Learning to commercialize deep learning
Neural network algorithm to

**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
Design new materials that fulfil **multiple target** criteria in yield, hardness, melting, oxidation, cost, density, fatigue, toughness, creep, and processibility.
Design new materials that fulfil multiple target criteria in yield, hardness, melting, oxidation, cost, density, fatigue, toughness, creep, and processibility.

Use a standard neural network to predict each property, combine results by multiplying likelihoods:

$$L_{\text{tot}} = L_{\text{yield}} \cdot L_{\text{hardness}} \cdot L_{\text{melting}} \cdot L_{\text{oxidation}} \cdot L_{\text{cost}} \cdot L_{\text{density}} \cdot L_{\text{fatigue}} \cdot L_{\text{toughness}} \cdot L_{\text{creep}} \cdot L_{\text{processibility}}$$
2012: Alloy designed: composition

Cr: 15.8  Co: 20.0  Mo: 0.5  W: 0.5  Ta: 4.9  Nb: 1.1  Al: 2.4

Ti: 3.0  Fe: 3.9  Mn: 0.2  Si: 0.2  C: 0.02  B: 0.06  Zr: 0.18

Ni: 47.2

900°C  30 hours
2012: Microstructure
2012: Predict the yield stress

Proposed theory

![Graph showing yield stress vs. temperature]

- **Yield stress / MPa**: 1250, 1000, 750, 500, 250, 0
- **Temperature / °C**: 0, 250, 500, 750, 1000

**Proposed theory**
2012: Test the yield stress
2012: Test the yield stress

Yield stress / MPa

Temperature / °C

Proposed theory
Proposed experiment
RR1000
2012: Test the oxidation resistance

![Graph showing mass gain over time for RR1000, Proposed theory, and Proposed experiment.](image-url)
2012: Alloys designed

**Cr-Cr₂Ta alloys**
Intermetallics, 48, 62

**Combustor alloy**
GB1408536

**RR1000 grain growth**
Acta Materialia, 61, 3378

**Discovery algorithm**
EP14153898
US 2014/177578

**Ni disc alloy**
EP14157622
US 2013/0052077 A2

**Mo-Hf forging alloy**
EP14161255
US 2014/223465

**Mo-Nb forging alloy**
EP14161529
US 2014/224885
2013: Property-property correlations
2013: Alloy for 3D printing: property-property correlations
Extrapolate ten results for processibility with weldability
Extrapolate ten results for processibility with weldability
2014: Further materials design

Battery design with DFT and experimental data
2014: Further materials design

Battery design with DFT and experimental data

Designing lubricants with DFT and experimental data
2014: Further materials design

Battery design with DFT and experimental data

Designing lubricants with DFT and experimental data

Identified and corrected errors in materials database
2015: Further capabilities

Extract information out of noise
Extract information out of noise

Merge two datasets together
2015: Further capabilities

- Extract information out of noise
- Merge two datasets together
- Train on encrypted data
2016: Understanding of business models

- Proposal: 5%
- Initial testing: 10%
- Certification: 100%
2016: Understanding of business models

- Proposal: 5%
- Initial testing: 10%
- Certification: 100%

- Proposal: 30%
- Initial testing: 70%
- Certification: 100%
2016: Drug discovery

Protein activity dataset from 0.1% complete

1000000 compounds

10000 proteins
2016: Drug discovery

Enhance protein activity dataset from 0.1% to 20% complete
2017: Startup Intellegens

Dr Gareth Conduit

Ben Pellegrini
2017: Startup Intellegens

Dr Gareth Conduit

Ben Pellegrini

Graham Snudden

Dr Elaine Loukes
2017: Startup Intellegens

Dr Gareth Conduit

Ben Pellegrini

Graham Snudden

Dr Elaine Loukes

Dr Thomas Whitehead

Gerald Fux
Drug discovery
2017: Startup: initial contracts

Drug discovery

Materials design

BenevolentAI

e-therapeutics
2017: Startup: initial contracts

Drug discovery

Materials design

Drug discovery
2018: Startup: plan to productize

| Input composition               | 52.93 | 0.2 | 1 | 2 | 9 | 10 | 4.5 | 2.1 | 0.07 | 1.2 | 10 | 4 | 1 | 2 | 1000 |
|---------------------------------|-------|-----|---|---|---|----|-----|-----|------|-----|----|---|---|---|-----|-------|
| Iron                            |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Carbon                          |       | 0   |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Manganese                       |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Silicon                         |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Chromium                        |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Nickel                          |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Molybdenum                      |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Vanadium                        |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Nitrogen                        |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Niobium                         |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Cobalt                          |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Tungsten                        |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Aluminium                       |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Titanium                        |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |
| Heat treatment                  |       |     |   |   |   |    |     |     |      |     |    |  |   |   |      |

### Predicted Output Properties

- **Yield stress**: 1220 MPa
- **Ultimate tensile strength**: 1951 MPa
- **Elongation**: 9%

![Graph showing the relationship between composition and properties](image)
2018: Exploring other verticals

Autonomous vehicles
2018: Exploring other verticals

Autonomous vehicles

Healthcare
2018: Exploring other verticals

Autonomous vehicles

Healthcare

Infrastructure
Conclusions

Develop technology motivated by problems

- 2012: Multiple targets, Superalloys
- 2013: Inter-property, 3D printing
- 2014: DFT-experiment, Batteries
- 2015: Merge datasets, Commercial data
- 2016: Business model, Drug discovery
- 2017: Angel investor, Drug discovery
- 2018: Productization, New verticals
- ?
Conclusions

Develop technology *motivated* by *problems*

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  - Multiple targets
  - Superalloys

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Flexibility to *adapt* to market need
Conclusions

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  - New verticals

Flexibility to **adapt** to market need

Willingness to take **risks** to enable greater returns