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Computational Design of Single-phase Face-centroid-cubic High Entropy Alloys using Machine Learning

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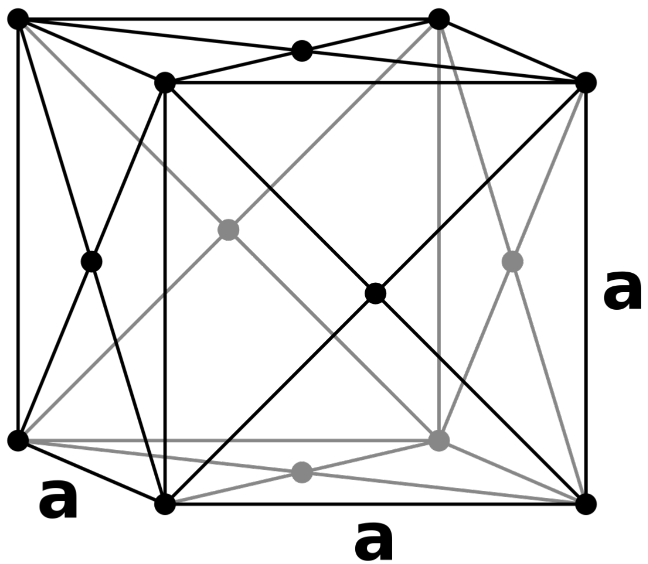
Motivations

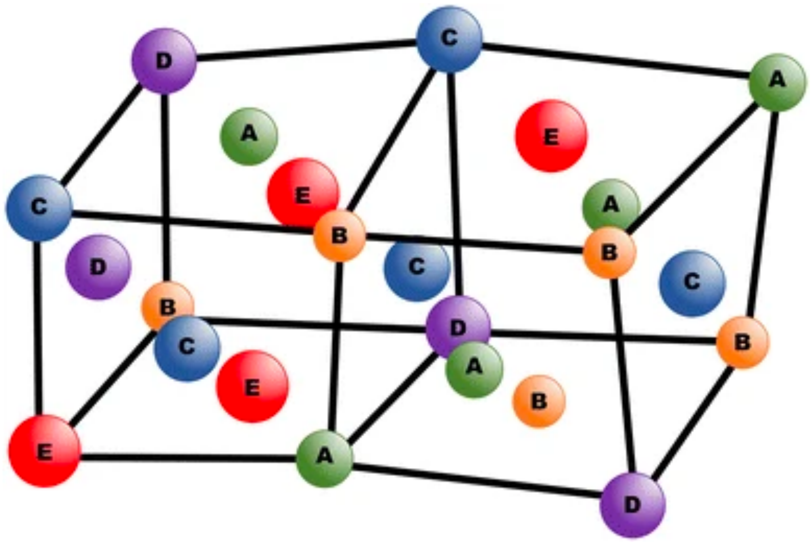
- High Entropy Alloy (HEA), 5 or more Principal elements with the concentration of each element being between 5% and 35%
- HEA has unique properties
- Single-phase HEA has homogeneous mechanical properties throughout the whole alloy

Motivations

- Properties of FCC structures: high tensile and plasticity



Face-centered-cubic (FCC) structure



A distorted face-centered-cubic structure

Motivations

- Infinite alloy composition designs
- There is a vast space to select elements and their proportions.

Pandat software

More than 10^9 calculations

	Start	End	# Steps
x%(Al)	0	50	10
x%(Co)	0	50	10
x%(Cr)	0	50	10
x%(Cu)	0	50	10
x%(Fe)	0	50	10
x%(Mn)	0	50	10
x%(Mo)	0	50	10
x%(Ni)	0	50	10
x%(Si)	0	50	10
x%(Ti)	-1	-1	-1

→ Machine Learning techniques

Project Scope

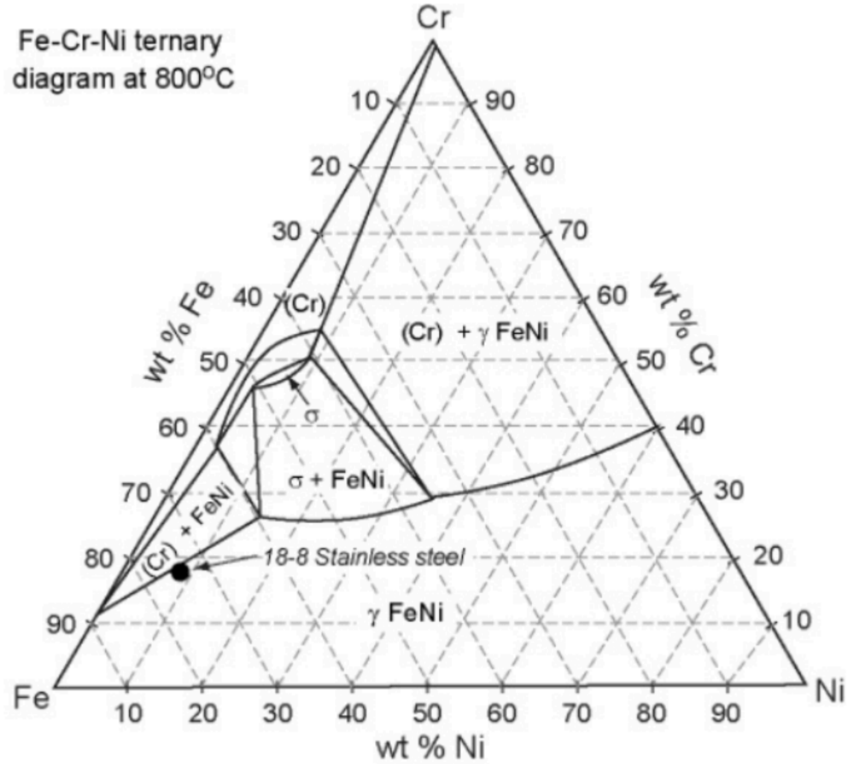
- Predict compositions of 5-component single phase FCC solid-solution High Entropy Alloy(HEA)
- using neural network classification and Genetic Algorithm

Implementation and Design

- Data preparations
- Neural network construction
  - Muti-task learning classification
  - Single-task learning classification
- Genetic Algorithm

Calculation of Phase Diagram (CALPHAD)

- A thermodynamic simulation method
- Phases of HEA are obtained by extrapolation method from binary and ternary phase diagrams



A ternary phase diagram

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Data Preparations

Step 1

Factorial design of experiment

Step 2

Data from literatures

Step 3

Search more data based on step 1

Process alloy formulas and verified in Pandat

$C_{15}^{5} = 3003$ records

With equimolar proportions, i.e. 20%

e.g. around those proportions which tend t
have high FCC ratios

High Throughput Calculations of Phase Diagram

- $C_{15}^{5} = 3003 \text{ records}$
- Every element is assigned to 20%
- T = 500, 700, 1000 and 1300 are used

Al	C	Co	Cr	Cu	Fe	Li	Mg	Mn	Mo	Ni	Si	Ti	V	Zr
x%														
20	20	20	20	20	0	0	0	0	0	0	0	0	0	0
20	20	20	20	0	20	0	0	0	0	0	0	0	0	0
20	20	20	20	0	0	20	0	0	0	0	0	0	0	0
20	20	20	20	0	0	0	20	0	0	0	0	0	0	0
20	20	20	20	0	0	0	0	20	0	0	0	0	0	0
20	20	20	20	0	0	0	0	0	20	0	0	0	0	0
20	20	20	20	0	0	0	0	0	0	20	0	0	0	0
20	20	20	20	0	0	0	0	0	0	0	20	0	0	0
20	20	20	20	0	0	0	0	0	0	0	0	20	0	0
20	20	20	20	0	0	0	0	0	0	0	0	0	20	0
20	20	20	20	0	0	0	0	0	0	0	0	0	0	20
20	20	20	0	20	20	0	0	0	0	0	0	0	0	0
20	20	20	0	20	0	20	0	0	0	0	0	0	0	0
20	20	20	0	20	0	0	20	0	0	0	0	0	0	0
20	20	20	0	20	0	0	0	20	0	0	0	0	0	0
20	20	20	0	20	0	0	0	0	20	0	0	0	0	0
20	20	20	0	20	0	0	0	0	0	20	0	0	0	0
20	20	20	0	20	0	0	0	0	0	0	20	0	0	0

Important features

FCC_num	T	f(@Fcc#1)	f(@Fcc#2)	f(@Fcc)	is_FCC	phase_num	x(Al)	x(C)	x(Co)	x(Cr)	x(Cu)	x(Fe)	x(Li)	x(Mg)	x(Mn)	x(Mo)	x(Ni)	x(Si)	x(Ti)	x(V)	x(Zr)
1	1109	0.0	0.0	1.0	1	1	10.0	0.0	0.0	18.0	18.0	18.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0	0.0
1	1129	0.0	0.0	1.0	1	1	10.0	0.0	0.0	18.0	18.0	18.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0	0.0
1	1139	0.0	0.0	1.0	1	1	10.0	0.0	0.0	18.0	18.0	18.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0	0.0
1	1143	0.0	0.0	1.0	1	1	10.0	0.0	0.0	18.0	18.0	18.0	0.0	0.0	0.0	0.0	18.0	0.0	0.0	0.0	0.0
1	317	0.0	0.0	1.0	1	1	0.0	0.0	20.0	0.0	0.0	20.0	0.0	0.0	20.0	0.0	20.0	0.0	0.0	20.0	0.0
1	400	0.0	0.0	1.0	1	1	0.0	0.0	20.0	0.0	0.0	0.0	0.0	0.0	20.0	0.0	20.0	0.0	0.0	20.0	0.0
1	500	0.0	0.0	1.0	1	1	0.0	0.0	20.0	0.0	0.0	0.0	0.0	0.0	20.0	0.0	20.0	0.0	0.0	20.0	0.0
1	600	0.0	0.0	1.0	1	1	0.0	0.0	20.0	0.0	0.0	0.0	0.0	0.0	20.0	0.0	20.0	0.0	0.0	20.0	0.0
1	800	0.0	0.0	1.0	1	1	0.0	0.0	20.0	0.0	0.0	0.0	0.0	0.0	20.0	0.0	20.0	0.0	0.0	20.0	0.0

The number of FCC phases

The ratios of FCC structures in the alloy

Whether the alloy is a single-phase FCC HEA

The number of phases present

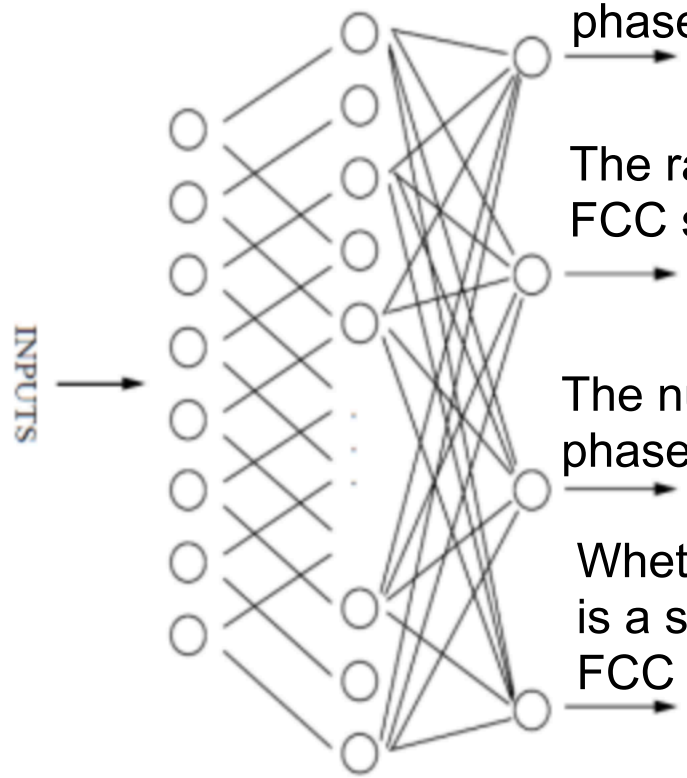
Ratios of each element in the alloy

Neural network classifier

- 16 inputs: temperatures and proportions
- Outputs: whether the alloy is FCC

Multitask Learning

Input neurons: 16



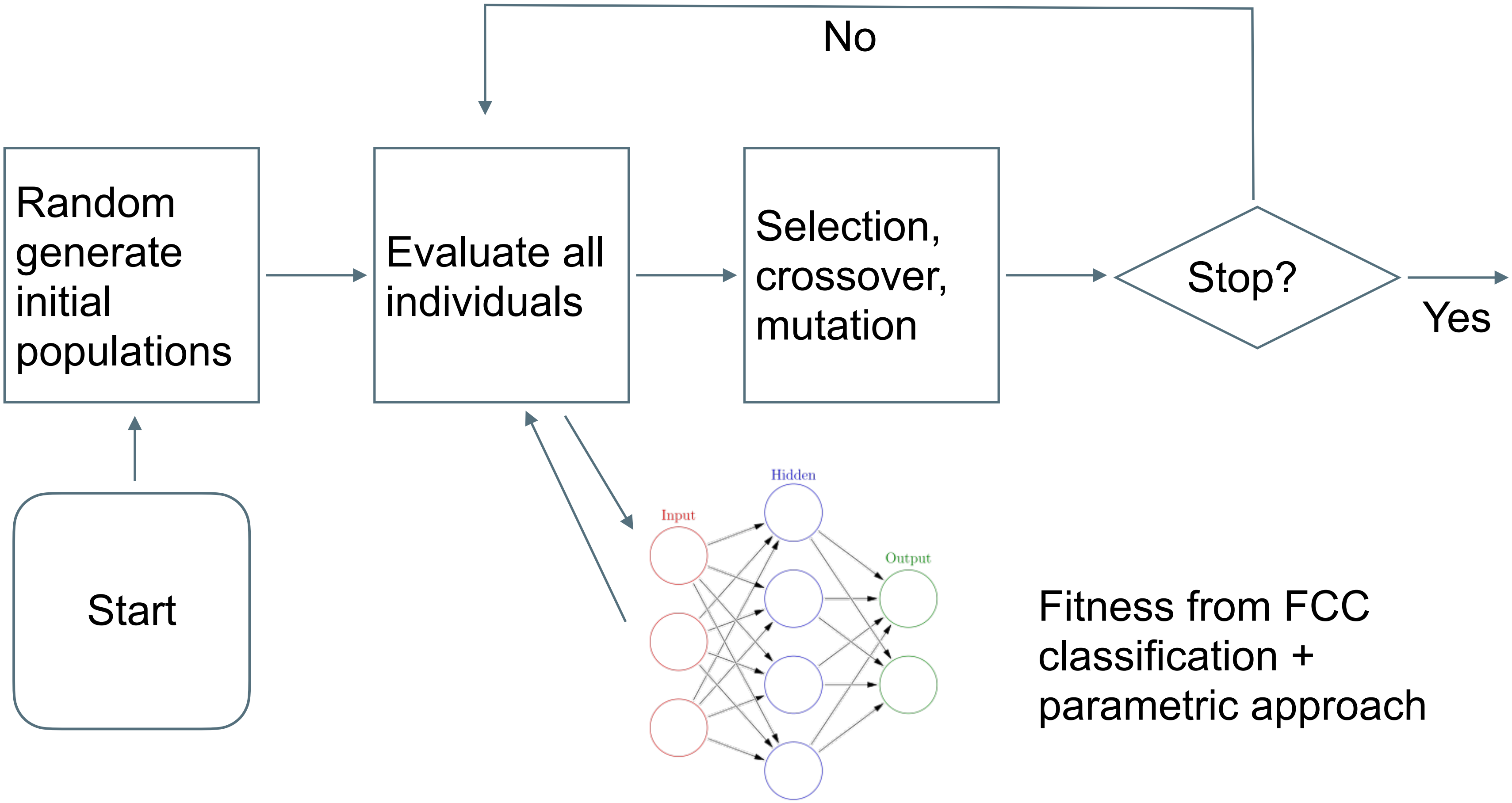
The number of FCC phases

The ratios of FCC structures

The number of phases present

Whether the alloy is a single-phase FCC HEA

Output neurons: 4

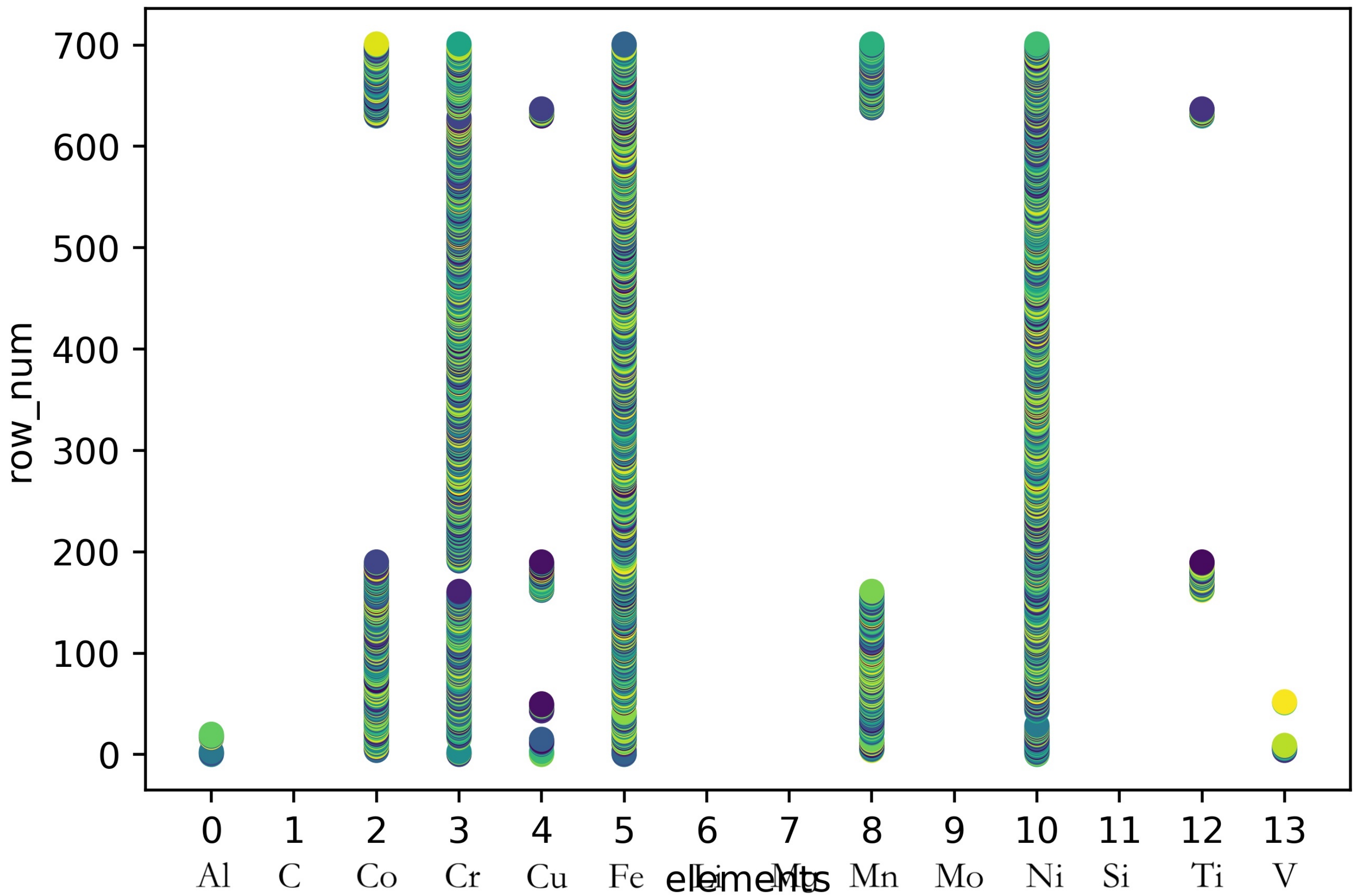

No
Random generate initial populations
Evaluate all individuals
Selection, crossover, mutation
Stop?
Yes
Start
Hidden
Input
Output
Fitness from FCC classification + parametric approach

Results

- Single task classification:
- ~ 98%, recall = 97.5%

- Muti task classification
- ~ 87%, recall = 0

Results: some discovered FCC HEA



Some discovered FCC HEA

T	Cr	Cu	Fe	Mn	Ni
975	15	13.76	14.28	29	27.96
T	Co	Cr	Fe	Mo	Ni
1025	23.08	23.45	23.35	6.87	23.25
1300	21.2	22.7	21.42	11	23.68

Element				
Cr	Cu	Fe	Mn	Ni
Al	Co	Cr	Fe	Ni
Al	Co	Cu	Fe	Ni
Co	Cu	Fe	Ni	Ti
Co	Cu	Fe	Mn	Ni
Co	Cr	Fe	Mo	Ni
Co	Cr	Fe	Mn	Ni
Co	Cr	Cu	Mn	Ni
Co	Cr	Cu	Fe	Ni
Co	Cr	Fe	Ni	Ti

Conclusion

- Classifier with good accuracy
- Discovered single-phase FCC HEA

- Add more positive cases (imbalanced data set)
- Improve the loss function to better utilize multi-task learning
- Combine the use of ML techniques and thermodynamic parameters in material science