Energy Market Analysis Using Kernel Methods

Master Thesis

L. Pernigo

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Advisor: Prof. Dr. M. Multerer

Co-Advisor: Dr. D. Baroli

Faculty of Informatics, USI Lugano

Abstract

The theory of kernel methods will be applied to the problem of point and probabilistic forecasting for the energy sector. Such choice is motivated by its interesting implications.

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Chapter 1

Problem Description

Individuals and organizations constantly face situations of uncertainty thus the need of robust forecasting methods. Such methods are crucial to the process of taking informed decision and to strategic planning.
The basic idea of forecasting is that we can extract knowledge from the past in order to make educated guesses about the future. Consequently, the range of fields where forecasting can be applied is very wide. In this thesis, our focus lies on applying forecasting techniques to the energy sector.
The reason of our decision to focus on the energy market is mainly motivated by the rapid changes it has undergone. Over the last decades, electricity markets have gone through an unprecedented transformation; this shift was driven by the liberalization of such markets, the development and integration of renewable energy sources, the increase of low carbon technologies and the adoption of smart meters. Events like the California electricity crisis help also motivating the choice of the electricity sector as subject of our studies, see [11]. Furthermore, the process of deregulation lead to an increasing interest in the field of electricity price forecasting (EF) within the academic community 2.2.
In addtion, the United Nations have identified the right to access affordable, reliable, sustainable and modern energy as one of their 17 SDGs [4].
Finally, the electricity market has a set of features that make it unique: electricity cannot be stored in an efficient way and supply and demand have to be matched instantly.

1.1 Motivation

The are mutliple reasons why the energy sector needs robust forecasting techniques. For power market companies, being able to predict prices with a low MAPE 4.3 results in increased savings [78]. Furthermore,the adoption

of smart meters provides power market companies with a ton of consumer data; this can enable them to better model consumer preferences.
Transmission system operators' main goal is to match supply and deman, generally TSO do so by increasing or decreasing the generation supplied. Thus, from their view point forecasting is critical for balancing the electricity netwrok.
Probabilistic forecasting may be useful to power producers, traders and consumers in order to improve their decision making process and managing risk(VaR). This holds in particular for traders, because probabilistic forecast enables them to simulate scenarios and carry out stress tests.
Other possible applications are: control of storage, demand side response, anomaly detection, network design and planning, simulating inputs and handling missing data.

1.2 Point vs probabilistic forecast

A distinction has to be made between two types of forecasting approaches: point forecasts and probabilistic forecasts. Point prediction, also called deterministic forecasting in the literature, is all about predicting a particular value in time. On the other hand, with probabilistic forecasting we aim at predicting either a prediction interval, quantiles or a probability distribution for each point in time. For this reason, probabilistic forecasts are more informative than point forecasts; and this is why the interest of the research community is shifting towards them. Note that a probabilistic forecast can be turned into a point forecast by simply taking its expecatation. Alternatively, a probabilistic forecast can be derived from a point one by modeling the residuals of the point prediction.

1.3 Aims and objectives

The scope of the thesis is analyzing state of the art forecasting methods in the energy market and to compare and to integrate them with ideas coming from the theory of kernel methods.

1.4 Outline

We start with a literature review and bibliometric analysis in section 2. Then the theory underlying kernel methods is covered in section 3. Following, section **??** introduces the state of the art methods in the context of both point and probabilistic forecasting. Section 5 explains the core features and terminology of the energy market and of the electricity newtork. Evaluation metrics necessary to rank the forecasting techniques are presented in section

4. Section 8 goes on with the ETL pipeline and the exploratory analysis. Implementation details are included in 9. Finally section 10 presents the experiments, the results and discusses models' strenghts, weaknesses and possible improvements.

Chapter 2

Literature Review

During the past 25 years a wide range of new ideas have been proposed for electricity point forecasting and for probabilistic forecasting.
The field benefitted greatly from the increse of computing power, the greater availability of dataset and the interest in data science. As a consequence, the forecaster's toolbox has grown in size and complexity.
Before delving into the literature review, it is important to make clear that at this point in time there is no superior method. Different solutions may outperform or underperform compared to other techniques depending on the problem settings. Thus, understanding the complexity, strenghts and weaknesses of each method is crucial for fitting the right model to the right setting.
Finally, within this research community, it emerged the need of more homogeneity in the choice of the error valuation metrics (section 4), data quality and in the way of comparing model performances [87]; as a solution, [54] proposes a checklist to aid evaluating the meaningfulness of new research. Hence, throughout this thesis work, we will stick to the proposed principles and best practices peculiar of the EF field.

2.1 Electricity forecasting classification

Electricity forecasting is a vague term and it is used in the literature to refer to the whole field. Thus, in order to introduce some clarity it is useful to classify the range of EF articles in terms of their core attributes.

2.1.1 Types

In the context of energy forecasting, the quantities of most interest are prices (EPF), loads (ELF) and renewables generation (mostly wind and solar).

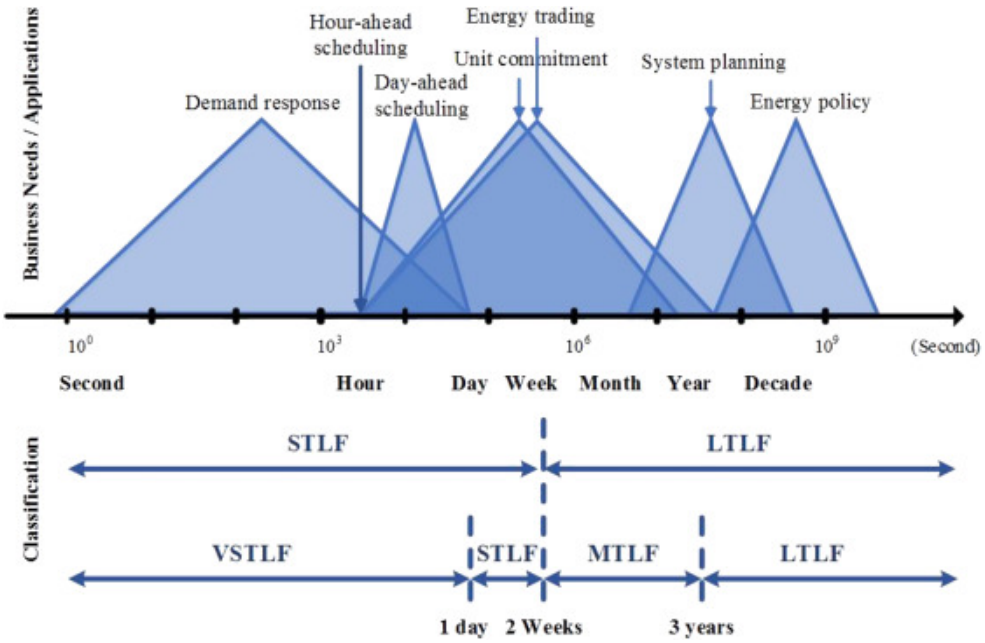


Figure 2.1: Time classsification [39]

2.1.2 Forecasting horizons

In terms of forecasting horizons, we can group EF into four major categories: very short term forcasting (VSTF), short term load forecasting (STF), medum term forecasting (MTF) and long term forecasting (LTF). Consensus in the literature is to use as cut off horizons one day, two weeks and three years respectilvely [38]; see 2.1 for a visualisation.

2.1.3 Size

Forecasts can either be for the whole target electricity network (system) or for a subset of it (zonal).

2.1.4 Point vs Probabilistic

Finally, EF literature distinguishes between point and probabilistic forecasts. Each of the two has its advantages and disadvantages; point forecasts are easier to generate and less computationally intensive while probabilistic forecast are more informative. Industry and research efforts have focused primarily on point forcasting. Nevertheless, interest in probabilistic forecasting has risen considerably over the last years due to renewable integration requirements, introduction of smart grids and increased market competitivness.

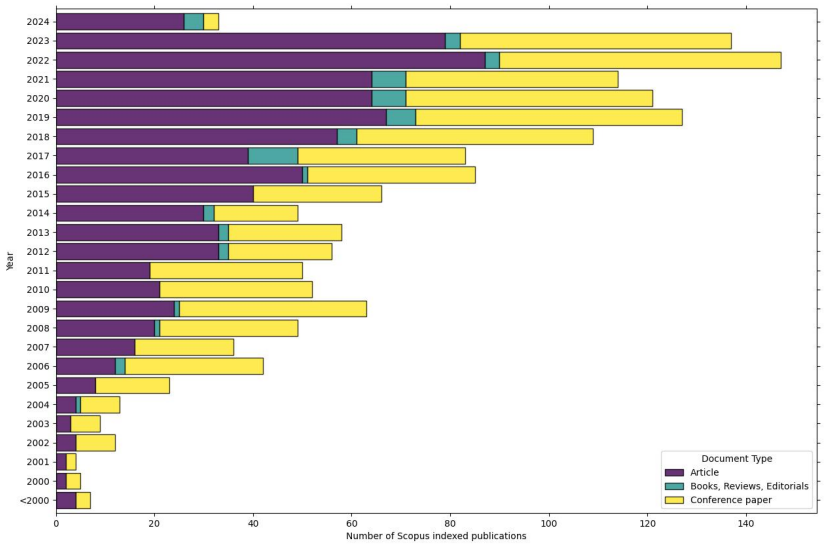


Figure 2.2: EF publications

2.2 Bibliographic analysis

This section presents the results of the bibliometric analysis we performed on March 6th 2024. This survey has been carried out by using the Scopus citation database. For details on the specific queries entered in Scopus, refer to A.6.

To get started, let us consider the evolution of the EF field over the years. This is visualized in figure 2.2, with results grouped by category; note, articles prior to the 2000 have been aggregated together due to their small number. Figure 2.2 shows the trend of an increasing interest in EF.

The next question was to compare the state of point versus probabilistic forecasting, this is visualized in figure 2.3. What it can be concluded is that probabilistic is less developed than point forecasting. To our mind this is due to the complexity of probabilistic forecast. Nevertheless, we can see a trend that suggests researchers are making an effort to fill this gap.

The EF literature is dominated by statistical and computational intelligence methods as can be seen from figure 2.4, with CI methods beign slightly preferred.

EF is an heterogenous field of research, its researchers come from a wide array of backgrounds, with electrical engineers and statisticians making up the top contributors; their different educational training may explain why the split between statistical and computational intelligence methods is so marked. Figure 2.5 depitcs the EF publications by subject area. What can be

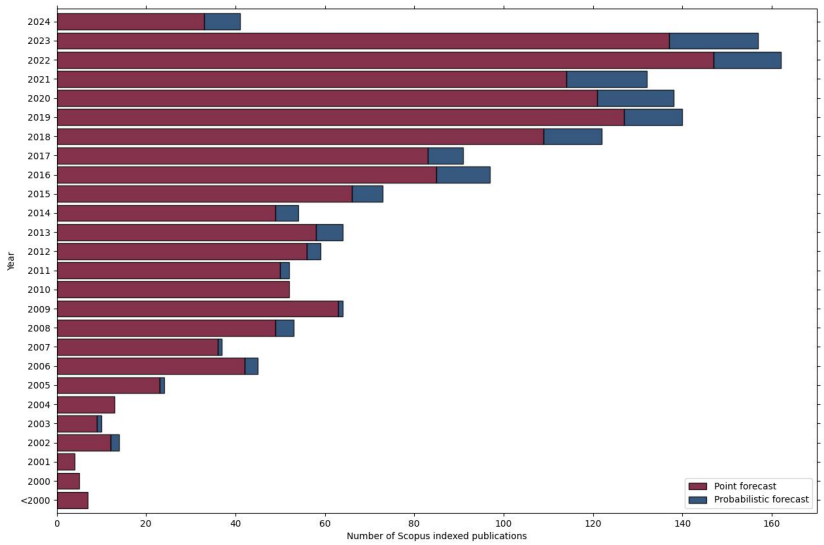


Figure 2.3: Point vs probabilistic pubblications

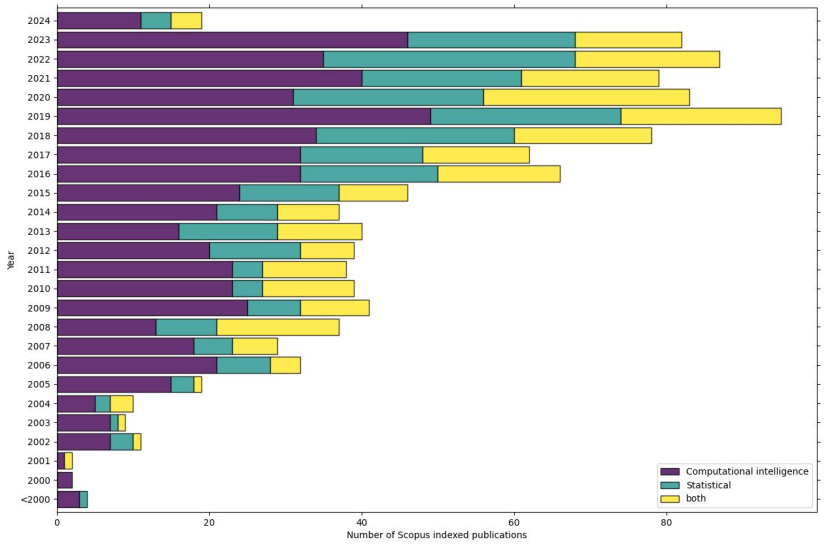


Figure 2.4: Pubblications by method

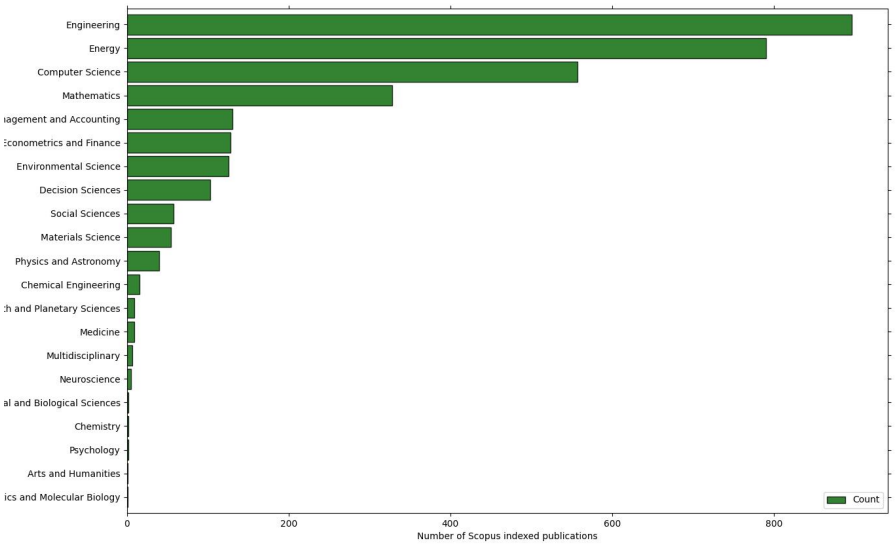


Figure 2.5: Pubblications by subject area

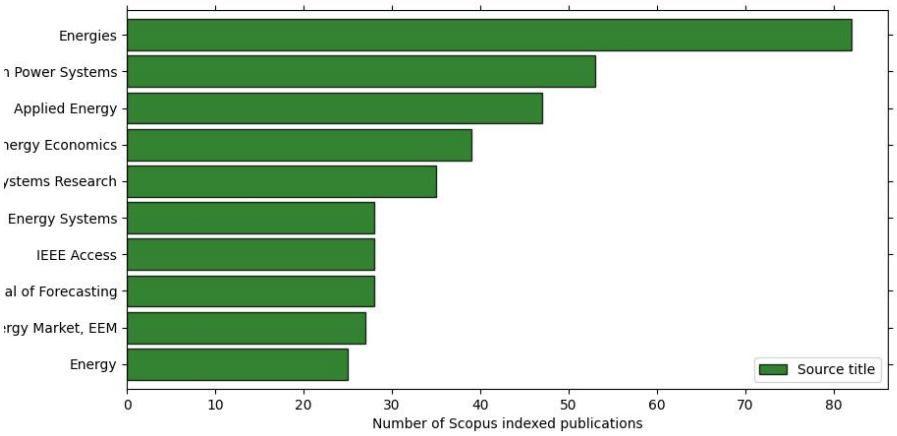


Figure 2.6: Most popolar sources/outlets

concluded, is that the bulk of pubblications come from engineering, computer science, mathematics and econometrics.
Finally, in order to refer to the most relevant source in the field, EF outlets have been ranked by popularity and plotted in figure 2.6.

2.3 EF literature review

To get started a few review articles were collected in order to understand conventions, best practicies and terminology of the EF community. Weron [87] reviews the state of the art for electricity price forecasting; beside analysing complexity of available solutions, strenghts and weaknesses it also stresses the need for objective comparative EPF studies. Specifically, it advocates for studies using similar datasets, using the same error evaluation metric and statistical testing model's outperformance. Hong et al. [39] discusses the state of the art in probabilistic electric load forecasting; it differentiates between techniques and methodologies. With techniques they refer to a family of models, like multiple linear regression or artificial neural networks. On the other hand, methodologies consist of general frameworks that can be incorporated into any method, for example variable selection mechanisms. Also this paper stresses the need for some guidelines to standardize research in the field. Nowotarski et al. [65] also carried out a thorough review of probabilistic forecasting. Weron et al. [54] offer a set of best practices when forecasting electricity prices in order to have a common framework to evaluate and compare future research. Zhang et al. [92] considers state of the art methods in wind power probabilistic forecasting and describes current challenges and possible future developments. Ziel et al. [95] provides detailed tables, grouping research papers by the time dimension 2.1.2 and objective 2.1.4 and reporting dataset, model and accuracy measures adopted. David et al. [19] adopt a combination of ARMA and GARCH in probabilistic forecasts of solar irradiance. Furthermore, they propose a recursive framework for parameter estimation. De Gooijer [20] reviews 25 years of time series forecasting for the period 1990-2005, highlighting the most influential works. He et al. [35] models multistep wind speed probabilistic forecasting by mixing CEEDMAN, LASSO and QRNN. In this work, CEEMDAN is used to decompose the wind speed time series, LASSO compresses high dimensional features, QR is used for obtaining quantile forecasts, finally KDE converts quantile forecasts into density estimates. Wan et al. [85] proposes a combination of QR and ELM to generate non parametric probabilistic forecasts of wind generation. Zhang et al. [93] forecasts wind speed by adopting QRMGM, which is a combination of QR with a minimal gated memory network. Hyndman et al. [45] explains kernel estimator of conditional density, analyses its asymptotic behaviour and covers an application for the daily temperatures of Melbourne. Kaur et al. [50] carries out a comparative study of techniques spanning ideas from statistic and artificial intelligence. Van der Meer et al. [80] provides another thorough anlysis of the probabilistic forecasting realm by covering recent advances and identifying research gaps. The IEEE Power and Energy Society provides also insightful lecture notes on probabilistic energy forecasting methodologies, implementations, and applications [1]. Marcjasz et al. [56] uses distributional neural networks to create probabilistic forecasts

for the day ahead electricity prices in the german market. Nowotarski et al. [64] introduce a method for constructing PI and call it quantile regression averaging. Their idea is weighting a set of models' prediction such that the pinball loss of the weighted model is minimized. The observed results is that QRA performed better compared to twelve individual models. Arora et al. [9] focus on modelling electricity smart meter data by proposing a non parametric probabilistic technique based on kernel density estimation and conditional kernel density estimation [69] [45]. Their conclusion is that kernel density methods are competitive against exponential smoothing when forecasting residential data. Conversely, exponential smoothing has still an edge in predicting SME data. Zhang et al. [91] introduce a framework based on quantile regression and kernel density estimation in the context of short term wind forecasting. The proposed methods behave well compared to an ARMA(1,1). Haben et al. [31] analyses a variety of techniques in terms of both probabilistic and point forecasting, within this study they focus on load forecasting at the low voltage level. Koochali et al. [53] reviews various existing methods for assessing probabilistic forecast models and discusses their advantages and disadvantages. Matheson et al. [57] develops classes of scoring rules for continuous probability distributions. Gneiting et al. [28] provides a thorough overview of the theory of proper scoring rules for interval and density forecasts. Gneiting et al. [26] covers theory and techniques state of the art in probabilistic forecasting. Zhang et al [90] proposes a two stage bootstrap sampling framework for probabilistic load forecasting. They test it for different regression models such as RF, GBRT, linear regression, and LSSVM regression. Jónsson et al. [48] introduces a density model for the day ahead market extending the adaptive QR framework of [60] by modelling the tails of the predicted density with an exponential distribution. Fatema et al. [22] considers gaussian process regression for point forecasting and prediction intervals prediction. Then, it inputs PI to KDE in order to estimate a probability distribution. Dudek [21] proposes a probabilistic forecasting model based on the Nadaraya Watson estimator [63] [86]. Huurman et al. [43] surveys the predictive power of weather variables for electricity prices in the danish market. Their empirical results suggest that weather is central for point forecasting day ahead prices. The opposite conclusion are drawn for density forecasting.

Lately, the idea of combining forecasts has gained popularity in the forecasting community [67]; in the literature, combined forecasts are called ensemble [27]. Experimental results have shown ensemble methods to outperform their component forecasts. Note that, the more the errors of the combined models are not correlated the more we can benefit from ensembles. It is also worth noting that older and simpler methods are still valuable (in combination with other models or on their own); these being less subject to overfitting than complex models.

A major step forward in EF was the creation of the global energy forecasting

competition (GEFCom) in 2012. Until then, no formal benchmarking process or data pool was established and new publications rarely reproduced the results from work done by others. Addressing these issues was the motivation behind the creation of GEFCom by the IEEE working group on energy forecasting. The EF field was positively affected by this competition; a number of ideas were tested on the same setting with only the best ones being published and it also contributed bridging the gap between industry practice and academic research. GEFCom 2012 had two tracks; the former about hierarchical load forecasting, the latter about wind power forecasting, see [40] for a comprehensive review.
The focus of GEFCom 2014 was on probabilistic forecasting, Hong et al. [41] discusses the problem tracks, the data and the winning methods. In this paragraph some of the winning entries of the 2014 GEFCom edition are discussed. Xie et al. [89] propose a two stage approach; in the first stage they use MLR to build a point forecast, then in the second stage they try different approaches for modelling the MLR residuals, among other they tried ESM, ANN and ARIMA. Maciejowska et al. [55] proposes a new probabilistic model extending the idea of QRA [64]. Haben et al. [30] mixes CKD and QR in their competition entry. Gaillard et al. [24] [25] combines quantile regression with generalized additive models [34]. Ziel et al. [94] estimates an AR model through the LASSO [79] instead of the standard OLS.
The last GEFCom was held in 2017, its focus was providing probabilistic load forecasts, see [42]. The GEFCom competition has also inspired the organization of other competitions such as the RWEnpower competition in the UK, the RTE competition in France, the Tokyo electric power company competition in Japan and the BigDEAL forecasting competitions.

A couple of considerations can be drawn from the above literature review. As already pointed out, the EF field is characterized by heterogeneity in its forecasting techniques; methods come from statisitics, mathematics, econometrics, electrical engineering and the artificial intelligence communities.
Every paper uses different datasets. Therefore, it is not possible to compare directly results from one paper to another without implementing the paper specific algorithms and then applying them to your dataset. An additional hurdle is that some datasets are not freely accessible.
Thus, a good understanding of state of the art methods in EF is required to carry out a rigorous comparison between methods. That is why the following chapters are devoted to summarising the mathematical theory underlying such techniques.

2.4 Kernel methods literature review

Kernel methods are a class of algorithms for patter analysis. With kernel methods we are able to apply linear methods with predictors in a high dimensional space, without having to explicitly evaluate the involved dot products of the features. Throughout this thesis work, we will address the performance of kernel methods in the context of EF.
Their name comes from the german word kern, which translates to core in english. Such term was first used by David Hilbert in his paper on integral equations [36] where he introduced the term of definite kernels. Following, Hilbert's and Schmidt's [70] work lead to the introduction of a new space, the Hilbert space. In 1909, James Mercer improved Hilbert's work by proposing his theorem [59]. This theorem underlies the power of kernel methods, that is the kernel trick. In 1938, Schoenberg [71] developed the mathematical results that allow us to find the kernel associated to a specific feature space metric. In 1941, Kolmogorov [52] carried out stuides on representing kernel in linear spaces. In 1950, Aronszajn [8] published the first work on RKHS; developing the general method for representing kernels in linear spaces. In 1964, Aizerman [7] further improved the theory of RKHS. It was in the nineties that theory of kernel methods got popular, particularly in the field of machine learning. Kernels have been used in various different tasks such as SVM [82] [81], Gaussian process classifiers [88], spline methods [84], neural networks [68] and principal component analysis [72]. Nevertheless kernel methods received very little attention in the specific setting of EF literature. The kernel theory needed for this thesis work is covered in section 3. For an introduction to kernel methods, we referred to [74] [37].
Kanagawa et Fukumizu introduces to the concept of kernel mean embedding [49]. Muandet et al. [61] surveys established results and new advances in the theory of Hilbert space distribution embeddings. It has to be said that, computing and storing such embeddings becomes prohibitive for large scale settings. Rudi et al. [16] proposes an efficient approximation procedure based on the Nyström method [66], providing also an upper bound for the approximation error. Article [17] presents kernel herding; basically, Smola et al. used the kernel trick to extend the herding algorithm to continous spaces. The result is an infinite memory deterministic process that takes in a collection of samples and learns to approximate a pdf.

Chapter 3

Kernel Theory

3.1 Kernel Mean Embedding of Distributions: A Review and Beyond

From this first paper [61], the notation and terms used in the theory of Reproducing Kernel Hilbert Spaces are summarized.
Many algorithms use the inner product as similarity measure between data instances $x, x' \in \mathcal{X}$. However, this inner product spans only the class of linear similarity measures.
The idea behind kernel methods is to apply a non-linear transformation φ to the data x in order to get a more powerful non linear similarity measure.

$$\begin{aligned} \varphi(x) : \mathcal{X} &\longrightarrow \mathcal{F} \\ x &\mapsto \varphi(x) \end{aligned}$$

Then we take the inner product in the high dimensional space $\mathcal{F}$ mapped by $\varphi(x)$.

$$k(x, x') := \langle \varphi(x), \varphi(x') \rangle_{\mathcal{F}}$$

$\varphi(x)$ is referred as feature map while k as kernel function.
Therefore, we can kernelize any algorithm involving a dot product by substituting $\langle x, x' \rangle_{\mathcal{X}}$ with $\langle \varphi(x), \varphi(x') \rangle_{\mathcal{F}}$
One would expect constructing the feature maps explicitly and then evaluate their inner product in $\mathcal{F}$ to be computationally expensive, and indeed it is. However, we do not have to explicitly perform such calculations. This is because of the existence of the kernel trick. To illustrate the idea behind the kernel trick consider the following example.
Suppose $x \in \mathbb{R}^2$ and assume to select $\varphi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$, then the

inner product in the feature space is $x_1^2 x_1'^2, x_2^2 x_2'^2 + 2x_1 x_2 x_1' x_2'$. Notice that this is the same of $\langle \varphi(x), \varphi(x') \rangle$; thus the kernel trick consists of just using $k(x, x') =: (x^T x')^2$.

3.1.1 RKHS

Following are the definitions that make up the basis for the theory of kernel methods.

Definition 3.1 *A sequence $\{v_n\}_{n=1}^{\infty}$ of elements of a normed space $\mathcal{V}$ is a Cauchy sequence if for every $\varepsilon > 0$, there exist $N = N(\varepsilon) \in \mathbf{N}$ such that $\|v_n - v_m\|_{\mathcal{V}} < \varepsilon \ \ \forall m, n \geq N$*

Definition 3.2 *A complete metric space is a metric space in which every Cauchy sequence is convergent.*

Definition 3.3 *A Hilbert space is a vector space $\mathcal{H}$ with an inner product $\langle f, g \rangle$ such that the norm defined by $\|f\| = \sqrt{\langle f, f \rangle}$ turns $\mathcal{H}$ into a complete metric space.*

Definition 3.4 *RKHS. A Reproducing Kernel Hilbert Space is an Hilbert space with the evaluation functionals $\mathcal{F}_x(f) := f(x)$ bounded, i.e. $\forall x \in \mathcal{X}$ there exists some $C > 0$ such that $\|\mathcal{F}_x(f)\| = \|f(x)\| \leq C\|f\|_{\mathcal{H}} \ \forall f \in \mathcal{H}$*

Theorem 3.5 *Riesz Representation. If $A : \mathcal{H} \to \mathbf{R}$ is a bounded linear operator in a Hilbert space $\mathcal{H}$, there exists some $g_A \in \mathcal{H}$ such that $A(f) = \langle f, g_A \rangle_{\mathcal{H}}$, $\forall f \in \mathcal{H}$.*

The Riesz representation theorem results in the following proposition for RKHS.

Proposition 3.6 *For each $x \in \mathcal{X}$ there exists a function $k_x \in \mathcal{H}$ such that $\mathcal{F}_x(f) = \langle k_x, f \rangle_{\mathcal{H}} = f(x)$*

The function k_x is the reproducing kernel for the point x. Furthermore, note that k_x is itself a function lying on $\mathcal{X}$

$$k_x(y) = \mathcal{F}_y(k_x) = \langle k_x, k_y \rangle_{\mathcal{H} = \langle \varphi(x), \varphi(x) \rangle_{\mathcal{H}}}$$

3.1.2 Kernel families

Table 3.1 contains popular kernel families in literature and applications.

3.2 Recovering Distributions from Gaussian RKHS Embeddings

This paper covers the RKHS embedding approach to nonparametric statistical inference [49]. The idea here is computing an estimate of the kernel mean

Table 3.1: Kernel types

Kernel function	Equation	Hyperparameters
Linear	$k(x_1, x_2) = x_1 x_2$	
Polynomial	$k(x_1, x_2) = (x_1^\intercal x_2 + c)^d$	c, d
Gaussian RBF	$k(x_1, x_2) = e^{-\frac{\|x_1 - x_2\|^2}{2\sigma^2}}$	σ
Exponential RBF/Laplacian	$k(x_1, x_2) = e^{-\frac{\|x_1 - x_2\|}{\gamma}}$	γ
Hyperbolic/Sigmoid Kernel	$k(x_1, x_2) = \tanh(\gamma x_1^\intercal x_2 + r)$	γ, r
Periodic	$k(x_1, x_2) = e^{\frac{-2sin^2\left(\frac{\pi}{p}\|x_1 - x_2\|\right)}{l^2}}$	p, l

in order to obtain an approximation of the underlying distribution of the observed random variable. The kernel mean embedding $\mu_{\mathbb{P}}$ of a probability $\mathbb{P}$ corresponds to the feauture map $\varphi(x)$ integrated with respect to the $\mathbb{P}$ measure.
That is $\mu_{\mathbb{P}} := \int_{\mathcal{X}} k(x, \cdot) d\mathbb{P}(x)$.
Kernel mean embedding serves as a unique representation of $\mathbb{P}$ in the RKHS $\mathcal{H}$. This holds provided that $\mathcal{H}$ is characteristic.

Definition 3.7 *The RKHS $\mathcal{H}$ and the associated kernel k are said characteristic, when the mapping $\mu : \mathbb{P} \to \mathcal{H}$ is injective.*

When the mapping is injective, we have that $\mu_{\mathbb{P}}$ is uniquely associated with $\mathbb{P}$; thus, $\mu_{\mathbb{P}}$ is a unique representation of $\mathbb{P}$ in $\mathcal{H}$.
Note that, by the reproducing property of RKHS $\langle f, k(x, \cdot)\rangle = f(x)$ we have:

$$E_{\mathbb{P}}[f(x)] = \langle f, \mu_{\mathbb{P}}\rangle_{\mathcal{H}}, \ \forall f \in \mathcal{H}$$

Proof

$$\begin{aligned} E_{\mathbb{P}}[f(x)] &= \int_{\mathcal{X}} f(x) d\mathbb{P}(x) \\ &= \int_{\mathcal{X}} \langle f, k(x, \cdot)\rangle_{\mathcal{H}} d\mathbb{P}(x) \\ &= \sum_{i=1}^{\infty} \langle f, k(x_i, \cdot)\rangle_{\mathcal{H}} \mathbb{P}(\mathcal{X}_i) \\ &= \langle f, \sum_{i=1}^{\infty} k(x_i, \cdot)\mathbb{P}(\mathcal{X}_i)\rangle_{\mathcal{H}} \\ &= \langle f, \mu_{\mathbb{P}}\rangle_{\mathcal{H}} \end{aligned}$$ □

The kernel mean embedding can be employed to estimate the density p at any fixed point x_0. Letting δ_{x_0} to be the dirac delta function we have:

$$p(x_0) = \int \delta_{x_0} p(x) dx = E_{\mathbb{P}}[\delta_{x_0}]$$

Therefore, the idea is to define an estimator for the expectation of δ_{x_0} through $\mu_{\mathbb{P}}$; this would result in an estimator of $p(x_0)$.
A kernel $k(x_0, \cdot)$ is used to approximate the delta function, furthermore applying theorem 1 of [49] we have that a consistent estimator of $E_{\mathbb{P}}[k(x_0, \cdot)]$ is given by $\sum_{i=1}^{n} w_i k(x_0, x_i)$
When the weigths are all $1/n$ we end up with the standard kernel density estimation.
Alternatively, the optimal weights can be found by minimizing the following problem $\|\hat{\mu} - \Phi w\|^2$ where $\Phi : \mathbb{R}^n \to \mathcal{H}$.

3.3 Super-Samples from Kernel Herding

Kernel herding is a deterministic sampling algorithm designed to draw "Super Samples" from probability distributions [17]. The idea of herding, is to generate pseudo-samples that greedily minimize the error betweeen the mean operator and the empirical mean operator resulting from the selected herding points.

Letting $p(x)$ be a probability distribution, kernel herding is recursively defined as follows:

$$x_{t+1} = \arg\max_{x \forall \mathcal{X}} \langle w_t, \varphi(x) \rangle$$
$$w_{t+1} = w_t + E_{\mathbb{P}}[\varphi(x)] - \varphi(x_{t+1})$$

w denotes a weight vector that lies in $\mathcal{H}$.
Here, by assuming that the inner product between weights and the mean operator is equal to a general functional f evaluated at x, that is $\langle w, \varphi(x) \rangle_{\mathcal{H}} =$

$f(x)$. We have:

$$\begin{aligned}
\langle w, \mu_{\mathbb{P}} \rangle_{\mathcal{H}} &= \langle w, \int k(x, \cdot) d\mathbb{P}(x) \rangle_{\mathcal{H}} \\
&= \langle w, \sum_{i=1}^{\infty} k(x_i, \cdot) \mathbb{P}(\mathcal{X}_i) \rangle_{\mathcal{H}} \\
&= \sum_{i=1}^{\infty} \langle w, k(x_i, \cdot) \rangle_{\mathcal{H}} \mathbb{P}(\mathcal{X}_i) \\
&= \sum_{i=1}^{\infty} f(x_i) \mathbb{P}(\mathcal{X}_i) \\
&= \int f(x) d\mathbb{P}(x) \\
&= \mathbb{E}_{\mathbb{P}}[f(x)]
\end{aligned}$$

Moreover, second assumption of the model is that $\|\varphi(x)\|_{\mathcal{H}} = R \quad \forall x \in X$. That is the Hilbert space norm of the feature vector is equal to a constant R for all states in the set $\mathcal{X}$.

This can be achieved by taking the new feature vector as $\varphi^{new}(x) = \frac{\varphi(x)}{\|\varphi(x)\|_{\mathcal{H}}}$. See A.1 for details.
By rewriting the formula for the weights we end up with

$$\begin{aligned}
w_{t+1} &= w_t + E_{\mathbb{P}}[\varphi(x)] - \varphi(x_{t+1}) \\
&= w_{t-1} + E_{\mathbb{P}}[\varphi(x)] + E_{\mathbb{P}}[\varphi(x)] - \varphi(x_{t+1}) - \varphi(x_t) \\
&= w_{t-2} + E_{\mathbb{P}}[\varphi(x)] + E_{\mathbb{P}}[\varphi(x)] + E_{\mathbb{P}}[\varphi(x)] - \varphi(x_{t+1}) - \varphi(x_t) - \varphi(x_{t-1})
\end{aligned}$$

Considering w_T, we have

$$w_T = w_0 + T E_{\mathbb{P}}[\varphi(x)] - \sum_{t=1}^{T} \varphi(x_t)$$

Note that $E_{\mathbb{P}}[\varphi(x)] = \int_{\mathcal{X}} \varphi(x) d\mathbb{P}(x)$ which corresponds to the definition of $\mu_{\mathbb{P}}$. That is μ is the mean operator associated with the distribution $\mathbb{P}$; it lies in $\mathcal{H}$.
Thus,

$$w_T = w_0 + T\mu_{\mathbb{P}} - \sum_{t=1}^{T} \varphi(x_t)$$

Notice we do not have to compute $\mu_{\mathbb{P}}$ explicitly, the terms involving $\mu_{\mathbb{P}}$ will be computed by applying the kernel trick.

Now we have everything we need in order to reformulate the original problem in a way such that it depends just on the states x. Plug the formula for

the weights in the formula for the x_t and use the kernel trick; we end up with

$$\begin{aligned} x_{T+1} &= \arg\max_{x \forall \mathcal{X}} \langle w_0 + T\mu_{\mathbb{P}} - \sum_{t=1}^{T} \varphi(x_t), \varphi(x) \rangle_{\mathcal{H}} \\ &= \arg\max_{x \forall \mathcal{X}} \langle w_0, \varphi(x) \rangle_{\mathcal{H}} + \langle T\mu_{\mathbb{P}}, \varphi(x) \rangle_{\mathcal{H}} - \langle \sum_{t=1}^{T} \varphi(x_t), \varphi(x) \rangle_{\mathcal{H}} \\ &= \arg\max_{x \forall \mathcal{X}} \langle w_0, \varphi(x) \rangle_{\mathcal{H}} + T\langle \mu_{\mathbb{P}}, \varphi(x) \rangle_{\mathcal{H}} - \sum_{t=1}^{T} k(x_t, x) \end{aligned}$$

Notice $\langle \mu_{\mathbb{P}}, \varphi(x) \rangle_{\mathcal{H}}$ can be rewritten in the following way

$$\begin{aligned} \langle \mu_{\mathbb{P}}, \varphi(x) \rangle_{\mathcal{H}} &= \langle \int_{\mathcal{X}'} \varphi(x') d\mathbb{P}(x'), \varphi(x) \rangle_{\mathcal{H}} \\ &= \langle \sum_{i=1}^{\infty} \varphi(x'_i) \mathbb{P}(\mathcal{X}'_i), \varphi(x) \rangle_{\mathcal{H}} \\ &= \sum_{i=1}^{\infty} \langle \varphi(x'_i), \varphi(x) \rangle_{\mathcal{H}} \mathbb{P}(\mathcal{X}'_i) \\ &= \sum_{i=1}^{\infty} k(x'_i, x) \mathbb{P}(\mathcal{X}'_i) \\ &= \int_{\mathcal{X}'} k(x', x) d\mathbb{P}(x') \\ &= E_{\mathbb{P}}[k(x', x)] \end{aligned}$$

Furthermore, by initializing $w_0 = \mu_{\mathbb{P}}$ we end up with the following function to be optimized, i.e.

$$\begin{aligned} x_{T+1} &= \arg\max_{x \forall \mathcal{X}} \langle w_0, \varphi(x) \rangle + T\langle \mu_{\mathbb{P}}, \varphi(x) \rangle - \sum_{t=1}^{T} k(x_t, x) \\ &= \arg\max_{x \forall \mathcal{X}} (T+1) E_{\mathbb{P}}[k(x', x)] - \sum_{t=1}^{T} k(x_t, x) \end{aligned}$$

Now consider the error term between the mean kernel operator and its estimation through herding samples

$$
\begin{aligned}
\varepsilon_{T+1} &= \|\mu_{\mathbb{P}} - \frac{1}{T+1}\sum_{i=1}^{T+1}\varphi(x_t)\|_{\mathcal{H}}^2 \\
&= \mathbb{E}_{x,x'\sim\mathbb{P}}[k(x',x)] - \frac{2}{T+1}\sum_{t=1}^{T+1}\mathbb{E}_{x\sim\mathbb{P}}[k(x,x_t)] + \frac{1}{(T+1)^2}\sum_{t,t'=1}^{T+1}k(x_t,x_{t'}) \\
&= \mathbb{E}_{x,x'\sim\mathbb{P}}[k(x',x)] - \frac{2}{T+1}\sum_{t=1}^{T+1}\mathbb{E}_{x\sim\mathbb{P}}[k(x,x_t)] + \frac{1}{(T+1)^2}\sum_{\substack{t=1\\t=t'}}^{T+1}k(x_t,x_{t'}) + \\
&\quad + \frac{2}{(T+1)^2}\sum_{\substack{t=1\\t\neq t'}}^{T+1}k(x_t,x_{t'})
\end{aligned}
$$

So ε_{T+1} depends on x_{T+1} only through $-\frac{2}{T+1}\mathbb{E}_{x\sim\mathbb{P}}[k(x,x_{T+1})] + \frac{2}{(T+1)^2}\sum_{t=1}^{T}k(x_t,x_{T+1})$
The term $k(x_{T+1},x_{T+1})$ is not included, because by assumption it is equal to the constant R.
Recognize that this term is the negative of the objective function maximized with respect to x. So the sample x_{T+1} minimizes the error at time step $T+1$, i.e. ε_{T+1}
During the iterative step of kernel herding we maximize the negative of this quantity, thus we are minimizing the error greedily. In the sense that at each iteration we choose the x that minimizes our current error; however this does not guarantee that the samples states are jointly optimal.
Intuitively, at each iteration, herding searches for a new sample to add to the pool; it is attracted to the regions where p is high and pushed away from regions where samples have already been selected.

- Explain kernel density estimation Explain under which conditions kernel mean embedding is equivalent to kernel density estimation. Kernel mean embedding generalization of kernel density estimation

- Other kernel theory concepts, I may need to restructure the structure of the kernel folder by putting in the right order the varies paper1,2,3,4

Chapter 4

Evaluation metrics

Proper evaluation methods guide researchers in choosing the model that best fits their needs; thus, this chapter is dedicated to the most common evaluation metrics adopted by academics in the field of EF. Error metrics and measures vary depending on wethter we are concerned with point or probabilistic forecasts. Additionally, note that the latter can take different forms which therefore requires different measures.

4.1 MAE

Consider the time series with actual values given by $\mathrm{L} = (L_{n+1}, L_{n+2}, \ldots, L_{n+h})$ and its h step ahead point forecast $\hat{\mathrm{L}} = (\hat{L}_{n+1}, \hat{L}_{n+2}, \ldots, \hat{L}_{n+h})$ the mean absolute error is defined as

Definition 4.1 $\mathrm{MAE}(\mathrm{L}, \hat{\mathrm{L}}) = \frac{1}{h}\|\mathrm{L} - \hat{\mathrm{L}}\|_1 = \frac{1}{h}\sum_{k=1}^{h} |L_{n+k} - \hat{L}_{n+k}|$

4.2 RMSE

Definition 4.2 $\mathrm{RMSE}(\mathrm{L}, \hat{\mathrm{L}}) = \frac{1}{\sqrt{h}}\|\mathrm{L} - \hat{\mathrm{L}}\|_2 = \sqrt{\frac{\sum_{k=1}^{h} (L_{n+k} - \hat{L}_{n+k})^2}{h}}$

MAE and RMSE posses the useful property of being expressed in the same units of the data thus enabling meaningful comparisons. However, a drawback of such measures is that we cannot use them to compare accuracy between time series wich have different magnitudes. For instance, a day ahead error of 1kWh is negligible when considering a daily demand of 100kWn while the same error is considerably big when daily demand is 2kWh. This consideration leads to relative accuracy scores, between those the MAPE is by far the most popular.

4.3 MAPE

.

Definition 4.3 $\text{MAPE}(\mathrm{L}, \hat{\mathrm{L}}) = \frac{100}{h} \sum_{k=1}^{h} \frac{|L_{n+k} - \hat{L}_{n+k}|}{|L_{n+k}|}$

4.4 RMSPE

Definition 4.4 $\text{RMSPE}(\mathrm{L}, \hat{\mathrm{L}}) = 100 \cdot \sqrt{\frac{1}{h} \sum_{k=1}^{h} \left(\frac{|L_{n+k} - \hat{L}_{n+k}|}{|L_{n+k}|} \right)^2}$

Note, MAPE and RMSPE may not be appropriate for series which have zero or very small values, for example, electricity demand at the household level; the result is a large score regardless of the absolute errors. Scaled errors constitute a robust family of scores.

4.5 MASE

Definition 4.5 $\text{MASE}(\mathrm{L}, \hat{\mathrm{L}}) = \frac{1}{h} \sum_{k=1}^{N} \frac{|L_{n+k} - \hat{L}_{n+k}|}{\frac{1}{h-1} \sum_{k=2}^{h} |L_k - L_{k-1}|}$

In the denominator we have the error of the naïve/persistence model. In this model, the current demand makes up the prediction for the next time step; that is $\hat{\mathrm{L}}_{n+1}^{\text{naive}} = \mathrm{L}_n$.

4.6 RMSSE

Definition 4.6 $\text{RMSSE}(\mathrm{L}, \hat{\mathrm{L}}) = \sqrt{\frac{1}{h} \sum_{k=1}^{N} \left(\frac{|L_{n+k} - \hat{L}_{n+k}|}{\frac{1}{h-1} \sum_{k=2}^{h} |L_k - L_{k-1}|} \right)^2}$

4.7 Pinball

The pinball score or quantile score is used to measure the accuracy of a quantile forecast.

Definition 4.7 $\text{Pinball}(L_t, \hat{L}_{t,q}, q) = \begin{cases} (1-q)(\hat{L}_{t,q} - L_t) & L_t < \hat{L}_{t,q} \\ q(L_t - \hat{L}_t, q) & L_t \geq \hat{L}_{t,q} \end{cases}$

The pinball loss is an asymmetric function, it weights its score differently depending on the error sign and on the quantile considered, see 4.1. By averaging all the pinball losses over all quantiles and over the whole forecast horizon, we obtain the pinball loss of the probabilistic forecast.

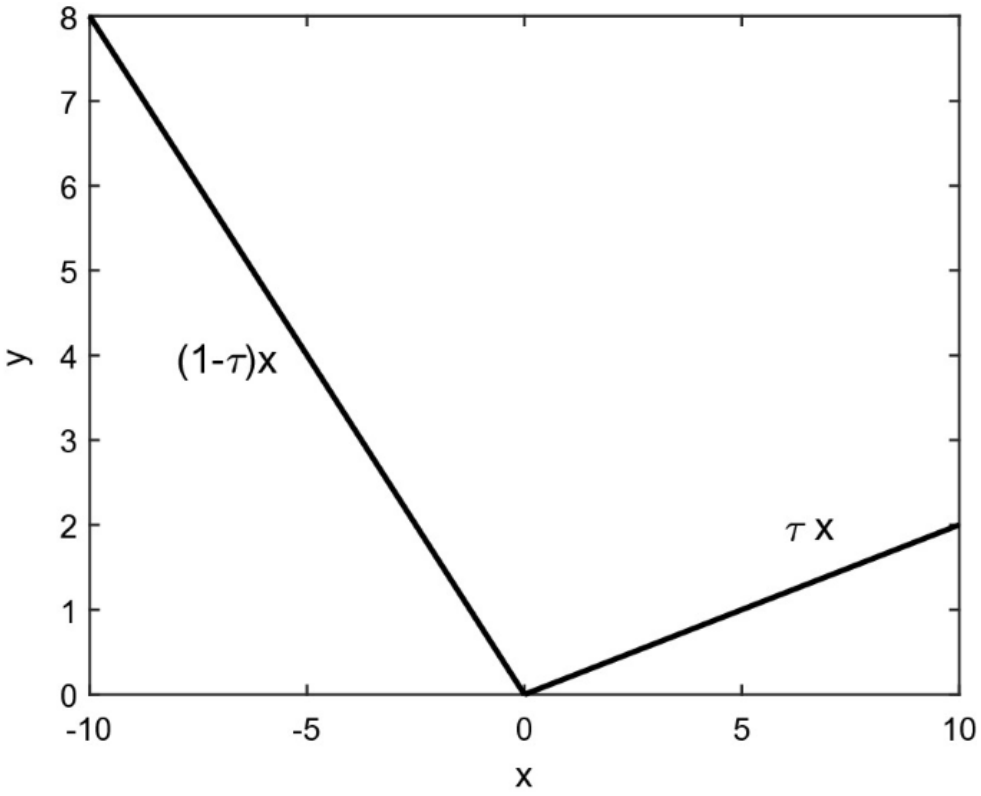


Figure 4.1: Pinball loss with q=0.2 [32]

4.8 Winkler

Definition 4.8 $\text{Winkler}_\alpha = \begin{cases} \delta & Low_t \leq L_t \leq Uppt \\ \delta + 2(Low_t - L_t)/\alpha & L_t < Low_t \\ \delta + 2(Lt - Upp_t)/\alpha & L_t \geq Upp_t \end{cases}$

Where delta is the PI width, that is $\delta = Upp_t - Low_t$. This score penalizes observations falling outside the PI and rewards narrow PI.

4.9 CRPS

The continous ranked probability score measures the differece between the estimated cumulative distribution $\hat{F}$ and the empirical Cdf.

Definition 4.9 $\text{CRPS}(L, \hat{F}) = \int_{-\infty}^{\infty} \left(\hat{F}(x) - \mathbb{1}(x - L)\right)^2 dx$

Nevertheless, we can evaluate the integral in closed form. Where the indicator

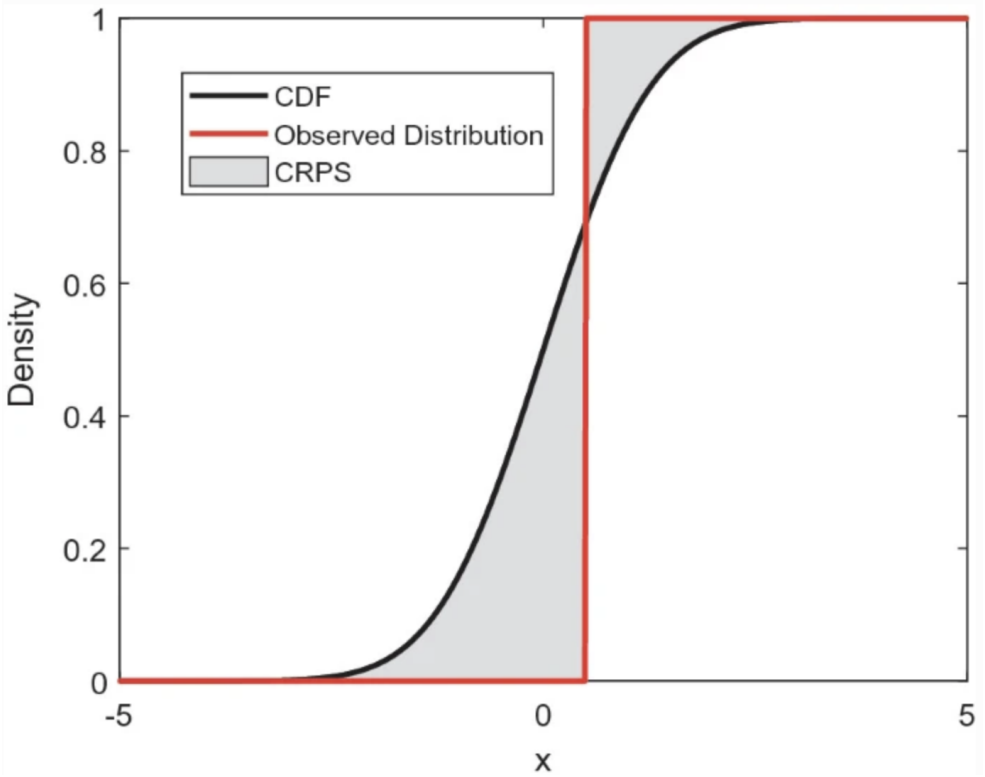


Figure 4.2: CRPS integral [32]

function is defined as $\mathbb{1}(z) = \begin{cases} 0 & z < 0 \\ 1 & z \geq 0 \end{cases}$
For a visualisation see, 4.2. The grey area is what contributes toward the CRPS score. The better the estimated cdf is the smaller the total CRPS score will be.
It is worth noting, that the CRPS integral can be rewritten in terms of expectations. This makes its evaluation easier, since we know that the sample mean converges to the expectation by the law of large numbers. This was first pointed out by [29], where authors take advantage of lemma 2.2 of [10] or equivalently identity 17 of [76].

Lemma 4.10 *Let* X_1, X_2, Y_1, Y_2 *be independent real random variables with finite expectations. Let* X_1, X_2 *be identically distributed with distribution function* F *and let* Y_1, Y_2 *be identically distributed with distribution function* G*. Then*

$$\mathbb{E}(|X_1 - Y_1|) - \frac{1}{2}\mathbb{E}(|X_1 - X_2|) - \frac{1}{2}\mathbb{E}(|Y_1 - Y_2|) = \int_{-\infty}^{\infty} (F(x) - G(x))^2 \, dx \tag{4.1}$$

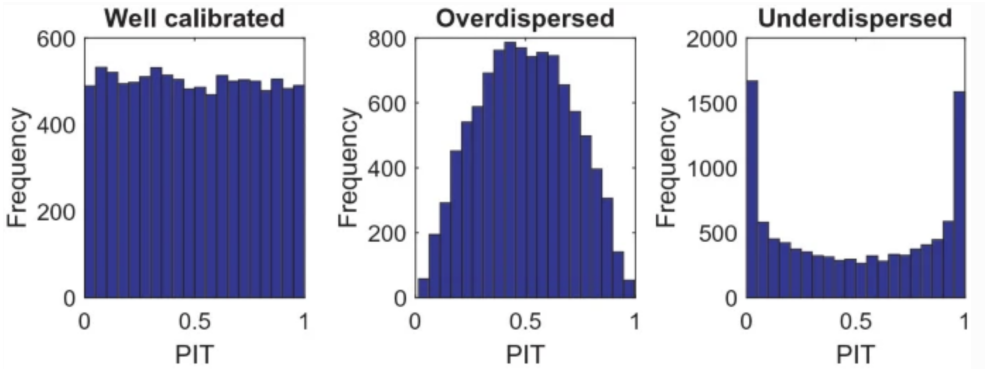


Figure 4.3: PIT types [32]

Notice that, in our case 4.9, the distribution G of Y_1 and Y_2 is degenerate, with all probability mass on a single point. It follows that, the third addend in the summation is zero. That is because the fact of Y_1 and Y_2 both following distribution G implies that $\mathbb{E}(|Y_1 - Y_2|)$ corresponds to the difference of two equal constant numbers.
Additionally, since Y_1 is just a constant, we have $Y_1 = L$.
Putting everything together we have obtained an alternative way of computing the CRPS score.

$$\int_{-\infty}^{\infty} \left(\hat{F}(x) - \mathbb{1}(x - L)\right)^2 dx = \mathbb{E}(|X_1 - L|) - \frac{1}{2}\mathbb{E}(|X_1 - X_2|) \tag{4.2}$$

4.10 PIT

The probability integral transform is a method to assess visually the quality of probabilistic forecasts. PIT is obtained by applying a cdf F to your data; if applying such cdf to the data results in a uniform distributed PIT then F is a valid prediction. If not, F is not the suited cdf for the considered data. Figure 4.3 provides an example, applying the true cdf results in a well calibrated PIT (left). Alternatively, applying a bad cdf results in either a overdispersed (middle) or underdispersed (right) PIT.

Chapter 5

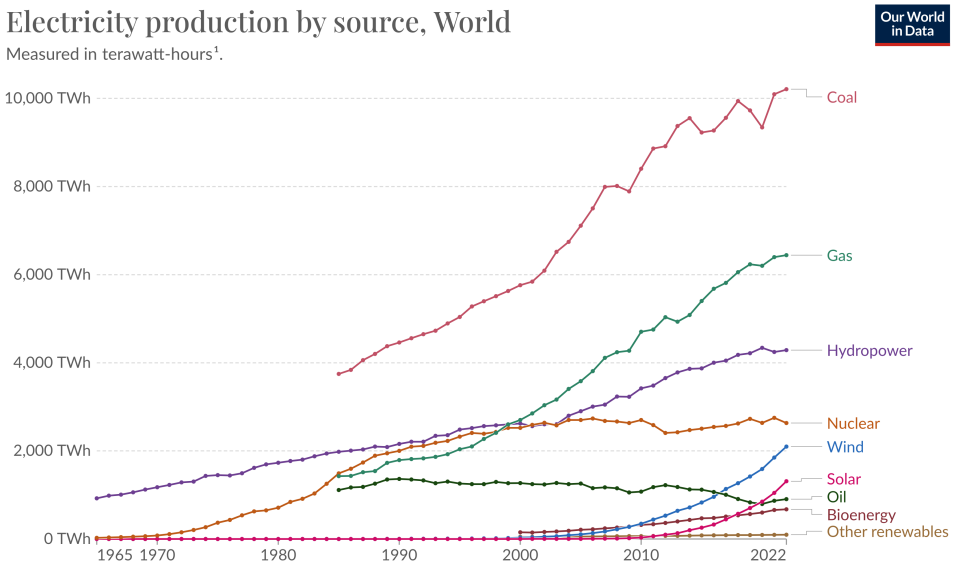
The Energy Market

Chapter explaining the energy market Chapter 9 of https://pubs.naruc.org/pub.cfm?id=536E10A7-2354-D714-5191-A8AAFE45D626

- what are smart grids?

- introduction of smart grids

- renewable integration requirements



Data source: Ember - Yearly Electricity Data (2023); Ember - European Electricity Review (2022); Energy Institute - Statistical Review of World Energy (2023)
Note: Other renewables include waste, geothermal and wave and tidal energy.
OurWorldInData.org/energy | CC BY

1. Watt-hour: A watt-hour is the energy delivered by one watt of power for one hour. Since one watt is equivalent to one Joule per second, a watt-hour is equivalent to 3600 Joules of energy. Metric prefixes are used for multiples of the unit, usually: - kilowatt-hours (kWh), or a thousand watt-hours. - Megawatt-hours (MWh), or a million watt-hours. - Gigawatt-hours (GWh), or a billion watt-hours. - Terawatt-hours (TWh), or a trillion watt-hours.

- How auctions work
- Difference intraday dayhead all other stuff
- EPEX Nordpool
- Prices can be negative

Chapter 6

Point forecasting

This chapter covers the theory of the most widely used method for point forecasting in the EF literature. Besides discussing the theory underlying these models, this and the following chapter include also a couple of worked examples in order to get acquainted with the practical applications of models.

6.1 Exponential smoothing

6.2 Multiple linear regression

6.3 Autoregressive models

explain their theory and how the procedure how they are used IMPORTANT: load series is not a stationary series so before applying AR we have to perform stationary tests or differencing steps

6.3.1 ARIMA

6.3.2 ARIMAX

6.3.3 SARIMA

6.3.4 SARIMAX

6.4 Generalized additive model

6.5 K-nearest neighbors

6.6 Support vector regression

Developed at the AT&T Bell Laboratories by Vapnik et al. [18], [83], support vector machines SVMs are one of the most popular techniques within the field of statistical learning.
The goal of support vector regression is finding a function f(x) with at most ε deviation from the actual observed data $y_i \ \forall i$ and as flat as possible. Put differently, we would like a model to keep error less than the ε threshold, In standard SVR we have

$$f(x) = \langle w, x \rangle + b \text{ with } w \in X, b \in R \tag{6.1}$$

Where X denotes the space of the input patters x_i. We can translate the flatness requirement into minimising the squared norm of w. Doing so we can formulate our problem as a convex optimisation problem.

$$\begin{aligned} \min \quad & \frac{1}{2}\|w\|^2 \\ s.t. \quad & y_i - \langle w, x_i \rangle - b \leq \varepsilon \\ & \langle w, x_i \rangle + b - y_i \leq \varepsilon \end{aligned} \tag{6.2}$$

Next, we need to introduce the slack variables ξ and ξ^*, in order to handle the above formulate optimisation problem. We obtain the following formulation

$$\begin{aligned} \min \quad & \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{l}(\xi_i + \xi_i^*) \\ s.t. \quad & y_i - \langle w, x_i \rangle - b \leq \varepsilon + \xi \\ & \langle w, x_i \rangle + b - y_i \leq \varepsilon + \xi^* \\ & \xi_i \geq 0 \\ & \xi_i^* \geq 0 \end{aligned} \tag{6.3}$$

The C constant trades off between ε deviation tolerance and flatness of the function f. We seek to minimise the epsilon insensitive loss function, defined

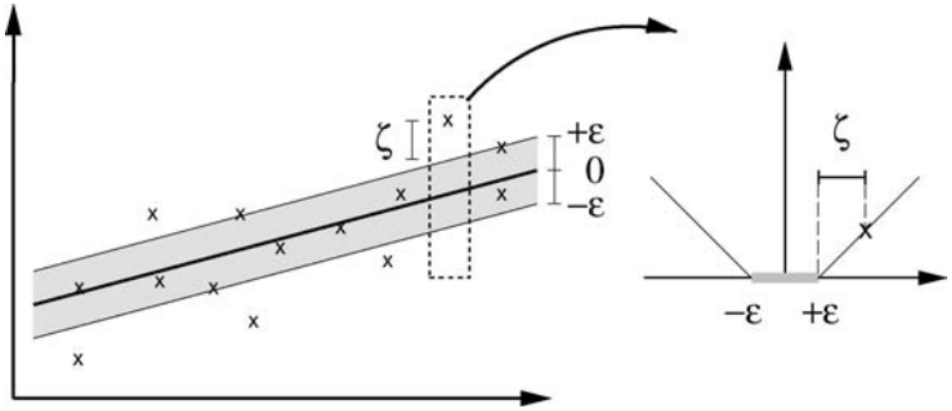


Figure 6.1: Support vector regression,[74]

as follows

$$\|\xi\|_\varepsilon := \begin{cases} 0 & \text{if } \|\xi\| \leq \varepsilon \\ \|\xi\| - \varepsilon & \text{if } \|\xi\| \leq \varepsilon \end{cases} \tag{6.4}$$

The model is depicted in figure 6.1. The gry band is called the epsilon insensitive tube, only the points outside it are accounted by the loss function. Smola et al. [75] point out that considering the dual formulation makes our optimisation problem easier to solve. Doing so we have

$$\begin{aligned} \max \quad & -\frac{1}{2}\sum_{i,j=1}^{l}(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\langle x_i, x_j\rangle + \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)(y_i - \varepsilon) \\ s.t. \quad & \sum_i = 1^l(\alpha_i - \alpha_i^*) = 0 \\ & \alpha_i, \alpha_i^* \in [0, C] \end{aligned} \tag{6.5}$$

Rearranging the gradient of the lagrangian with respect to w, we obtain the so called support vector expansion.

$$w = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)x_i \tag{6.6}$$

That means that w can be completely described as a linear combination of the training features x_i. Notice, the complexity of the function representation is independent of the feature space dimensionaly but depends only on the number of support vectors; that is those point i for which $(\alpha_i - \alpha_i^*) \neq 0$ Notice that, we do not needd to compute w explicitly in order to evaluate f(x). Furthermore, equation 6.6 implies

$$f(x) = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)\langle x_i, x\rangle + b \tag{6.7}$$

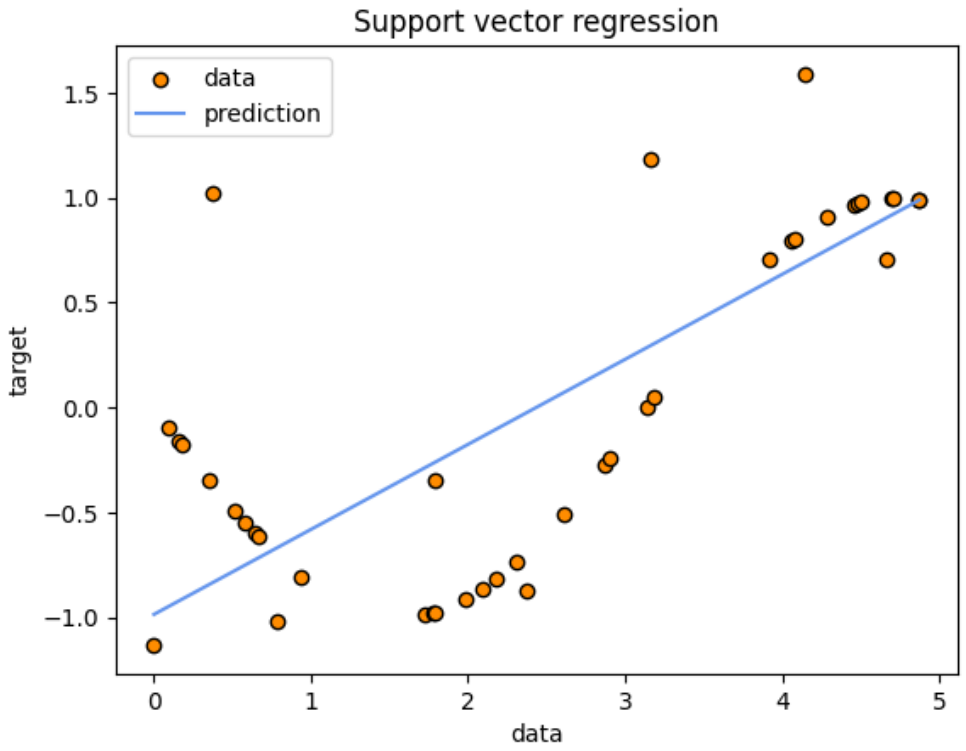


Figure 6.2: support vector regression

Employ the Karush-Kuhn-Tucker conditions, b can be retrieved easily. Particularly, use the condition that the product between the constraints and the dual variable has to vanish. These implies that the lagrange multipliers α_i, α_i^* may be nonzero only for the samples inside the epsilon insensitive tube. Consequently for any of these data points, the equality $b = y_i - \langle w, x_i - \varepsilon \rangle$ holds. To get an idea, see figure 6.2 for a how support vector regression handles a sinusoidal function with noise.

6.7 Artificial neural networks

6.7.1 DNN

6.7.2 LSTM

6.7.3 DeepAr

6.7.4 AR Net

6.8 Kernel methods

6.8.1 Kernel regression

6.8.2 Kernel support vector regression

Support vector regression can be kernelized by swapping the R2 euclidean dot product of data x with the dot product in the higher feature space F. Doing so, the optimisation problem can be restated as

$$\begin{aligned} \max \quad & -\frac{1}{2}\sum_{i,j=1}^{l}(\alpha_i - \alpha_i^*)(\alpha_i - \alpha_i^*)k(x_i, x_j) + \sum_{i=1}^{l}(y_i - \varepsilon)(\alpha_i - \alpha_i^*) \\ s.t. \quad & \sum_{i=1}^{l}(\alpha_i - \alpha_i^*) = 0 \\ & \alpha_i, \alpha_i^* \in [0, C] \end{aligned} \tag{6.8}$$

Our regressor f is then given by

$$\sum_{i=1}^{l}(\alpha_i - \alpha_i^*)k(x_i, x) + b \tag{6.9}$$

Notice, in this setting w is no longer given explicitly and we seek for the flattest function in the feature space not the input space. See figure 6.3 and figure 6.4 for two examples. In the former we have used a polynomial kernel while in the latter the standard radial basis function kernel.

Comparing theese pictures with figure 6.2, it can be concluded that introducing kernels allows support vector regression to handle non linearities in the data.

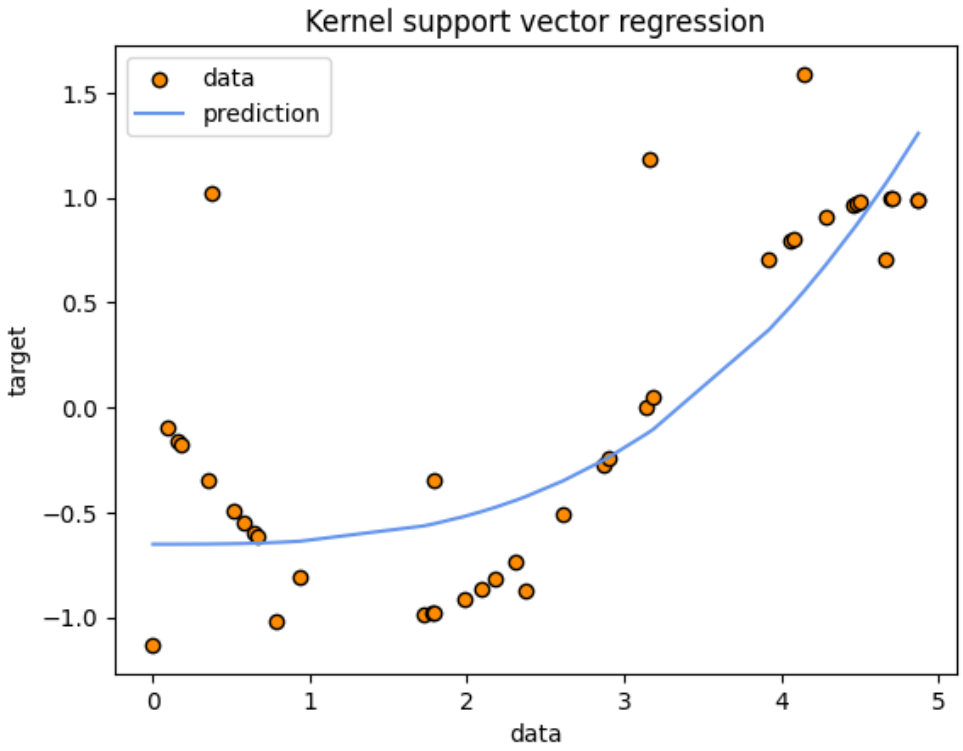


Figure 6.3: polynomial support vector regression

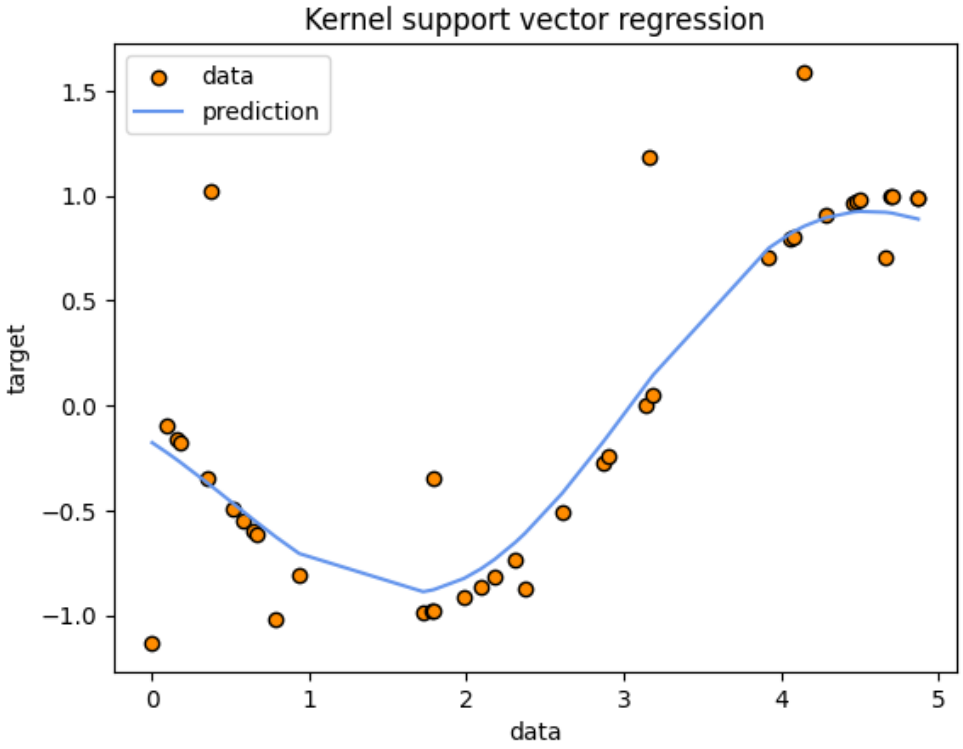


Figure 6.4: rbf support vector regression

Chapter 7

Probabilistic forecasting

When it comes to probabilistic forecasting, there are a couple of standard practical approaches; conceptually they can be grouped into two main categories. The former class of approaches tries modelling the distribution of the observed data directly. The latter family of approaches constructs first a point forecast and then learns the distribution of the model's errors.

7.1 Quantile regression

Quantile regression can be interpreted as an extension of standard regression. In this setting, you basically slice the dependent variables into quantiles and then fit a regression for each quantile. With standard regression, we build a model for the conditional mean, conversely, with quantile regression we model the conditional quantile function for any desired quantile. Therefore, with quantile regression we are able to study the impact of covariates on quantiles directly.

Definition 7.1 *For any real valued random variable Y, we define its associated quantile function.*

$$Q(q) = \inf\{y : F(y) \geq q\} \tag{7.1}$$

Alternatively, in order to ease the posing of the quantile regression problem, we can formulate quantiles as the solutions to simple optimization problems. For any $0 < q < 1$ consider the pinball loss function from section 4.7, $\rho_q(u) = u(q - \mathbb{1}_{\{u<0\}})$. Such loss is minimized by the quantile $Q(q)$. Thus,we can estimate quantiles by minimizing the expectation of $\rho_q(Y - g(x, \beta))$ with respect to the parameter β.
Note, that in the special case $q = \frac{1}{2}$, quantile regression corresponds exactly to standard regression with an absolute value loss function.
It follows that the conditional linear quantile function $Q_Y(q|X = x) = x_i\beta(q)$,

can be estimated by solving

$$\hat{\beta}(q) = \arg\min_{\beta} \sum \rho_q(y_i - x\beta) \tag{7.2}$$

Notice that, this cost function is not differentiable, therefore there is no analytical solution to the quantile regression problem. Nevertheless, we can easily solve it by employing linear programming and convex optimisation [12].
Furthermore, we can extend this framework to non linear quantile regression by choosing a non linear model in place of $x\beta$ in the above equation 7.2.

7.2 Quantile forest

Meinshausen [58] extends the idea of random forest [13] generalising it, the result is the quantile forest algorithm. Quantile forest allows us to estimate conditional quantiles in a non parametric fashion.
In order to understand this algorithm, it is first necessary to first cover the theory of decision trees and random forests.

7.2.1 Decision trees

Decision trees methods partition recursively the feature space in a set of binary rectangles and then fit a simple model in each of those partitions (the most straightforward is fitting just a constant). To get started, we first split the space into two disjoint regions, then we model the response variable by the mean of the observed predicted variables with associated features falling in that specific region. Our goal is selecting the best features and best split point such that to achieve the best generalizing fit. For an example/visualisation consider the pictures 7.1 and 7.2 taken from [33], where the decision tree algorithm is visualised for a regression problem with two independent variables X_2 and X_1.

Suppose to partition the feature space into M regions $R_1, \ldots, R_M$, then the model reads as follows.

$$f(x) = \sum_{m=1}^{M} c_m \mathbb{I}_{\{x \in R_m\}} \tag{7.3}$$

It follows that the function minimising the sum of squares is the one with $\hat{c}_m = mean(y_i | x_i \in R_m)$. Finding the best split in terms of minimum sum of squares is computationally infeasible in practice. Therefore we approximate a solution by approaching the problem in a greedy fashion. Let j denote the splitting variable and s be the the split point we define the two half planes

$$R_1(j,s) = \{X | X_j \leq s\} \quad R_2(j,s) = \{X | X_j \, s\} \tag{7.4}$$

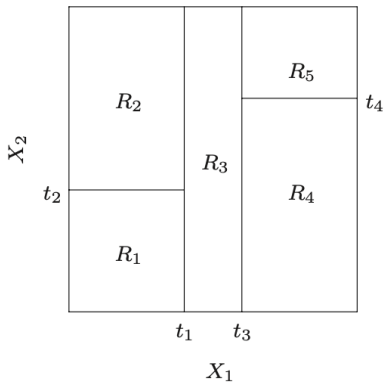


Figure 7.1: two-dimensional feature space partitioned by recursive binary splitting

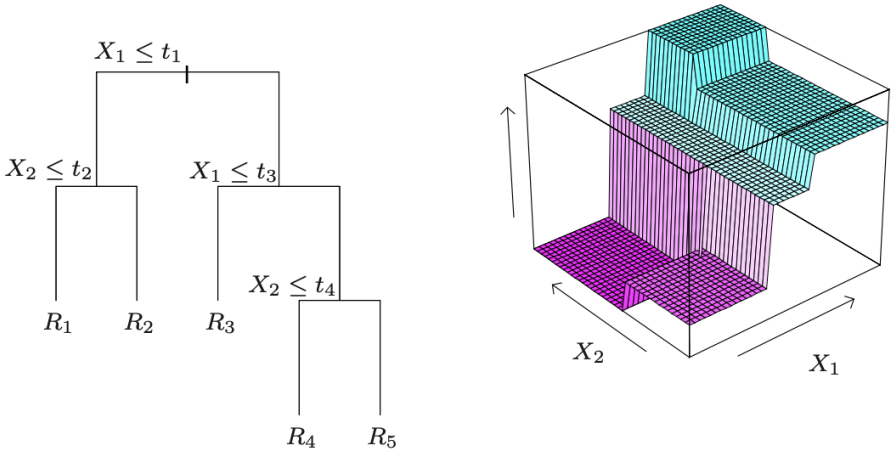


Figure 7.2: partition tree and regression model

Then we search for the s and j that solve

$$\min_{j,s} \left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2 \right] \tag{7.5}$$

The inner problem is easy, as already pointed out we will have

$$\hat{c}_1 = mean(y_i | x_i \in R_1) \quad \hat{c}_2 = mean(y_i | x_i \in R_2) \tag{7.6}$$

For the outer problem, we scan through all the (j,s) tuples and pick the best pair. Next, one or both of these regions from the previous step are split into two more regions; we recurse this process until some stopping condition is triggered (max number of branches, max deth of tree, threshold on the MSE,

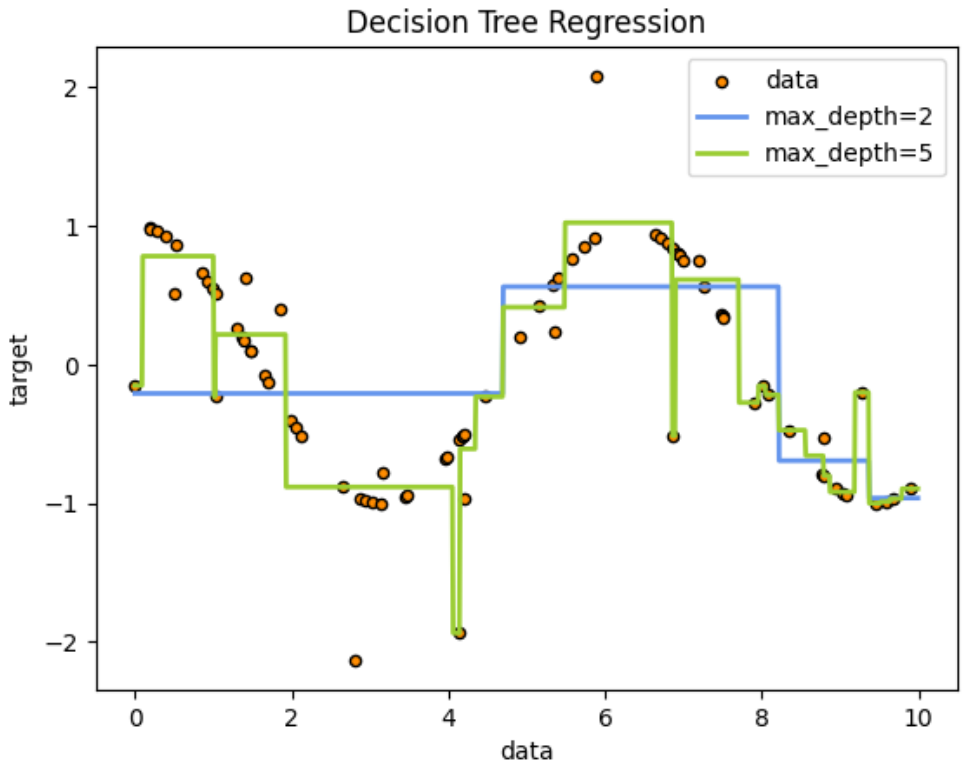


Figure 7.3: decision tree regression

minimum number of observation in each leaf node). Notice, this being a greedy algorithm implies that our final solution is guaranteed to be just a local optimum not a global one. Even though their simplicity, these models have proved themselves to be really powerful. See figure 7.3 for a example where decision tree with different hyperparameters are fitted to a sine wave plus noise. The most popular among these model is the CART [14] tree, its name comes from the fact that it can handle both classification and regression problems.

7.2.2 Bootstrap

The idea behind boostrapping is to randomly sample from the training set with replacement B times and then fitting B models to each of the ”artificial” datasets. Boostrapping can serve different tasks; we can use it to assess the accuracy of a parameter estimate or of a prediction but also to improve their estimates.

7.2.3 Bagging

Bagging stands for boostrap aggregation. The bagging estimate is dafined by $\mathbb{E}_P[\hat{f}^*]$ where P is the empirical distribution putting equal probability on each data point of the training set. Basically, for each bootstrap fitted model $\hat{f}^{*b}(x)$, we compute the bagging estimate by

$$\hat{f}_{bag}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}^{*b}(x) \tag{7.7}$$

Bagging is particularly useful in reducing the variance of decision trees, resulting in an improved prediction(tradeoff bias variance). Note, this improvement comes from the fact that averaging reduces variance and leaves biases unchanged.

7.2.4 Random forest

Decision trees are characterised by high variance and low bias, thus, they can benefit extremely from bagging. Furthermore, every decision tree generated through bagging will be identically distributed (i.d.), thus the expectation of an average of B trees is probabilistically equivalent to the expectation of any such trees. As a consequence, the bias will stay fixed since the bias of the bagged estimator is the same as that of each individual tree.
Consider positively correlated i.d. random variables, then the variance of their average is

$$\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2 \tag{7.8}$$

The second term disappears as B increases, while the first term depends heavily on the correlation between bagged trees. Random forest consists in is reducing the correlation between the trees by randomly selecting m of the p features as candidates for splitting; m tipically takes a value in the order of $\sqrt{p}$ or even 1 with default value $m = \lfloor \frac{p}{3} \rfloor$, while a good minimum node size is around five.
Letting $T(x;\Theta_b)$ be the bth bagged tree where Θ_b denotes the randomness characterizing its splits, cutpoints and terminal node values, we have that the random forest regressor is given by

$$\hat{f}_{rf}^{B} = \frac{1}{B}\sum_{b=1}^{B}T(x;\Theta_b) \tag{7.9}$$

For a simple visualisation compare figure 7.4 with 7.3

7.2.5 Quantile forest

The key observation here is noting that random forests approximates the conditional mean $\mathbb{E}(Y|X=x)$ by a weighted average over the observed Y.

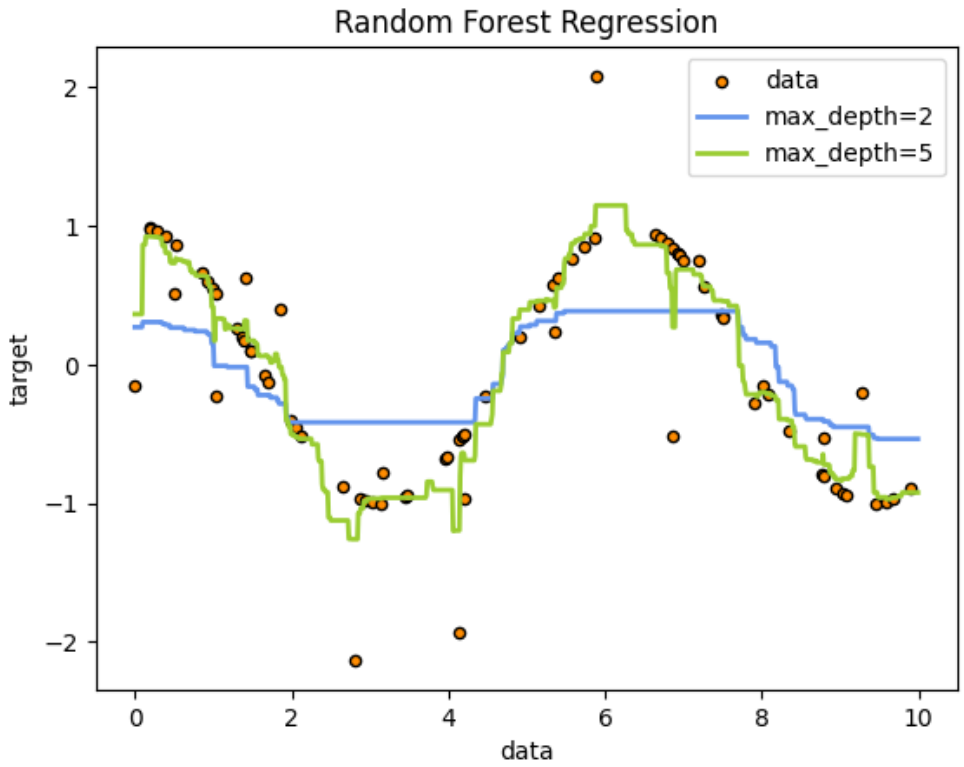


Figure 7.4: random forest regression

Hence, we can extend this idea to the full conditional distribution by

$$F(y|X=x) = P(Y \leq y|X=x) = \mathbb{E}(\mathbb{I}_{\{Y\leq y\}}|X=x) \tag{7.10}$$

All we have to do is approximating $\mathbb{E}(\mathbb{I}_{\{Y\leq y\}}|X=x)$ by a weighted mean over the random variable $\mathbb{I}_{\{Y\leq y\}}$

$$\hat{F}(y|X=x) = \sum_{i=1}^{n} \omega_i(x)\mathbb{I}_{\{Y_i\leq y\}} \tag{7.11}$$

By swapping $F(y|X=x)$ with $\hat{F}(y|X=x)$ in the defintion of conditional quantiles we obtain their respective random forest estimator

$$\hat{Q}_q = \inf\{y : \hat{F}(y|X=x) \geq q\} \tag{7.12}$$

7.3 Quantile gradient boosting machine

7.3.1 Boosting

With boosting we fit an additive expansion of elementary basis functions; with M basis functions we have

$$f(x) = \sum_{m=1}^{M} \beta_m b(x; \gamma_m) \tag{7.13}$$

where $b(x; \gamma)$ are the basis functions while β_m are the coefficients of the expansion. Boosted models are fitted by minimizing a loss function over the training data

$$\min_{\beta_m, \gamma_m} \sum_{i=1}^{N} L\left(y_i, \sum_{m=1}^{M} \beta_m b(x_i; \gamma_m)\right) \tag{7.14}$$

However, such problem is highly intensive in terms of computation. Therefore, what is done in the literature is approximating its solution by iteratively adding new basis function to the current expansion. That is, we construct f_m by solving for the optimal basis function and coefficients to add to f_{m-1}. Considering the square loss, we would have

$$L(y_i, f_{m-1}(x_i) + \beta_m b(x_i; \gamma)) = (e_{im} - \beta_m b(x_i; \gamma))^2 \tag{7.15}$$

7.3.2 Boosted trees

We combine several trees obtaining the boosted tree model

$$f_M(x) = \sum_{m=1}^{M} T(x; \Theta_m) \tag{7.16}$$

Thus, at each step of the iterative optimisation procedure, we have to solve

$$\hat{\Theta}_m = \arg\min_{\Theta_m} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + T(x_i; \Theta_m)) \tag{7.17}$$

Remember, Θ_m referes to the parameters of the mth tree, $\Theta_m = \{R_{jm}, \gamma_{jm}\}_1^{J_m}$

7.3.3 Gradient boosting

In order to robustly solve 7.17, gradient boosting considers the following problem

$$\tilde{\Theta}_m = \arg\min_{\Theta} \sum_{i=1}^{N} (-g_{im} - T(x_i; \Theta))^2 \tag{7.18}$$

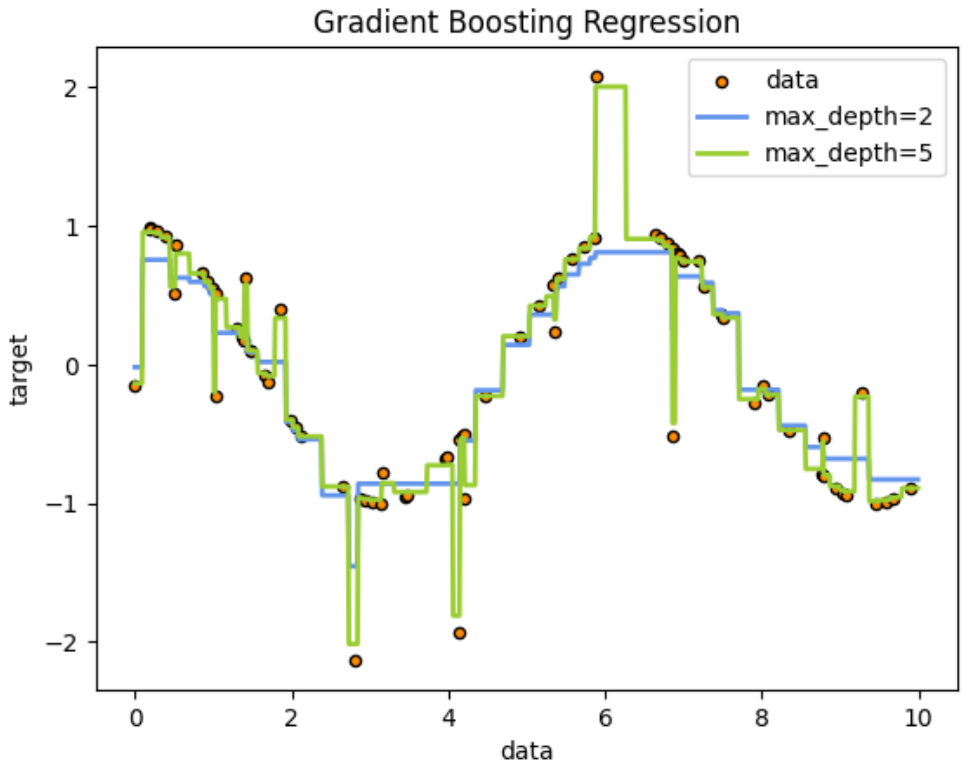


Figure 7.5: gradient boosting regression

where g_{im} is the gradient of $L(f) = \sum_{i=1}^{N} L(y_i, f(x_i))$ evaluated at f_{m-1}. Put simply, we are fitting the m-th tree to the negative of the gradient values of f through least squares. In order to solve our quantile regression tasks through gradient boosting, all we need to do is specifying the pinball loss as our criterion to guide the minimisation algorithm. See figure 7.5 for a visualisation

7.4 Kernel methods

7.4.1 Kernel quantile regression

The idea of quantile regression has been extended to kernel methods by Takeuchi et al. [77]. There, they minimize a risk plus regularizer defined as follows.

$$R[f] := \frac{1}{m} \sum_{i=1}^{m} \rho_q(y_i - f(x_i)) + \frac{\lambda}{2} \|g\|_{\mathcal{H}}^2 \tag{7.19}$$

where $f = g + b$, $g \in \mathcal{H}$ and $b \in R$. Using the link between RKHS and feature spaces, we can rewrite $f(x) = \langle w, \varphi(x) \rangle + b$. Moreover, note that

the RKHS norm is defined as follows $\|f\|_{\mathcal{H}} = \inf\{\|w\|_F : w \in F, f(x) = \langle w, \varphi(x)\rangle_F, \forall x \in X\}$, where F is the feature space. Doing so we obtain a minimization problem equivalent to minimizing equation 7.19.

$$\min_{w,b} \quad C\sum_{i=1}^{m} q(y_i - \langle w, \varphi(x)\rangle - b) + (1-q)(-y_i + \langle w, \varphi(x)\rangle + b) + \frac{1}{2}\|w\|^2 \tag{7.20}$$

Note the division by λ so that $C = \frac{1}{\lambda m}$.
We can next rephrase the optimisation in 7.20 by introducing the slack variables ξ_i and ξ_i^*.

$$\begin{aligned} \min_{w,b,\xi_i,\xi_i^*} \quad & C\sum_{i=1}^{m} q\xi_i + (1-q)\xi_i^* + \frac{1}{2}\|w\|^2 \\ \text{s.t.} \quad & y_i - \langle w, \varphi(x)\rangle - b \leq \xi_i \\ & -y_i + \langle w, \varphi(x)\rangle + b \leq \xi_i^* \\ & \xi_i \geq 0 \\ & \xi_i^* \geq 0 \end{aligned} \tag{7.21}$$

In order to make it more compact, we rewrite equation 7.21 in matrix notation.

$$\begin{aligned} \min_{w,b\xi,\xi^*} \quad & Cq\xi^\intercal \mathbb{1} + Cq(\xi^*)^\intercal \mathbb{1} + \frac{1}{2}w^\intercal w \\ \text{s.t.} \quad & y - \Phi^\intercal w - b \preceq \xi \\ & -y + \Phi^\intercal w + b \preceq \xi^* \\ & \xi \succeq 0 \\ & \xi^* \succeq 0 \end{aligned} \tag{7.22}$$

Consider now, the lagrangian L associated to 7.22

$$\begin{aligned} L(w,b,\xi,\xi^*) =& Cq\xi^\intercal \mathbb{1} + Cq(\xi^*)^\intercal \mathbb{1} + \frac{1}{2}w^\intercal w - \alpha^\intercal(\xi - y + \Phi^\intercal w + b) - (\alpha^*)^\intercal(\xi^* + y - \Phi^\intercal w - b) \\ & - \nu^\intercal \xi - (\nu^*)^\intercal \xi^* \end{aligned} \tag{7.23}$$

The next step is deriving its dual formulation, since it is easier and more efficient to solve. This because the dual problem has the useful property of being always convex.

Definition 7.2 *The dual function associated to the lagrangian $L(x,\lambda)$ is given by $g(v) = \inf_x L(x,\lambda)$*

where λ is called the lagrange multiplier of the optimization problem. Such dual formulation has an useful property, that is

$$g(\lambda) \leq p^* \tag{7.24}$$

where p^* is the optimal value of your optimization problem. Consider a simple lagrangian $L(x, \lambda) = f(x) + \sum \lambda_i r_i(x) + \sum v_i h_i(x)$, where $r_i(x)$ are inequality constraints while $h_i(x)$ are equality constraints of the problem. Then it can be noted that, the lower bound on p^* is non trivial only when the lagrange multiplier $\lambda \succeq 0$. Therefore, the idea is that by maximizing the dual function subject to the contraint $\lambda \succeq 0$, we can obtain an approximate or perfect solution to the primal problem.
To explain why we may or not be able to attain the best solution to the primal problem by maximizing its dual, we have to introduce the concept of duality. We use d^* to denote the optimal value of the lagrange dual problem; we can think of it as the best lower bound on p^*.
The inequality 7.24 is called weak duality. The difference $p^* - d^*$ is said the optimal duality gap; it is the gap between the optimal value of the primal problem and the best lower bound on it that can be obtained from the Lagrange dual function. Moreover, note that the optimal duality gap is always nonnegative.
We say that strong duality holds, when the optimal duality gap is zero; in other words, the lagrange dual bound is tight.
Constraint qualifications are condtions under which strong duality holds; one of the most popular is Slater's condition.

$$\begin{aligned} \exists x \in \text{relint } D \text{ s.t. } r_i(x) < 0, \quad i = 1, \dots, m \\ h_i(x) = 0 \end{aligned} \tag{7.25}$$

Where relint D is the relative interior of $D := \cap_{i=0}^{m} \text{dom}(r_i)$
Slater's theorem naturally follows.

Theorem 7.3 *If Slater's condtion holds and the problem is convex then strong duality holds.*

We can now check that our optimization problem posseses strong duality by checking Slater's condition.
In our case we don't have any equality constraint, so we do not have to worry about the $h_i(x) = 0$ term in 7.25. All we have to check is the convexity of our problem and that there exist a x such that $r_i(x) < 0$. For convexity, a sufficient condition is the positive definiteness of Q in the quadratic programming problem

$$\begin{aligned} \min \quad & x^\intercal Q x + c^\intercal x \\ s.t \quad & Ax \preceq b \end{aligned} \tag{7.26}$$

In our case, equation 7.23, we have $w^\intercal w$, thus Q is just the identity matrix which satisfies the positive definiteness requirement. Therefore, our problem is convex. Next we check that Slater's condition holds. Considering first the two non negative constraints on ξ and ξ^*, we conclude that ξ and ξ^* have to be greater or equal to zero for the existence of an x satisfying Slater's

condition. Thus, let us suppose that $0 \leq \xi \leq \alpha$ and $0 \leq \xi^* \leq \alpha$.
Next, let us consider the other two inequalities and make the following ansatz.

$$\begin{aligned} w =& \Phi^\intercal (\Phi\Phi^\intercal)^{-1} y \\ b <& \alpha \end{aligned} \tag{7.27}$$

We then have

$$\begin{aligned} -\xi + y - \Phi\Phi^\intercal(\Phi\Phi^\intercal)^{-1} y - b <& 0 \\ -\xi^* - y + \Phi\Phi^\intercal(\Phi\Phi^\intercal)^{-1} y + b <& 0 \end{aligned} \tag{7.28}$$

Hence, we conclude that our problem satisfies Slater's condition. Therefore the solution of the dual and primal problem are equivalent.
We end this section with the derivation of the dual problem; that is the convex problem, we will solve in order to get the quantiles prdeiction of our quantile kernel algorithm.
First, derive the dual function of 7.23.

$$\begin{aligned} g(\alpha, \alpha^*, \nu, \nu^*) &= \inf_x L(x, \lambda) \\ &= \inf_{\xi, \xi^*, w, b} L(w, b, \xi, \xi^*) \end{aligned} \tag{7.29}$$

Setting its derivates to zero

$$\begin{cases} \frac{\partial L}{\partial w} = 0 \implies w = \Phi^\intercal(\alpha - \alpha^*) \\ \frac{\partial L}{\partial b} = 0 \implies (\alpha - \alpha^*)^\intercal \mathbb{1} = 0 \\ \frac{\partial L}{\partial \xi} = 0 \implies Cq\mathbb{1} - \alpha - \nu = 0 \\ \frac{\partial L}{\partial \xi^*} = 0 \implies C(1-q)\mathbb{1} - \alpha^* - \nu^* = 0 \end{cases} \tag{7.30}$$

As pointed out previously, the lower bound resulting from the dual formulation is non trivial only when the lagrange multipliers are $\succeq 0$. Looking at the last two equations of the system 7.30, this implies the following two constraints $\alpha \in [0, Cq\mathbb{1}]$ and $\alpha^* \in [0, C(1-q)\mathbb{1}]$.
Substitute the conditions for an optimum into 7.23, we obtain the dual formulation.

$$\begin{aligned} g(\alpha, \alpha^*) =& \xi^\intercal(Cq\mathbb{1} - \alpha - \nu) + (\xi^*)^\intercal(C(1-q)\mathbb{1} - \alpha^* - \nu^*) - (\alpha - \alpha^*)^\intercal \Phi\Phi^\intercal(\alpha - \alpha^*) \\ &+ (\alpha - \alpha^*)^\intercal y - (\alpha - \alpha^*)^\intercal b + \frac{1}{2}(\alpha - \alpha^*)^\intercal \Phi\Phi^\intercal(\alpha - \alpha^*) \end{aligned}$$

$$\begin{aligned} g(\alpha, \alpha^*) =& 0 + 0 - \frac{1}{2}(\alpha - \alpha^*)^\intercal \Phi\Phi^\intercal(\alpha - \alpha^*) + (\alpha - \alpha^*)^\intercal y - 0 \\ g(\alpha, \alpha^*) =& -\frac{1}{2}(\alpha - \alpha^*)^\intercal \Phi\Phi^\intercal(\alpha - \alpha^*) + (\alpha - \alpha^*)^\intercal y \end{aligned} \tag{7.31}$$

Defining $\mathrm{a} = (\alpha - \alpha^*)$ and letting K the kernel matrix, we have that the dual optimisation problem reads as follows

$$\begin{aligned} \max_{\mathrm{a}} \quad & -\frac{1}{2}\mathrm{a}^\intercal K \mathrm{a} + \mathrm{a}^\intercal y \\ \text{s.t.} \quad & C(q-1)\mathbb{1} \preceq \mathrm{a} \preceq Cq\mathbb{1} \\ & \mathrm{a}^\intercal \mathbb{1} = 1 \end{aligned} \tag{7.32}$$

Switching sign, we rephrase it as a minimisation problem, which is the common practice in convex optimisation.

$$\begin{aligned} \min_{\mathrm{a}} \quad & +\frac{1}{2}\mathrm{a}^\intercal K \mathrm{a} - \mathrm{a}^\intercal y \\ \text{s.t.} \quad & C(q-1)\mathbb{1} \preceq \mathrm{a} \preceq Cq\mathbb{1} \\ & \mathrm{a}^\intercal \mathbb{1} = 1 \end{aligned} \tag{7.33}$$

The kernel quantile regression estimator is then given by

$$f(x) = \sum_i \mathrm{a}_i k(x_i, x) + b \tag{7.34}$$

Since our optimisation problem possesses strong duality and it is differentiable in both the objective and the constraint, we have that it must satisfy the Karush Kuhn Tucker conditions, see section 5.5.3 [12]. Thanks to the KKT conditions on the primal optimisation problem we have that $f(x_i) = y_i$ for $\mathrm{a}_i \notin \{C(q-1), Cq\}$. To see this, we have to consider the KKT conditions.

$$\begin{aligned} \lambda^* r_i(x^*) &= 0, \quad i = 1, \dots, m \\ \nabla L(x^*) &= 0 \end{aligned} \tag{7.35}$$

In our setting we have

$$\begin{aligned} \alpha_i(\xi_i - y_i + r_i) &= 0 \\ \alpha_i^*(\xi_i^* + y_i - r_i) &= 0 \\ \nu_i \xi_i &= 0 \\ \nu_i^* \xi_i^* &= 0 \\ \nabla L &= 0 \end{aligned} \tag{7.36}$$

Using the gradient of the lagrangian of equation 7.30 we end up with

$$\begin{aligned} \alpha_i(\xi_i - y_i + r_i) &= 0 \\ \alpha_i^*(\xi_i^* + y_i - r_i) &= 0 \\ (Cq - \alpha_i)\xi_i &= 0 \\ (C(1-q) - \alpha_i)\xi_i^* &= 0 \end{aligned} \tag{7.37}$$

Now, let us break into cases

$$\begin{cases} \alpha_i = Cq,\ \alpha_i^* = 0 & \implies \alpha_i - \alpha_i^* = Cq, \xi_i \leq 0, \xi^* = 0 \implies \xi_i - y_i + f_i = 0 \\ \alpha_i = 0,\ \alpha_i^* = C(1-q) & \implies \alpha_i - \alpha_i^* = C(q-1), \xi_i = 0, \xi^* \leq 0 \implies \xi_i^* + y_i - f_i = 0 \\ 0 \leq \alpha_i \leq Cq,\ 0 \leq \alpha_i^* \leq C(1-q) & \implies \xi_i = 0, \xi_i^* = 0 \implies -y_i + f_i = 0,\ y_i - f_i = 0 \end{cases} \tag{7.38}$$

Therefore in order to retrieve b we simply have to choose an index i such that $a_i \notin \{C(q-1), Cq\}$ and let

$$b = y_i - \sum_i a_i k(x_i, x) \tag{7.39}$$

7.4.2 Weather quantiles

In order to get acquainted with the inner workings of the presented methods, this section covers an application explaining practical details and comparing results.
The dataset used is the Melbourne daily maximum temperatures [46]. It contains the daily maximum temperatures in Melbourne, Australia, from 1981-1990, excluding leap days, see figure 7.6. Due to the bimodality of the data, such dataset is commonly used to give a difficult quantile regression problem [45], thus why we chose it. The observed bimodality is that a hot day is likely to be followed by either an equally hot day or one much cooler. Hereafter, the results of the four presented methods on the Melbourne dataset are reported, see figure 7.7 for a visualisation. Hyperparameter tuning have been optimised through cross validation, see A.2.

Table 7.1: Pinball loss Melbourne data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
Pinball loss	11.278895	10.317612	10.340842	10.031708

As already pointed out, the quantile regression with q=0.5 corresponds to the standard regression problem, hence we can compare the proposed methods also in terms of the mean absolute error. From these tables, we can see that kernel quantile regression outperformed the simple quantile regressor as well as the more complex models like quantile forest and gradient boosting quantile regression for the Melbourne temperatures dataset. Not only kernel quantile regression was the best in terms of total pinball loss but also the best in terms of each quantile pinball loss and mean absolute error. Comparison has been carried out on further datasets, yielding similar conclusion as the one of above, to know more see A.3.

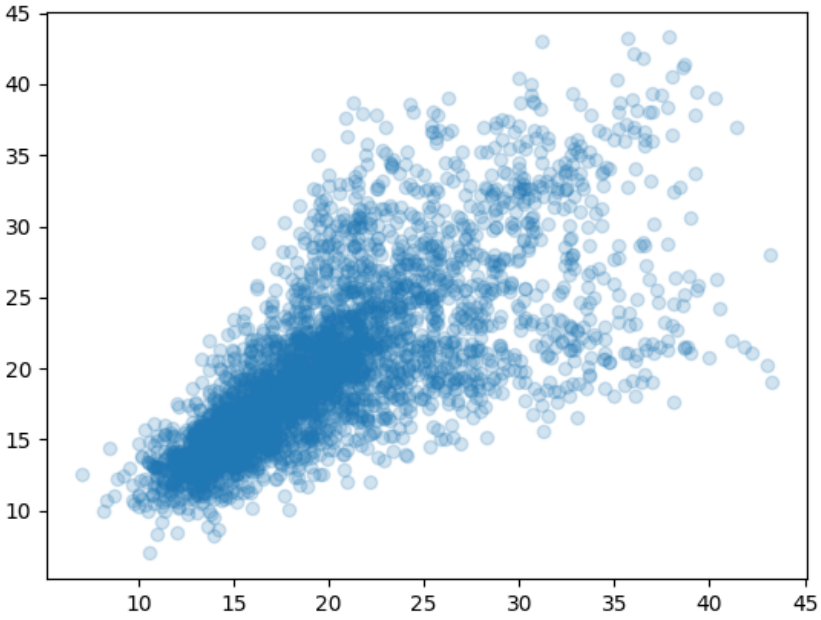


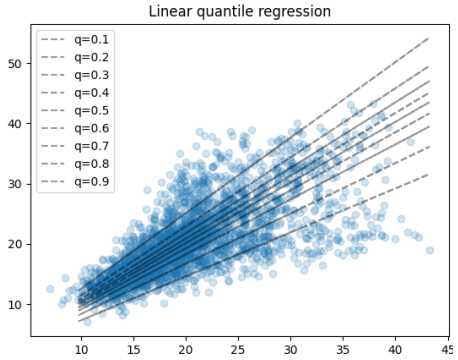
Figure 7.6: Melbourne temperatures dataset

Table 7.2: Pinball loss quantile-wise Melbourne data

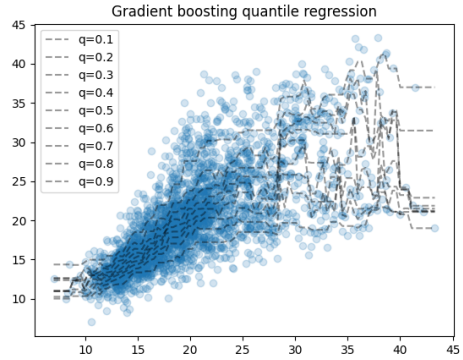
Quantiles	Linear qr	Gbm qr	Quantile forest	Kernel qr
0.100000	0.710644	0.549232	0.562888	0.540235
0.200000	1.155014	0.938561	0.946712	0.903213
0.300000	1.417805	1.212671	1.222407	1.173803
0.400000	1.540108	1.399925	1.409293	1.367943
0.500000	1.574957	1.517281	1.484589	1.455849
0.600000	1.525114	1.498608	1.495474	1.447470
0.700000	1.397918	1.372183	1.362173	1.331503
0.800000	1.170140	1.115077	1.123195	1.096606
0.900000	0.787195	0.714075	0.734112	0.715085

Table 7.3: MAE Melbourne data

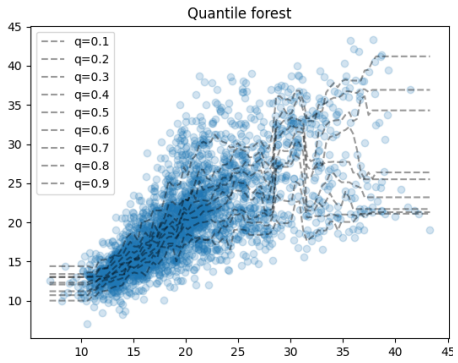
	Linear qr	Gbm qr	Quantile forest	Kernel qr
MAE	3.253882	3.134805	3.095041	3.024336



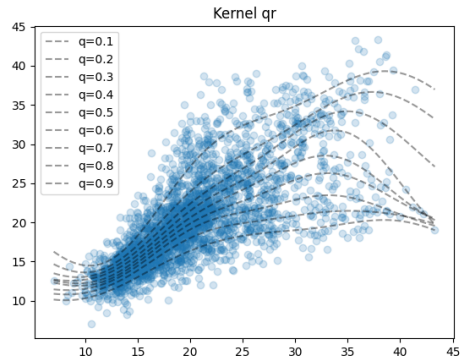
(a) Linear quantile regression



(b) Gradient boosting quantile regression



(c) Quantile forest



(d) Kernel quantile regression

Figure 7.7: Quantile regressors

7.5 Kernel density estimation

- Explain the framework of kernel density estimation.

- Explain how it is applied in the literature.

- Extend to Conditional kernel density estimation and how it is applied in the literature

- there is sample in sklearn kde, so we can use it to create a method of the kde class that computes its crps.

- Do a simple showcase with an example

7.6 Ensemble methods

- Explain the idea of ensemble methods.

- The most popular framework is based on autoregressive processes

- simple example

7.7 DMLP

7.8 DeepAR

7.8.1 Kernel herding

Select the best point forecasting method and create a probabilistic forecast by modelling its model errors with kernel herding (do something like the residual bootstrap ensembles if it is meaningful and possible to implement).

Chapter 8

Exploratory Analysis and Data ETL

- Explain how data has been retrieved.

- Data provider EPEX(entsoe retrieves its data)

- Explain the ETL(Extract Transform Load) pipeline I set up.

- Explore data in order to get useful insights for how to tune the models to get the most of them.

- correlation between temperatures and load

- Correlation and auto correlation plots

- Split train and test dataset Explain carefully why it is important to carry out an out of sample test and not in sample. In sample test involves look ahead bias because we are fitting the model on the data we want to predict, thus it overfits on the data considered but it does not generalize well.

This section covers the datasets used in our experiments, attributes and features will be thoroughly described. Next, we will explain the ETL pipeline that we set up in order ease the workflow of our comparison studies. Finally, in order to to bettern understand patters within the data, detect outliers and discover interesting patterns we carry out an exploratory data analysis.

8.1 GEFCom2014

The chosen dataset for probabilistic load forecasting, was the data from the GEFCom 2014 competition. The data is freely hosted on Dr. Hong blog [41]. Contestant were asked to provide one month ahead hourly probabilistic forecasts on a rolling basis for 15 consecutive round. To get started, in the first round, organizers provided 69 months of hourly load data and 117 months of hourly temperature data. As the competition task went on, the real observed data of the previous tasks was made available. The GEFCom2014 Data

contains five zip files. We are interested in the probabilistic load forecasting data, which is contained in the GEFCom2014-L_V2 zip file. Within this subfolder, we a txt with the competition instructions and 15 folders one for each of the consecutive tasks. For each of those we have the prediction of the competition benchmark model and the train file upon which we will fit our model.
Each data from the various task folders are shifted by one months between others.
In order to compare our model performance with the winning entries of the GEFCom2014 competition we will refer to the Provisional_Leaderboard_V2 file contained also in the GEFCom2014 Data directory. Notice a quick premise, within this xsls file the authors opted for various scores to compare the entries performance. This choice was motivated by the need to give a proportial weight to each task when averaging between them; that is in order to not penalise too much the tasks with higher point spreads. Furthermore, additional factors such as frequency of benchmark outperformance, and robustness and clarity in methodology explaination.
Since we are only interested in the load forecasting track, we can directly compare between models by comparing their pinball scores. Such scores are stored inside the subtab L-score-0/L-score-2 of Provisional_Leaderboard_V2.

Chapter 9

Implementation

This section is inteneded to explain and aid for reproducibilty studies. Hereafter the specific libraries used and the custom implementatios are thoroughly documented.
For the list of python packages needed see the requirement.txt file.

Section documenting code - indicate computer specifics

- Explain how methods' implementation has been adapted to my specific setting.

- Explain in detail how to my src code has been implemented its rationale and how to use it.

- As I explain code scripts go over the test, to explain better my ideas.

9.1 Linear quantile regression

The implementation of statsmodels.regression.quantile_regression.QuantReg has been used. The model is fitted through iterative reweighted least squares.

9.2 Quantile gradient boosting machine

The implementation of sklearn.ensemble.GradientBoostingRegressor as been used.

9.3 Quantile forest

The implementation of quantile_forest.RandomForestQuantileRegressor as been used. This estimator is compatible with scikit-learn.

9.4 Kernel quantile regression

Kernel quantile regression had no previously implemented open source library, thus the need of implementing our own version.
The scikit-learn team provides a project template for the creation of estimators compatible with scikit-learn functionalities. Therefore, the KQR class is derived from the scikit-learn BaseEstimator and the mixin class RegressorMixin. Our KQR class is initialized by providing a quantile, the regularization term C and the rbf kernel bandwidth gamma; the latter are the two hyperparameters of our custom estimator.
In the fit method, we set up and solve the convex optimisation problem by using the cvxopt library. When using this library, it is important to keep two things in mind. First this library assumes the quadratic term of the optimisation problem to be multiplied by the 0.5 factor, thus we just have to provide the Q matrix with no 0.5 in front. Secondly, in order to specify multiple inequalities we have to stack them an provide as a unique matrix.
Once a solution to the convex problem has been found, we create a mask for the support vectors of the estimator in order to estimate the constant term of our kernel quantile regressor.
In the predict method, we pass a matrix X_eval of independent variables, next we compute the kernel matrix between X_train and X_eval and obtain y_eval with the formula $y = \alpha^\intercal K + b$.
This estimator is compatible with useful scikit-learn in built methods like gridsearch, crossvalidation and scoring rules.
Up to now, there are only two open source implementation of the quantile kernel regression. Nevertheless they are both in R, that is there exists no python, matlab or julia open source implementation. Following are reported the results of a comparative study between our own implementation and the one of the R library kernlab(i guess it is in C or C++ and then binded to R).

9.4.1 Python vs R implementation

In this section, a comparison study has been carried out in order to inspect the competitiveness of our implementation with the existing one for the R programming language.

Chapter 10

Experiments Analysis

Analysis of experiments and results
Building on the theory introduced in 6 and 7, this section covers the experiments carried out and the results obtained.

- Comments
- Comparison
- Table of loss scores

Plots:
- Plots for visualizing timeseries with quantiles bounds
- Other plots that will come up to mind

10.1 Quantile forecasting

In this subsection we compare performance of quantile regressor considering the GEFCom2014 dataset.
- experiment for quantile estimator on gefcom2014 and we are good

List of Symbols

ANN	Artificial neural network
AR	Autoregressive model
ARMA	Autoregressive moving average model
ARIMA	Autoregressive integrated moving average model
ARX	Autoregressive exogenous model
CI	Computational intelligence
CKD	Conditional kernel density
CRPS	Continous ranked probability score
DDNN	Distributional neural network
EDA	Exploratory data analysis
EF	Electricity forecasting
ELF	Electricity load forecasting
EMD	Empirical mode decomposition
EPF	Electricity load forecasting
ESM	Exponential smoothing models
ETL	Extract transform load
EVs	Electric vehicles
GBRT	Gradient boosting regression tree
GEFCom	Global energy forecasting competition
GPR	Gaussian process regression
HWT	Holt-Winters-Taylor exponential smoothing method
KDE	Kernel density estimation
LCTs	Low carbon technologies
LSSVR	Least squares support vector regression
LV	Low voltage
MAE	Mean absolute error
MASE	Mean absolute scaled error

MAPE	Mean absolute percentage error
MGM	Minimal gated memory network
MLR	Multiple linear regression
OLS	Ordinary least squares
RF	Random forest
RKHS	Reproducing kernel hilbert space
RMSE	Root mean squared error
PI	Prediction interval
PF	Price Forecasting
PPF	Probabilistic Price Forecasting
QR	Quantile regression
QRA	Quantile regression averaging
SME	Small and medium-sized enterprises
SNARX	Smoothed nonparametric ARX
SDGs	Sustainable development goals
SVMs	Support vector machines
TOU	Time of use tariffs
TSO	Transmission system operator
d^*	dual optimum
$\mathbb{E}$	expectation
$\Phi(x)$	feature matrix
F	feature space
$\varphi(x)$	feature vector
$g(v)$	dual function
$\mathbb{I}$	Indicator function
K	kernel matrix
$k(x, x')$	kernel function
L	lagrangian
ρ_q	pinball loss
p^*	primal optimum
relint	relative interior
$\mathcal{H}$	reproducing kernel hilbert space
$\mathbb{1}$	vector of ones

Appendix A

Appendix

A.1 Feature Map Normalization

Proof

$$\begin{aligned}
\|\varphi^{new}(x)\|_{\mathcal{H}}^2 &= \|\frac{\varphi(x)}{\|\varphi(x)\|_{\mathcal{H}}}\|_{\mathcal{H}}^2 \\
&= \|\frac{\varphi(x)}{\sqrt{k(x,x)}}\|_{\mathcal{H}}^2 \\
&= \langle\frac{\varphi(x)}{\sqrt{k(x,x)}}, \frac{\varphi(x)}{\sqrt{k(x,x)}}\rangle_{\mathcal{H}} \\
&= \frac{1}{\sqrt{k(x,x)^2}}\langle\varphi(x), \varphi(x)\rangle_{\mathcal{H}} \\
&= 1
\end{aligned}$$

□

A.2 Cross validation

A.3 Quantile regressor extensive comparison

A.3.1 Boston housing dataset

The Boston housing dataset https://www.kaggle.com/datasets/altavish/boston-housing-dataset contains information about various attributes for suburbs in Boston. There are 13 indipendent variables:

- CRIM per capita crime rate by town
- ZN proportion of residential land zoned for lots over 25,000 sq.ft.
- INDUS proportion of non-retail business acres per town.

Table A.1: Pinball loss Boston housing data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0	13.785678	11.418540	10.587686	10.297572

Table A.2: Pinball loss quantile-wise Boston data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0.100000	0.729749	0.771714	0.588441	0.578898
0.200000	1.122582	1.033442	0.932824	0.869145
0.300000	1.479486	1.170642	1.153765	1.142783
0.400000	1.712577	1.436263	1.352667	1.331955
0.500000	1.911385	1.344361	1.408333	1.396300
0.600000	1.989514	1.448885	1.464902	1.431705
0.700000	1.938362	1.508741	1.427912	1.382772
0.800000	1.658058	1.497901	1.275059	1.245288
0.900000	1.243965	1.206591	0.983784	0.918725

Table A.3: MAE Boston data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0	3.826326	2.845989	2.965490	2.810494

- CHAS Charles River dummy variable (1 if tract bounds river; 0 otherwise)
- NOX nitric oxides concentration (parts per 10 million)
- RM average number of rooms per dwelling
- AGE proportion of owner-occupied units built prior to 1940
- DIS weighted distances to five Boston employment centres
- RAD index of accessibility to radial highways
- TAX full-value property-tax rate per 10,000
- PTRATIO pupil-teacher ratio by town
- B $1000(Bk - 0.63)^2$ where Bk is the proportion of afroamericans by town
- LSTAT lower status of the population

The dependent variable is MEDV, that is the median value of owner occupied homes in $1000's

Table A.4: Pinball loss Abalone data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0	5.613975	5.531938	5.212990	5.252491

Table A.5: Pinball loss quantile-wise Abalone data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0.100000	0.277903	0.290531	0.274079	0.269287
0.200000	0.469361	0.488079	0.453110	0.457286
0.300000	0.621961	0.625633	0.580766	0.596791
0.400000	0.729757	0.715875	0.689904	0.691310
0.500000	0.794695	0.766185	0.735945	0.740834
0.600000	0.810691	0.785769	0.744928	0.746636
0.700000	0.769587	0.730318	0.700287	0.710392
0.800000	0.667776	0.656913	0.609378	0.608334
0.900000	0.472244	0.472635	0.424593	0.431621

Table A.6: MAE Abalone data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0	1.627627	1.574179	1.499522	1.498583

A.3.2 Abalone dataset

The abalone data https://archive.ics.uci.edu/dataset/1/abalone consist of measurements of abalone molluscs, the goal is predicting their age by building a model for estimating its number of rings; age is the number of rings plus 1.5 The data has 8 attributes:

- Sex Categorical variable either male, female or infant
- Length
- Diameter
- Height
- Whole height
- Shucked height
- Viscera weight
- Shell weight

Table A.7: Pinball loss Vehicle data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0	4.054449	2.289554	2.844410	2.204343

Table A.8: Pinball loss quantile-wise Vehicle data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0.100000	0.254649	0.139849	0.170489	0.182490
0.200000	0.403772	0.236339	0.285875	0.223165
0.300000	0.548820	0.244086	0.357375	0.242963
0.400000	0.576918	0.263169	0.389305	0.262835
0.500000	0.554367	0.306123	0.410738	0.295878
0.600000	0.563046	0.335363	0.398125	0.306062
0.700000	0.516019	0.287490	0.326572	0.283716
0.800000	0.407742	0.261882	0.313698	0.235793
0.900000	0.229115	0.215253	0.192233	0.171440

Table A.9: MAE Vehicle data

	Linear qr	Gbm qr	Quantile forest	Kernel qr
0	1.117714	0.606971	0.752197	0.594292

A.3.3 Vehicle dataset

This data contains info about used cars https://www.kaggle.com/datasets/nehalbirla/vehicle-dataset-from-cardekho, the predictors are:

- Year
- Present_price ex showroom price
- Kms Driven
- Fuel type
- Seller type
- Transmission
- Owner number of previous owners

The dependent variable is the selling price.

What can be concluded from these numerical examples is that, on average kernel quantile regression yields better results than quantile forest [58] and gradient boosting machine quantile regression [23] in terms of the pinball loss as well as in terms of the mean absolute error.

A.4 Cross validation

Cross validation directly estimates the expected test error

$$Err = \mathbb{E}\left[L\left(Y, \hat{f}(X)\right)\right] = \mathbb{E}\left[Err_{\mathcal{T}}\right] \tag{A.1}$$

$Err_{\mathcal{T}}$ is the prediction error over an independent test sample

$$\mathbb{E}_{\mathcal{T}} = \mathbb{E}\left[L\left(Y, \hat{f}(X)\right)|\mathcal{T}\right] \tag{A.2}$$

That is *Err* is the average over everything that is random: X,Y and the training set $\mathcal{T}$ used to learn $\hat{f}$. Hence, our interest lies in estimating the *Err* quantity in order to guide model selection.

A.4.1 K-fold cross validation

K-fold cross validation splits the data into K roughly equally sized parts, then K models are trained. For k from 1 to K we train the kth model on the whole dataset except the kth partition. Next, the prediction error of the kth fitted model is computed. Finally averaging all the k prediction erros we obtain an estimate for the expected test error. We select the model which performs best in terms of expected prediction error.
Usually, K is set equal to 5 or 10. Leave-one-out cross validation is the case when K is set equal to the size of the data.

A.4.2 Gridsearch

Model performance depends higly on the choice of hyperparameters. Notice, there is no way to get to know them in advance, therefore, all we can do is trying a lot of combinations until we fit a good enough set of hyperparameters. Essentially, gridsearch carries out hyperparameter tuning by performing a search over a predefined hyperparemeters grid. During its search, it tries all possible combination and evaluates the different models using cross validation. For example, suppose that the grid contains 100 possible candidates and that we are doing 5-fold cross-validation, then the gridsearch algorithm will carry out 500 iterations. Therefore, we get an estimate of prediction error for each considered model and this guides us in hyperparameters (model) selection.

A.4.3 Randomized search

Randomized search controls the number of steps by choosing smartly the hyperparameters to try in each iterations. Let us say, there are 100 candidates and we set the number of iterations to 20 then the search will stop after the 20th iteration and return the best set among the hyperparameters observed.

The advantage is that it is much more quicker than gridsearch, but on the other hand its performance is worse than gridsearch.

A.4.4 Halving gridsearch

Gridsearch has been the to go choice for hyperparameters tuning for the past years. However, such method is brute forcing all possible combinations, hence it is highly computationally intensive, especially when it comes to large datasets.
The scikit-learn team addressed this disadvantage of gridsearch by introducing the halving gridsearch method [3] (2020). Such technique has proved itself to greatly speed up hyperparameter tuning. The ground concept underlying this method is successive halving. During the first iteration of halving gridsearch, all candidates are trained on a small subset of the training set. Next, we keep only the candidates which performed best and compare them again on a bigger subset of the training set. As the iterations pass, the surviving candidates will be given more and more training samples. The algorithm stops when we are left with only the best set of hyperparameters.

A.4.5 Cross validation for time series data

When data points are dependent on preceding values, we cannot use standard K-fold cross validation. The rationale is that K-fold will randomize the order of the data, thus it might happen to use future data to predict the past; we want to avoid such behaviour in a time series setting. When carryout out any kind of cross validation, we must keep consistency in the way we evaluate our predictors during model selection and in the way we perform evaluation of the test data. Hence, for time series crossvalidation we have the timeseries split procedure, see figure A.1 for a visualisation; the blue observations make up the training sets while the orange observations form the test sets. We then average all the observed losses in order to get an estimate for Err. Notice, in the literature this procedure is sometimes also referred to evaluation on a rolling forecasting origin. This comes from the fact that at each iteration we push forward the origin of our forecast. The same concept applies for multi step ahead forecasting, see picture A.2. That is in predicting $\hat{L}_{N+m}$ we use as inputs $L_1, L_2, \ldots, \hat{L}_N, \hat{L}_{N+1}, \ldots, \hat{L}_{N+m-1}$; where $\hat{L}_N, \hat{L}_{N+1}, \ldots, \hat{L}_{N+m-1}$ are one step ahead forecasts.

A.5 Kernel methods best practices

Following, are reported a couple of considerations important to keep in mind when working with kernel methods.

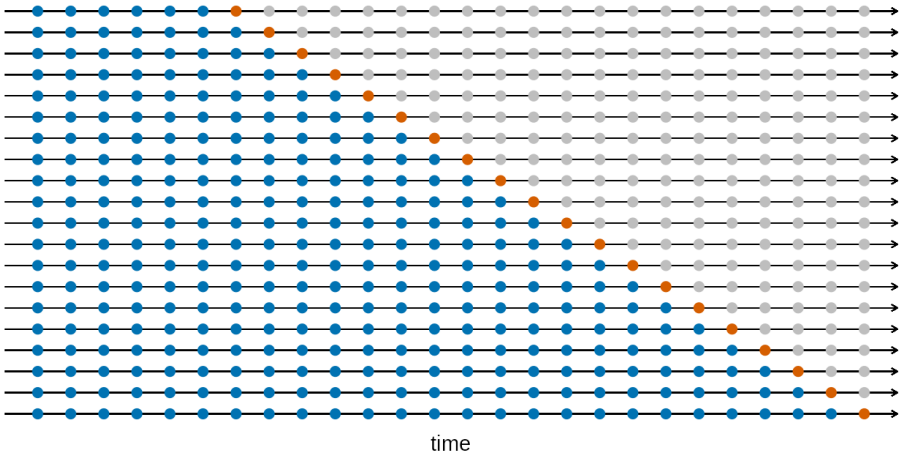


Figure A.1: Cross validation for one step ahead timeseries data [44]

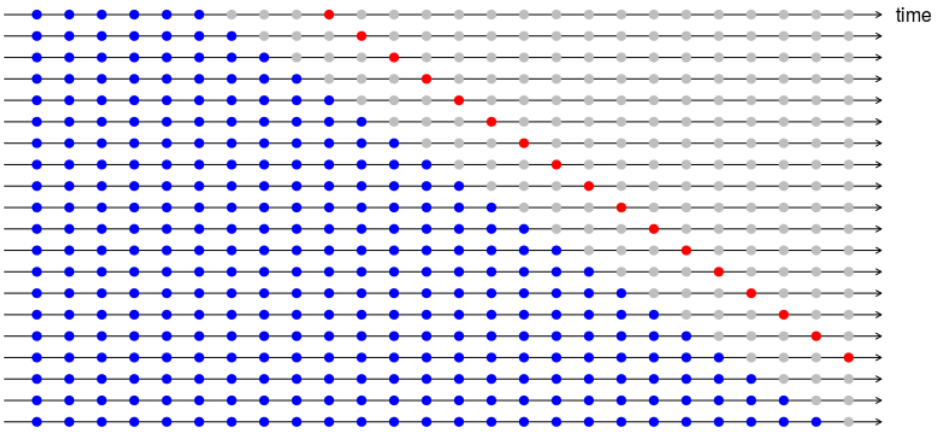


Figure A.2: Cross validation for m step ahead timeseries data [44]

A.5.1 Data normalization

With data normalization we transform the range of the feautures to a standard scale. Such preprocessing step is essential when employing distance based algorithms like svm or k-nearest neighbors. The rationale behind it is that by normalizing data we give an uniform weight to each feature in the learning process; in this way we do not favour larger scale features. Examples of the most popular features scaling are:

- Standard scaler= it computes the standard score z of a sample x z=$\frac{x-\mu}{\sigma}$.
- MinMax scaler= it maps every data sample to the range 0, 1. $\frac{x-\min(X)}{\max(X)-\min(X)}$

- Robust scaler= it scales features using statistics that are robust to outliers. Essentially, it subtracts the median and then scales the data according to the interquantile range.

Many other data scaling algorithms exists, we refer the reader to a thorough comparison [5].
We conclude this subsection with a custom example that motivates the need of feature scaling [2]. The idea is to compare the results of modelling the data with k nearest neighbors on the unscaled data against the scaled data. The considered data is the wine recognition dataset https://archive.ics.uci.edu/dataset/109/wine. The goal for this dataset is recognising from whose cultivator the wine comes based on two features with a completely different scale. The first feature has values in the [0,1000] range while the second feature has values contained in [1,10]. The unscaled and scaled version are compared in figure A.3 What

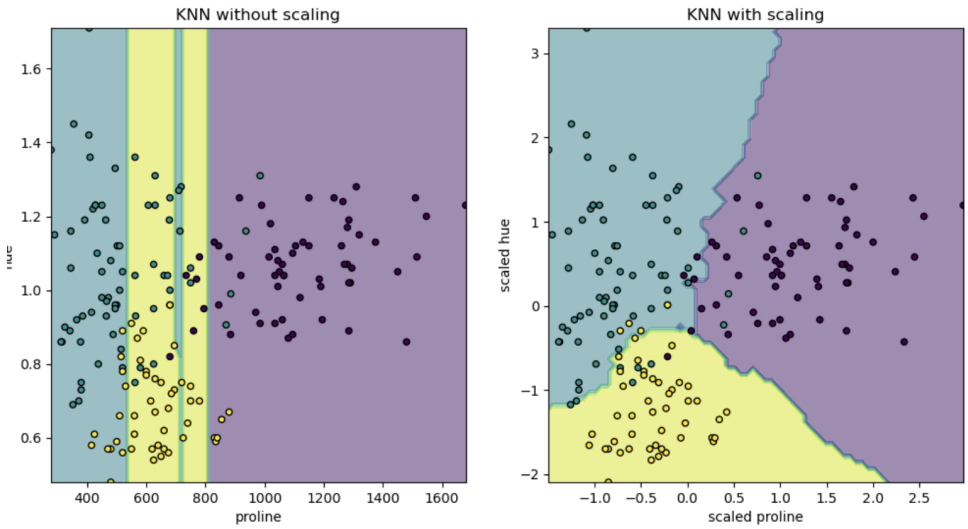


Figure A.3: importance of feature scaling

we can conclude from the image is that, the model trained on scaled data is greatly better than the other. On the left, we can see that distances between categories are impacted solely by the larger scale feature. Conversely, on the right, we have that the two features contributing equally in determining the neighbors.

A.5.2 Data compression

When the number of points n is large, kernel methods suffer from high computational costs. Using kernel methods, we have that the storage cost is of the order of $O(n^2)$ while the computational cost for finding the solution is of the order $O(n^3)$. A significant speed up can be obtained thanks to low

rank approximation.

Nystrom decomposition

The Nyström approximation involves storing a submatrix of the whole kernel matrix. Thus, storage and computational cost are reduced to $O(nm)$ and $O(nm^2)$ respectively. Nyström works by selecting $m < n$ points, callled representative points; it approximates K as

$$\tilde{K} = K_{n,m} K_{m,m}^{-1} K_{n,m}^{\mathsf{T}} \tag{A.3}$$

Pivoted Cholesky decomposition

Pivoted Cholesky approximate the Cholesky decomposition of a matrix. Since kernel matrices are positive definite, they can decomposed in terms of the Cholesky decomposition. Hence, we have that pivoted Cholesky can be used to approximate the full kernel matrix.

A.6 Src code

The whole code for the project is hosted on https://github.com/luca-pernigo/ThesisKernelMethods.

- query: folder containing Scopus data and scripts to generate bibliometric survey plots in section 2
- kqr.py: file implementing our custom kernel quantile regression

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