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Life cycle thinking and machine learning for urban metabolism assessment and prediction

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ABSTRACT

The real-world urban systems represent nonlinear, dynamical, and interconnected urban processes that require better management of their complexity. Thereby, we need to understand, measure, and assess the structure and functioning of the urban processes. We propose an innovative and novel evidence-based methodology to manage the complexity of urban processes, that can enhance their resilience as part of the concept of smart and regenerative urban metabolism with the overarching intention to better achieve sustainability. We couple Life Cycle Thinking and Machine Learning to measure and assess the metabolic processes of the urban core of Lisbon's functional urban area using multidimensional indicators and measures incorporating urban ecosystem services dynamics. We built and trained a multilayer perceptron (MLP) network to identify the metabolic drivers and predict the metabolic changes for the near future (2025). The prediction model's performance was validated using the standard deviations of the prediction errors of the data subsets and the network's training graph. The simulated results show that the urban processes related to employment and unemployment rates (17%), energy systems (10%), sewage and waste management/treatment/recycling, demography & migration, hard/soft cultural assets, and air pollution (7%), education and training, welfare, cultural participation, and habitat-ecosystems (5%), urban safety, water systems, economy, housing quality, urban void, urban fabric, and health services and infrastructure (2%), consists the salient drivers for the urban metabolic changes. The proposed research framework acts as a knowledge-based tool to support effective urban metabolism policies ensuring sustainable and resilient urban development.

1. Introduction

It can be argued that urbanization and globalization are accelerated by technological advancements. These are often, the main drivers that influence and change the spatial and functional structure of the urban areas today. These two main drivers -urbanization and globalization- appear interdependent in how their influence upon urban systems, resulting in the increase of the global urban population. Specifically, the urban global population has grown rapidly from 751 million (30% of the world's population) in 1950 to 4.2 billion (55% of the world's population) based on recent data from 2018 and it is projected to reach 6.7 billion (68% of the world's population) by 2050 (United Nations (UN) 2018). It has been well documented that much of the world's economic activities are now concentrated in urban areas, generating 80% of the global gross domestic product (GDP) (Ferrao & Fernandez, 2013) while simultaneously demanding nearly 75% of energy consumption (UN-Habitat, 2021) to support this activity. Therefore, urban areas are now responsible for metabolizing or consuming a vast proportion of natural resources in support of their inhabitants' needs, generating a high rate of pollution and waste, and stress upon society. On the other hand, urban cores areas facilitate research and development, economic and social development while simultaneously providing the necessary infrastructure to support health care and well-being by employing a variety of advanced technologies.

As part of the context of urban metabolism, an urban core area can be seen as a complex ecosystem requiring a neverending exchange of materials, energy, and information between its processes/systems and as a consequence must expand beyond its boundary in order to function and grow. This means that urban core areas require more "space" to survive than they typically encompass, perhaps suggesting that they lack

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efficiency. Thus if one were to make urban sustainability, a priority, one must find ways to cope with the environmental, social, and economic challenges initiated by the increased demand for more resource extraction and consumption, that generates excess waste production. By doing so, it is essential to understand, measure, and therefore assess the complexity of the different urban metabolic processes/systems and the services they deliver that are critical for human survival and well-being. Different methodologies have been proposed and applied to measure urban metabolism with the intention of creating a more sustainable society since 1965, when it was first introduced by Wolman. In Section 2, we provide a detailed analysis of the applied methodologies, highlighting their benefits and deficiencies. Summarizing the main shortcomings of these methodologies, we identify challenges related to the determination of the urban processes/systems' boundaries and the lack of an integrated and multi-impact approach, including the lack of the impact of the ecosystem services on urban sustainability.

Attempting to address the above-stated limitations, we propose an original methodology that assesses the multidimensional urban metabolic processes by coupling Life Cycle Thinking (LCT) with Machine-Learning (ML) from an ecosystem services perspective. We build and assess a smart and regenerative metabolic scenario that can simultaneously assess the main drivers for changes in purchasing power per capita in our study area, the urban core of the functional urban area of Lisbon (UCL) indicating, in which *degree, where* metabolic changes will occur in the near future and the level of impact on the overall urban system. We accept that the urban metabolism is derived indirectly from GDP changes expressed in purchasing power per capita (IpC) when the analysis is at an urban core area scale as in our study area. The methodological approach applied in this study is described in detail in the Research framework Section 3, followed by the Results Section 4. These sections have raised several hypotheses and issues that we summarize in Section 5, Discussion. Finally, we highlight the main findings and novelty of our study in the Conclusions Section 6.

The objectives of this study are based on five key methodological steps. They are 1) to identify the main limitations of previously applied methodologies of urban metabolism (UM), 2) to introduce a new and novel methodology that addresses these limitations and contributes to the extent of state-of-art thinking, 3) to create evidence-based knowledge from the multidimensional metabolic methodology under the perspective of ecosystem services 4) to identify the main drivers for urban metabolic changes; and 5) to predict metabolic changes for a near future. This newly developed methodology should be considered as a tool for optimizing planning and design, in support of critical policy-making by measuring and assessing urban metabolism and thus ensuring urban sustainability.

2. Background

The concept of urban metabolism (UM) has been evolved and adapted over time in response to scientific and technical changes. Based on the literature, the concept of UM appeared first using Material flow Analysis (MFA), then the Emergy (embodied energy) method influenced by the work of Odum, 1983 or occasionally the Ecological Footprint (EF) method, and most recently coupled with Life Cycle Assessment (LCA) (Goldstein, Birkved, Quitzau & Hauschild, 2013). UM's first approach is related to Industrial Ecology incorporating tools of MFA to assess material, water, food, and nutrient fluxes and stocks within urban systems and the resulting outcomes to other systems in the form of pollution, waste, or exports (Sahely, Dudding & Kennedy, 2003 as cited in Pincetl, Bunje & Holmes, 2012). MFA is based on the principle of mass balance (mass in = mass out + stock changes), where matter cannot either be created or destroyed. Zhang, 2013 supports that by directly adding the weight of different materials, the quality differences among these materials are ignored. Moreover, the role of energy flows that drive all material flows throughout the urban metabolic process is also ignored. Scholars attempting to understand metabolic processes thoroughly have combined MFA along with energy flow analysis (EFA), focusing on physical material and energy flows in urban ecosystems, under one analytical framework (MEFA) (Kennedy, Pincetl & Bunje, 2011 as cited in Zhang, Lu, Tam & Feng, 2018).

Moving the focus beyond mass, UM's emergy-based accounting method (EMA) ensures that the emergy (solar energy) used directly or indirectly for the creation and flow of all products or services is accounted. Hence the qualitative differences of the materials and energy flows that were ignored previously are now highlighted (Pincetl et al., 2012; Zhang, 2013). The Emergy method, initially originated by Odum in 1988, is based on ecology, thermodynamics, and general systems theory fields, emphasizing the fundamental dependence of cities on ecological processes that can occur only due to solar energy. Emergy is measured in solar emergy joules (seJ) and emphasizes standard units for all materials, energy, nutrient, and waste flows in biophysical systems (Pincetl et al., 2012). The main challenge of this method and, therefore, its limitation relies on the difficulty of converting materials and energy flows of different units to the seJ metric (Pincetl et al., 2012).

In line with Goldstein et al. (2013), these first generations of UM methods fail to fully quantify the environmental impacts of larger-scale systems. In an attempt to face the limitations of the first generations of UM, in the last decade, authors have coupled UM with LCA assessing the environmental consequences of cities (Goldstein et al., 2013; Loiseau, Roux, Junqua, Maurel & Bellon-Maurel, 2014; Peuportier & Herfray, 2010) and various urban processes (Ramos & Rouboa, 2020). In general, life-cycle assessment (LCA) is a cradle-to-grave standardized method accounting the associated environmental impacts of products or services over their different life cycle phases. Pincent, 2012 states that LCA provides methodologies and tools appropriate to quantify the materials or UM, including processes generating inputs and outputs.

However, various shortcomings of LCA applications have been pointed out. Beloin-Saint-Pierre et al., (2017) in their review of the methodological choices of UM studies, found out that besides the fact that Life cycle modeling is essential for sustainability assessment, "the life cycle of complex system like UM is not clearly framed in most UM studies under review". Mirabella, Allacker & Sala, (2018) reviewing the application of LCA at the city scale, affirms that "no applications of comprehensive LCA at urban scale exist to date", in other words, "no complete urban LCA studies exist so far". The conventional LCA methodologies provide only relative sustainability evaluation since they ignore ecosystem services' role in supporting human activities (Bakshi, Ziv & Lepech, 2015 as cited in Liu, Charles & Bakshi, 2019). Another essential deficiency relies on system boundary determination; the results may reflect the authors' subjectivity in system boundary, leading to errors or contradictory results. Moreover, LCA is data-dependent. Therefore, if the life cycle inventory is not complete may not return the total environmental impact of the process/product under analysis. As LCA uses a single standard approach ignoring multiple factors (environment, technology, and capital) that may affect the target process, its environmental assessment lacks a multi-angle approach (Wang et al., 2020).

Hybrid modeling approaches coupling different urban metabolism methodologies have been developed to cope with the shortcomings of the applied methods previously described. Authors have integrated Emergy and LCA to assess sustainability in urban systems under study (Cano Londoño et al., 2019; Li et al., 2020; Santagata, Zucaro, Fiorentino, Lucagnano & Ulgiati, 2020) to reach maximum environmental benefits as well as the most cost-effective technologies according to the financial limits (Falahi & Avami, 2019). Wang et al., 2020 reviewed the EMA and LCA methods and suggested their coupling development to be based on three aspects; the aggregate emergy flow table, the indicator system construction, and indicator evaluation methods to exert the maximum functional advantages of each method. Westin et al., 2020 have combined MFA and LCA to identify environmental hotspots of urban consumption. García-Guaita et al., (2018) integrated MFA and LCA under UM approach for urban environmental evaluation. The main limitations of this study include a lack of local data and the absence of social and economic indicators in the analysis. Attempting to describe the links between the different variables of UM, authors have coupled the network approach (NE) with MFA, with ecological network analysis (ENA), Environmentally-Extended Input-output analysis (EE-1/O), and LCA (Berloin et al., 2017). This type of methodologies are data-driven, allowing comparisons and recognition of future trends. Urban systems' metabolic patterns have been studied using the Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM) accounting method relating fluxing and funds, and therefore offering applicable and coherent indicators (Rallo† and Zucaro, 2019; Perez-Sanchez et al., 2019). However, this method appears to be static, allowing the observation of a system's evolution but not its dynamics (Ginard-Bosch and Ramos-Martín, 2016). LCA has also been combined with agent-based models (ABM) make it suitable to evaluate the sustainability of complex systems through behavior-driven modeling (Marvuglia, Navarrete Gutiérrez, Baustert & Benetto, 2018; Walzberg, Dandres, Merveille, Cheriet & Samson, 2019; Micolier et al., 2019). Baustert and Beneto, 2017 categorize the coupling of ABM and LCA based on the direction of the information flow as; *ABM-enhanced LCA* with the ABM to feed the LCA model, *LCA-enhanced ABM* opposite to the previous, and as *ABM/LCA symbiosis* when the information is looping between the two models (Marvuglia et al., 2018). Although there are already examples of using ABM for simulating LCA, there is still a long road to be made in order to make them more user-friendly and less computing expert-oriented.

3. Research framework

In this study, we couple Life Cycle Thinking (LCT) and Machine Learning (ML) adopting smart and regenerative urban metabolism to assess purchasing power per capita (IpC) changes driven by the multidimensional metabolic processes of our study area UCL (Fig. 1). IpC indicator is a composite indicator drawn from the factor analysis calculation based on 16 variables selected by Statistics Portugal (Table C in Annex). The IpC is the main factor resulting from the factor analysis, as it explains more than 45,6% of the 16 variables' total variation after rotation. The indicator explains the purchasing power expressed on a daily basis, in per capita terms using the figure of Portugal as a reference (STATISTICS PORTUGAL, 2017). Purchasing power by definition is "the quantity of goods and services that can be bought with a monetary unit," observing the real economic activity trends (production, consumption) globally concentrated in urban core areas as mentioned in the introduction. Therefore indirectly, it can give a perception of the flows of materials, energy, and information representing the holistic and multidimensional perspective of urban metabolism associated with the production of waste and environmental impacts.

We understand LCT as a systematic approach that offers a holistic vision of all generated impacts of an urban system, improving its multidimensional performance throughout its entire value chain. Adopting LCT to study urban metabolism allows coping with urban sustainability from both macro and micro scale points of view. UM requires large-scale data and life cycle assessment, as standardized methodology requires more detailed data (Maranghi, Parisi, Facchini, Rubino & Basosi, 2020). Coupling LCT with Artificial Intelligence (AI) and Machine Learning (ML) methods enables us to adopt a data-driven and bottom-up-based methodology capable of building knowledge from the systems dialectic in an iterative way. AI is the development of a certain type of computational technique that can perform tasks simulating human intelligence and behavior to solve practical problems (Goodfellow, Bengio & Courville, 2016; Openshaw & Openshaw, 1997). AI is powered by ML. ML consists of algorithms that learn by example using historical data to predict outcomes and uncover patterns not easily identified by humans. The obtained knowledge can be used by ML algorithms to make predictions about future trends. ML is found in literature associated with different names such as; pattern recognition, statistical modeling, data mining, knowledge discovery, predictive analytics, data science, adaptive systems, and self-organizing systems (Domingos, 2015). ML algorithms based on the learning role fall into three categories; supervised learning, unsupervised learning, and reinforcement learning (Graves A. 2012; Sathya & Abraham, 2013). The supervised ML algorithms reveal insights, patterns, and relationships from a labeled (classified) training dataset (input-output pairs) using regression or classification techniques. On the contrary, unsupervised ML algorithms infer patterns from a dataset without reference to known or labeled outcomes. Reinforcement learning (RL) reflects ideas from psychology. The RL algorithms learn using trial and error and related reward interactions with their environment to find optimal policies without being taught by examples (Fu, Liu, Ling & Cui, 2014).

Artificial neural network (ANN) techniques have been extensively applied overall the last thirty years in several areas, e.g., medicine (diagnosis and decoding brain signals), security (face recognition), Linguistics (language recognition and translations), governance (decision support systems and smart cities), Banking and Insurance (loans and insurance attribution), Pharmaceutical (risk analysis), non-renewable resources exploration (prediction), advertising and marketing (customer profiling), remote sensing (automatic and semiautomatic analysis of satellite images), human and physical geographical studies (spatial data pattern & data relationships analysis), Landscape and urban planning (conflict management and urban growth simulation), and so forth (Bação, Lobo & Painho, 2005; Fischer, 1998, 2006; Henriques, Bação & Lobo, 2012; Openshaw & Openshaw, 1997; Venugopal & Baets, 1994). With the advent of big data, and more specific geoBig data, and the increased parallel computing, ANN methods, and techniques, also commonly known as the Neurocomputing field of studies, have gained more and more applicability across all types of scientific domains, ranging from art, social sciences & humanities to more philosophical and ethics studies. To the best of authors' knowledge, coupling LCT and ML to study urban metabolism changes has not been applied before.

Our research framework is understood from an ecosystem services perspective. Specifically, under the urban metabolism concept, an urban core area could be seen as an ecosystem where biotic components are in conjunction with abiotic components of their environment, developing circular and ongoing complex relationships. Studying the functional aspects of an ecosystem responsible for the flows of energy and the cycles of materials and the beneficial ecosystem services to human well-being, we are able to apply this knowledge for the design and planning of the urban environment. Therefore, maintaining the urban ecosystem services is the key to sustain urban places, reinforce system resilience, ensuring public health and well-being.

After defining the goal and the scope of our study, we start implementing our research framework by conducting the Life Cycle Inventory (LCI). The LCI is the first phase to implement a LCT methodology. By definition, LCI is the quantification of inputs (material and energy flows) and outputs (emissions to air, water, or soil) of a system under study. In this phase, all the processes involved in the life cycle of a product/process/or system of processes have to be identified along with the data related to these processes, and their system boundaries need to be determined (Khanali, Mobli & Hosseinzadeh-Bandbafa, 2017; Nabavi-Pelesaraei, Rafiee, Mohtasebi, Hosseinzadeh-Bandbafha & Chau, 2018). Doing the LCI, we identify the indicators representing the smart and regenerative urban metabolic processes, and we set their system boundaries by defining the dimensions and subdimensions. Last, we selected the related measures (Data components) to these urban metabolic processes and again classified them under the urban ecosystem services perspective. We use for case study the urban core of the functional urban area (FUA) of Lisbon, Portugal, and its administrative boundaries as overall system boundary to test the proposed methodology. Having finished the LCI, we couple it with ML to obtain evidence-based knowledge on the drivers and dynamics of the metabolic processes of our study area.

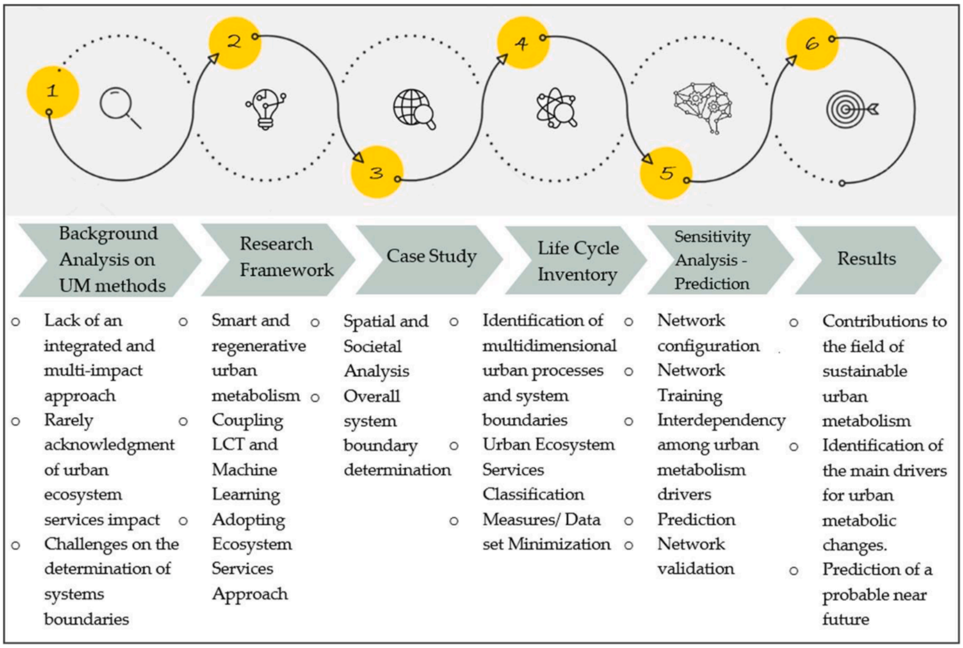

Fig. 1. Research framework flow.

3.1. Case study analysis

In this subsection, we delineate our study area by setting the overall system boundary for our study and analyze it by conducting spatial and societal analysis. Hence, in this paper, we use the urban core of the functional urban area (FUA) of Lisbon city to assess and predict its smart and regenerative urban metabolism. FUAs consist of densely urban zones with more than 50,000 inhabitants (Copernicus, 2018). Using the core area of Lisbon FUA (UCL), we delimit the area of strong metabolic influence of the city of Lisbon.

The UCL is located in the country's center, crossed by the Tagus River and it is met by the Atlantic Ocean to the west (Fig. 2). The UCL, is divided into nine municipalities: Lisbon, Loures, Odivelas, Amadora, Oeiras, Cascais in the northern margin of the Tagus River and Almada, Seixal and Barreiro in the southern margin. The UCL covers approximately 1040 (1036.847397) square kilometers, of which 19% is classified as agricultural, 27.3% is covered by forest, natural areas, and urban green areas, and 51% by the built environment (Copernicus Programme, 2018). It has an annual average air temperature of 16,4°C (Celsius), a maximum of 22 °C, and a minimum of 11,6°C and the annual precipitation of the region of Lisbon is 692,3 mm (Statistics Portugal (INE), 2018).

The total resident population of UCL is 1690,014 inhabitants (equal to 16% of the total population of Portugal), with a population density of 1629.9 inhabitants per square kilometer (Statistics Portugal (INE) 2011). The 49% of the total population of UCL constitutes the labor force almost equally divided by sex (24,19% male and 24,87% female). Nearly 14,5% of the population is classified as young people under the age of 15, while elderly people over the age of 65 make up account for 20% of UCL's population (Statistics Portugal (INE) 2011). The UCL has an aging index of 120 elderly per 100 young people. The percentage of the foreign population as the total resident population of the area is 9% (Statistics Portugal (INE) 2011).

The regional economic activities are based mainly on the tertiary sector, and the primary and manufacturing activities are low. In 2018, the tertiary sector contributed to 87.0% of the regional gross value added (GVA), the secondary sector (including construction) to 12.6%, and only 0.4% of the GVA comes from the primary sector (EC, 2021). The region of Lisbon comprises a science and tech hub concentrating the highest expenditure on Research and Development (R&D) activities, 1.62% of GDP whilst the national average is 1.35%. In addition, it concentrates the highest share of personnel and researchers in R&D, 16.6% per 1000 active inhabitants whereas the average for Portugal is a bit lower at only 11.1% (PORDATA, 2018). Looking at the index purchasing power per capita of UCL, we see that the municipality of Lisbon has the greatest purchasing power (219.6) in-country, with Portugal as reference value 100. Six to nine municipalities of UCL, including the municipality of Lisbon, have purchasing power above the national average and three (Loures, Seixal, and Odivelas) below (PORDATA 2018).

Finishing our analysis, we examine a couple more urban metabolism parameters related to energy and material flows. The total electricity consumption in the study area is 4198.2 kgwatt-hour per inhabitant, while the national electricity consumption is 4754.4 kWh/inhab. The municipality of Seixal has the highest consumption 7072.70 kWh/inhab., following Lisbon with 6038.40 kWh/inhab. The overall waste selectively collected[1] of the UCL (not including the municipality of Odivelas) is 154 kg per inhabitant while the national average value is 103 kg/inhab. The municipality of Cascais has more than double the national value (250 kg/inhab.), following Almada with 191.5 kg/inhab. and Lisbon with 179.8 kg/inhab. (PORDATA, 2018).

[1] Waste selectively collected in eco-points, door-to-door, recycling yards and special circuits of various materials and biodegradable urban waste selected for organic recovery the energy consumption (INE, 2018)

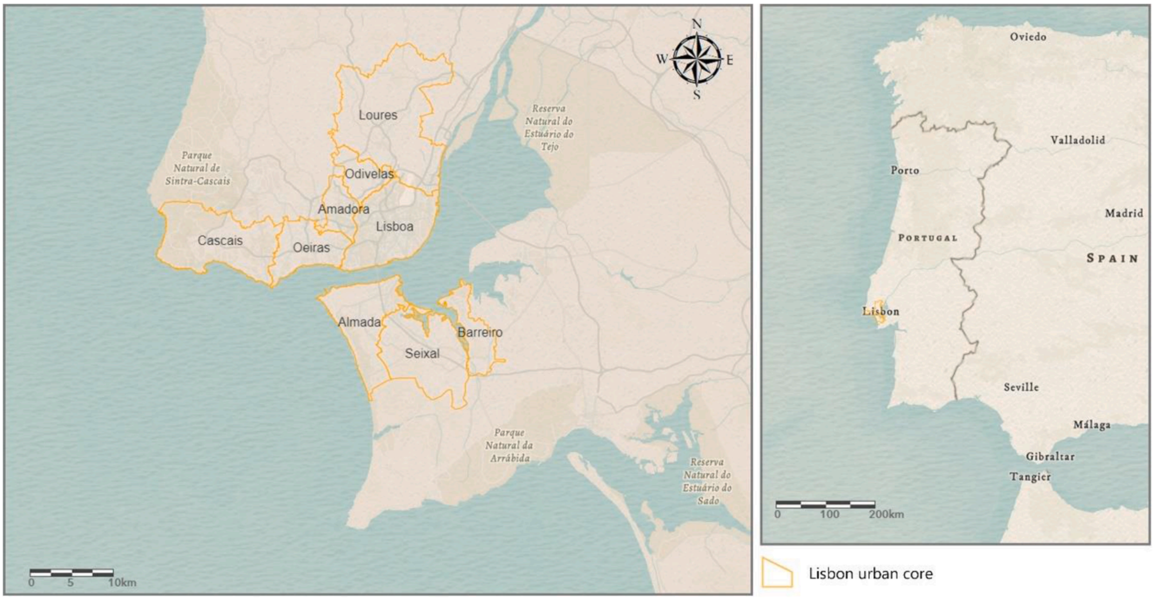

Fig. 2. Geographical position of the study area.

Table 1
Multidimensional metabolic analysis in the perspective of urban ecosystem services.

Dimensions	Subdimensions	Indicators of urban processes	Urban Ecosystem Services
Social	Urban Governance	Public participation and stakeholder engagement in decision making	Cultural services
	Human Capital	Demography and migration	Regulating services
		Fertility and Mortality	Supporting services
		Education and training	Cultural services
	Economic Capital	Welfare	Provisioning services
		Employment-unemployment rates	Supporting services
		Economy	Provisioning services
		Touristic attractiveness	Cultural services
		Social inventions	Provisioning services
	Health system	Healthcare services and infrastructure	Regulating services
Cultural	Cultural mapping	Hard/ Soft cultural assets	Cultural services
	Cultural Participation	Cultural participation	Cultural services
	Urban agriculture	Urban agriculture	All ecosystem services
Technological	Housing	Housing quality	Supporting services
	Mobility-Accessibility	Road network	Supporting services
		Railway	Supporting services
		Maritime transport	Supporting services
	Urban structure	Urban fabric	Supporting services
		Urban void	No ecosystem services
	Innovation	Research and development	Cultural services
	Utility systems and infrastructure	Sewage and Waste management/treatment/recycling	Regulating services/ Supporting services
		Energy systems	Provisioning Services
		Water systems	Provisioning Services
		Urban safety	Regulating services
Ecological	Habitat-ecosystems	Habitat-ecosystems	All ecosystem services
	Environmental protection	Environmental protection	All ecosystem services
	Environmental quality	Air pollution	All ecosystem services
		Air temperature	All ecosystem services
		Soil exploitation	All ecosystem services
		Water quality	All ecosystem services

3.2. Life cycle inventory in urban ecosystem services perspective

Under the smart and regenerative concept, the metabolic processes are not just the linear consumption of energy and materials that generate waste, but instead, they are circular, ongoing, and co-evolutionary, eliminating waste by regenerating resources using technology (Peponi & Morgado, 2020). As urban cores are metabolic complex systems that exist through the interactions and interdependencies of all social-cultural-technological-ecological urban processes, a holistic, multidimensional systematic network approach is essential to evaluate their urban metabolism.

The social dimension of an urban metabolism includes all urban processes related to urban governance, human capital, economic capital, and health system. The focus is to plan and design a smart and regenerative social structure that improves and even eliminates situations perceived as social problems (social exclusion, inequalities, poverty, limited health care access, and so on). The cultural dimension of urban metabolism contains processes related to the hard and soft cultural

Table 2
Dataset for measuring smart and regenerative urban metabolism. (Where U.E.S. = urban ecosystem services, C.S.= cultural services, R.S.= regulating services, S.S.= supporting services, P.S.= provisioning services, N.S.= no services, A.S.= all ecosystem services.).

	Indicators	Data components/ measures	Timespan	U.E.S.
Social	Public participation and stakeholder engagement in decision making	Registered voters in the elections for the Local Authorities: voters and abstention	2009, 2017	C.S.
	Demography and migration	Resident population, according to the Census by major age group and sex:(0–14, 15–64, 65+)	2001, 2011	R.S.
		Annual population growth (Individual): (Natural increase, Migration net increase)	2011, 2018	R.S.
		Foreign population with legal resident status as a% of the resident population by sex (Proportion%)	2011, 2018	R.S.
		Population density (Ratio- Average no. of individuals/ Km^2)	2011, 2018	R.S.
	Fertility and Mortality	Crude birth rate - ‰	2011, 2018	S.S.
		Crude death rate - ‰	2011, 2018	S.S.
	Education and training	Enrolled students in higher education by sex: (Males, Females)	2011, 2018	C.S.
		Enrolled students in pre-school, primary, lower secondary, and upper-secondary education by sex: (Males, Females)	2011, 2018	C.S.
		Schools in pre-school, primary, lower secondary, and upper-secondary education	2011, 2018	C.S.
		Teaching staff in pre-school, primary, lower secondary, and upper-secondary education	2011, 2018	C.S.
	Welfare	Total dependency rate (Ratio -%)	2011, 2018	P.S.
		Proportion of buying power (Proportion -%)	2011, 2017	P.S.
		Purchasing power per capita - Index (number) -%	2011, 2017	P.S.
		Average monthly earnings of employees by the level of education and by sex: (Upper-secondary and post-secondary non-tertiary; Higher)	2011, 2018	P.S.
	Employment- unemployment rates	Activity rate, according to the Census: by age group (25–34, 35–44) and by sex (total) (Rate -%)	2001, 2011	S.S.
		Unemployment rate, according to the Census: by age group (25–34, 35–44) and by sex (total) (Rate -%)	2001, 2011	S.S.
		Employment rate, according to the Census: by age group (25–34, 35–44) and by sex (total) (Rate -%)	2001, 2011	S.S.
	Economy	Value of goods imported and exported by enterprises: (Imports, Exports) (€)	2011, 2018	P.S.
		Industrial, commercial, public, military, and private units (sqkm) (class 12,100, urban atlas)	2012, 2018	P.S.
		Survival rate of Enterprises born 2 years before (Rate-%)	2011, 2018	P.S.
	Touristic attractiveness	Guests in tourist accommodations per 100 inhabitants (Ratio -%- individual)	2011, 2018	C.S.
		Total incomes of tourist accommodations: total (€ - Thousands)	2011, 2018	C.S.
	Social inventions	Public Administration Retirement Fund: retirees and pensioners	2011, 2018	P.S.
		Social Security and Public Administration Retirement Fund pensions in total of the resident population aged 15 and over (Rate -%)	2011, 2018	P.S.
	Healthcare services and infrastructure	Inhabitants per doctor and pharmacist (Ratio)	2011, 2018	R.S.
		Pharmacies and mobile medicine depots	2011, 2018	R.S.
		National Health Service: beds in general and specialist hospitals	2011, 2018	R.S.
Cultural	Hard/ Soft cultural assets	Live shows: performances	2011, 2018	C.S.
		Live shows: box-office revenue (€ - Thousands)	2011, 2018	C.S.
		Cinema: screenings	2011, 2018	C.S.
		Cinema: box-office revenue (€)	2011, 2018	C.S.
		Museums: Number	2013, 2018	C.S.
		Art galleries and others temporary exhibition spaces (No.)	2011, 2018	C.S.
		Art galleries and other places for temporary exhibitions: exhibitions	2011, 2018	C.S.
		Cultural facilities: Number	2011, 2019	C.S.
		Town Council expenditure on culture and sports as a% of total expenditure: (Proportion -%)	2011, 2018	C.S.

(*continued on next page*)

Table 2 (*continued*)

	Cultural participation	Museums: total visitors (individual)	2013, 2018	C.S.
		Cinema spectators (No.)	2011, 2018	C.S.
		Live shows spectators (No.)	2011, 2018	C.S.
		Sports and leisure facilities (sqkm) (class 14,200, urban atlas)	2012, 2018	C.S.
	Urban agriculture	Arable land (annual crops), Permanent crops, Pastures (sqkm) (classes 21,000, 22,000, 23,000, urban atlas)	2012, 2018	A.S.
Technological	Housing quality	Licensed buildings by type of building work (New constructions- Extensions, alterations, and reconstructions)	2011, 2018	S.S.
		Buildings, according to the Census by type: Mainly residential - Mainly non-residential	2001, 2011	S.S.
		Conventional dwellings: total (Dwelling)	2001, 2018	S.S.
		Average bank valuation of flats by type: (Dwelling typology 2-berdoom, 3-bedroom) (Mean- €)	2011, 2018	S.S.
	Road network	Fast transit roads, other roads and associated land (sqkm) (classes 12,210, 12,220 urban atlas)	2012, 2018	S.S.
	Railway	Railways and associated land (sqkm) (class 12,230, urban atlas)	2012, 2018	S.S.
	Maritime transport	Port areas (sqkm) (class 12,300, urban atlas)	2012, 2018	S.S.
	Urban Fabric	Continuous urban fabric (S.L. > 80%) (sqkm) (class 11,100, urban atlas)	2012, 2018	S.S.
		Discontinuous dense urban fabric (S.L. 50% - 80%) and Discontinuous medium density urban fabric (S.L. 30% - 50%) (sqkm) (classes 11,210, 11,220, urban atlas)	2012, 2018	S.S.
	Urban void	Land without current use (sqkm) (class 13,400, urban atlas)	2012, 2018	N.S.
	Research and development	Employees in high technology sectors: by economic activity (research activities)	2011, 2018	C.S.
	Sewage and Waste management/ treatment/recycling	Urban waste by type of destination t (tonne): (Landfill, Energy recycling, Organic recycling, Recycling)	2011, 2018	S.S. R.S.
		Urban waste selective collection per inhabitant (Ratio-kg/ inhab.)	2011, 2018	S.S. R.S.
		Urban waste collection per inhabitant (Ratio-kg/ inhab.)	2011, 2018	S.S. R.S.
		Dwellings connected to sewerage systems (Proportion -%)	2011, 2018	S.S. R.S.
	Energy systems	Electricity consumption per inhabitant by type of consumption kWh (kilowatt-hour) / inhab. - Ratio: (Street Lighting, State Buildings, non-Domestic, Domestic, Industry, Agriculture)	2011, 2018	P.S.
		Natural gas consumption per inhabitant (Ratio - Nm^3/ inhab.)	2011, 2018	P.S.
		Fuel sales for consumption t(ton): (Butane gas, Propane gas, Liquefied petroleum gas (LPG), Unleaded petrol 98, Unleaded petrol 95, Fuel diesel)	2011, 2018	P.S.
	Water systems	Water supplied/consumed per inhabitant (ratio- m3/ inhab.)	2011, 2018	P.S.
	Urban safety	Inhabitants per firemen (Ratio- individual)	2011, 2018	R.S.
		Crimes registered by the police: total and for some categories of crime: (Domestic violence against spouse or similar; Motor vehicle theft; Burglary in residence; Burglary in commercial or industrial building; Total)	2011, 2018	R.S.
		Deaths in road traffic accidents	2011, 2018	R.S.
		Injuries in road traffic accidents	2011, 2018	R.S.
		Pedestrian accidents deaths	2011, 2018	R.S.
		Pedestrian accidents	2011, 2018	R.S.
Ecological	Habitat-ecosystems	Urban Atlas (classes 3, 4, 5 including green urban areas)	2012, 2018	A.S.
	Environmental Protection	Expenditure by municipalities on the environment: by environmental management and protection domains (Euro-Thousands): (Protection of biodiversity and landscape; Protection against noise and vibrations; Waste management; Other areas)	2011, 2018	A.S.
		Expenditure of municipalities in environment as% of total expenditure (Proportion-%)	2011, 2018	A.S.
		Environmental Non-Governmental Organizations (ENGO): Number	2011, 2018	A.S.
	Air pollution	Annual mean concentration of PM10 particles (μg/ m^3); Annual	2013, 2018	A.S.
		Annual mean concentration of CO (8 h) (mg/m3)	2014, 2018	A.S.
		Annual mean concentration of O3 (hourly) (μg/m3)	2013, 2018	A.S.
		Annual mean concentration of NO2 (VL=40 μg/m3) (ug/m3)	2013, 2018	A.S.

(*continued on next page*)

Table 2 (*continued*)

	Air temperature	Annual mean air temperature (°C)	2012, 2018	A.S.
	Soil exploitation	Mineral extraction and dump sites (class 13,100, urban atlas) and Constructions sites (sqkm) (class 13,300, urban atlas)	2012, 2018	A.S.
	Water pollution	Quality for human consumption (Proportion%)	2011, 2018	A.S.

assets of the area under study, their accessibility, and public participation. The hard-cultural assets are publicly owned, and the soft-cultural assets are found within communities (e.g., artists and creative people), businesses (e.g., creative industry), and other stakeholders' groups. In the cultural dimension of urban metabolism, we include processes related to urban agriculture, highlighting its beneficial role in building community cohesion, providing a place where community members can come together, interact, and strengthen their bonds. The smart and regenerative cultural planning refers to the planning and implementation of strategies that highlight the unique hard and soft cultural assets of a place, boosting the local and regional competitiveness (urban art interventions, collaborative community projects and networks, urban culture inheritance, and the creation of the contemporary city culture). The technological dimension of urban metabolism lies in implementing advanced technologies in urban planning and design, which is required to solve the technical issues of supplying energy, water, materials, construction, planning, and design and do it while regenerating the urban metabolisms. Examples of this implementation are applying the Internet of Things (IoT) and the Information and Communication Technology (ICT) to support interconnection among heterogeneous systems, laser cleaning technologies, sensors for data collection, barriers to prevent floods, management, and disposal of the city's waste. The ecological dimension of urban metabolism refers to understanding and mimicking organisms and ecosystems (including their functions and services). By learning from ecosystem processes, we apply this knowledge to regenerate the exploitation of natural resources, the human and social capital, the economy, mobility, and governance and how they interact with each other.

Having defined the metabolic dimensions and subdimensions establishing the boundaries of their related urban processes, we identify their representative indicators as shown in Table 1. Adopting the ecosystem services perspective, we classify these indicators according to four well-known groups; provisioning services, regulating services, supporting services, and cultural services proposed by the Millennium Ecosystem Assessment (MA), 2005 classification system. Pedersen Zari, 2012 provides a list (Table A in Annex) with the main ecosystem services of each category after conducting a comparative survey of the existing research. In line with this list, we classify the urban processes of a smart and regenerative urban ecosystem into these four categories, transferring the ecological knowledge to the built environment aiming to maintain the overall health and resilience of the urban ecosystem as a whole (Table 1). Therefore, the provisioning services offered by a holistic smart and regenerative urban ecosystem are related to the welfare, economy, social inventions, energy and water systems, and all urban ecological processes, including processes related to urban agriculture. The regulating services regulate environmental media or processes, such as pollination and dispersal, climate regulation, biological control decomposition, and disturbance prevention and moderation of extremes. Thus, the regulating services are provided by urban processes related to demography and migration, Healthcare services and infrastructure, urban agriculture, sewage and waste management, treatment and recycling, urban safety processes, and all urban ecological processes. Following the supporting services are these ecosystem processes and functions that support other services like soil formation, soil retention, renewal of fertility, quality control, nutrient cycling, habitat provision, and species maintenance. Therefore, the supporting services are provided by urban processes related to fertility and mortality, employment- unemployment rates, urban agriculture, mobility - accessibility, urban fabric, sewage and waste management, treatment and recycling, and all urban ecological processes. Finally, the cultural services are the services offered by the urban ecosystem responsible for covering cultural or spiritual needs, such as artistic inspiration, education, and knowledge, esthetic value, cultural diversity and history, recreation and tourism, creation of sense of place, spiritual and religious inspiration, relaxation and psychological well-being (Table 1, Table A).

We finish the life cycle inventory phase by building the dataset reflecting these urban processes and functions responsible for smart and regenerative metabolism and circularity of resources, information, and waste emissions in all dimensions for two different years (2011, 2018). The built dataset consists of 254 measures. These measures represent the biophysical characteristics of the ULC, for instance, land use and land cover, the UCL's socioeconomic profile, as population growth and density, economic prosperity, lifestyle practices, access to services, and quality of life. Moreover, we include measures representing the material and energy flows, including energy, water, waste flows. Some of these measures could be used for more than one indicator/ urban process of different metabolic dimensions. Still, to avoid data redundancy, we chose to use them once to measure the urban process they represent more generally.

For our analysis, we set the year 2011 as the oldest year and the year 2018 as the most recent year to study the metabolism of ULC before the COVID-19 pandemic; 2018 was the year with the majority of the available data. When a specific dataset was not available for the target years 2011 and 2018, we chose the closest year to them available. The Census data were only available for the years 2001 and 2011. We retrieved statistical data from the Database of Contemporary Portugal (PORDATA), Statistics Portugal (INE), and the Urban Atlas land use and land cover (Copernicus Programme, 2012, 2018).

Overall, the built dataset consists of 4 dimensions organized in 15 sub-dimension, comprising 29 indicators and 254 measures, for two time periods focusing on the system dynamics over time and space (Table 2).

3.3. Urban metabolism sensitivity analysis and prediction

Coupling LCI and ML, we support the application of the smart and regenerative urban metabolism concept. The LCI under the ecosystem services perspective enables the smart and regenerative aspect of the system dynamics. ML allows us to capture the feedback effect coming from the different urban processes and system dynamics components. In this way, we encapsulate the circularity of urban metabolism, adopting a data-driven methodology. From the ML algorithms, we have used Artificial Neural Networks (ANN) to accomplish this task. ANN is an information processing technique that mimics the way in which a biological nervous system operates. It uses a variety of highly connected processing units that co-work to process information and generate meaningful results.

Specifically, in the STATISTICA software[2] environment, we developed an algorithmic representation of the urban metabolism of our study

[2] STATISTICA software is an advanced analytical package for data analysis, management, mining, statistics, ML, text analytics, data visualization. It can be used for predictive modeling, clustering, and classification. More details regarding the tools and applications of the software can be found on (StatSoft Inc., 2004).

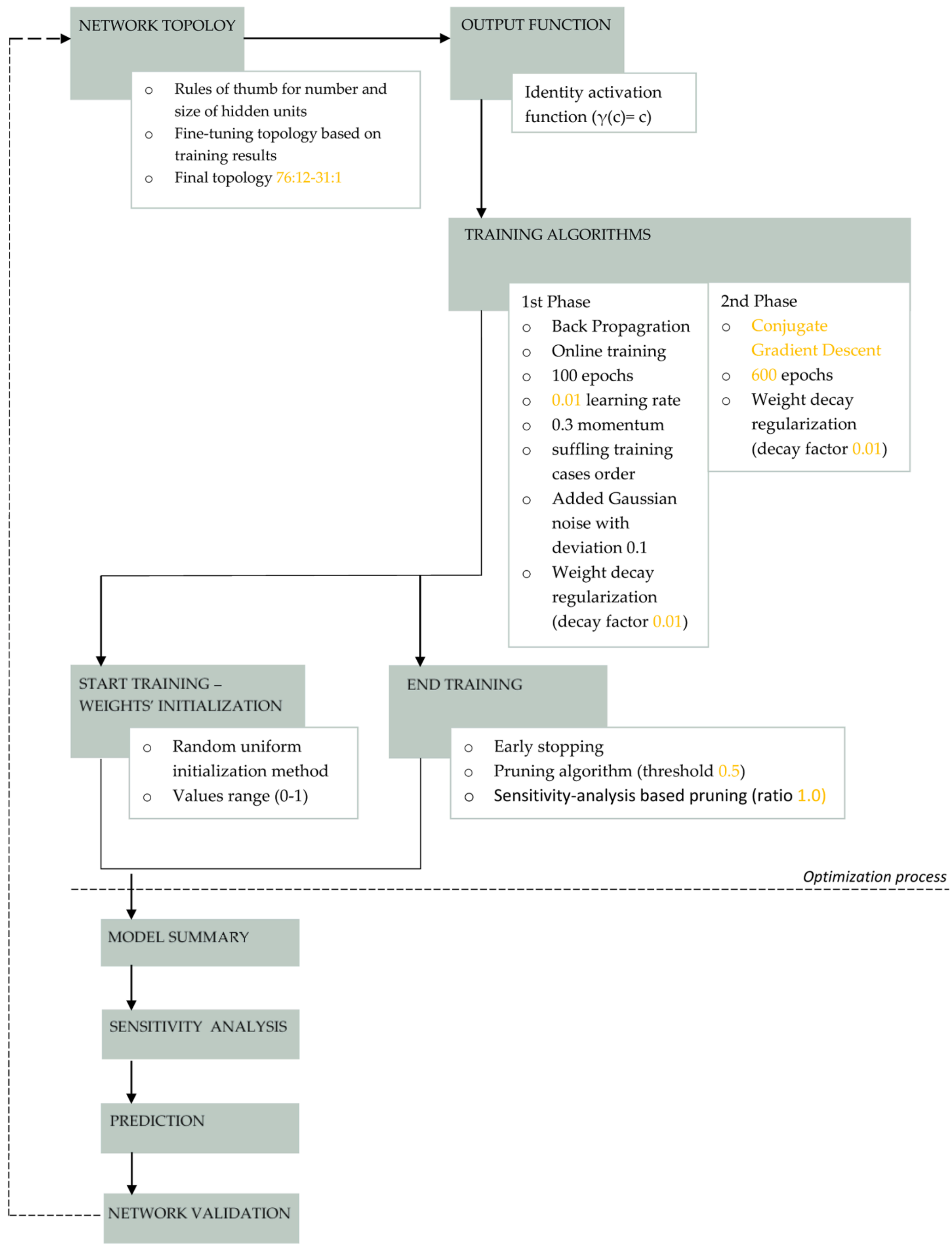

Fig. 3. Flowchart of MLP network training.

area, using the Multilayer Perceptron (MLP) a supervised algorithm of ANN, and create a network of 253 input units and one output unit (the dependent variable) where here represents the purchasing power per capita for the year 2018. MLPs are often identified as the most common neural network architecture that produces predictive models for one or more dependent (target) variables based on the values of the predictor (independent) variables (Lievano & Kyper, 2006). MLP training procedure starts by setting a layered feedforward topology (input layer-hidden layer(*s*)-output layer). Then training algorithms using optimization functions set the network's weights and thresholds and update the network parameters at every iteration of the training aiming to minimize the prediction error[3] made by the network. Ultimately, a network is appropriately trained when it has learned to model the function that relates the input variables to the output variables. Therefore, it can be used to make predictions where the output is unknown (Lievano & Kyper, 2006). For explanatory or causal forecasting problems as of this study, the functional relationship of predictors and the dependent variable is of the form $y = f(x_1, x_2, \ldots, x_p)$ where $x_1, x_2, \ldots, x_p$

[3] An error function combines all the differences between the actual outputs and the target outputs of all training cases and gives the networks error. For regression problems the error function is usually the sum of the squared errors.

Table 3
Model summary.

Profile	Train Perf.	Select Perf.	Test Perf.	Train Error	Select Error	Test Error	Training/ Members	Inputs	Hidden nodes (1)	Hidden nodes (2)
MLP 76:76–12–31–1:1	0.488857	0.837801	0.803547	0.216065	0.104959	0.352127	BP100, CG593b	76	12	31

are p predictors and y the target variable (Zhang, Patuwo & Hu, 1998). Another important output that we can perform once the network is trained, is the sensitivity analysis on the network inputs. From this analysis, we can examine the inputs' interdependencies and obtain information regarding the variables of the data set that most affect the output of our analysis, or in other words the network's performance. To do so, sensitivity analysis rates the input variables according to the deterioration in network's performance that occurs if that variable is "unavailable" to the network. STATISTICA software has a missing value substitution procedure allowing forecasting where the value of one or more input variables v is missing. To define the sensitivity of a variable v, the network initially runs using a set of test cases, and the network error is accumulated. Then network runs again using the same test cases and replacing the observed values v with the estimated value by the missing value procedure and the network error is accumulated again. The variables are rated based on the ratio of the error with the missing value substitution to the original error; greater the ratio means greater the expected deterioration in error and therefore the network is more sensitive to the specific v input variable (StatSoft Inc., 2004).

To train the network, we typically divide the original data set into training, selection, and testing sets. The training set is normally the biggest in size and is used to learn the parameters of the model during the training process. The selection test or validation test is used to tune the parameters of the model (network configuration, regularization techniques, and so on) and eventually to select the "best" model. Finally, when the model has been trained, the testing set is used to evaluate its performance, ensuring that it can generalize well to unseen data.

We adopted an explorative approach to train our network, trying different sizes of hidden layers and units, learning algorithms and parameters aiming to find an affective network configuration for our study (Fig. 3). Starting with the network's topology, we tested various approaches-rules of thumb suggested by the literature for choosing the number and the size of hidden units. One approach suggests that a hidden layer should never be more than twice as large as the input layer (Berry & Linoff, 1997). Another tested approach was that the number of hidden units should be 2/3 the size of the input units plus the output unit. We also tested the default configuration of STATISTICA software of one hidden layer with the number of hidden units equal to half of the sum of the input and output units. Another rule of thumb that we tied suggests that the second hidden layer has to be at least three times the size of the first hidden layer (Lippmann, 1987). Moreover, we also tested random sizes of hidden units, increasing or decreasing them according to the network's performance.

After setting the network's topology, we selected the linear approach to map the output variable using the identity activation function ($\gamma(c) = c$). This function takes real-valued arguments and returns them unchanged, supporting a substantial amount of extrapolation, although not unlimited (the hidden units will saturate eventually) (StatSoft Inc., 2004). We randomly assigned five out of nine (total) training cases to the training set, two to the selection set, and two to the testing set.

To start the training process, we followed a two-phased standard training procedure for MLPs. We used the Backpropagation learning algorithm for the first phase of 100 epochs. We tried different powerful algorithms for the second phase of 600 epochs Quasi-Newton (BFGS), and Levenberg-Marquardt, and the Conjugate Gradient Descent. The BFGS (Broyden–Fletcher–Goldfarb–Shanno) algorithm belongs to the Quasi-Newton methods. It is a local search optimization algorithm that approximates the inverse Hessian matrix. The approximation at first follows the line of steepest descent and later follows the estimated Hessian more closely. The BFGS's main drawback is that it needs O(n2) memory to store the inverse Hessian Matrix, making it impractical for most sophisticated ML models with millions of parameters. To decrease the memory cost, the Limited Memory BFGS (L-BFGS) extension can be applied to avoid storing the complete inverse Hessian approximation matrix (StatSoft, Inc. 2004); Goodfellow et al., 2016). The following tested optimization algorithm was the Levenberg-Marquardt (LM), a fast convergence algorithm for small networks, able to solve nonlinear least-square problems. LM combines the gradient descent and Gauss-Newton minimization algorithms. When the parameters of the network are far from their optimal value, LM acts more like a gradient-descent, and when the parameters are closer to their optimal value, it acts more like a Gauss-Newton (Gavin, 2019). The main disadvantage of LM algorithm is that can be very slow to converge when the network has more than ten parameters (Waterfall et al., 2006), and for flat functions can be lost in parameter space (Transtrum & Sethna, 2012). The last optimization algorithm tested was the Conjugate Gradient Descent that we eventually selected for the second phase of the training phase showing the best results for our network. The Conjugate Gradient Descent is an advanced optimization algorithm to train MLP recommended for networks with a large number of weights and/or multiple output units. The technical details on how the optimization algorithms carry out the network training process, how they update the network weights and minimize the prediction error are presented in the supplementary material.

For the first phase of training, we used a learning rate of 0.01 (initial and final) on each epoch. The learning rate is the amount that the weights are updated during the training; how far to move the weights in the direction opposite of the gradient. During the training, the backpropagation algorithm estimates the amount of error for which a node's weights in the network are responsible. Then the node's weight is updated based on learning rate-scaled error instead of the full amount of error. Using 0.01 learning rate, the weights of the network are updated 0.01 times the estimated weight error. To give faster training and better predictive accuracy to the network, we used a momentum value of 0.3. During the training, the gradient keeps changing direction and slower the process of training. Introducing the training momentum (a history of weights), the weights are adjusted to one direction smoothing the variations and making the training faster without losing information caused by highspeed convergence. We used the online type of training of Backpropagation that updates the weights of the network when each training case is presented. If all training cases are presented, and none of the stopping rules has been met, the process continues by recycling them. We shuffled the order of the presentation of the training cases at each epoch. The last parameter added for the first training phase was the Gaussian noise with a deviation of 0.1 to the output value on each training case. For the second phase of the training process no shuffle option was available since Conjugate Gradient Descent is a batch update algorithm that updates the weights once at the end of each epoch based on the average gradient of the error surface across all cases. For the same reason to avoid adding noise the learning rate and momentum are not available either (StatSoft Inc., 2004).

At the beginning of the training, we used the random-uniform method to initialize the network's weights normally-distributing small random values within a range of minimum and maximum values (0–1). We applied a pruning algorithm at the end of the training to prune neurons in input and hidden layers with fan-out weights below 0.05

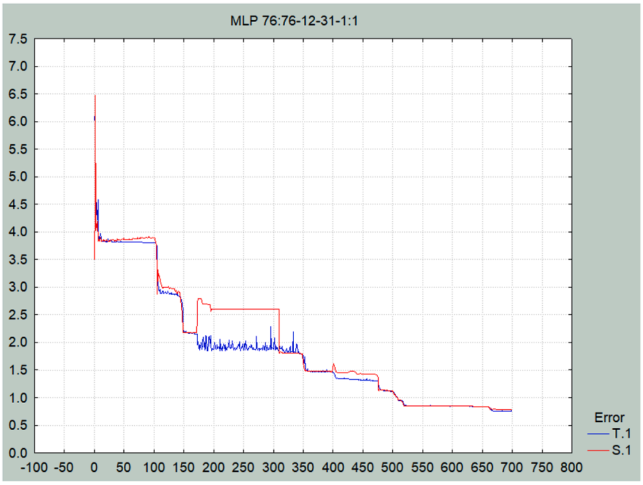

Fig. 4. Network's training graph: training (T.1) and selection (S.1) error, axis (x) shows epochs, and axis(y) shows the error function.

since they don't significantly contribute to the network's performance. We also used sensitivity analysis with a ratio of 1.0 to perform input pruning. Considering that large weights make the network unstable, we applied a weight decay regularization to both training phases using a decay factor of 0.01. Overall, this parameterization road map forges the best network for the case study.

After training more than 300 networks, we found the most effective model that generalizes well (Table 3). We trained the model with 76 input variables of the 253 having two hidden layers with 12 and 31 hidden units, respectively. Backpropagation with 100 epochs and Conjugate Gradient Descent (CG) were used to find the best network with the lowest selection error on the 593rd epoch of CG. The network's performance on the different data subsets used during the training process is shown in Table 3. The performance for regression networks like ours is the Standard Deviation Ratio. When the network's performance equals 1, the network performs as a simple average, and a lower ratio implies a better estimate. In Table 3, we can also find the network error on the subsets as the root mean squared (RMS) errors generated by the error function (sum-squared differences between the target and actual output values on each output unit). Based on a rule of thumb, when RMS error is greater or equal to 0.5, the model does not generalize well.

Another way to validate the model and assess its generalization ability in combination with the model summary is the graph of the training and selection errors on each epoch (Fig. 4.). The training should stop when the training error curve and the selection error curve are close to each other. Flat lines or noisy values of relatively high error indicate that the model was unable to learn for the training dataset. The same applies when the training error curve continues to decrease at the end of the graph. In the opposite case, when the model has learned the training dataset too well (including noise or random fluctuations), while the training error curve continues to decrease through epochs and the selection error curve decreases up to a point and then starts to increase again. When the selection dataset does not provide enough information to evaluate the model's generalization ability, the selection error curve shows noisy movements around the training error curve even if the training error curve indicates a good fit. The selection dataset is unrepresentative also when the selection error curve is lower than the training error curve. On the other hand, when the training dataset is unrepresentative, both training and selection error curves show improvement, but there is a large gap between them. Our model's graph shows a good fit with the training and selection error curves to decrease to the point of stability with a very small gap between them.

4. Results

ANN - MLP network training provided us with two main outcomes. First, as a result of the sensitivity analysis, we obtained the main drivers representing the urban processes that most influence the predicted urban metabolism changes (the dependent variable) in terms of IpC changes. Second, we predicted where and to which degree these changes in urban metabolism will occur in the near future.

In Table B (Annex), we present the output variables of our model's sensitivity analysis ranked by descendent order, from higher sensitivity

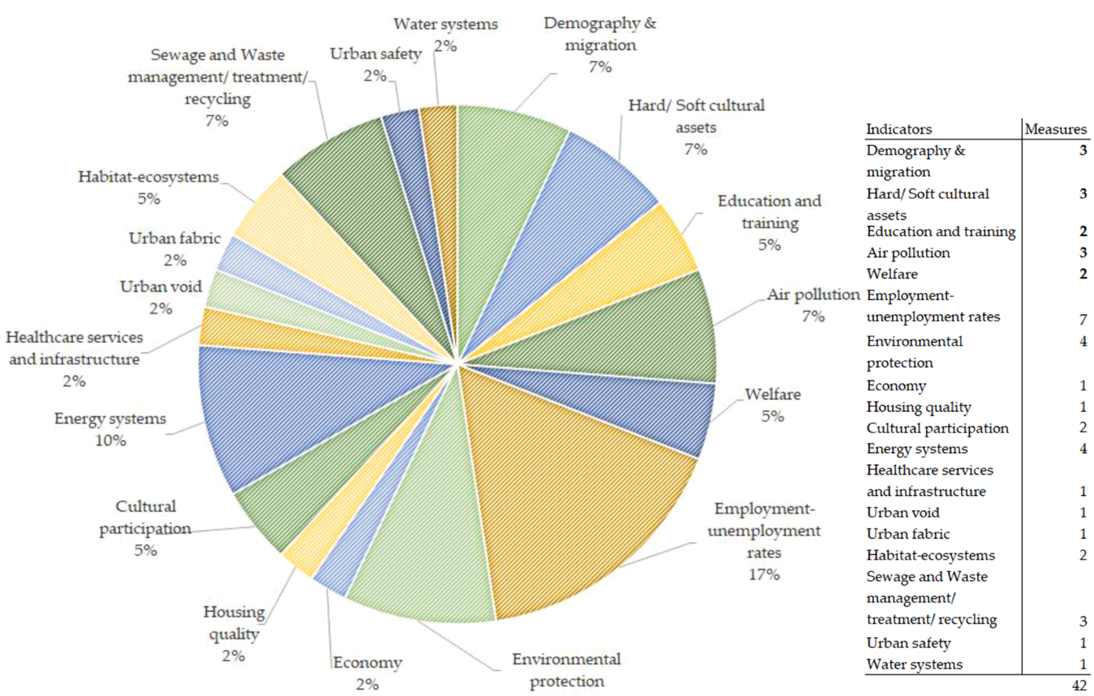

Fig. 5. Occurrence of data components/ measures per indicator with high sensitivity to urban metabolism changes (%).

Table 4
Important measures to urban metabolic changes under the perspective of ecosystem services.

Dimensions	Sub-dimensions	Indicators of Urban processes	Data components/ measures	Year	Code	Rank	U. E.S
Social	Human capital	Demography & migration	Resident population, according to the Census male 65+	2001	ml65_01	1	R. S.
Cultural	Cultural Mapping	Hard/ Soft cultural assets	Cinema: box-office revenue (€)	2011	cn_bxof11	2	C. S.
Social	Human capital	Demography & migration	Resident population, according to the Census female 65+	2011	fml65_11	3	R. S.
Social	Human capital	Education and training	Teaching staff in pre-school	2011	tch_pre11	4	C. S.
Ecological	Environmental quality	Air pollution	Annual mean concentration of NO2 (VL=40 μg/m3) (ug/ m3)	2013	N02_13	5	A. S.
Social	Economic capital	Welfare	Average monthly earnings of male employees by Upper-secondary and post-secondary non-tertiary level of education	2011	ernml_upp11	6	P.S.
Ecological	Environmental quality	Air pollution	Annual mean concentration of PM10 particles (μg/ m^3); Annual	2013	PM10_13	7	A. S
Cultural	Cultural Mapping	Hard/ Soft cultural assets	Live shows: box-office revenue (€ - Thousands)	2001	lv_bxof01	8	C. S
Social	Economic capital	Employment- unemployment rates	Employment rate, according to the Census by age group (%) (35–44)	2011	empl3544_11	9	S. S
Ecological	Environmental protection	Environmental protection	Expenditure by municipalities on Protection against noise and vibrations (€ -Thousands)	2018	exp_noise18	10	A. S
Social	Economic capital	Economy	Industrial, commercial, public, military, and private units (sqkm) (class 12,100, urban atlas)	2012	ind_ua12	11	P. S
Technological	Housing	Housing quality	Non-residential buildings, according to the Census	2001	tb_nrsd01	12	S. S
Social	Economic capital	Employment- unemployment rates	Unemployment rate, according to the Census male (%) (total)	2011	unmpl_ml11	13	S. S
Social	Economic capital	Employment- unemployment rates	Employment rate, according to the Census male (%) (total)	2011	empl_ml11	14	S. S
Cultural	Cultural participation	Cultural participation	Cinema spectators (No.)	2011	cn_spct11	15	C. S.
Technological	Utility systems and Infrastructure	Energy systems	Electricity consumption per inhabitant by type of consumption kWh (kilowatt-hour) / inhab. – Ratio: (street lighting)	2011	elc_strligh11	16	P. S
Social	Health system	Healthcare services and infrastructure	National Health Service: beds in general and specialist hospitals	2018	bed_hspt18	17	R. S
Technological	Utility systems and Infrastructure	Energy systems	Fuel sales for consumption t(ton): (propane gas)	2018	propn_18	18	P. S
Social	Economic capital	Employment- unemployment rates	Employment rate, according to the Census female (%) (total)	2011	empl_fml11	19	S.S.
Technological	Urban structure	Urban void	Land without current use (sqkm) (class 13,400, urban atlas)	2012	ncuse_ua12	20	N. S.
Technological	Urban structure	Urban fabric	Continuous urban fabric (S.L. > 80%) (sqkm) (class 11,100, urban atlas)	2012	cntufb_ua12	21	S.S.
Ecological	Habitat-ecosystems	Habitat- ecosystems	Urban Atlas classes 3,4,5 included urban green areas	2012	ecstm_12	22	A. S.
Ecological	Habitat-ecosystems	Habitat- ecosystems	Urban Atlas classes 3,4,5 included urban green areas	2018	ecstm_18	23	A. S.
Ecological	Environmental quality	Air pollution	Annual mean concentration of CO (8 h) (mg/m3)	2014	CO_14	24	A. S.
Social	Economic capital	Employment- unemployment rates	Unemployment rate, according to the Census female (%) (total)	2011	unmpl_fml11	25	S.S.
Social	Economic capital	Welfare	Average monthly earnings of female employees by higher level of education	2011	ernfml_hgh11	26	P.S.
Social	Economic capital	Employment- unemployment rates	Unemployment rate, according to the Census female (%) (total)	2001	unmpl_fml01	27	S.S.
Technological	Utility systems and Infrastructure	Energy systems	Electricity consumption per inhabitant by type of consumption kWh (kilowatt-hour) / inhab. – Ratio: (agriculture)	2011	elc_agr11	28	P.S.
Technological	Utility systems and Infrastructure	Energy systems	Fuel sales for consumption t(ton): (fuel diesel)	2011	fueldsl_11	29	P.S.
Technological	Utility systems and Infrastructure	Sewage and Waste management/ treatment/ recycling	Urban waste collection per inhabitant (Ratio – kg/ inhab.)	2011	uw_clct11	30	R. S.
S.S.							
Technological	Utility systems and Infrastructure	Sewage and Waste management/ treatment/ recycling	Urban waste by type of destination t (tonne): (organic)	2018	uw_orgrcl18	31	R. S.
S.S.							
Social	Economic capital	Employment- unemployment rates	Employment rate, according to the Census by age group (%) (25–34)	2011	empl2534_11	32	S.S.
Cultural	Cultural participation	Cultural participation	Live shows spectators (No.)	2011	lv_spct11	33	C. S.

(continued on next page)

Table 4 (*continued*)

Dimensions	Sub-dimensions	Indicators of Urban processes	Data components/ measures	Year	Code	Rank	U. E.S
Social	Human capital	Education and training	Teaching staff in pre-school	2018	tch_pre18	34	C. S.
Technological	Utility systems and Infrastructure	Sewage and Waste management/ treatment/ recycling	Urban waste selective collection per inhabitant (Ratio – kg/ inhab.)	2011	uw_slctv11	35	R. S.
S.S.							
Technological	Utility systems and Infrastructure	Urban safety	Crimes registered by the police (motor vehicle theft)	2011	thfmoto11	36	R. S.
Technological	Utility systems and Infrastructure	Water systems	Water supplied/consumed per inhabitant (ratio- m3/ inhab.)	2011	water_cons11	37	P.S.
Social	Human capital	Demography & migration	Annual population growth (individual): (natural increase)	2018	grth_natu18	38	R. S.
Cultural	Cultural Mapping	Hard/ Soft cultural assets	Art galleries and other places for temporary exhibitions: exhibitions	2011	art_exh11	39	C. S.
Ecological	Environmental protection	Environmental protection	Environmental Non-Governmental Organizations (ENGO): number	2011	engo_11	40	A. S.
Ecological	Environmental protection	Environmental protection	Expenditure by municipalities on the environment (€ -Thousands) by environmental management and protection domains: (others)	2018	exp_oth18	41	A. S.
Ecological	Environmental protection	Environmental protection	Expenditure by municipalities on protection of biodiversity and landscape (€ -Thousands)	2018	exp_biolsc18	42	A. S.

Table 5
Purchasing power per capita by municipality for the years 2018 and 2025.

Municipalities	IpC 2018	IpC 2025
Lisboa	219.6	172.1422
Loures	92.3	104.6195
Odivelas	89.3	104.1329
Amadora	100.6	100.6236
Oeiras	156.5	173.5109
Cascais	122.1	89.2158
Almada	108.7	91.0583
Seixal	89.7	106.8435
Barreiro	100	162.4113

(1) to lower sensitivity (76) based on their ratio. Focusing on the measures with a ratio of about one, we summarize the occurrence of the different data components/ measures (variables) per indicator (Fig. 5). The summarized occurrence of the measures per indicator shows us to which urban processes the metabolic changes are more sensitive, examining holistically all the measures of the different metabolic dimensions of the study area. We see that the *Employment- unemployment rates* indicator measures have the greatest percentage of occurrence (17%) among the variables that most affect the network's performance. Second in place come the indicators Environmental protection, and *Energy systems* with 10% measures' occurrence. The indicators *Sewage and Waste management/treatment/recycling, Demography & migration, Hard/Soft cultural assets,* and *Air pollution* appear with 7% of measures occurrence followed by the *Education and training, Welfare, Cultural participation,* and *Habitat-ecosystems* indicators' measures with 5%. Last is the group of measures with 2% occurrence for the *Urban safety, Water systems, Economy, Housing quality, Urban void, Urban fabric*, and *Health services and infrastructure* indicators.

The output of the sensitivity analysis shows evidence of the multidimensionality of a smart and regenerative urban metabolism. The most important measures (predictor variables) to urban metabolism changes cover all four metabolic dimensions, eleven out of fifteen subdimensions and eighteen out of 29 indicators (Table 4). Therefore, these indicators and related measures show a system-based representation of the interdependencies between different urban metabolic processes responsible for resource use, materials, energy and information circulation, waste production, and their associated performance throughout their entire value chain. These urban processes provide all urban ecosystem services benefiting human well-being.

The second output obtained from our model was the prediction with high accuracy of the urban metabolic changes in terms of IpC changes for the UCL for the year 2025. The year 2025 is calculated by adding to the present year (2018) the number of years (7) between the two time periods of the input data (2018, 2011). Looking at Table 5, we can observe that the degree to the UCL's urban metabolism at the municipality level either increases, decreases, or stays stable in 2025. In order to have a spatial visualization upon where the forecasting metabolic changes in 2025, we mapped the current metabolism of our study area (Fig. 6) and the prediction results of the urban metabolism (Fig. 7) at the municipality level.

Results show that Lisbon's metabolism decreased dramatically, followed by Cascais' and Almada's in 2025. On the other hand, Loures, Odivelas, and Seixal show an increased metabolism of the same class (Fig. 6, 7). The municipality of Oeiras has one of the highest urban metabolism in 2018, and it continues to have for the year 2025. Amadora municipality does not show any significant metabolic changes for the near future, contrary to Barreiro's municipality that presents an intensive metabolism.

From our previous analysis, the main drivers of these metabolic changes are the urban processes related to the 42 higher ranks of higher sensitivity (Table 4). Therefore, those with decision responsibility can either stabilize, increase, or decrease the metabolism of the study area by activating these key metabolic drivers. Knowing the degree, the spatial distribution of the future metabolic changes, and the key drivers of change provides important information to link with potential urban development strategies related to urban governance. Provided by specific guidance coming from our model, we can enhance the relevant urban metabolic functions and services in a way to plan and manage resilient and sustainable urban development.

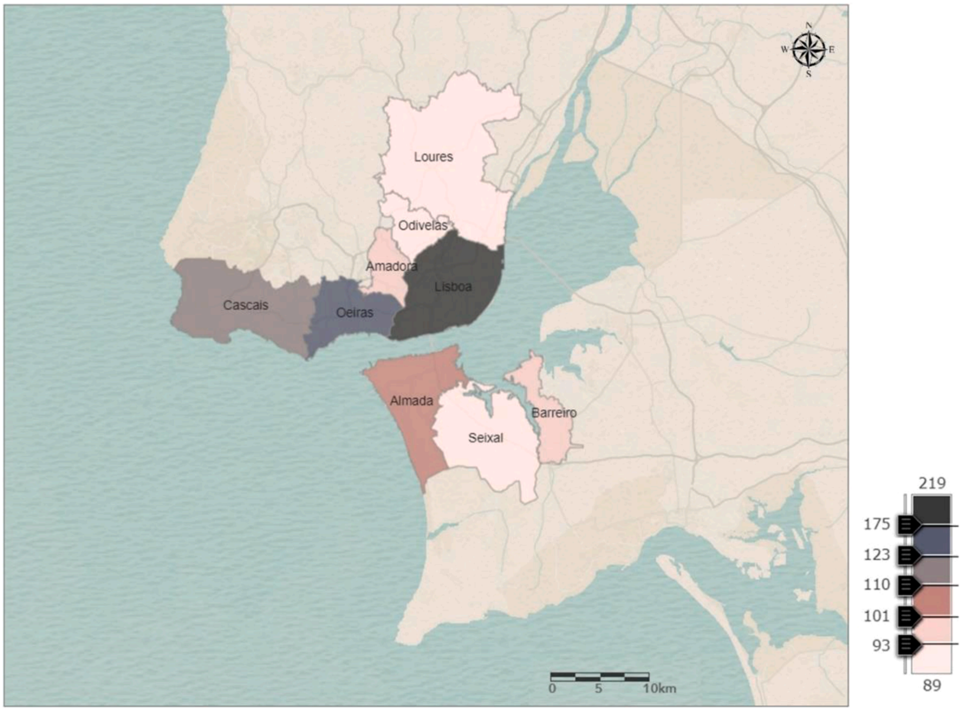

Fig. 6. Urban metabolism per municipality for the year 2018.

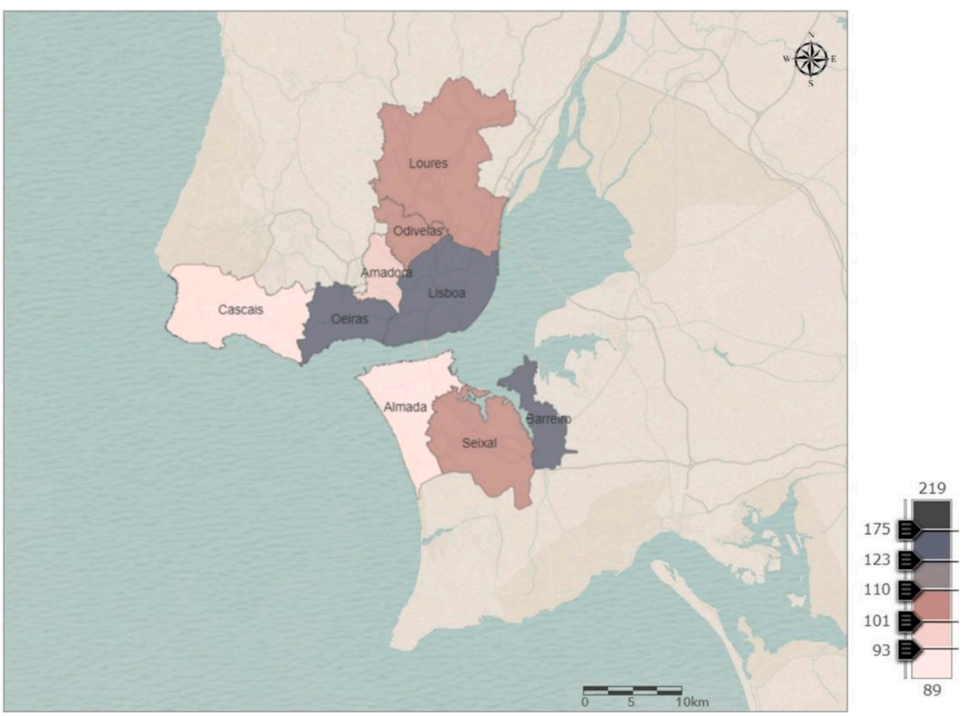

Fig. 7. Urban metabolism per municipality for the year 2025.

5. Discussion

Urban cores are complex systems where various urban processes are responsible for resource use, flows of materials-energy-information, and waste emissions, establishing social, cultural, technological, and ecological relationships. Therefore, urban cores have their own metabolism, requiring a systematic approach that encapsulates its complexity and assess its sustainability. Adopting the concept of smart and regenerative urban metabolism, we describe the urban processes and their relationships as circular ongoing, co-evolutionary, focusing on eliminating waste by regenerating resources using technology. The urban processes represent different sub-systems of the urban system of which they are part. They are delimited by flexible and open boundaries that allow communication channels between the sub-systems and beyond the system boundary enabling their interdependence. In line with the UM framework, we treat the urban systems like ecosystems and the services offered by the different urban processes as ecosystem services. Natural ecosystems provide functions and services essential to human welfare and long-term survival. Studying the structure and services of ecosystems, we obtain guidance on how to achieve system resilience. In this way, we can build a research framework supporting a holistic understanding of how urban systems function, considering their multiple dimensions. Therefore, we can design a methodology able to capture the metabolic dynamics highlighting the impact of urban ecosystem services on urban sustainability.

We proposed a novel methodology that couples LCT and ML under ecosystem services perspective. LCT is the way of thinking of the consequences in the environmental, economic, and social dimensions of a product/process/system of processes throughout its entire life, meaning the effects on ecology, resources, and human health (Farjana, Parvez Mahmud & Huda, 2021). It facilitates the links between the different dimensions of urban processes aiming to reduce resource use, waste production and improve a process's socioeconomic performance through its entire cycle. The main limitations when applying LCT and mostly LCA at the city level are the definition of system boundaries giving insights into the fundamental urban dynamics, the appropriate functional units, and the use of data that capture the complexity of urban systems at micro and macro scales. Indeed, to measure and access UM at a local scale demands data with a high level of granularity produced and or collected systematically through time and space and with ground truth. Unfortunately, the type of multidimensional data meeting such requirements is scarce, affecting knowledge-based analysis due to uncertainty and data gaps.

Coupling LCT with ML, we are able to overpass/minimize these limitations, modeling a neural network of the different urban processes. ML algorithms have proven to be suitable for dealing with problems of data scarcity, where are uncertainty and unpredictable system dynamics. Although the demand for quality data at a local and even human scale still remains to be fulfilled, ML algorithms can work with data gaps and help the network perform better, enhancing its integrated systematic multidimensionality. For instance, while preparing the input dataset for implementing the proposed research framework at municipality level, we faced difficulties to encounter crucial data to measure important urban metabolic processes related to food consumption, construction materials, air quality measures at human scale, noise pollution, number of passengers transported by public transportation, domestic material consumption, number of people exposed to conditions beyond a critical threshold, among others.

Moving to the network training process's limitations, we must confront the general nonconvex case during the training. When training neural networks, ML traditionally avoids the general optimization problems by designing the objective function and constraints to guarantee that the optimization problem is convex. Although, even convex optimization comes with complications (Goodfellow et al., 2016). There are a few main challenges involved when optimizing convex functions—starting with the ill-conditioning of the Hessian matrix a common problem in numerical optimization where the Stochastic Gradient Decent (SGD) is "stuck" meaning that even very small steps of the gradient increase in cost function, the learning is very slow regardless a strong gradient (Goodfellow et al., 2016). Another important optimization issue is the convergence to a local minima when the training algorithm stops in a low point (the lowest of the surrounding terrain) rather than continuing to seek for the global minima, and therefore, it has not learned the entire training set. Plateaus, Saddle Points, and Other Flat Regions are common nonconvex optimization problems. In these points or regions on the landscape, the gradient is zero (very flat), which means it does not know which direction to move to optimize the model; therefore, the iterative algorithm is stuck mimicking local minima (Bishop, 1995).

An important task of neural networks is to have a final model that can perform well both on the training dataset and the unseen dataset (test dataset). When the predictive model has learned from the details of the training set (noise in the data) instead of the general behavior (the underlying function), it has overfitted the training dataset, and therefore, it is not able to perform the same with the testing set. Overfitting is a typical cause of poor generalization of the model, having high generalization error. A predictive model can underperform when it has learned too little from the training dataset and does not perform well on the testing dataset (underfitting).

In order to tackle these challenges while training neural networks, we looked for the optimum network topology (structure), and configuration we tried different training algorithms. We used regularization methods (parameters) to control the complexity of the network. Going through the literature, we noticed that there is not a consensus regarding the number of hidden layers and hidden units to be used, we tested the related rules of thumb. We trained the network using a two-phased MLP designed to address problems related to convergence to local minima and network overfitting. More precisely, the first stage is a light run on backpropagation in conjunction with a soft training rate in order to perform the raw convergence. This first stage could be sufficient to solve simple problems. Due to the complexity of the systems under analysis, the first phase is not enough. Therefore, we moved to the second more powerful training phase, using an extended run of conjugate gradient descent. As it benefits from the backpropagation performance first stage, this algorithm is less likely to bump into convergence problems.

We tried different learning rates for the first phase of training until finding the best for our network. If the learning rate is very low, the training process will take too much time with no significant updates to the weights. On the other hand, if the training rate is too high, it results in an undesirable divergent function behavior. We also added Gaussian noise to the output value on each training case to reduce the network's tendency to overfit. We used smaller weights and early stopping to reduce the problem of overfitting. We shuffled the order of the presentation of the training cases at each epoch, so the training algorithm to be less prone to stuck in a local minima. We applied a sensitivity analysis-based pruning algorithm, using a threshold ratio equal to 1.0. In this way, we excluded the input variables with sensitivity analysis below 1.0 to not compromise the network's performance since it most likely constitutes a by-product of overfitting.

We conclude that the network optimization process cannot be based on rules of thumb but by conducting an exploratory procedure consisting of fine-tuning the network parameters based on the previous training results. It is worth mentioning that the complexity of the network under study is based on the complexity of the dataset.

When the optimization process was successfully completed, we performed sensitivity analysis on the network's input to identify the most influential indicators and their related measures for the urban metabolism changes (Table 4, Table B). It is essential to highlight that the rate of the indicators' sensitivities does not occur in an absolute manner; instead, it is measured considering the interdependencies between the input variables. Therefore, the obtained results regarding the importance of particular indicators concern the specific network considering the specific dataset used. The metabolic changes in this study are expressed in terms of purchasing power per capita (IpC) changes. As mentioned before, the IpC is a composite indicator provided by STATISTICS Portugal as a result of a factorial analysis using 16 variables. Using IpC for two time periods in our analysis it is important to say that there is a risk that the variation in IpC values could be a result of using associated variables that do not totally match between the different years or to use different reference periods for the associated data. For the purpose of this study, we assume that the IpC values of the two different years have been calculated using the same associated variables with the same year of reference. Knowing the key indicators causing metabolic changes, the degree of these changes, and their spatial location, one step further would be to qualitatively assess the metabolic changes. For instance, an increase in the urban metabolism in terms of IpC is predicted to happen in the municipality of Barreiro for the year 2025. What does this increase mean? that consumption and production in the area are going to increase due to increased migration? or due to individual earnings increase? or due to poor environmental protection policies that do not promote circular economy principles of reuse, reduce, recycle? Insights can be drawn by studying the dynamic changes of the key indicators as a result of the current study in the two different years of study (2011, 2018) individually and as a sum.

The proposed methodology can be applied to evaluate the multidimensional urban metabolism of urban areas and compare the metabolism of different urban areas at different levels; neighborhood-place; parish; municipality; metropolitan; country depending on the scale of the available data to be used for the analysis. The methodological framework and the proposed workflow are reproducible and can be used in different geographies to identify the main drivers for the urban metabolism changes, as well as to enable an alternative vision of the future. This approach contributes to both evidence-based policymaking and for professionals to adopt a new urban planning paradigm, more in line with the environmental and societal challenges cities are facing.

6. Conclusions

This study carries out a UM-LCT-ANN methodological framework from an ecosystem services perspective to overcome the limitations of previously applied UM methodologies and extend the state of the art of the subject. The proposed framework is applied to the urban core of Lisbon's functional urban area allowed us to obtain evidence-based knowledge on the complex metabolism of the different urban processes. The study results demonstrated the main drivers causing urban metabolic changes, and in which degree, and where. We were also able to forecast/predict urban metabolism changes for the near future, providing a data-based vision of how urban metabolism unfolds. Even though different urban processes require different dimensions and scales of analysis to measure and assess their metabolism accounting for the flows and storage of energy-material-information and their socioeconomic and environmental impacts, it is of utmost importance to design a framework that can be applied at various temporal and spatial scales. The proposed research framework has the ability to investigate the interdependencies of the urban metabolic processes of different dimensions holistically through time and space. Along with its main findings, we have shown that our methodology can be used as a tool to develop efficient policies for improving and fostering urban sustainability and contribute to a change of paradigm for urban planners and urban designers practitioners. Further research would be to build different scenarios based on experts, stakeholders, and local communities' visions, on how a city should be.

CRediT authorship contribution statement

Angeliki Peponi: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing – original draft, Writing – review & editing, Visualization, Supervision, Project administration. **Paulo Morgado:** Conceptualization, Methodology, Data curation, Writing – review & editing, Supervision. **Peter Kumble:** Conceptualization, Writing – review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.scs.2022.103754.

Annex

Table A
Ecosystem Services (Pedersen Zari, 2012).

Provisioning services	Regulating services	Supporting services	Cultural services
Food: Human (land/fresh water/ marine) Forage	Pollination and seed dispersal	*Soil*: Formation Retention Renewal of fertility Quality control	Artistic inspiration
Biochemicals: Medicines Other	*Biological control*: Pest regulation Invasive species resistance Disease regulation	*Fixation of solar energy*: Primary production/plant growth (above ground, below ground, marine, fresh water)	Education and knowledge
Raw materials: Timber fiber Stone Minerals	*Climate regulation*: Greenhouse gas (GHG) regulation Ultraviolet light (UV) protection Moderation of temperature	*Nutrient cycling*: Regulation of biogeochemical cycles Retention of nutrients	esthetic value
Fuel: Biomass Mineral Other	*Prevention of disturbance and the moderation of extremes*: Wind/wave force modification Mitigation of flood/drought Erosion control	*Habitat provision*: Refugium Nursery function	Culture diversity and history
Fresh water: Consumption Irrigation Industrial processes	*Decomposition*: Waste removal	*Species maintenance*: Biodiversity Natural selection Self-organization	Recreation and tourism
Ornamental resources Genetic information	*Purification*: Water/air/soil		Spiritual and religious inspiration Creating of sense of place Relaxation and psychological well-being

Table B
Sensitivity analysis of input variables (authors).

ml65_01	cn_bxof11	fml65_11	tch_pre11	NO2_13	ernml_upp11	PM10_13	
1.381698	1.327549	1.232948	1.139873	1.101623	1.100816	1.045264	Ratio
1	2	3	4	5	6	7	Rank
lv_bxof01	empl3544_01	exp_noise18	ind_ua12	tb_nrsd01	unmpl_ml11	empl_ml11	
1.036905	1.028956	1.02440	1.01827	1.01532	1.01367	1.01254	Ratio
8	9	10	11	12	13	14	Rank
cn_spct11	elc_strligh11	bed_hspt18	propn_18	empl_fml11	ncuse_ua12	cntufb_ua12	
1.01199	1.01109	1.01082	1.00942	1.00843	1.00831	1.00818	Ratio
15	16	17	18	19	20	21	Rank
ecstm_12	ecstm_18	CO_14	unmpl_fml11	ernfml_hgh11	unmpl_fml01	elc_agr11	
1.00792	1.00692	1.00619	1.00604	1.00521	1.00435	1.00424	Ratio
22	23	24	25	26	27	28	Rank
fueldsl_11	uw_clct11	uw_orgrcl18	empl2534_11	lv_spct11	tch_pre18	uw_slctv11	
1.00407	1.00284	1.00177	1.00131	1.00118	1.00110	1.00087	Ratio
29	30	31	32	33	34	35	Rank
thfmoto11	water_cons11	grth_natu18	art_exh11	engo_11	exp_oth18	exp_biolsc18	
1.00081	1.00064	1.00037	1.00036	1.00035	1.00031	1.00020	Ratio
36	37	38	39	40	41	42	Rank
scrt_pens18	cn_spct18	fueldsl_18	inh_phrm11	fml0_14_01	empl2534_01	cn_src18	
0.99991	0.99957	0.99953	0.99953	0.99947	0.99934	0.99919	Ratio
43	44	45	46	47	48	49	Rank
bnk_dw218	empl3544_11	LPG_18	O3_18	dm_viol18	agr_ua12	ppldns18	
0.99907	0.99855	0.99775	0.99767	0.99757	0.99743	0.99729	Ratio
50	51	52	53	54	55	56	Rank
act3544_11	uw_clct18	firefght18	ppldns11	ernfml_hgh18	firefght11	NO2_18	
0.99711	0.99699	0.99689	0.99663	0.99622	0.99598	0.99556	Ratio
57	58	59	60	61	62	63	Rank
dw_swgstm18	butn_18	airtemp_18	CO_18	art_sp11	uw_land18	ml15_64_01	
0.99511	0.99143	0.99086	0.99038	0.98698	0.98338	0.97367	Ratio
64	65	66	67	68	69	70	Rank
exp_biolsc11	lv_perf11	elc_agr18	petr95_18	fml15_64_01	rd_ua12		
0.96218	0.93563	0.90899	0.81710	0.75047	0.70421		Ratio
71	72	73	74	75	76		Rank

Table C
Associated variables for the calculation of the IpC indicator through factorial analysis (STATISTICS PORTUGAL, 2017).

Variables	Description
IRS	Personal income tax
Gross income	It's the reported income for taxes purposes
Value of domestic purchase through ATMs, per capita	The value is drawn by the location of the ATMs
Value of the payment transactions (services and special services) through ATMs, per capita	The value is drawn by the location of the ATMs
Value of domestic withdrawals from ATMs	The value is drawn by the location of the ATMs
Loans granted for housing purposes, per capita	The value is drawn based on the location of the real estate
Monthly earnings of full-time full-paid employees	The value is drawn by company location/municipality
Population living in places with over 5 K inhabitants as a proportion of the resident population	Drawn from the Census
Number of cars sold according to the place of residence of owners, per capita	The value is drawn based on the location of the car owners
Companies' turnover according to their location, per capita	The retail market only, with exception of cars and motorbikes business)
Value of international withdrawals from ATM	The value is drawn by the location of the ATMs
Value of international purchases from ATMs	The value is drawn by the location of the ATMs
Municipal tax on onerous transfers of real estate, per capita	The value is drawn by the location of the houses
Municipal property (real estate) tax	The value is drawn based on the location of the real estate
Corporate turnover of catering business, per capita	The value is drawn based on the location of the real estate

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