Neural Networks

Prof. Daniel R. Cassar

Ilum School of Science

Outline

Outline

Famous models based on Neural Networks

AlphaFold

AlphaGo

ChatGPT

Midjourney

DALL·E

STABLE DIFFUSION

Claude

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Study material

See https://github.com/drcassar/bam2024

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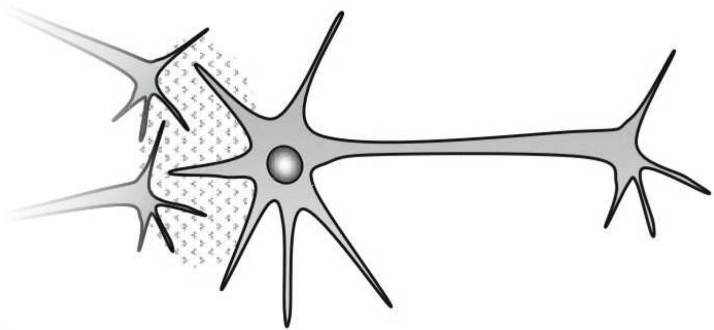
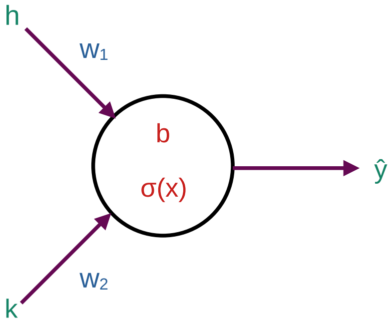
Neurons and synapses



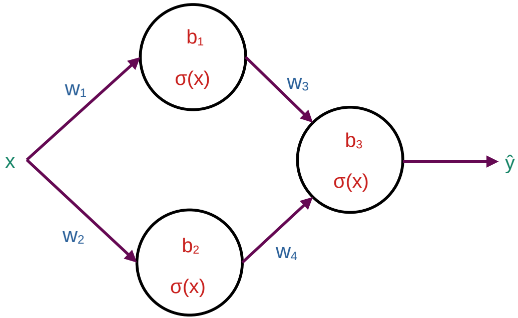
da Silva, I.N., Hernane Spatti, D., Andrade Flauzino, R., Liboni, L.H.B., and dos Reis Alves, S.F. (2017). Artificial neural networks: a practical course

Artificial neurons and artificial synapses (Perceptron)



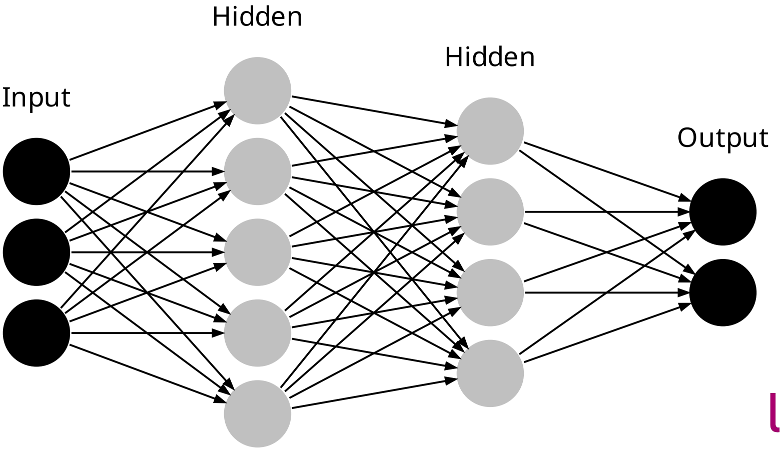
$$\hat{y} = \sigma\left(hw_1 + kw_2 + b\right)$$

Artificial neurons in series and in parallel



$$\hat{y} = \sigma\Big(\sigma\big(xw_1 + b_1\big) \cdot w_3 + \sigma\big(xw_2 + b_2\big) \cdot w_4 + b_3\Big)$$

Multilayer Perceptron Neural Networks



Outline

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GlassNet — multitask deep learning model

Composition (input): $2\,SiO_2 \cdot CaO \cdot MgO$

$T_0 = 1702\,\mathrm{K}$
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Building GlassNet: data pipeline

Query:

- SciGlass database
- 85 properties
- Minor chemical filtering (H to Bi)

Before deduplication:

- $\sim$ 280 000 entries

After deduplication:

- $\sim$ 220 000 entries (10% reserved for testing!)

https://github.com/epam/SciGlass

Feature engineering — physicochemical elemental properties

- Atomic number
- Atomic radius*
- Atomic volume
- Atomic weight
- BCC lattice parameter+
- Bandgap energy+
- Boiling point
- Covalent radius
- C_6 coefficient
- Density
- Dipole polarizability
- Effective nuclear charge
- Electron affinity
- Electronegativity*
- Energy per atom+
- Energy to remove the first electron
- FCC lattice parameter+
- Fusion enthalpy
- Glawe's number
- Heat of formation
- Magnetic moment+
- Mass number of the most abundant isotope
- Maximum ionization energy
- Melting point
- Mendeleev's number
- Number of electrons
- Number of filled d valence orbitals
- Number of filled f valence orbitals
- Number of filled p valence orbitals
- Number of filled s valence orbitals
- Number of neutrons
- Number of oxidation states
- Number of protons
- Number of unfilled d valence orbitals
- Number of unfilled f valence orbitals
- Number of unfilled p valence orbitals
- Number of unfilled s valence orbitals
- Number of unfilled valence orbitals
- Number of valence electrons
- Pettifor's number
- Single-bond covalent radius
- Van der Walls radius*
- Volume per atom+

Mendeleev: `https://mendeleev.readthedocs.io`
Magpie data: Ward, L. et al. (2016). Npj Computational Materials 2, 16028.

Feature engineering

Composition: SiO_2
Property: atomic number
Element order: $\begin{bmatrix} \mathrm{H} & \mathrm{O} & \mathrm{Na} & \mathrm{Si} \end{bmatrix}$

$$\boldsymbol{C} = \begin{bmatrix} 0 & 0.67 & 0 & 0.33 \end{bmatrix}$$

$$\boldsymbol{S} = \begin{bmatrix} 1 & 8 & 11 & 14 \end{bmatrix}$$

Feature engineering

Composition: SiO_2
Property: atomic number
Element order: $\begin{bmatrix} \mathrm{H} & \mathrm{O} & \mathrm{Na} & \mathrm{Si} \end{bmatrix}$

$$\boldsymbol{C} = \begin{bmatrix} 0 & 0.67 & 0 & 0.33 \end{bmatrix}$$

$$\boldsymbol{S} = \begin{bmatrix} 1 & 8 & 11 & 14 \end{bmatrix}$$

$$\boldsymbol{C} \circ \boldsymbol{S} = \begin{bmatrix} 0 & 5.36 & 0 & 4.62 \end{bmatrix}$$

$\circ$: Hadamard product

Feature engineering

Composition: SiO_2
Property: atomic number
Element order: $\begin{bmatrix} \mathrm{H} & \mathrm{O} & \mathrm{Na} & \mathrm{Si} \end{bmatrix}$

$$\boldsymbol{C} = \begin{bmatrix} 0 & 0.67 & 0 & 0.33 \end{bmatrix}$$
$$\boldsymbol{S} = \begin{bmatrix} 1 & 8 & 11 & 14 \end{bmatrix}$$

$$\boldsymbol{C} \circ \boldsymbol{S} = \begin{bmatrix} 0 & 5.36 & 0 & 4.62 \end{bmatrix}$$

$$\mathrm{mean}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 4.99$$
$$\max\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 5.36$$
$$\min\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 4.62$$
$$\mathrm{sum}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 9.98$$
$$\mathrm{std}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 0.37$$

$\circ$: Hadamard product
Calculations disregard the zero-valued elements of $(\boldsymbol{C} \circ \boldsymbol{S})$

Feature engineering

Composition: $Na_2O \cdot SiO_2$
Property: atomic number
Element order: $\begin{bmatrix} \mathrm{H} & \mathrm{O} & \mathrm{Na} & \mathrm{Si} \end{bmatrix}$

$$\boldsymbol{C} = \begin{bmatrix} 0 & 0.5 & 0.33 & 0.17 \end{bmatrix}$$
$$\boldsymbol{S} = \begin{bmatrix} 1 & 8 & 11 & 14 \end{bmatrix}$$

$$\boldsymbol{C} \circ \boldsymbol{S} = \begin{bmatrix} 0 & 4 & 3.63 & 2.38 \end{bmatrix}$$

$$\mathrm{mean}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 3.34$$
$$\max\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 4$$
$$\min\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 2.38$$
$$\mathrm{sum}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 10.01$$
$$\mathrm{std}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 0.69$$

$\circ$: Hadamard product
Calculations disregard the zero-valued elements of $(\boldsymbol{C} \circ \boldsymbol{S})$

Feature engineering — features for clustering

Composition: $Na_2O \cdot SiO_2$
Property: atomic number
Element order: $\begin{bmatrix} \mathrm{H} & \mathrm{O} & \mathrm{Na} & \mathrm{Si} \end{bmatrix}$

$$\boldsymbol{C} = \begin{bmatrix} 0 & 0.5 & 0.33 & 0.17 \end{bmatrix}$$

$$\lceil \boldsymbol{C} \rceil = \begin{bmatrix} 0 & 1 & 1 & 1 \end{bmatrix}$$

$$\boldsymbol{S} = \begin{bmatrix} 1 & 8 & 11 & 14 \end{bmatrix}$$

Feature engineering — features for clustering

Composition: $Na_2O \cdot SiO_2$
Property: atomic number
Element order: $\begin{bmatrix} \mathrm{H} & \mathrm{O} & \mathrm{Na} & \mathrm{Si} \end{bmatrix}$

$$\boldsymbol{C} = \begin{bmatrix} 0 & 0.5 & 0.33 & 0.17 \end{bmatrix}$$

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$$\mathrm{mean}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 11$$

$$\max\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 14$$

$$\min\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 8$$

$$\mathrm{sum}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 33$$

$$\mathrm{std}\left(\boldsymbol{C} \circ \boldsymbol{S}\right) = 2.45$$

Feature engineering — features for clustering

Composition: $Na_2O \cdot 2\,SiO_2$
Property: atomic number
Element order: $\begin{bmatrix} \mathrm{H} & \mathrm{O} & \mathrm{Na} & \mathrm{Si} \end{bmatrix}$

$$\boldsymbol{C} = \begin{bmatrix} 0 & 0.56 & 0.22 & 0.22 \end{bmatrix}$$
$$\lceil \boldsymbol{C} \rceil = \begin{bmatrix} 0 & 1 & 1 & 1 \end{bmatrix}$$
$$\boldsymbol{S} = \begin{bmatrix} 1 & 8 & 11 & 14 \end{bmatrix}$$

$$\lceil \boldsymbol{C} \rceil \circ \boldsymbol{S} = \begin{bmatrix} 0 & 8 & 11 & 14 \end{bmatrix}$$

$$\operatorname{mean}(\boldsymbol{C} \circ \boldsymbol{S}) = 11$$
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Feature engineering — feature selection

Starting point:

elemental fraction (composition)	77
regression physicochemical properties	275
clustering physicochemical properties	275
TOTAL	627

Feature engineering — feature selection

Starting point:

elemental fraction (composition)	77
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TOTAL	627

After Variance Inflation Factor (VIF) selection:

elemental fraction (composition)	64
regression physicochemical properties	12
clustering physicochemical properties	22
TOTAL	98

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GlassNet: the pipeline

Multitask learning:

- Chemical composition $\rightarrow$ 98 features $\rightarrow$ Neural network $\rightarrow$ 85 properties

Note:

- Not limited to oxide glasses

Finding a reasonable neural network architecture (NP-hard)

- Hyperparameter tuning
  - Two runs testing 1000 different architectures
  - Tree-structured Parzen Estimator search
  - With Asynchronous Successive Halving Algorithm (ASHA)
- Cross-validation
  - 10-fold cross-validation
- Training the final model

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Li, L. et al. (2020). A System for Massively Parallel Hyperparameter Tuning. (arXiv)
Bergstra, J., Yamins, D., and Cox, D. (2013). In International Conference on Machine Learning (ICML 2013).

GlassNet — new multitask deep learning model

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Property groups

1. Viscosity
2. Optical properties
3. Dielectric properties
4. Electrical properties
5. Mechanical properties
6. Thermal properties
8. Density
9. Crystallization
10. Liquidus temperature
11. Surface tension
12. Thermal shock resistance

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Was the multitasking approach beneficial?

Yes and no!

- Better results for 24 properties measured in different conditions
- No statistical difference for 29
- Worse results for 24 properties measured in only one condition with more than 10k data points

- Solution: hybrid model (multitask + single-task)

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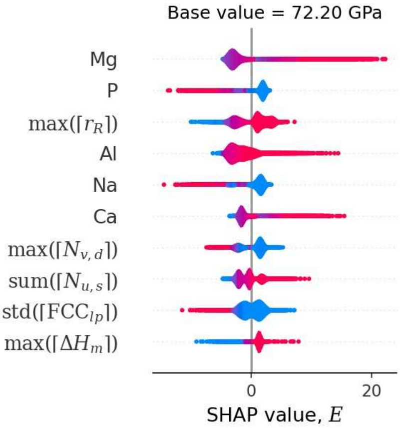
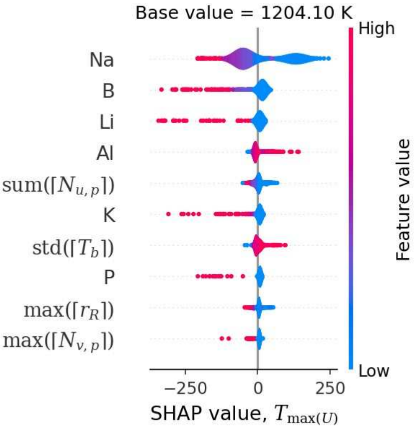
Opening the black-box with SHAP





https://github.com/slundberg/shap
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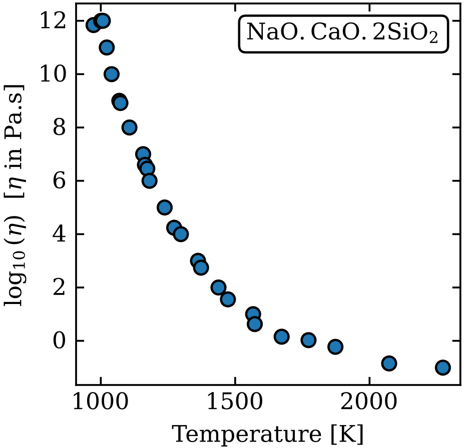
Most important features for glass design (SHAP analysis)

Viscosity	Optical	Mechanical	Crystallization
B	Pb	$N_{u,s}$	$N_{f,p}$
Na	N_u	Na	$N_{u,p}$
Al	Bi	ΔH_m	ΔH_m
K	$N_{f,d}$	FCC_{lp}	B
Li	$N_{f,p}$	P	Na
Pb	Ti	Mg	Se
$N_{f,s}$	Nb	Ca	S
Ca	$N_{f,f}$	r_R	Te
ΔH_m	La	$N_{f,d}$	T_b
P	Ge	Al	V

Building on top of GlassNet: Viscosity prediction



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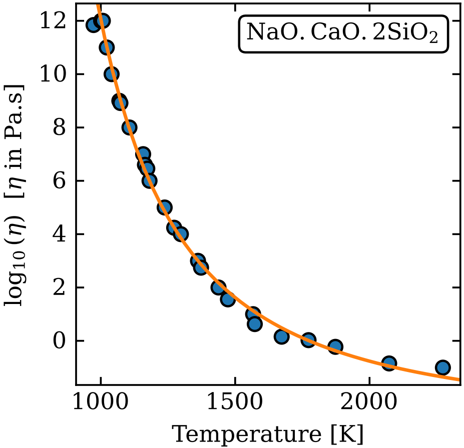

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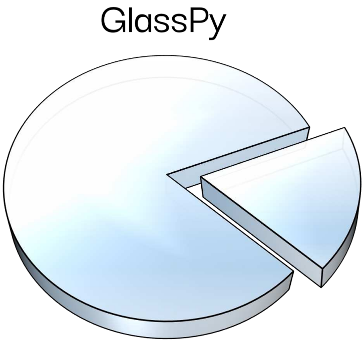
Open Science

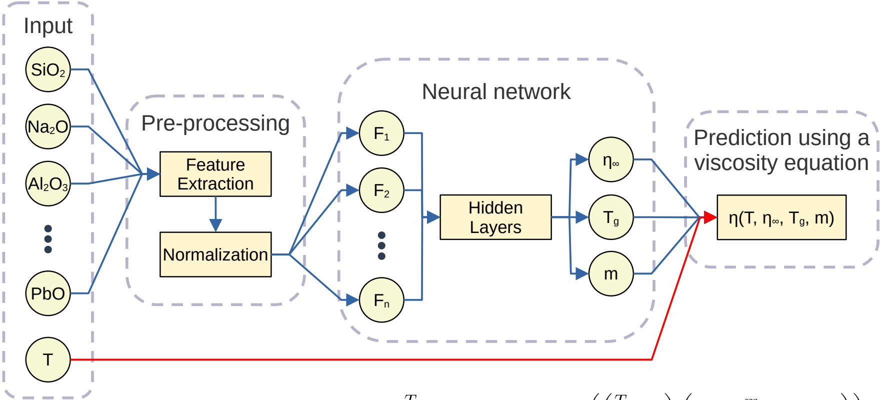


- Python module
- Free and open source
- Ready-to-use GlassNet
- SciGlass data as a pandas DataFrame

`https://github.com/drcassar/glasspy` (GPLv3 license)
`https://glasspy.readthedocs.io/` (documentation)

Outline

ViscNet — physics-informed neural network



$$\log_{10}\left(\eta\left(T,\eta_\infty,T_g,m\right)\right)=\log_{10}\left(\eta_\infty\right)+\frac{T_g}{T}\left(12-\log_{10}\left(\eta_\infty\right)\right)\exp\left(\left(\frac{T_g}{T}-1\right)\left(\frac{m}{12-\log_{10}\left(\eta_\infty\right)}-1\right)\right)$$

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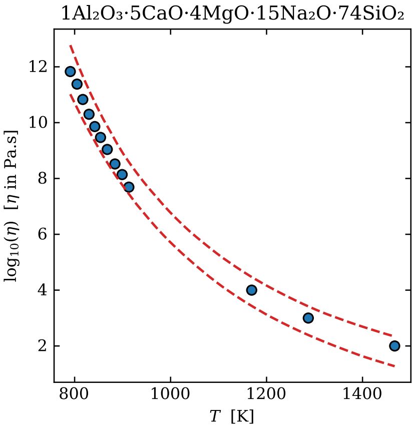
ViscNet — prediction and extrapolation



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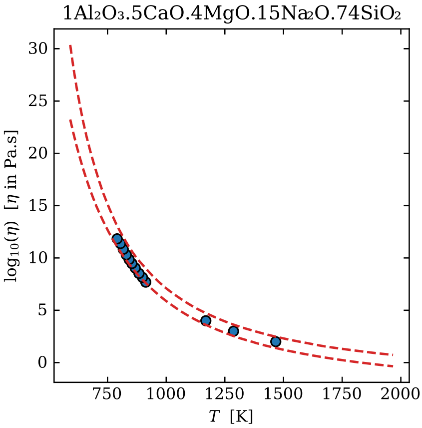
ViscNet — prediction and extrapolation



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Outline

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Acknowledgments

BAM
Bundesanstalt für Materialforschung und -prüfung

INCT/CNPq
MATERIALS INFORMATICS

CNPq
Conselho Nacional de Desenvolvimento Científico e Tecnológico

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CNPEM

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