Characterising Uncertain Long-term Decarbonisation Pathways with Clustering Algorithms

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Outline

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- Uncertain long-term decarbonisation pathways
 - Energy System Modelling Environment (ESME)
- Clustering algorithms
 - (K-means, hierarchical clustering, Gaussian mixture model, spectral clustering, density-based clustering)
- Proximity matrix and transformation
- Performance evaluation of clustering algorithms
- Representative long-term pathways
- Coevolution of metrics
- Conclusions

What if we have a huge number of decarbonisation pathways?

Distribution of metrics in 2030 and 2050 across pathways



TCAR-OIL(2050) TCAR-BFL(2050) BLD-ELC(2050) BLD-OIL(2050) BLD-DH(2050) BLD-SOL(2050) BFL-DOM(2050) [AS-GAS(2050) TAS-OIL(2050) TAS-BFL(2050) TCAR-ELC(2050) [CAR-GAS(2050) TCAR-H2(2050) THGV-GAS(2050) THGV-BFL(2050) TGV-ELC(2050) TLGV-H2(2050) ELC-WND(2050) ELC-NUC(2050) ELC-CCS(2050) ELC-ORE(2050) ELC-FOS(2050) BLD-BIO(2050) BLD-GAS(2050) H2-BCCS(2050) H2-CCCS(2050) H2-ELC(2050) H2-GCCS(2050) H2-GAS(2050) IND-BIO(2050) IND-COA(2050) IND-ELC(2050) IND-GAS(2050) IND-H2(2050) IND-0IL(2050) THGV-ELC(2050) THGV-H2(2050) THGV-OIL(2050) TLGV-OIL(2050) TLGV-BFL(2050)

Scatter plots showing relationship between key metrics in 2050





Motivation

- Whole energy system models, such as UK TIMES (~2000 techs), Irish TIMES (1700 techs), are essential tools to help policy-makers decide long-term decarbonisation pathways
- However, future is highly uncertain! Model is extremely sensitive to input assumptions!
 - Technology cost, resource availability, etc.
- Uncertainty analysis
 - Global sensitivity analysis (Fais et al., 2016; Pye et al., 2015)
 - Modelling to generate alternatives (Price and Keppo, 2017; Li and Trutnevyte, 2017; DeCarolis et al., 2016)
- Unmanageable number of pathways!
- How can we find patterns out of these to support policy-making?
 - Representative pathways
 - Represent the whole set of pathways
 - Different enough from each other
 - Relationship between technologies
- Challenges: extremely high-dimensional and unlabeled!!
- Clustering algorithms come to help!



Research Procedure



SMF

Energy System

Modelling Environment



Energy System Modelling Environment

Spatially explicit UK regions

Systems optimisation via linear programming





Uncertain Long-term Decarbonisation Pathways

- Taken from existing study (Pye et al., 2019)
- -80% GHG reduction in 2050 (rel. to 1990), -53% in 2030
- Uncertain characteristics
 - Capital costs
 - Commodity costs
 - Build rates
 - Resource availability
- Variation of parameters

(by 2050)

- Mature: +/-10%
- New: +/-30%
- Novel/emerging: +/-50%
- Monte Carlo technique
- 600 pathways



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Pye, S, Li, P-H, Keppo, I, O'Gallachoir, B. 2019. Technology interdependency in the United Kingdom's low carbon energy transition, Energy Strategy Reviews, 24, 314-330.



Clustering algorithms in action



Source: <u>George Seif</u>, The 5 Clustering Algorithms Data Scientists Need to Know. <u>https://towardsdatascience.com/the-5-clustering-algorithms-data-scientists-need-to-know-a36d136ef68</u> https://rstudio-pubs-static.s3.amazonaws.com/199446_36b75293d1544636a278369aefd9a094.html



Proximity Matrix

- Proximity matrix: representing the similarity between pathways for clustering analysis
- Proximity: summation of differences of metrics between pathways over modelling years

$$\Box d_{i,j} = \sqrt{\sum_{y} \sum_{m=1}^{M} (x_{i,y,m} - x_{j,y,m})^2}$$

Only consider 2030 and 2050 for simplification

- Issues
 - Pathway might be dominated by a few key metrics, such as nuclear
 - Need pathway sets with various distribution characteristics for robustness testing
- Metric transformation is thus applied!



Metric Transformation

Difference between transformed metric and average metrics



Standarisation





Reduce the influence of metrics with extreme high values Sectoral standarisation



Treat every metric within a sector equally



Influence of Metric Transformation on Clustering

Metric transformation	Characteristics of clustered metrics
None	 All metrics are close to averages in 2030 Power sector is the only sector with obvious variation in 2050, as shown in Figure 6(a)
Power	 Influence of high variance of a few metrics, such as those in the power sector, is mitigated Variation of some metrics becomes more obvious, such as bioenergy consumption in the buildings (BLD-BIO) in 2030 and hydrogen production by gas and CCS (H2-GCCS) in 2050
Standardisation	 Variance of every metric is treated equally Variance of many clustered metrics is more obvious in both 2030 and 2050
Sectoral standardisation	 Relatively high variance of metrics in a sector are more likely to be revealed Trade-off between metrics in a sector is clearer, such as oil cars (TCAR-OIL) and EVs (TCAR-ELC) in 2050, as shown in Figure 6(b)



Performance evaluations and the choice of number of clusters

- No predefined categories for evaluation
- Criteria: cohesion and separation

Indicator	Sum of squared error (SSE)	squared (SSE) Davies-Bouldin (DB) Calinski- Harabaz (CH)		Calinski- Harabaz (CH) Dunn (DN)	
Formula	$\sum_{c=1}^{C}\sum_{i\in c}\sum_{m=1}^{M}\ x_{i,m}\ $	$\frac{1}{C} \sum_{c=1}^{C} \max_{c'} \left\{ \frac{S_c + S_{c'}}{\ \bar{x}_c - \bar{x}_{c'}\ } \right\}$	$\frac{\sum_{c=1}^{C} n_c \ \bar{x}_c - \bar{x}_g\ ^2 / (C_c)}{\sum_{c=1}^{C} \sum_{i \in c} \ x_i - \bar{x}_c\ ^2 / (C_c)}$	$\frac{\min_{i \in c, j \in c'} \ x_i - x_j\ }{\max_{i, j \in c} \ x_i - x_j\ }$	$\frac{1}{N} \sum_{c=1}^{C} \sum_{i \in c} \frac{b_i - a_i}{\max\{b_i, a_i\}}$
Improvement direction	\rightarrow	\downarrow	1	↑	↑

- Elbow measure
 - Turning point
 - Ideal number of clusters



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Performance comparison of clustering algorithms

Metric	Clustering	Clustering validity index							
transformation	algorithm	SSE	DB	CH	DN	SL			
	KM	1	1	1	2	1			
Nono	HC	2	1	2	1	2			
None	GMM	3	3	3	3	3			
	SC	4	4	4	4	4			
	KM	1	1	1	2	1			
Dowor	HC	3	2	3	1	3			
Power	GMM	2	3	2	3	2			
	SC	4	4	4	4	4			
	KM	11	2	1	2	2			
Standardiastian	HC	3	1	3	1	1			
Standardisation	GMM	2	4	2	3	3			
	SC	4	3	4	4	4			
	KM	1	2	1	2	1			
Sectoral	HC	3	1	3	1	3			
standardisation	GMM	2	3	2	3	2			
	SC	4	4	4	4	4			

Performance of clustering algorithms



Distribution of pathways across identified clusters by clustering algorithm





Representative Long-term Decarbonisation Pathways

- Elbow measure:
- 5 clusters could be ideal for pathway characterisation



• Centroid pathways of clusters as representative pathways!

Average deviation of Metrics in representative pathways





Identified Representative Pathways (2030 and 2050)

Key characteristics				Higher High lov Higher	district hea w carbon e H2	ating elc		Higher e More CO More oil	CS and BE	ng ICCS			
Rey characteristics		Lower CCS High low ca	S arbon elc			Higł Higł	ner CCS ner EV			Similar But mo	to #4 bre fossil	fuel in 2030	
	Sector		Clus	ter 1	Clus	ter 2	Clus	ster 3	Clus	ster 4	Clust	er 5	
	Sector		2030	2050	2030	2050	2030	2050	2030	2050	2030	2050	
		BIO	+				-		+		-		
		DH			+	++	+		-		-		
Buildi	ing	ELC				-				+		+	
		GAS	-		-				-		+		
		SOL				+							
		CCS						++	-	++		+++	
		FOS	-				+						
Electri	city	NUC		+++	+	+++		-			-		
		ORE	+	++		++							
		WND		++		++		++					
		BCCS		-		-			+	+++		++	
Hydro	gen	CCCS				+		+	-			-	
		GCCS		-		+		+		-		-	
	Δ٧	GAS			+						+		
	Αv	OIL	++		-	-				+	-	+	
		ELC				-	+	+++				-	
	CAR	H2		+		++		-		-		-	
Trans-port —		OIL	+		+				+	+++	+	+++	
	GAS	GAS		-									
	110 V	OIL		+									
		ELC				+				-		-	
	LGV H2	H2				+							
		OIL	+				+			+	-	+	

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Correlation between key metrics in 2050



Coevolution of metrics across pathways with hierarchical clustering



Cluster	Cluster name	Cluster metrics	Negatively correlated
colour			clusters
Orange	H_2 production with gas for	H ₂ production (via gas steam methane reforming (SMR)) and	Brown (-0.51)
	transport	use in the transport sector.	
Green	Renewable generation	Renewable power generation options, costs metrics, selected	Brown (-0.48)
		transport electrification.	
Sky blue	Passenger car	Passenger transport electrification; system electricity; aviation	Brown (-0.66)
	electrification	biofuels.	
Brown	H_2 with bio CCS, car oil	Biomass resource; H ₂ production with CCS & bioenergy; oil in	Orange (-0.51), Green (-
	use	cars; system oil use; H2 and oil use in industry.	0.48), Sky blue (-0.66)
Pink	Building electrification,	Electrification of buildings – as per the description in Table 2;	Blue (-0.94)
	power gen. w/ CCS	CCS in power sector, and system gas use.	
Blue	District heating	District heating (and storage). Clustered with transport biofuel	Pink (-0.94)
		use but weak correlation.	

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Pye, S, Li, P-H, Keppo, I, O'Gallachoir, B. 2019. Technology interdependency in the United Kingdom's low carbon energy transition, Energy Strategy Reviews, 24, 314-330.



Conclusions

- Performance of clustering algorithms is highly sensitive to the distribution of pathways
- For evenly distributed pathways (generated by Monte Carlo approach for uncertainty analysis), k-mean is the most robust choice
- Sectoral standarisation can emphasise key metrics in a sector without being overshadowed by a few key metrics with extremely high values in other sectors
- For coevolution of metrics across pathways, hierarchical clustering is useful to identify highly correlated metric sets
- More detailed technologies can be taken into account!
- Can be applied to characterise pathways from various models
- Future tasks: characterise pathways with strong constraints, such as no CCS





Thanks for your attention!

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UCL Energy Institut	Metric	Definition	Units		
<u> </u>	ELC-WND	Wind generation level	TWh		
	ELC-NUC	Nuclear generation level	TWh		
	ELC-CCS	CCS generation level	TWh		
	ELC-ORE	Other renewable generation level	TWh		
	ELC-FOS	Fossil generation level	TWh		
	BLD-BIO	Building bioenergy consumption	TWh		
	BLD-ELC	Building electricity consumption	TWh		
	BLD-GAS	Building gas consumption	TWh		
	BLD-OIL	Building oil consumption	TWh		
	BLD-DH	Building district heating consumption	TWh		
	BLD-SOL	Building solar energy consumption	TWh		
	H2-BCCS	H2 production by biomass gasification with CCS	TWh		
	H2-CCCS	H2 production by coal gasification with CCS	TWh		
	H2-ELC	H2 production by electrolysis	TWh		
	H2-GCCS	H2 production by gas (SMR) with CCS	TWh		
	H2-GAS	H2 production by gas (SMR)	TWh		
	IND-BIO	Industry bioenergy consumption	TWh		
	IND-COA	Industry coal consumption	TWh		
	IND-ELC	Industry electricity consumption	TWh		
	IND-GAS	Industry gas consumption	TWh		
	IND-H2	Industry hydrogen consumption	TWh		
	IND-OIL	Industry oil consumption	TWh		
	TAS-GAS	Aviation & shipping - gas	TWh		
	TAS-OIL	Aviation & shipping - oil	TWh		
	TAS-BFL	Aviation & shipping - biofuel	TWh		
	TCAR-ELC	Cars - electricity	TWh		
	TCAR-GAS	Cars - gas	TWh		
	TCAR-H2	Cars - H2	TWh		
	TCAR-OIL	Cars - oil	TWh		
	TCAR-BFL	Cars - biofuels	TWh		
	THGV-ELC	Heavy goods vehicles - electricity	TWh		
	THGV-GAS	Heavy goods vehicles - gas	TWh		
	THGV-H2	Heavy goods vehicles - H2	TWh		
	THGV-OIL	Heavy goods vehicles – oil	TWh		
	THGV-BFL	Heavy goods vehicles - biofuels	TWh		
2019 Internationa	TLGV-ELC	Light goods vehicles - electricity	TWh		
	TLGV-H2	Light goods vehicles - H2	TWh		
	TLGV-OIL	Light goods vehicles - oil	TWh		



Comparison between clustering algorithms

MiniBatchKMea A \$	nityPropagatio	n MeanShift	SpectralClustering	Ward Ag	lomerativeCluster	ingDBSCAN	OPTICS	Birch	GaussianMixture
<u>()</u> .01s	<u>60</u> 5.40s	0	s <u>.395</u>	0		<u>()</u>	<u>O</u>	0,025	<u>()</u> .01s
.02s	6.06s		s	A	.125	O1 .01s	.75s	O .025	.01s
.03s	3.67s		is .14s	.53	.405	.01s	.74s	.025	.015
.025	3.0 9 s		.205		205		.745	.028	.ots
	*	*	*					**	
.02s	* 2.88s	. 1	<u>.s</u> <u>.25s</u>	. 15	.10s	• .02s	. 75s	.02s	.01s
.01s	2.56s	.1 av Workshor	<u>is .20s</u>	.09	.06s	01s	.75s	.02s	01s

Source: scikit-documentation: 2.3 clustering https://scikit-learn.org/stable/modules/clustering.html