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Predicting the Momentum Flux- Profile Relationship from Macro Weather Parameters

EMILIO DORIGATTI



KTH Information and
Communication Technology

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EMILIO DORIGATTI

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External Supervisor: Gunilla Svensson
Academic Supervisor: Seif Haridi
Examiner: Jim Dowling

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Abstract

The study of climate heavily relies on simulations. For efficiency reasons, many important phenomena cannot be simulated, and have to be parametrized, i.e. their effect must be described based on macro parameters. The turbulence resulting from the interaction between the atmosphere and the surface is an example of such phenomena. One of the quantities of interest arising from turbulence is the momentum flux-profile relationship, which relates the transport of momentum (flux) and the change of wind speed with altitude (profile). This quantity can be computed following the Monin-Obukhov Similarity Theory (Obukhov 1971). However, this theory requires parameters that are hard to measure, both in real life and in the simulations, is only applicable in a restricted range of conditions, and produces predictions that are accurate only up to 20-30% (Foken 2006).

The goal of this thesis is to compute the momentum flux-profile relationship using only macro weather parameters, which are readily available in climate simulations; this is done using Data Mining techniques on 17 years of weather data collected from the Cabauw meteorological tower in the Netherlands. Moreover, we asses the impact of different sets of features on the prediction error.

Results show that even the simplest linear models are able to compete with the similarity theory, and complex methods such as gradient boosted trees can reduce the mean squared error by almost 50%. Furthermore, these methods are applicable to a much wider range of conditions compared to the similarity theory, while providing roughly the same predictive performance achieved by this theory *in its validity range*. These results are obtained using wind speed and air temperature at different levels, the soil temperature, and the net radiation at the surface; the improvement offered by the heat fluxes is significant, but of low magnitude. The soil heat flux, the dew point, and the hourly trend of the features do not have a tangible impact on the performance.

Referat

Klimatstudier är till stor del beroende av simulationer. Av effektivitetsskäl så kan många betydande fenomen inte simuleras och måste parametreras, exempelvis beskrivs då fenomenets effekt baserat på makroparametrar. Turbulensen som resulterar i interaktionen mellan atmosfären och jordytan är ett exempel på ett sådant fenomen. En av de mängder av möjliga intressanta simulationer som uppstår av turbulens är Flux-Profile förhålladen som sätter i relation transport av momentum (flux) och ändringar i vindhastighet i relation med höjden (profile). Denna mängd kan beräknas med Monin-Obukhov likhetsteori (Obukhov 1971). Denna teori kräver vissa parametrar som är svåra att mäta både i verkligheten och i simulationer. Teorin är endast applicerbar i ett begränsat antal situationer och resulterar i förutsägelser med endast 20-30% träffsäkerhet (Foken 2006).

Målet med denna uppsats är att beräkna Flux-Profile förhållandet enbart med makroväder parametrar som är tillgängliga i klimatsimulationer; detta görs med informationsutvinnning på 17 års väderdata insamlat från Cabauw väderstation i Nederländerna. Olika kombinationer av egenskaper kommer att användas för att utvärdera felet på förutsägelserna.

Resultaten visar att även de enklaste linjära modellerna är jämförbara med likhetsteorin, och komplexa metoder såsom gradient boosted trees kan reducera medel-kvadratfel med nästan 50%. Dessutom är dessa metoder applicerbara på en större mängd av villkor jämfört med likhetsteorin, samtidigt som de ger liknande träffsäkerhet som likhetsteorin i dess validitetsintervall. Dessa resultat erhölls genom att använda vindhastighet och lufttemperatur på olika höjder, jordtemperatur, nettostrålningen på jordytan, förbättringen genom att använda värmeflöden är markant, men har låg magnitud. Jordens värmeflöden, daggpunkten och den timvisa trenden över egenskaperna hade inte en märkbar påverkan på prestandan.

Declaration

I hereby certify that I have written this thesis independently and have only used the specified sources and resources indicated in the bibliography.

Stockholm, 07. June 2018

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Emilio Dorigatti

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Chapter 1

Introduction

This chapter briefly introduces the area for this project, and formally defines and motivates the problem that is tackled. Section 1.1 introduces Climate Science, Machine Learning and Data Mining, then section 1.2 formally defines the research questions that this work sets to answer and why it is relevant, and section 1.3 explains how the research questions will be answered. Next, section 1.4 discusses potential ethical issues and sustainability aspects of this project, then section 1.5 explains the research methodology followed to answer the research questions, and, finally, section 1.6 describes how the remainder of the report is organized.

1.1 Background

Climatology, or climate science, studies the long-term average weather conditions. In the last few decades, climate scientists found evidence of ongoing changes in Earth's climate, most notably, a general increase in average temperature; in the long run, this and other changes can potentially have a devastating impact on life on our planet. Regardless of the causal effect of human activities on it, having a solid understanding of the climate allows us to find the best way to mitigate its change, and to preserve our planet.

Climate science is an extremely difficult field, for a number of reasons. First, climate is evident, by definition, only over long periods of time and large distances, making the usual scientific approach of testing hypotheses by conducting experiments inapplicable; instead, climate scientists have to rely on historical data. Second, the atmosphere is a complex and chaotic system, which must be described through systems of nonlinear differential equation. They can be used to create numerical simulations, such as the atmospheric model of GFDL-CM3 (Donner et al. 2011), HadCM3 (Gordon et al. 2000) and others, and the resulting predictions compared to historical data to assess the accuracy of the theory. Furthermore, the chaotic character of the atmosphere makes it impossible to study parts of it in isolation from others, as small scale phenomena affect large scale ones, and vice versa. These simulations, called General Circulation Models (GCMs), use equations

describing fluid dynamics to simulate the behavior of the atmosphere. These equations are discretized by using a grid whose horizontal resolution varies between tens and hundreds of kilometers, depending on the simulation; the smaller the grid, the more precise the simulation is, but the higher computational resources are needed. Grids of this size are too large to simulate some phenomena, such as clouds and turbulence, which have to be "summarized" with simpler theories (a process called *parametrization*).

The atmosphere can be vertically divided in several regions with different characteristics. The lowest such region, the troposphere, contains most of the air mass in the atmosphere, and occupies the lowest 10 to 12 kilometers of the atmosphere. This is where weather happens, and it can be further divided in a number of sub-layers, the lowest of which is the *atmospheric boundary layer*: it is the region of the atmosphere that is affected by the conditions of the surface. Most human activities happen in this layer, and it is responsible for a large part of the diffusion and transport of aerosol such as, among others, pollutants. Yet, the physics governing the atmospheric boundary layer is not fully understood, and the theory is lacking. This means that its parametrization in GCMs is inaccurate.

Recent developments in information technology made bottom-up approaches feasible, in contrast to the traditional, top-down approach of science. In this new way of thinking, existing data is used to automatically infer the "best" explanation for the measurements at hand, the underlying laws that originated that data. The field that makes this possible is called *Machine Learning*: it takes advantage of several methods coming from statistics, information theory, optimization theory, etc., to make computers learn from examples. Together with Natural Language Processing and Automated Planning, it is one of the three main branches of Artificial Intelligence, the sub-field of Computer Science that studies ways of making machines behave intelligently.

An even broader field, called *Data Mining*, is concerned with finding interesting patterns, structures, and regularities in large datasets, where the definition of interesting depends on the specific goals. Data Mining makes use of techniques from Machine Learning, as well as other statistical models such as ANOVA, and visualization techniques.

1.2 Problem Statement and Purpose

One important issue in the study of the atmospheric boundary layer is the derivation of flux-profile relationships for wind and temperature: they essentially relate the transport of momentum and heat by the turbulence (flux) with the change of wind speed/temperature with altitude (profile). The state of the art relationships are defined by the Monin-Obukhov similarity theory (?) in terms of a parameter describing instability; difficulties in measurements of relevant quantities make this theory accurate only up to 20-30% (Högström 1996), and applicable in a restricted set of conditions.

1.2. PROBLEM STATEMENT AND PURPOSE

Optis et al. (2014) shows that, at least in difficult conditions, several simulation models produce flux estimates that are highly inaccurate, presenting low correlation (mostly below 0.3) and errors that are as large as the fluxes themselves. On the contrary, Ronda et al. (2003) and Dimitrova et al. (2016) show that other simulation models are able to provide accurate estimates of the fluxes at the price of biased surface temperature estimates. Intuitively, this trade-off arises because of the deep relationship between the net radiation, the surface fluxes and the surface temperature: one can choose which two quantities to estimate accurately, and sacrifice accuracy on the remaining one. Basu & Lacser (2017) raise awareness on the fact that the lowest grid level used in many simulations recent simulations is too low, outside of the validity region of the Monin-Obukhov similarity theory, although no quantitative measure of the issues caused is presented. In the atmospheric model of the GFDL-CM2 and CM3 models, the wind speed used to calculate the fluxes is artificially adjusted to correctly include the contribution from turbulence, and the predictions from the similarity theory are adjusted to prevent excessive surface cooling of the land surface during winter (Anderson et al. 2004). Since errors in the simulation accumulate over time, even slight improvements can greatly improve the accuracy of the results after years of simulated time.

In spite of its drawbacks, the Monin-Obukhov similarity theory is still widely used in most GCMs; limitations of its validity are not believed to be a likely explanation for the high scatter that is found in experimental studies, unless in highly stable conditions, where measurement challenges arise (Högström 1996). With the availability of macro- and micro-meteorological data such as the Cesar database, and the recent developments in Machine Learning, this conjecture can be finally put to the test. More specifically, we pose the following

Research Question 1: How can the data from the Cesar database be used to predict the momentum flux-profile relationship more accurately than the Monin-Obukhov similarity theory, by using only macro weather parameters?

Research Question 2: What impact do different macro-weather parameters have on the quality of the predictions obtained?

A positive and successful answer to the research questions would help in producing one or more estimators that can be incorporated in general circulation models in order to provide more accurate predictions of the momentum flux-profile relationship. This, in turn, would lead to more precise long term climate forecasts, ultimately advancing our understanding of the impact of human activities on the planet.

1.3 Goals

The first research question is answered by proposing one or more Data Mining methods, i.e. feature selection and extraction, and a Machine Learning model, that obtain sufficient predictive performance, whereas the second research question is answered by a quantitative comparison of the performance of the models when using certain subsets of features.

1.4 Ethics and Sustainability

Carrying out this project posed no ethical issues: data collection was mostly automated and performed by a third party, and there is no evidence that such activities were performed in unethical and/or unlawful manner. Privacy and confidentiality are not relevant issues either, since no test subjects were needed to perform the research, and the data is free and open to everybody.

The author strongly aligns with the Open Science movement, according to which scientific research should be made as open and accessible as possible, so that it can be examined, extended and improved by as many people as possible (Fecher & Friesike 2014). This is what allowed mankind to become what it is today, and it should not change. For this reason, this work was performed entirely with Free and Open Source tools, providing a low barrier to entry, and focusing on reproducibility of the results. The entirety of the analysis and its historical record, from the very data to the generation of plots and tables, is openly accessible¹ and can be performed by anyone with enough computational resources.

Some of the analysis performed in this work required a considerable amount of computational resources, in the order of hundreds of cores and terabytes of memory. Such resources are power hungry and require electricity to run and to be kept at an appropriate temperature, as well as proper support infrastructure, e.g. for networking. In an effort to reduce the energy requirements, only the necessary experiments were performed, and care was taken not to do unnecessary work, for example by reusing results of previous experiments where possible. Moreover, this project strongly aligns with the thirteenth goal, *take urgent action to combat climate change and its impacts*, of the Sustainable Development Goals set by the United Nations.² The Paris agreement³ is a formal document where adhering nations set goals to limit the global rise of temperature well below 2 °C. The main contribution of this project is to aid the development of accurate climate simulations, thanks to which nations can set realistic targets, monitor their progress towards the goals, etc.

¹<https://github.com/e-dorigatti/mscthesis>

²<https://www.un.org/sustainabledevelopment/>

³<https://unfccc.int/process-and-meetings/the-paris-agreement/the-paris-agreement>

1.5. RESEARCH METHODOLOGY

1.5 Research Methodology

Following the taxonomy of Håkansson (2013), this project aligns with the positivist school of thought, and follows the quantitative research methodology by applying a deductive approach in order to answer the research questions. The data is collected through field measurements, and processed and analyzed with mathematical and statistical tools, that provide strong reliability and replicability guarantees.

The two most widely used research methodologies in Data Mining are CRISP-DM, the cross-industry standard process for data mining, by Chapman et al. (2000), and KDD, knowledge discovery in databases, by Fayyad et al. (1996). Despite the difference in terminology, they essentially describe the same process for extracting useful information, or *patterns*, from one or more raw data sources. This process is composed by the following steps (we use the nomenclature of CRISP-DM):

1. *Business Understanding*: Get familiar with the application domain, obtaining necessary background knowledge, then identify the goals of the process from the customer's perspective and translate them to data mining tasks;
2. *Data Understanding*: Obtain and clean the data that is necessary to conduct the data mining tasks, appropriately dealing with empty, missing and outlier values, and conducting simple analyses and visualizations to inspect the overall quality and gain further understanding of the data itself;
3. *Data Preparation*: Transform the data in the format needed to conduct the data mining tasks, e.g. by performing feature selection and/or extraction, such as joins, aggregates, etc.
4. *Modeling*: Conduct the data mining tasks, using the data prepared in step 3;
5. *Evaluation*: Interpret and evaluate the results obtained in step 4, both from a data mining perspective and from a business perspective, and quantify to what extent the goals defined in step 1 were achieved;
6. *Deployment*: Act on the outcome of the data mining tasks, report it and possibly take action based on the results and/or deploy models to support live decision making, etc.

It is important to mention that these steps are not strictly sequential, but heavily interact with one another: insights gained from the data can give rise to new questions, the evaluation of the results can highlight flaws in earlier steps, etc.

1.6 Outline

The thesis is organized as follows: in chapter 2, we introduce the relevant background in Climate Science and Machine Learning, then, in chapter 3, we describe

CHAPTER 1. INTRODUCTION

how the data is collected and used to answer the research question, chapter 4 contains the results of such investigation, and, finally, chapter 5 discusses the results, pointing out limitations and possible directions for expanding this work.

Chapter 2

Background

This chapter introduces the basic concepts the reader should be qualitatively familiar with, in order to understand the content of this thesis. It is assumed readers are already knowledgeable of simple mathematical concepts, such as calculus, linear algebra, statistics, and probability theory. We first describe fluid dynamics, with a focus on the boundary layer (section 2.1), then use that knowledge to describe the atmospheric boundary layer and the Monin-Obukhov similarity theory (section 2.2), and finally describe the Machine Learning algorithms that will be used to answer the research questions (section 2.3).

The most important section is 2.2.4, since it introduces the state of the art which this work tries to improve upon, but readers should feel free to skip the sections they are already familiar with.

2.1 Fluid Dynamics

Fluid dynamics is the discipline that studies the flow of fluids; it has several branches that study different fluids, such as aerodynamics (the study of air motion) and hydrodynamics (the study of water motion). These disciplines are routinely applied when designing cars, airplanes, ships, pipelines, etc.

2.1.1 Laminar and Turbulent flow

There are two distinct ways in which particles in a fluid can move: laminar flow and turbulent flow. In the former, all the particles move orderly, perhaps with a different speed, but all in the same direction, whereas in the latter the movement of particles is highly chaotic and unpredictable, and tends to give rise to eddies of varying sizes. People are most familiar with the distinction between the two through the smoke rising from a cigarette, which starts smooth and becomes turbulent shortly thereafter, as in figure 2.1. The kind of flow in under specific conditions can be predicted using the Reynolds number Re , which is the ratio between inertia forces,

Figure 2.1: Smoke from a cigarette, and the transition from laminar to turbulent flow.



favoring turbulent flow, and viscosity forces, stabilizing the fluid towards laminar motion:

$$Re = \frac{\rho u L}{\mu} = \frac{u L}{\nu}$$

With ρ the density of the fluid, u its velocity, L a characteristic linear dimension of the system under consideration, μ and ν the kinematic and dynamic viscosity of the fluid. The viscosity describes, intuitively, how much the molecules of the fluid tend to stick together and resist motion by generating drag. For example, water has low viscosity, and honey has high viscosity.

Since turbulence is random, it is usually studied in terms of the statistical properties of physical quantities through the Reynolds decomposition; given a scalar quantity $a(s, t)$ which varies in space and time, we can compute its average

$$\bar{a}(s) = \frac{1}{T} \int_{T_0}^{T_0+T} a(s, t) dt$$

and the deviation from the average

$$a'(s, t) = a(s, t) - \bar{a}(s)$$

By definition, $\bar{a}' = 0$, which means that all the effects of turbulence are contained in a' . Common statistical properties such as variance and covariance are expressed respectively as $\overline{a' a'}$ and $\overline{a' b'}$.

2.1.2 The Boundary Layer

In the context of fluid dynamics, the boundary layer is the region where a fluid flows close to a solid surface. Imagine a laminar flow close to a solid surface; because of viscosity, the molecules flowing near the surface move slower, and, in the limit, the

2.1. FLUID DYNAMICS

velocity of the molecules in direct contact with the surface is 0 (this is called the *non-slip condition*). Thus, the velocity of the fluid increases smoothly, continuously and monotonously with the distance from the solid, until it reaches the *free-flow* velocity, after which it stays constant. The region close to the surface, where the fluid moves slower, is called the *boundary layer*, and is the region where the viscosity of the fluid influences its motion. Its height δ can be defined when the local velocity surpasses a certain threshold, such as 99% of the free-flow velocity.

The variation of velocity with distance from the surface, $\partial\bar{u}/\partial z$, is called *shear*, and, together with viscosity, determines the materialization of turbulence in the flow. Every layer of fluid is squeezed between a faster moving layer above and a slower moving below; in high shear conditions, this causes high stress on the particles, and prevents them from moving orderly, thus leading to turbulent motion. Figure 2.2 shows turbulence forming close to the wall in a canal, where the water flows from right to left. Viscosity and the no-slip condition prevent this phenomenon to arise in a region very close to the solid surface, called the *laminar (or viscous) sub-layer*, where we still find laminar motion.

The strength of the turbulence is proportional to $u_{rms} = (\overline{u'^2})^{1/2}$, which is, in turn, proportional to the shear. Again, because of the no-slip condition, u_{rms} is zero at $z = 0$, increases in the laminar sub-layer, and decreases to 0 at the end of the boundary layer, assuming laminar flow outside of it. Higher free-stream velocity generates higher shear, more turbulence, and a thinner laminar sub-layer. The strength of turbulence can be written in units of velocity, resulting in the *friction velocity*, computed as $u_* = (\tau/\rho)^{1/2} = (\nu \cdot \partial\bar{u}/\partial z)^{1/2}$, where τ is the shear stress, ρ is the density of the fluid, $\nu = \mu/\rho$ is the kinematic viscosity, and μ the dynamic viscosity. Therefore, the friction velocity increases with shear and viscosity, and decreases with density; it is proportional to the free-stream velocity and the turbulence strength, and inversely proportional to the height of the laminar sub-layer. Expressing the shear τ in terms of the horizontal kinematic momentum fluxes $\overline{u'w'}$ and $\overline{v'w'}$, we obtain an equivalent formulation of u_* :

$$u_* = \left(\overline{u'w'}^2 + \overline{v'w'}^2 \right)^{1/4} \quad (2.1)$$

Under this light, u_* essentially represents the degree by which turbulence moves air around, hence its second name of *momentum flux*: the larger the momentum flux, the more air is moving disregarding the mean flow, hence the stronger turbulence. On the contrary, with little turbulence, air tends to follow the mean flow with little deviations, causing the terms u' , v' and w' to be of small magnitude.

The mean velocity \bar{u} increases linearly within the laminar sub-layer, then logarithmically until the end of the boundary layer, thus the shear decreases further away from the surface. In the logarithmic sub-layer, the velocity is computed as $\bar{u}(z) = u_*(\log z - \log z_0)/\kappa$, where z_0 is the characteristic roughness of the surface, and κ is the von Karman's constant, whose value is around 0.4 Högström (1996). The characteristic roughness depends on the texture of the surface, and its relationship with the height δ_s of the laminar sub-layer; if the roughness scale is smaller

Figure 2.2: Turbulent boundary layer at the edge of a canal; water flows from right to left. Colors are inverted to make the patterns more visible. Picture taken by the author.



than δ_s , the logarithmic velocity profile is not affected by the texture, because the laminar sub-layer completely covers the variations on the surface, and we have the so-called smooth turbulent flow. If, on the contrary, the bumps in the surface are larger than δ_s , the laminar sub-layer follow the profile of the surface, and the logarithmic velocity profile is altered depending on the texture, a regime called rough turbulent flow.

2.2 The Atmospheric Boundary Layer

The atmosphere is composed by air, which behaves like a fluid. Therefore, close to the Earth's surface, in the region called *atmospheric boundary layer* (ABL), we find the same effects described in the previous section. Additionally, there are other phenomena that complicate things further, such as the temperature of the surface, which changes widely from day to night and from Summer to Winter, the rotation of the Earth, the varying roughness of the surface, due to cities and vegetation, etc. The effect of the surface on the first few hundred meters of the atmosphere is the main focus of *Boundary Layer Meteorology*.

This section gives a high level introduction of the main topics in Boundary Layer Meteorology: we start from an overview of the role of turbulence in the ABL in section 2.2.1, then examine the main mechanisms which produce turbulence and their effect on the transport of heat in section 2.2.2. Next, section 2.2.3 considers the exchange of energy between the atmosphere and the Earth surface, and, finally, section 2.2.4 formally introduces the Monin-Obukhov similarity theory.

2.2.1 Turbulence in the Atmospheric Boundary Layer

The height of the ABL typically varies between 100 and 1000 meters, highly depending on the conditions, and it is always turbulent. There are two main instabilities driving turbulence in the ABL:

- Shear instability: caused by shear, the mechanism described in the previous section. This happens at high Reynolds number, and, by using typical values for the ABL, we find Re well above 10^6 .

2.2. THE ATMOSPHERIC BOUNDARY LAYER

- Rayleigh-Bernard (also known as buoyancy driven) instability: is caused by the decrease of potential density¹ with height, or, in other words, when warm fluid is below cold fluid; the warm fluid will rise, and the cold fluid will drop, a phenomenon called *convection*. During hot Summer days, the surface is much warmer than the air, thus the air close to the surface will heat and tend to rise.

Turbulence has the very important role of transport and mix of air properties, such as heat, moisture, particles, aerosols, etc. This is especially true in *unstable* conditions, when the air moving upward (e.g. because it is warmer) is less dense than the air moving downward. On the contrary, when the air closer to the surface is denser (e.g. because it is colder), turbulence is weaker, and the ABL is called *stable*.

The ABL can be divided in two main sub-layers: the inner surface layer and the outer Ekmann layer. This distinction is mainly done based on the scale of the dominating turbulent eddies: they are much smaller than the height of the ABL in the surface layer, and of comparable size in the outer layer.

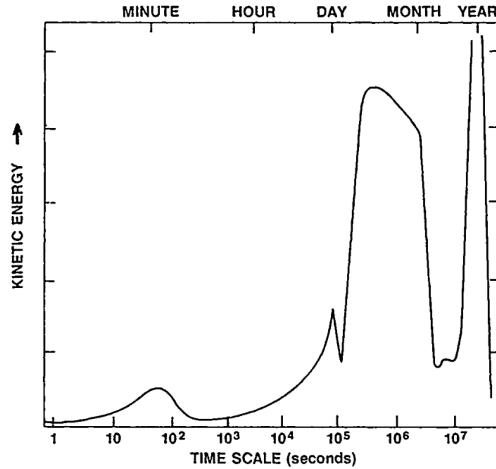
It is very important to have a macroscopic understanding of the turbulent processes in the ABL, because they happen at length and time scales too small to be simulated in global climate models. The process of expressing the result of turbulence as a function of large scale parameters is called parametrization; having realistic models is essential in order to conduct precise simulations of the global climate in the scale of tens or hundreds of years, because errors tend to accumulate and amplify as the simulation goes on. Other fields that benefit from the study of the ABL are urban meteorology (interested in the dispersion of pollutants), agricultural meteorology (interested in the formation of frost and dew, the temperature of the soil, etc.), aviation (predict fog and strong winds), and so on.

2.2.2 The Turbulence Kinetic Energy Budget

Kinetic energy is energy stored in form of movement: faster or heavier objects have more kinetic energy than slower or lighter ones. The Reynolds decomposition allows us to decompose the kinetic energy of turbulent flows in two terms: one caused by the mean flow, and one caused by turbulence. This decomposition can be justified by examining the temporal spectrum of kinetic energy, shown in figure 2.3. Four peaks are visible, corresponding to different sources of kinetic energy: turbulence, day-night cycle, synoptic scale variability, lows and highs passing, and seasons. Importantly, there are few sources of kinetic energy in the 30 minutes to one hour time scale; this so-called spectral gap allows us to separate between turbulence and other sources of fluctuations in the atmosphere.

¹The potential density is the density that a parcel of air would attain if brought at a standard reference pressure adiabatically, i.e. disallowing exchanges of heat with its surroundings. Potential density is useful to compare densities irrespectively of pressure, i.e. altitude.

Figure 2.3: Long term average of atmospheric kinetic energy at different time-scales. The peaks in the scale of days and months and years are due to the day-night and Summer-Winter cycles, the peaks in the monthly scale are due to baroclinic instability in the mid-latitude westerlies, and the peaks at one minute are due to convection and atmospheric turbulence (Scorer 1992, Vinnichenko 1970)



From now on, we will use a coordinate system with the x axis aligned to the average horizontal wind direction, the y axis perpendicular to it, and the z axis pointing away from the surface. Then, we will use the letters u , v and w to denote the components of the wind along the axes x , y and z respectively; clearly, $\bar{v} = 0$. Eddy fluxes can then be described in terms of covariances: let θ denote the potential temperature,² then $\overline{w'\theta'}$ is the turbulent heat flux, i.e. the sensible heat flux in the vertical due to turbulence. Usually the ABL is studied assuming homogeneous horizontal conditions, because they vary on a length scale larger than the height of the ABL. Because of this, the horizontal eddy correlations $\partial\overline{u'a'}/\partial x$ and $\partial\overline{v'a'}/\partial y$ are usually of negligible intensity, and are thus ignored; this is to say that the vertical fluxes are assumed to be horizontally constant. Note that this is not necessarily true when clouds are involved.

It is important to notice that turbulence is dissipative in nature. Consider a hot Summer day, where air is warmer close to the surface, and a circular eddy moving some air up and some down, so that the average motion is zero. The parcel of air moving up ($w' > 0$) ends up being warmer than its surroundings ($\theta' > 0$), while the one moving down ($w' < 0$) will be colder ($\theta' < 0$); the result is a net transport of heat through the eddy: $\overline{w'\theta'} > 0$. On the contrary, imagine a cold night, where the air close to the surface is colder; the same eddy would transport a colder parcel of air upward, and a warmer one downward. In both cases, the end result would be a

²The potential temperature is final temperature after bringing a parcel of air to a standard pressure adiabatically, i.e. not allowing exchange of temperature with the surroundings. It is a useful mean to compare temperatures irrespectively of pressure, i.e. altitude.

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net transport of heat without transport of mass, since the same mass of air that is moved upwards is also moved downwards. As a result, the eddy must lose energy, and thus dissipate over time.

Since turbulence changes over time, we are more interested in the change of kinetic energy, the *turbulent kinetic energy budget*. A full derivation is out of the scope of this work, but its final form (Högström 1996) can be derived from prime physical principles, resulting in

$$\frac{\partial \overline{e'^2}}{\partial t} = \underbrace{\overline{u'w'} \frac{\partial \bar{u}}{\partial z}}_P - \underbrace{\frac{g}{T} \overline{w'\theta'}}_B + \underbrace{\frac{\partial}{\partial z} \frac{\overline{w'e'^2}}{2}}_{T_t} + \underbrace{\frac{1}{\rho} \frac{\partial p'w'}{\partial z}}_{T_p} + \epsilon \quad (2.2)$$

where $e'^2 = u'^2 + v'^2 + w'^2$. The P term is the production due to shear, B is the production due to buoyancy, T_t is the turbulent transport of TKE by large-scale eddies, T_p is the transport due to pressure, and ϵ is molecular dissipation due to viscosity. P and B are the most prominent terms, and the transport terms are close to zero in neutral conditions (Högström 1996).

The P term is always positive, as energy is taken from the mean flow to the turbulent one (in other words, turbulence can only generate kinetic energy). The contribution from buoyancy B can be either positive or negative, depending on the difference of temperature between a parcel of air moved by the turbulence and the surrounding air. When $\overline{w'\theta'}$ is negative, the turbulence is moving cold air upward and warm air downward; these parcels of air will try to undo the effect of turbulence, thereby increasing the overall kinetic energy. A similar reasoning goes for when the heat flux is positive.

2.2.3 Surface Fluxes

A flux measures the amount of a physical quantity that flows through a surface. In the context of boundary layer meteorology, we are interested in the heat that flows through the surface of earth, because, through it, the surface and the atmosphere exchange energy; the unit of measurement is, therefore, W m^{-2} . The main source of energy for the surface is short-wave radiation coming from the sun, and long-wave radiation coming from the atmosphere and the clouds. A small amount of long-wave radiation is emitted from the surface, therefore let the net radiative flux be R , positive when the surface gains energy.

The main fluxes by which the surface gains or loses energy to the atmosphere are called the turbulent flux of *sensible heat* H , also called kinematic heat flux, and the turbulent flux of *latent heat* λE , also called kinematic flux of water vapor/moisture. The difference between the two is that the former causes an actual change of temperature, whereas the latter does not affect temperature.³ The main

³Imagine a pot of boiling water; selecting a higher temperature on the stove will not increase the temperature of water above 100 °C, but will make it boil faster. The additional heat introduced in the system is dissipated through increased evaporation.

causes of sensible heat fluxes are conduction and convection, whereas the main cause of latent heat fluxes is water movement: condensation, evaporation, melting, etc.

The final flux of interest is the soil heat flux G , which is the heat transferred into or out of the deeper layer of the soil and not given back to the atmosphere. These four fluxes are linked by the surface energy balance equation:

$$R = H + \lambda E + G$$

which states that the total incoming energy R must be equal to the energy given back to the atmosphere $H + \lambda E$ (not counting long-wave radiation, which is accounted to in R) plus the energy absorbed by the surface G , assuming the temperature is constant. When the temperature is not constant, one can write a budget equation relating the changes in these quantities.

The turbulent fluxes H and λE are constant in the surface layer. Experimentally, the energy balance is not always achieved (Bosveld 2018) because of the difficulty in measuring fluxes. Section 3.1.1 talks about their measurement in more detail.

2.2.4 Monin-Obukhov Similarity Theory

One of the quantities of interest is the momentum flux-profile relationship, computed as follows:

$$\frac{\partial \bar{u}}{\partial z} \frac{\kappa z}{u_*} \quad (2.3)$$

where κ is the von Karman constant, which roughly equals 0.4. The profile is expressed by the $\partial \bar{u} / \partial z$ term, and the momentum flux is contained in the friction velocity u_* according its interpretation in equation 2.1.

One of the factors to distinguish laminar from turbulent flow is the length scale L of the system. This length scale for the ABL was derived by Obukhov (1971), and forms the basis of the similarity theory. According to this theory, the normalized wind profile of equation 2.3 can be expressed as an unique *universal* function of $\xi = z/L$, with

$$L = -\frac{u_*^3}{\kappa \frac{g}{\theta_v} \frac{Q}{\rho c_p}} \quad (2.4)$$

where

- $g = 9.81 \text{ m s}^{-2}$ is the acceleration due to Earth's gravity
- θ_v is the virtual temperature,⁴ obtained as

$$\theta_v = \theta \frac{1 + r_v/\epsilon}{1 + r_v} = \theta(1 + 0.61 \cdot q) \quad (2.5)$$

⁴Potential temperature of dry air if it had the same density as moist air. It allows to use formulas for dry air when the air is not dry.

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where θ is the air temperature, r_v is the mixing ratio, $q = r_v/(1 + r_v)$ the specific humidity, and ϵ is the ratio of the gas constants of dry air and water vapor, roughly 0.622.

- Q is the buoyancy flux, approximated by $H + 0.07\lambda E$ and measured in W m^{-2}
- ρ is the air density, computed from the pressure P and the specific gas constant for dry air $R = 287.058 \text{ J kg}^{-1} \text{ K}$ as

$$\rho = \frac{P_0}{RT_v}$$

- c_p is the specific heat of dry air, $1005 \text{ J kg}^{-1} \text{ K}^{-1}$ at 300 K

The stability parameter ξ is positive for stable conditions, where wind shear dominates the production of TKE, and negative for unstable conditions, where buoyancy is the main contributor to turbulence. It approaches 0 in the limit of neutral stratification (i.e. $\partial\bar{\theta}/\partial z = 0$), because the temperature flux goes to 0 causing L go to infinity.

The universal function must be determined experimentally. This is no easy task, and considerable effort has been devoted to it; one of the greatest difficulties lies in obtaining accurate and unbiased measurements, especially the fluxes. Högström (1988) is a meta-study that aggregates and improves many previous results, and suggests the following expressions:

$$\phi_m(\xi) = \begin{cases} (1 - 19.3\xi)^{-1/4} & -2 < \xi < 0 \\ 1 + 6\xi & 0 \leq \xi < 1 \end{cases} \quad (2.6)$$

The Monin-Obukhov similarity theory (MOST) is only applicable in the surface layer, at heights much larger than the aerodynamic roughness length, and with $|\xi| < 2$; intuitively, when $|\xi|$ is too large, the eddies do not feel the effect of the surface anymore. For example, under very stable stratification ($\xi \gg 1$), vertical motion is severely limited, so the height z does not play a role; as a result, the flux-profile relationship does not depend on ξ . Even under ideal conditions, the predictions of this theory are accurate up to 10-20% (Foken 2006). Some works, such as Yaglom (1977), argue that the poor agreement between data and experiments, and even among experiments themselves, can be largely attributed to difficulties in measuring the necessary quantities. Recent attempts, such as (Grachev et al. 2007, Mcnaughton 2006, Wilson 2008, Hatfield et al. 2005), try to extend, improve, or altogether replace, this similarity theory or pars thereof.

2.3 Statistics and Machine Learning

The goal of Machine Learning is to develop algorithms that allow computers to learn from examples. Learning is intended as the ability of inferring general rules from

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the available examples, so that new, previously unseen examples can be correctly characterized. The set of samples from which the computer is supposed to learn is called the *training set*, and each sample is a sequence of numbers describing its attributes, or *features*. There are three approaches in machine learning:

- *Supervised* learning: in this setting, the examples are composed of an input and a desired output, and the goal is to build a model that can correctly predict the output given the input. There are different algorithms depending on the type of output: *regression* algorithms predict continuous output, while *classification* algorithms predict discrete output.
- *Unsupervised* learning: in this setting, no output is available. The task of the algorithm is to figure out hidden relationships between the samples in the training set, for example whether they form clusters, or there are anomalous samples, or the correlation between features of the examples.
- *Reinforcement* learning: in this setting, the computer is free to act in an environment and to observe how the environment responds to its actions. Additionally, it receives a *reward* for every action it takes, and the goal of the computer is to learn a sequence of actions that maximizes the received reward. Reinforcement learning is often applied in control theory Lewis et al. (2012) and game playing (Silver et al. 2017).

A supervised machine learning model uses a set of parameters to compute the output value starting from the input features. The actual parameters values are learned from the training set in a process called *training*. This process is controlled by another set of parameters called hyper-parameters, whose value can be found from the training data as well. Whereas the parameters control the relationship between input and output, hyper-parameters control the "character" of the learning algorithm, such as how eager or conservative it is in learning minute details in the features. Learning too many details can be detrimental, because some differences can be due to noise, rather than actual differences.

In the remaining of this chapter, we describe the theory of learning, justifying the general methodology followed in Machine Learning (section 2.3.1), then we explain how to make sure a model is able to generalize to unseen data (section 2.3.2). Following, we explain how to actually find the optimal values for parameters of a regression model (section 2.3.3) and its hyper-parameters (section 2.3.4), next we introduce four regression models that are used to answer the research questions: Ridge regression (section 2.3.5), k-Nearest Neighbors (section 2.3.6), Gradient Boosted Trees (section 2.3.7) and Gaussian Processes (section 2.3.8). Finally, we describe how several samples can be compared in order to find the one with the smallest, or largest, mean (section 2.3.9).

Notation: Scalars are denoted in *italic*, vectors (always column) and matrices in **bold**. The training set contains N training samples, indexed by n , and each sample

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is a pair of feature vector $\mathbf{x}_n \in \mathbb{R}^D$ and a target value $t_n \in \mathbb{R}$. The feature vectors are grouped in the $N \times D$ matrix $\mathbf{X} = [\mathbf{x}_1 \cdots \mathbf{x}_N]^\top$ and the target values in the $N \times 1$ vector $\mathbf{t} = [t_1, \dots, t_N]^\top$. Models are parametrized by a parameter vector $\boldsymbol{\theta}$ and their output for the feature vector \mathbf{x}_n is $f_n = f(\mathbf{x}_n; \boldsymbol{\theta})$, while the hyper-parameters are contained in the vector $\boldsymbol{\Theta}$.

2.3.1 Learning Theory

The goal of supervised learning is to use the training examples $\mathcal{D} = (\mathbf{X}, \mathbf{t})$, independent and identically distributed according to an unknown distribution p_{XT} , to find a good prediction rule $\hat{f} : \mathcal{X} \rightarrow \mathcal{Y}$ among a family of available functions \mathcal{F} . In most practical cases, $\mathcal{X} = \mathbb{R}^D$ and \mathcal{Y} is either \mathbb{R} for regression or a subset of \mathbb{N} for classification. The goodness of a prediction rule f is measured through a *loss function* $\ell : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ that tells, given a target value t and a guess $y = f(x)$, how much the guess is off. The *risk* of an estimator f is simply its expected loss:

$$R(f) = \mathbb{E}_{(x,t) \sim p_{XT}} [\ell(f(x), t) | f] \quad (2.7)$$

The ideal situation is to find the estimator f^* that has the lowest risk; unfortunately this is not possible, because the distribution p_{XT} is unknown. Since the training data is a sample from this distribution, we can compute the *empirical risk* of f on this set of examples instead:

$$\hat{R}(f) = \mathbb{E}_{(x,t) \sim D} [\ell(f(x), t) | f] = \frac{1}{N} \sum_{n=1}^N \ell(f(x_n), t_n) \quad (2.8)$$

We can now use the empirical risk as a surrogate for the true risk, selecting the estimator

$$\hat{f} = \operatorname{argmin}_{f \in \mathcal{F}} \hat{R}(f) \quad (2.9)$$

as our best guess. This procedure is called *empirical risk minimization*. Note that \hat{f} is a random function, because it depends on \mathcal{D} , which is a random variable. An interesting question to ask is how good \hat{f} actually is, or, in other words, what is its expected true risk $\mathbb{E}[R(\hat{f})]$ and how it compares to the lowest attainable risk $R(f^*)$. This latter quantity can be decomposed as

$$\mathbb{E}[R(\hat{f})] - R(f^*) = \left(\mathbb{E}[R(\hat{f})] - \inf_{f \in \mathcal{F}} R(f) \right) + \left(\inf_{f \in \mathcal{F}} R(f) - R(f^*) \right) \quad (2.10)$$

where the first term is the *estimation* error incurred by not selecting the best possible estimator in \mathcal{F} , and the second term is the *approximation* error caused by searching a good estimator in \mathcal{F} and not somewhere else. They usually have opposite behavior:

- the estimation error is high when \mathcal{F} is too complex for the data at hand, where complexity refers to the range of phenomena that can be accurately modeled

by these functions. In other words, \mathcal{F} contains many valid explanations that are equally good on the training set (they have low empirical risk \hat{R}), but are not accurate models of the underlying phenomenon p_{XT} , i.e. they do not generalize well (they have high risk R);

- the approximation error is high when \mathcal{F} cannot adequately model the phenomenon that we are trying to describe, i.e. when it does not contain any good explanation for it.

This decomposition is often referred to as the *bias-variance decomposition*, where bias and variance refer to, respectively, approximation and estimation error.

A common way of building \mathcal{F} is to fix the form of the models it contains, and allow their behavior to be controlled through a series of *parameters*. Then, equation 2.9 reduces to finding a good set of parameters; this process can also be governed by other parameters, called *hyper-parameters*. The fundamental problem is to find a class of functions that is powerful enough to model p_{XT} , but not too powerful so as to contain too many good explanations, because we would not be able to choose. Equivalently, we want to find a good model, one that can explain the data we have, and generalize to new examples. This problem is known as *model selection*, and is important to distinguish between model selection for *identification*, and model selection for *estimation*. In the former case, the goal is to obtain a model and its parameters, to be used on new prediction problems, whereas the goal of the latter is to obtain a realistic estimate of the performance that can be obtained on new data. This problem can be approached in two ways: by directly estimating approximation and estimation errors using hold-out sets, or by penalizing complex models in order to favor simpler explanations, even though they might have slightly higher empirical risk. The next sections describe these two approaches.

2.3.2 Cross Validation

The idea behind hold-out methods is to partition the available data in two smaller sets D_T and D_V , usually of size 2/3 and 1/3 of the total, and use the *training* set D_T to choose \hat{f} and D_V to estimate its risk. Since \mathcal{D} is assumed to be a representative sample from p_{XT} , if the two partitions contain independent and identically distributed samples, the empirical risk on the *validation set* D_V can give us a glimpse on the generalization power of \hat{f} . This is because the validation set contains new samples that were not used to choose \hat{f} , thus the empirical risk on this set is an unbiased estimate of the true risk of the discovered model. This allows us not only to be confident about the performance of the estimator on unseen data, but also to compare different estimators. The problem of a single hold-out set is the variance of its estimate of the risk, which depends on the size of the validation set. This means that we are faced with a trade-off: use a lot of data to select a good estimator, but have high uncertainty in its estimated performance, or use less data and select a less powerful estimator, but have a more accurate picture of its performance.

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The solution to this problem is to repeatedly perform this partitioning procedure so as to obtain many estimates of the risk, each on a different subset of validation samples, and average these results together. This can be done in a number of different ways:

- In random subsampling, the procedure above is simply repeated many times, by using two thirds random examples for training, and the remaining one third for validation;
- In bootstrapping (Efron & Tibshirani 1993), the training set is created by taking $N = |D|$ examples *with replacement* from \mathcal{D} , and using the remaining examples for validation. This means that the validation set contains on average approximately 36.8% of the samples in \mathcal{D} , and the training set the remaining 63.2%, with many duplicates;
- In k -fold cross validation (Geisser 1975), \mathcal{D} is partitioned in k subsets, and each of them is used in turn as validation set, while the others are used for training. This produces k estimates of the true risk, coming from the k subsets.

Regardless of the method used, the final estimate of the performance is the average of the estimates obtained from the individual trials. Every method has different properties regarding both the bias and the variance of the estimates, and there is considerable controversy on which method should be used in which situation. For example, Kohavi (1995) recommends using 10-fold CV for comparing models, because, although its estimate of the performance is biased, it has lower variance compared to bootstrapping; however, Bengio & Grandvalet (2004) show that it is not possible to obtain an universal unbiased estimate of the variance of k -fold CV. Zhang & Yang (2015) further discusses this issue, and debunks some myths and commonly held misconceptions about CV, including the belief, consequent Kohavi (1995), that 10-fold cross validation is always the best choice. Generally, there is a trade-off in choosing the value of k , as high values yield estimates with lower bias, but higher variance (Arlot et al. 2010), and are more computationally intensive.

Cross validation can be used to perform two distinct tasks: *estimation* and *identification*. The goal of the former is to accurately estimate the best performance attainable on a prediction problem, whereas the goal of the latter is to identify the parameters and hyper-parameters that give rise to the best possible estimators. Consequently, when the goal is estimation we want to eliminate bias, whereas in identification we need low variance. Estimation is best performed with nested CV (Stone 1974, Varma & Simon 2006), in which there is an inner CV loop done on every training fold of the outer CV loop. This procedure is formalized in algorithm 1, where random hyper-parameter search (Bergstra & Bengio 2012) is used in the inner CV loop to find good values for the hyper-parameters. Krstajic et al. (2014) advocates for repeating nested CV, since plain nested CV produces estimates with fairly high variance, but the computational cost of such procedure can be prohibitively high.

Algorithm 1 Nested cross validation with random hyper-parameter search.

Input:

\mathcal{D} Dataset
 K_O Number of outer folds
 K_I Number of inner folds
 R Number of random combinations to try
 $model$ Model to train
 $distrs$ Distribution of each hyper-parameter

Output: Summary statistics computed on each outer validation fold

```

for  $k_o \leftarrow 1 \dots K_O$  do                                 $\triangleright$  Outer  $K_O$ -fold cross validation
    Generate  $k_o$ -th outer fold ( $D_T^o, D_V^o$ ) from the dataset  $\mathcal{D}$ 
     $best\_mse \leftarrow \infty$ 
     $best\_params \leftarrow \perp$ 
    for  $r \leftarrow 1 \dots R$  do                       $\triangleright$  Find best hyper-parameters on  $D_T^o$ 
         $params \leftarrow$  a random hyper-parameter combination from  $distrs$ 
         $params\_mse \leftarrow 0$ 
        for  $k_i \leftarrow 1 \dots K_I$  do           $\triangleright$  Evaluate  $params$  with  $K_I$ -fold CV
            Generate  $k_i$ -th inner fold ( $D_T^i, D_V^i$ ) from  $D_T^o$ 
             $model \leftarrow$  a new instance of the model with parameters  $params$ 
            Train  $model$  on  $D_T^i$ 
             $mse \leftarrow$  result of the evaluation of  $model$  on  $D_V^i$ 
             $params\_mse \leftarrow params\_mse + mse$ 
        end for
        if  $params\_mse < best\_mse$  then       $\triangleright$  Keep best result on inner CV
             $best\_mse \leftarrow params\_mse$ 
             $best\_params \leftarrow params$ 
        end if
    end for
     $model \leftarrow$  a new instance of the model with parameters  $best\_params$ 
    Train  $model$  on  $D_T^o$ 
    Evaluate  $model$  on  $D_V^o$  and compute evaluation metrics
end for
Compute summary of the metrics obtained in the outer loop

```

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2.3.3 Parameter Estimation for Regression

In this section, we describe a general framework, rooted in Bayesian statistics, for estimating the parameters of a regression model, while controlling overfitting. An advantage of Bayesian methods is that they offer a sound theoretical foundation for model selection, without requiring repeated experiments to choose among candidate models, although this mathematical rigor is not free from practical difficulties (Wasserman 2000, Chipman et al. 2001).

A common assumption in the regression setting is that the observations are corrupted by additive Gaussian white noise, i.e. $t_n = y_n + \epsilon_n$, where y_n is the "true" value, and $\epsilon_n \sim \mathcal{N}(0, \beta^{-1})$ is the noise. Let $f_n = f(\mathbf{x}_n; \boldsymbol{\theta})$ be the model's prediction for the sample \mathbf{x}_n , then we can write the probability of observing t_n , assuming that $f_n = y_n$, as:

$$p(t_n | \mathbf{x}_n, \boldsymbol{\theta}, \beta) = \mathcal{N}(t_n | f(\mathbf{x}_n; \boldsymbol{\theta}), \beta^{-1}) \quad (2.11)$$

This probability is called *likelihood* of the observation t_n , under the model $f(\cdot; \cdot)$ with parameters $\boldsymbol{\theta}$. Since the training data is assumed to be independent and identically distributed, the likelihood of the whole training set is

$$p(\mathbf{t} | \mathbf{X}, \boldsymbol{\theta}, \beta) = \prod_{n=1}^N \mathcal{N}(t_n | f(\mathbf{x}_n; \boldsymbol{\theta}), \beta^{-1}) \quad (2.12)$$

and the predicted value t for a new sample \mathbf{x} is distributed as

$$p(t | \mathbf{x}, \mathbf{X}, \mathbf{t}) = \int p(t | \mathbf{x}, \boldsymbol{\theta}, \beta) \cdot p(\boldsymbol{\theta}, \beta | \mathbf{t}, \mathbf{X}) d\boldsymbol{\theta} d\beta \quad (2.13)$$

In practice, it is not feasible to compute this integral, and its value is dominated by the values of $\boldsymbol{\theta}$ and β close to the one that maximizes equation 2.12 anyways; this is the gist of *maximum likelihood estimation* (MLE). Note that, since the goal is to predict y_n , there is a high probability that the "true" parameters would *not* be the ones with maximum likelihood. When a model learns the noise in the training data, it cannot generalize well to new, unseen data, because the noise is random. This situation is known as *overfitting*, and tends to happen when the model is too complex relative to the amount of data available for training, and is related to high estimation error mentioned previously.

The risk of overfitting can be reduced with a number of *regularization* strategies. A widely used strategy consists in including a prior distribution on the parameters of the model, and maximizing their posterior distribution, computed using Bayes theorem:

$$\begin{aligned} p(\boldsymbol{\theta} | \mathbf{t}, \mathbf{X}) &= \frac{p(\mathbf{X}, \mathbf{t} | \boldsymbol{\theta}) \cdot p(\boldsymbol{\theta})}{p(\mathbf{X}, \mathbf{t})} \\ &\propto p(\mathbf{t} | \mathbf{X}, \boldsymbol{\theta}) \cdot p(\mathbf{X} | \boldsymbol{\theta}) \cdot p(\boldsymbol{\theta}) \\ &\propto p(\mathbf{t} | \mathbf{X}, \boldsymbol{\theta}) \cdot p(\boldsymbol{\theta}) \end{aligned} \quad (2.14)$$

where we removed $p(\mathbf{X}, \mathbf{t})$ and $p(\mathbf{X}|\boldsymbol{\theta}) = p(\mathbf{X})$ because they are constant for a given dataset, and we are not interested in the exact probability, but where it reaches its maximum value. This parameter estimation procedure is called *maximum a posteriori* (MAP). Two commonly used prior distributions are the multivariate Laplace and the multivariate Normal, leading respectively to L1 and L2 regularization, when centered and symmetrical/spherical. Note that MAP reduces to MLE when we assume an uniform prior $p(\boldsymbol{\theta})$.

The maximization of the posterior can be done conveniently by maximizing its logarithm; this gives expressions that are easier to handle analytically, and give less numerical problems when computed. The MAP problem can be formulated as follows:

$$\boldsymbol{\theta}^* = \operatorname{argmax}_{\boldsymbol{\theta}} \log p(\mathbf{t}|\mathbf{X}, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta}) \quad (2.15)$$

If we assume a Gaussian likelihood like the one in equation 2.12, and a spherical Gaussian prior distribution $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, \lambda \mathbf{I})$, the MAP estimation of equation 2.15 becomes, after removing unnecessary constant terms,⁵

$$\boldsymbol{\theta}^* = \operatorname{argmin}_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) = \operatorname{argmin}_{\boldsymbol{\theta}} \sum_{n=1}^N (f(\mathbf{x}_n, \boldsymbol{\theta}) - t_n)^2 + \lambda \boldsymbol{\theta}^\top \boldsymbol{\theta} \quad (2.16)$$

where L is the *loss function*, in this case the sum-of-squares error. It is customary to use the mean squared error instead of the sum of squares because it results in smaller numbers and is readily interpreted; being only a constant factor away from 2.16, it does not transcend the essence of MAP estimation. Note that we assumed the hyper-parameter λ to be fixed, but a fully Bayesian treatment would allow its estimation, too, by introducing a *hyper-prior* distribution for it. To avoid an endless chain of priors, the hyper-prior is assumed to be *non-informative*, e.g. uniform. Designing good hyper-priors and their philosophical consequences is a fascinating topic by itself, but out of scope for this thesis, see Syversveen (1998) for an introduction.

Depending on the model $f(\cdot; \cdot)$, 2.16 can be solved analytically to yield a closed-form solution for $\boldsymbol{\theta}$. When this is not possible, iterative optimization methods are employed. A widely used approach is called *gradient descent*: the gradient of a function computed at a given location "points" to the steepest direction where the function's value increases. By repeatedly following the gradient, it is possible to reach a local maximum, or, in the opposite direction, a local minimum:

$$\boldsymbol{\theta}_{n+1} := \boldsymbol{\theta}_n - \eta \cdot \nabla f(\mathbf{x}_n) \quad (2.17)$$

The series $\boldsymbol{\theta}_1, \dots, \boldsymbol{\theta}_n$ is guaranteed to converge to the local optimum at a rate of $O(n^{-1})$ if certain conditions are met (Gitman et al. 2018). Nocedal & Wright

⁵These terms depend on β , but do not contain $\boldsymbol{\theta}$. Obviously, they should be included if one is interested in finding the optimal value of β .

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(1999) describes more advanced optimization techniques that use the gradient and, possibly, the Hessian, such as Newton's. The gradient of $L(\boldsymbol{\theta})$ is

$$\nabla_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta} | \mathbf{t}, \mathbf{X}) = 2 \sum_{n=1}^N (f(\mathbf{x}_n; \boldsymbol{\theta}) - t_n) \cdot \nabla_{\boldsymbol{\theta}} f(\mathbf{x}_n; \boldsymbol{\theta}) + 2\lambda \boldsymbol{\theta} \quad (2.18)$$

and its Hessian is

$$\begin{aligned} \nabla_{\boldsymbol{\theta}}^2 \log p(\boldsymbol{\theta} | \mathbf{t}, \mathbf{X}) &= 2 \sum_{n=1}^N \left[(\nabla_{\boldsymbol{\theta}} f(\mathbf{x}_n; \boldsymbol{\theta})) (\nabla_{\boldsymbol{\theta}} f(\mathbf{x}_n; \boldsymbol{\theta}))^\top \right. \\ &\quad \left. + (f(\mathbf{x}_n; \boldsymbol{\theta}) - t_n) \nabla_{\boldsymbol{\theta}}^2 f(\mathbf{x}_n; \boldsymbol{\theta}) \right] + 2\lambda \mathbf{I} \end{aligned} \quad (2.19)$$

In some cases, the gradient and the Hessian can be approximated using a random subset of the training set, and, in extreme cases, a single sample. These variants are called *minibatch* gradient descent and *stochastic* gradient descent respectively. They both compute a noisy approximation to the true gradient, which can actually improve convergence and generalization of high-dimensional, non-convex loss functions such as those found in deep learning (Neelakantan et al. 2015, Smith & Le 2017). Vanilla gradient descent can be greatly improved with a number of techniques, such as momentum (Rumelhart et al. 1986), adaptive learning rate (Duchi et al. 2011, Zeiler 2012, Kingma & Ba 2014), and so on, see Ruder (2016) for an overview.

2.3.4 Hyper-parameters Optimization

The previous section discussed some methods to find the best parameters for a model. The behavior of most models, though, is governed by other *hyper-parameters*, such as λ in equation 2.16. In practice, finding good values for the hyper-parameters is often as important as fitting the model, since these hyper-parameters often control the learning process itself. As mentioned in section 2.3.3, one possibility is to introduce a non-informative hyper-prior for the hyper-parameters, such that the hyper-prior does not have parameters itself, or is invariant to their values; this road is only followed by the brave, though. The others are left with simpler approaches.

An unsophisticated solution to this problem is to choose some possible values for each hyper-parameter, try all the possible combinations, and pick the one that works best. Alternatively, one can sample each hyper-parameter from a probability distribution, and try many random combinations of values; Bergstra & Bengio (2012) showed that this latter method is surprisingly effective at this task, and scales much better than the former. Unfortunately, this procedure can overfit, too, so it has to be paired with some resampling technique such as cross validation. The procedure is simply to test every hyper-parameter combination on every fold, so that 50 combinations tested with 10-fold cross validation require to fit the model 500 times.

More sophisticated techniques treat hyper-parameter optimization as a regression problem, and use supervised machine learning to predict the performance of a given hyper-parameter combination, and to guide the search accordingly (Bergstra et al. 2011). Clearly, one should use models that are not sensitive to their own hyper-parameter setting, or the problem is just moved! For this reason, popular algorithms that are used for this are evolutionary algorithms and Bayesian non-parametric models.

2.3.5 Ridge Regression

A linear regression model has the form $f(\mathbf{x}_n; \boldsymbol{\theta}) = \boldsymbol{\theta}^\top \mathbf{x}_n$; ridge regression is simply L2-regularized linear regression. This model is simple enough that the solution for equation 2.16 can be found analytically in closed form:

$$\boldsymbol{\theta}^* = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^\top \mathbf{t} \quad (2.20)$$

Notice that the term *linear* in linear regression refers to linearity with respect to the parameters, not the features. In fact, new features can be added through the use of a possibly non-linear feature mapping $\phi : \mathbb{R}^D \rightarrow \mathbb{R}^M$, such that $\mathbf{x}'_n = \phi(\mathbf{x}_n)^\top = [\phi_1(\mathbf{x}_n), \dots, \phi_M(\mathbf{x}_n)]^\top$. Then, the model parameters can be fitted to the augmented training set $\Phi = \mathbf{X}'$, where Φ is called the *design matrix*. A typical feature added is a bias $\phi_1(\mathbf{x}) = 1$.

2.3.6 k-Nearest Neighbors

The k-Nearest Neighbor model (Stone 1977) predicts a value for a sample \mathbf{x} by averaging the target values of the K training samples that are closest to \mathbf{x} , possibly weighted by distance or some other metric. Let $\mathbf{t}_{(1)}, \dots, \mathbf{t}_{(K)}$ be the target values of the K training samples closest to \mathbf{x} according to a distance metric $d : \mathbb{R}^D \rightarrow \mathbb{R}$, then we have

$$f(\mathbf{x}) = \sum_{k=1}^K w_{(k)} \cdot \mathbf{t}_{(k)} \quad (2.21)$$

Note that the kNN algorithm does not have parameters, only hyper-parameters: K itself, the distance function, and the weighting scheme. Typical distance functions are the Manhattan distance $d(\mathbf{u}, \mathbf{v}) = \sum_{d=1}^D |u_d - v_d|$ and the squared Euclidean distance $d(\mathbf{u}, \mathbf{v}) = \sum_{d=1}^D (u_d - v_d)^2$, and typical weights are uniform $w_{(k)} = 1/K$ and based on distance $w_{(k)} = d(\mathbf{x}, \mathbf{x}_{(k)}) / \sum_{k'=1}^K d(\mathbf{x}, \mathbf{x}_{(k')})$.

2.3.7 Gradient Boosted Trees

Gradient boosting (Breiman 1997) is a general method of combining several weak predictors in order to obtain a stronger one. The final prediction for a sample is obtained as a weighted average of the predictions of the individual models:

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$$f_M(\mathbf{x}) = \sum_{m=1}^M \beta_m h(\mathbf{x}; \boldsymbol{\theta}_m) \quad (2.22)$$

Each model parameters $\boldsymbol{\theta}_m$ and the weight β_m are found by improving the predictions of f_{m-1} :

$$(\beta_m, \boldsymbol{\theta}_m) = \underset{\boldsymbol{\theta}, \beta}{\operatorname{argmin}} \sum_{n=1}^N L(t_n, f_{m-1}(\mathbf{x}_n) + \beta h(\mathbf{x}_n, \boldsymbol{\theta})) \quad (2.23)$$

where L is the loss function, such as the squared error loss introduced previously. This optimization problem can be challenging, depending on the specific form of h and L . Actually, equation 2.23 is equivalent to gradient descent in function space⁶ (Mason et al. 1999, Friedman 2001). This gradient can be computed explicitly on the N training points, but we do not know how to compute it on the other points that are not in the training set.⁷ The fundamental idea is to find a model that can predict this gradient, by training it on the dataset. This model is exactly h with parameters $\boldsymbol{\theta}_m$:

$$\boldsymbol{\theta}_m = \underset{\boldsymbol{\theta}}{\operatorname{argmin}} \sum_{n=1}^N [-g_m(\mathbf{x}_n) - h(\mathbf{x}_n, \boldsymbol{\theta})]^2 \quad (2.24)$$

with g_m being the gradient of L with respect to f_{m-1} :

$$g_m(\mathbf{x}_n) = \frac{\partial L(t_n, f_{m-1}(\mathbf{x}_n))}{\partial f_{m-1}(\mathbf{x}_n)} \quad (2.25)$$

Then, the step size β_m is obtained by line search, i.e. minimizing the loss function in the direction of the gradient:

$$\beta_m = \underset{\beta}{\operatorname{argmin}} \sum_{n=1}^N L(t_n, \beta h(\mathbf{x}_n, \boldsymbol{\theta}_m)) \quad (2.26)$$

This is now a tractable problem, since 2.25 can be computed easily, and both 2.24 and 2.26 are simple regression problems.

If $L(y_n, t_n) = (y_n - t_n)^2/2$, we have that $-g_m(\mathbf{x}_n) = f_{m-1}(\mathbf{x}_n) - t_n$, or, in other words, we are creating a new model by counteracting the errors of the current model! Other popular loss functions are the least absolute deviation, $L(y_n, t_n) = |y_n - t_n|$, in which case $-g_m = \operatorname{sign}(t_n - f_{m-1}(\mathbf{x}_n))$, and the Huber loss:

$$L_\delta(t_n, y_n) = \begin{cases} \frac{1}{2}(y_n - t_n)^2 & |y_n - t_n| \leq \delta \\ \delta(|y_n - t_n| - \frac{1}{2}\delta) & |y_n - t_n| > \delta \end{cases} \quad (2.27)$$

⁶This means that you actually modify the function itself, not its parameters, as we did in section 2.3.3. This is true provided that the parametric function h is able to represent the gradient.

⁷This is the essence of gradient descent in function space, since a function is defined for every point (at least the functions we consider in Machine Learning are).

which is robust to outliers as least absolute deviation, but does not penalize small errors too much, like least squares. In this case,

$$-g_m(\mathbf{x}_n) = \begin{cases} t_n - y_n & |t_n - y_n| \leq \delta \\ \delta \cdot \text{sign}(t_n - y_n) & |t_n - y_n| > \delta \end{cases} \quad (2.28)$$

In summary, the gradient boosting algorithm starts with a simple prediction f_0 , such as the average of the true values, builds a model of the form in equation 2.22 by iteratively applying equations 2.24 and 2.26.

A popular choice is to use decision trees for h . Often, an additional *learning rate* parameter is introduced to shrink the β coefficients. Other hyper-parameters for this algorithm are M , the number of boosting steps to perform, the number of examples to use to compute equations 2.24 and 2.26, the number of features used to build the trees, their maximum depth, and so on.

A popular extension to vanilla gradient boosting is *extreme gradient boosting* (Chen & Guestrin 2016), which essentially adds both L1 and L2 regularization to the loss function, helping to reduce overfitting, and provides better scalability, and a more recent option is LightGBM (Ke et al. 2017), that further improves scalability by carefully selecting which samples and features to use for building each tree.

2.3.8 Gaussian Processes

A Gaussian Process (GP) is a collection of an infinite number of random variables, such that the joint distribution of any finite subset of them is Gaussian. Intuitively, this allows us to define a distribution over functions, since there is a random variable for every point of the input space. We can sample a function out of a GP by obtaining the random variables at the points of interest; their distribution is a (multivariate) Gaussian, with a certain mean and covariance, and a sample from this distribution contains the values of the sampled function at the points we queried. This process is expressed as follows:

$$p(\mathbf{y}|\mathbf{X}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{X})d\mathbf{f} \quad (2.29)$$

where \mathbf{X} are the query points, \mathbf{f} a function sampled from the GP, and \mathbf{y} the value of the function at the query points. By definition of GP, all the distributions in equation 2.29 are Gaussian, since the Gaussian distribution is self-conjugate.⁸ Simplistically, a GP is just a way of computing the mean and covariance of \mathbf{f} given \mathbf{X} , i.e. $p(\mathbf{f}|\mathbf{X})$; \mathbf{f} is then a multivariate Gaussian, which we can manipulate as usual.

Consider the setting of ridge regression described in section 2.3.5, where $\mathbf{y} = f(\mathbf{X}; \boldsymbol{\theta}) = \Phi\boldsymbol{\theta}$, with Φ being the design matrix. Recall that in section 2.3.3 we

⁸Referring to equation 2.14, the prior is said to be conjugate to the likelihood if the posterior has the same algebraic form of the prior; the Gaussian distribution is self-conjugate, because a Gaussian prior with a Gaussian likelihood results in a Gaussian posterior. Conjugate distributions are mostly used for algebraic convenience.

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introduced the Maximum A Posteriori estimation method by using a prior distribution on the model parameters $\boldsymbol{\theta}$; this makes \mathbf{y} a random variable itself. If we use an isotropic Gaussian for $\boldsymbol{\theta}$, we have that the distribution of \mathbf{y} is again Gaussian with mean

$$\mathbb{E}[\mathbf{y}] = \mathbb{E}[\Phi\boldsymbol{\theta}] = \Phi\mathbb{E}[\boldsymbol{\theta}] = \mathbf{0} \quad (2.30)$$

and covariance

$$\text{cov}[\mathbf{y}] = \mathbb{E}[\mathbf{y}\mathbf{y}^\top] = \Phi^\top\mathbb{E}[\boldsymbol{\theta}^\top\boldsymbol{\theta}]\Phi = \alpha^{-1}\Phi^\top\Phi = \mathbf{K} \quad (2.31)$$

where α is the precision of the prior on $\boldsymbol{\theta}$. This is a simple GP with zero mean, and whose covariance between any two points can be computed as the dot product of their features.

In general, we can use any function k to compute the covariance between two input points, as long as the resulting matrix \mathbf{K} , with $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$ is symmetric and positive semi-definite.⁹ We call any such function *kernel*, a function $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ that, intuitively, expresses the similarity of any two input vectors. Mercer's theorem guarantees that for every symmetric positive-definite kernel there exists a basis function ϕ , such that the kernel corresponds to the dot product in the space generated by ϕ . In practice, this means that we do not have to explicitly define ϕ , and that we can even use basis functions that create an infinite dimensional space. Commonly used kernels are the radial basis function kernel:

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\sigma^2}\right) \quad (2.32)$$

where $\|\mathbf{x} - \mathbf{x}'\|^2 = \sum_d (\mathbf{x}_d - \mathbf{x}'_d)^2$ is the squared Euclidean distance, and which incidentally corresponds to an infinite dimensional basis function, and the linear kernel:

$$k(\mathbf{x}, \mathbf{x}') = \sigma^2 \mathbf{x}^\top \mathbf{x}' \quad (2.33)$$

Furthermore, certain operations on a kernel generate another valid kernel, and kernels can be combined in certain ways to produce new kernels. For example, the product of a kernel with a positive constant is a valid kernel, the sum and product of two kernels are valid kernels, etc. Generally, a kernel can have parameters, which we denote, as usual, as $\boldsymbol{\theta}$.

In order to use a Gaussian Process for inference (in the regression setting), we need to compute the predictive distribution $p(\mathbf{y}|\mathbf{X}, \mathbf{t}, \mathbf{X}^*, \boldsymbol{\theta})$, where \mathbf{X}^* is the matrix containing the vectors for which we want to predict the value \mathbf{y} . We know that the predictive distribution is Gaussian, therefore its mean $\boldsymbol{\mu}_{\mathbf{y}}$ and covariance $\boldsymbol{\Sigma}_{\mathbf{y}}$ can be obtained relatively easily, resulting in:

⁹This means that $\mathbf{K}^\top = \mathbf{K}$ and $\mathbf{v}^\top \mathbf{K} \mathbf{v} \geq 0$ for any \mathbf{X} (used to compute \mathbf{K}) and \mathbf{v} . This condition is necessary for \mathbf{K} to be a valid covariance matrix.

$$\boldsymbol{\mu}_y = K_{\theta}(\mathbf{X}^*, \mathbf{X}) K_{\theta}(\mathbf{X}, \mathbf{X})^{-1} \mathbf{t} \quad (2.34)$$

$$\boldsymbol{\Sigma}_y = K_{\theta}(\mathbf{X}^*, \mathbf{X}^*) - K_{\theta}(\mathbf{X}^*, \mathbf{X})^T K_{\theta}(\mathbf{X}, \mathbf{X})^{-1} K_{\theta}(\mathbf{X}, \mathbf{X}^*) \quad (2.35)$$

where $K_{\theta}(\mathbf{A}, \mathbf{B})$ is a matrix whose (i, j) cell equals to $k(A_i, B_j; \theta)$. From these formulas, note that in order to use GPs, one needs to remember the kernel matrix, of size N^2 and invert it, an operation which has a computational complexity of $O(N^3)$; this makes GPs, and any method based on kernels, hard to scale up.

Up until now, we assumed the kernel was fixed, and treated θ as hyper-parameters. We could use one of the cross validation methods described in section 2.3.2 to find their values, but the Bayesian framework that we used to derive GP allows us to find θ , too, by maximizing $\log p(\mathbf{t} | \mathbf{X}, \theta)$ ¹⁰ with respect to θ . This function often has many local maxima, and is usually optimized by means of gradient descent.

Finally, the derivative of a GP is itself a GP, whose mean is obtained simply by deriving equation 2.34 (McHutchon 2013):

$$\frac{\partial \mathbf{y}}{\partial \mathbf{X}_*} = \frac{\partial K_{\theta}(\mathbf{X}_*, \mathbf{X})}{\partial \mathbf{X}_*} K_{\theta}(\mathbf{X}, \mathbf{X})^{-1} \mathbf{t} \quad (2.36)$$

We invite the reader to refer to (Bishop 2006, Chapter 6) for an in-depth treatment of kernel methods, including Gaussian Processes.

2.3.9 Robust Effect Size

The effect size is a statistic used to compare the means of two populations, usually called *control* and *treatment*, that is computed as the standardized difference of the means:

$$\delta = \frac{\mu_t - \mu_c}{\sigma} \quad (2.37)$$

where μ_t and μ_c are the means of the treatment and control groups respectively, and σ is a normalizer that can be computed in essentially three ways: when the standard deviations of the control and treatment populations can be assumed to be equal, then σ should be the pooled standard deviation,¹¹ otherwise it should be the standard deviation of either the control or treatment group. Generally, the effect size is computed to be positive when the treatment group represent an improvement over the control group.

Recently, there is a departure from the standard procedure of reporting p-values, test statistics and critical values resulting from hypothesis testing towards reporting effect sizes and their confidence intervals, in addition or in alternative to the usual statistics, see for example Wilkinson (1999) and *Standards for Reporting on*

¹⁰Obtained as in equation 2.29, usually called log-marginal-likelihood, since we marginalized \mathbf{f} .

¹¹The average standard deviation of the control and treatment groups, weighted by the degrees of freedom (one less than the number of observations) of each group.

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Empirical Social Science Research in AERA Publications (2006). However, effect sizes can be as misleading as significance testing when the assumptions underlying its expression are violated; commonly used effect size measures, such as Cohen's d (Cohen 1988), assume both populations are normally distributed and have the same standard deviation.¹² Alternatives that do not assume equal standard deviation exist (Shieh 2013, Algina et al. 2006, Bonett 2008), but they all require normality, and generally use approximate distributions of the standard error and/or the CI (or both).

In order not to assume normality, we compute the CI for the effect size using the bootstrap percentile method. This method estimates the population value of any statistic θ and its CI using a single sample of N observations, by extracting M new samples (with replacement) of size N from it and computing θ on each resample. The population statistic is estimated by the average of the M sample statistics, and the extremes of the (central) $100(1 - \alpha)\%$ CI are respectively the $100(\alpha/2)$ and $100(1 - \alpha/2)$ percentiles of those values. Usually M is in the order of 10^2 or 10^3 , enough to guarantee a certain degree of stability in these estimates.

The sample effect size of equation 2.37 is not robust to outliers when it is computed with the sample means and standard deviations. Since we do not assume normality outliers are expected, therefore we use measures of location that are not heavily affected by them: the sample trimmed mean and the sample Winsorized standard error. The $100\gamma\%$ trimmed mean \bar{X}_γ of a sample X_1, \dots, X_N is simply the mean of that sample after discarding the $100\gamma\%$ largest and the $100\gamma\%$ smallest observations;¹³ a common value for γ is 0.2. The standard error of the sample trimmed mean is obtained from the Winsorized sample standard deviation; let $X_{(\gamma)}$ and $X_{(1-\gamma)}$ be the 100γ and $100(1 - \gamma)$ percentiles, and define the Winsorized observations as follows:

$$W_n = \begin{cases} X_{(\gamma)} & \text{if } X_n \leq X_{(\gamma)} \\ X_{(1-\gamma)} & \text{if } X_n \geq X_{(1-\gamma)} \\ X_n & \text{otherwise} \end{cases} \quad (2.38)$$

then we have the Winsorized sample mean

$$\bar{X}_W = \frac{1}{N} \sum_{n=1}^N W_n \quad (2.39)$$

the Winsorized sample variance

$$\hat{\sigma}_W^2 = \frac{1}{N-1} \sum_{n=1}^N (W_n - \bar{X}_W)^2 \quad (2.40)$$

and the estimated variance of the trimmed mean

¹²A property called *homoscedasticity* (contrary: heteroscedasticity).

¹³This is common practice, for example, when scoring in sports such as the modern Olympiads, where the smallest and largest scores are discarded.

CHAPTER 2. BACKGROUND

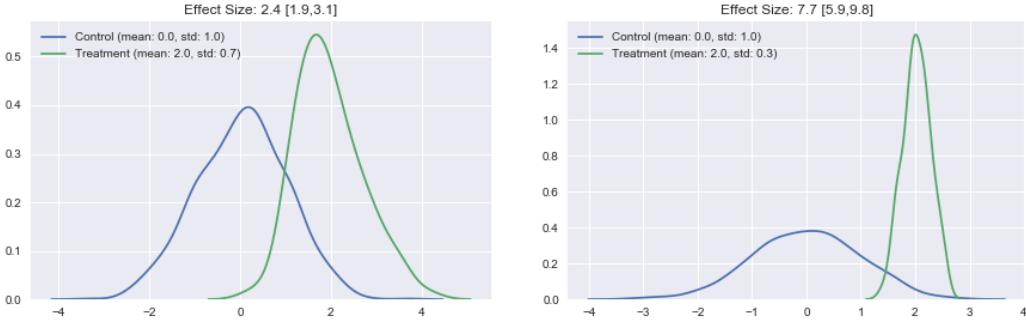


Figure 2.4: Graphical explanation of why the effect size is normalized with the standard deviation of the treatment, when the control has a mean of 0 and standard deviation of 1 and the treatment has a mean of 2; inarguably, the treatment in the right figure the best of the two. Of course, one could perform the same experiment but keeping the treatment fixed and varying the standard deviation of the control: in that case, the effect size would not change. Refer to the main text for a discussion.

$$\text{Var}[\bar{X}_\gamma] = \frac{\hat{\sigma}_W^2}{N(1-2\gamma)^2} \quad (2.41)$$

The standard error of \bar{X}_γ is the usual $(\text{Var}[\bar{X}_\gamma]/N)^{1/2}$. Plugging everything into equation 2.37 and normalizing with the treatment Winsorized sample standard error gives the sample effect size

$$\hat{\delta} = (\bar{T}_\gamma - \bar{C}_\gamma) \cdot \sqrt{\frac{N}{\text{Var}[\bar{T}_\gamma]}} = (1-2\gamma) \frac{\bar{T}_\gamma - \bar{C}_\gamma}{\hat{\sigma}_W} \quad (2.42)$$

where T_1, \dots, T_N and C_1, \dots, C_M are the *independent* samples of treatment and control groups respectively. See Wilcox & Keselman (2003) and Wilcox (2010) for an introduction to robust statistical methods, including the ones just described.

Figure 2.4 shows the effect size computed according to 2.42, and tries to provide an intuitive explanation as to why we normalize with the treatment standard deviation. Note that we cannot use an average (weighted or unweighted) as normalizer since it corresponds to assuming homogeneity of *population* variances, an assumption that we wanted to avoid in the first place. Since the goal is to assess the improvement caused by the treatment, it would not make sense to normalize with the standard deviation of the control group, because it would not allow us to discriminate between treatments with the same mean but different standard deviations: given two treatments with the same mean, we prefer the one with the smaller standard deviation. Of course, this reasoning can be applied in the opposite direction: normalizing by the control standard deviation would give a larger effect size when the control group has a smaller standard deviation, which is certainly a

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desirable property, since a control group with a smaller standard deviation is more clearly separated from the treatment. However, we consider the control group to be fixed, and we will never need to compare two control groups against the same treatment.

Chapter 3

Method

This chapter describes how the data is collected (section 3.1) and used to re-create the flux-profile relationships (section 3.2), as well as their prediction based on the Monin-Obukhov similarity theory (section 3.3). Then, we describe the main contribution of this thesis, namely how their prediction can be improved using machine learning techniques (section 3.4). Finally, we describe how the evaluation is performed (section 3.5), and explicitly state the necessary criteria for a successful answer to the research questions (section 3.6).

3.1 Data Collection and Preparation

The Cabauw Experimental Site for Atmospheric Research¹ (Cesar) is a consortium formed by eight Dutch institutes and universities, which collaborate to operate and maintain an observatory for micro-meteorological conditions near the village of Cabauw, the Netherlands. The data collected characterizes the state of the atmosphere and the soil, and their interaction via radiation and surface fluxes.

The observatory is surrounded by fields and no urban agglomerations is present within 15 kilometers; the land is flat with changes of altitude within a few meters over 20 kilometers. The main mast, is 213 meters high and offers measurement levels every 20 meters (see figure 3.1); at each level there are three booms of length 10 meters that allow observations as unobstructed by the main mast as possible, although some disturbance remains. There are three additional smaller masts of height 10 and 20 meters located close to the main mast, in order to obtain undisturbed measurements at the lower levels, and facilities to perform soil and surface observations.

The main focus of this project is on the wind profile and the turbulent fluxes of sensible and latent heat. Additional variables, such as temperature and humidity, are needed to compute quantities of interest, most importantly the Obukhov length, and as possible predictors for the universal functions. There is one measurement for each variable every ten minutes, and missing measurements are gap-filled with

¹<http://www.cesar-database.nl/>

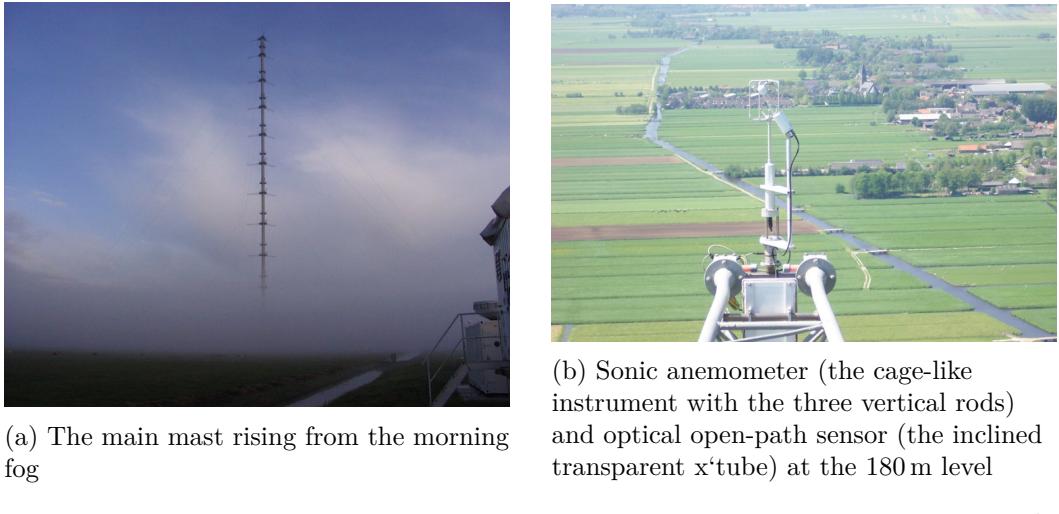


Figure 3.1: The Cabauw main mast (3.1a, from the Cesar Observatory website²) and some measurement instruments it supports (3.1b, from the KNMI website³)

a number of techniques. The data collected is always visually validated by an operator, which marks suspect or invalid sections of data.

Following, we describe the instruments used to collect the measurements (section 3.1.1), the techniques used to impute missing or invalid measurements (section 3.1.2), and the criteria applied to filter low quality data (section 3.1.3).

3.1.1 Measurement

The Cesar observatory provides full information regarding data collection,⁴ see in particular Bosveld (2018), what follows is a brief summary of the sections in that document that are relevant for this work.

Wind Speed Measurement

Wind speed and direction are measured at heights of 200, 140, 80, 40, 20 and 10 meters, in either two or all three booms available. The wind vane that measures direction has a resolution of 1.5° , and the cup anemometer that measures wind speed has an accuracy of the largest between 1% and 0.1 m s^{-1} . Monna (1978) studied the threshold sensitivity of both instruments, and found it lower than 0.5 m s^{-1} , even though the measurements are inaccurate up to 3 m s^{-1} .

For every ten minutes interval, the measurement comes from the instrument that is best exposed to the wind, and less affected by the obstruction caused by the

⁴<http://projects.knmi.nl/cabauw/insitu/observations/documentation>

3.1. DATA COLLECTION AND PREPARATION

mast. Corrections are then applied to the raw measurements to further attenuate the disturbance by the tower, following Wessels (1983).

Eddy Correlation

The eddy correlation technique is used to compute the turbulent surface fluxes of sensible and latent heat H and λE , as well as the momentum flux, starting from fluctuations in wind, temperature, humidity, and CO_2 content.

These measurements are obtained with a sonic anemometer and an optical open-path sensor, shown in figure 3.2. Sonic anemometers measure the wind speed by leveraging the fact that the speed of sound in free air is affected by the speed of the air itself; since the speed of sound is known, the wind speed can be easily recovered from the time a sound impulse takes to travel a short distance. By measuring the wind velocity along three orthogonal paths, the full wind vector can be recovered. This measure can then be used to compute the temperature, by leveraging the fact that the speed of sound is affected by the temperature of the medium it travels in. Optical open-path sensors quantify the amount of water vapor and carbon dioxide in the air by emitting a ray of infrared light and measuring its intensity 10 to 20 centimeters further. H_2O and CO_2 molecules in the air absorb electromagnetic radiation at known frequencies, thus the concentration of water vapor and carbon dioxide can be inferred by measuring the attenuation at these wavelengths.

All these instruments can take up to 100 measurements per second, necessary in order to compute the turbulence. The eddy correlation technique measures fluxes by computing their sample covariance with the vertical wind speed. Let w_t be the vertical wind speed at time t , then the turbulent vertical flux for the quantity a is computed as follows:

$$F_a = \frac{1}{T_2 - T_1} \sum_{t=T_1}^{T_2} (w_t - \bar{w})(a_t - \bar{a})$$

where \bar{w} and \bar{a} are the averages of w_t and a_t for $T_1 \leq t \leq T_2$. The fluxes in the Cesar database are computed every ten minutes, with 10 measurements per second.

The eddy correlation technique is far from perfect, and is known to be imprecise especially in stable conditions, see e.g. Lee et al. (2004), Loescher et al. (2006), de Roode et al. (2010) etc.

Air Temperature and Dew Point Measurement

Both air temperature and dew point⁵ are measured at heights of 200, 140, 80, 40, 20, 10 and 1.5 meters, and the dew point is computed from the air temperature and the humidity obtained with the open-path sensor described previously. The instruments at the highest four levels are located on the main tower, whereas 20

⁴<http://www.cesar-observatory.nl/>

⁴<https://www.knmi.nl/research>

⁵The temperature the air needs to be to reach a relative humidity of 100%.

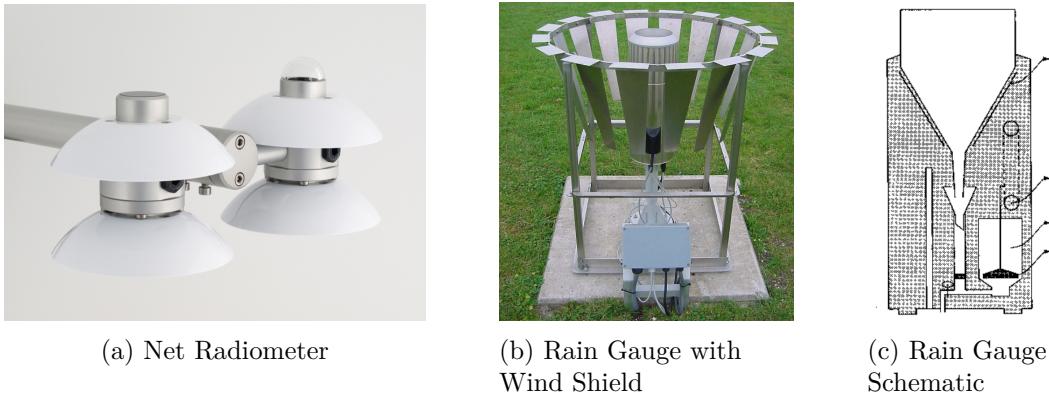


Figure 3.2: Some instruments used at the Cabauw observatory. Credits: picture a - Wikimedia Commons⁶, picture b - Wauben (2004), picture c - Babington (2000).

and 10 meters are measured in the smaller mast, and 1.5 meters is measured by the weather station. The resolution of the instruments is of $0.1\text{ }^{\circ}\text{C}$, whereas the accuracy is $0.1\text{ }^{\circ}\text{C}$ for temperature and 3.5% of relative humidity for the dew point (1.5% after 2014). Low wind speed and high irradiation can result in a few $0.1\text{ }^{\circ}\text{C}$ overestimate of the temperature (Meijer 2000), whereas the humidity can be over estimated when drying after dew, fog, or rain (Bosveld 2018).

Net Radiation Measurement

The Cabauw observatory measures both incoming and outgoing long- and short-wave radiation, and the net radiation is simply the combination of these four components. The basic operating principle of an instrument that measures radiation is to have a device coated with paint that is highly absorbing towards a certain range of frequencies; the temperature difference between the surface of this sensor and the body of the whole instrument generates an electrical potential that is proportional to the radiation absorbed by the sensor, after appropriate corrections. The instruments that measure short-wave radiation are called *pyranometers*, while long-wave radiation is measured by *pyrgeometer*. The instrument used to measure the net radiation has a pair of pyrgeometers, one facing up and one facing down, to measure the net long-wave radiation, and a pair of pyranometers arranged similarly to measure net short-wave radiation (see figure 3.2a).

This instrument is positioned at 1.5 m height, and is ventilated and heated to prevent formation of dew, that can make the measurements invalid.

Surface Soil Heat Flux

The surface soil heat flux, measured in W m^{-2} , is extrapolated from the average fluxes measured at depths of 5 cm and 10 cm; under the assumption of homogeneous

⁶https://en.wikipedia.org/wiki/File:Hukseflux_netto_radiometer_nr01_photo.jpg

3.1. DATA COLLECTION AND PREPARATION

soil, the amplitude of the flux in the frequency domain decays exponentially with depth. In order to increase the temporal resolution, the amplitude of the surface soil heat flux is then related to the amplitude of the soil temperature gradient, obtained as the difference between the soil temperature at 0 cm and 2 cm. An inverse Fourier transform converts this surface soil heat flux into the time domain (Holtslag & Bruin 1988, Appendix A). The heat flux is computed by dividing the temperature difference at the top and bottom sides of a plate-shaped sensor⁷ with the horizontal area of the sensor. A *thermocouple* is a device that generates a voltage proportional to this temperature difference, and self-calibrating sensor converts this voltage into a heat flux measurement in W m^{-2} (Gainsford 2006).

Rain Amount

The KNMI electronic rain gauge (Babington 2000, Wauben 2004) records the average precipitation intensity of the last 12 seconds in mm s^{-1} every 12 seconds, and the rain amount, in mm, is derived for every 10 minutes interval. The rain gauge is composed by a heated container in which precipitation accumulates and which is emptied every 12 seconds; the flow of outgoing liquid is measured by a floater connected to a potentiometer, and its value divided by 12 gives the precipitation intensity. The accuracy of the precipitation meter is 0.2 mm, and the precision is 0.1 mm. Figure 3.2b shows the rain gauge with the wind shield (Wauben 2004), and figure 3.2c shows a diagram of the instrument (Babington 2000).

3.1.2 Gap Filling

With gap-filling, missing measurements are replaced by synthetic values (Bosveld 2014). The gap-filling method depends on the missing parameter and the duration of the period where data is not available. There are two classes of parameters: forcing parameters, which include wind, temperature, specific humidity, incoming radiation and rain, and validation parameters, which include the surface fluxes, outgoing radiation, and friction velocity.

For less than two hours of missing measurements, both forcing and evaluation parameters are gap-filled by interpolation of nearby values. For longer periods, forcing parameters are derived by transforming measures obtained from the nearby site of De Bilt, which are themselves gap-filled, if necessary. Evaluation parameters are computed with a vegetation model⁸ instead. The gap-filling procedure is performed by the Cesar consortium, and we do not impute the remaining missing values, since we believe there is a good reason why these values were not gap-filled in the first place.

⁷Because of conduction, the temperature of the sensor would tend to homogenize; the higher the difference in temperature, the more energy is hitting the warmer side.

⁸A model that considers vegetation and solves the surface energy balance equation given the forcing parameters, then computes the validation parameters.

3.1.3 Data Filtering

Following other works in this field, such as Korrell et al. (1981) and Höglström (1988), we exclude all the records where any of the following conditions applies:

- The sensible heat flux H is smaller than 10 W m^{-2} ;
- The friction velocity u_* is smaller than 0.1 m s^{-1} ;
- The wind speed \bar{u} is lower than 1 m s^{-1} .

The reason for this is that the measures are too inaccurate to be of use.

3.2 Momentum Flux-Profile Relationship

Since the turbulent fluxes and the friction velocity are measured at the surface level, we can compute the momentum flux-profile relationships only at 10, 20 and 40 meters, because these quantities can be assumed constant only within the surface layer. It is very hard to know the exact height of the surface layer, because it depends on the weather and no exact formulas are known, but it is usually assumed to be 10% as high as the boundary layer. Based on the typical height of the boundary layer, the surface layer is often higher than 40 meters and lower than 80. JW Verkaik (2006) indeed reports that a large number of observations from Cabauw at 20 m are inside the surface layer, the 100 m level is already outside of the surface layer, and Korrell et al. (1981) used the observations at 50 m in their analysis, but not those at 100 m. Moreover, Braam (2008) reported that the observations at 60 m are outside of the surface layer only in the early morning; the height of the boundary layer starts growing at around 6 AM, and reaches 600 m between 9.30 AM and 10.30 AM, and reaches its maximum height, between 1800 m and 2000 m, at the end of the day. Unfortunately, there is no mention of the 40 m level in Braam (2008). Note that these measures were obtained in May, therefore they are likely to be smaller in Winter, and larger in the Summer. This evidence seems to support the fact that 40 m is inside the surface layer most of the time.

3.2.1 Obukhov Length

The Obukhov length is computed as in equation 2.4, reported here:

$$L = -\frac{u_*^3}{\kappa \frac{g}{\theta_v} \frac{Q}{\rho c_p}}$$

The flux of virtual potential temperature can be computed following the formulas in section 2.2.4, as the data contains all the necessary quantities; u_* is given, as well as the specific humidity and the pressure. The Obukhov length is computed at each height level using the corresponding air temperature measurement, and the fluxes measured at the surface.

3.2. MOMENTUM FLUX-PROFILE RELATIONSHIP

3.2.2 Gradients

The momentum flux-profile relationship is in equation 2.3, reported here for the reader's convenience:

$$\phi_m(\xi) = \frac{\partial \bar{u}}{\partial z} \frac{kz}{u_*}$$

In order to compute it from the data, we need to compute the derivative of the wind speed with respect to the altitude. In general, the derivative can be obtained by fitting a model on the observations, and computing the derivative using the model. The simplest option is to use a piecewise linear function that passes through the measurements; let the observations be sorted by height and y_i the measurement at height z_i , then for $z \in [z_i, z_{i+1}]$ we have:

$$f(z) = y_i + (z - z_i) \frac{y_{i+1} - y_i}{z_{i+1} - z_i} \quad (3.1)$$

The derivative of this function at height z_i is then the average of the slope of the segments that start and end at z_i :

$$\begin{aligned} f'(z_i) &= \lim_{h \rightarrow 0} \frac{f(z_i + h) - f(z_i - h)}{2h} \\ &= \frac{1}{2} \cdot \lim_{h \rightarrow 0} \left(\frac{f(z_i + h) - f(z_i - h)}{h} \right) \\ &= \frac{1}{2} \cdot \lim_{h \rightarrow 0} \left(\frac{y_i}{h} + \frac{y_{i+1} - y_i}{z_{i+1} - z_i} - \frac{y_i}{h} + \frac{y_i - y_{i-1}}{z_i - z_{i-1}} \right) \\ &= \frac{1}{2} \cdot \left(\frac{y_{i+1} - y_i}{z_{i+1} - z_i} + \frac{y_i - y_{i-1}}{z_i - z_{i-1}} \right) \end{aligned} \quad (3.2)$$

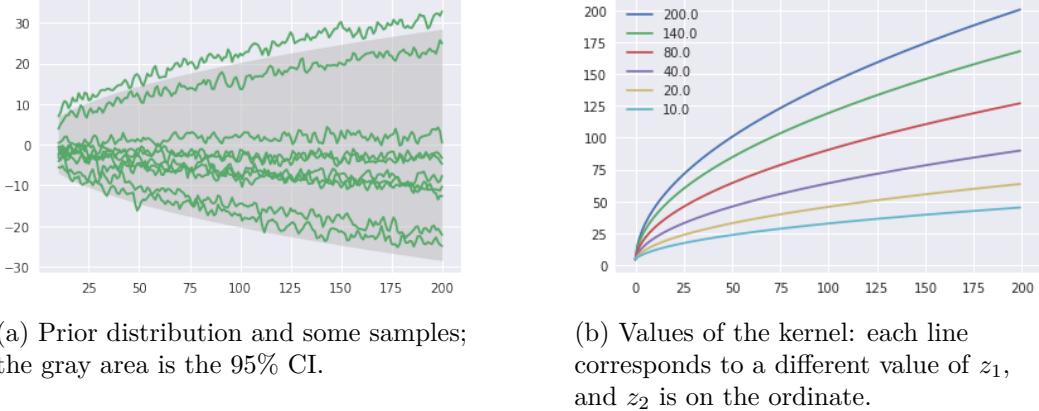
In order to compute this derivative at the lowest measured level $z_1 = 10$ m, we can exploit the no-slip condition and introduce an artificial observation $y_0 = 0$ m s⁻¹ at z_0 . The value of the *roughness length* z_0 depends on the properties of the surface, and, although no unambiguous value is known for the Cabauw observatory, its value is likely between 10^{-1} m and 10^{-2} m (JW Verkaik 2006, Baas et al. 2017), therefore it is reasonable to conclude that its effect is negligible on the final gradient.

A more complicated model, introduced by Nieuwstadt (1984), is

$$f(z) = a + bz + cz^2 + d \ln z \quad (3.3)$$

The model is linear in its parameters, therefore equation 2.20 can be used to compute the coefficients, using the feature mapping $\phi(z) = [1, z, z^2, \ln z]^\top$ and regularization parameter $\lambda = 0$. Once the coefficients are known, the gradient is trivial to compute:

$$f'(z) = b + 2cz^2 + d \frac{1}{z} \quad (3.4)$$



(a) Prior distribution and some samples; the gray area is the 95% CI.

(b) Values of the kernel: each line corresponds to a different value of z_1 , and z_2 is on the ordinate.

Figure 3.3: Behavior of the kernel in equation 3.5, where the altitude is on the x axis, and the predicted value on the y axis. Notice the approximate logarithmic profile with which the predicted value changes with altitude; this is caused by the square root term in the kernel, and emulates the effect of the $\ln z$ term in equation 3.3.

After removing the observations for which this model has a $R^2 < 0.9$, Nieuwstadt (1984) estimates the uncertainty of this gradient to be around 30%. Note that some works, such as Yagüe et al. (2006), do not use the squared term, and others, such as Steeneveld et al. (2005) add squared and even cubic logarithmic terms $\ln^2 z$ and $\ln^3 z$.

Finally, a third method of computing the gradient is to fit a Gaussian process to the profile using the following kernel:

$$k(z_1, z_2) = \exp\left(-\frac{(z_1 - z_2)^2}{2\sigma_0^2}\right) + \sqrt{\sigma_1^2 + z_1 z_2} + \sigma_2^2 \mathbb{1}[z_1 = z_2] + \sigma_3^2 \quad (3.5)$$

where $\mathbb{1}[P]$ is an indicator function whose value is 1 if the predicate P is true, and 0 otherwise, and the parameter σ_2 controls the noise in the measurement. Unfortunately, this noise is not constant, and does not depend on the altitude level; for example, for the wind speed u , the precision of the instrument is $\max(0.1, 0.01 \cdot u)$. Therefore, all the parameters must be found by optimizing the marginal likelihood. Figure 3.3 shows the prior distribution of a Gaussian process with this kernel, as well as the value of the kernel for some choices of z_1 and z_2 .

Our final goal is to obtain the derivative of the predictive posterior mean, which can be done using equation 2.36; for this we need to derive equation 3.5 with respect to z_1 :

$$\frac{\partial k(z_1, z_2)}{\partial z_1} = \frac{z_2 - z_1}{\sigma_0^2} \exp\left(-\frac{(z_1 - z_2)^2}{2\sigma_0^2}\right) + \frac{z_2}{2\sqrt{\sigma_1^2 + z_1 z_2}} + \sigma_2^2 \mathbb{1}[z_1 = z_2] \quad (3.6)$$

3.3 MONIN-OBUKHOV SIMILARITY THEORY

3.3 Monin-Obukhov Similarity Theory

Even though there is agreement on form of the momentum flux-profile relationship, there is still debate on the exact values of the coefficients, with different experiments resulting in different values (Högström 1988). In order to ensure a fair comparison with the results of this work, we fit the universal functions to the data from the Cesar database. Their general form is:

$$\phi(\xi) = \begin{cases} a + b\xi & \xi \geq 0 \\ a(1 - c^2\xi)^d & \xi < 0 \end{cases} \quad (3.7)$$

where a is close to 1, b is positive, and d is negative. Since d is negative, the base of the power must be positive, hence the squared c . Following the approach outlined in section 2.3.3, the coefficients a , b , c and d can be found by minimizing the L2-regularized mean squared error using equations 2.18 and 2.19; in this case, the parameter vector is $\boldsymbol{\theta} = [a, b, c, d]^\top$. The gradient of 3.7 is:

$$\nabla_{\theta}\phi(\xi)|_{\xi \geq 0} = \begin{bmatrix} 1 \\ \xi \\ 0 \\ 0 \end{bmatrix} \quad \nabla_{\theta}\phi(\xi)|_{\xi < 0} = \begin{bmatrix} \tau^d \\ 0 \\ -2acd\xi\tau^{d-1} \\ a\tau^d \ln \tau \end{bmatrix} \quad (3.8)$$

where $\tau = 1 - c^2\xi$. The Hessian of 3.7 when $\xi \geq 0$ is simply 0, because it is a linear function in all parameters, while, in the negative case, we have:

$$\nabla_{\theta}^2\phi(\xi)|_{\xi < 0} = \begin{bmatrix} 0 & 0 & -2cd\xi\tau^{d-1} & \tau^d \ln \tau \\ 0 & 0 & 0 & 0 \\ -2cd\xi\tau^{d-1} & 0 & \frac{2ad\xi\tau^d}{c^4\xi^2+\tau} (2c^2d\xi - c^2\xi - 1) & -2ac\xi\tau^{d-1} (d \ln \tau + 1) \\ \tau^d \ln \tau & 0 & -2ac\xi\tau^{d-1} (d \ln \tau + 1) & \tau^d \ln^2 \tau \end{bmatrix} \quad (3.9)$$

Analytical computation of the Hessian allows us to use the Newton conjugate gradient descent algorithm, which provides super-linear convergence rate, unlike other conjugate gradient methods whose rate of convergence is only linear (Nocedal & Wright 1999). This model is then fitted to the data using L2 regularization, and evaluated as the other regression models. In the remainder of the report, we will refer to this model as the *MOST Estimator*.

3.4 Prediction

In this section, we discuss how we use the data from the Cesar database to predict the momentum flux-profile relationship.

3.4.1 Features

All features come from the Cesar database, but the two research questions are answered with different sets of features. The first research question essentially asks if we can use this data to obtain more accurate predictions than the similarity theory, therefore it makes sense to use as many macro features as possible, leaving aside the features related to turbulence. A single sample contains, then: altitude z , wind speed at z , 10 m, 20 m and 40 m, air temperature at z , 10 m, 20 m and 40 m, soil temperature, dew point, specific humidity, relative humidity, air pressure, rain amount, net radiation, soil heat flux, air density, and virtual air temperature, for a total of 19 features. Note that there are three samples, one at each altitude level, for every 10-minutes interval, but each sample contains wind and air temperature from all the three altitude levels. The reason for this is that, according to early experiments, predicting the gradient is very difficult without measurements at different levels.

The second research question asks to quantify the importance of different features. This is done by partitioning some of the features mentioned previously into five sets, and comparing the performance of the model that performed best on the first research question on these five sets. The five sets are:

- F1: altitude z , wind speed at z , 10 m, 20 m and 40 m, air temperature at z , 10 m, 20 m and 40 m and soil temperature;
- F2: Soil heat flux;
- F3: Net radiation;
- F4: Rain amount, dew point;
- F5: Turbulent kinetic heat flux H , turbulent latent heat flux λE ;

These sets are used cumulatively in the order they are listed, meaning that F2 is used in conjunction with F1, F3 with F2 and F1, and so on.

We also create a second version of each feature set, augmented with the hourly trend of each variable, except for the altitude z . The reason for including the trend is that it can possibly give an indication of, for example, the time of the day, or other complex phenomena for which there is no measurement. The trend is computed simply as the difference between the current value and the value measured one hour before, divided by one hour. Given the goal of this work, namely to produce a model to be used in climate simulations, it would not make sense to use future values to compute the trend. The interval of one hour was chosen because it is long enough to capture local variations, but not too long so as to contain irrelevant information.

Finally, each feature is centered and standardized so as to have zero mean and unit standard deviation:

$$T_{ij} = \frac{X_{ij} - \hat{\mu}_j}{\hat{\sigma}_j} \quad (3.10)$$

3.4. PREDICTION

where i is the sample index and j is the feature index; obviously, every $\hat{\mu}_j$ and $\hat{\sigma}_j$ are computed only on the training data, and used to normalize both training and testing data. This method is not robust to outliers, since they heavily affect mean and standard deviation; this can be prevented by subtracting the median and normalizing with the interquartile range instead. These two methods give similar results in our datasets, therefore we follow equation 3.10, since it is the most widely used in practice.

Note that standardization is applied to all features, both for the first and the second research question, whereas the trend and the five feature sets are only used to answer the second research question.

Motivation

This partitioning was decided based on the knowledge of a domain expert, so that the level of a feature reflects both its expected impact on the performance and how desirable it is to include it. An example of the former reasoning is with F4, where the effect of moisture is expected to be already captured by the soil heat flux (in F2), and to be generally negligible in all but the most extreme conditions. An example of the latter reasoning is with F5, because turbulent fluxes are hard to measure accurately, and some of the current simulation models are known to be quite inaccurate in their estimation of these fluxes (Optis et al. 2014). Similarly, the friction velocity was not included, because the point of predicting ϕ_m is to use it to estimate u_* from the wind gradient, which is readily measured both in real life and in simulations. JW Verkaik (2006) has shown that the direction of the wind affects the universal functions at Cabauw, because of the different covers of the surface, changing the roughness length, and disturbances by the main mast, preventing accurate wind speed measurement. Nonetheless, we decided not to include the wind direction in the features, as this is very specific to the Cabauw observatory, and would reduce the generality of our models.

The five sets only include the most fundamental quantities, while features that can be computed from others, such as the virtual temperature, are not included. The reason is that using derived features would make it difficult to compare the sets, since it is not possible to attribute the improvement to the fundamental quantities or to the derived ones. Improvement caused by derived features indicate that the predictive model is not good enough and needs to be helped (since derived features are deterministic), but such an improvement would lead to the wrong conclusion that one or more fundamental features are relevant for the prediction.

Note that we cannot interpret a fitted model to obtain the importance of the features (e.g. the coefficients of linear regression, or the mean decrease in the split criterion for random forests), as this method is not reliable when some of the features are correlated (Strobl et al. 2007, 2008), which is a very relevant issue in our case. Trivially, the wind speeds at different levels are very strongly correlated (Pearson's r is above 0.95), and there are other, more complex, correlations, such as between the net radiation and the soil heat flux, or between the soil temperature

and the dew point (Pearson's r is respectively 0.75 and 0.79). Other non-parametric methods, such as Permutation Importance (Altmann et al. 2010), have enormous computational requirements that make them unfeasible. Filter methods, e.g. using the Mutual Information, compare the target variable with only one feature at a time, and thus do not consider the impact of groups of features, or the relation between a group of features conditioned on the fact that we already know other features. Both of them are important in our case, since F4 explicitly contains the effect of humidity, but it is believed that F4 provides little information over F1, F2 and F3 combined, since humidity can be inferred from other variables. Unfortunately, such complex requirements rule out most of the traditional feature selection methods (Chandrashekhar & Sahin 2014). Moreover, it is difficult to provide a qualitative interpretation of the importance of variables based only on these scores: what is the threshold below which a variable is not important anymore? Is a mutual information of 0.1 high enough? What about 0.3? Is being better than half of the other features enough to be considered important? Comparing the performance of a model on different feature sets provides a clear-cut answer: either including a feature improves performance, or it does not.

3.4.2 Estimators

The models that we use are ridge regression, k-nearest neighbors and gradient boosted trees. Due to the size of the dataset, we cannot use kernel-based algorithms such as SVM and Gaussian processes, as they require $\Theta(N^2)$ memory to store the kernel matrix, and $O(N^3)$ time to invert it.

All models are fitted using cross validation with random hyper-parameter search. This procedure detailed in section 3.5, but we list here the distributions of the hyper-parameters that we use in the random search:

- Ridge regression and MOST estimator: the only hyper-parameter to tune is the regularization coefficient, for which we use a \log_{10} -uniform distribution⁹ from 10^{-6} to 10^1 .
- k-nearest neighbors: the hyper-parameters to tune are the number of neighbors, chosen uniformly from 1 to 15, the distance function, either L1 or L2 norm, and the weights of the neighbors, either uniform or directly proportional to the distance to the query point.
- Gradient boosted trees: the distributions are shown in table 3.1. Note that δ , for the Huber loss, refers to the percentile of the residuals, so that $\delta = 0.25$ uses L2 loss for the smallest 25% and L1 loss for the largest 75%.

We use log-uniform distributions for parameters with a high range of possible values to reflect the intuition that small values are as likely as large values, and to

⁹A random variable X has a \log_β -uniform distribution from β^a to β^b if $\log_\beta X$ is uniformly distributed between a and b . Equivalently, if Y is uniform between a and b , then β^Y is \log_β -uniform.

3.5. PERFORMANCE EVALUATION

Table 3.1: Distribution of the hyper-parameters for gradient boosted trees

Hyper-parameter	Distribution	Values
Number of estimators	Log ₁₀ -uniform	From 10^1 to 10^3
Learning rate	Log ₁₀ -uniform	From 10^{-3} to 10^0
Number of features	Uniform	All possible values
Maximum depth	Uniform	From 4 to 12
Sub-sampling factor	Uniform	From 25% to 100%
Loss function	Uniform	Least squares, least absolute deviation, Huber loss (equation 2.27)
δ (for the Huber loss)	Uniform	From 1% to 99%

avoid the samples being dominated by the larger values. Samples from an uniform distribution from 10^0 to 10^3 are ten times more likely to be from $[10^2, 10^3]$ than from $[10^1, 10^2]$, and, on average, only one in 100 samples will be in $[10^0, 10^1]$. Log₁₀-uniform distributions do not have this problem, and a sample is equally likely to belong to any of the three intervals.

3.5 Performance Evaluation

The goal of performance evaluation is to obtain a realistic estimate of the performance of a model on unseen data. Because the similarity theory is only valid in the $-2 \leq \xi \leq 1$ range, we will use this data as the primary target for evaluation, and call it the *MOST dataset*. We will also evaluate the models on the full dataset, to see what kind of performance can be expected in the general case.

3.5.1 Evaluation Procedure

The two research questions require different evaluation procedures. The first question essentially entails finding what kind of performance is possible to achieve: this is best done using nested cross-validation, so that the estimate is not biased, albeit with higher variance. The second research question is about comparing alternatives; in this case, using a biased evaluation procedure is not a problem, but it is important to have low variance estimates, therefore we use repeated cross-validation. In both cases we use random search (Bergstra & Bengio 2012) to optimize the hyper-parameters of the models.

A fundamental assumption underlying hold-out evaluation methods is that the samples in the training set are independent and identically distributed, so that the distribution in the two partitions are equal. This is not our case, since there is a inherent time dependency in the data, meaning that samples obtained close in time are very similar. This can be confirmed by training and evaluating a k-nearest neighbors regressor with $k = 1$ on random splits: the resulting mean squared error

is in the order of 10^{-3} , which is clearly unrealistic. To circumvent this problem, the CV folds are created on *months*: all the samples in a given month/year combination are either in the training set or in the validation set. We choose months instead of days because the weather often does not change significantly in the span of 24 hours, whereas in a month there are at least three weeks worth of samples that are independent from the conditions at the start and end of the month.

For nested CV, we use 10 outer folds and 10 inner folds, and try 10 random hyper-parameter combination; since there are two datasets, every model is fit a total of $2 \cdot (10 \cdot 10 \cdot 10 + 10) = 2020$ times. Repeated CV is done using the best estimator found with nested CV, using 10 folds and 25 hyper-parameters combinations, and repeating the procedure $2 \cdot 5$ times, for a total of 2500 fittings.

According to the model and its hyper-parameters, fitting can take from a few seconds up to 8 hours or more; in order to reduce the total time needed, we implemented both plain and nested CV using Apache Spark (Zaharia et al. 2016). Since the number of stragglers is very low,¹⁰ running multiple cross validation jobs at the same time can reduce the duration of the whole process by five to ten times.

3.5.2 Evaluation Metrics

The main evaluation metric is the mean squared error, since that is what we are optimizing for, and we also compute the following metrics to get a more complete idea of the performance of the estimators:

- Mean Squared Error (MSE);
- Mean Absolute Error (MAE);
- Median Absolute Error (mAE);
- Mean Absolute Percent Error (MAPE);
- Median Absolute Percent Error (mAPE);
- R^2 Score:

$$1 - \frac{\sum(f_n - t_n)^2}{\sum(t_n - \bar{t})^2}$$

where f_n is the predicted value for the test sample x_n with true value t_n , the squared error is $(f_n - t_n)^2$, the absolute error is $|f_n - t_n|$, and the absolute percent error is $100|1 - f_n/t_n|$. We present both mean and median scores because the former are heavily skewed by outliers. We also present both absolute and percent errors

¹⁰For k-nearest neighbors, the slowest method, the median fitting time in our experiments is around 10 minutes, the third quartile is around half an hour, and the maximum is between 8 and 12 hours.

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because the latter are easier to interpret, but tend to explode when the true value is very small,¹¹ a condition that happens frequently in our dataset.

3.6 Success Criteria

The differences needed to answer the research questions are quantified by comparing the MSE using the effect size. We prefer the effect size over the average MSE because the effect size allows us to consider the standard deviation together with the mean; this could lead us to prefer models with slightly worse average MSE, but more consistent and reliable performances. Since we are looking for an improvement, we compute the right 95% confidence interval for the population effect size. In other words, besides providing a point estimate for the population effect size δ_{pop} , we also provide an interval $[\delta_{low}, \infty)$ that contains it 95% of the times. We say the treatment is better than the control if $\delta_{low} > 0$, and the best treatment is the one with the largest δ_{low} . In the tables, the effect size is formatted as $[\delta_{low}, \delta_{pop}]$; the right square bracket is dropped to indicate that the interval is unbounded in that direction.

A successful answer to the first research question entails finding a model and hyper-parameters whose right confidence interval bound δ_{low} is larger than 0, where the effect size is computed by using the MOST estimator as control. The second research question is answered by comparing the MSE obtained on the ten feature sets (F1 to F5, with and without trend). All these effect sizes are computed on the MOST dataset.

¹¹Predicting 1 for a true value of 100 gives a percent error of 99%, but predicting 100 for a true value of 1 gives, somewhat unfairly, a percent error of 9900%, whereas their absolute error is identical.

Chapter 4

Results

This chapter presents the results obtained following the procedures outlined in chapter 3. Section 4.1 describes the dataset and shows some of its peculiarities, then section 4.2 identifies the best method to compute the gradient of the profile. Next, section 4.3 shows the momentum flux-profile relationship obtained on the dataset and its predictions by the MOST estimator, and finally sections 4.4 and 4.5 present the performance of the other estimators and the importance of the feature sets.

All the processing was done using the Python programming language¹ version 3.6.5, and the usual Data Science stack, in no particular order: Pandas 0.23.0 (McKinney 2010), scikit-learn 0.19.1 (Pedregosa et al. 2011), SymPy 1.1.1 (Meurer et al. 2017), Matplotlib 2.2.2 (Hunter 2007), Seaborn 0.8.1,² NumPy 1.14.2 (Walt et al. 2011), Jupyter Notebook 5.5.0 (Kluyver et al. 2016), IPython 6.4.0 (Pérez & Granger 2007), Spark 2.2.0 (Zaharia et al. 2016), with the crucial support of Hopsworks (Ismail et al. 2017)

4.1 Exploratory Data Analysis

The dataset consists of 17 years of measurements, from January 2001 to December 2017, for a total of 3,436,416 observations. The Cesar database contains one tar-gzipped archive for every month, whose content is a single data file in the netCDF format (Unidata 2018). The archives contain a subset of related variables, and we used the datasets containing surface fluxes, tower meteorological profiles, meteorological surface data, and soil heat, for a total of 816 datasets covering 204 months.

Unfortunately, most of these observations contain unreliable measurements, as per section 3.1.3, leaving only 1,561,973 usable records. Additionally, the turbulent fluxes measured in March 2016 exhibit a much wider range than the March measurements of other years. Roughly 15 to 20% of the measurements in that month are suspicious; since the Cesar database contains a separate dataset every month that is manually reviewed, we decided to completely exclude the dataset of March

¹<https://www.python.org/>

²<https://doi.org/10.5281/zenodo.883859>

CHAPTER 4. RESULTS

Table 4.1: Basic descriptive statistics of the features in the Cesar database. H , λE , the net radiation and the soil heat flux are measured in W m^{-2} , u_* and the wind speed in m s^{-1} , the CO_2 flux in $\text{mg m}^{-2} \text{s}^{-1}$, the temperatures in K, the air pressure in hPa, the air density in kg m^{-3} , the rain amount in 6 mm h^{-1} , and the specific humidity is in g kg^{-1} .

	Mean	Std.	Min.	25%	50%	75%	Max.
H	3.7	47.3	-460.0	-25.8	-14.7	28.2	479.6
λE	74.5	114.1	-534.8	-5.0	23.7	132.4	748.7
u_*	0.3	0.1	0.1	0.2	0.3	0.4	1.8
CO_2 Flux	-0.1	0.3	-7.5	-0.2	0.0	0.1	6.1
Wind Speed	5.9	2.6	1.0	4.0	5.4	7.2	29.4
Air Temp.	284.7	6.4	259.6	280.1	284.8	289.4	306.9
Soil Temp.	284.4	5.7	271.9	279.6	284.3	289.1	302.6
Dew Point	280.3	6.1	188.0	276.6	280.6	284.7	296.7
Spec. Hum.	6.6	2.5	-0.9	4.8	6.4	8.3	17.8
Rel. Hum.	76.5	15.2	0.0	66.9	79.2	88.3	133.7
Air Press.	1,009.6	69.0	960.9	1,008.3	1,014.8	1,020.7	1,046.4
Rain Amount	0.0	0.1	0.0	0.0	0.0	0.0	15.1
Net Rad.	81.8	167.2	-158.5	-35.4	-3.0	172.5	7,775.4
Soil Heat Flux	2.9	15.6	-77.8	-6.5	-0.7	8.9	1,139.0
Air Dens.	0.3	0.1	0.1	0.2	0.3	0.3	2.8
Virt. Air T.	1,443.8	454.9	124.8	1,104.2	1,391.0	1,753.2	3,506.0

Table 4.2: Number of measurements by gap filling method. Due to inconsistencies in the Cabauw Documentation (Bosveld 2014), we cannot be sure of the meaning of the columns, but this is our interpretation: 0 - Unknown, 2 - Cabauw In situ, 3 - Automatic Weather Station in Cabauw, 4 - Computed from profiles, 5 - Interpolated, 6 - Cabauw-based model, 7 - De Bilt-based model.

	0	2	3	4	5	6	7
H	-	1,192,346	-	-	17,291	97,720	1,005
λE	-	1,180,434	-	-	18,503	97,846	11,579
u_*	-	1,174,593	-	132,461	465	618	225
CO_2 Flux	-	964,749	-	-	48,983	287,855	6,775
Wind Sp.	-	1,302,308	2,338	-	879	331	2,506
Air Temp.	-	1,298,075	-	-	2,419	5,959	1,909
Spec. H.	-	1,292,626	-	-	3,149	10,693	1,894
Air Press.	7,096	-	1,298,205	-	654	-	2,407
Rain Am.	7,096	1,181,167	117,844	-	346	-	1,909
Net Rad.	-	1,274,106	-	20,962	1,715	-	11,579
Soil H. Fl.	-	1,232,822	-	-	-	72,256	3,284

4.1. EXPLORATORY DATA ANALYSIS

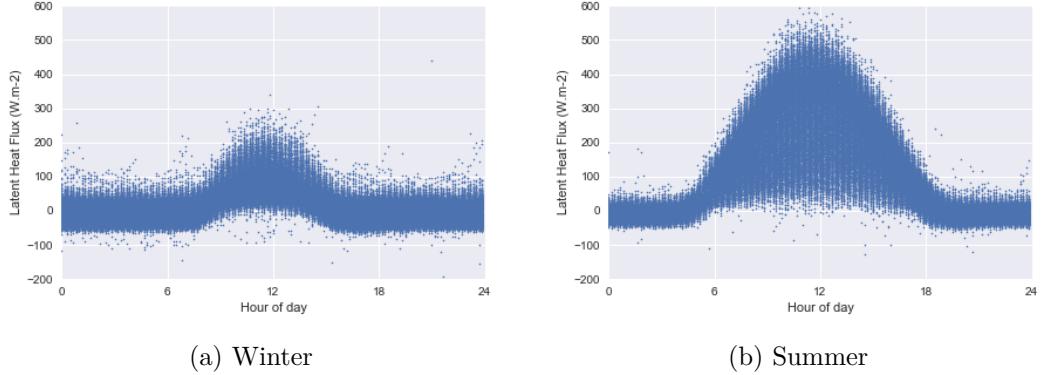


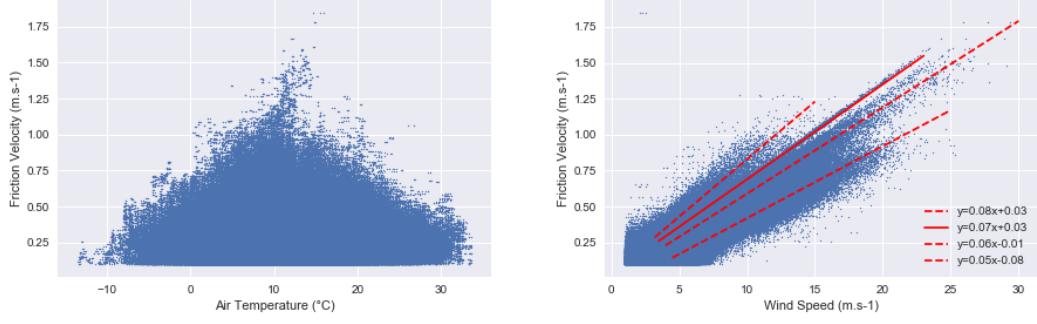
Figure 4.1: Turbulent latent heat flux versus hour of day in Winter (left) and Summer (right). One can see both the difference in day duration, and the effect of increased temperature on evaporation and transpiration. The sensible heat flux follows a very similar pattern, with lower absolute values.

2016, fearing for a systematic error somewhere in the process. Moreover, 6 measurements of the turbulent latent heat are way above the acceptable range, 4,538 do not have a dew point, and 247,656 do not have a soil temperature; this leaves 1,308,362 usable records, of which 1,082,035 (83%) are in the MOST validity range. Table 4.1 summarizes the weather parameters that were used to compute the similarity functions and/or as features for the models, and table 4.2 presents the number of observations that were gap-filled with each method, for the measurements for which this information was provided.

Figure 4.1 shows the turbulent latent heat flux versus hour of day both in Winter and Summer, whereas figure 4.2 shows the friction velocity as a function of air temperature and wind speed. The dependency of u_* with the wind speed of figure 4.2b is quite complicated: there are three clear regions with different constant of proportionality and correlation coefficient. The group where the two quantities are almost perfectly correlated corresponds to imputed values for the friction velocity, derived from the wind speed. The three other groups differ widely in the values of the fluxes and radiation; for example, fitting an ordinary least squares model to 1000 bootstraps of the observations with negative net radiation yields an average proportionality coefficient of 0.051 with standard deviation 1.52×10^{-5} , whereas the same procedure on the complementary set yields an average of 0.046 with standard deviation 1.40×10^{-5} . Note that this dependency might be related to the observed imbalance in the surface energy budget, usually around 15% during day time and 100% during night time at the Cabauw observatory; Bosveld (2018) notes that the imbalance seems to depend on the speed of wind.

Talking about speed of wind, figure 4.2b shows some measurements exceeding 25 m s^{-1} ; according to the Beaufort scale, holding umbrellas and walking become hard at 15 m s^{-1} . Slightly less than 5% of the samples are above 11 m s^{-1} , and only 656 observations (0.04%) are above 20 m s^{-1} . Those measurements are not issues

CHAPTER 4. RESULTS



(a) Air temperature. Curiously, the momentum flux is low when the air temperature is high; intuitively, one would expect to have large u_* in that situation, since it tends to happen in stable conditions.

(b) Wind, and eyeballed line fits for different groups of data. The legend shows the equation of the lines from highest to lowest.

Figure 4.2: Friction velocity versus air temperature (left) and wind speed (right). Figure 4.2b shows four distinct groups of data with different proportionality between \bar{u} and u_* . The solid line shows almost perfect correlation: this is because of the gap-filling technique discussed in section 3.1.2. The samples in the three other groups differ widely in fluxes, radiation, and altitude.

with the data: figure 4.4 shows the highest wind speed present in the Cesar database to date, corresponding to cyclone Jeanett.

Figure 4.3 shows the result of the t-SNE dimensionality reduction algorithm (van der Maaten & Hinton 2008) applied to 250,000 samples (19.2% of the total), using the same features of table 4.1, plus z , L , ξ , the wind and virtual temperature gradients, ϕ_m , the month of the year and hour of day. The 250,000 samples were chosen uniformly at random and standardized with equation 3.10 before fitting, but the colors were computed using the raw features on a perceptually uniform color scale, after excluding the top and bottom 1% values. Overall, the points cluster in a relatively uniform blob, which is not surprising once you consider that the measurements were taken continuously, meaning that all physical quantities change smoothly, thus all points close in time are also close in feature space. The colors reveal some structure, though: the left-hand side of the blob contain measurements taken in the Summer, and the right-hand side contains measurement in Winter (see the air temperature in figure 4.3e and month in figure 4.3v). Moreover, unstable conditions are clustered in a stripe, centered vertically, that runs from left to right (see the fluxes of figures figs. 4.3b, 4.3c and 4.3t, the radiation in figure 4.3u, and the hour of day in figure 4.3w). In figure 4.3h we also see a cluster on the top with all the observations at 40 meters, whereas the two lower levels are mixed somewhat uniformly in the bottom part of the plot. Finally, figure 4.3x shows the result of k-means clustering in the standardized feature space, using $k = 2$

4.1. EXPLORATORY DATA ANALYSIS

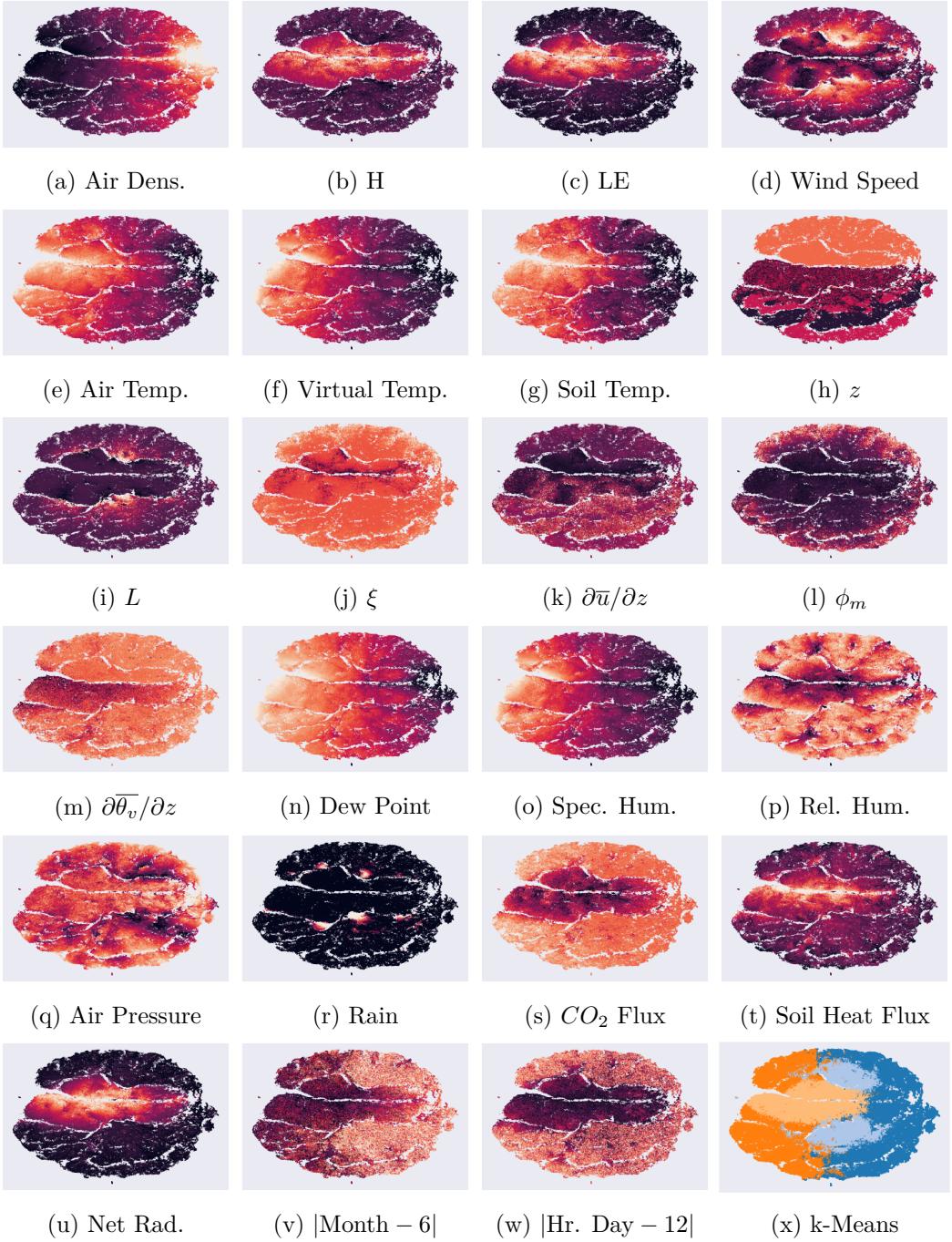


Figure 4.3: Results of the t-SNE dimensionality reduction algorithm; every figure uses a different feature to color the points (darker points have smaller values), except figure 4.3x, where the colors represent the result of 2-means clustering (blue/orange) and 4-means clustering (the four shades). The colors are consistent, in the sense that light and dark shades of blue are placed in the same cluster by 2-means clustering, ditto for orange. Figures 4.3v and 4.3w use respectively the month and hour of day as feature values, but are colored using the values transformed with the formula in their caption. The points were drawn in random order. (Best viewed in color)

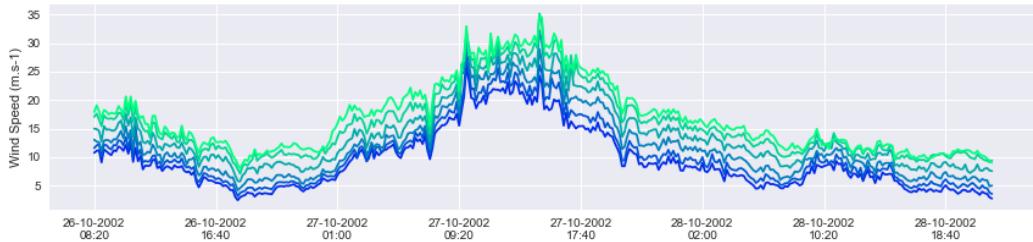


Figure 4.4: Wind speed measurements during Cyclone Jeanett, which struck northwest Europe in October 2002, causing 33 fatalities. Every line corresponds to a different altitude, with brighter colors for higher altitudes. The top speed registered at Cabauw is 35.2 m s^{-1} , but the cyclone registered winds up to 42.5 m s^{-1} in other parts of Europe!

(blue/orange) and $k = 4$ (the four shades). This clustering is consistent with the qualitative division above, with the dark orange and blue clusters corresponding to Summer and Winter respectively, light orange corresponding to unstable conditions with considerable vertical movement of air, and light blue corresponding to strong horizontal winds with little movement in the vertical. Stably stratified conditions seem to occur at the boundary of the blob, where ϕ_m takes the highest values (see figure 4.3l). This is also not surprising, since stable stratification tend to happen at night throughout the year, unlike free convection or z-less scaling, which only happen in specific conditions.

4.2 Gradient Computation

Section 3.2.2 introduced three different ways to compute the gradient, but we need to choose one to compute the universal functions. In this section, we refer to the finite differences method in equation 3.2 as *FD*, the logarithm-based model of equation 3.4 as *LG* and the Gaussian Process-based model of equation 2.36 as *GP*.

By analyzing the Pearson correlation between the three methods at each altitude level, we see that the FD gradient is poorly correlated with the other two methods at the 10 meters level, but is very well correlated with the LG gradient at the other levels. The LG and GP gradients disagree on the lower levels, but it appears their predictions converge as altitude increases. It is clear that the FD gradient is inadequate at the lowest level, which can be explained by considering that equation 3.2 with $z = 10$ reduces to the wind speed at 20 meters divided by 20.

The error that LG and GP incur in predicting the wind speed is independent of the altitude level, and the predictions from GP are closer to the true wind speed, except for a few large outliers. Therefore, it is reasonable to conclude that FD predictions of the gradient at 10m are wrong. If we examine the prediction error as a function of the wind speed, we see that GP becomes more and more reliable as the wind speed increases; not only does its error decrease, so does the variance of

4.3. FLUX-PROFILE RELATIONSHIP

the error. LG's error, however, decreases until a certain wind speed, after which it stabilizes to 1%. This can be explained by considering that the measurement error of the wind speed is the maximum between 0.1 m s^{-1} and 1%, therefore the error of LG can be attributed almost entirely to uncertainty in the data, whereas GP is overfitting high wind speeds.

Finally, we can compare the error when predicting ϕ_m with the similarity theory (equation 2.6), using the three methods of computing the gradient. FD is slightly better than LG if we do not consider the 10 m level, but way worse if we include it. GP is significantly worse than FD in the MOST validity region, but only slightly worse on the whole dataset; this suggests that GP is weak when $|\xi|$ is small.

To conclude, although FD (equation 3.2) is the most accurate way of computing the profile gradient, it does not allow us to use data at the 10 m level. Considering that LG (equation 3.4) is just slightly worse, but allows us to include that level (increasing the data available by 50%!), all the results presented from now on make use of it.

Appendix A contains detailed tables and charts supporting the arguments made in this section.

4.3 Flux-Profile Relationship

Figure 4.5 shows the wind shear versus the instability parameter, together with the commonly accepted flux-profile relationship in green and the relationship fitted on our dataset in red. Qualitatively, the scatter plot looks as expected, going to zero as ξ decreases, linearly increasing in the $0 \leq \xi \leq 1$ interval, and leveling off after that, possibly approaching the $\xi^{1/3}$ form proposed by Grachev et al. (2007). There seem to be a lot of scatter, but more than half of the data is enclosed in the box $-0.5 < \xi < 0.5, 0 < \phi_m < 2$.

The performance of the MOST estimator is shown in table 4.3; we see a considerable increase in the MSE when the full dataset is used; this is not surprising, considering that, with $\xi > 1$, ϕ_m tends to level off, and there are a considerable number of outliers in the range $-20 \leq \xi \leq -2$ (see figure 4.5a) that cannot be fitted by the MOST estimator. Figure 4.5 shows ϕ_m as a function of ξ as computed in our dataset, as well as the predictions of equation 2.6 and the fitted MOST estimator.

Table 4.3 shows the values of the coefficients in equation 3.7, when fitted to the region of data where the Monin-Obukhov similarity theory is valid. We note a big difference with the values recommended in Högström (1988), as well as most studies on the topic. However, Bouwman (1990) studied the stable, nocturnal boundary layer at Cabauw, and reported values varying between 0.81 and 0.95 for a and between 2.7 and 3.2 for b , depending on the direction of the wind; there is no known explanation for this discrepancy. Although Bouwman (1990) used the same method that we applied to find the coefficients, no goodness of fit statistics, such as MSE or R^2 , were reported.

CHAPTER 4. RESULTS

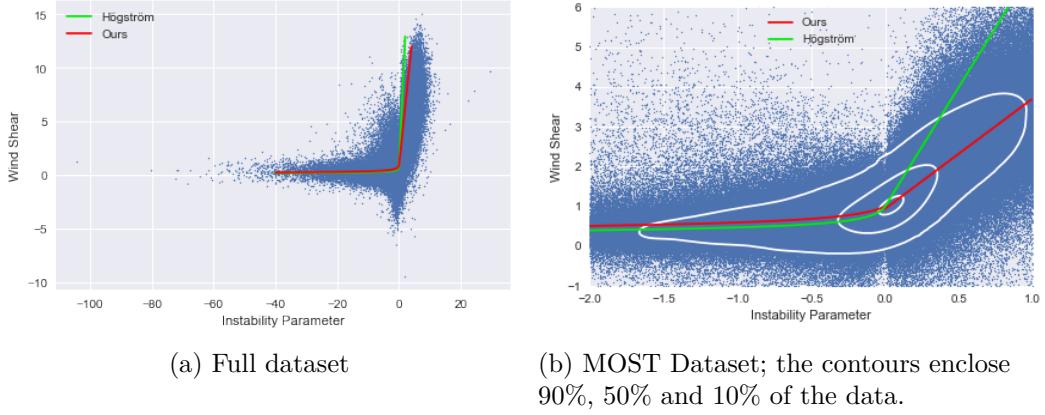


Figure 4.5: Wind shear ϕ_m versus the instability parameter ξ , with the prediction according to equation 2.6 in green, and our predictions, following equation 3.7 with the coefficients being the median values in table 4.4, in red.

Table 4.3: Evaluation metrics for the MOST estimator on both datasets obtained with nested cross-validation. The first number is the average over the 10 outer folds, followed by the standard deviation in parentheses.

Metric	Full Dataset	MOST Dataset
MSE	0.64 (0.04)	0.32 (0.02)
R^2	0.71 (0.01)	0.61 (0.01)
MAE	0.53 (0.01)	0.39 (0.01)
mAE	0.37 (0.01)	0.28 (0.01)
MAPE	257.80 (207.39)	178.30 (68.99)
mAPE	28.48 (0.81)	24.44 (0.81)

Table 4.4: Values of the coefficients of the MOST estimator of equation 3.7 fitted on the MOST dataset. The minimum values for c and d seem to be outliers, as well as the next smallest value, but the other 8 values are closely clustered together within an interval of about 0.15.

	Mean	Std.	Min.	25%	50%	75%	Max.
a	0.94	0.00	0.94	0.94	0.94	0.95	0.95
b	2.77	0.01	2.76	2.77	2.77	2.78	2.78
c	2.45	0.47	1.25	2.61	2.65	2.67	2.71
d	-0.30	0.11	-0.60	-0.26	-0.26	-0.26	-0.25

4.4. PERFORMANCE OF THE MODELS

Table 4.5: Descriptive statistics of the MSE achieved by each estimator with nested CV, and effect size comparing it with the MOST baseline (control). Gradient boosted trees perform better in both datasets, and Ridge regression beat the MOST estimator on the MOST dataset.

Dataset	Model	Mean	Std.	Min.	50%	Max.	Effect Size
Full	MOST	0.64	0.04	0.58	0.63	0.71	-
	GBT	0.36	0.04	0.31	0.36	0.42	[3.5, 7.1]
	kNN	0.61	0.05	0.56	0.58	0.73	[-0.3, 0.6]
	Ridge	0.62	0.06	0.55	0.62	0.72	[-0.9, 0.2]
MOST	MOST	0.32	0.02	0.29	0.32	0.34	-
	GBT	0.17	0.02	0.16	0.17	0.22	[3.6, 12.0]
	kNN	0.32	0.03	0.27	0.32	0.36	[-4.0, 0.1]
	Ridge	0.27	0.02	0.24	0.28	0.30	[1.1, 3.4]

4.4 Performance of the Models

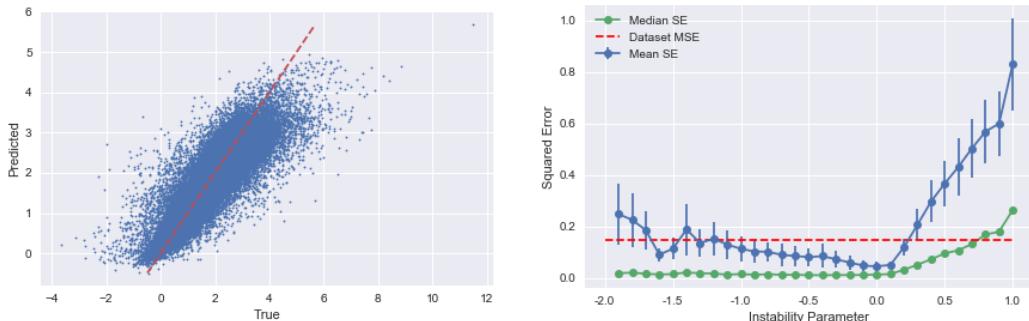
The first research question asked *how can the from the Cesar database be used to predict the momentum flux-profile relationship more accurately than the Monin-Obukhov similarity theory, by using only macro weather parameters?*

Table 4.5 shows descriptive statistics of the MSE obtained by the best combination of features and trend, for each estimator and for each datasets, as well as the effect size comparing it with the MOST baseline. The scores were obtained with the nested cross validation procedure, and are also shown in figure 4.8. Gradient Boosted Trees always perform significantly better than the MOST estimator, obtaining roughly half of its MSE in both datasets. Moreover, even the simple Ridge estimator managed to obtain significantly lower MSE in the MOST dataset. Table 4.6 shows the values of all the evaluation metrics computed on the outer validation folds on both datasets. Figure 4.6 shows the predictions obtained with the GBT estimator on one of the outer validation folds of the MOST dataset, and the squared error as a function of the instability parameter. Its behavior is consistent with what is widely known in the literature, and is caused by imprecision in the measurement and in the eddy correlation technique used to compute the turbulent fluxes (see section 3.1.1).

Appendix B reports the optimal hyper-parameters found during nested CV for the MOST estimator and the estimators that beat it.

Table 4.6: Descriptive statistics of all the metrics obtained by the gradient boosted trees estimator in the nested CV procedure, for both datasets.

Dataset	Metric	Mean	Std.	Min.	50%	Max.
Full	R^2	0.84	0.01	0.82	0.84	0.85
	MAE	0.35	0.02	0.31	0.35	0.38
	MAPE	105.34	77.54	60.41	69.33	296.47
	MSE	0.36	0.04	0.31	0.36	0.42
	Train MSE	0.32	0.03	0.28	0.33	0.36
	mAE	0.19	0.01	0.16	0.19	0.20
MOST	mAPE	16.74	0.90	15.18	16.68	18.23
	R^2	0.79	0.02	0.73	0.79	0.80
	MAE	0.26	0.02	0.24	0.26	0.30
	MAPE	87.62	57.80	50.59	63.66	228.67
	MSE	0.17	0.02	0.16	0.17	0.22
	Train MSE	0.15	0.03	0.12	0.15	0.22
	mAE	0.16	0.02	0.14	0.15	0.20
	mAPE	15.10	1.10	13.87	14.78	17.49



(a) Predicted value (y -axis) versus true value (x -axis), $R^2 = 0.803$; we see a tendency to overestimate small values and underestimate large ones.

(b) Squared error versus ξ . The error is smallest during neutral stratification, and grows larger as conditions stabilize.

Figure 4.6: Behavior of the GBT estimators on one of the outer validation folds of the MOST dataset, containing 107,932 samples.

4.5. IMPORTANCE OF THE FEATURES

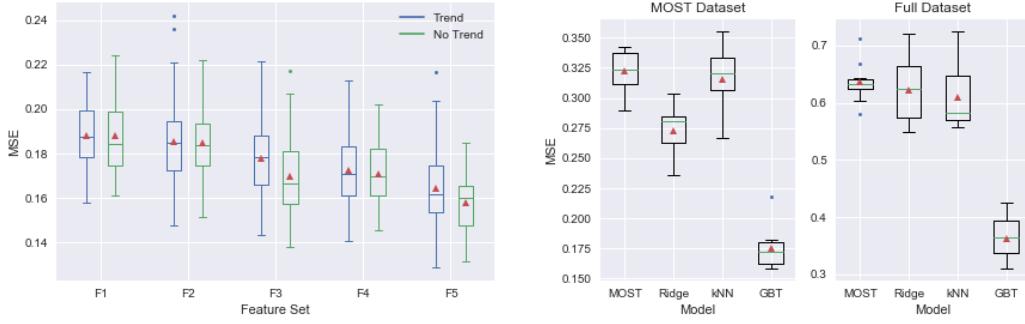


Figure 4.7: MSE obtained via repeated CV by the GBT estimator on the MOST dataset, for each of the five feature sets with and without trend.

Figure 4.8: MSE obtained via nested CV by the models, for the MOST dataset (left) and the full dataset (right).

4.5 Importance of the Features

The second research question asked *what impact do different macro-weather parameters have on the quality of the predictions obtained?*

Table 4.7 reports descriptive statistics about the MSE obtained by the GBT estimator in each validation fold of repeated CV on the MOST dataset. These scores are summarized in figure 4.7, while tables 4.8 and 4.9 quantify the difference using the effect size. The figure might give the impression that the samples are normally distributed, but a Shapiro-Wilk normality test on F1 without trend gives a p-value of 0.0519 ($W = 0.954$), and a p-value of 0.140 ($W = 0.965$) on F3 (without trend); we feel there is not enough evidence to deem *all* ten groups normally distributed, hence our use of the non-parametric bootstrap CI method to compare them.

Table 4.8 compares each feature set with and without trend, for the MOST dataset and the GBT estimator. Essentially, the table shows that the features augmented with trend do not provide a significant improvement over those without trend. On the contrary, not including the trend is sometimes beneficial. Table 4.9 compares the five feature sets without trend. The only feature sets that do not improve over the previous sets are F2 (soil heat flux) over F1, and F4 (rain amount and dew point) over F3; in all other cases, adding features gives statistically significant improvements, reducing the error by 5 to 10%. This is likely not to be true for the features augmented with trend, where the improvements from one feature set to the next are not significant, because of the higher variance in the scores. However, even the features with trend show a reduction in error moving from F1 to F5.

CHAPTER 4. RESULTS

Table 4.7: Descriptive statistics of the MSE used to produce figure 4.7, table 4.8 and table 4.9. Y and N in the trend row indicate the versions with and without trend, respectively.

Features	F1		F2		F3		F4		F5	
	Trend	N	Y	N	Y	N	Y	N	Y	N
Mean	0.19	0.19	0.19	0.19	0.17	0.18	0.17	0.17	0.16	0.16
Std.	0.02	0.01	0.02	0.02	0.02	0.02	0.01	0.02	0.01	0.02
Min.	0.16	0.16	0.15	0.15	0.14	0.14	0.15	0.14	0.13	0.13
50%	0.18	0.19	0.18	0.18	0.17	0.18	0.17	0.17	0.16	0.16
Max.	0.22	0.22	0.22	0.24	0.22	0.22	0.20	0.21	0.18	0.22

Table 4.8: Effect sizes comparing the MSE scores of each feature set with and without trend. Using the trend does not improve the performance, and sometimes not using the trend is better.

Treatment	F1	F2	F3	F4	F5
Not Trend	[-0.3, 0.1]	[-0.4, 0.0]	[-0.0, 0.5]	[-0.5, 0.1]	[-0.1, 0.3]
Trend	[-0.7, -0.1]	[-0.4, -0.0]	[-1.2, -0.5]	[-0.5, -0.0]	[-0.7, -0.3]

Table 4.9: Effect sizes comparing the MSE scores of all pairs of feature sets without trend. The control is on rows, and the treatment is on columns. The only feature sets that do not bring an improvement are F2 over F1 and F4 over F3.

Features	F1	F2	F3	F4	F5
F1	-	[-0.3, 0.1]	[0.4, 1.0]	[0.4, 1.0]	[1.2, 2.0]
F2	[-0.5, -0.1]	-	[0.3, 0.8]	[0.3, 0.8]	[1.2, 1.8]
F3	[-1.6, -0.9]	[-1.6, -0.9]	-	[-0.7, -0.2]	[0.1, 0.7]
F4	[-1.3, -0.8]	[-1.3, -0.8]	[-0.3, 0.2]	-	[0.4, 0.9]
F5	[-2.3, -1.4]	[-2.3, -1.5]	[-0.9, -0.5]	[-1.3, -0.8]	-

Chapter 5

Conclusion

The Monin-Obukhov similarity theory is an important component in many climate simulation models. In this work we reproduced the similarity theory using the data from the Cesar database, and investigated whether it is possible to improve its predictions by using macro weather parameters instead of parameters describing turbulence. This was done both within the validity range of the similarity theory ($-2 \leq \xi \leq 1$) and on the full dataset, to assess the performance of the models in the general case. Moreover, we identified which of these macro weather parameters are important in order to obtain good predictions.

As shown in table 4.5, we could improve the predictions of the similarity theory even with a simple regularized linear model, and more complex methods can reduce the MSE by almost 50%. Moreover, the error we achieved on the full dataset is comparable with the error achieved by the MOST estimator in the restricted dataset. Table 4.8 shows that no useful information can be obtained from knowing the value of a feature one hour earlier than the prediction, possibly because of overfitting. Finally, table 4.9 shows that, besides the heat fluxes, the net radiation is an important predictor, whereas the dew point and the soil heat flux do not contribute significantly to the predictive performance.

We conclude this thesis by commenting on several aspects of the present work (section 5.1), briefly describing related works and how this project compares with them (section 5.2), and finally giving some suggestions as how to build on the foundation laid here (section 5.3). In the following sections, we will comment on the estimators, samples and features used, as well as important aspects to consider during deployment.

5.1 Discussion

An obvious, but perhaps easy to ignore, fact is that the models presented are black boxes that cannot be easily interpreted. This approach is very different from the traditional methodology in Physics and related fields, in which theories offer predictions by *explaining* the phenomena at hand. Interpretability is a weak point of

current methods in Machine Learning (Doshi-Velez & Kim 2017), but when the problem is formulated explicitly as uncovering certain physical laws, intriguing results arise, see for example Raissi & Karniadakis (2018), Martius & Lampert (2016) etc.

In the following sections we examine several aspects of this work, namely the estimators, the features, and the training samples, as well as deployment related issues.

5.1.1 Estimators

Ridge was chosen because it is a simple model that is often used as baseline, and in this case it proved to be a viable alternative in spite of its simplicity.

kNN is another simple model that can nonetheless adapt to complex, non-linear phenomenon. However, in this case it proved to be a relatively weak estimator, since its performance is on par with the state of the art that we were trying to beat. Its high resource requirements at prediction time make it a poor replacement for the MOST estimator. Early experiments showed that, interestingly, its best performances are achieved with F1, where it could beat Ridge regression, and gradually degrade as more features are added. This behavior could be explained by considering figure 4.2b, which shows that the friction velocity and the wind speed are well correlated; as more and more features are added, it is harder and harder for kNN to relate u_* and \bar{u} .

The GBT is one of the most flexible and advanced algorithms in Machine learning, and its performance in this task prove it. Furthermore, highly optimized implementations exist, for example xgboost (Chen & Guestrin 2016) and LightGBM (Ke et al. 2017). Both of them use GPUs for training and prediction, making them lightning fast and serious contenders.

Due to the size of the dataset, we had to discard kernel based methods such as SVMs and Gaussian processes, although a possible approach would be to create an ensemble of models trained with small subsets of the data. Furthermore, the high amount of resources needed to train deep neural networks prevented a thorough evaluation.

5.1.2 Features

The features used for prediction play a very important role, since they affect the ability to generalize to different conditions, and the ease with which the model can be applied to new situations. This is especially noteworthy since no feature engineering was performed, except for standardization. This means, for example, that the model could have incorporated biases coming from the instruments used at Cabauw, thereby hurting performance when using samples coming from different instruments (newer version, different maker, different measuring principle, etc.). The features that are computed with the eddy correlation method are particularly

5.1. DISCUSSION

susceptible to this issue: since the shortcomings of such procedure are well known, it is likely that better methods will be developed in the future.

Although our experiments showed that measurements in the past do not improve the performance, the method we used was quite crude. Advanced methods explicitly based on time series analysis, such as ARIMA, could be tried. We performed some informal experiments with recurrent neural networks, but the results are discouraging, since they had difficulties even in properly fitting the dataset (see appendix C.1)

In this project, we focused on the Monin-Obukhov similarity theory, which defines the flux-profile relationships in term of the Obukhov length L ; the instability parameter $\xi = z/L$ can then be used to distinguish between stable ($\xi \gg 0$), unstable ($\xi \ll 0$) and neutral ($\xi \approx 0$) conditions. An alternative approach is to use the Richardson number, defined as:¹

$$Ri = \frac{g}{T} \frac{\partial \theta / \partial z}{(\partial \bar{u} / \partial z)^2} \quad (5.1)$$

which is, essentially, the ratio between production of turbulence due to buoyancy and to wind shear, and qualitatively behaves as ξ . In fact, there are deep connections between the Obukhov length and the Richardson number (Obukhov 1971), so much so that some GCMs use Ri instead of L to parametrize the atmospheric boundary layer (Anderson et al. 2004, Donner et al. 2011). It would then be interesting to apply the methodology used in this project to this different parametrization of turbulence, in hope of achieving better performance.

Feature importance

We derived the importance of the different feature sets by comparing the performance of a model when using these sets. Obviously, this makes the importance tied to the specific model, in this case Gradient Boosted Trees, and we cannot exclude that different models can make different use of the features, thereby altering their importance. In general, highly flexible models would manage to make use of every relevant feature, regardless of its actual importance, and less flexible models would not be able to use any but the simplest and clearest pieces of information available.

H , λE and the net radiation have the highest mutual information with ϕ_m , of 0.28, 0.36 and 0.35 respectively, whereas the soil heat flux, rain and dew point have a MI of 0.17, 0.03 and 0.02; these scores are very well correlated with the respective effect sizes in table 4.9 ($r = 0.986$, $p = 0.012$). Similarly, the scores of the trend variables are all below 0.11. For comparison, the scores of L and ξ are 0.58 and 0.71. The high MI of H , λE and the radiation, and the low MI of rain and the dew point makes it unlikely that different models would manage (not to) make use of them. However, the soil heat flux has an intermediate mutual information score, thus it is possible that some other model would manage to successfully make use of it.

¹http://glossary.ametsoc.org/wiki/Richardson_number

Even though we showed that the dew point and the soil heat flux are not important predictors, we cannot rule out the possibility that the model was able to figure out the information contained in these features using features from earlier sets, or, on the contrary, needed features from later sets make sense of them. For example, the soil heat flux could have had an impact only when the model could relate it to the turbulent fluxes in F5. Similarly, perhaps the model was able to figure out the dew point by relating the air temperature and the net radiation with the soil heat flux (to estimate humidity). The opposite is also possible, namely these measures could have been not informative enough, and the model needed more features, such as the virtual temperature, to make sense of them.

Micro parameters

One of the biggest obstacles in applying the similarity theory lies in accurately measuring the quantities it relies on. Examples are the von Karman's constant κ , the roughness length z_0 , the turbulent fluxes H and λE , the friction velocity u_* , and so on. The advantage of using only macro parameters to predict ϕ_m is that accurately measuring these quantities becomes less important, in the sense that we can force models to find explanations that do not rely on them.

A downside of not using micro parameters is that the resulting models do not generalize well in conditions that are different to those presented in the training set, especially if it contains measures coming from a single location, such as in our case. Training with data coming from different locations would certainly produce more general models, as long as the data contains features that are informative and general enough to allow the model to differentiate between the different conditions. For example, the properties of the surface, such as its roughness, have a large impact on turbulence: what our model thinks is the normal behavior of turbulence might in fact be largely determined by the surface around the measurement site. But our model is completely unaware of the effect of the surface, so it might not be able to give accurate predictions at sites with different surface characteristics. See Beljaars (1982) and JW Verkaik (2006) for a discussion on how the obstacles around the Cabauw tower affect the flux-profile relationships measured there; in particular, the turbulence behaves differently depending on the wind direction. A training set with relevant features and diverse samples can alleviate this problem. For example, features could be extracted from satellite images of the surroundings; a very crude approach would be to classify the surface into one of several categories, and use a lookup table with precomputed roughness lengths.

5.1.3 Training Samples

As mentioned earlier, having training samples from multiple sites would certainly increase the generality of the models, but there are other sources of samples that can be used, too.

5.1. DISCUSSION

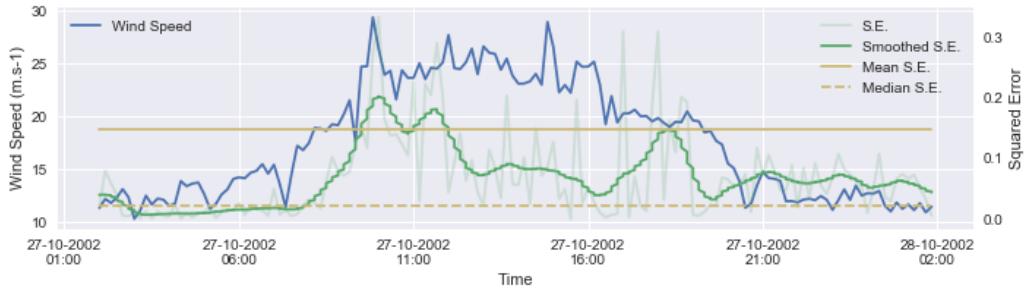


Figure 5.1: Wind speed and squared error during cyclone Jeanett (light green is the average of the three altitude levels, solid green is a smoothed time average of that). Throughout the storm, the error is larger than the median, and many peaks are larger than the mean. Moreover, the variations in the prediction seem to be larger, indicating that the model is less confident about its predictions.

Surface layer

Although the Cabauw tower takes measurements until 200 m, one of the issues we had to deal with is that the height of the surface layer is difficult to determine. We chose to use the measures at 10, 20 and 40 meters only, which comprise only half of the available data. There is evidence that some of the samples at 40 meters are anomalous: in figure 4.3h, the samples at 40 meters are clearly separated from the other two levels, which are well mixed, and in figure 4.5a there are some outliers in the range $-20 < \xi < 0$ that deviate significantly from the assumed relationship, and that could explain the difference between the coefficients found in the literature and those in table 4.4. These outliers mostly belong to the 40 m level. On the other hand, it is very likely that in some situations, especially in the afternoon and before sunset, the samples at 80 m, and perhaps even 100 m, are in the surface layer.

Altitude levels

In this project we used the same altitude levels at which measurements are taken at the Cabauw site. It is possible to generate synthetic samples at different altitude levels by interpolating the measures that change with height (i.e. wind speed, temperature, and humidity). This is not too hard, since we are already fitting a curve to the profiles of wind and temperature (see section 3.2.2), and becomes essential when building a training set with samples coming from different sources, and when training a model to be included in a simulation. For example, the atmospheric model of the GFDL-CM2 and CM3 only use wind and temperature at 30 m and at the surface to compute the turbulent fluxes (Anderson et al. 2004). One has to keep in mind, of course, that samples generated in such a way increase uncertainty in the resulting models, since the modeled profile might be different from the actual profile.

Surface type

Most GCMs use different parametrizations for land, ocean and sea-ice (Anderson et al. 2004, Donner et al. 2011, Gordon et al. 2000), since they behave very differently. This project was focused on land, but the same methodology can be used to develop models that work for the other surface types, too, provided that there is data.

Extreme weather events

Figure 4.4 shows the wind speed measured during cyclone Jeanett; these measurements are unique, since such extreme events are rare in Europe. This is the strongest cyclone in the dataset, but there are around 10 other events registering winds above 20 m s^{-1} , for a total of 654 samples, i.e. 0.04% of the total.

Figure 5.1 shows the prediction error during cyclone Jeanett: although the error increases during the storm, it is still at acceptable levels. The figure shows 432 samples, and, since the test set contained 134,044 samples, the average error is not determined only by this event. In fact, the average error without these samples decreases by less than 0.2%. This is pleasantly surprising, but it is impossible to guarantee that the models will be this well behaved in all circumstances.

5.1.4 Deployment

As mentioned in section 1.2, the point of this project is to produce estimators that, eventually, will replace the similarity theory in GCMs. It is therefore very important to develop models that can be easily integrated with such simulations.

Technology

The technologies (programming language, libraries and frameworks) used in this project are not necessarily the same that are used to develop in GCMs. Additional development effort is therefore needed to embed the predictors shown in this project in the simulators. To verify that this re-implementation is correct, the developers can run the same analyses that were performed in this project, and ensure they get the same results.

Performance

Current GCMs are computationally very demanding, and a single simulation requires weeks on specialized high performance clusters. Therefore, one of the requirements that were not considered in this project, but are of high practical relevance, is the performance of the estimator. Table 4.5 shows that a simple linear model is already more accurate than the similarity theory, and in appendix C.2 we further explore this aspect by presenting an ensemble of linear models whose performance rivals that of gradient boosted trees. This is a notable achievement since

5.2. RELATED WORK

the predictions from a linear model is obtained with a scalar product, therefore they have the potential to compete with the similarity theory in terms of computational complexity,

5.2 Related Work

Although there have been a number of works aimed at validating (Businger et al. 1971, Högström 1996, Dyer 1974, Yagüe et al. 2006) and extending (Grachev et al. 2007, Mcnaughton 2006, Wilson 2008, Hatfield et al. 2005) the similarity theory, to the best of our knowledge this is the first work that applies Machine Learning, instead of theories based on Physics, to predict turbulence parameters. However, there are some works that are similar, in spirit, to this one. As a reminder, our best results are a RMSE of $\sqrt{0.18} = 0.42$ and a correlation coefficient of $\sqrt{0.79} = 0.89$.

Ulden & Holtslag (1985) introduce two methods to compute u_* : either from the profile (the method used by Nieuwstadt (1978)) or by leveraging the surface energy budget. Venkatram (1980) then provides the empirical relationship $L \sim u_*^2$. The profile method is widely used in the literature, either directly or as a starting point, and uses the similarity theory to model the wind speed u at altitude z as

$$u(z) = \frac{u_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) + \beta \frac{z - z_0}{L} \right] \quad (5.2)$$

Irwin & Binkowski (1981) compare estimates of the Obukhov length computed using profiles and the Richardson number to its value computed with turbulent fluxes (i.e. equation 2.4).

Hurley & Luhar (2009) use TAPM to predict several turbulence parameters, including u_* , H and λE and compares them with the Cabauw data of 2005. TAPM is a simulation based on numerical solutions of equations of atmospheric flow, thermodynamics, moisture conservation, turbulence and dispersion on a horizontal grid that goes down to 300 m, and uses a parametrization of the momentum flux that improves upon the similarity theory in stable conditions. This gives predictions of u_* with an RMSE of 0.14 and a correlation of 0.76.

Weber (1999) predicts u_* using the standard deviations of the horizontal and vertical wind components $\overline{u'u'}^{1/2}$ and $\overline{v'v'}^{1/2}$, as well as the mean horizontal wind \bar{u} by doing a simple line fit, similarly to what we did in figure 4.2b. The resulting RMSEs are respectively 0.07, 0.07 and 0.1, although the data does not come from Cabauw.

Holtslag & van Westrhenen (1991) use the values computed by an atmospheric model at a grid point close to Cabauw to derive several boundary layer parameters, including u_* . Unfortunately, they only provide a chart comparing their predictions with the measurements, and conclude that "the agreement with model prediction and analyses is good" without giving any quantitative measure.

Nieuwstadt (1978) derives the wind profile from u_* , and predicts u_* by minimizing the squared difference between the reconstructed and true profiles. They

validate this method using measurements at the 20 m level of the Cabauw tower for three different wind directions, obtaining correlation coefficients of 0.84 for wind between South and West and 0.89 for wind between North and South-East.

Holtslag (1987) uses an iterative method to jointly estimate the Obukhov length, the sensible heat flux and the friction velocity. The procedure starts from an initial guess of L and iteratively refines the estimates, alternating improvements of u_* and H with improvements of L , while keeping the other variables fixed.

Most works are focused on the friction velocity, rather than the full momentum flux-profile relationship, and obtain errors that are between 20 and 40% of ours.² However, all of them are based on physical models with restrictive assumptions about stability, humidity, etc., and make extensive use of empirical constants and simplifying assumptions. In this light, our main contribution is to provide a model-free and assumption-free method of computing the momentum flux-profile relationship that works in all conditions.

5.3 Future Work

The path ahead is quite clear: by using more datasets, the models can be made general and applicable in a wider range of conditions, making them suitable to completely replace the component that predicts the turbulent fluxes in GCMs. Trying different machine learning techniques could also be important, since they can bring further performance improvements. Although we focused on the momentum flux-profile relationship, the similarity theory predicts similar relationships for temperature and moisture, as well: they need to be predicted, too, in order to produce a complete replacement. We tested the estimators on their predictive power, but the real test is to actually assess their impact when used in a GCM; this will pose a further challenge, since the samples will come from imperfect and approximate simulations instead of measurement instruments.

In appendix C, we outline some experiments that were performed, and that could form the basis for more advanced applications of Machine Learning to the prediction of the momentum flux-profile relationship.

²Keep in mind that our models had to predict the wind gradient, too.

Appendix A

Gradient Computation

Tables and charts supporting the arguments in section 4.2.

Table A.1: Pearson correlation coefficient between the gradients predicted by the different methods, divided by level. The FD gradient is poorly correlated with the other two methods at the 10 meters level, but is very well correlated with the LG gradient at the other levels. The LG and GP gradients disagree on the lower levels, but it appears their predictions converge as altitude increases.

z	FD / GP	LG / FD	LG / GP
10	0.192	0.480	0.317
20	0.645	0.991	0.640
40	0.863	0.981	0.835

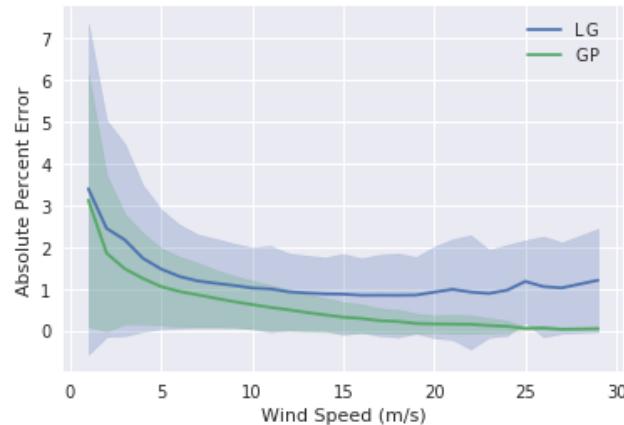


Figure A.1: Mean absolute percent error of the wind modeled by the LG and GP models as a function of the true wind speed; the shaded regions enclose the average plus or minus the standard deviation. Also see figure A.2.

APPENDIX A. GRADIENT COMPUTATION

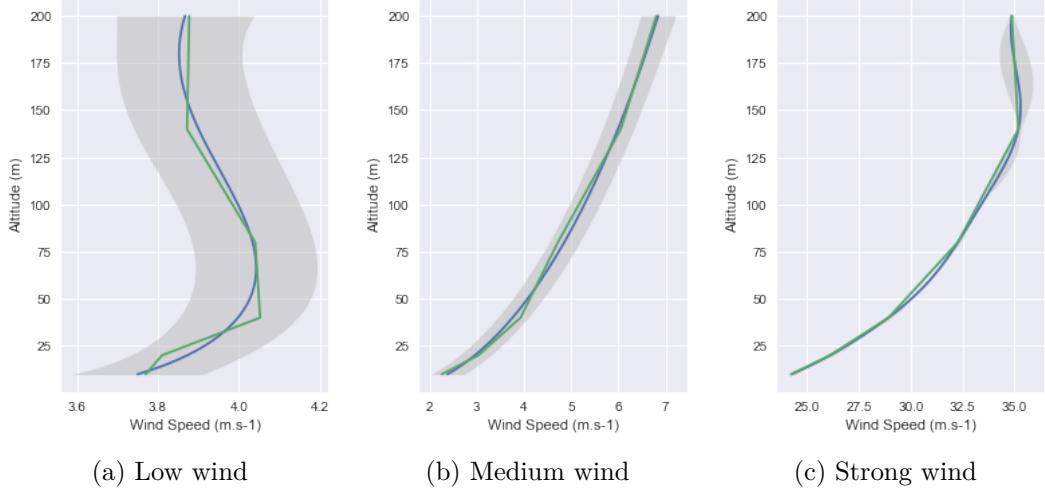


Figure A.2: Profile predicted by GP as the wind speed increases.

Table A.2: MSE obtained on two datasets when predicting ϕ_m using the commonly accepted momentum flux-profile relationship (equation 2.6) for the three methods of computing the gradient. The errors in the second line were computed after discarding the data at the 10 meters level, because we argued the FD method is not reliable in that situation.

	MSE (MOST Dataset)	MSE (Full dataset)
FD	1.994	9.322
FD (z is 20/40)	0.627	11.832
LG	0.660	8.498
GP	1.213	8.899

Table A.3: Absolute percent error of the wind speed modeled by the LG and GP methods at each altitude level. The altitude does not affect the error, and the GP wind speed is closer to the true wind speed than the LG model in the vast majority of cases, although the difference is negligible, often less than a few percents.

	z=10		z=20		z=40	
	LG	GP	LG	GP	LG	GP
Mean	1.23	1.03	2.26	1.42	1.39	1.04
Std.	1.40	1.12	2.34	1.47	1.48	1.12
Min.	0.00	0.00	0.00	0.00	0.00	0.00
25%	0.37	0.32	0.74	0.46	0.47	0.3
50%	0.82	0.76	1.62	1.06	1.03	0.73
75%	1.55	1.42	2.96	1.97	1.84	1.41
Max.	53.75	212.4	106.56	192.94	80.35	43.47

Appendix B

Hyper-Parameters

This appendix lists the hyper-parameters that were found in the nested CV procedure, as well as the MSE on the corresponding validation fold, for the MOST estimator (tables B.1 and B.2) and those estimators that performed better than it, specifically the Ridge estimator on the MOST dataset (table B.3) and the GBT estimator on both datasets (tables B.4 and B.5).

Regularization for the MOST estimator is always very low, in the order of 10^{-4} and 10^{-5} . This is not surprising, considering its high bias. We remind the reader that the primary purpose of nested CV is *not* to identify the optimal hyper-parameters; however, inspecting their values can give useful indications on possible improvements and fallacies of the algorithms.

Table B.1: Optimized hyper-parameters and validation MSE for the MOST estimator on the MOST dataset for each outer fold of nested CV.

	1	2	3	4	5	6	7	8	9	10
(MSE)	0.30	0.31	0.33	0.34	0.31	0.31	0.34	0.33	0.29	0.34
Reg.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table B.2: Optimized hyper-parameters and validation MSE for the MOST estimator on the full dataset for each outer fold of nested CV.

	1	2	3	4	5	6	7	8	9	10
(MSE)	0.63	0.58	0.63	0.60	0.62	0.63	0.67	0.71	0.64	0.64
Reg.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

APPENDIX B. HYPER-PARAMETERS

Table B.3: Optimized hyper-parameters and validation MSE for the Ridge estimator on the MOST dataset for each outer fold of nested CV.

	1	2	3	4	5	6	7	8	9	10
(MSE)	0.30	0.29	0.28	0.28	0.28	0.28	0.26	0.24	0.24	0.28
Alpha	6.97	5.46	7.00	3.64	3.21	3.94	2.83	4.59	4.25	2.01

Table B.4: Optimized hyper-parameters and validation MSE for the GBT estimator on the MOST dataset for each outer fold of nested CV.

	1	2	3	4	5	6	7	8	9	10
(MSE)	0.18	0.17	0.18	0.17	0.16	0.22	0.18	0.16	0.16	0.18
Alpha	0.22	-	-	0.38	-	0.10	-	-	0.44	0.71
Depth	8	7	8	7	7	4	8	9	7	5
Feat.	0.86	0.70	0.57	0.74	0.72	0.40	0.68	0.38	0.62	0.61
L.R.	0.07	0.10	0.03	0.10	0.07	0.05	0.05	0.05	0.10	0.05
Loss	Hu	LAD	LS	Hu	LS	Hu	LS	LAD	Hu	Hu
Subs.	0.28	0.85	0.74	0.83	0.55	0.54	0.47	0.56	0.30	0.62
Trees	447	425	738	327	622	276	294	235	941	692

Table B.5: Optimized hyper-parameters and validation MSE for the GBT estimator on the full dataset for each outer fold of nested CV.

	1	2	3	4	5	6	7	8	9	10
(MSE)	0.31	0.36	0.37	0.42	0.37	0.33	0.40	0.34	0.32	0.40
Alpha	0.18	-	0.83	0.32	-	-	0.64	-	-	-
Depth	7	5	6	8	6	5	6	9	8	7
Feat.	0.99	0.66	0.88	0.24	0.77	0.94	0.44	0.69	0.84	0.39
L.R.	0.09	0.05	0.02	0.09	0.05	0.08	0.05	0.09	0.07	0.07
Loss	Hu	LS	Hu	Hu	LS	LS	Hu	LS	LS	LAD
Subs.	0.48	0.90	0.57	0.94	0.90	0.94	0.94	0.91	0.29	0.91
Trees	807	574	728	164	775	656	413	101	107	203

Appendix C

Further Experiments

In this appendix, we briefly describe some experiments that approach the problem using more advanced Machine Learning techniques. In section C.1 we use deep neural networks, section C.2 uses an ensemble of linear models, and section C.3 uses more advanced hyper-parameters optimization techniques.

C.1 Prediction with Deep Neural Networks

The reason why this is not included in the main report is that time and resources constraint prevented a formal and thorough evaluation of these results. That said, this approach is definitely promising and worth pursuing in the future.

Methods: The features were obtained in the same way as for the other estimators discussed in the main report. The validation set used all the samples belonging to 18 months, and a new random validation set was created for every experiment performed. The configuration of the networks was obtained manually:

- **Architecture:** Fully connected layers only, number of neurons halved at every layer. The first layer with 1 neuron was the output layer, and the first hidden layer had either 128, 256 or 512 neurons, resulting in 7 to 9 hidden layers;
- **Activation Function:** linear for the output layer, PReLU (He et al. 2015) for the hidden layers;
- **Regularization:** Dropout ($p = 0.5$, only when the first layer had 256 neurons or more);
- **Optimizer:** Adam (Kingma & Ba 2014) with initial learning rate 10^{-3} ;
- **Batch Size:** 1024 (1165 batches per epoch);
- **Learning Rate Schedule:** Divide by 10 if the validation loss had not decreased by at least 10^{-4} in the last 10 epochs;

APPENDIX C. FURTHER EXPERIMENTS

Table C.1: MSE obtained by neural networks compared to the MOST estimator and gradient boosted trees. The features included the trend.

Dataset	MOST	GBT	F1	F2	F3	F4	F5
Full	0.64	0.36	0.31	0.29	0.26	0.24	0.21
MOST	0.32	0.18	-	-	-	-	0.13

- **Early Stopping:** if the validation error did not improve in the last 25 epochs, or if the learning rate was reduced below 10^{-6} .

Results: The results are shown in table C.1. Neural networks show promising results, but one needs to keep in mind the anecdotal nature of these results, since they are a point estimate, and not an average of different validation scores.

Other experiments were performed using all the observations in the hour preceding the sample to predict, and using up to three GRU layers, followed by up to four fully connected layers, with the other parameters as detailed above. The performances were discouraging, with the network struggling to go below 0.15/0.20 training MSE and 0.7/0.8 validation MSE on F4 and full dataset.

C.2 Prediction with an Ensemble of Linear Models

We can relax the constraints needed to answer the research questions, in particular the second one, and perform additional feature engineering. In order to minimize the computational resources needed, we apply Ridge linear regression to the MOST dataset.

Methods: Instead of restricting ourselves to the five feature sets, we use all the quantities shown in table 4.1, except for the turbulent heat fluxes, and, in light of the results shown in the main report, we do not use the trend. We add polynomial features, then standardize the dataset, apply PCA, and fit the Ridge estimator. This whole procedure, including feature engineering, is performed separately for a number of random subsets of samples (with replacement) and features, and the final prediction is the average of the predictions obtained by the different models. We then optimize the parameters of every steps with random search and cross validation. This means that, although all the steps share the same hyper-parameters, they are fit on different subsets of the full dataset, and thus have different parameters. This improves generalization, since the best performing hyper-parameters were able to extract good features and use them to obtain good predictions on different independent subsets. Table C.2 shows the distribution of the hyper-parameters, which were optimized with 10-fold cross validation by sampling 250 values, as well as the optimal values found in the procedure.

C.3. MORE HYPER-PARAMETER OPTIMIZATION

Table C.2: Distribution of the hyper-parameters used in the random search and optimal value found.

	Hyper-P.	Distribution	Values	Optimal
Base Est.	Polynomial Degree	Uniform	1 or 2	2
	Polynomial Interactions	Uniform	Yes or No	Yes
	PCA Target Dimension	Uniform	2 to 19	19
	Ridge Regularization	Log ₁₀ -uniform	10 ⁻⁷ to 10 ¹	2 × 10 ⁻⁵
Bag Est.	Number of B.E.	Uniform	5 to 100	13
	Samples per B.E.	Uniform	5% to 25%	11%
	Features per E.E.	Uniform	4 to 20	20

Results: The average MSE obtained on the 10 validation folds is 0.187 with a standard deviation of 0.022, which is just slightly worse than the best results obtained by the gradient boosted trees on F3. All the other metrics are within one standard deviation, too.

Discussion: The linear models use all the available features, and the effect of PCA is only to decorrelate the features. However, they use few samples and weak regularization; in spite of this, the MSE on the training folds is almost identical to the MSE on the validation folds, indicating that the linear models do not overfit and suggesting that the ensemble is not needed to reduce variance.

C.3 More Hyper-parameter Optimization

By foregoing nested cross-validation and focusing on a particular dataset (MOST) and set of features (table 4.1 without H and λE), we can reduce the computational resources needed for more involved hyper-parameter tuning procedures.

Methods: We optimized the hyper-parameters of extreme gradient boosted trees (Chen & Guestrin 2016) using both HyperBand (Li et al. 2017) and the Python library GPyOpt.¹ For Hyperband, we use the default parameters suggested in the paper, i.e. $\eta = 3$ and $R = 81$, with each unit of budget corresponding to 15 trees. The Bayesian optimization procedure is based on Gaussian Processes with the RBF kernel, using the integrated expected improvement as acquisition function. Integration is performed over the posterior of the hyper-parameters, approximated with MCMC sampling (Snoek et al. 2012), in order to improve the accuracy of the proposed hyper-parameters. The dataset was randomly split in three smaller sets: a training set of 162 months, a validation set of 20 months, and a test set of 20 months. The training set was used to train the models, and the hyper-parameter

¹<http://github.com/SheffieldML/GPyOpt>

APPENDIX C. FURTHER EXPERIMENTS

Table C.3: Distribution of the hyper-parameters used and best values found by the two optimization procedures. NoT is the number of trees, LR the learning rate, MCW the minimum child weight, γ the minimum decrease in loss for adding a new split, and NoF the number of features.

Hyper-P.	Distribution	Range	Best (Hyperband)	Best (GPyOpt)
NoT	Log ₁₀ -Uniform	10^1 to 10^3	1000	1000
LR	Log ₁₀ -Uniform	10^{-4} to 10^0	8.86×10^{-3}	4.34×10^{-2}
Max. Depth	Uniform	2 to 12	12	12
MCW	Uniform	1 to 10	9	10
Subsample	Uniform	10% to 100%	64.6%	49.3%
γ	Uniform	0 to 1	0.194	0
α (L1 reg.)	Log ₁₀ -Uniform	10^{-20} to 10^0	1.87×10^{-11}	1.70×10^{-7}
λ (L2 reg.)	Log ₁₀ -Uniform	10^{-20} to 10^0	2.46×10^{-10}	5.96×10^{-5}
NoF	Uniform	10% to 100%	22.7%	12.5%
Loss	Uniform	MSE or MAE	MAE	MAE

optimization procedure optimized the scores on the validation set; the test set is used at the end to evaluate the optimal configuration. Table C.3 shows the distribution of the hyper-parameters used in the search, and the optimal values found by the two methods.

Results: The MSEs of the best configuration found by Hyperband, after 200 steps, were 0.08250, 0.1613, and 0.1676 on the training set, validation set, and test set respectively. The scores of best configuration found by GPyOpt, after 18 steps, were 0.04756, 0.1606, and 0.1670. These results are very similar to what was obtained with random search and nested cross validation. Informal experiments show that these parameters also yield comparable performance on the full dataset.

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