Quantum leap for machine learning

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Materials and pharmaceuticals market

Materials enabler for new technology, advanced materials market estimates at $1.5 trillion per year

Pharmaceuticals at heart of human health, worth $1 trillion per year

Improvements to materials or pharmaceuticals offer significant impact

Ripe for disruption – new formulations found after ~20 years of experimental driven trial and improvement
Challenge of machine learning in experimental sciences

Train from **sparse** datasets, typically found in experimental sciences

<table>
<thead>
<tr>
<th>COMPOSITION</th>
<th>PROCESS</th>
<th>PROPERTIES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iron</td>
<td>Carbon</td>
<td>Mn</td>
</tr>
<tr>
<td>Steel 1</td>
<td>99.1</td>
<td>0.27</td>
</tr>
<tr>
<td>Steel 2</td>
<td>98.6</td>
<td>0.9</td>
</tr>
<tr>
<td>Steel 3</td>
<td>0.42</td>
<td></td>
</tr>
<tr>
<td>Steel 4</td>
<td>98.4</td>
<td>0.55</td>
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</tbody>
</table>
Challenge of machine learning in materials

Train from **sparse** datasets, typically found in experimental sciences

**Merge** simulations, physical laws, and experimental data

**Reduce** the need for expensive experimental development

**Accelerate** discovery of new formulations

**Generic** with applications in materials and pharmaceuticals
Jet engine
Jet engine combustor
Target properties

- Elemental cost: $< 25 kg^{-1}$
- Density: kgm^{-3} < 8500
- $\gamma'$ content: wt% < 25
- Oxidation resistance: mgcm^{-2} < 0.3
- Processability: defects < 0.15%
- Phase stability: wt% > 99.0
- $\gamma'$ solvus: °C > 1000
- Thermal resistance: KΩ^{-1}m^{-3} > 0.04
- Yield stress at 900°C: MPa > 200
- Tensile strength at 900°C: MPa > 300
- Tensile elongation at 700°C: % > 8
- 1000hr stress rupture at 800°C: MPa > 100
- Fatigue life at 500 MPa, 700°C: cycles > $10^5$
Direct laser deposition
Machine learning prediction of direct laser deposition
Machine learning prediction of crack formation
Predict direct laser deposition from crack formation
## Composition Designed

<table>
<thead>
<tr>
<th>Element</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Cr</td>
<td>19%</td>
</tr>
<tr>
<td>Co</td>
<td>4%</td>
</tr>
<tr>
<td>Mo</td>
<td>4.9%</td>
</tr>
<tr>
<td>W</td>
<td>1.2%</td>
</tr>
<tr>
<td>Zr</td>
<td>0.05%</td>
</tr>
<tr>
<td>Nb</td>
<td>3%</td>
</tr>
<tr>
<td>Al</td>
<td>2.9%</td>
</tr>
<tr>
<td>C</td>
<td>0.04%</td>
</tr>
<tr>
<td>B</td>
<td>0.01%</td>
</tr>
<tr>
<td>Ni</td>
<td></td>
</tr>
<tr>
<td>Expose</td>
<td>0.8</td>
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<tr>
<td>$T_{HT}$</td>
<td>1300°C</td>
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</tbody>
</table>
Microstructure
Measuring the defect density

![Graph showing the relationship between exposure parameter and percent defects.](image)

Other materials designed

Nickel and molybdenum

Steel for welding

Experiment and DFT for batteries
Other materials designed

Lubricants with molecular dynamics and experiments

Drug design

Open Source Malaria competition
Applications of quantum computing to machine learning

**Accelerated** implementation of **standard** algorithms in machine learning

Development of **new machine learning** methods, quicker and better at handling missing data

Enhance underlying **first principles** predictions
Specific standard algorithm library improvements
Specific standard algorithm library improvements

Neural network requires **matrix multiplication**

Random forest requires **sorting**
Ambitious improvements in machine learning

Handling **unknown** values through superposition of quantum states

Accurate understanding of **uncertainty** in predictions

Allow organizations to **share** information but retain **privacy** of data

**Explainable** machine learning
Improved first principles quantum simulations leads to better inputs for machine learning to guide extrapolation of experimental data.
Conclusion

Opportunity for predictive technologies in material sciences and pharmaceuticals

Apply quantum implementations of standard algorithms used in machine learning

Improve first principles calculations used to augment experimental data