

Load and Demand Side Flexibility Forecasting

Rocio Alvarez Merce

Etta Grover-Silva

Johanna Le Conte

Ecole Polytechnique
Palaiseau Cedex, France

Eco CO2
Nanterre, France

Eco CO2
Nanterre, France

Email: rocio.alvarez-merce@ecoco2.com

Email: etta.grover-silva@ecoco2.com

Email: johanna.leconte@ecoco2.com

Abstract—Recent developments in energy metering technologies have allowed electric load data to be more easily accessible. Services that use this data to inform customers can raise awareness about electricity consumption and provide suggestions to encourage energy efficient behavior. Quantifying the flexibility of the demand combined with accurate predictions of the total electric load allow information services to provide suggestions to end-users on how to reduce electric consumption that are appliance and time specific. With the arrival of new electric generation technologies, such as photovoltaic or wind energy, demand side flexibility will play an important role in the optimization of the future electric system. The accurate prediction of demand flexibility at a building level, therefore can contribute to the optimization of load scheduling. This study presents an effective multi-step technique to forecast the average hourly demand flexibility for a household, using neural networks, unsupervised clustering techniques and an optimization algorithm, combined with statistical studies. The model is mainly based on the historical electric use of a building and does not require significant computational capacity, thus making it widely applicable and informative for residential customers, helping them improve their behavior to be more energy efficient in the future.

Keywords—non-intrusive load monitoring; demand flexibility; long short-term memory; recurrent neural network.

I. INTRODUCTION

Worldwide, the energy sector is increasing the penetration of decentralized renewable power generation systems and therefore, reducing more traditional centralized fossil fuel generation. This transition presents several challenges, such as moving from a more stable and controllable power generation to a more volatile and less predictable one. Mitigating this volatility and simultaneously decreasing the number of conventional power generators makes it harder to balance out supply and demand in order to ensure a stable and reliable grid. In addition, emissions from buildings have risen in the last few years, reaching an all-time high in 2018 [1], making this transition even more challenging. In particular, households in the European Union (EU) represented one-fourth of its total final energy consumption [2]. This results from several factors, including extreme weather conditions that increase energy demand for heating and cooling and inefficient behavioral habits that result in high energy use which is unnecessary for the comfort of building inhabitants.

Accordingly, demand side management is important to reduce overall emissions of buildings while guaranteeing end-user comfort. Accurate forecasts of individual building electric loads are crucial to effectively inform end-users about their

energy consumption habits. The willingness of end-users to change their energy use habits can therefore provide demand flexibility. Accurate predictions of the energy demand and demand flexibility at a building level can help encourage energy efficient behavior, stabilize the electricity grid and reduce the electricity bill, while accelerating the sustainable energy transition.

Recent developments in technology have allowed energy consumption data to be more easily accessible. Several studies show that real-time feedback about appliance specific energy use in energy efficiency awareness programs results in the highest energy savings [3]. In this regard, an awareness raising project has been put in place by the company Eco CO2 in the context of a public tender in France put forth by ADEME related to a funding mechanism called Investissement d'avenir [4]. This awareness raising service called Tableau de Bord de l'Habitat (TBH) Alliance aims to test different interfaces with varying information about the electric load of each user to encourage energy efficient behaviour. A digital tablet and a website is available for users to observe their electric load data, load profile analysis metrics and suggestions to reduce their consumption. In this context, quantifying demand flexibility combined with accurate predictions of the total electric load can lead to services that provide action plans to reduce energy consumption that are appliance and time specific.

Models used in building energy analysis can be grouped into two categories: the top-down approach, and the bottom-up approach [5]. Top-down approaches do not consider the occupant behavior inside, and very little information is needed about the building, they rely mostly on historical consumption data. Bottom-up techniques take into consideration the physical characteristics of a building and occupant behavior resulting in more detailed models. The bottom up approaches require a significant amount of detailed input information about each building and often require complex models that require a high computational time. Therefore, a pure bottom-up approach is not feasible for the assessment of a large group of end-users where detailed information is not available.

Many different top-down methods have been developed for load forecasting, such as curve fitting using numerical methods or machine learning algorithms [6]–[9]. Load forecasting is a complex multi-step time series regression problem. Some forecasting techniques, such as curve fitting using numerical methods, do not provide accurate results as they often fail to track seasonality and trends accurately. Machine learning algorithms, such as neural networks are more effective at integrating seasonal trends. In particular, they can be applied

to energy consumption data to forecast electric load profiles. In spite of new developments in literature and applied modeling, this remains to be a difficult problem [6].

Traditional machine learning algorithms are often ineffective at predicting sequential data, where each data point represents an observation at a certain point in time. The algorithm assumes that the data is non-sequential, and that each data point is independent of the others. As a result, the inputs are analyzed independently, without the intrinsic temporal dependencies. Consequently, some models are successful at predicting a single value, but they fail to attain multi-step forecasting. A benefit of neural network models over many other machine learning techniques is that they are able to compute multi-step predictions. This is useful in time series forecasting as the forecasts are multiple future time steps. In the field of building energy consumption forecasting methods, Artificial Neural Networks (ANN) are the most commonly used models for making load and energy use predictions [7]. ANN modeling techniques have been used to estimate energy consumption in multiple studies [6], [8], [10], [11] using Convolutional, Nonlinear Autoregressive and Feed Forward Neural Networks.

Recurrent Neural Network (RNN) has been proven to be a powerful tool for modeling sequential data as a regression time-series problem. The RNN is able to remember the analysis that was done up to a given point by maintaining a state, considering past observations. The state can be thought of as the memory of the RNN, which captures information about what's been previously calculated and is integrated into each step in the training process. This allows RNNs to process information sequentially and exhibit temporal behavior for a time sequence while retaining information from the past. Nonetheless, there are a few challenges in the effective implementation of this algorithm. Recurrent networks are computationally intensive since they keep track of past states. Some other common issues that may appear during the training phase are the vanishing or exploding gradient. As a result, the simple Vanilla RNN is not useful for long sequences of data. To solve these problems, a specific type of RNN that maintains a strong gradient over many time steps is used, thus being able to efficiently work with long sequences: the Long Short-Term Memory (LSTM) model.

Once accurate predictions of the load profile are acquired, it is necessary to then assess the flexibility of this future load. Several strategies to quantify the demand response of the residential sector to optimize electricity consumption are present in literature. Furthermore, the individual flexibility of different smart appliances has been quantified. Sancho Tomas et al. [12] applied a time-inhomogeneous Markov process to model energy variations over time for different appliances. Laicane et al. [13] investigated the potential for demand side management to reduce peak load. Load shifting algorithms were developed by Dlamini and Cromieres [14] to achieve significant household load reduction. DHulst et al. [15] presented a demand response flexibility analysis based on measurements from appliances within a large-scale implementation of smart grid technologies in a distribution grids project. These studies allow for the quantification of the flexibility of individual appliances.

In this paper, a LSTM model is used to predict the load profile of individual households. This predicted load profile

is then decomposed into specific load categories using a combination of both top-down and bottom-up non-intrusive analysis. The prediction of appliance specific load profiles then allows for the forecast of total demand response potential of a household and the associated flexibility. Firstly, limited information about households is gathered through a questionnaire about the building energy systems and operational set points. Then, an effective supervised learning algorithm is used to forecast the energy consumption of the households, using historical load profile data. Thirdly, in a top-down approach, a decomposition algorithm is used to partition the predicted load profile into two main categories: active (manual control of appliances by inhabitants) and inactive (appliances that cycle automatically and are not controlled directly by inhabitants) loads. These categories are then further separated by applying statistical studies of typical appliance uses to provide an estimate of the expected energy use per device [16]. Finally, an optimization algorithm is used to reconstruct a load forecast and the average flexibility of the demand is determined for each hour of the day. This multi-step hybrid approach is applied to a case study of three residential clients and the results are presented. The following sections of this paper are composed of Section II describing the methodology of the algorithm including Section II-A detailing the forecasting algorithm, Section II-B describing the estimation of the load flexibility and Section II-C presenting details on the evaluation of the load predictions. It is followed by Section III, which describes the case study where results are presented in Section IV and final conclusion in Section V.

II. METHODOLOGY

The electric load data used for this study was collected through the services offered by the company Eco CO2. Using a LSTM model, total load profiles were forecasted for each household. These forecasted load profiles are then analyzed with a non-intrusive load decomposition technique. Additionally, an optimization algorithm is used to reconstruct the hourly load profile for each appliance type. Finally, the hourly flexibility potential for each household is determined.

A. Forecasting

For the load forecasting, an LSTM model was used. The RNN has two hidden layers: a 200-neuron LSTM layer, and a 100-neuron dense layer, implemented in python with the TensorFlow and Keras sequential model packages. To determine the best choice of hyperparameters for the model, a sensitivity test was performed on multiple hyperparameters of the LSTM algorithm. Different architectures of LSTM networks were compared, each one with different hyperparameters, reaching an optimal compromise between forecasting accuracy and low computational time. The number of time steps used as input was $n_{input} = 24$ prior observations, and both the input and output layers have the same number of time steps ($n_{input} = n_{output}$).

The network was trained on 43 weeks of historical data in each run. This 43 week period was chosen based on the maximum historical data available for all users. This was repeated four times in order to obtain 1 full month of load predictions for each user. The default number of epochs and batch size for all analysis was $n_{epochs} = 400$ and $n_{batch} = N/25$, respectively, being N the total number of training samples.

Finally, the rectifier (ReLU) was chosen as the activation function, and ADAM (Adaptive Moment Estimation [17]) as the optimizer.

B. Energy Flexibility

To determine the flexibility potential of a 24-hours period for a household, a two-step approach was applied to the load forecasts. The load category partitioning algorithm published in [3] is applied to forecasted profiles obtained from the LSTM model to classify the total weekly energy use into eight categories listed in Table I. Active load periods are classified as the time intervals with a relatively high value and high variance.

TABLE I. HOUSEHOLD CHARACTERISTICS

Active load categories	Inactive load categories
Cooking	Domestic Hot Water (DHW)
Lighting	Refrigeration
Multimedia active	Multimedia standby
Washing	Continuous Mandatory Ventilation (CMV)

The load categories classified as inactive were assumed to be a constant percentage of the inactive load profile for the whole week period. The load categories classified as active required an optimization algorithm to assign the active consumption to different time periods of the active load profile. Therefore, identifying the expected times of use of each category. This was achieved by minimizing the objective function:

$$\min \sum_t^T X_{act,t} * p_{act} - b_{act,t} \quad (1)$$

where $X_{act,t}$ is the unknown binary variable matrix where each column corresponds to a specific active load category time series, $b_{act,t}$ is a column vector with the forecasted total energy use of each category for the week, and p_{act} is a column vector with the average hourly power values for each category. These last values were collected from statistical household energy consumption studies [18]–[21]. In addition, four constraints were defined, one per each active load category:

$$\sum_t^T j_t \leq j_{tot} \quad (2)$$

where j_t is the value of the active category j corresponding to timestep t and j_{tot} is the weekly energy use obtained in the previous step, corresponding to the same category j of the active consumption.

With this two-step approach, hourly load profiles were obtained for each consumption category. The average hourly flexibility potential was then determined. Flexibility depends on both the total load value and the end use device or category. For categories labeled as inactive, reducing consumption entails changing the temperature set-point for different inactive appliances or reducing the consumption of phantom loads. Literature studies show that Domestic Hot Water (DHW) demand response potential can be reduced 3% by decreasing the set-point by 3°C, while refrigeration can attain a 40% reduction by increasing its set-point by 3°C [15]. Standby or

phantom loads from the multimedia category have shown a 17% flexibility potential if devices are unplugged when not in use [22]. For categories labeled as active, demand side flexibility correlates more with postponing the cycle of active appliances: 1 washing event over 3 can be shifted in order to increase flexibility potential [15].

C. Forecasting evaluation

Different criteria can be used to evaluate the performance of the regression forecasting model. Commonly used metrics are the coefficient of determination (R-squared, R^2), the Root Mean Square Error (RMSE), and the Mean Absolute Error (MAE). These error measures are defined in (3), (4) and (5), respectively.

$$R^2 = \frac{\sum_{i=0}^N (y_i - \hat{y}_i)^2}{\sum_{i=0}^N (y_i - \bar{y})^2} \quad (3)$$

$$RMSE = \sqrt{\frac{\sum_{i=0}^N (y_i - \hat{y}_i)^2}{N}} \quad (4)$$

$$MAE = \frac{1}{N} \sum_{i=0}^N |y_i - \hat{y}_i| \quad (5)$$

where y_i denotes the observed values from the test set, \hat{y}_i the predicted values, and \bar{y} the mean of the observed data as defined in (6).

$$\bar{y} = \frac{1}{N} \sum_{i=0}^N y_i \quad (6)$$

The RMSE is the most used evaluation metric for regression models. On the other hand, averaging values makes MAE more robust to outliers while the RMSE gives a relatively high weight to large errors. For the coefficient of determination, high values are preferable. However, even a model with low R^2 can be accurate if the RMSE is low [23].

III. CASE STUDY

The data used for this study was collected through the services offered by the company Eco CO2. Load data from 3 French households was collected through sensors that are capable of reading and transmitting the total electric load data for each household. Additionally, limited information about the households was gathered through a questionnaire. The characteristics of the case study households is summarized in Table II.

TABLE II. HOUSEHOLD CHARACTERISTICS

	Household 1	Household 2	Household 3
Surface (m^2)	100	110	160
Heating type	Natural gas	Natural gas	Natural gas
DHW	electric	electric	electric
CMV	yes	no	yes
Cooking	electric	electric	electric
Refrigeration	2	3	3 + freezer
Washing	3	3	3
Multimedia	6	6	7
Annual consumption (kWh)	5786	10193	4172

Household 1 shows an annual electric consumption of 5786 kWh. Household 3 presents the lowest measured value, roughly exceeding 4000 kWh, whereas household 2 uses more than 10000 kWh per year. The maximum consumption attained for one-hour period ranges between 4 kWh to almost 7 kWh, for users 2 and 3, respectively.

All households present gas heating, electric cooking devices and roughly the same number of washing and multimedia appliances. Regarding the refrigeration category, household 1 presents the lowest number of appliances (two). Both households 2 and 3 have three refrigeration devices, taking into consideration that, for the latter, one of these appliances is a freezer. User 3 is the only one without electric DHW and user 2 does not have a Continuous Mandatory Ventilation (CMV) system. For this reason, these end-use appliances will not be considered for these users during the decomposition algorithm. In addition, the studied households present different surface dimensions. This variation is taken into account in the optimization model when applying normalized values of statistical household energy consumption studies. For example, the lightning category is highly dependent on the area of the household.

IV. RESULTS

The LSTM model used to forecast electricity consumption was efficient after finding the optimal hyper-parameters. Error measure results are shown in Table III.

TABLE III. PERFORMANCE OF FORECASTING MODEL

Household ID	R^2	RMSE	MAE
1	0.692	0.432	0.334
2	0.625	0.464	0.402
3	0.496	0.157	0.125

R-squared values were calculated for the monthly time series forecasts for each user. The calculated values ranged from 0.496 to 0.692, showing a good fit to the test values. The calculated RMSE and MAE showed low values for all cases. Household 3 showed smaller results not because of under fitting issues, but because its average electricity consumption was lower than the other two cases, hence leading to smaller forecasted values and metric results.

The optimization algorithm was then applied to determine the partitioned consumption forecast as shown in Figure 1. Active and inactive loads are highlighted in shades of gray. An example day for each user is presented in Figure 1 with the associated partitioned load curve for the different categories presented in Table I.

Of the three users analyzed, household 3 did not have electric domestic hot water and household 2 did not have a CMV. Accordingly, during the decomposition algorithm, these end use appliances were not considered for these users. The variability of the total consumption may change according to each user and their energy behavior. However, an overall decrease of global consumption occurs for all studied cases during nighttime hours, around 12am, or between 1am and 3am.

Overall, most of the consumption corresponds to the inactive category, reaching 60% and up to 78% of the total consumption. This is mainly caused by the use of DHW,

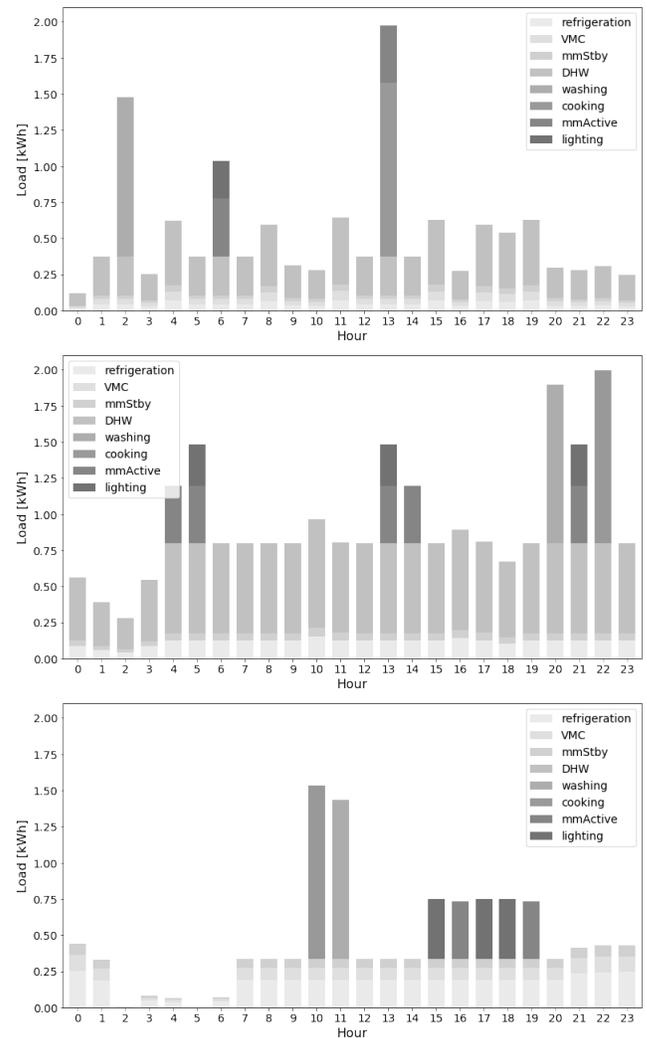


Figure 1. Example electric load forecasts partitioned into appliance categories for a 24-hour period for household 1 (top), household 2 (middle) and household 3 (bottom). Inactive load categories are shown at the bottom of each graph, while active loads are shown at the top of the stacked bars

one of the highest consumption appliances, followed by the refrigeration category. As could be expected, inactive load consumption stays almost constant for all forecasted periods, while active consumption changes depending on user behavior.

The consumption of the active part is dominated by the multimedia and lighting categories, showing consumption peaks several times a day. The washing and cooking categories are only active approximately once every 24 hours. For all end-users, active periods corresponding to multimedia and lightning categories usually occur during the same intervals. These intervals are often between 4am and 6am, or during the afternoon between 1pm and 19pm. With respect to the cooking and washing categories, they occur more often between 10am and 1pm or between 8pm to 10pm.

It is important to notice when these forecasted active and peak inactive periods occur during the day, considering that these could be the possible periods where demand response programs could be more efficiently deployed.

The final average forecasted flexibility potential for each

household is shown in Figure 2. These results are based on the possible consumption savings obtained from the different guidelines mentioned in Section II-B: for inactive loads, reducing consumption entails diminishing the consumption of phantom loads or changing the temperature set point; for active loads, demand side flexibility correlates more with postponing the cycle of active appliances.

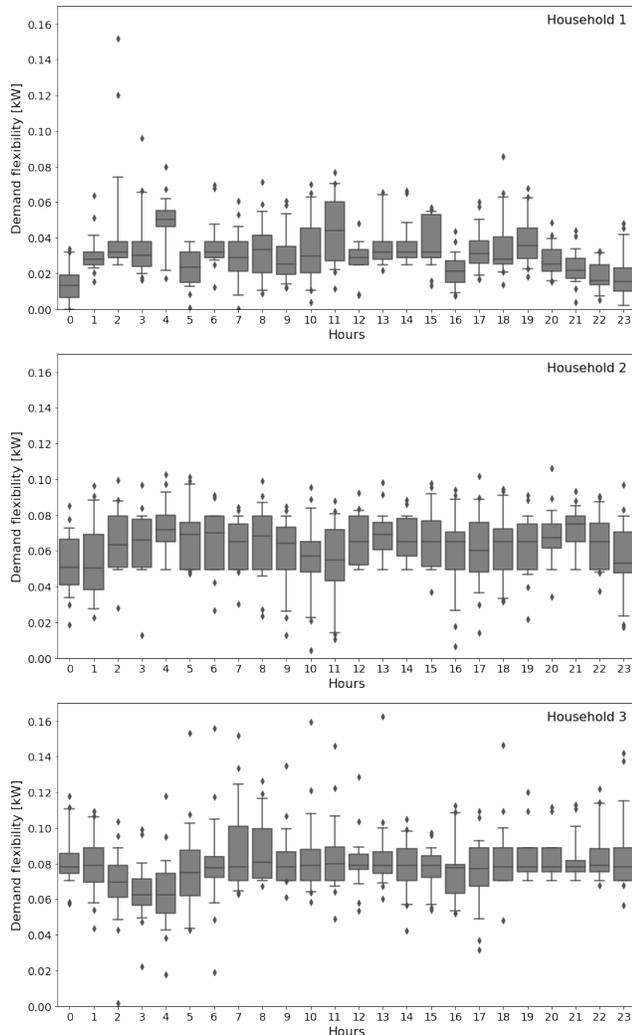


Figure 2. Average demand flexibility values for the three households for a 24-hour period

Average flexibility potential is dependent on the household characteristics, time of day and inhabitant behavior. For all cases, the smallest values for a 24-hour period are found around midnight, between 11pm and 1am, or during the early morning, between 3am and 4am.

Household 1 shows the lowest flexibility values, mostly between 0 and 0.08 kW. This is explained by the characteristics of the household, such as having the lowest number of refrigeration appliances (see Table II) and refrigeration consumption values of all study cases. The adjustment of refrigeration temperature set points results in the largest flexibility in the inactive category, thus not allowing for significant load flexibility in this particular case. Moreover, flexibility associated with changing domestic hot water temperature set points result

in only 3% savings. Therefore, for this household, where 70% of the inactive load corresponds to the use of DHW, this results in overall lower flexibility potential.

On the contrary, household 3 presents the highest flexibility values, around 0.08 kW for every hour. This household has the lowest total electricity consumption of all three and does not have electric DHW, usually responsible of a large percentage of the inactive loads. Additionally, more than 50% of his inactive consumption corresponds to the refrigeration category, resulting in a possible 40% inactive load flexibility.

Finally, household 2 shows the greatest variability in the flexibility potential values since it is the household with the highest total consumption. Besides, during all the studied period, the percentage of the active load is higher and more variable, providing a higher active load flexibility but a lower inactive load flexibility.

V. CONCLUSION

This paper has presented an effective multi-step technique to forecast the average hourly demand flexibility of a household. This model is widely applicable, does not require high computational capacity, and is also compatible with the type and resolution of data available through the massive deployment of smart meters. This solution allows for end-users to learn about their energy use and receive behavior adjustment suggestions for future possible use to encourage energy efficient behavior in advance.

The average demand flexibility values vary between 0.015kW and 0.08kW for each hour depending on the household characteristics, time of day and user behavior. For all cases, the smallest values for a 24-hour period are found around midnight, between 11pm and 1am, or during the early morning, between 3am and 4 am, where it has been noted that the load is relatively low.

The largest flexibility comes from the inactive part of the consumption: changes of temperature set points and unplugging unused multimedia devices causing phantom loads that increase total consumption. Particularly, the adjustment of refrigeration set points results in the largest flexibility values in the inactive category, while DHW usage leads to smallest values: domestic hot water appliances are often responsible of a large percentage of the inactive consumption but its temperature set point change results in only 3% savings. Active consumption appliances contribute to smaller flexibility values since it concerns end-user active behavior, rescheduling activities, postponing appliances or actively changing consumption habits.

Overall, the individual demand flexibility of each user is limited, between 15W and 80W every hour, but the aggregate demand flexibility is interesting to exploit in a massive deployment program. With the arrival of new electric generation technologies, such as photovoltaic or wind energy, demand side flexibility will play an important role in the optimization of the future electric system.

REFERENCES

- [1] "Buildings sector CO₂ emissions in the sustainable development scenario," International Energy Agency, 2019, URL: <https://www.iea.org/> [accessed: 2019-10-02].
- [2] "Statistical office of the european union," European Commission, 2019, URL: <https://ec.europa.eu/eurostat> [accessed: 2019-10-02].

- [3] K. C. Armel, A. Gupta, G. Shrimali, and A. Albert, "Is disaggregation the holy grail of energy efficiency? the case of electricity," *Energy Policy*, vol. 52, 2013, pp. 213–234.
- [4] T. Alliance. *Projet tbh*. [Online]. Available: <https://www.projet-tbh.fr/> (2015)
- [5] L. G. Swan and V. I. Ugursal, "Modeling of end-use energy consumption in the residential sector: A review of modeling techniques," *Renewable and Sustainable Energy Reviews*, vol. 13, no. 8, 2009, pp. 1819–1835.
- [6] K. Amarasinghe, D. L. Marino, and M. Manic, "Deep neural networks for energy load forecasting," in *2017 IEEE 26th International Symposium on Industrial Electronics (ISIE)*, June 2017, pp. 1483–1488.
- [7] S. Seyedzadeh, F. P. Rahimian, I. Glesk, and M. Roper, "Machine learning for estimation of building energy consumption and performance: a review," Springer International Publishing, 2018.
- [8] F. S. et al., "Predictive models for building's energy consumption: An artificial neural network (ann) approach," in *2015 XVIII AISEM Annual Conference*, Feb 2015, pp. 1–4.
- [9] P. A. Gonzalez and J. M. Zamarreo, "Prediction of hourly energy consumption in buildings based on a feedback artificial neural network," *Energy and Buildings*, vol. 37, no. 6, 2005, pp. 595–601.
- [10] R. Platon, V. R. Dehkordi, and J. Martel, "Hourly prediction of a building's electricity consumption using case-based reasoning, artificial neural networks and principal component analysis," *Energy and Buildings*, vol. 92, 2015, pp. 10–18.
- [11] J. Yuan, C. Farnham, C. Azuma, and K. Emura, "Predictive artificial neural network models to forecast the seasonal hourly electricity consumption for a university campus," *Sustainable Cities and Society*, vol. 42, 2018, pp. 82–92.
- [12] A. S. Toms, M. Sumner, S. Lamparter, and D. Robinson, "On the energy demands of small appliances in homes," *Energy Procedia*, vol. 78, 2015, pp. 3384–3390, 6th International Building Physics Conference, IBPC 2015.
- [13] I. Laicane, D. Blumberga, A. Blumberga, and M. Rosa, "Reducing household electricity consumption through demand side management: The role of home appliance scheduling and peak load reduction," *Energy Procedia*, vol. 72, 2015, pp. 222–229, international Scientific Conference Environmental and Climate Technologies, CONECT 2014.
- [14] N. G. Dlamini and F. Cromieres, "Implementing peak load reduction algorithms for household electrical appliances," *Energy Policy*, vol. 44, 2012, pp. 280–290.
- [15] R. Dhulst, W. Labeeuw, B. Beusen, S. Claessens, G. Deconinck, and K. Vanthournout, "Demand response flexibility and flexibility potential of residential smart appliances: Experiences from large pilot test in belgium," *Applied Energy*, vol. 155, 2015, pp. 79–90.
- [16] E. Grover-Silva, E. Magliaro, and J. L. Conte, "Electric load profile non-intrusive analysis to guide energy efficient behavior for residential clients," no. 163. Bucharest, Romania: 2019 IEEE PES Innovative Smart Grid Technologies Europe, Oct. 2019, pp. 1–5.
- [17] D. P. Kingma and J. Ba, "Adam: A method for stochastic optimization." *ICLR 2015: International Conference on Learning Representations*, jan 2017.
- [18] Enertech, "Lighting appliance measurement campagne for 100 households in france (campagne de mesures de l'eclairage dans 100 logements en france)," Electricite de France et Agence de l'Environnement et de la Maitrise de l'Energie, Tech. Rep., 2004.
- [19] T. Kreitz, "Refrigeration, washing machines and ac appliance measurement campagne (campagne de mesures des appareils de production de froid, des appareils de lavage et de la climatisation)," ADEME, Tech. Rep., 2016.
- [20] Enertech, "Load measurements for residential multi-media appliances and information technology devices (mesure de la consommation des usages domestiques de laudiovisuel et de linformatique)," ADEME, Tech. Rep., Jul 2008.
- [21] O. Sidler, "Knowledge and management of electrical appliances for the residential sector (connaissance et maitrise des usages specifiques de l'electricite dans le secteur residentiel)," Enertech, Tech. Rep., 2009.
- [22] R. Y. et al., "Quantifying flexibility of commercial and residential loads for demand response using setpoint changes," *Applied Energy*, vol. 177, 2016, pp. 149–164.
- [23] D. Alexander, A. Tropsha, and D. A. Winkler, "Beware of R^2 : Simple, unambiguous assessment of the prediction accuracy of QSAR and QSPR models," *Journal of Chemical Information and Modeling*, vol. 55, 2015, pp. 1316–1322.