 patches of the very image itself. Parameter $\nu = 0.1$ is set to allow at most 10% outliers. Images from a texture data set [11] (row one, two and four) and PatternNet [61]; top image is altered by us. For every image, we show *Left:* input image; *Middle* decomposition of one-class SVM; *Right* Sobel filter for reference. All images were resized to 256 pixels width.

[Kaufmann, Müller, Montavon 2018]

Semi-final Conclusion

- explaining & interpreting nonlinear models is essential
- orthogonal to improving DNNs and other models
- need for opening the blackbox …
- understanding nonlinear models is essential for Sciences & AI
- new theory: LRP is based on deep taylor expansion
- compare the right thing

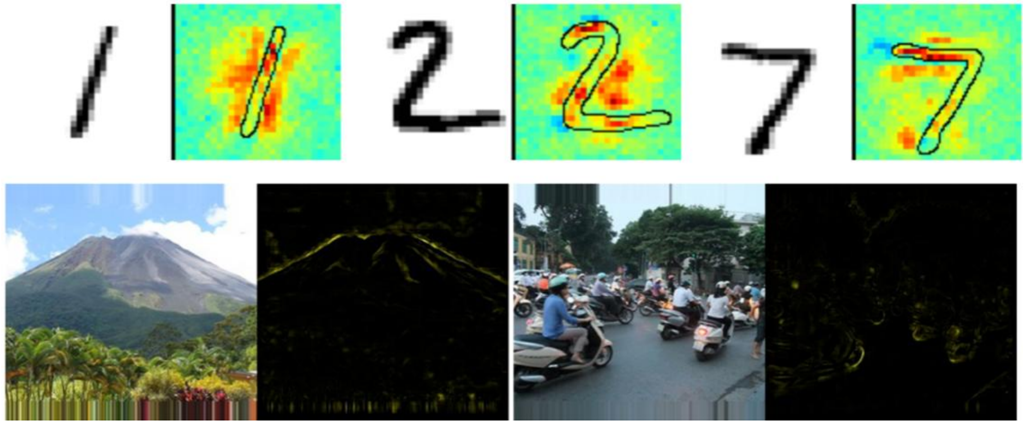
www.heatmapping.org

Thank you for your attention

Visit:

`http://www.heatmapping.org`

- Tutorials
- Software
- Online Demos

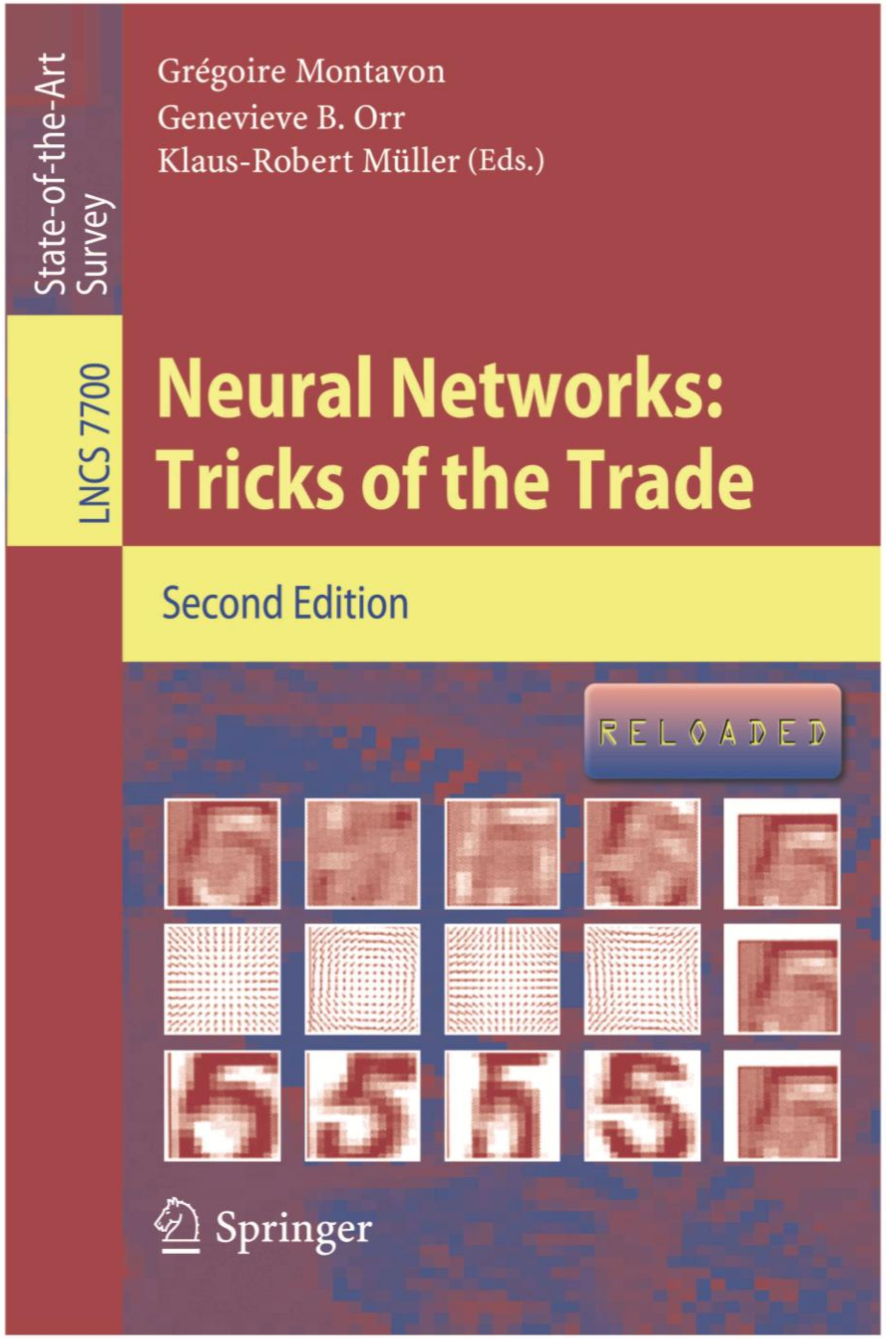


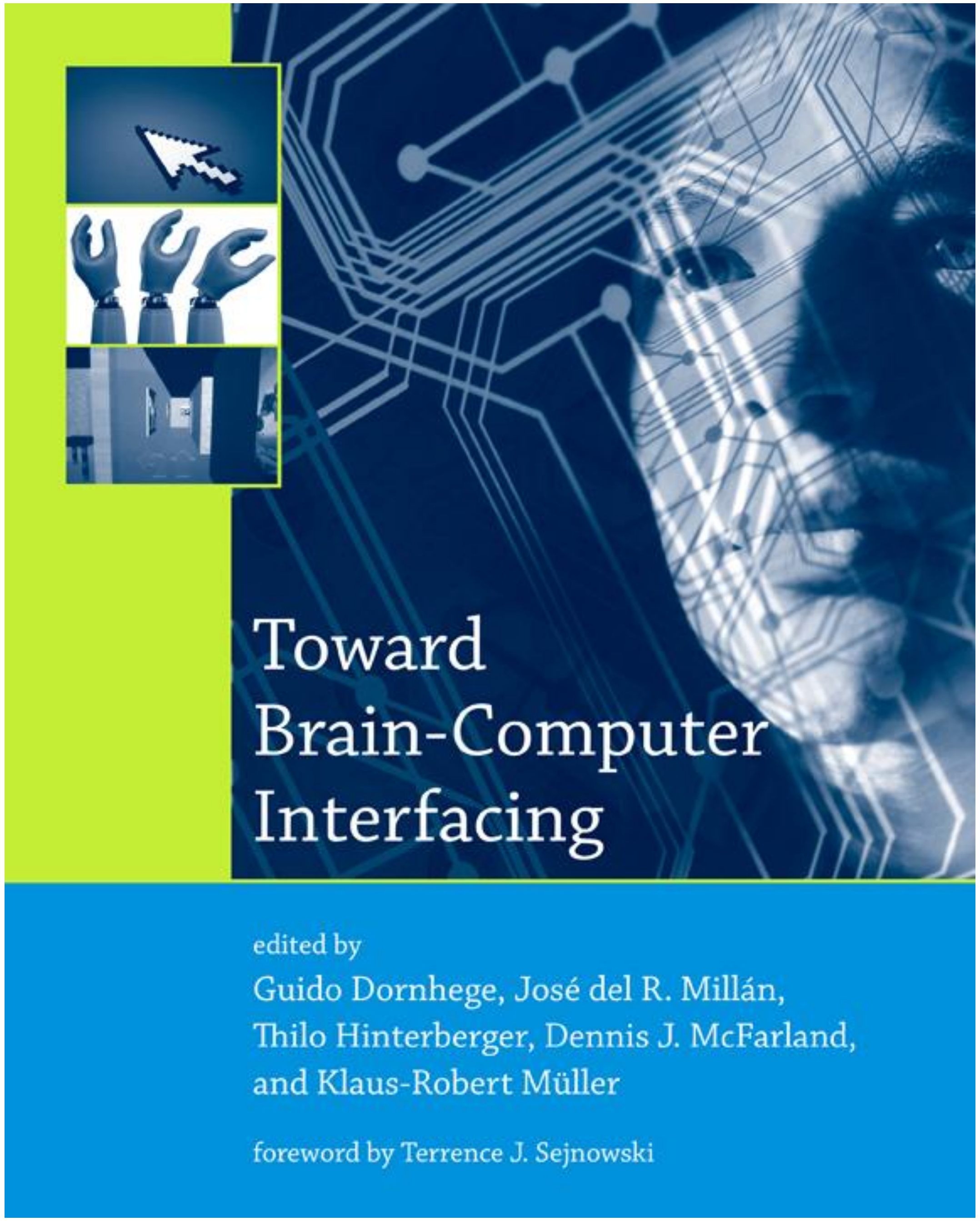
Tutorial Paper

Montavon et al., “Methods for interpreting and understanding deep neural networks”, Digital Signal Processing, 73:1-5, 2018

Keras Explanation Toolbox

https://github.com/albermax/innvestigate


State-of-the-Art Survey
LNCS 7700
Grégoire Montavon
Genevieve B. Orr
Klaus-Robert Müller (Eds.)
Neural Networks: Tricks of the Trade
Second Edition
RELOADED
Springer


Toward Brain-Computer Interfacing
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Thilo Hinterberger, Dennis J. McFarland,
and Klaus-Robert Müller
foreword by Terrence J. Sejnowski

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Further Reading I

Bach, S., Binder, A., Montavon, G., Klauschen, F., Müller, K. R., & Samek, W. (2015). On pixel-wise explanations for non-linear classifier decisions by layer-wise relevance propagation. PloS one, 10, e0130140 (7).

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