UNIVERSITY OF CAMBRIDGE

The modern day blacksmith

Gareth Conduit

Theory of Condensed Matter group

Neural network algorithm to

Train from sparse datasets

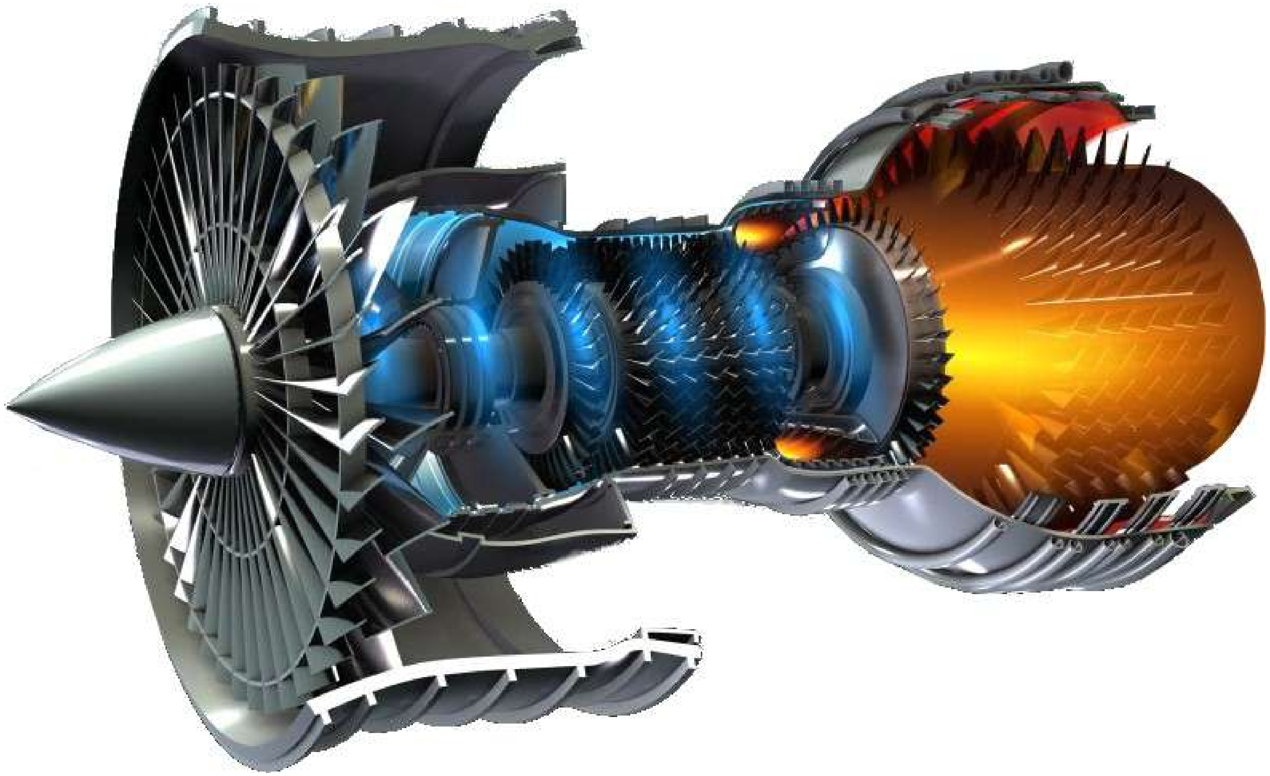
Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

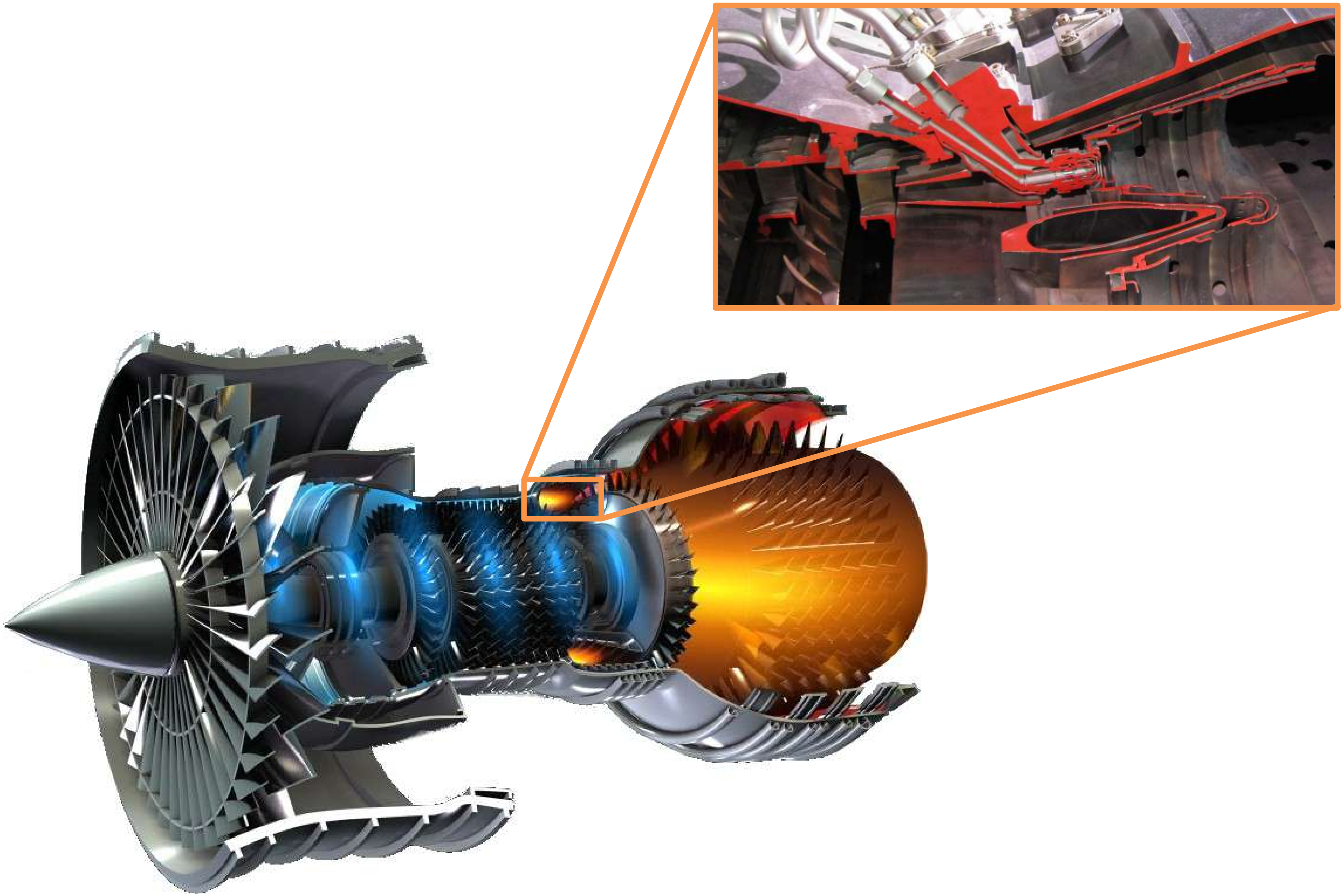
Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

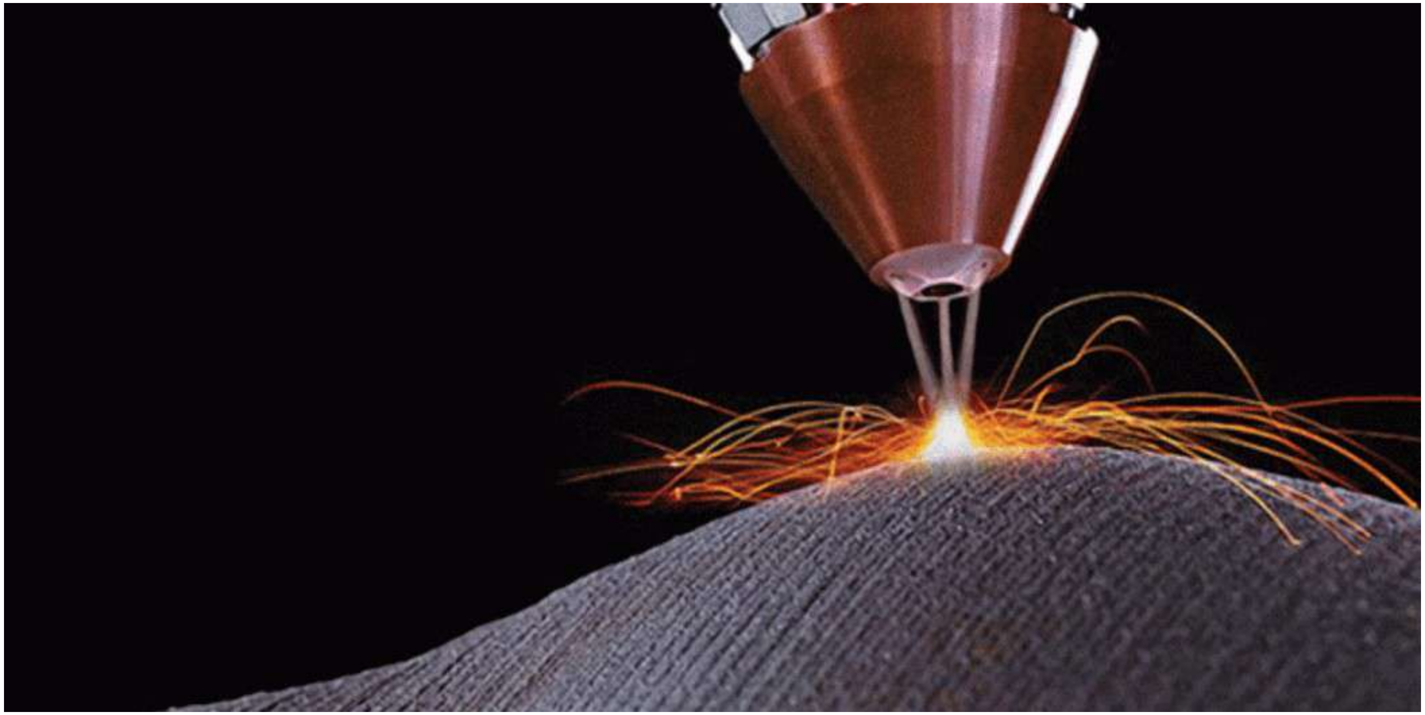
Schematic of a jet engine



Combustor in a jet engine

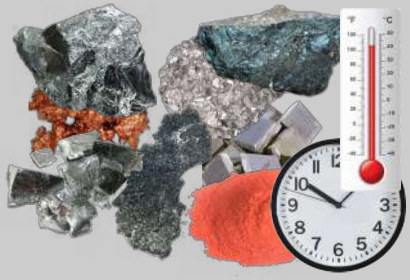


Direct laser deposition requires new alloys



Neural networks for materials design

Composition



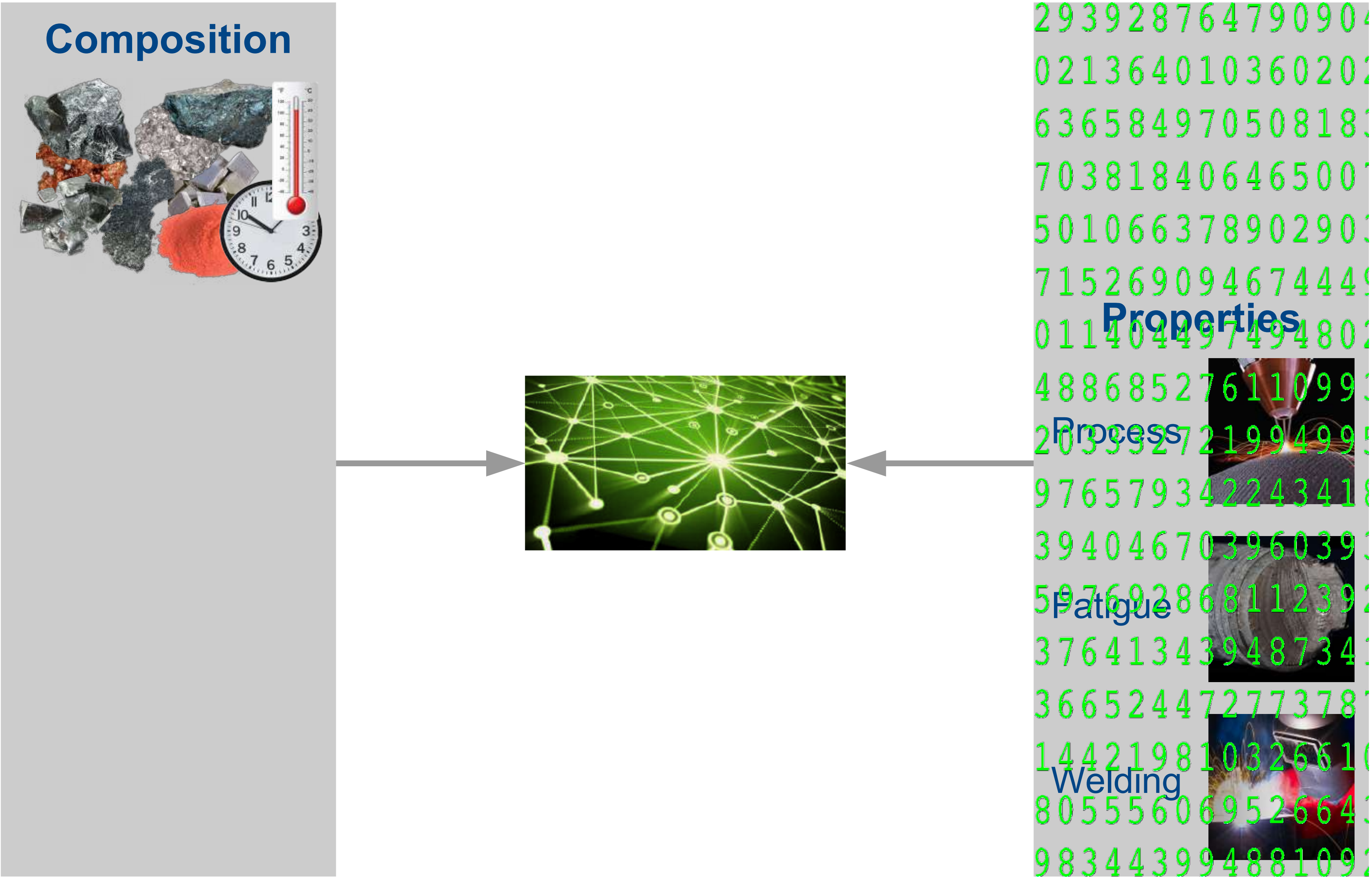
Properties

Process

Fatigue

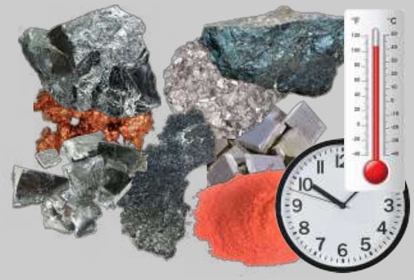
Welding

Neural networks for materials design



Neural networks for materials design

Composition



Properties

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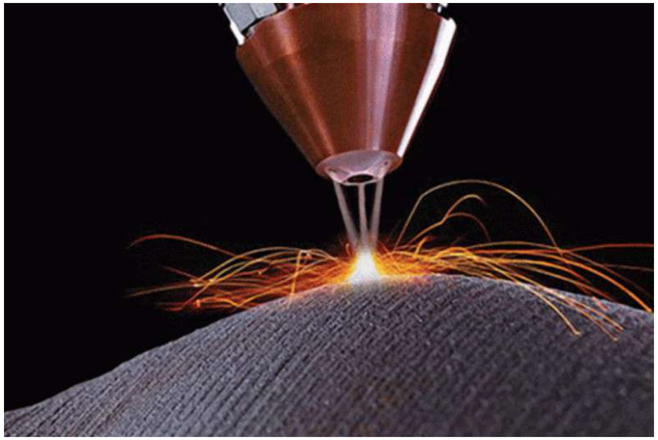
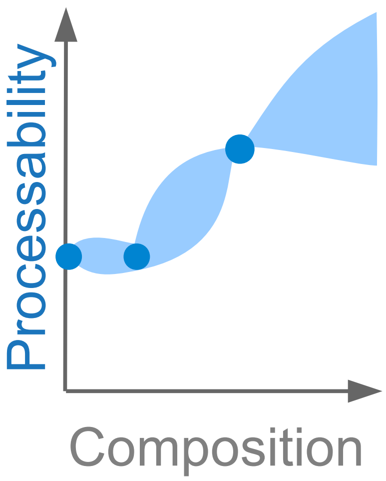


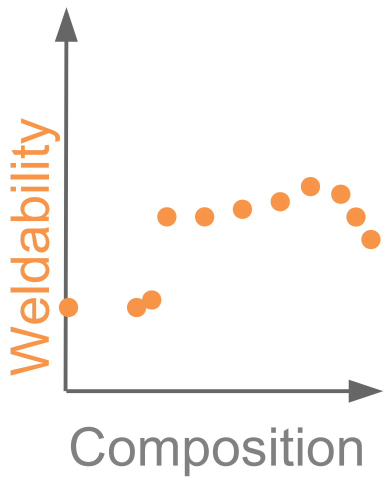
Laser

Electricity

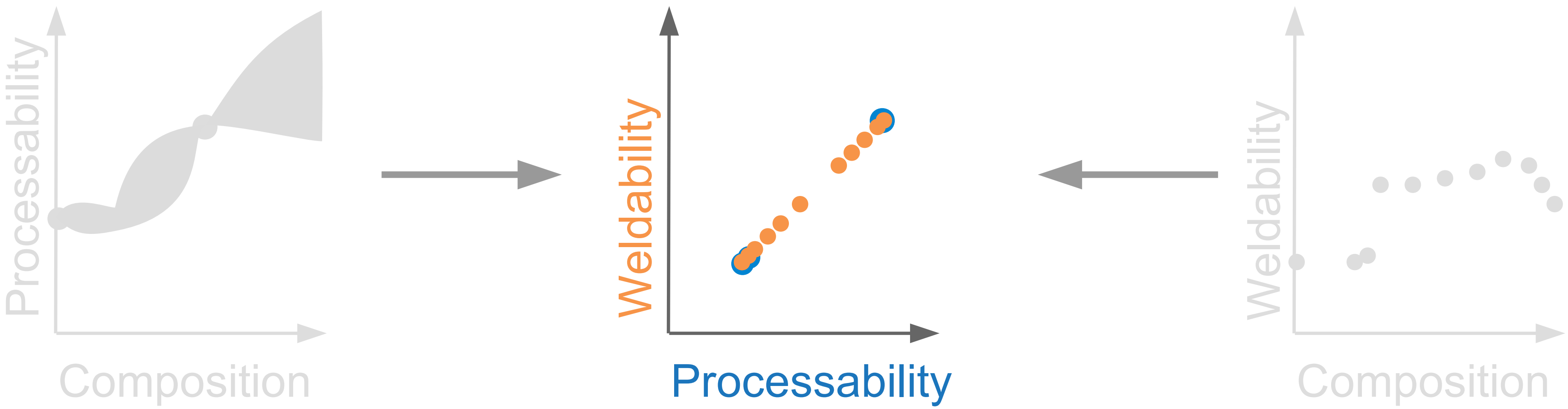
Insufficient data for processability



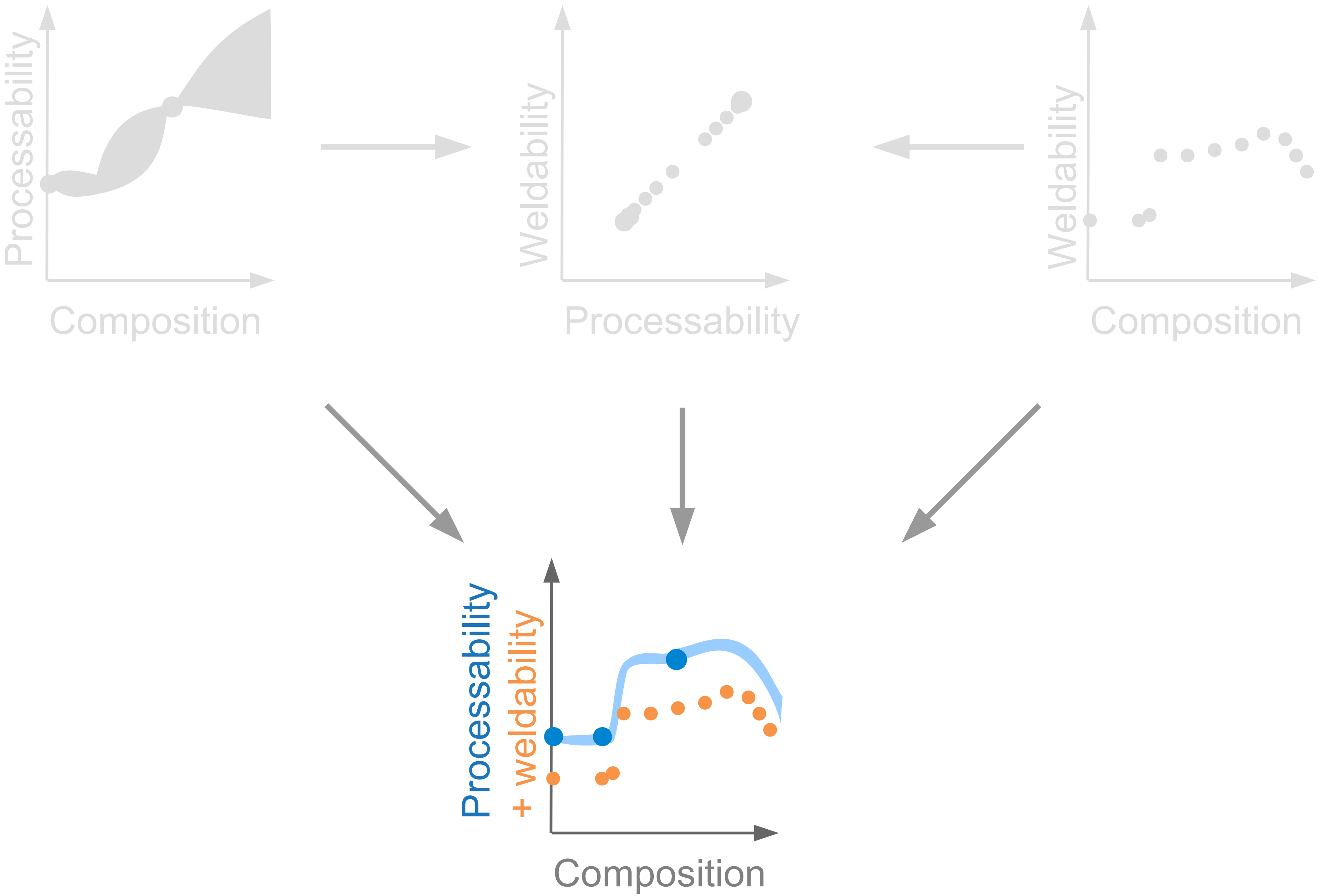
Welding is analogous to direct laser deposition



Simple processability-welding relationship

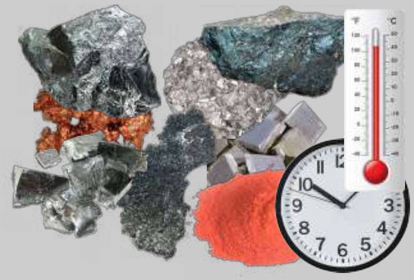


Merging properties with the neural network



Neural networks for materials design

Composition



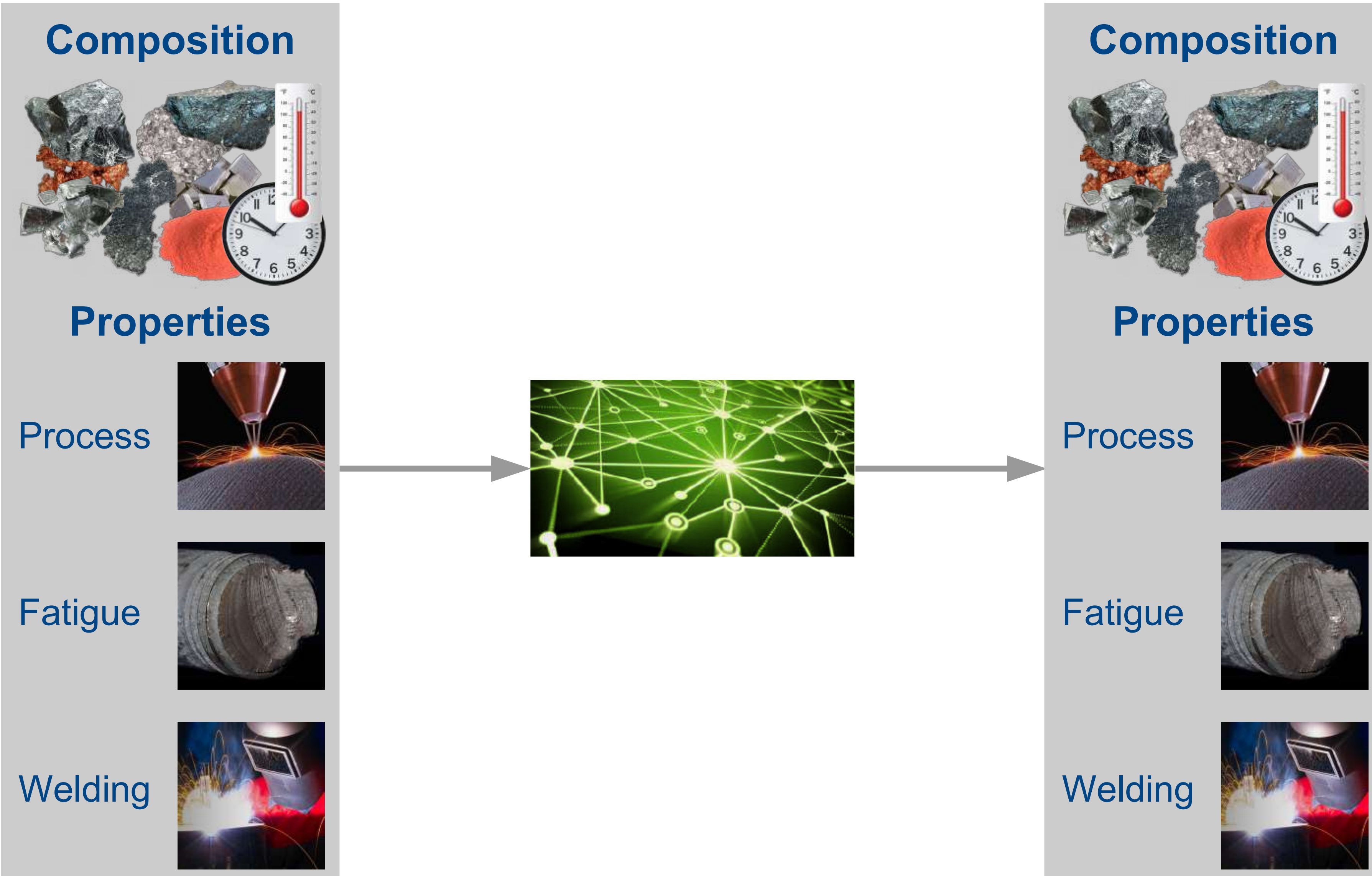
Properties

Process

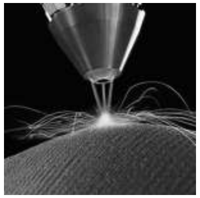
Fatigue

Welding

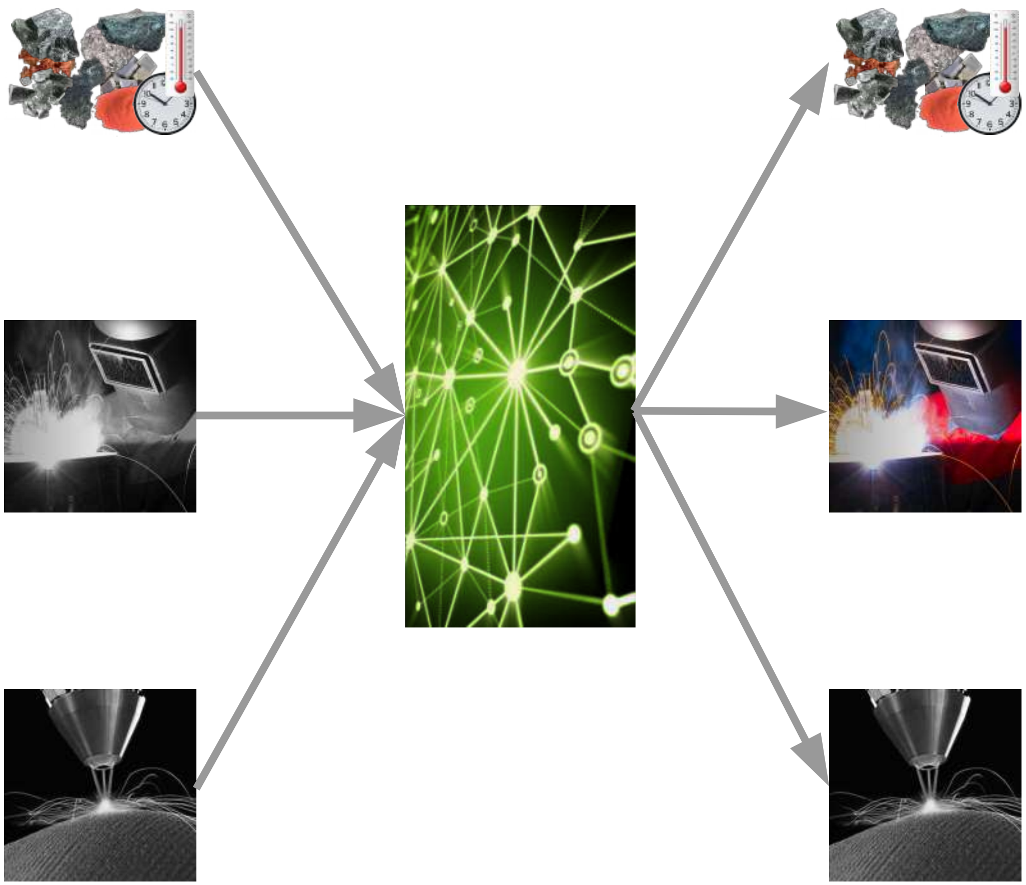
Neural networks for materials design



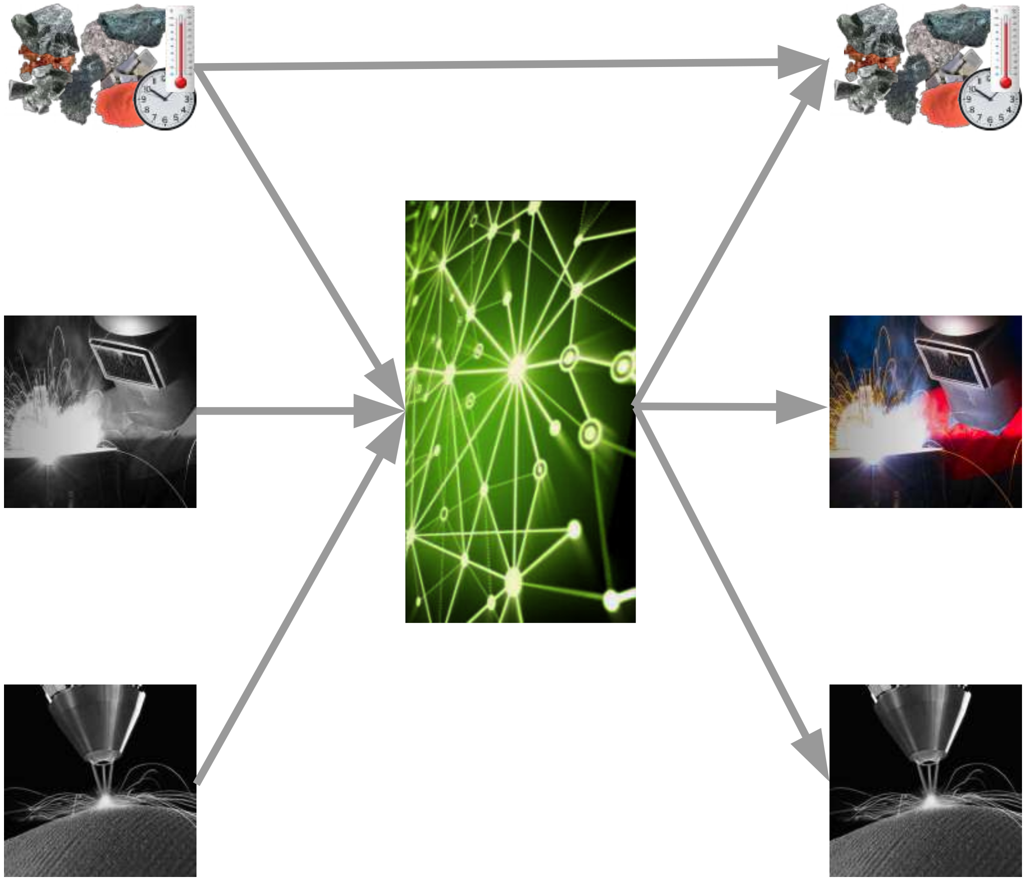
Filling in missing values



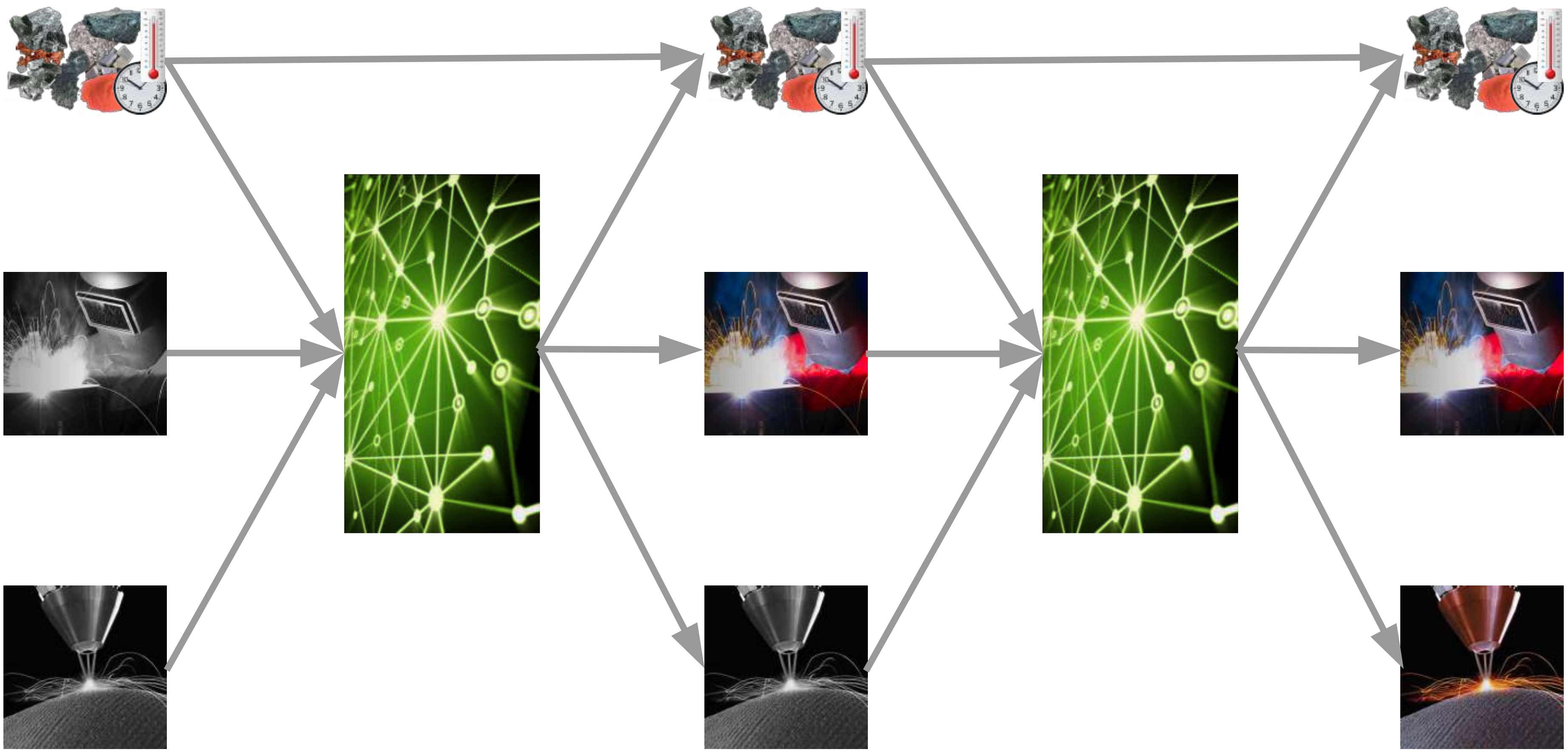
Filling in missing values



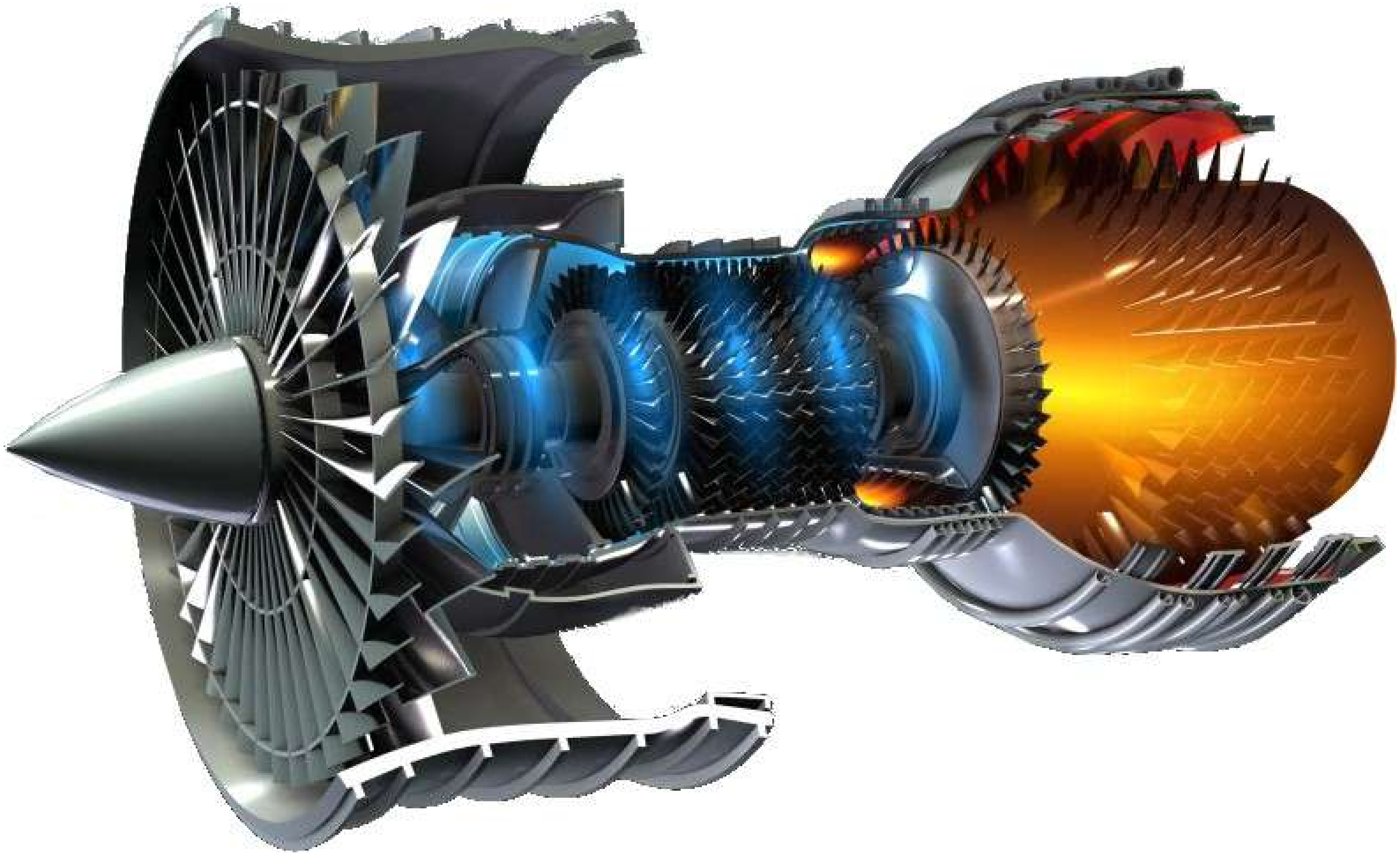
Pass through present value



Second pass to fill in missing values



Schematic of a jet engine



Target properties

Elemental cost	< 25 $\$kg^{-1}$
Density	< 8500 kgm^{-3}
γ’ content	< 25 wt%
Oxidation resistance	< 0.3 $mgcm^{-2}$
Processability	< 0.15% defects
Phase stability	> 99.0 wt%
γ’ solvus	> 1000˚C
Thermal resistance	> 0.04 $K\Omega^{-1}m^{-3}$
Yield stress at 900˚C	> 200 MPa
Tensile strength at 900˚C	> 300 MPa
Tensile elongation at 700˚C	> 8%
1000hr stress rupture at 800˚C	> 100 MPa
Fatigue life at 500 MPa, 700˚C	> 10^5 cycles

Composition

Cr: 19%

Co: 4%

Mo: 4.9%

W: 1.2%

Zr: 0.05%

Nb: 3%

Al: 2.9%

C: 0.04%

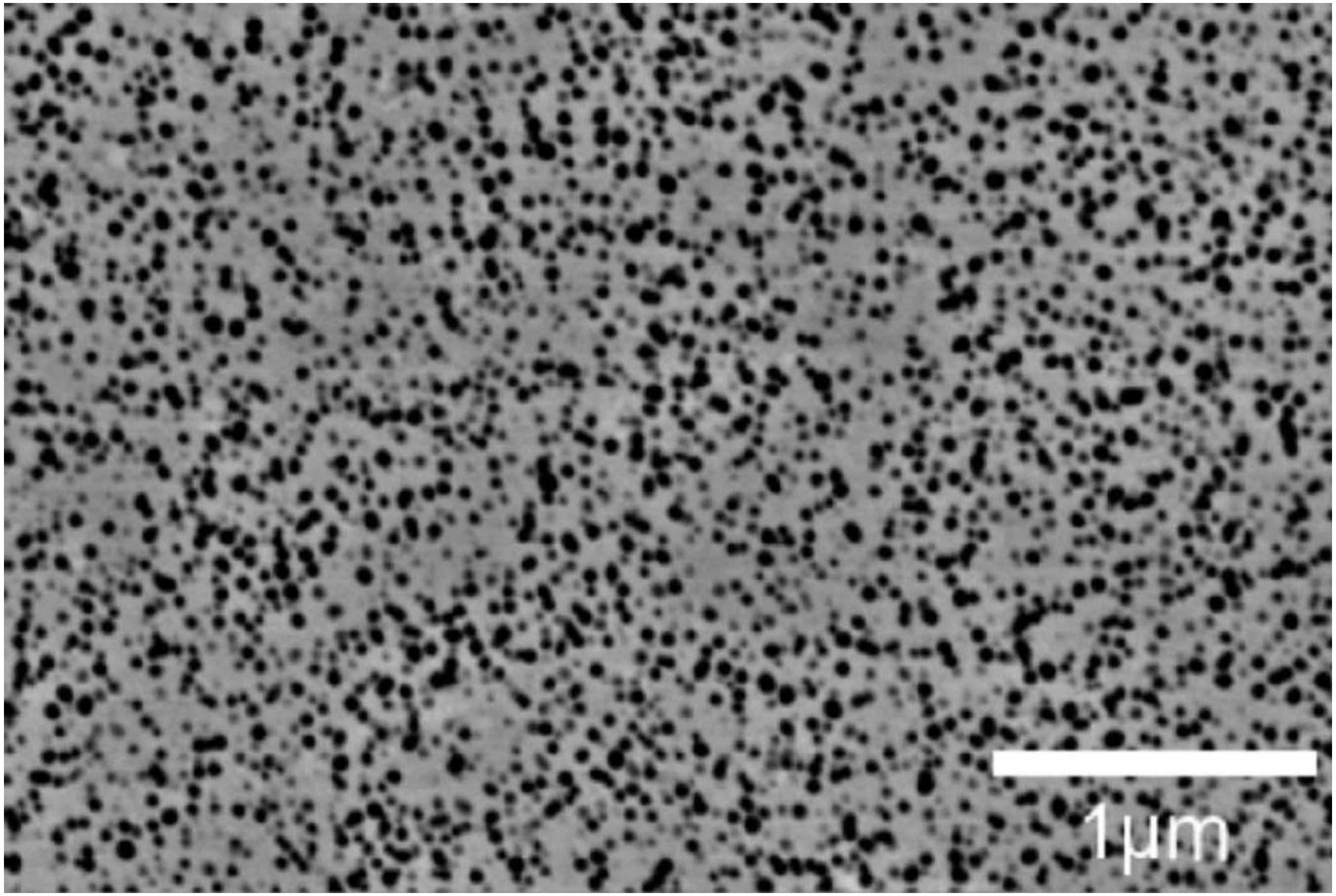
B: 0.01%

Ni

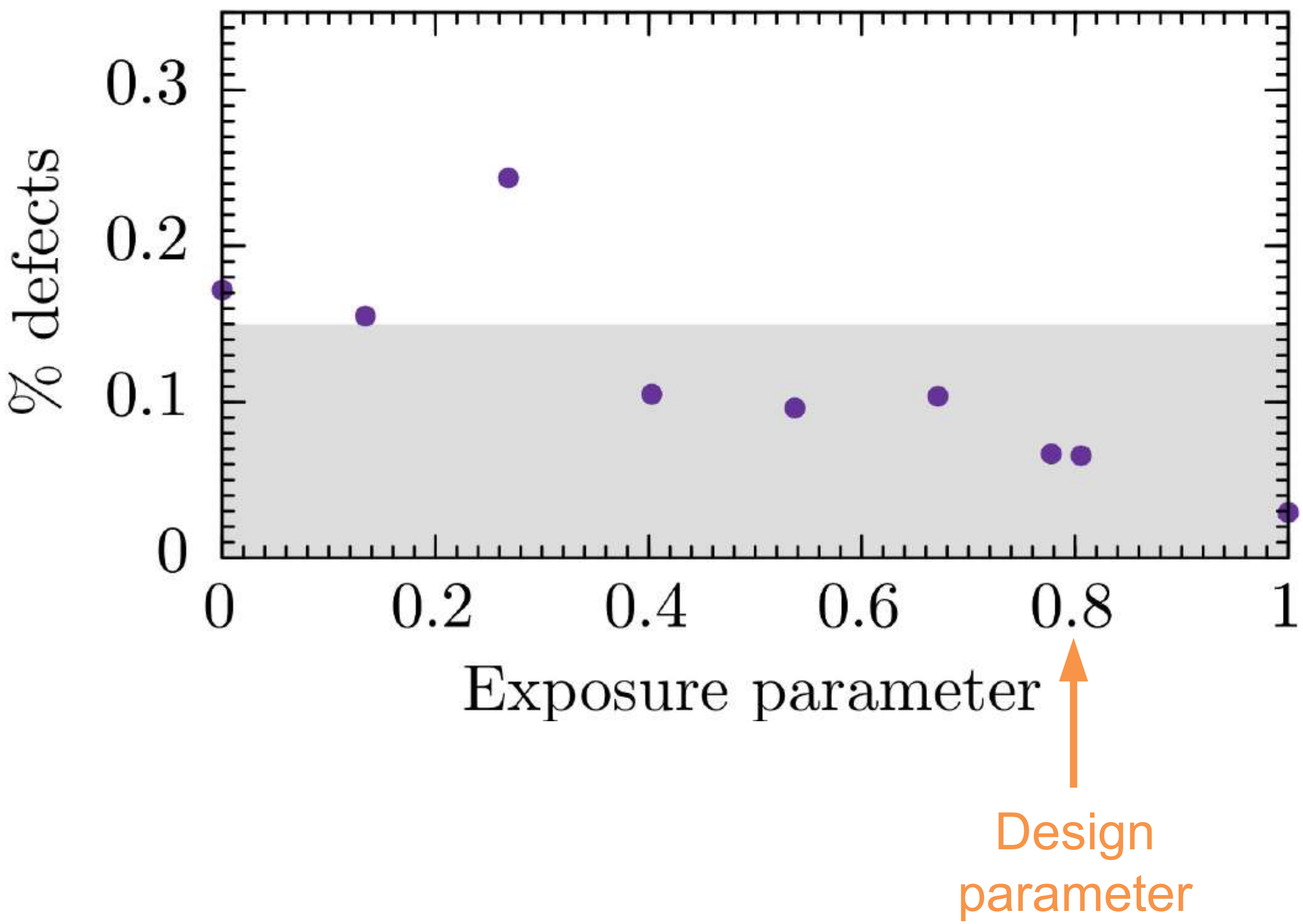
Expose 0.8

T_{HT} 1300ºC

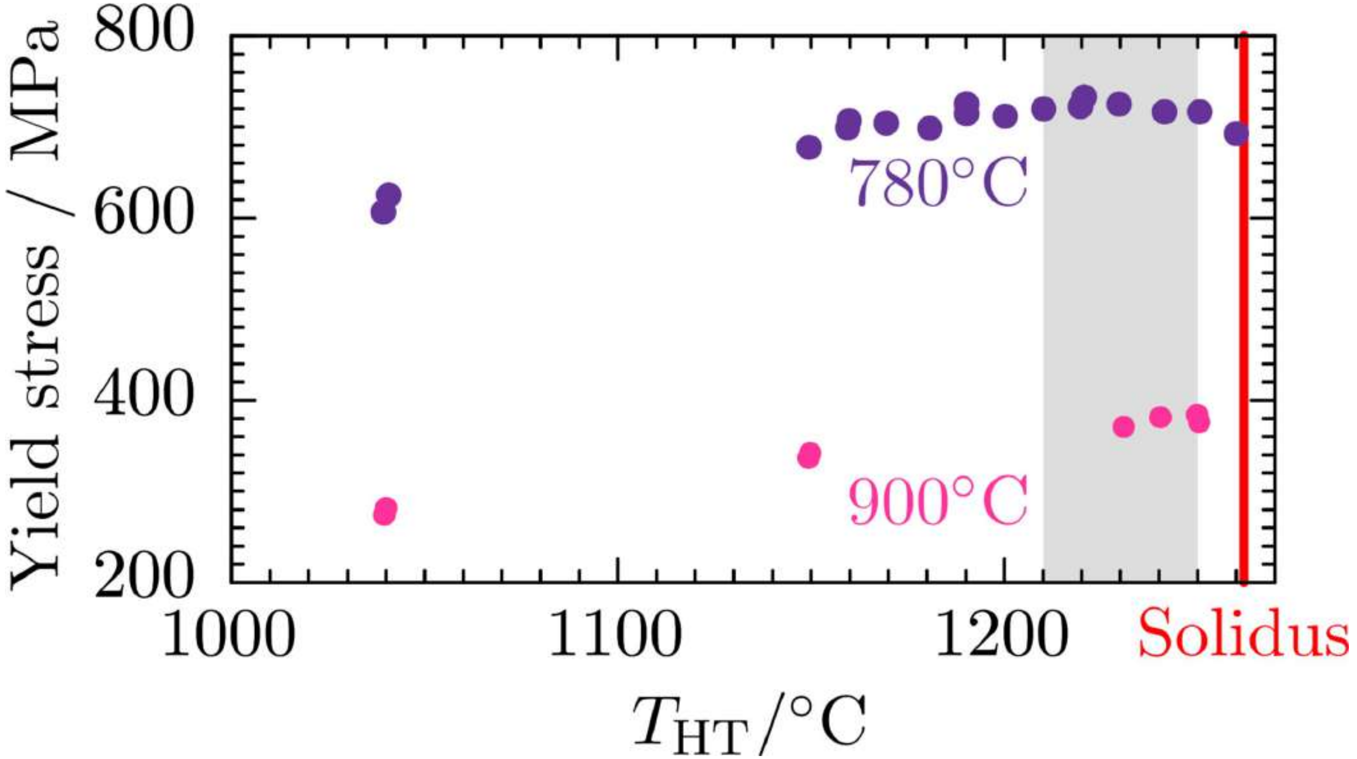
Microstructure



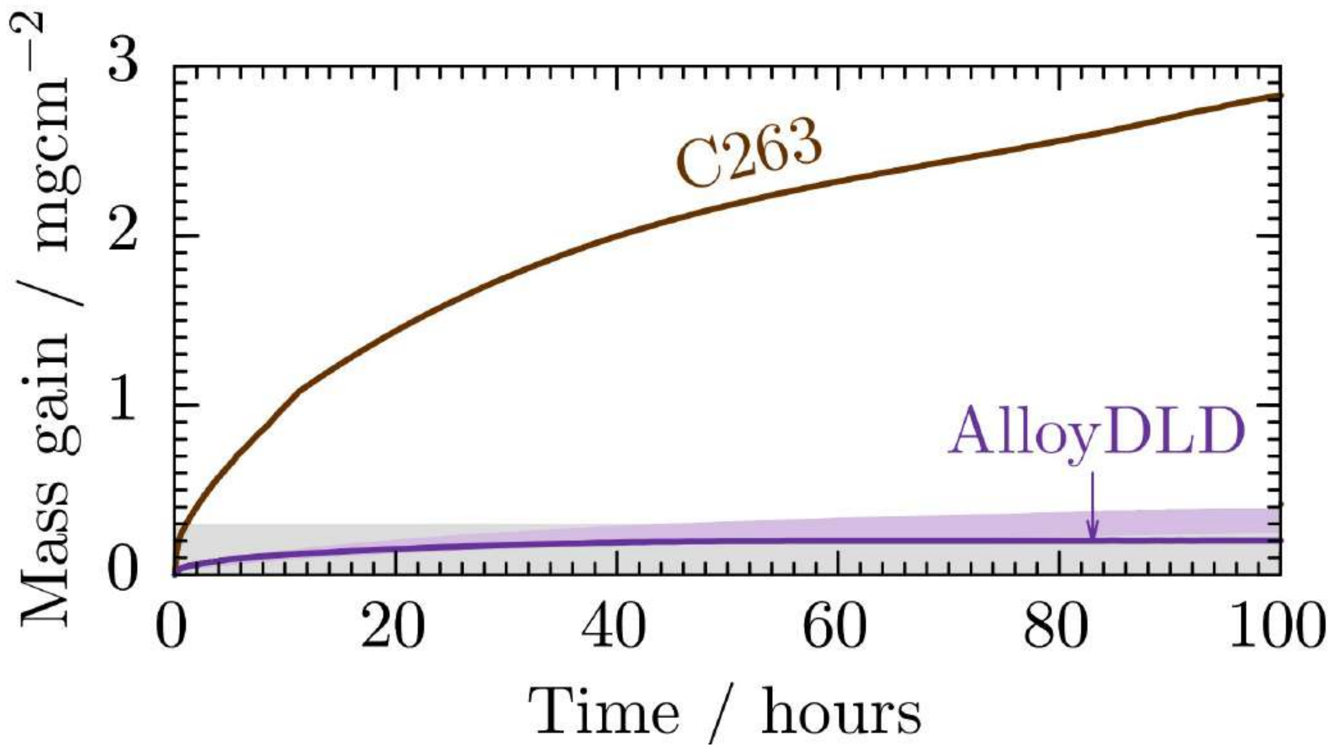
Testing the processability: horizontal printing



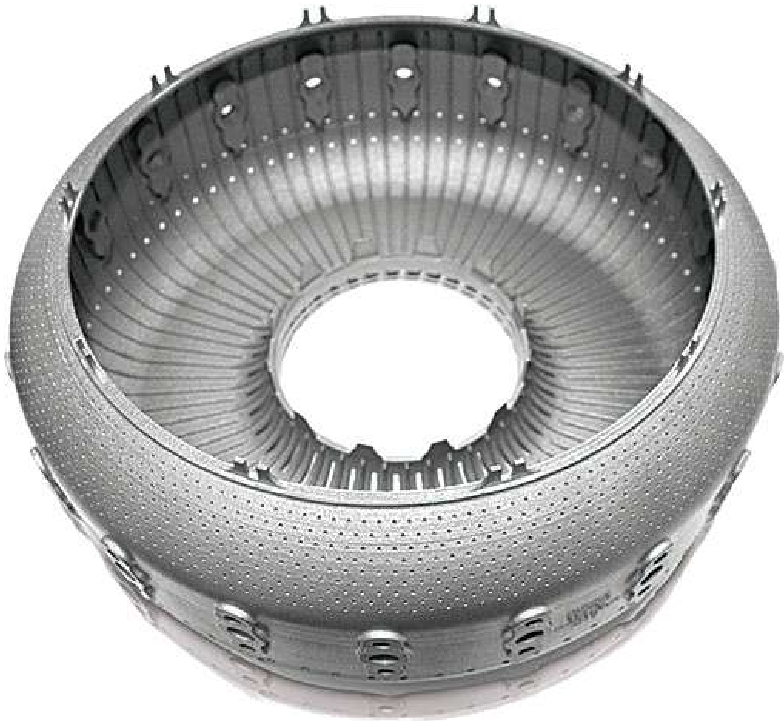
Testing the processability: horizontal printing



Testing the oxidation resistance



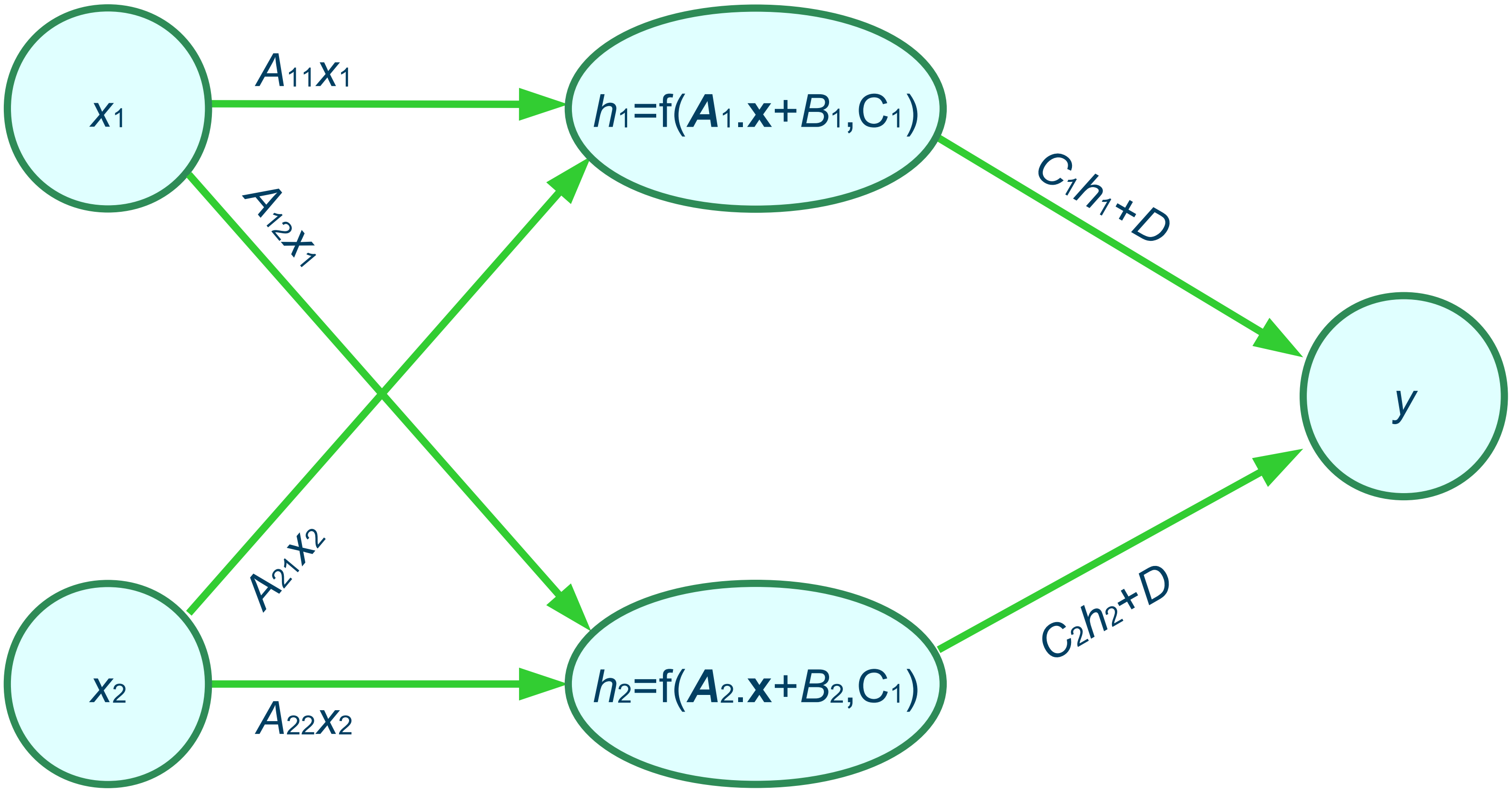
Printing components for an engine



Materials Solutions

ROLLS ROYCE

Underlying neural network



Neural network of multiple variables

$$y = D + C \frac{\vec{A}.\vec{x} + B}{\left|\vec{A}.\vec{x} + B\right| + |C|}$$

Taylor expand the neural network

$$y = D + C\,\frac{\vec{A}.\vec{x}+B}{\left|\vec{A}.\vec{x}+B\right| + |C|}$$

$$= \begin{cases} D + \vec{A}.\vec{x}+B & \left|\vec{A}.\vec{x}+B\right| \ll |C| \\ D + C\,\mathrm{sign}\left(\vec{A}.\vec{x}+B\right) & \left|\vec{A}.\vec{x}+B\right| \gg |C| \end{cases}$$

Physical formulae with multiplication

$$\mu = \frac{\tau_{\mathrm{i}}}{3\sigma_{\mathrm{y}}}$$

$$\kappa = \frac{6E_{\mathrm{d}}'h\sigma_{\mathrm{d}}}{E_{\mathrm{s}}'H^2}$$

$$i_L = \frac{ZFDC}{\delta}$$

$$E = \frac{1}{2}kx^2$$

$$\sigma = \frac{3FL}{2bd^2}$$

$$V = IR$$

$$PV = nk_{\mathrm{B}}T$$

$$\rho = \frac{AR}{L}$$

$$\lambda = \left(\frac{m}{ne^2\mu_0}\right)^{1/2}$$

Physical formulae with addition and multiplication

$$\mu = \frac{\tau_{\mathrm{i}}}{3\sigma_{\mathrm{y}}}$$

$$\kappa = \frac{6E_{\mathrm{d}}'h\sigma_{\mathrm{d}}}{E_{\mathrm{s}}'H^2}$$

$$i_L = \frac{ZFDC}{\delta}$$

$$E = \frac{1}{2}kx^2$$

$$\sigma = \frac{3FL}{2bd^2}$$

$$\omega = \left(\frac{k(m_1 + m_2)}{m_1 m_2} \right)^{1/2}$$

$$i_{\mathrm{A}} = i_0 \exp\left(\frac{azF\eta}{RT} \right)$$

$$V = IR$$

$$V = I(R_1 + R_2)$$

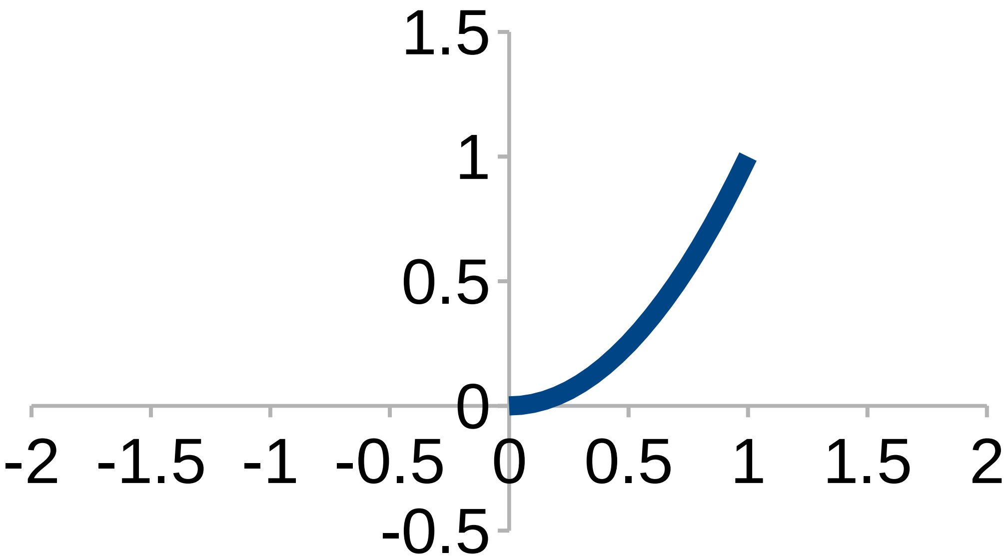
$$PV = nk_{\mathrm{B}}T$$

$$\rho = \frac{AR}{L}$$

$$\lambda = \left(\frac{m}{ne^2\mu_0} \right)^{1/2}$$

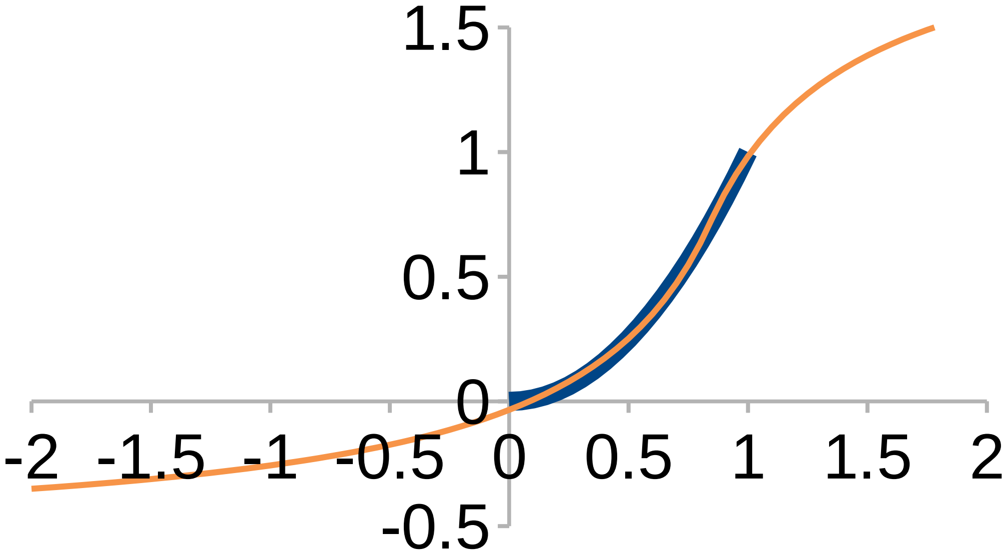
$$\epsilon = A\sigma^n \exp(-Q/RT)$$

Training data to enable multiplication



Neural network to replicate the parabola

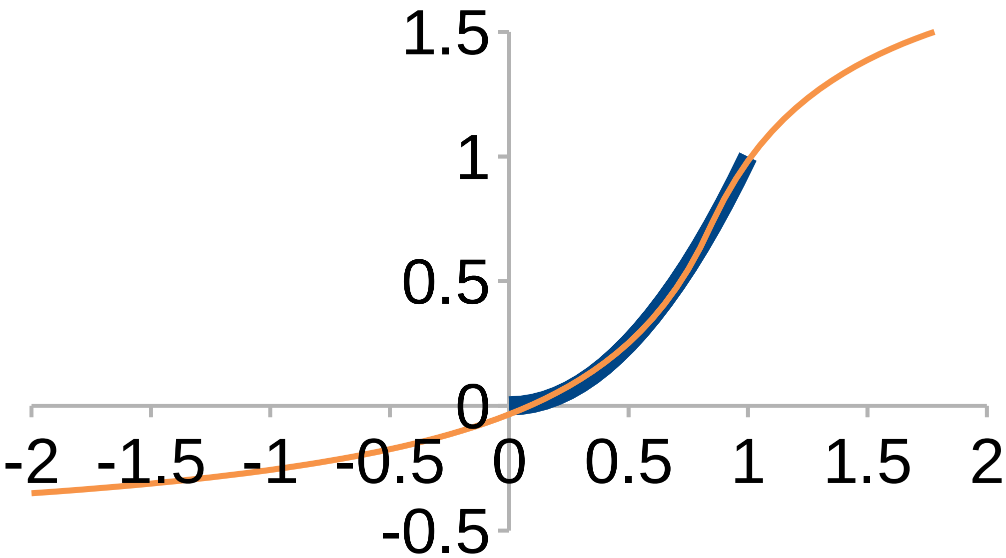
1) Shift the activation function into squared region



$$y = 0.57 + \frac{1.2(2.01x - 1.85)}{|2.01x - 1.85| + 1.2}$$

Neural network to replicate multiplication

1) Shift the activation function into squared region



$$y = 0.57 + \frac{1.2(2.01x - 1.85)}{|2.01x - 1.85| + 1.2}$$

2) Combine two activation functions in the square region

$$y = \underbrace{\left(\frac{x_1}{2} + \frac{x_2}{2}\right)^2}_{\text{Node 1}} - \underbrace{\left(\frac{x_1}{2} - \frac{x_2}{2}\right)^2}_{\text{Node 2}} = x_1 x_2$$

Can we do better with logarithms?

$$\log y = \underbrace{\left(\log x_1 + \log x_2\right)}_{\text{Node 1}} = \log\left(x_1 x_2\right)$$

$$y = x_1 x_2$$

Becomes tricky when x<0, and cannot recover addition

Blend addition and multiplication into one kernel

$$y = D + \bar{\alpha}\,\bar{y} + \sum_i \frac{\alpha_i C_i \left(\vec{A}_i . \left(\vec{x} - \vec{\bar{x}} \right) + B_i \right)}{\left| \vec{A}_i . \left(\vec{x} - \vec{\bar{x}} \right) + B_i \right| + \left| C_i \right|}$$

Blend addition and multiplication into one kernel

$$y = D + \bar{\alpha}\,\bar{y} + \sum_i \frac{\alpha_i C_i \left(\vec{A}_i . (\vec{x} - \bar{\vec{x}}) + B_i\right)}{\left|\vec{A}_i . (\vec{x} - \bar{\vec{x}}) + B_i\right| + |C_i|}$$

$$-\left[\prod_j \operatorname{sign}(x_j)\right] \sum_i \frac{(1-\alpha_i) C_i B_i \prod_j |x_j|^{A_{ij}}}{|B_i| \prod_j |x_j|^{A_{ij}} + |C_i|}$$

Recover addition

$$y = D + \bar{\alpha}\,\bar{y} + \sum_i \frac{\alpha_i C_i \left(\vec{A}_i . (\vec{x} - \bar{\vec{x}}) + B_i\right)}{\left|\vec{A}_i . (\vec{x} - \bar{\vec{x}}) + B_i\right| + |C_i|}$$

$$- \left[\prod_j \operatorname{sign}(x_j)\right] \sum_i \frac{(1 - \alpha_i) C_i B_i \prod_j |x_j|^{A_{ij}}}{|B_i| \prod_j |x_j|^{A_{ij}} + |C_i|}$$

When α=1 and for small x recover addition

$$y = D + \bar{y} + \sum_i \left[\vec{A}_i . (\vec{x} - \bar{\vec{x}}) + B_i\right]$$

Recover multiplication

$$y = D + \bar{\alpha}\,\bar{y} + \sum_i \frac{\alpha_i C_i \left(\vec{A}_i . \left(\vec{x} - \vec{\bar{x}}\right) + B_i\right)}{\left|\vec{A}_i . \left(\vec{x} - \vec{\bar{x}}\right) + B_i\right| + \left|C_i\right|}$$

$$- \left[\prod_j \operatorname{sign}(x_j)\right] \sum_i \frac{(1-\alpha_i) C_i B_i \prod_j |x_j|^{A_{ij}}}{|B_i| \prod_j |x_j|^{A_{ij}} + |C_i|}$$

When α=0 and for small x≥0 recover multiplication

$$y = D - \sum_i B_i \prod_j x_j^{A_{ij}}$$

Addition-multiplication merging improves performance

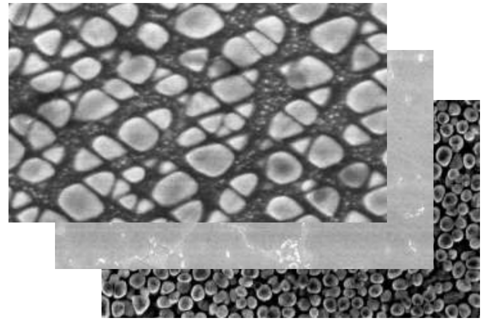
$$y = D + \bar{\alpha}\,\bar{y} + \sum_i \frac{\alpha_i C_i \left(\vec{A}_i . \left(\vec{x} - \bar{\vec{x}}\right) + B_i\right)}{\left|\vec{A}_i . \left(\vec{x} - \bar{\vec{x}}\right) + B_i\right| + \left|C_i\right|}$$

$$- \left[\prod_j \text{sign}\left(x_j\right)\right] \sum_i \frac{\left(1 - \alpha_i\right) C_i B_i \prod_j \left|x_j\right|^{A_{ij}}}{\left|B_i\right| \prod_j \left|x_j\right|^{A_{ij}} + \left|C_i\right|}$$

Addition-product merging improves performance by ~50%

Materials designed

Nickel and molybdenum

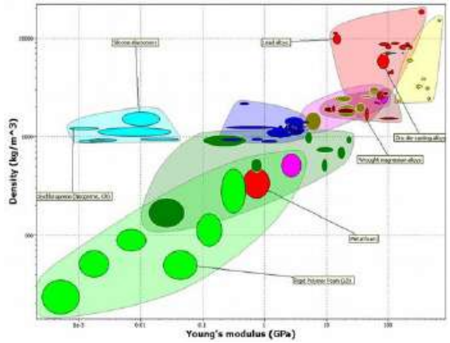


Experiment and DFT for batteries

Steel for welding

More materials

Identified and corrected errors in materials database



GRANTA
MATERIAL INSPIRATION

Lubricants with molecular dynamics and experiments

bp

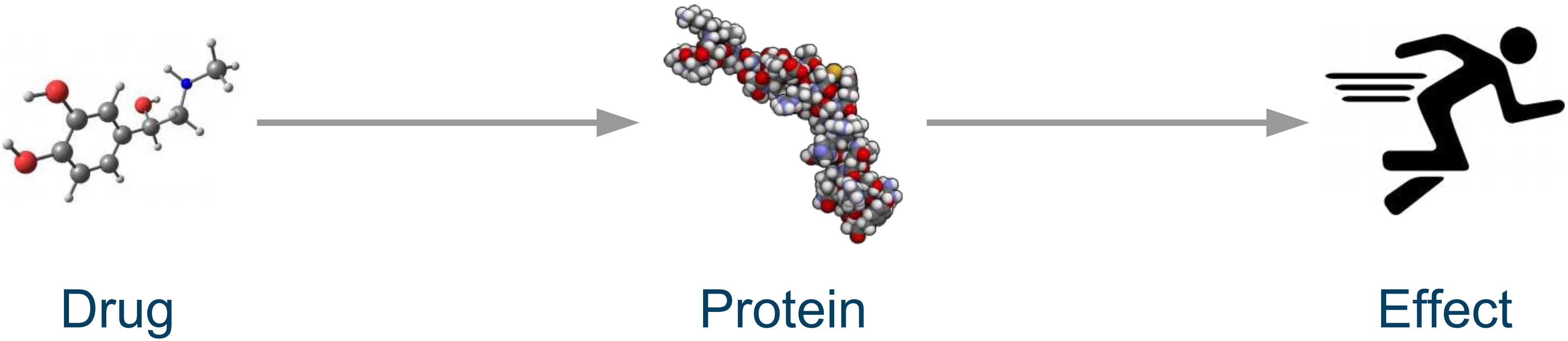
Drug design

e-therapeutics

optibrium

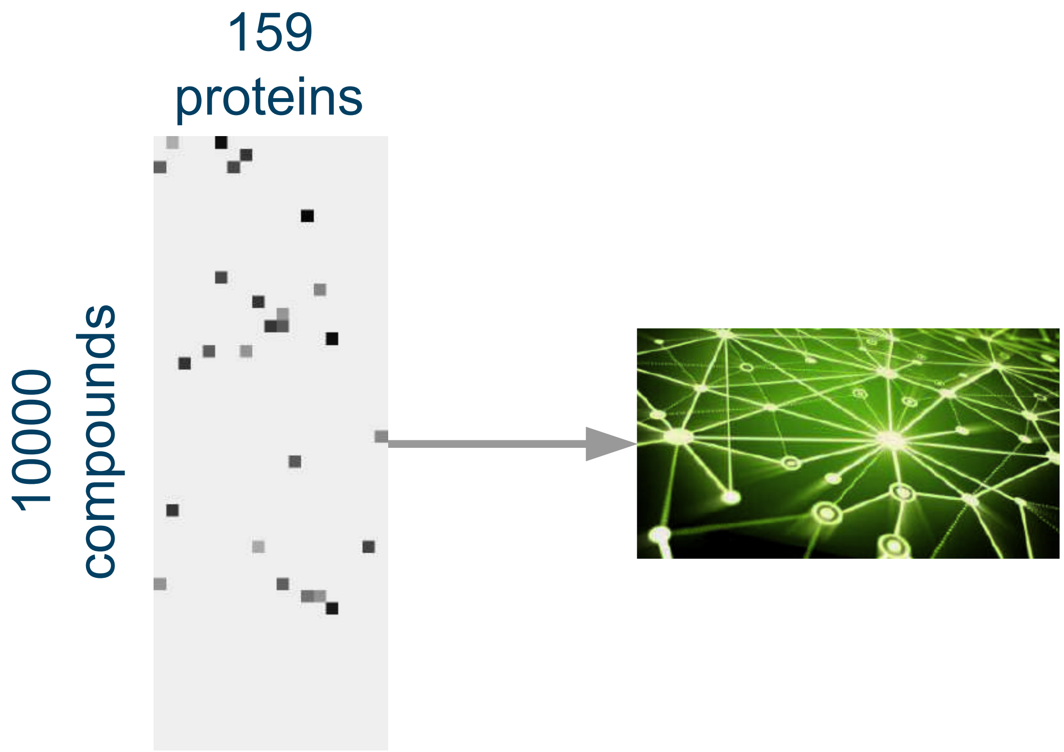
Takeda

Action of a drug



Novartis dataset to benchmark machine learning

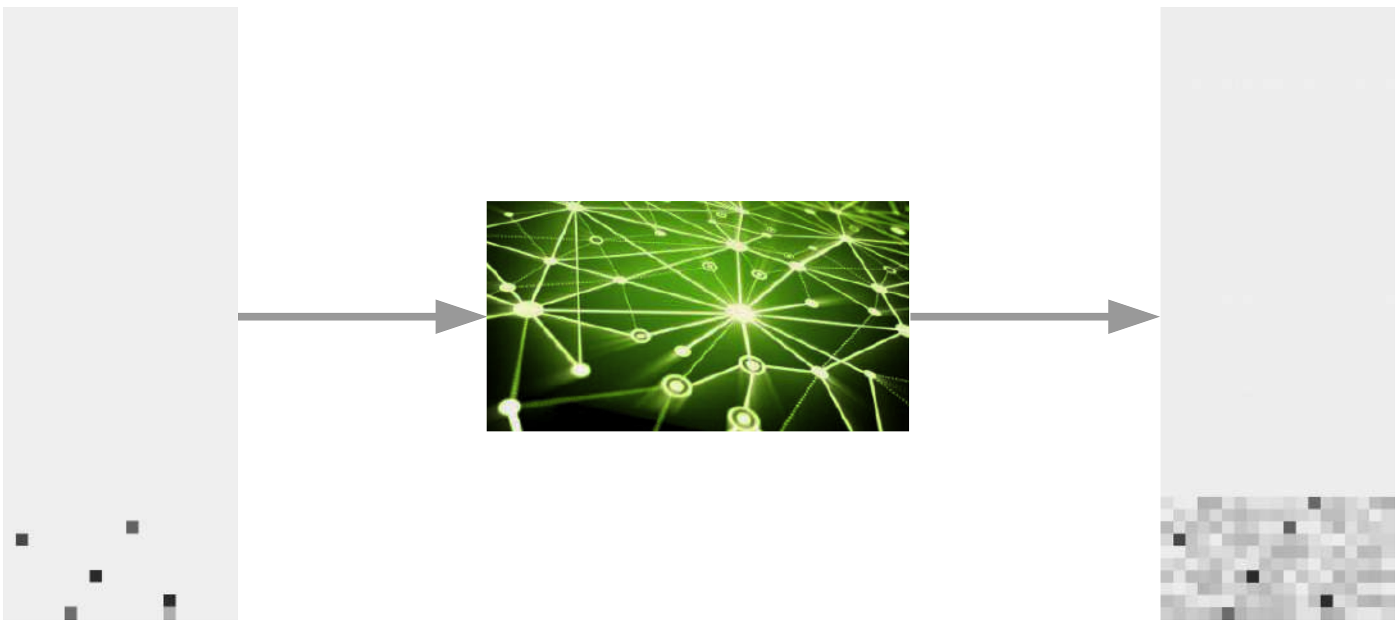
159 kinase proteins, 10000 compounds, data 5% complete



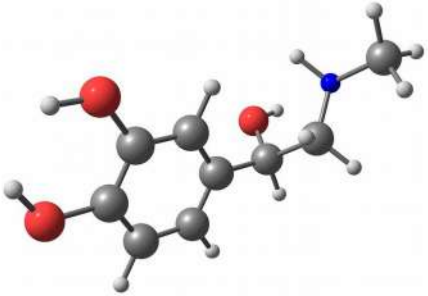
Data from ChEMBL
Martin, Polyakov, Tian, and Perez,
J. Chem. Inf. Model. 57, 2077 (2017)

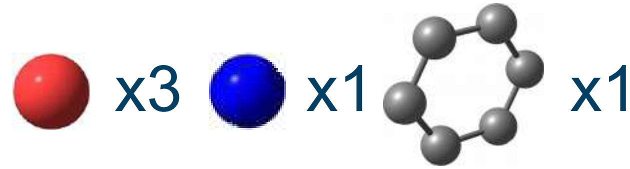
Impute missing entries to validate

Validate using a realistically split holdout data set, extrapolate to new chemical space

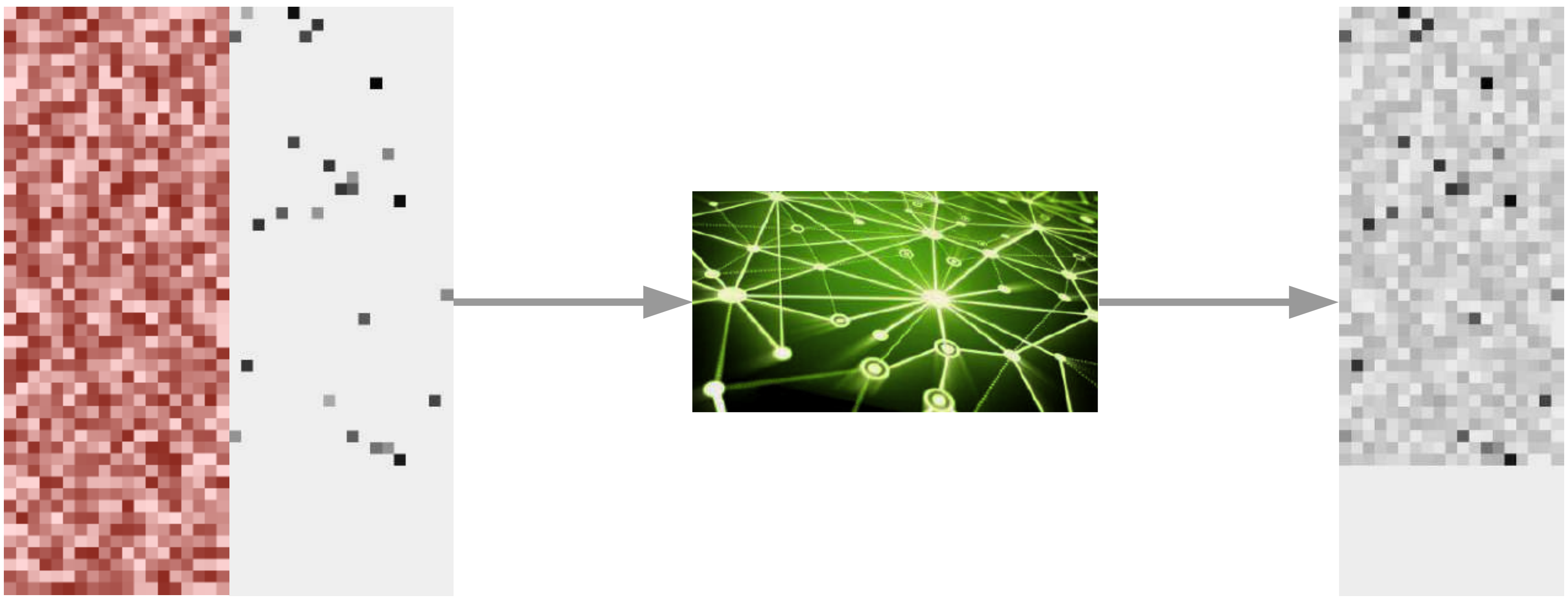


Quantitative structure-activity relationships

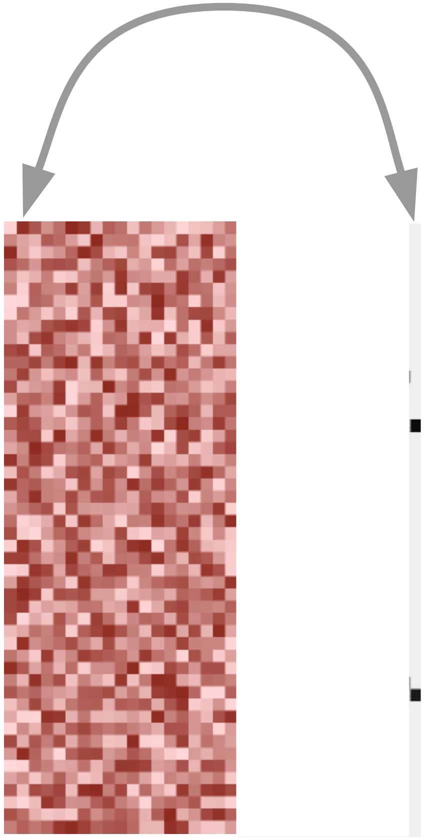




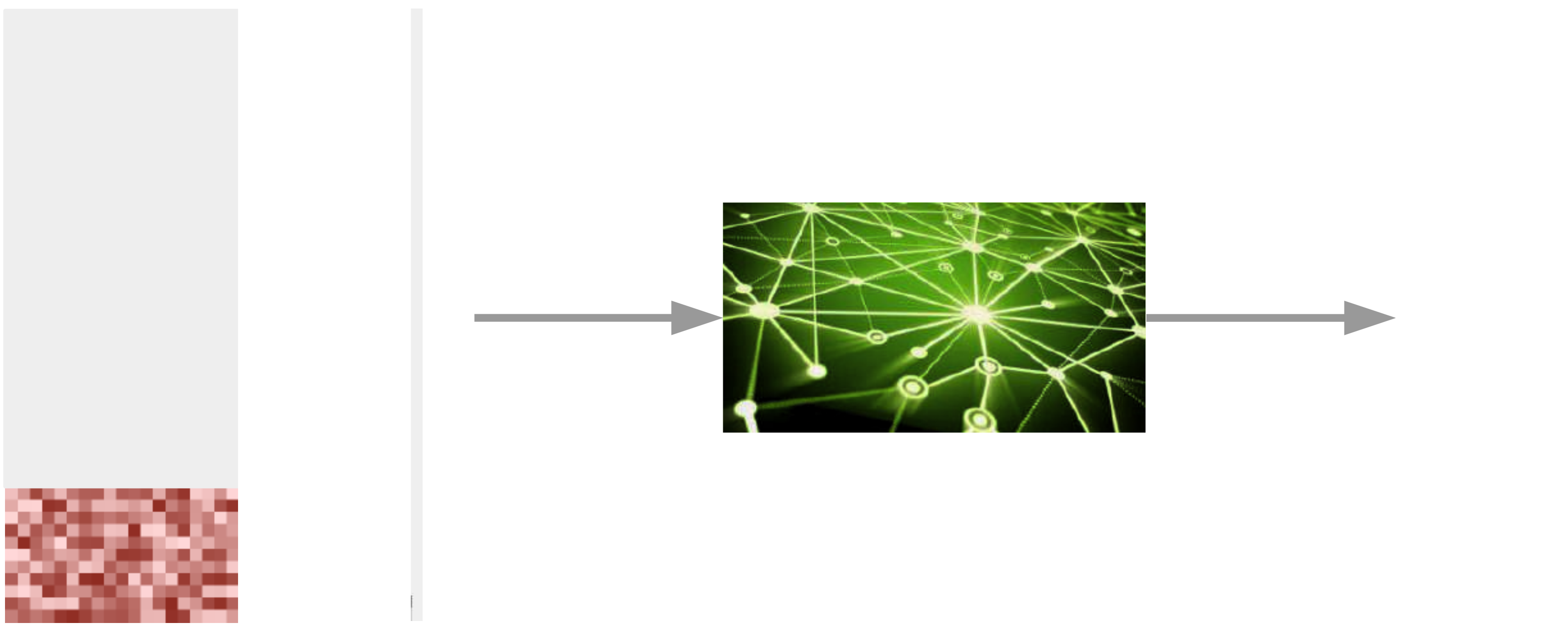
Molecular weight=183 Da



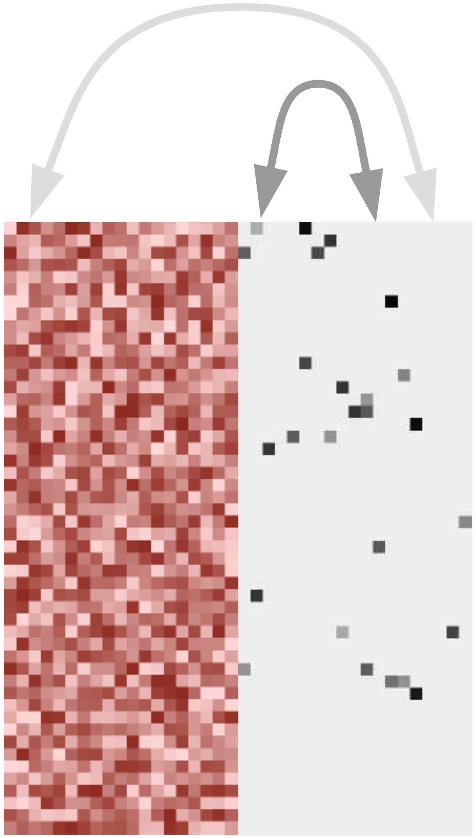
Quantitative structure-activity relationships



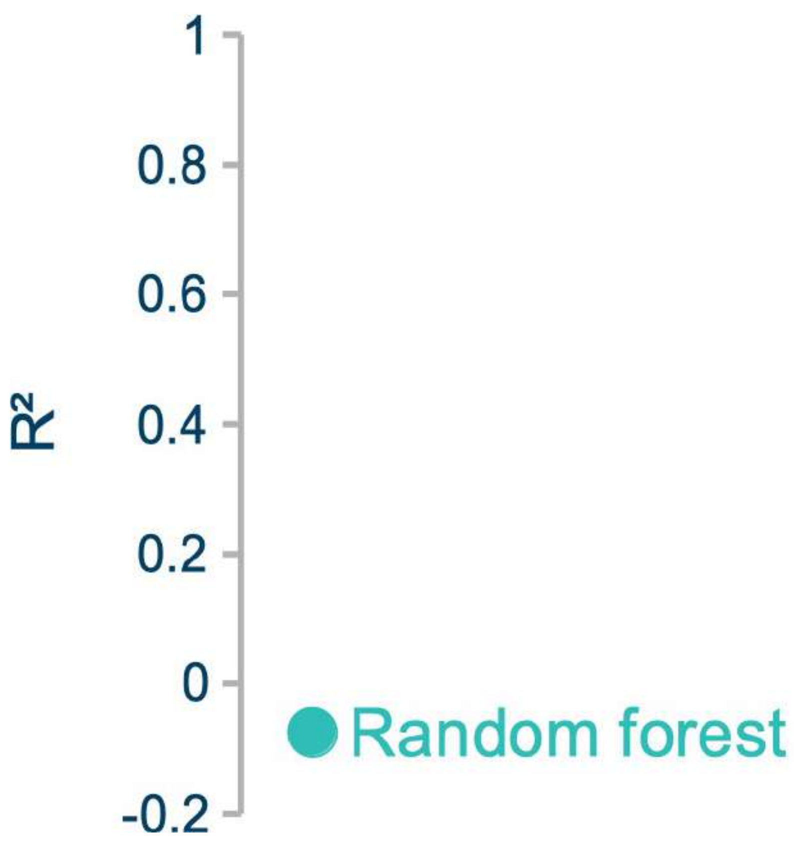
Predict one column at a time



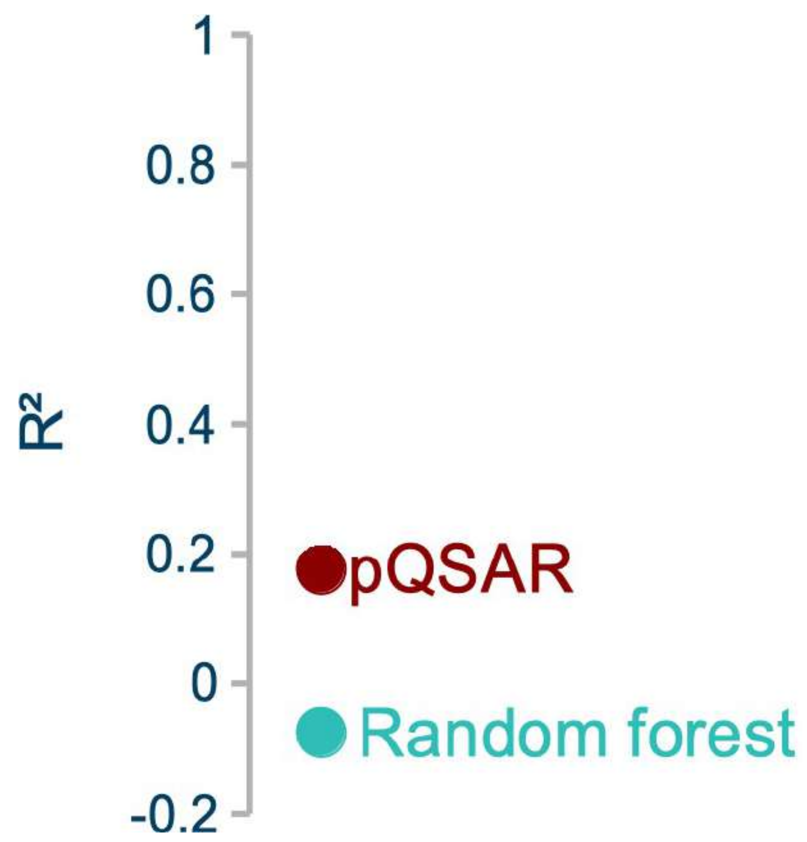
Learn protein-protein correlations



Random forest

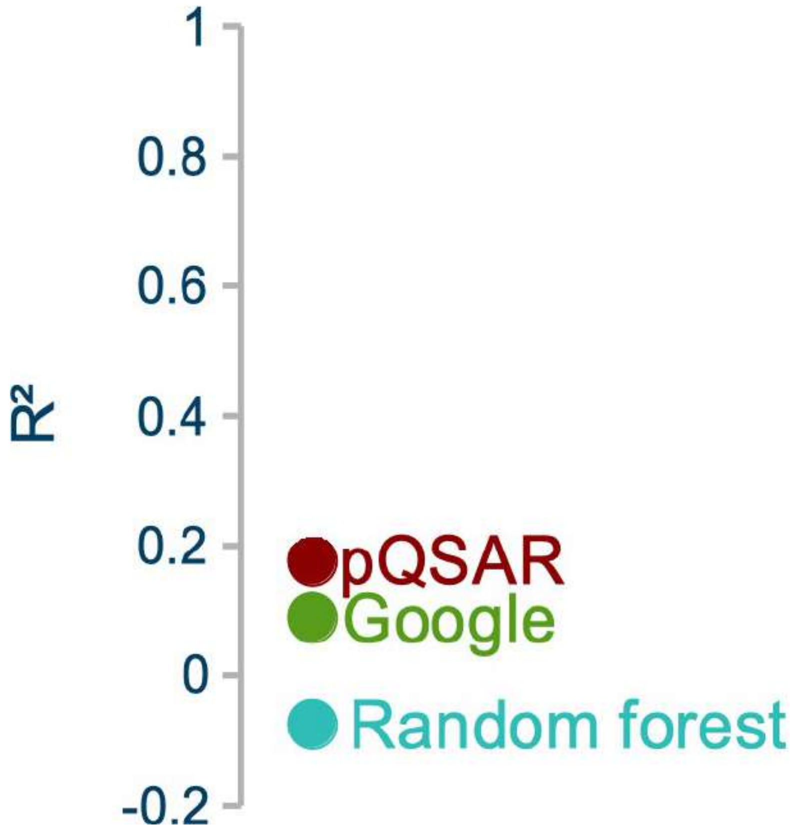


Predictions from pQSAR

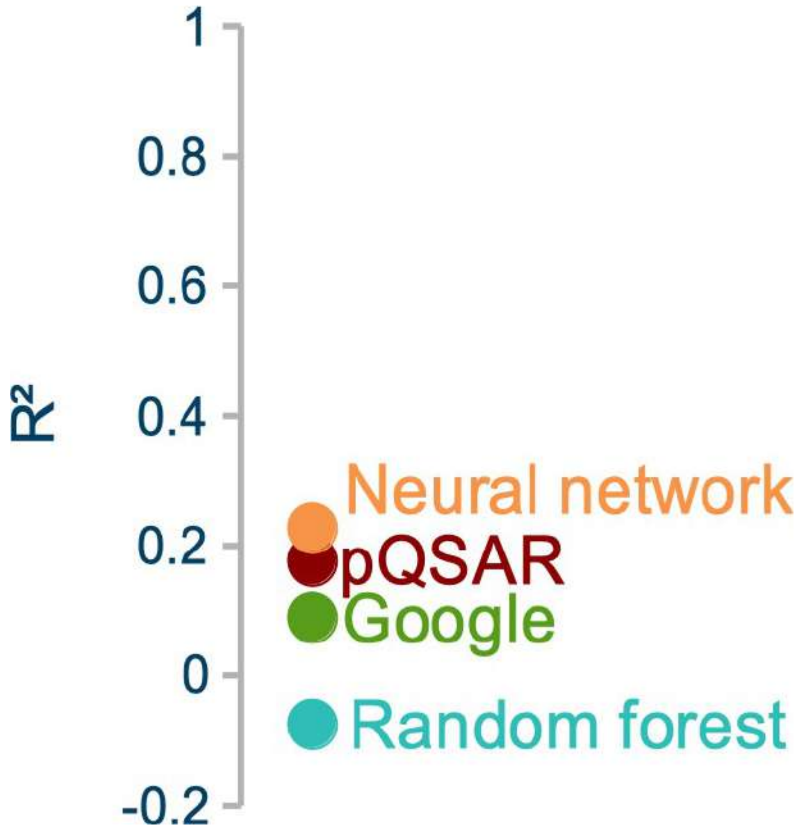


Martin, Polyakov, Tian, and Perez,
J. Chem. Inf. Model. 57, 2077 (2017)

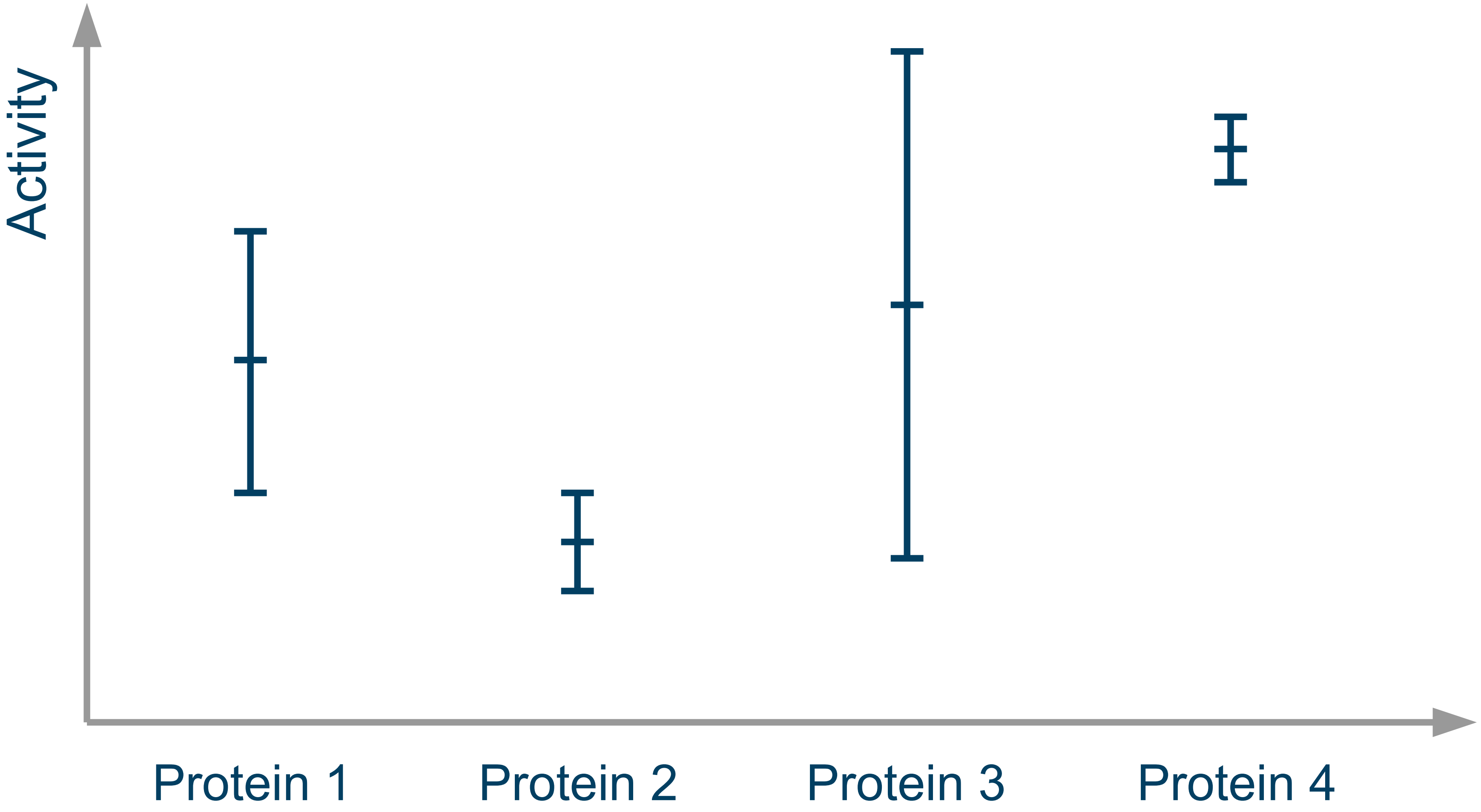
Google's attempt



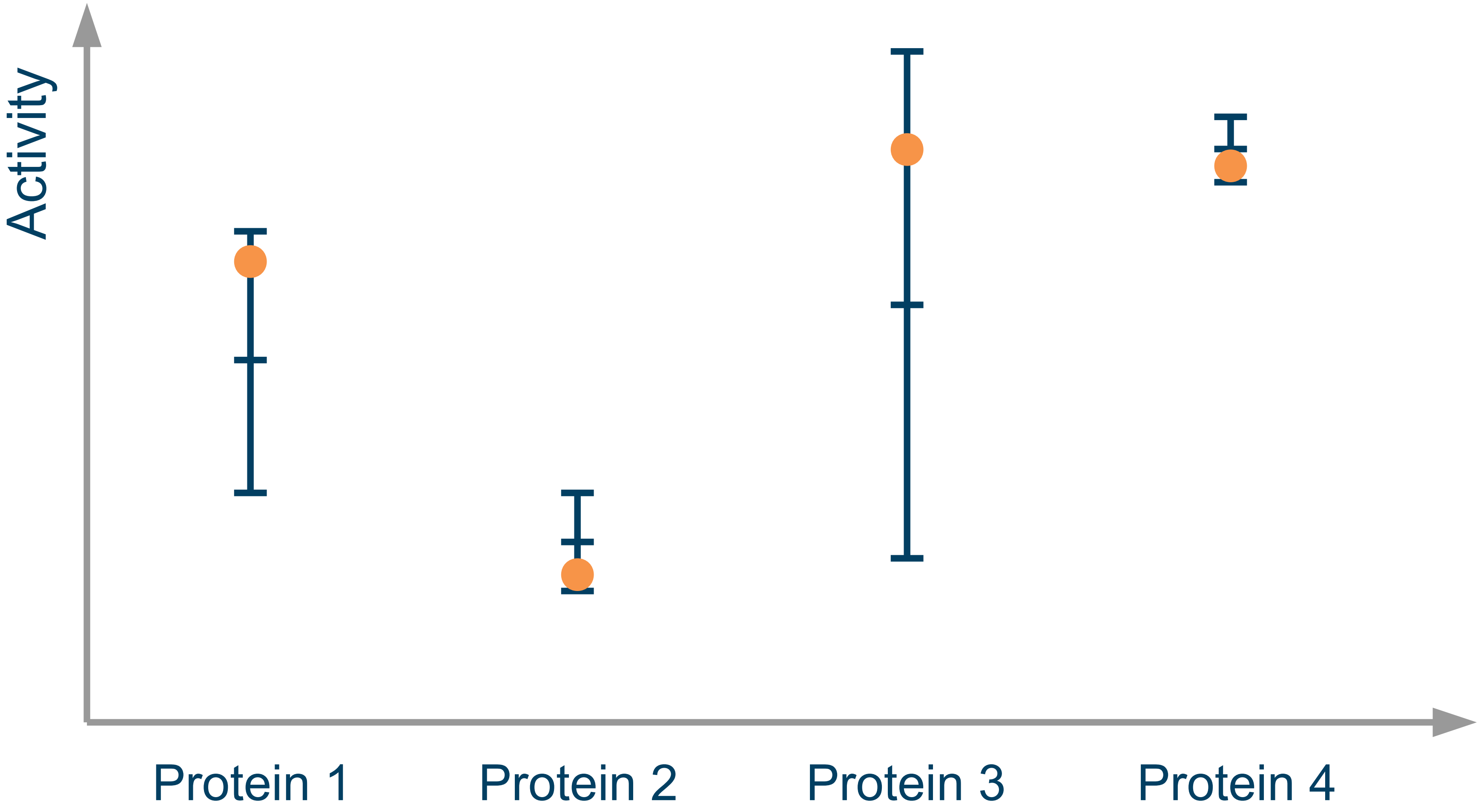
Neural network with missing data



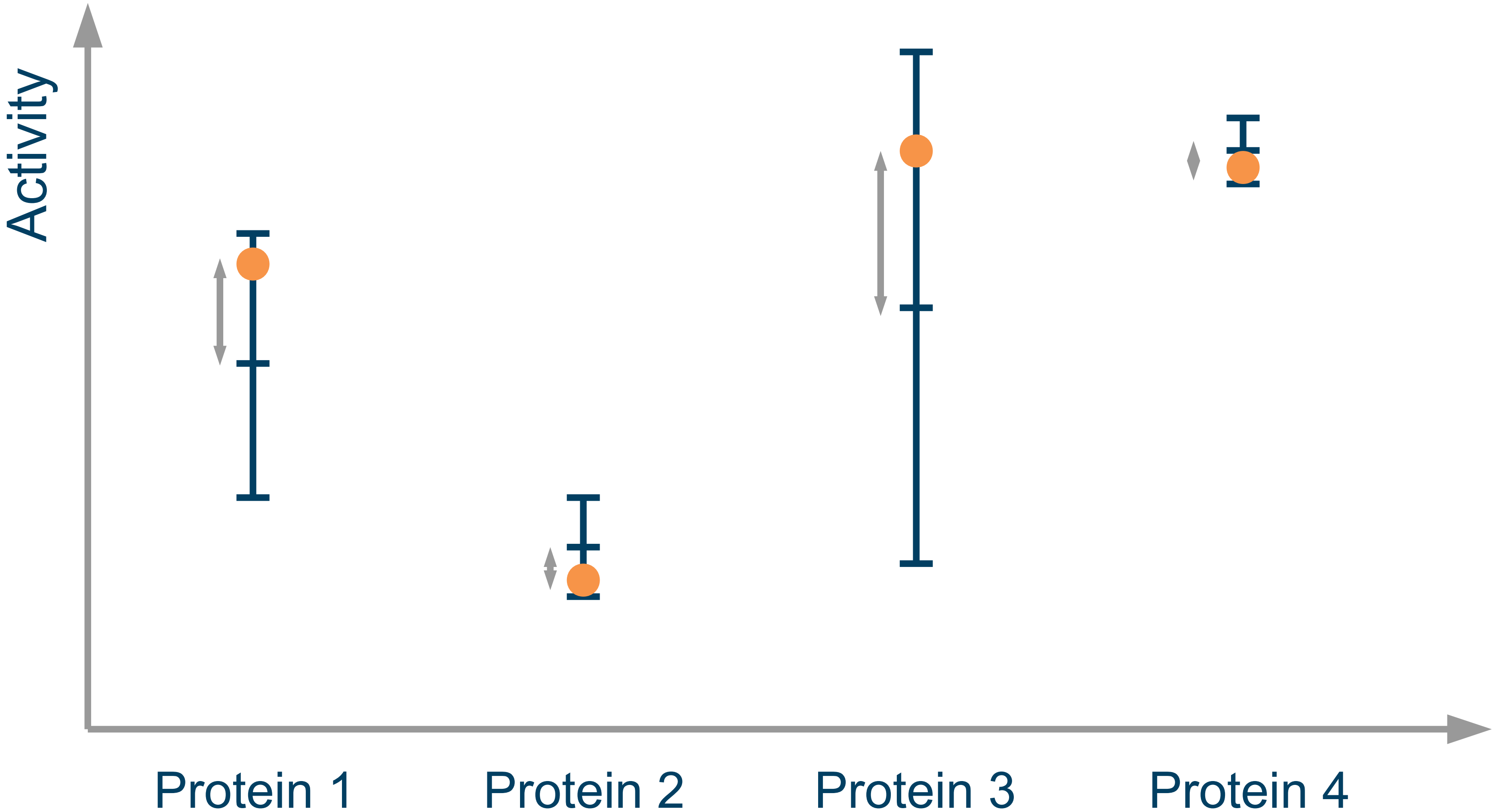
Predictions have an uncertainty



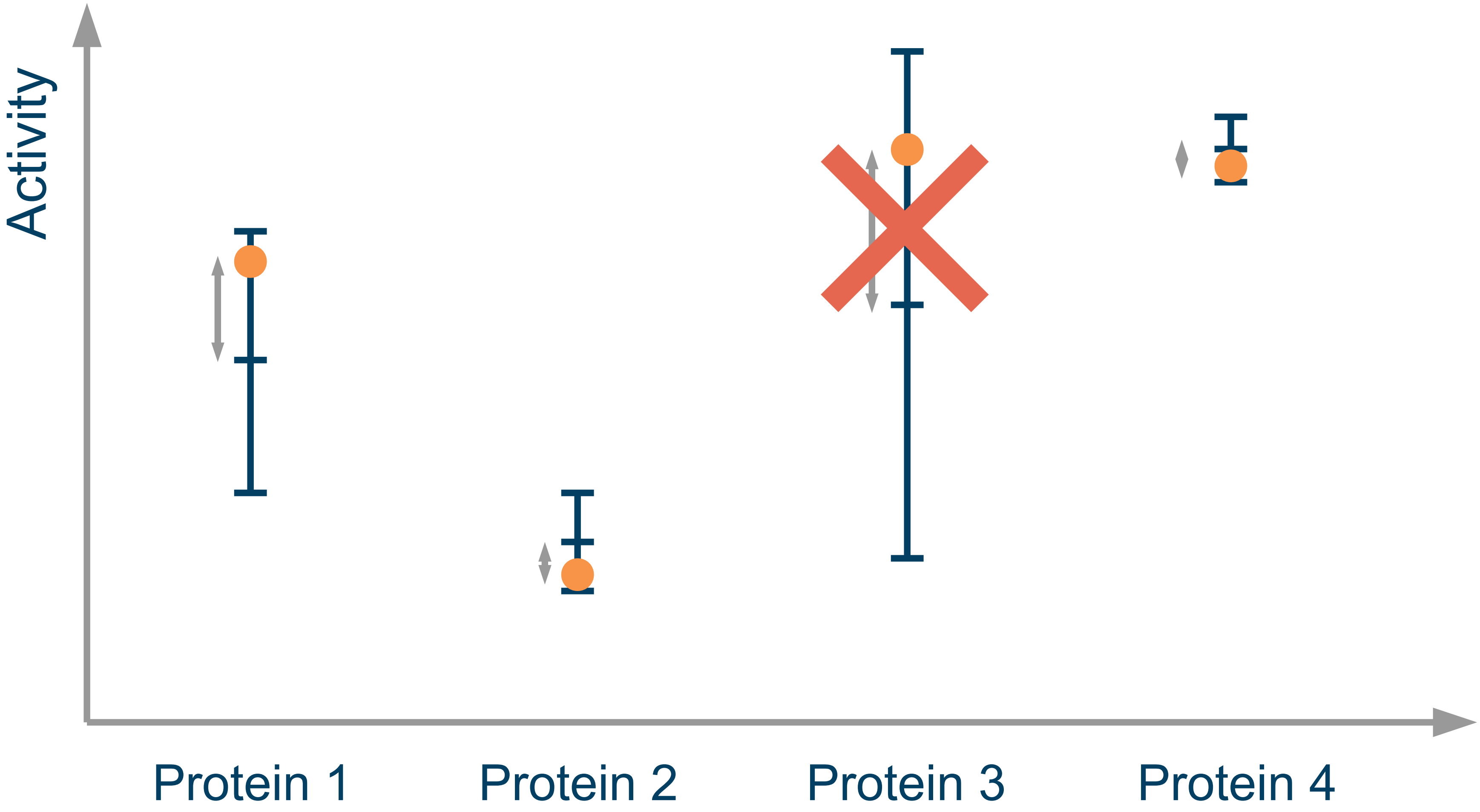
Validation data typically within one standard deviation



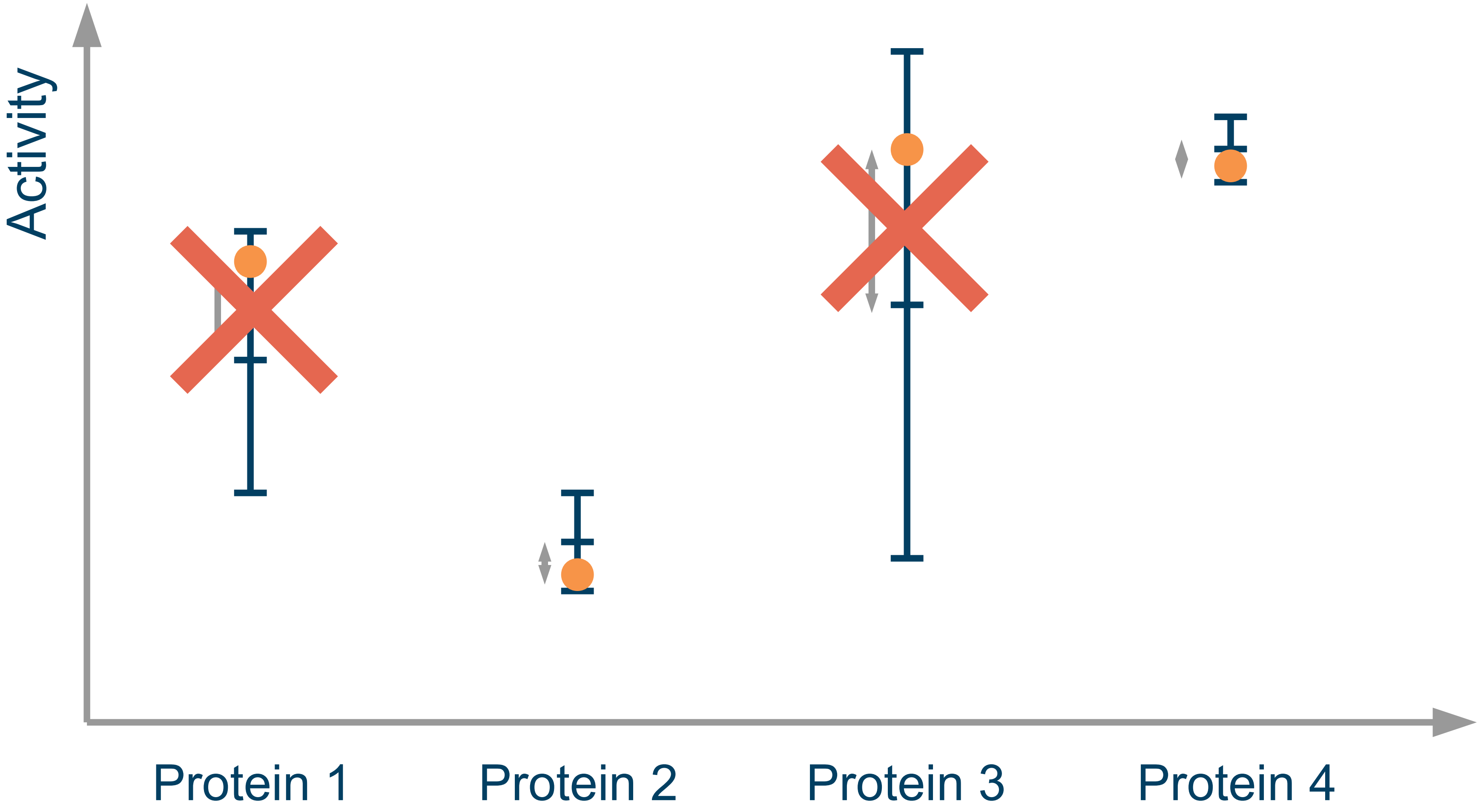
R^2 metric calculated with difference from mean



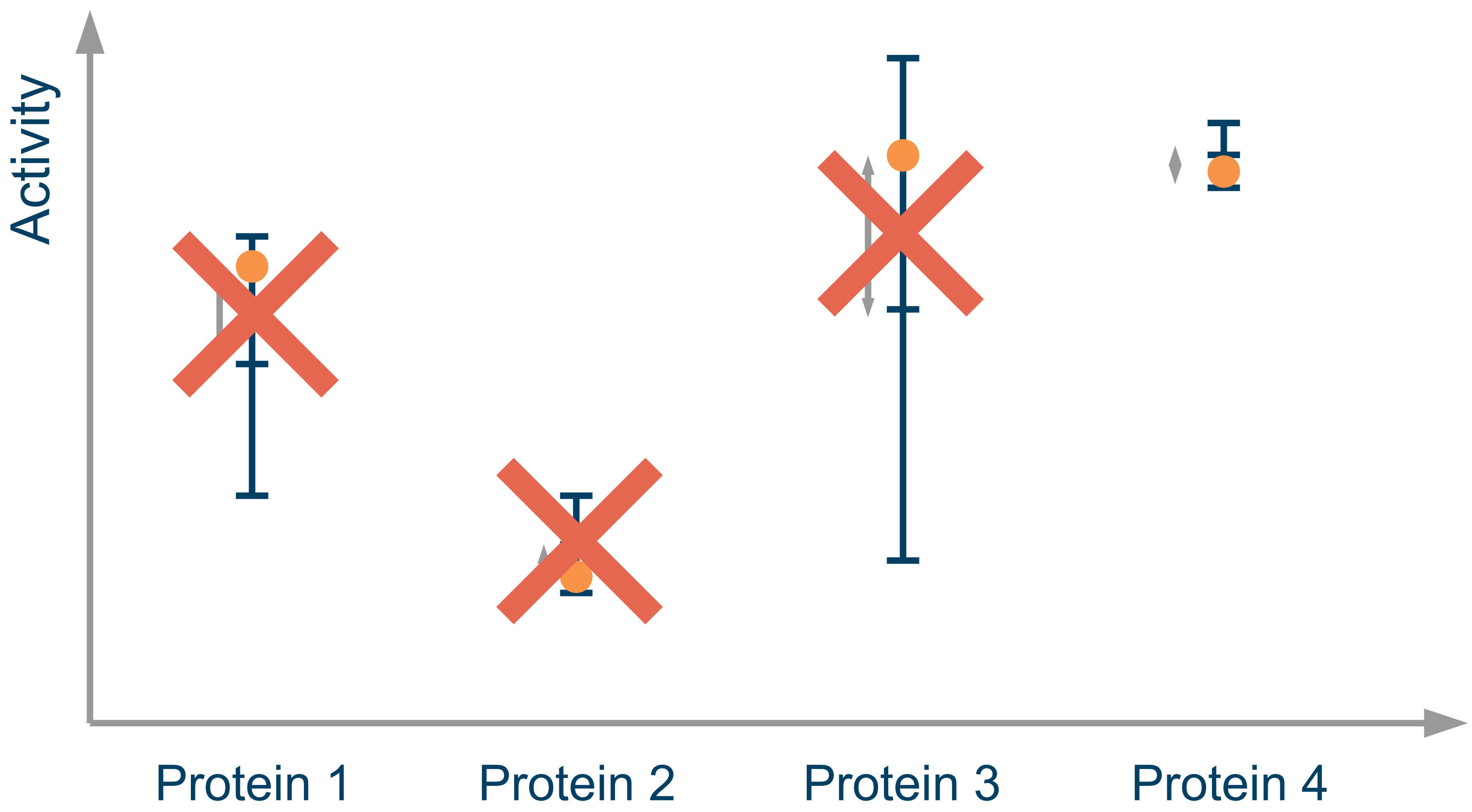
Impute 75% of data with smallest uncertainty



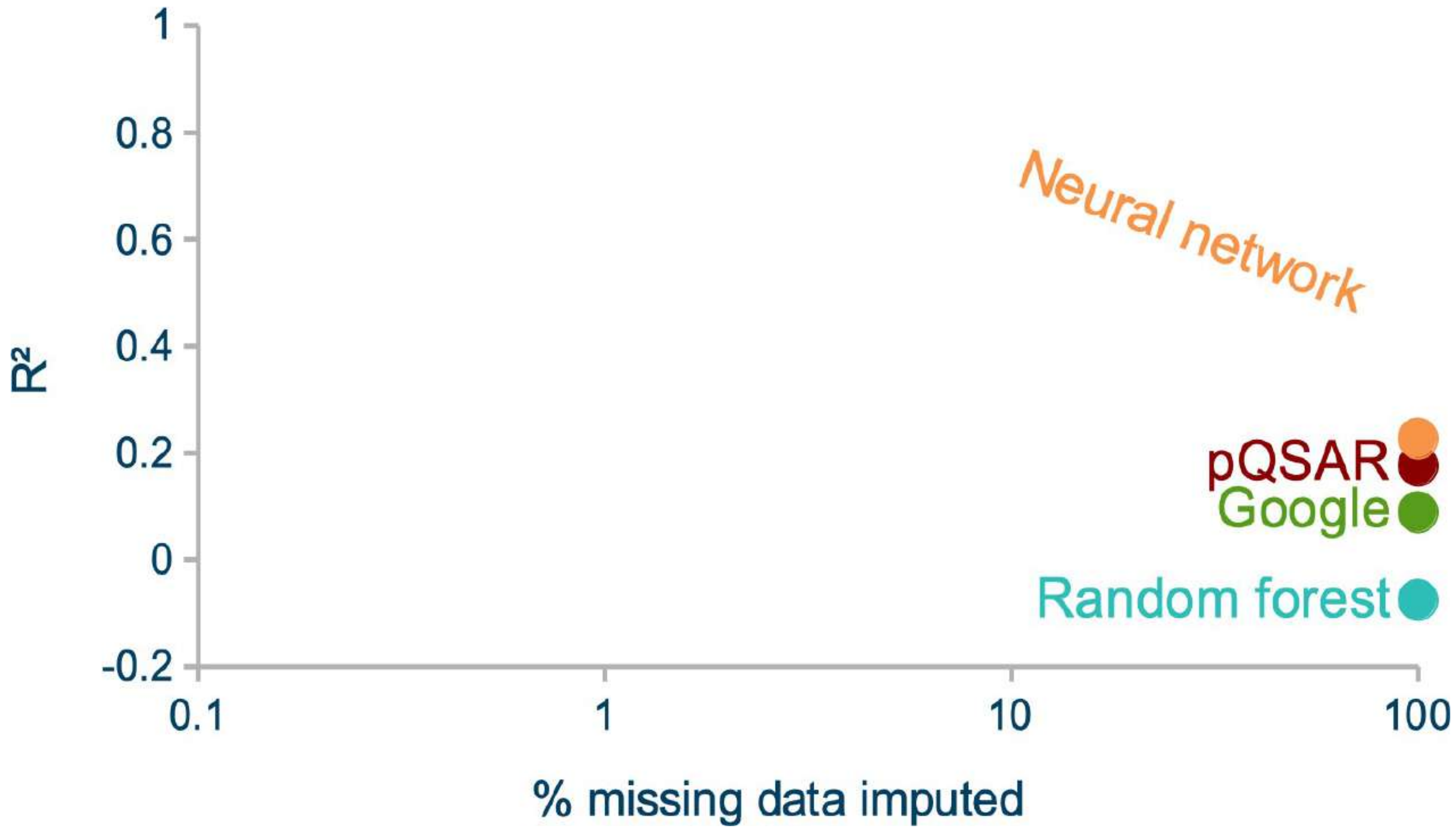
Impute 50% of data with smallest uncertainty



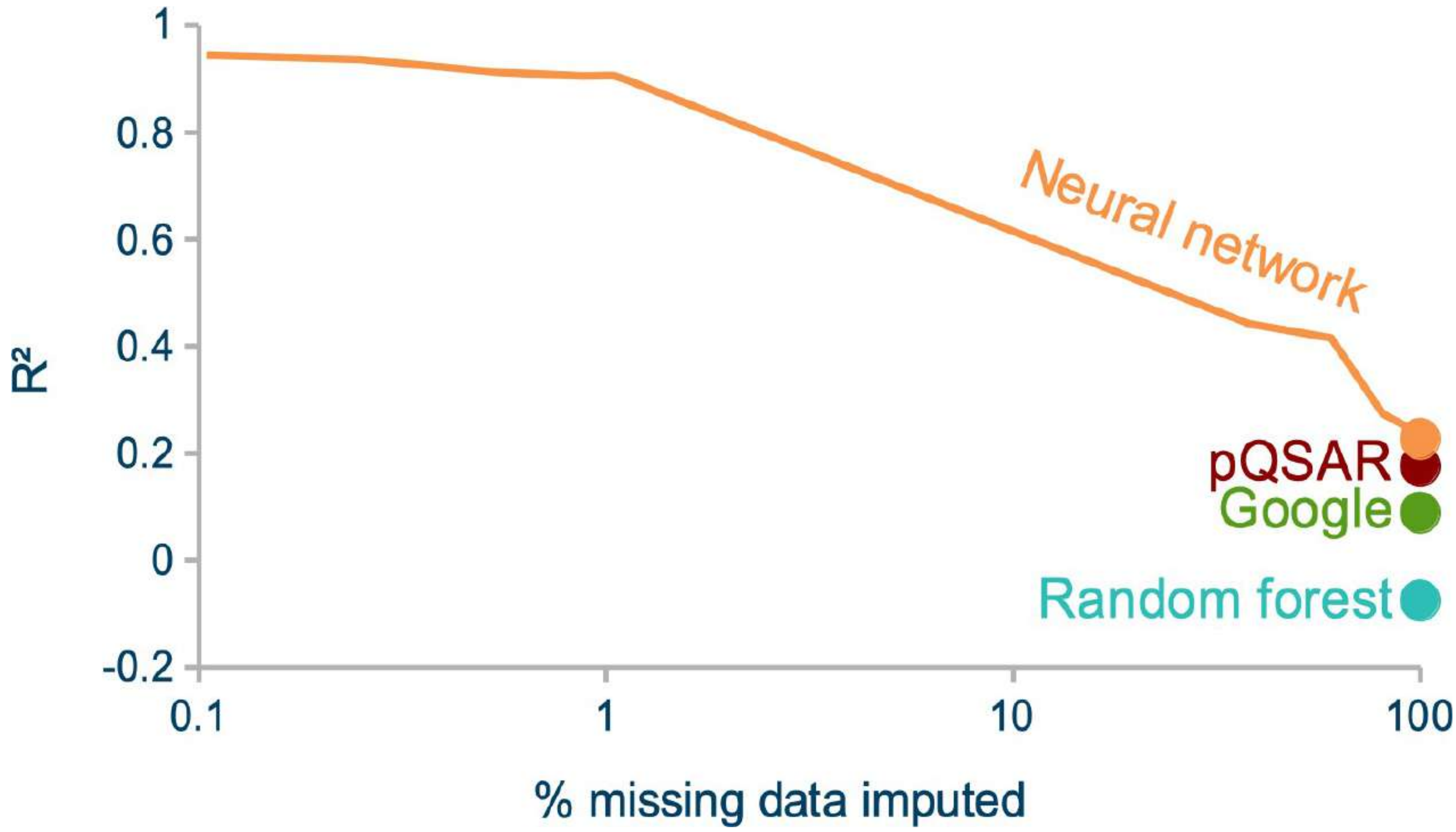
Impute 25% of data with smallest uncertainty



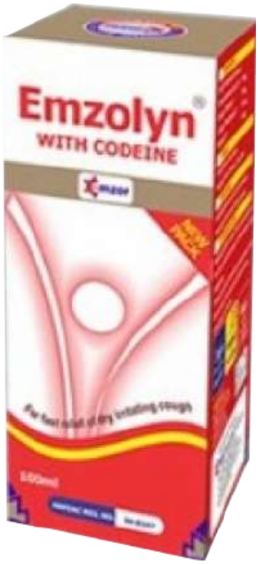
Improved performance by exploiting uncertainty



Improved performance by exploiting uncertainty



Different drugs can treat the same ailment



Roadmap to productization

Reseller agreement with drug discovery software company **Optibrium**

Machine learning tool embedded into next generation of Optibrium software for release in **October 2020**

Summary

Merge different experimental quantities and computer simulations into a holistic design tool

Exploit mathematical knowledge about physical relationships

Designed and experimentally verified alloy for direct laser deposition

Improved predicability of drug design from R^2=0.18 to R^2=0.93