AlloyInter: Visualising Alloy Mixture Interpolations in t-SNE Representations

Benedikt Kantz†, Peter Waldert, Stefan Lengauer, Tobias Schreck

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Institute of Visual Computing, Graz University of Technology
†Corresponding author, benedikt.kantz@tugraz.at

Motivation: SciVis Contest 2025

Figure: Me being lost at (the east) sea. (Deadline +2 days)

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- Scrap metal recycling is crucial!
- Mixture of scraps influences outcomes.
- Task: enable material scientists to explore combinations effectively!

... and steer them towards their goal!

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Related Works

Parallel Coordinates in Manufacturing

- Goguelin et al. [1]: additive manufacturing with parallel coordinates
- Yang et al. [2]: hierarchical displays of parallel coordinates for exploration

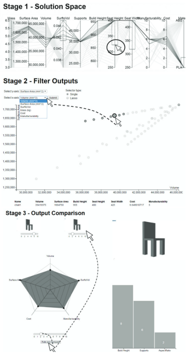

Figure: Goguelin et al. [1]

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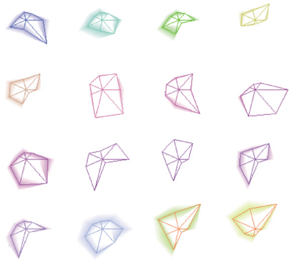

Figure: Yang et al. [2]

Related Works

Exploring the Pareto Front

- Cibulski et al. [3]: Pareto front with parallel coordinates
- Chen et al. [4]: Self-Organizing Maps (SOM) in combination with Pareto front for optimal strategies.

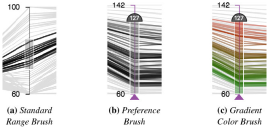

Figure: Cibulski et al. [3]

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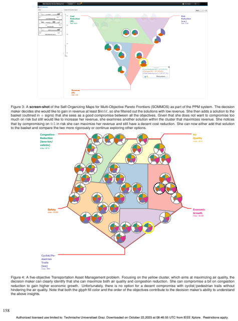
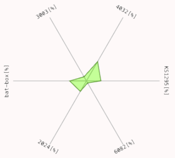


Figure: Chen et al. [4]

AlloyInter

Overview

a. Input selection ($\boldsymbol{x}$)



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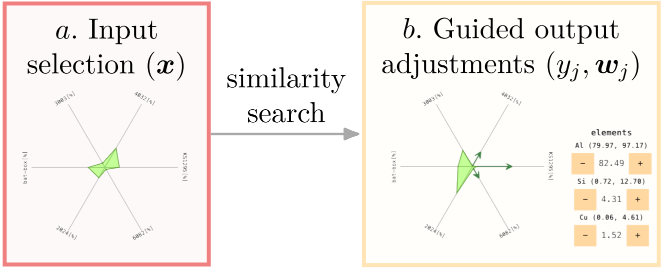

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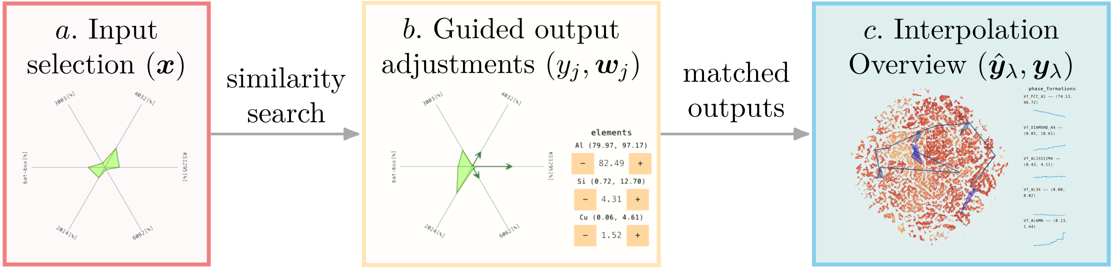

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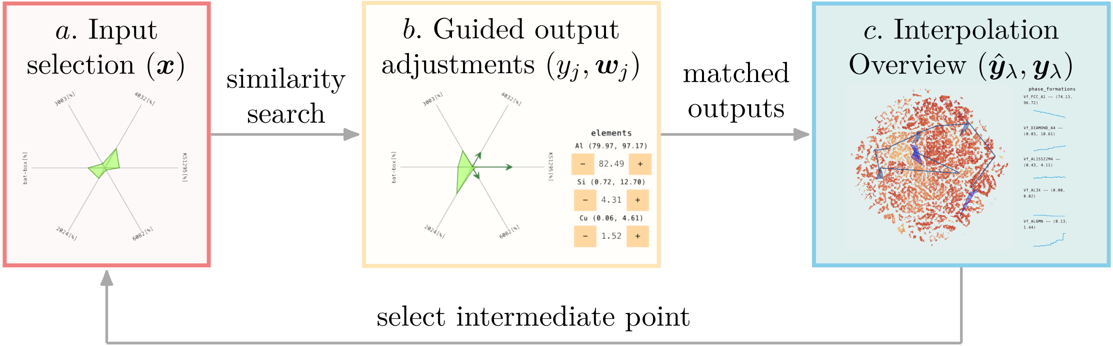
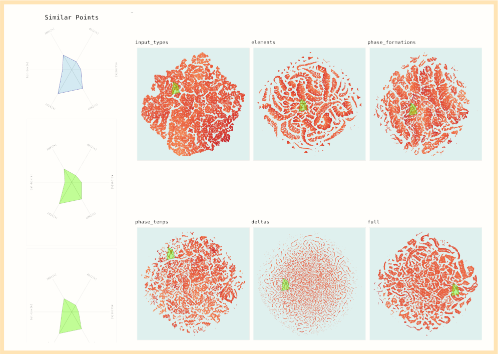


AlloyInter

a. Input selection ($\boldsymbol{x}$)

- Adjust $\boldsymbol{x} \in \Delta_6$
- Similar points from input dataset $\boldsymbol{X}$ retrieved
- Shown in t-SNE $\hat{\boldsymbol{Y}}$



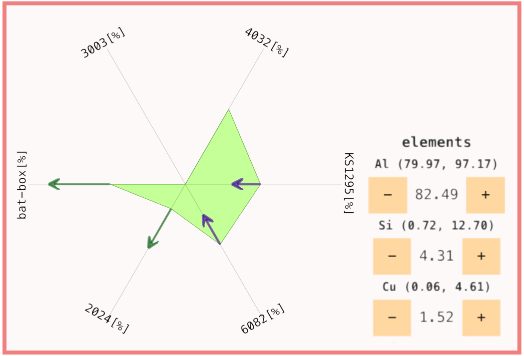
AlloyInter

b. Guided output $\boldsymbol{y}$ selection

- Adjust output $\boldsymbol{y} \in \boldsymbol{Y}$
- Suggestions using XAI[1] [5, 6]

$$\boldsymbol{w} = \Phi_{f^*}(\boldsymbol{x})$$

- Search for similar output $\boldsymbol{y} \in \boldsymbol{Y}$, hovered selection shown in t-SNE $\hat{\boldsymbol{Y}}$



[1] Using Light Gradient Boosting Machine (LightGBM), prior research indicates good performance.

AlloyInter

c. Interpolation Overview $\hat{\boldsymbol{y}}_\lambda, \boldsymbol{y}_\lambda$

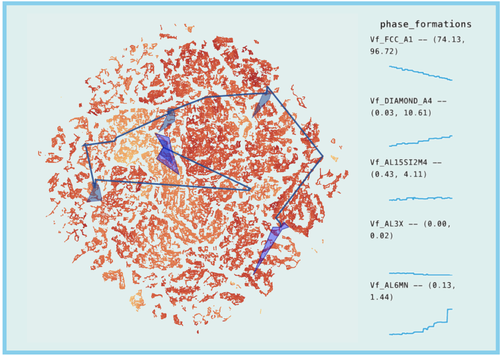
- Interpolation between selections

$$\boldsymbol{x}_\lambda = \lambda \boldsymbol{x}_0 + (1-\lambda)\boldsymbol{x}_1 .$$

- Use learned

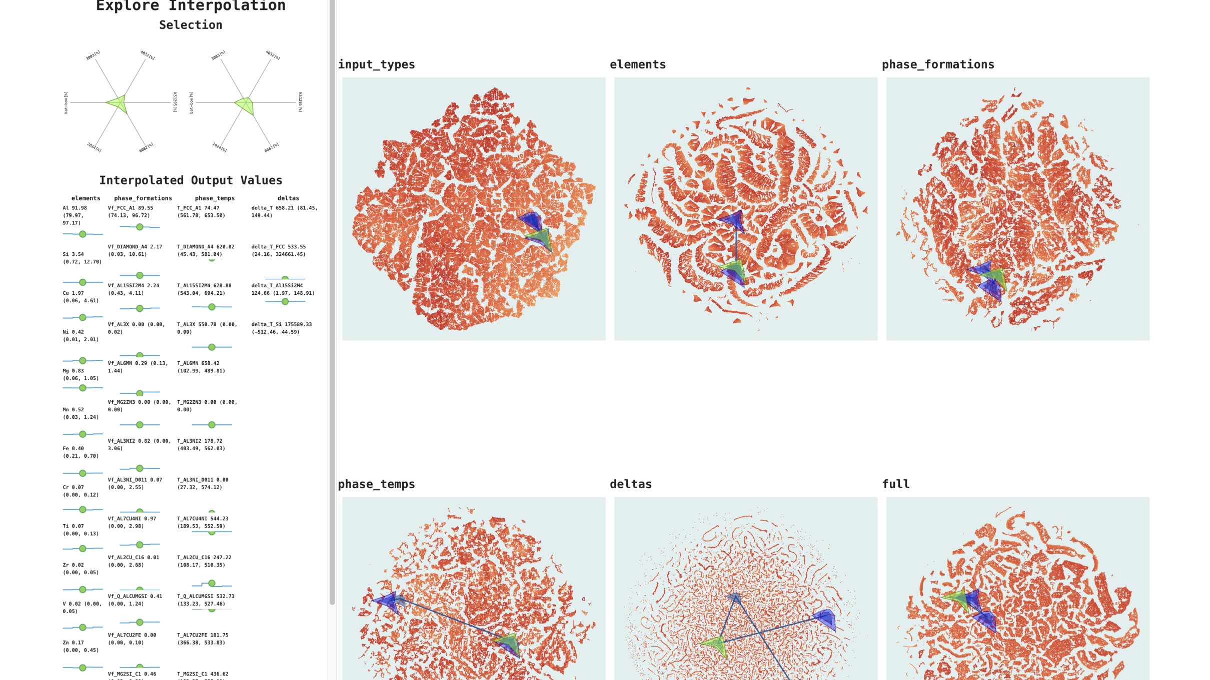
$$\boldsymbol{y}^*_\lambda = \boldsymbol{f}^*(\boldsymbol{x}_\lambda)$$

& find closest matches $\boldsymbol{y}_\lambda \in \boldsymbol{Y}$.



Demo Time!

Demo: http://hereditary.cgv.tugraz.at/alloy-inter



Explore Interpolation
Selection
3003[%]
4032[%]
KS1295[%]
6082[%]
2024[%]
bat-box[%]
Interpolated Output Values
elements
phase_formations
phase_temps
deltas
Al 91.98 (79.97, 97.17)
Si 3.54 (0.72, 12.70)
Cu 1.97 (0.06, 4.61)
Ni 0.42 (0.01, 2.01)
Mg 0.83 (0.06, 1.05)
Mn 0.52 (0.03, 1.24)
Fe 0.40 (0.21, 0.70)
Cr 0.07 (0.00, 0.12)
Ti 0.07 (0.00, 0.13)
Zr 0.02 (0.00, 0.05)
V 0.02 (0.00, 0.05)
Zn 0.17 (0.00, 0.45)
Vf_FCC_A1 89.55 (74.13, 96.72)
Vf_DIAMOND_A4 2.17 (0.03, 10.61)
Vf_AL15SI2M4 2.24 (0.43, 4.11)
Vf_AL3X 0.00 (0.00, 0.02)
Vf_AL6MN 0.29 (0.13, 1.44)
Vf_MG2ZN3 0.00 (0.00, 0.00)
Vf_AL3NI2 0.82 (0.00, 3.06)
Vf_AL3NI_D011 0.07 (0.00, 2.55)
Vf_AL7CU4NI 0.97 (0.00, 2.98)
Vf_AL2CU_C16 0.01 (0.00, 2.68)
Vf_Q_ALCUMGSI 0.41 (0.00, 1.24)
Vf_AL7CU2FE 0.00 (0.00, 0.10)
Vf_MG2SI_C1 0.46
T_FCC_A1 74.47 (561.78, 653.50)
T_DIAMOND_A4 620.02 (45.43, 581.04)
T_AL15SI2M4 628.88 (543.04, 694.21)
T_AL3X 550.78 (0.00, 0.00)
T_AL6MN 658.42 (102.99, 489.81)
T_MG2ZN3 0.00 (0.00, 0.00)
T_AL3NI2 178.72 (403.49, 562.03)
T_AL3NI_D011 0.00 (27.32, 574.12)
T_AL7CU4NI 544.23 (189.53, 552.59)
T_AL2CU_C16 247.22 (108.17, 510.35)
T_Q_ALCUMGSI 532.73 (133.23, 527.46)
T_AL7CU2FE 181.75 (366.38, 533.83)
T_MG2SI_C1 436.62
delta_T 658.21 (81.45, 149.44)
delta_T_FCC 533.55 (24.16, 324661.45)
delta_T_Al15Si2M4 124.66 (1.97, 148.91)
delta_T_Si 175589.33 (-512.46, 44.59)
input_types
elements
phase_formations
phase_temps
deltas
full

Complete System

- Optimization of alloy mixture using interactive exploration.
  - Select one input $\boldsymbol{x}_0$.
  - Select another input $\boldsymbol{x}_1$ based on close output by adjusting target $\boldsymbol{y}$.
  - Interpolate $\boldsymbol{x}_\lambda$ to explore intermediate suitable compositions.
- All in an integrated web view using t-Distributed Stochastic Neighbor Embedding (t-SNE).

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Future Work

- Exploring the Pareto Front

... by allowing custom composition of target costs.

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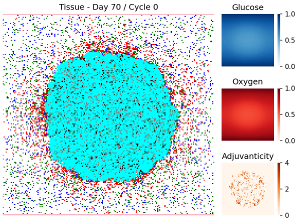

Figure: Simulation of a Tumor cell [7].

Acknowledgments

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HEREDITARY

https://ivc.tugraz.at

https://hereditary-project.eu/

Thanks for coming by :) [1]

Paper: https://arxiv.org/abs/2509.19202v1

[1] Feel free to come by the poster!

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More Ideas?