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Sandia National Laboratories

An Investigation into the Potential for Fusel Alcohol Mixtures from Biomass Feedstocks to Improve the Efficiency of Gasoline Blends

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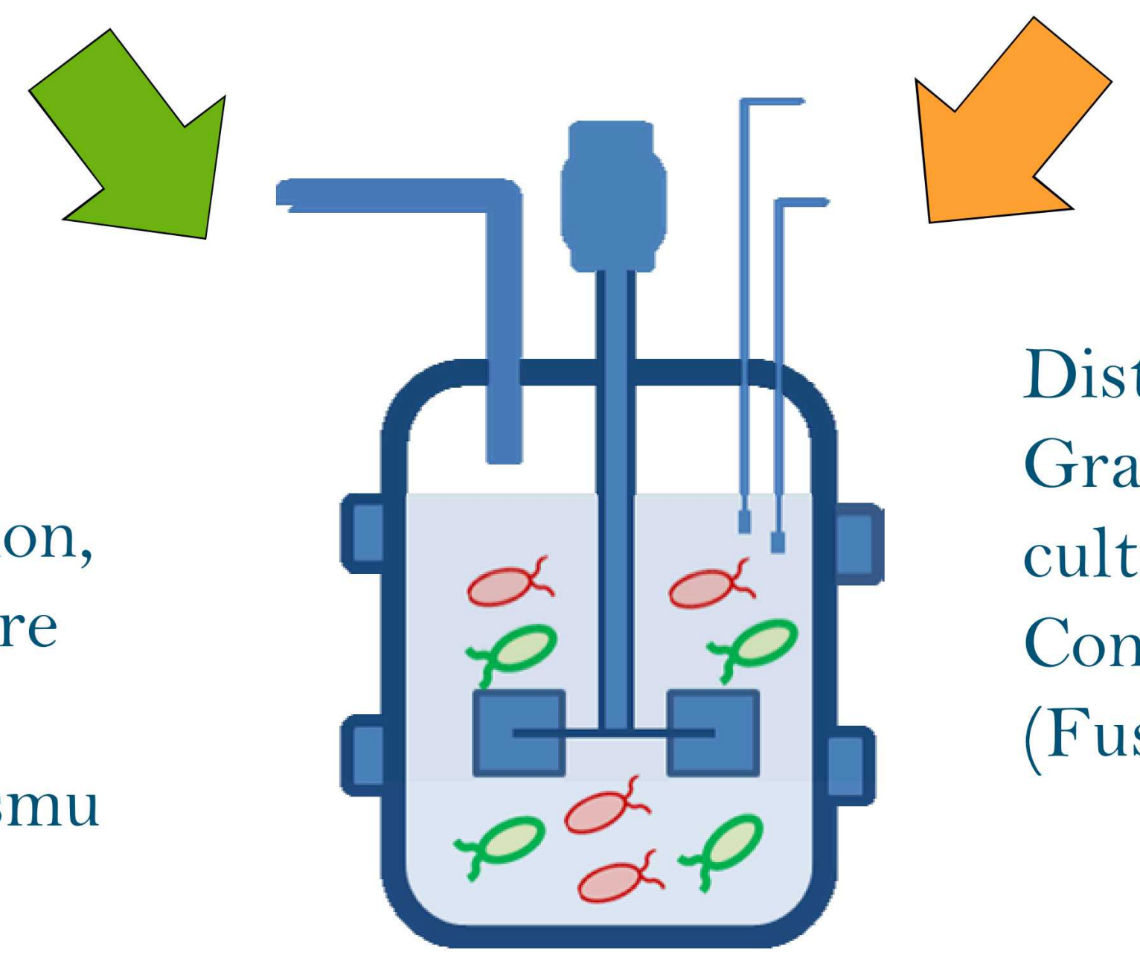
Introduction

With the intention of lessening environmental deterioration due to the effects of gasoline, bioethanol production reached 25.7 billion gallons in 2015. As a result of bioethanol production distiller's grains, a waste product rich in polysaccharides, proteins, and oils, is produced in plentiful amounts. In response, Sandia has worked to utilize this distillers grain waste product, along with other viable low cost biomass feedstocks such as algae, to produce fusel alcohol mixtures with the potential to improve efficiency of gasoline blends. Co-cultures of engineered strains of E. coli or Corynebacterium were obtained to yield fusel alcohol mixtures to then blend with various gasoline BOBs. The performance of these mixtures were measured through the use of the merit function develop under the Co-Optima program; the mixtures made the top 10 list for biomass feedstocks that improve efficiency for gasoline blends. As a continuation of this work, an investigation into the optimization of the fusel alcohol mixtures produced by the co-cultures is underway, with the intention of maximizing merit score. Then the initial co-culture reaction will be tuned to generate the optimal blend or blends deemed to maximize gasoline efficiency

7 AFFORDABLE AND CLEAN ENERGY

13 CLIMATE ACTION

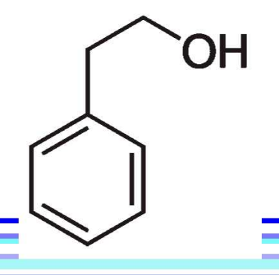
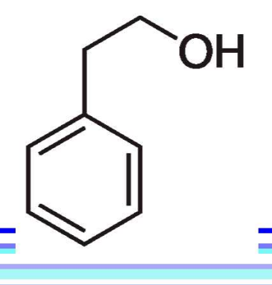
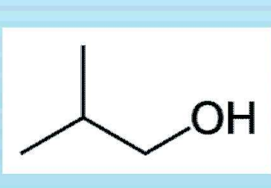
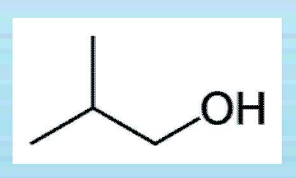
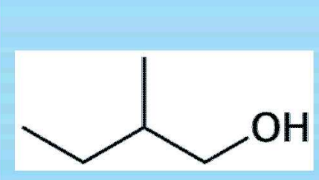
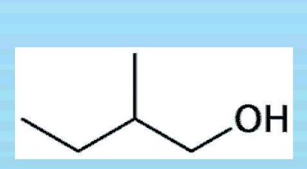
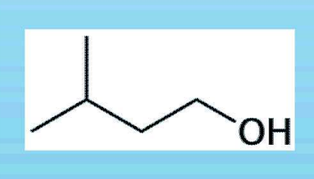
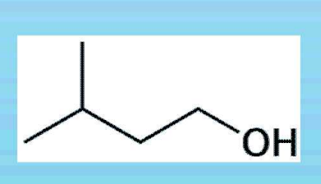
Methodology



ABY2 Algae Conversion, Co-culture on Scenedesmus, (Fusel Blend 4)

Distillers Grains Co-culture Conversion, (Fusel Blend 5)

Fermentation Process

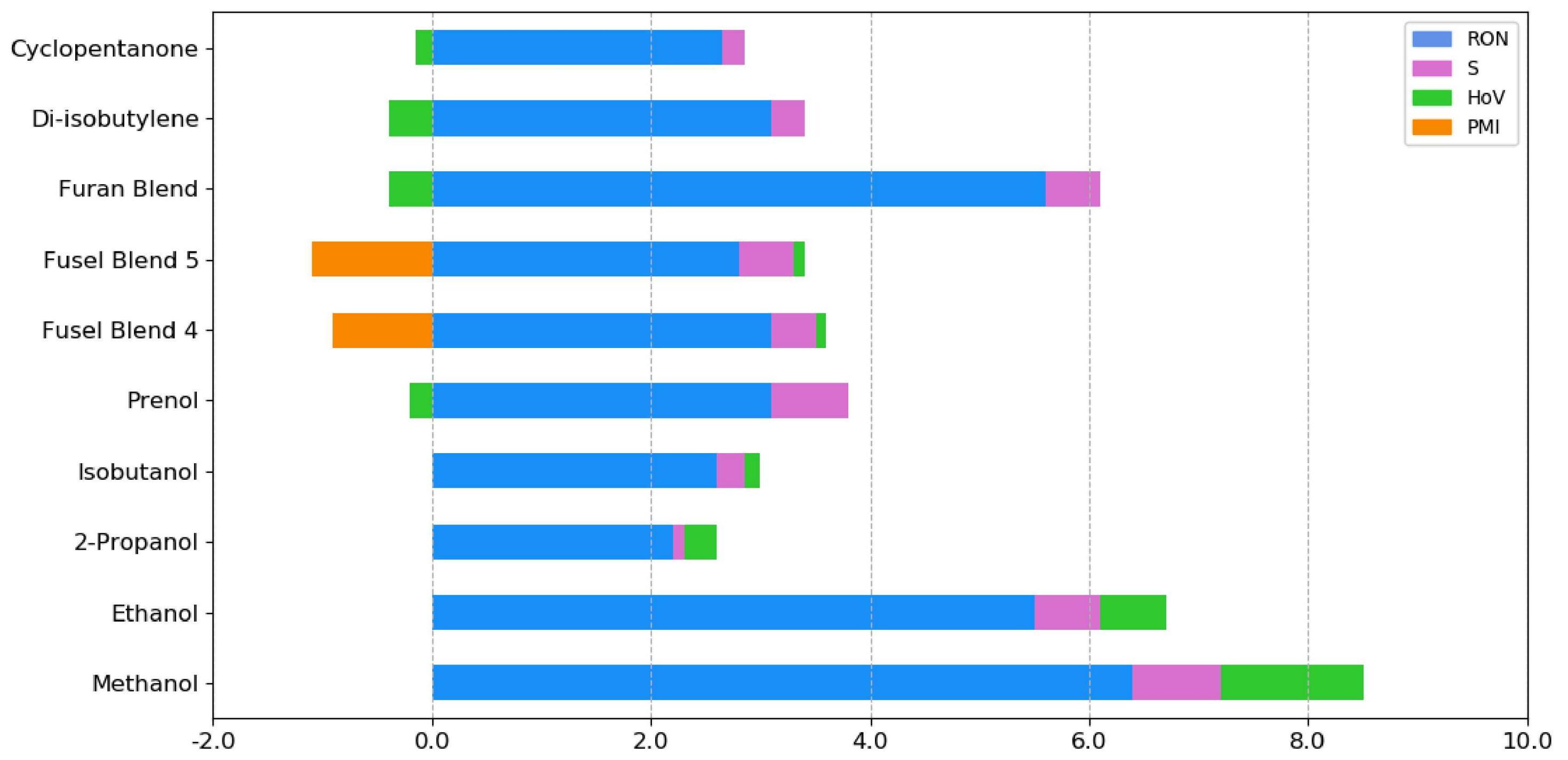
	11 %	2-Phenylethaol	8%	
	17 %	Ethanol	19 %	
	55 %	Isobutanol	57 %	
	5%	2-methyl-1-butanol	5%	
	12 %	3-methyl-1-butanol	11 %	

Results

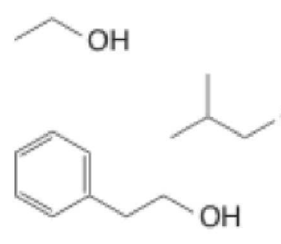
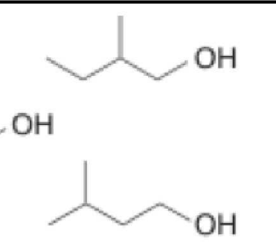
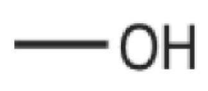
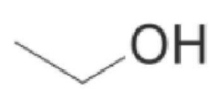
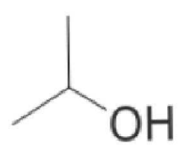
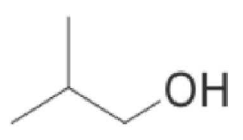
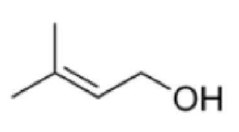
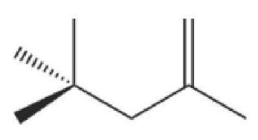
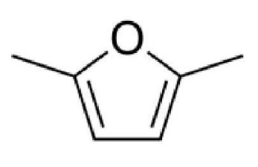
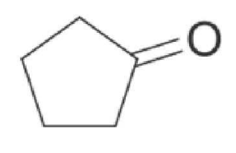
- Predicted the performance of the fusel alcohol mixtures blended with various gasoline BOB's using the Merit Function
- Compared the potential efficiency of our fusel alcohol mixtures to other Co-Optima top 10 biomass derived blendstocks

$$
\begin{aligned}
Merit = {} & \frac{(RON_{mix}-91)}{1.6} - K\frac{(S_{mix}-8)}{1.6} \\
& + \frac{0.085[ON/kJ/kg]\cdot((HoV_{mix}/(AFR_{mix}+1))-(415[kJ/kg]/(14.0[-]+1)))}{1.6} \\
& + \frac{((HoV_{mix}/(AFR_{mix}+1))-(415[kJ/kg]/(14.0[-]+1)))}{15.2} \\
& + \frac{(S_{L\,mix}-46[cm/s])}{5.4} \\
& - H(PMI_{mix}-1.6)[0.7+0.5(PMI_{mix}-1.4)] \\
& + 0.008\,{}^{\circ}C^{-1}\left(T_{c,90,conv}-T_{c,90,mix}\right)
\end{aligned}
$$

Merit function developed under the Co-optima program, dependent upon the properties (Ron, OS, HoV, S_L, PMI, and T_C) for the total blended mixture. It is used to calculate the potential increase in efficiency for varying gasoline blends.



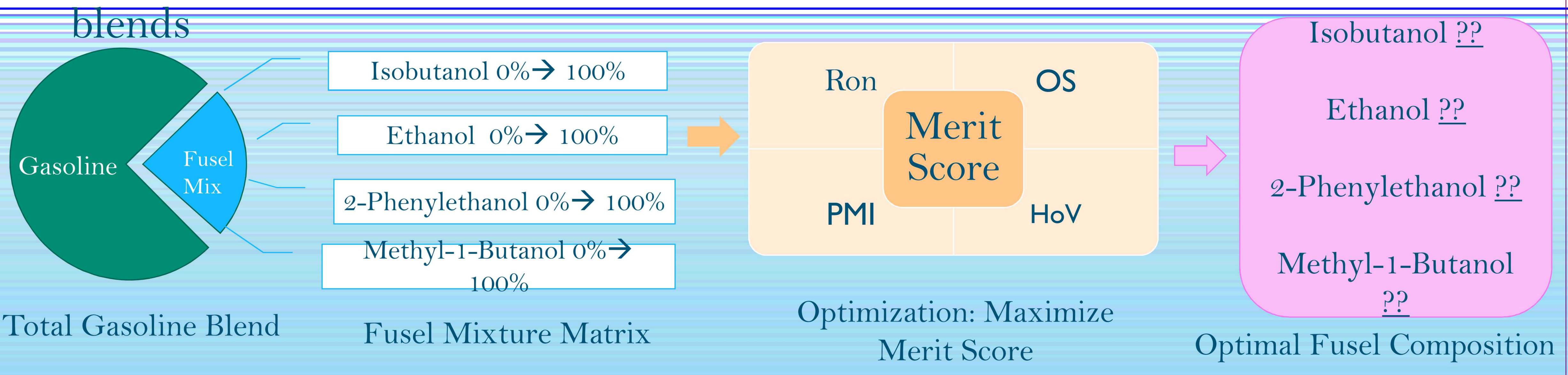
The above plot shows the merit function score of the Co-Optima top 10 blendstocks. It portrays the fuel property contribution (positive or negative) to the overall merit score of the blendstock blended at 20% in sBOB gasoline.

🟩 Strong Performance 🟦 Good Performance 🟧 Marginal Performance 🟥 Poor Performance	Algae Fusel Alcohol Blend	Distillers Grains Fusel Alcohol Blend	Methanol	Ethanol	Isopropanol	Isobutanol	Prenol	Diisobutylene	Furan Mixture	Cyclopentanone
Chemical Structure										
Blending RON	127	126	143	130	122	109	140	130	146	125
Octane Sensitivity	32	31	44	35	17	25	38	29	41	22
Heat of Vaporization [kJ/kg]	691	691	1173	919	744	508	508	318.2	355	504
Particulate Matter Index	1.8	2.0	0.05	0.06	0.08	0.17	0.17	0.57	0.57	0.74
Sooting index	32.7	32.7	6.6	10.3	19.2	26.2	26.2	68.5	NA	22
Merit Function Score at 20 vol%	4.7	4.2	11.9	9.1	2.7	4.2	6.6	4.5	8.8	3.4
Energy Density [MJ/kg]	35.2	35.2	20.1	26.8	30.7	33.1	34.4	44.3	34	32
Blending Vapor Pressure	Low	Low	High	High	High	Moderate	Low	Low	-	-
Water solubility [g/L]	237	215	1000	1000	1000	85	17	0.004	2.2	60.8
Stability Issues	Minimal	Minimal	Minimal	Minimal	Minimal	Minimal	Significant	Significant	Severe	Moderate
Infrastructure Compatability	Moderate	Moderate	Poor	Poor	Poor	Moderate	Moderate	Moderate	Moderate	Very Poor

The above figure demonstrates the viability of fusel alcohol blends 4&5 as a gasoline blendstock in comparison to other top 10 blendstocks. Fusel mixtures 4&5 generally do not illustrate properties that contribute to poor performance, while other blendstocks have at least one poor performing property.

Present & Future Work

- Identify optimal mixtures of fusel alcohols to maximize the merit function for different blending percentages
- Investigate the potential costs and benefits of properties not included in the merit function
- Tune fusel alcohol mixture production reactions to yield seemingly optimal blends



Gasoline

Fusel Mix

Isobutanol 0%→ 100%

Ethanol 0%→ 100%

2-Phenylethanol 0%→ 100%

Methyl-1-Butanol 0%→ 100%

Ron

OS

Merit Score

PMI

HoV

Isobutanol ??

Ethanol ??

2-Phenylethanol ??

Methyl-1-Butanol ??

Total Gasoline Blend

Fusel Mixture Matrix

Optimization: Maximize Merit Score

Optimal Fusel Composition

Flow chart depicting future workflow, beginning with the generation of a matrix containing the possible compositions of alcohol blends. The computational calculation of mixture properties will respectively generate a merit score for the wide range of mixtures to ultimately identify an optimal mixture or pareto front.

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