

BUILDING A FOUNDATION FOR PROFITABLE DIGITAL TRANSFORMATION IN SCI-TECH R&D

Artificial intelligence may be hot right now, but the smart money is investing in data

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Everywhere you look these days, it seems someone is talking about the impact of digital technologies on the future of your industry.

It is the story on every magazine cover and the keynote topic at every conference. Artificial intelligence, machine learning, natural language processing, deep learning, big data, blockchain, data science, predictive analytics, smart machines – the sheer volume of digitalization buzzwords can leave one dizzy. Worse yet, overhyped benefits or a poorly considered digital strategy can lead to a crisis born from disappointing returns and unmet expectations. Within the next decade, it is predicted that **70 percent of businesses will attempt to transform themselves digitally,¹ but only 30 percent will succeed.** These daunting statistics reveal both the competitive urgency and the investment risks inherent in undertaking a digital transformation.

With almost all leading R&D organizations perceiving that digital technologies should be a priority for their business, it is paramount to fully understand the opportunities and risks of digitalization so that you can make smart investments when implementing these programs. This whitepaper discusses the current state of digitalization in R&D, outlines the realistic benefits your organization can achieve through digital transformation, and provides advice for ways you can ensure a solid basis for long-term digital success while avoiding common pitfalls.

WHAT IS DIGITALIZATION?

Digitalization (aka digital transformation) is the implementation of digital technologies such as artificial intelligence (AI), machine learning, and predictive analytics to improve business outcomes, processes, and/or profitability. Though often used interchangeably, digitalization should not be confused with digitization (the act of converting analog data into a digital format), which is often a critical component of a larger digitalization project.

70%
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TRANSFORM THEMSELVES DIGITALLY**

30%
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THE DISRUPTIVE PROMISE OF DIGITAL TECHNOLOGIES

All of the hype about digitalization is not without good reason. Well-implemented investments in digital initiatives are already delivering significant returns across a wide range of disciplines, from drug delivery to agriculture.

For example, over the past few years a number of highly publicized incidents and recalls have tainted the promise of lithium-ion battery technology due to the flammability of the liquid electrolyte required. However, a predictive AI-derived model built at Stanford expedited the path to finding innovative solutions² by supporting rapid screening of over 12,000 solid electrolyte alternatives, allowing researchers to rapidly identify 21 highest potential materials for full laboratory testing. In this case, AI is supporting increased safety, while greatly reducing the time and investment required in the R&D process to achieve it.

Blue River's LettuceBot,³ is another AI implementation that has delivered immediate return for its inventors. This technology is revolutionizing agriculture by reducing pesticide and fertilizer use. After analyzing a massive dataset of plant images, this technology can differentiate crops from weeds, and assess the health of a crop plant to determine if fertilizer or pesticide is needed and the optimal application dose. When integrated with agricultural equipment in the field, the outcome is an increased margin for farmers and environmental benefits for the local watershed as well.

In the drug discovery realm, a team of graduate students and faculty from the University of Toronto won a contest held by Merck to identify molecules that could lead to new drugs by using deep learning to zero in on the molecules most likely to bind to their targets.⁴



AI will also soon be helping organic chemists synthesize those drug molecules more efficiently when CAS launches retrosynthetic capabilities based on ChemPlanner⁵ in SciFinderⁿ. This technology will help organic chemists find and compare possible novel synthetic pathways to speed up drug discovery.⁶

These early success stories show the potential of emerging digital technologies to solve critical problems and enhance business outcomes. But really the digitalization wave is just getting started, and the potential impact of these technologies for R&D-focused organizations is astounding. Have you considered the possibilities in your organization and industry?

Digitalization programs can deliver a wide array of competitive advantages for the companies that implement them successfully. While some seek to reduce operational costs, free up human time to work on more complex tasks or gain other workflow efficiencies, others are focusing digitalization efforts on driving innovation and finding new opportunities. There is a wide array of potential applications within the technical,

operational and business programs of R&D-focused organizations. Additionally, a comprehensive program of digitalization helps form connections between the technical, operational and business functions that allow companies to evolve in real time to keep pace with the dynamic market.

Let's consider, for example, a global animal health company that has traditionally held a leading market position in agricultural feed and medicine and has recently launched a line of holistic foods for companion animals (pets). A company such as this could benefit from implementing digitalization programs in a number of ways. For example, as consumer preferences shift toward organic foods and meat raised without antibiotics, they may need to accelerate their innovation cycle to maintain market leadership and identify other products that can help keep livestock healthy without antibiotics. They would likely also benefit from applying digital technologies to optimizing the efficiency of their pet food manufacturing processes, as margins are slim and any efficiencies they can gain would provide an important advantage. Finally, they may want to optimize their product mix and strategy by predicting demand curves in various global markets based on demographic and market data.

This example shows tangible digitalization projects an R&D-focused company such as this could seek to implement in a reasonable timeframe that could provide a significant positive impact for their business success.



HEADWINDS SLOWING DIGITALIZATION IN SCI-TECH R&D

With two-thirds of the CEOs of Global 2000 companies⁷ placing digital transformation at the center of their corporate strategy, this digital revolution is poised to permanently change industries worldwide.

While interest in digitalization is at an all-time high, and opportunities are many, most companies report that they feel behind the curve or are not ready to take advantage of current digital technologies. If you are in that boat, you are not alone. In truth, many organizations report struggling with where to begin. A recent Gartner survey showed that **59% of organizations are still gathering information to build their AI strategies.**⁸ Further, a more targeted Accenture survey of US and European R&D top executives at pharmaceutical firms⁹ showed that **55% classified their organization's degree of digital technology adoption as "already adopting", while 42% characterized their firm's situation as "exploring", and 3% are "waiting and seeing".** A similar survey of life science professionals by the Pistoia Alliance¹⁰ reported that **44% of respondents are already using or experimenting with AI.**

Multiple factors are creating headwinds to digitalization progress. First, there is a plethora of potential opportunity and a never-ending supply of data, which can make it hard to decide where it is best to focus investment. Also, the required initial investments are high and **current success rates are estimated to be as low as 15%,¹¹** making it difficult to justify a positive ROI projection on many of these projects. Further, sci-tech leaders acknowledge they are facing daunting gaps in areas such as technology, talent, knowledge, resources, content and culture. In fact, **27% of companies cite a skills gap¹² as a major impediment to data initiatives.** Also, with digital technologies evolving so rapidly, if not carefully considered, a project that begins today could already be out of date by the time it is completed.

When facing all these challenges, it is not surprising that some leaders are staying on the sidelines, hesitant to jump into a digital transformation. However, not doing so could put your organization at a competitive disadvantage. In the following sections, we will provide suggestions based on our experience to help you invest wisely and realistically, outline some of the pitfalls to watch out for, and show how, with a robust system in place, the right digitalization projects can help you gain a competitive edge in the marketplace.



27%

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TO DATA INITIATIVES**



SUCCESSFUL DIGITALIZATION STARTS WITH THE DATA

The largest and most fundamental need in the hierarchy of digitalization is data. Having a robust data foundation is crucial for implementation of digital technologies like AI, predictive analytics, and machine learning. However, respondents to the Pistoia Alliance survey¹⁰ stated that access to data and data quality were two of the biggest barriers to digitalization projects such as AI and machine learning within their organisation.

Data science adviser Monica Rogati discusses the importance of a healthy data foundation in more detail in an article on the data science hierarchy of needs.¹³ Rogati suggests these elements take the form of a pyramid: data collection sits at the bottom as the fundamental first step, followed by data storage, exploration/transformation, aggregation, labelling and finally optimization. Only after these steps have been considered and implemented can technology such as an AI algorithm begin to extract meaning from the dataset.

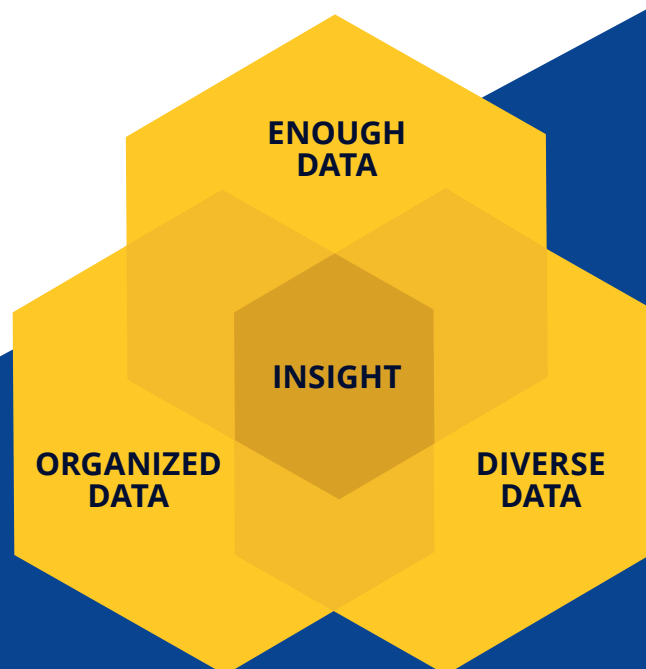
Thus, building a high-quality data foundation for your organization is the first step to take when initiating a digital transformation. The definition of what makes data “high-quality” is broad, but we’ve identified three main factors to consider when

initiating a data collection process: have enough data, make sure the data collection is sufficiently diverse to meet your objectives, and then structure and curate the collection carefully.



YOU LIKELY NEED MORE DATA THAN YOU THINK

A first priority for your sci-tech R&D company to consider is that it must have enough data – both quantity and richness are important. Digital technologies are hungry for as much data as you can give them, because it is only with a large dataset that they can come to accurate conclusions. As an example, **facial recognition software from Facebook now has an accuracy rate of 97.35 percent,¹⁴** which is closely approaching human performance, but this achievement was only made possible by giving the system access to a dataset of 4 million Facebook users. In a chemistry example, a deep learning neural network was trained on 50,000 crystal structures¹⁵ of inorganic materials to acquire the ability to recognize chemical similarities and predict new materials.



The amount of data your sci-tech R&D company will need depends on the complexity of the problems you are trying to tackle. In other words, the depth and breadth of data you have readily available will determine which AI applications are even achievable. As an example, machine learning requires parameters to train a model – a simple model with a few thousand parameters will require much less data than a model with several million parameters. In cases like this, **the difference between models could require 100 or 1000 times as much data to effectively train it**, so one must consider the needs of your intended future applications when defining your data requirements.

It is also important to have sufficient depth in key areas that are most important to your industry, as sparse data in an important segment could greatly hinder your success. For example, if the animal health company mentioned earlier had a large data collection in the agricultural space, as a result of their long-term work in that segment, but lacked sufficient data on their target growth segment, companion animals, any conclusions drawn from the data could lack relevance for their new segment hindering their growth opportunity.

If a lack of relevant data is a problem, it is possible to acquire, license, or borrow additional datasets

from commercial partners, government sources, or public repositories. Partnering in this way expedites the process of data collection and data structuring, which can often be the limiting factors in digitalization; licensed data has usually already crossed the many data barriers that are commonly encountered, so you don't have to. There is also emerging research on applying deep learning when only small amounts of data are available,¹⁶ such as during early stage drug discovery.



DATA DIVERSITY DRIVES INNOVATION AND OPPORTUNITY

Having a broad and deep data collection related to an organization's core competencies and markets is critical. However, if you intend to use digital technologies to look for growth and innovation opportunities, diversity of data is also very important. If all the data you have is about an area you already know well, technologies such as network analysis or AI are not likely to find you many new opportunities. Thus, it is important to identify and include data collections that are adjacent to your core focus.



THE DIFFERENCE BETWEEN MODELS COULD REQUIRE

100 OR 1000

TIMES AS MUCH DATA

If we again consider the animal health example, such an organization may have lots of data on agriculture and companion animals but may also derive value from data about zoo animals or wild animals. They may also want to look to studies of human patients that may have relevance in some areas. It may even be valuable to look farther afield into materials data that could support innovation in areas such as drug delivery or veterinary medical devices that may provide other long-term growth paths for the company. To assess these growth opportunities, market and financial data are likely to also be required for these new markets.

As discussed above, a data acquisition strategy is often needed to bring greater diversity to your data collection. The sources for these new types of data may be very different than those an organization has traditionally pulled from, and there are many approaches depending on your needs. The terminology or format used may not match up with that which is common in your core fields, thus necessitating curation to allow the data to be married seamlessly.

Though the volume and diversity of data needed for your intended long-term applications of digital technologies may feel like a daunting mountain to climb, the good news is that you don't have to do it all at once. Your data collection is something you can continue building over time to address the needs of your evolving organization. The key is to identify any gaps and prioritize filling them in tandem with choosing the specific digitalization projects and targets you will pursue to ensure you have the necessary data to make those projects successful. It is important to ensure that the cost to acquire any additional data needed is incorporated in the overall ROI assessment of each digitalization project.

WELL ORGANIZED DATA IS THE KEY TO EFFICIENT IMPLEMENTATION

Having large amounts of relevant, diverse data is advantageous for digitalization purposes, but to be useful for drawing actionable insights, it is crucial



that the data are well organized. In this case, organization encompasses building an overarching data structure and curating and cleaning up the specific data to be effective within that structure. These steps of data maintenance and management add real value to your data collection that would otherwise go unrealized and save valuable time when implementing technology later. The sheer amount of relevant data that can be sourced means that indexing and standardization are becoming more crucial for knowledge extraction than ever before.¹⁷ In the end, the quality of the insights you can extract directly depends on the robustness of your curation process and the quality of the resulting data collection.

The first step is developing an extensible data structure or data model that creates a common framework into which data will fit and a common language to describe the data elements. This can be particularly challenging for R&D companies, as scientific data is uniquely complex and often disconnected. For example, if we consider the case of the animal health company again, relevant data elements that must be accounted for include: text content, chemical structures, drug/target relationships, taxonomic animal names (kingdom, phylum, genus etc.), financial values, along with schematics, graphs and charts, and many others. It is important that data models are detailed enough to provide clarity and utility while allowing for flexibility to evolve and augment data for what will be a numerous and diverse set descriptive and predictive efforts over time.

Data modeling provides a standard mechanism of defining and analyzing data within an organization. These investments pay off in the form of increased data use and lower costs when leveraging data assets. Business analysts, researchers, engineers, and managers will have access and clarity on data elements and how they relate to one another. Developers, testers, and technologists can efficiently integrate data for internal systems and external products. Without published and well-maintained models your ability to get value from your data will be limited and more expensive.

While statistical analyses and computational algorithms can be of some use in organizing and enriching your large datasets, it is important that you also allow for human curation within your data governance process as well. Human auditing of data collections is critical to validating and correcting errors. Data quality issues can introduce bias, noise, or lead to low model accuracy. Furthermore, scientists and technicians with experience in relevant fields such as chemistry, biology, and data science can extract and interpret information elements that AI cannot. This type of intellectual indexing requires greater investment, but also makes critical data far more valuable and useful for many years to come. Partnering with an

organization, such as CAS, that can provide human expertise and technology resources specialized for indexing and curating of sci-tech content can often allow this important process to be achieved more quickly and cost effectively.



PLANNING FOR MAINTENANCE ENSURES LONG-TERM SUCCESS

Just like a home or a vehicle, your data collection requires maintenance to preserve its value over time. Key activities include hardware maintenance, database software upgrades, data model updates, and referential and entity consistency checks. External expertise is often valuable in structuring and executing a long-term maintenance and governance model for your data collection to ensure it remains up to date and compatible with the newest technologies.

To ensure that maintenance of your collection is allotted appropriate resources, include costs for this on-going need in your project financials. It is also important to ensure clear ownership and accountability for content maintenance and on-going acquisition in the long term among the business, technology, research, and other stakeholders that utilize the data collection.

KEY TAKEAWAY

Though development of your dataset can feel like a blocker to progress, it is a foundational investment that is vital to the success of any digitalization project. Though the newest digital technologies get all the attention, today's smart investment is to start with the data. Specifically, it is necessary to ensure you have enough data breadth and depth, a diverse data set covering core areas as well as adjacent opportunity areas, and that your data is well organized and curated to maximize its utility and project efficiency.

This is really a case of go slow now, to go fast later. Big data technology is evolving rapidly and will continue to change frequently.

However, **a solidly built data foundation will continue to pay dividends into the future** and allow you to more efficiently implement each new technology as it comes along. That is a sustainable advantage that will continue to provide return over and over for many years to come.

If timelines are tight and patience for technology implementation is short, consider consulting external expertise to build your data foundation more quickly. Outsourcing for expertise lets you model your approach from similar datasets to accelerate your project, offer new insights to your desired outcome, and ensure a stable foundation for digitalization.

ADDITIONAL STRATEGIC CONSIDERATIONS FOR DIGITALIZATION IN R&D ORGANIZATIONS

Digitalization offers an opportunity to enhance your business in many ways, but only if the entire workforce, including leadership, has a shared vision of these opportunities and the desired outcome that helps them embrace the digital mindset, and a commitment to the on-going investment required.

Almost as important as building the data collection and implementing the technology is fully integrating these capabilities and the related processes into the culture of your organization to maximize the return on your investments. Too often, misinformation surrounding digitalization can put the success of digital projects at risk. In fact, **despite 86% of enterprise decision makers⁷ feeling that their digitalization efforts must have an impact within two years to avoid financial ramifications, only 38% of executives¹² strongly feel that their business leaders are currently taking full advantage of their existing initiatives.** To build a robust foundation for successful organizational outcomes, leaders and decision makers must understand the importance of managing organizational expectations and implementing necessary change management processes to ensure organizational alignment at all levels.



DON'T LET UNREALISTIC EXPECTATIONS GET A FOOTHOLD

Digital technology strategies have a key commonality with your product, marketing, or overall business strategy – you have to have a clear vision of what you want to accomplish before you set out a plan. Digital technologies are certainly powerful, but sometimes they can be perceived as the proverbial genie in a bottle that can grant all wishes.



**STRATEGIC
CONSIDERATIONS**

**DATA
CONSIDERATIONS**

Strategic considerations, alongside data considerations form the foundations of digitalization success

The truth is that AI, machine learning, or digital analytics are not a cure-all for a sparse innovation pipeline or an all-encompassing solution to inefficiency or productivity problems.¹⁸ These technologies can, however, provide important gains in these areas when used in a targeted way.

If allowed to persist, unrealistic expectations can lead organizations to execute an overly broad implementation of digital technologies that target many business challenges simultaneously.¹⁹ These projects often struggle to serve a diverse set of stakeholders and fail to deliver meaningful ROI by spreading their focus too wide. Instead, selective and careful application of these technologies is key. By focusing your resources on what differentiates your business from others, you can extend your advantage in that area.

In order to manage organizational expectations around digitalization projects, make sure to gain

alignment around clear and measurable goals. Then manage scope creep aggressively. Also, beware of overhyping the potential outcomes and benefits when justifying budget allocation. Though this may help make your case for funding stronger at the time, if that vision cannot be realized it will come back to bite you later.



DON'T PUT EXCESSIVE TRUST IN THE DATA

The real power of digital technologies is that they allow your company to perform high-volume, high-accuracy functions not possible with traditional programming, which allows far more possibilities to be considered and compared. AI is adept at assessing and analyzing data to find patterns far more quickly than people can, but it can't make complex judgements and business decisions that require incorporation of broader context that would be simple for a human. Instead, its purpose is to execute on proven methodologies that don't require higher-level human intelligence, so that the user is free to perform other, more cognitive pursuits, such as formulating R&D strategies and critical thinking.

The input data feeding the algorithms and models which underpin these technologies are often extremely dynamic and influenced by a multitude of changing external factors.

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If your data is not carefully monitored and maintained, these changes can cause failures, or more concerning will silently erode the accuracy and effectiveness of the system over time. In this way, blind reliance on a purely AI-generated conclusion can be risky, so you should take reasonable steps to ensure the data in the pipeline is fresh and is monitored via human oversight on an on-going basis.

It is very important that the people across the ranks of an organization undergoing digital transformation understand these realities. This is important for two reasons. First, it will give those utilizing results from these systems confidence to question the conclusions if they have concerns. Creating a situation wherein humans feel uncomfortable questioning AI data poses big risks for your organization and also demotivates your staff.

Second, understanding the limitations of digital technologies addresses one of the biggest misconceptions that often arises during digital transformation – the perception that the goal of these projects is to replace humans with “smart machines”. This concern is common and can be very detrimental to organizations achieving the full potential of their digital investments. If the people fear the technology, they are likely to do whatever they can to oppose it. Alternatively, if they see value in the results and believe that it will make their work more interesting and their organization more successful, they are likely to embrace it.

Thus, making sure human intellect remains respected and encouraging teams to remain open to, but also skeptical of, AI-generated conclusions is a key pillar of successful digital transformation.



COMMUNICATE EFFECTIVELY TO GAIN ALIGNMENT

One of the most fundamental tenants to change management in any organizational context is communicate, communicate, communicate. The bigger your company, the harder it is to ensure alignment around common objectives and expectations for digital transformation and the role of each unit in making that vision a success.

In the case of digitalization in R&D organizations, this is particularly important as many different stakeholders from areas such as technology, business, and research are usually involved in delivering the return on these investments. Beyond the cultural concerns and misconceptions noted above, organizational silos and disagreements often arise that can make implementation of digitalization projects particularly problematic. These can surface as arguments over data structures and guidelines that may require some units to change long-standing practices. It can also present as data hoarding, wherein groups are resistant to sharing data repositories they have built with the broader project.

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To minimize the impact of these and similar types of resistance, first broadly communicate about the “Why?” of the project. What needs, internal and external, are driving the project and how will the organization and individuals benefit from the outcomes? What does success look like 1, 3, and 5 years from now? Be sure to address “What’s in it for me?”

Once you can measurably demonstrate that your organization understands the vision, next comes the “How?”. It is important that your digitalization approach and related processes, data guidelines, etc. are universally understood and adopted, keeping in mind that it is important not only to communicate what will change, but also what will stay the same. Effective documentation of key requirements, specifications, and timelines is very helpful to ensure alignment for the project. Published data catalogs and data models are often a good first step. CAS has also successfully utilized a “data steward” role on key projects as a sort of “translator” to help departments within the organization map their content and processes to new models.

A key pitfall to avoid is un-resourced mandates. Asking stakeholders to make major changes to their processes without providing the support needed to achieve these targets on the desired timeline is likely to cause frustration, resistance, and delays in your project. To avoid this situation, to the extent they can be anticipated these costs should also be included in your initial project proposal and ROI.

KEY TAKEAWAY

To ensure organizational alignment around digitization projects, it is critical to manage expectations and ensure broad awareness of benefits and limitations. Clear communication of the why and the how, along with thorough documentation, can optimize implementation commitment and efficiency to maximize the return and impact of your organization's investment.

CONCLUSION

The wheels of digitalization are already in motion. As such, science and technology R&D companies need to adjust their strategies and invest accordingly, or risk disruption from competitors that have fully embraced these digital opportunities. To ensure a positive return on these digitalization investments, company leaders and decision makers must plot a careful strategy and implement best practices around data and management.

First, invest in building a robust data collection that is abundant and diverse enough to fully encompass your digitalization opportunity space. Then invest the time to structure and curate that data to maximize the value that can be efficiently gained from it and optimize the speed of future project implementations. Finally, allot appropriate resources to support on-going data maintenance to maintain quality and timeliness, and ensure clear accountability for those tasks. This whole effort can be time consuming and costly for a company without digitalization expertise or specialized technology. Therefore, relying on an experienced partner, such as CAS, to help address your data needs, can give you a head start in your digitalization program.

Beyond the data and technology, it is critical to engage all employees with your digital strategy and vision for the potential of these technologies to transform your organization. Ensuring widespread understanding of the capabilities, limitations and benefits of such projects is critical to ensuring uptake and success. These strategic and cultural aspects can be just as challenging as the technology build itself and are often overlooked, especially for companies with a longstanding history of success in the previous analog paradigm.

These elements will provide your organization with a strong foundation for a successful digitalization strategy to drive efficiency, accelerate innovation and deliver real differentiating competitive advantages to your business. Once they are in place, you will be ready to implement each wave of technology as advances continue to constantly keep your organization ahead of the curve.

1

**INVEST IN BUILDING
A ROBUST
DATA COLLECTION**

2

**TAKE TIME
TO STRUCTURE AND
CURATE THAT DATA**

3

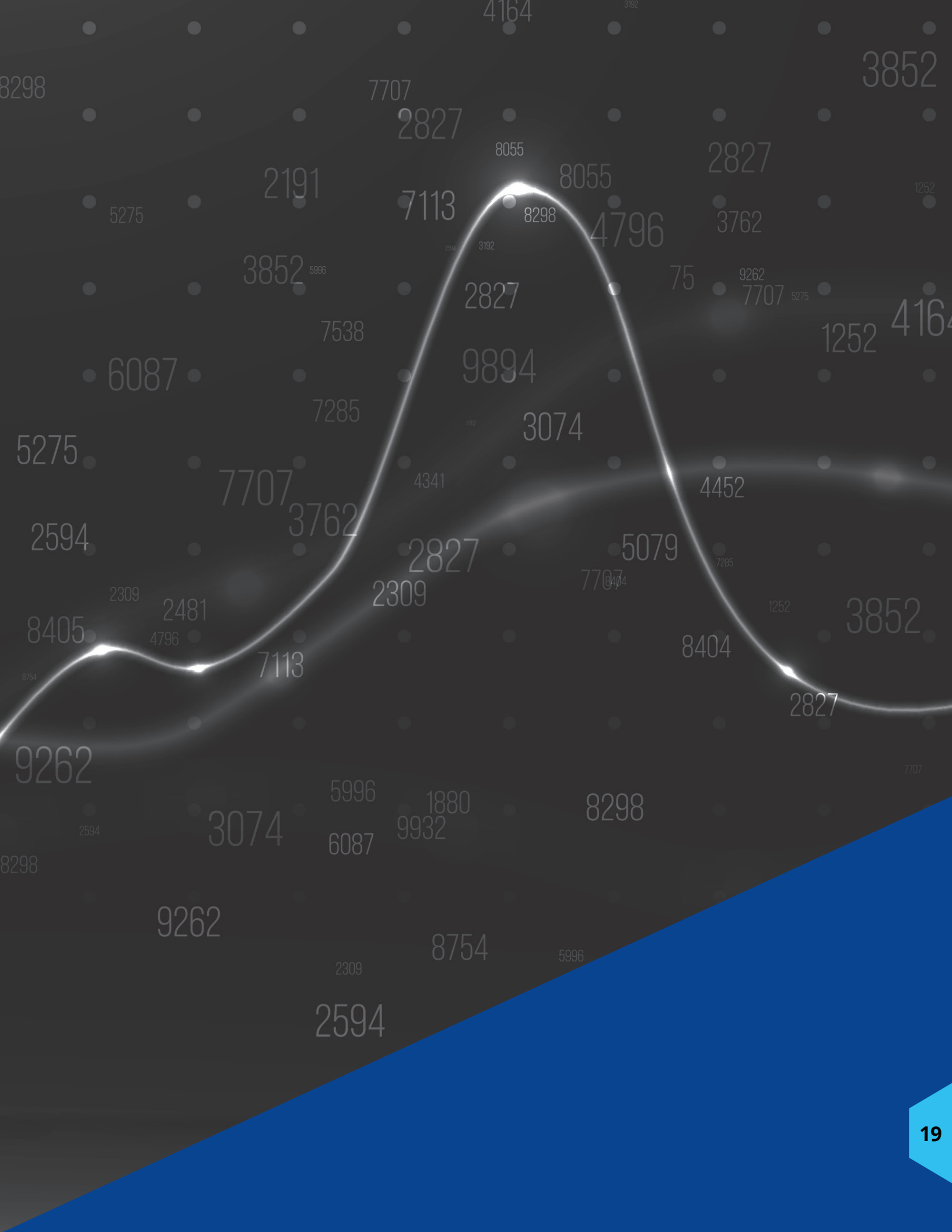
**ALLOT APPROPRIATE
RESOURCES TO
SUPPORT ON-GOING
DATA MAINTENANCE**

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