IDENTIFICATION OF FACTORS AFFECTING DAIRY SIRE SEMEN PRODUCTION AND OPTIMIZATION OF THE AI SUPPLY CHAIN

By

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TABLE OF CONTENTS

IDENTIFICATION OF FACTORS AFFECTING DAIRY SIRE SEMEN PRODUCTION AND

OPTIMIZATION OF THE AI SUPPLY CHAIN

LIST OF TABLES

LIST OF FIGURES

ABSTRACT

This dissertation focused on product forecasting and optimization of the dairy sire artificial

insemination (**AI**) supply chain. Three main chapters explore different aspects in the supply

chain, bull-level sperm production prediction, herd ranking and valuation for culling decisions,

and global product allocation. The first chapter explored the predictive ability of machine

learning (**ML**) algorithms in forecasting total sperm (**TSp**) using management factors and bull

demographics. When using random forest (**RF**), at least 85% accuracy was achieved when

predicting up to 4 months out. The most influential factors were collection frequency, TSp in

previous months, and age at collection. The second chapter provided a framework to model herd

replacement decisions and predict net present value (**NPV**) of Holstein bulls. The Markov Chain

(**MC**) modeled the steady state proportion of bulls within a herd across 330 iterations, with

aggregated NPV calculated after each time point, which steady state was reached at 310

iterations. In a case study, 49% of bulls were recommended for culling based on negative

BullVal$ (bull's NPV minus NPV of replacement). A bull's NPV was influenced primarily by

market allocation and pricing, as well as the interaction of sperm production with genetic merit.

The final chapter focused on global allocation of semen units, utilizing a linear program

optimization model. Constraints considered were regional demand, bulls' semen production

supply, and company's supply. Most limiting constraints to the solution were regional demands,

as supported by a sensitivity analysis, with the largest change in objective function value per unit

increase assigned to regional demand. This dissertation achieved the goal of leveraging ML,

Markov chains, and optimization models in decision-making processes of the AI supply chain.

Forecasting weekly TSp using a RF model could enhance the operational efficiency of semen

processing, collection scheduling, and inventory control. In conjunction with an accurate

monthly TSp forecast, an AI company can use the global allocation tool to assign product for the

coming trimester. The results can then be used in culling and collection decisions. The global

allocation tool's sensitivity analysis would be beneficial for an AI company to negotiate bounds

and constraints. BullVal$ tool would be most beneficial in culling decisions as well as being tied

into the product allocation and collection scheduling processes. Bulls with negative BullVal$

should be culled before high BullVal$ bulls (barring any health issues), to make way for more

profitable replacements. Prioritization of high BullVal$ bulls in collection scheduling would

allow an AI company to maximize profit and market potential.

CHAPTER 1: LITERATURE REVIEW

1.1   Introduction

Dairy farming in the United States was transformed in 1938 with the establishment of Artificial

Insemination (**AI**) cooperative in New Jersey (Foote, 2002) . Cooperatives allowed farmers to

remove bulls from herds, thereby reducing sexually transmitted diseases and injuries to cows and

humans and increasing genetic progress within the herd (as a farmer could select multiple,

genetically superior bulls to inseminate cows based on needs for each cow, individually). Bulls

are now raised and collected by genetics companies, whose goals are to provide farmers with

high-quality semen to impregnate their cows and heifers to produce profitable offspring to

populate their herds in the next generation. Shortening the generational interval has sped genetic

progress, both on the sire and dam sides of the pedigree (García-Ruiz et al., 2016). We have

nearly reached the sire's biological threshold of shortening the generation interval, as semen

collected from bulls as soon as they hit puberty at 8-10 mo of age is used to create the next

generation. Prior to genomics, a bull's worth was first determined by parent average, then

officially validated by progeny testing, with many bulls having performance records of 1,000 or

more daughters contributing to their genetic trait predictions. This process took several years, so

precise estimates of a bull's genetic worth and his entry into the national or global semen

marketplace did not occur until nearly 5 yr of age. With the introduction of whole-genome

prediction, bulls just weeks old already have genomic predictions of their merit for key traits that

are as reliable as those based on progeny testing, allowing companies to determine at a very

young age if a bull's semen should be collected and marketed widely.

The race to collect semen from potentially profitable bulls at a young age has outpaced research

on the male reproductive physiology of these young sires. Age at puberty and initial sperm

production capacity are unpredictable in these young bulls, with scrotal circumference and testes weight historically used to predict potential sperm production (Hahn et al., 1969). Most research on best management practices of AI sires took place in the pre-genomic era, focusing on mature bulls (i.e. Foote, 1978; Mathevon et al., 1998). Published research of young sires, including management factors that might contribute to optimal sperm production and methods to forecast future semen production in these young sires, is limited. This knowledge would allow AI companies to raise bull calves in an optimal manner, plan staffing for semen collection and processing, and generate accurate estimates of the amount of product that will be available to customers.

Customers select bulls based on a portfolio of traits, which are often combined into a selection index. These indexes provide a single metric for the overall genetic potential of a bull's offspring regarding health, reproduction, and production traits. However, to our knowledge, there are no published studies on valuation of individual bulls based on their expected contributions to future net profit of an AI company. Extensive research has been published on cow valuation, replacement policies, and optimization of herd structure (De Vries, 2004; Kalantari et al., 2010; Cabrera, 2012). There is an opportunity to apply similar methods to an AI company's bull herd for a more objective, all-encompassing valuation and ranking system that could be used for culling and product allocation decisions.

Another task that could potentially benefit from objective decision-support or forecasting tools is that of allocation of product to customers. Dairy genetics companies market their product to customers all over the world. However, each region differs in the types of bulls that are of interest to farmers, country-specific regulations on the importation of animal products, product pricing (e.g., ability to pay for a premium product), and quantity of units needed. Global

marketing of young genome-tested bulls' semen is problematic, as individual bulls' production

capacity is inconsistent and difficult to estimate at an early age. Product allocation among

competing markets is currently a very intensive and subjective process that takes place multiple

times a year, typically corresponding to the release of national genetic evaluations, such as the

Council on Dairy Cattle Breeding (Bowie, MD).

With the use of machine-learning (ML) algorithms and optimization modeling, there is an

opportunity to reduce the subjectivity in these challenging operational processes within an AI

company. New to the dairy research realm, particularly in the dairy bull segment, ML algorithms

and optimization modeling can significantly aid routine supply chain decisions.

The purpose of this review is to discuss the factors influencing semen production and summarize

published research regarding semen production and bull management, historical valuations of

bulls, global breeding objectives, dairy replacement policies, and product allocation studies, to

provide a justification for the research described in subsequent chapters.

1.2   Dairy bull physiology and semen production factors

1.2.1   Bull Physiology

Semen production and sperm quality and output are influenced by many factors, including bull

breed, age, health, management, environment, and genetics. Before diving into these factors, a

basic understanding of bull physiology and collection procedures is provided.

Seminiferous tubules within the testes are lined with Sertoli cells, which support developing

spermatocytes. In the spaces between the seminiferous tubules are Leydig cells, which produce

testosterone in the presence of luteinizing hormone (**LH**). Gonadotropin-releasing hormone

(**GnRH**) is released from the hypothalamus in response to multiple inputs. GnRH initiates the

release of follicle-stimulating hormone (**FSH**) and LH from the pituitary. FSH is a glycoprotein

hormone that induces Sertoli cells to proliferate, produce androgen-binding protein (**ABP**), and secrete inhibin, and it modulates fluid secretions of the Sertoli cells into the tubule lumen. In the immature bull, FSH initiates testicular development at puberty, and in the adult bull, it initiates spermatogenesis. The glycoprotein LH specifically targets Leydig cells to start producing testosterone, which maintains spermatogenesis, ABP production, and Sertoli-cell fluid secretion. ABP binds to testosterone, and then moves to the epididymis, where this complex supplements the systemic supply of testosterone. Inhibin, a protein secreted by Sertoli cells, has negative feedback on the pituitary, reducing FSH secretion, whereas testosterone has direct negative feedback on hypothalamic GnRH secretion and pituitary LH. Sertoli cells convert testosterone to estradiol-17B (Leydig cells also produce estradiol-17B), which gives negative feedback to the hypothalamus and pituitary (Fayrer-Hosken, 1997).

Once sperm are produced in the seminiferous tubules, they are transported through the rete testes and efferent ducts to the epididymal duct (Schenk, 2018). The epididymis is divided into three compartments: 1) the caput (head) removes water and secretes sperm maturation compounds, 2) the corpus (body) is where sperm maturation and acquisition of fertility occurs, and 3) the cauda (tail) stores and maintains fertile sperm (Schenk, 2018). Sperm are voided through the epididymis during ejaculation or urination via the deferent duct and urethra. Accessory glands (seminal vesicles, prostate, and bulbourethral glands) secrete fluids that are vital for sperm motility initiation and nutrition and provide a supportive environment for spermatozoa. These secretions are combined with spermatozoa to produce semen. At birth, the penis is attached by connective tissue and blood vessels. As the calf approaches puberty, these connections disappear (Fayrer-Hosken, 1997). After puberty, seminiferous tubules elongate and widen as the lumen forms, caudal epididymal capacity increases, and testes continue to grow rapidly. This allows for

increased spermatogenesis, thus increasing sperm produced daily per gram of testis (Schenk, 2018).

On average, a bull ejaculates 4 mL (range 1-15mL depending on age, breed, and genetic predisposition) with 300 to 2,500 x 10^6 (1,200 x 10^6 average) sperm cells/mL (Fayrer-Hosken, 1997). Maximum sperm production per gram of testis is reached about 20 wk after puberty (Schenk, 2018). Improvements in motile sperm and sperm morphology are seen within 10 wk post-puberty, possibly related to the normalization of spermatogenesis and epididymal function (Schenk, 2018). In a sexually-rested, mature bull, the cauda can store 5-6 d of sperm production, however, it is ideal to collect mature bulls 2 d per wk and collect young bulls 3 non-consecutive d per wk, to reduce sperm abnormalities and maximize sperm harvest (Almquist and Amann, 1961; Almquist, 1982).

Testicular size is a widely accepted method to forecast a bull's sperm production capacity, because greater sperm production is associated with larger testes. Testicular size is dependent on bull's age, breed, and plane of nutrition. Bulls' testes continue to grow through 2-3 yr of age (Almquist and Amann, 1976; Almquist, 1982; Schenk, 2018). Some studies describe puberty as when a bull's scrotal circumference (**SC**) reaches 26 or 28 cm (Wolf et al., 1965; Fortes et al., 2012), but body weight is the primary influence in puberty attainment (Fayrer-Hosken, 1997). Other factors influencing sperm production are covered in the subsequent pages of this chapter.

1.2.2 Collection Procedures

Semen-collection processes vary between AI company, however, there are general practices that are implemented by all. Each bull has its own preferences for sexual arousal, which the bull collection team takes into consideration. Bulls are often brought into the collection area prior to collection and housed in a holding area, such that they can watch other bulls' collections.

Another arousal technique involves being teased near a mounting steer. At the time of collection, bulls mount either a live steer or a mounting block. The collection team allows two to four false mounts, where the bull mounts an animal or block but is not collected. On the collection mounts, a team-member inserts the bull's penis into a warmed artificial vagina to collect the bull's ejaculate. Between ejaculates, bulls are given short breaks. A team member does a preliminary examination of the ejaculate in a lab adjacent to the collection area, and then the collection is sent to another lab for further testing and processing.

1.2.3 Factors influencing semen production

With the introduction and utilization of genomic selection, AI companies can predict a bull's genetic worth as early as in utero, via biopsy, but they generally wait to collect a tissue sample for genotyping until after the bull calf is born. This early and reliable prediction has transformed the AI industry over the past decade. It is no longer necessary to wait until a bull is "proven", via progeny testing at four to five yr of age, to collect large quantities of semen for customers. Bulls are now collected as early as possible, with product (semen) being sold prior to 1.5 yr of age. It is estimated that, at present, more than half of bulls advertised and collected are less than 15 mo of age (Harstine, 2018; Schenk, 2018). About 15-20% of bulls have difficulty obtaining enough high-quality sperm due to physical limitations or low libido (Schenk, 2018), so despite customers' interest in purchasing semen from these young sires, only limited quantities are available. This imbalance between supply and demand for semen of elite young dairy sires has generated increased interest in research focused on understanding puberty and sexual maturity (Kenny et al., 2018). Prior to genomic selection, the vast majority of research on bull management and semen production focused on proven bulls $\geq$ 4 yr of age (e.g. Everett et al., 1978; Mathevon et al., 1998).

That said, research studies in the pre- and post-genomic era agree on many factors influencing semen production. Recent studies have focused on hastening onset of puberty via nutritional, managerial, and hormonal interventions applied to bull calves (Byrne et al., 2018; Kenny et al., 2018). Enhancing nutrition prior to 6 mo of age hastens puberty, maturation, and increases availability of saleable semen, regardless of what happens later in life (Byrne et al., 2017). However, an enhanced plane of nutrition up to 6 mo of age does not affect semen quality, sperm motility (Dance et al., 2015, 2016).

The same research group as Byrne et al. (2018) looked at the DNA methylation differences under two different planes of nutrition (high versus medium) for the first 24 wk of age, followed by continuation of the medium plane through 16 mo of age (Perrier et al., 2020). On average, bulls on high plane of nutrition during the study period reached puberty one mo earlier than those on the medium plane. Hierarchical clustering showed inter-individual variability not related to diet or age led DNA methylation profiles. Although age revealed no change in methylation, they observed 580 differentially methylated CpGs (**DMCs**) between the nutritional planes, most of which were hypermethylated in the high plane group and "enriched in endogenous retrotransposons, introns, intergenic regions, and shores and shelves of CpG islands" (Perrier et al., 2020). Genes involved in spermatogenesis, Sertoli cell function, and the hypothalamic–pituitary–gonadal axis were differentially methylated in high and medium groups at 15 mo of age, suggesting roles in early puberty onset. At 16 mo, the medium group had genes enriched for ATP-binding molecular function that reflect changes to sperm methylome and were persistent even after both groups reached sexual maturity. Overall, a high plane of nutrition early in life seemed to provide "modest but persistent changes in sperm DNA methylation profiles after puberty" (Perrier et al., 2020).

To maximize a bull's sperm production potential at an early age via management and environment, AI companies are now producing a greater proportion of young bulls internally through nucleus breeding programs and bringing in acquired (contract) bull calves from commercial farms as young as possible. Contrary to the pre-genomic era, where bulls were brought into the stud beyond 1 yr of age and housed in groups, young bulls are now brought in at a young age and primarily housed independently, with the goal of minimizing social stress and competition. This individualized management approach aids in raising bulls at the highest quality of care and allows them to reach their full potential (Harstine, 2018). The widespread availability of accurate genomic predictions for young bull calves, coupled with management practices designed to hasten puberty and enhance sperm production, has led to a drastic shortening of the generation interval, from about 7 yr to 2.5 yr, which is nearing the biological threshold (García-Ruiz et al., 2016).

Collection teams comprised of a bull handler and semen collector can also significantly affect semen production (Mathevon et al., 1998; Fuerst-Waltl et al., 2006). Mathevon et al. (1998) stated that, although collection team accounts for less than 10% of the variance in sperm production, it significantly affects semen volume, total sperm (**TSp**), and motility for both young and mature bulls. A successful collection team relies heavily on bull-specific measures, because one protocol does not suit every bull, reminding us that bulls are biological creatures with specific behavioral preferences.

Another important factor in semen production is the amount of semen per ejaculate. Murphy et al. (2018) found that the first ejaculates in a given collection had greater semen production and pre-freeze motility than second ejaculates; however, there was no difference in post-thaw motility. Subsequent ejaculates of bulls < 1 yr old did not differ in semen production or motility

when compared with those from older bulls (Murphy et al., 2018). The authors concluded that collecting two ejaculates from a young bull in a given collection event would be an effective strategy in maximizing production without decreasing post-thaw motility (Murphy et al., 2018). Similar results have been observed with proven bulls, as demonstrated by Everett et al. (1978) and Fuerst-Waltl et al. (2006). First ejaculates yield greater volume, sperm concentrations, and total number of sperm per ejaculate compared with subsequent ejaculates (Fuerst-Waltl et al., 2006). Furthermore, sperm concentration varies more than ejaculate volume and has greater influence on the variation observed in total sperm harvested per ejaculate (Everett et al., 1978). Ejaculate volume increases with age, consequently increasing total number of sperm (Everett and Bean, 1982; Murphy et al., 2018), which emphasizes the need to revisit collection strategies as the AI industry shifts to predominantly marketing semen from young genome-tested bulls. Collection interval (time between successive collection dates) and ejaculation frequency are major factors in TSp collected from a bull across time (Everett et al., 1978; Fuerst-Waltl et al., 2006; Murphy et al., 2018). This is a tricky balance, and at face value, these factors appear contradictory. The more rest time provided to a bull between collections, the greater its semen production and quality. Previous studies vary regarding the ideal collection interval; highest number of motile sperm per ejaculate is achieved with intervals of 4-5 d between collections, as compared with 1-6 d for sperm concentration, and 4-9 d for percentage of viable sperm (Mathevon et al., 1998; Fuerst-Waltl et al., 2006). In an earlier study, increasing the interval between collections from 2 to 6+ d resulted in 45.9% more sperm per ejaculate, 31.0% more sperm per ml, and 14.0% greater volume, with daily sperm output highest when bulls ejaculated more frequently (Everett et al., 1978).

Temperature and season have been known to affect a bull's sperm production, but results are conflicting (Everett et al., 1978; Mathevon et al., 1998; Brito et al., 2002; Fuerst-Waltl et al., 2006; Murphy et al., 2018), perhaps due to differences in geographical location and breed of cattle used in these studies. It is well-accepted that the testis is susceptible to heat stress, even for short durations (2-3 hr), causing sperm defects (Fayrer-Hosken, 1997). A Brazilian study found that, "neither ambient temperature and humidity nor month (season) significantly affected sperm production and semen quality" for bulls in Ribeirao Preto, Sao Paulo and Uberaba, Minas Gerais (Brito et al., 2002). Temperature and humidity were not significantly different across time in those two locations. Studies based in New York and Ireland found that winter months yielded the lowest sperm production and the highest in spring or summer months (Everett et al., 1978; Murphy et al., 2018). Mathevon et al. (1998) concluded the opposite, with winter yielding more favorable semen production traits in young bulls and no significant effects on mature bulls in Ontario. Solunar periods have no effect on semen output (Everett et al., 1978), and studies of temperature effects yielded conflicting or insignificant results (Everett and Bean, 1982; Fuerst-Waltl et al., 2006). Fuerst-Waltl et al. (2006) found the optimal ambient temperature for semen production is 5-15°C.

It is widely acknowledged that as age increases, so does semen production (e.g. Everett et al., 1978; Murphy et al., 2018); however, studies disagree on specific effects of age and the influence of management factors on the sperm production curve (Amann et al., 1974; Everett and Bean, 1982; Van Os et al., 1997; Brito et al., 2002). Figure 1 shows the general curve of sperm production by age (Van Os et al., 1997). All studies indicate an increase in sperm per ejaculate, number of viable sperm, and ejaculate volume with age (Amann et al., 1974; Van Os et al., 1997; Brito et al., 2002), but the timing of the sperm per ejaculate plateau differs from 2 to 7.5 yr

(Everett and Bean, 1982; Van Os et al., 1997; Murphy et al., 2018). Amann et al. (1974) found

that sperm per ejaculate increased with age until 7.5 yr, then decreased. The plateau is driven by

a decrease in percentage of motile sperm and sperm concentration and an increase in volume

(Amann et al., 1974; Fuerst-Waltl et al., 2006). Other studies show an increase in TSp with age

(with relation to increase of ejaculate volume) until 4 yr (Everett and Bean, 1982; Murphy et al.,

2018).
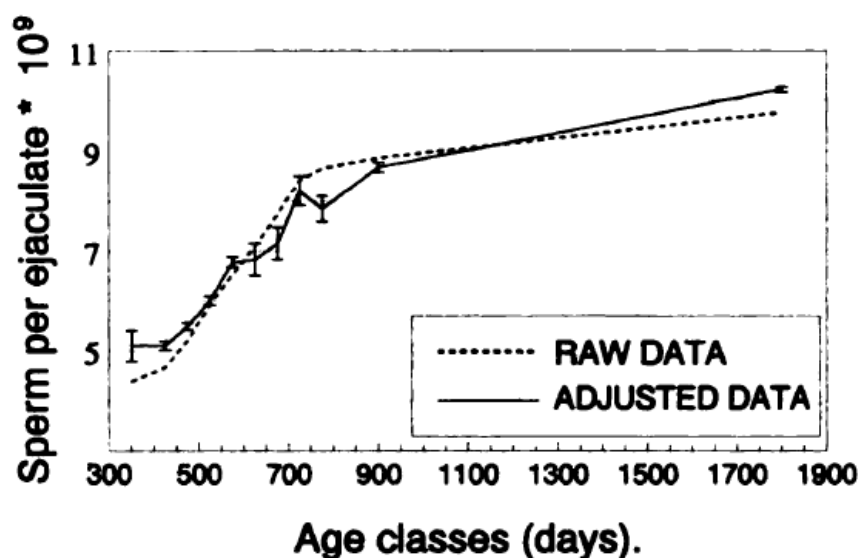
FIG. 1. Sperm output per ejaculate in relation to bull age.

Figure 1.1. Age by sperm per ejaculate. Figure from Van Os et al., 1997.

Between bulls, large differences in all measures of semen output exist between first and second

ejaculates within a collection, as well as between-collection intervals (Everett and Bean, 1982).

The first ejaculate contains nearly 50% more sperm than second ejaculates (Everett et al., 1978).

Pre-pubertal bulls have smaller ejaculate volumes than mature bulls, and the time period around

puberty is marked by rapid increases in body weight and testicular size (Aponte et al., 2005).

Semen-producing capacity of a young bull in his first yr of production is 30-50% of that of a

mature bull (Amann and DeJarnette, 2012). The definition of puberty for a bull is widely

accepted as when it reaches a SC of 28 cm and produces an ejaculate containing $50x10^6$ sperm

with 10% motility (Wolf et al., 1965). However, several papers have noted that SC should not be

the only indicator of puberty, as it is greatly influenced by environment and breed (Lunstra and

Echternkamp, 1982). On average, Holsteins tend to be 9-11 mo of age at onset of puberty

(Harstine, 2018; Murphy et al., 2018).

Genetic parameters of reproductive capacity measures have been explored across many cattle

breeds. Berry et al. (2014) performed a meta-analysis of reproductive performance in dairy and

beef cattle and reported heritability estimates for 8 traits in a meta-analysis of 25 published

studies. Most noteworthy were SC (number of studies (n) =12, $h^2 = 0.42\pm0.0002$), sperm number

(n =8, $h^2 = 0.222\pm0.018$), sperm concentration (n=13, $h^2 = 0.169\pm0.028$), and semen volume

(n=11, $h^2 = 0.197\pm0.019$) (Table 1.1). These traits show moderate heritability, but the studies

present a wide range of values. The authors do not report breed trends among these values;

however, in other studies (Chase et al., 2001; Lunstra and Cundiff, 2003; Casas et al., 2007), *Bos

indicus* cattle had slower testicular growth than *Bos taurus*. Additionally, they summarized

pooled genetic correlations among traits (Table 1.1). Reported genetic correlations "suggest that

larger SC is associated with a greater volume and concentration of sperm, a larger proportion of

live sperm with greater motility, and a larger proportion of normal sperm. Greater sperm

concentration was associated with greater sperm motility and the proportion of normal sperm but

only weakly associated with volume, although in some studies the genetic correlation was

strongly negative," (Berry et al., 2014). The moderate heritability and strong genetic correlations

of SC with desirable traits such as sperm concentration and mobility may allow for genetic

selection of bulls with larger SC to increase TSp production and the amount of product available

for marketing. However, testicular size should not be the only focus or indicator of bull fertility.

Table 1.1. Pooled mean heritability (diagonal), pooled genetic correlations, and standard errors, adapted from Tables 4 and 6 of Berry et al., 2014.

Trait	Scrotal circumference	Sperm concentration	Sperm mobility	Sperm number	Volume
Scrotal circumference	0.42±0.0002				
Sperm concentration	0.77	0.169±0.028			
Sperm mobility	0.76 ± 0.07	0.61 ± 0.10			
Sperm number		0.60 ± 0.07	0.50 ±0.13	0.222±0.018	
Volume		-0.16 ± 0.10	0.06 ±0.13	0.83± 0.13	0.197±0.019

Studies have found a few genes associated with sperm production (Fortes et al., 2012; Liu et al.,

2017). Fortes et al. (2012) focused a genome wide association study (**GWAS**) on age at puberty

and age at which SC reached 26 cm in Brahman bulls. They detected several genes (CA8,

CHD7, CSF2RA, FAM110B, IMPAD1, NSMAF, PCMTD1, PENK, RLBP1, RP1, SDR16C,

SNTG1, TOX and XKR4) on *Bos taurus* autosome (**BTA**) 14 for age at puberty. A total of 32

single nucleotide polymorphisms (**SNPs**) on BTA14 were implicated for both age at SC= 26 and

puberty between 21.95 Mb and 28.4 Mb, suggesting this region plays a role in pubertal

development in Brahman cattle. This work was published prior to the *Bos indicus* assembly, as

they used the UMD3.0 Bovine assembly for their analysis. Using the *Bos taurus* assembly for

Bos indicus animals could skew results, leading to overestimation of genome homozygosity

(Utsunomiya et al., 2019). When comparing phylogenetic trees and principal component analysis

plots, ascertainment bias has been shown to contribute to low variability among zebu breeds

(Utsunomiya et al., 2019).

Stafuzza et al. (2020) addressed these concerns by genotyping Nelore cattle on Clarifide®

Nelore 2.0 (Zoetis) and performed a GWAS for age at puberty. Genomic regions explaining

more than 0.5% of the additive genomic variance included genes related to spermatogenesis

functions (ADAM11, BRCA1, CSNK2A, CREBBP, MEIOC, NDRG2, NECTIN3, PARP2,

PARP9, PRSS21, RAD51C, RNASE4, SLX4, SPA17, TEX14, TIMP2 and TRIP13).

"Enrichment analysis by DAVID also revealed several GO terms related to spermatogenesis,

such as DNA replication (GO:0006260), male meiosis I (GO:0007141), double-strand break

repair (GO:0006302), base excision repair (GO:0006284), apoptotic process (GO:0006915),

cell–cell adhesion (GO: 0098609) and focal adhesion (GO:0005925)," (Stafuzza et al., 2020).

Genomic studies of Holstein bulls' sperm production capabilities are prevalent. Thirteen markers

were significant for sperm concentration, including SNPs located close to protein arginine

methyltransferase 6 (PRMT6), Sel1 repeat containing 1 (SELRC1), triple QxxK/R motif

containing (TRIQK) and zinc finger homeobox 3 (ZFHX3) genes (Hering et al., 2014a). Some

significant markers were located near candidate genes with known roles in production of male

germ cells (histone deacetylase 9 (HDAC9), an inhibitor of DNA binding 2 (ID2) and

glutathione S-transferase theta 1 (GSTT1)), and sperm concentration or biochemistry (Vav3,

GSTM1, CDK5, NOS3, PDP1 and GAL3ST1) (Hering et al., 2014a). The same group performed

a genomic analysis of semen volume (**SV**) and TSp (Hering et al., 2014b). They identified three

markers located on BTA 22 (rs41625599, rs41584616, rs42012507) with high significance for

both traits, with three genes in the same vicinity (DCP1A, SFMBT1, TMEM110). Marker

rs110109069 on BTA 25 was significantly associated with TSp and marker rs42438348 located

on BTA 10 associated with SV. Additional candidate genes for both traits included GALC,

PRKCD, PHF7, TLR9, and SPATA7 (Hering et al., 2014b).

In 2017, Liu and colleagues identified 20 SNPs that played roles in one or more semen production traits (semen volume per ejaculate, initial sperm motility, number of sperm per ejaculate, and number of motile sperm per ejaculate) in Chinese Holsteins. One SNP was located downstream of PDGFRB, and three SNPs were located in the promoter of MARCH1. MARCH1 had high expression in sperm cells, and one SNP in a regulatory region of MARCH1 had a significant effect on gene expression (Liu et al., 2017).

1.3   Basics of Machine Learning: Applications in Animal and Dairy Sciences

Researchers in the animal and dairy sciences have recently embraced the power machine learning algorithms can provide in data analysis and interpretation relative to traditional statistical models. Machine learning algorithms offer greater flexibility than linear models and can capture nonlinear relationships between outputs and potential explanatory variables, with fewer assumptions about the distributions of variables or restrictions on missing values (Kuhn and Johnson, 2013). They have been used in a wide range of cases, such as prediction of genomic breeding values (Yao et al., 2016), early postpartum health disorders (Pralle et al., 2018), and insemination outcomes (Shahinfar et al., 2014), forecasting of future milk yield (Murphy et al., 2014), and analysis of images to determine body condition scores (Rodríguez Alvarez et al., 2018).

Linear models (**LM**) are the most widely used methodology as a baseline for prediction of continuous outcomes in our field. They allow a detailed understanding of how various explanatory variables affect the outcome through coefficients.

Random forest (**RF**) is an ensemble method comprised of decision trees that tend to provide robust predictions and resist bias in the presence of messy data and missing values (Breiman, 2001). They are known to be extremely successful in prediction, due to performing a very large

number of iterations across all possible tree configurations, and they can provide a variable

importance ranking. RF can predict both continuous and categorical outcomes, as well as linear

and non-linear relationships. However, RF can suffer from overfitting, as demonstrated by

Dallago et al. (2019) in prediction of first test day milk yield of primiparous dairy cows. They

found that artificial neural networks (**ANN**) were most successful in predicting milk yield

compared with RF and multivariate linear regression (Dallago et al., 2019).

Another tree-based algorithm is the model tree. As opposed to RF's many trees, a model tree is a

single tree with linear regression models at the leaf nodes. Model trees handle missing data

effectively and capture non-linear relationships through tree-building, whereas end nodes can

capture linear relationships. The M5P algorithm constructs, prunes, and smooths a model tree,

allowing efficient learning and computational feasibility in high-dimensional tasks (Quinlan,

1992). In explaining conception and service rates in dairy cows, M5P was used to develop

models (Schefers et al., 2010). The authors concluded that, although the M5P provides a benefit

over MLR when handling missing data, it did not perform significantly better than MLR

(Schefers et al., 2010).

The popularity of ANN has increased exponentially in animal sciences and many other fields in

recent years, as they are able to accommodate highly complex and non-linear relationships

(Kuhn and Johnson, 2013). The most basic of ANN algorithms, the multilayer perceptron (**MLP)**

is a feed-forward ANN with one or more hidden layers, trained using back-propagation (Reed

and Marks, 1999). The simplicity of this model prevents over-fitting, and it can be used as a

starting point when comparing different ANNs. The MLP was successful in predicting monthly

composite somatic cell count (**SCC**) of dairy cows when combined with five-fold cross-

validation, with model performance similar to a generalized linear model and better than a RF (Anglart et al., 2020).

Extreme learning machine (**ELM**) is a basis function method that is often used in time-series analyses, including applications in soil science (Liakos et al., 2018). It is known for computational efficiency and resistance to over-fitting, due to its simple structure and lack of need for tuning (Huang et al., 2012). A kernel ELM prediction model accurately estimated indicators of diet energy digestion of dairy cows, performing better than a LM (Fu et al., 2020). Bayesian-regularization neural network (**BRNN**) is a back-propagation network that uses ridge regression in the objective function and a Bayesian decision framework to end training (Burden and Winkler, 2008); it is robust and resistant to over-fitting, but computational time can be a limitation (Burden and Winkler, 2008; Pérez-Rodríguez et al., 2013).

Resampling techniques are used to estimate the best parameters for model performance. In general, one subset is used to fit a model and the remaining data are used to test efficacy of the model. This is repeated multiple times, and results are aggregated and summarized (Kuhn and Johnson, 2013). K-Fold Cross-Validation is widely used and accepted. The training data is split into k sets of equal size, and a model is fit using all the samples excluding the first subset ("fold"). The sample held out in the first fold is then used to estimate the model performance. In the next iteration, the first subset is returned to the larger set and the next subset is removed. The process repeats itself until all subsets have been tested (Kuhn and Johnson, 2013).

1.4   Conclusions for bull physiology and semen production factors

Research over the past 70 years has focused on proven bulls' semen production, though more recent studies have focused on genomic relationships of semen production and puberty for both *Bos indicus* and *Bos taurus*. With the shift towards collecting young genome-tested bulls as

early as possible, the number of studies and depth of knowledge regarding the semen production characteristics of these young bulls are lacking. This literature review covered what is already known about the management, feeding, and genetics of young sires, as well as the power machine learning algorithms can bring to prediction and modeling in animal and dairy sciences. With these new tools, we can explore the impact of management factors on sperm quantity in young sires, and we can use these factors to forecast total sperm production one or more months into the future. This knowledge would help genetics companies with scheduling and allocating human and material resources more precisely for semen collection and processing. Such methods could also provide more reliable forecasts of product availability and facilitate allocation of this product to global customers. Additionally, the industry will gain insight into the optimal management conditions to allow young bulls to achieve maximum sperm production.

1.5   Bull Valuations and Ranking

Valuation and rankings of bulls based on predicted genetic merit of offspring are used by farmers to select the best sires for the next generation of replacement heifers, with future production, health, and fertility in mind. A large selection of bulls are provided by the AI industry and farmers make varying choices to drive the genetic improvement of their dairy cattle. Selection index is a composite of animals' predicted breeding values for various traits that is used to forecast total economic merit (**TEM**) of their offspring, and these are used widely to aid both AI companies and farmers in selection decisions (Shook, 2006).

Selection indexes can be formed using predicted transmitting ability (**PTA**) values of traits, which are the average values of genes transmitted from the individual to its progeny, and these are derived from the performance of an animal and its known relatives (Shook, 2006).

Index selection drives genetic improvement, as it encompasses many traits and balances them with economic weights to derive a single value that can be used in selection decisions. Selection index is more effective than tandem selection and independent culling levels (Hazel and Lush, 1942). Hazel and Lush (1942) showed that, "selection for a total score or index of net desirability is much more efficient than selection for one trait at a time," and "selection on independent culling levels is less efficient than selection on total score, but in some cases, permits earlier selection without waiting until all traits are mature." Hazel (1943) further described index selection for livestock, by defining phenotypic and genetic correlations that were needed for the construction of multiple-trait selection indexes and describing how they could be estimated. The goal in using a selection index is to improve one or more traits, referred to as the selection objective, by ranking and choosing mates using a combination of those or related traits, known as the selection criterion (Cole and VanRaden, 2018).

Henderson (1963) proposed the separation of the selection index into two steps: 1) estimate individual breeding values for each trait included the aggregate breeding value, and 2) apply relative economic weights to these estimated breeding values. This allowed for best linear unbiased prediction (**BLUP**) techniques to estimate individual breeding values for specific biological traits. It also allowed comparison of individuals of different age classes, allowing for easier selection decisions between young and progeny-tested sires to maximize genetic gains (Dickerson and Hazel, 1944b; a). BLUP models are very popular, with the animal model eventually gaining the most acceptance, as it can provide greater accuracy by accounting for all known genetic relationships (VanRaden and Wiggans, 1991).

In the beginning stages of genetic evaluation, statistical theory and model-development out-paced data collection. As the industry enhanced their recording systems and increased

development of computational technology, they were able to capitalize on index selection. Even more recently, the access to bovine genome accelerated genetic gains.

USDA's first widely published selection index, predicted difference dollars (**PD$**) was introduced in 1971 (Van Raden et al., 2021). PD$ only consisted of milk and fat yields. In 1974, a sire model (Modified contemporary comparison, **MCC**) was used to evaluate yield by the USDA-AIPL (Beltsville, MD). The MCC was an improvement over the previously used herdmate comparison, as it considered the merit of herdmates that performed under the same management and environmental conditions. However, it could not match the benefits of the animal model, which considered all relatives, evaluated all animals within a breed simultaneously, and improved accounting for nonrandom bull use effects (Powell and Norman, 2006).

In 1975, Sweden introduced the total merit index (**TMI**), comprised of 12 traits including milk production, growth rate, female fertility, stillbirth rate, milking ease, temperament, and six conformation traits (Philipsson et al., 1975). This index integrated AI and milk-recording schemes and the concept of discounted gene flow as a basis for derivation of economic weights. The TMI was the leading international development at its time, capitalizing on the most important traits, in which each country could tailor to its own economic values (Philipson et al., 1994).

To reflect market and breeding goal differences, USDA introduced cheese yield price (**CY$**) and protein price (**MFP$**) in 1977 and 1984, respectively (Norman et al., 1979; Norman, 1986). In 1994, PL and SCS were added to yield traits to create NM$ (VanRaden and Wiggans, 1995). "The NM$ measures additional lifetime profit that is expected to be transmitted to an average daughter but does not include additional profit that will be expressed in granddaughters and more

remote descendants," (VanRaden et al., 2021). Since NM\$ introduction, roughly every three years, the index is revised to reflect industry trends, introducing new traits and adjusting economic values. This includes an increased focus on health and fertility, with decreased emphasis on yield traits. Protein yield has increased in importance along with fitness traits, with a decrease in emphasis on milk yield. Furthermore, in 1999, CY\$ and MFP\$ were replaced by more complete merit indexes, cheese merit (CM\$) and fluid merit (FM\$).

In the 2000 NM\$ revision, type composites were included with yield and health traits (VanRaden, 2000). Prior to this, breed association indexes tended to include type traits as indicators of fitness, while NM\$ included direct measures of health and longevity. In 2003, cow fertility and calving ease were added to NM\$ (VanRaden and Seykora, 2003). The most recent changes include the addition of cow health traits in 2018, and the addition of feed saved, early first calving, and heifer livability in 2021 (VanRaden et al., 2018; VanRaden et al., 2021). Genomic selection, also known as whole-genome selection, refers to the computation of genomic PTAs (**GPTAs**) as the sum effects of genetic markers (or haplotypes of markers) dispersed widely across the genome, with the objective of capturing the unknown quantitative trait loci (**QTL**) that contribute to a trait's variation (Hayes et al., 2009). Genomic selection can replace pedigree-based selection, if all animals in the population are genotyped, or augment pedigree-based selection if they are not. Reliabilities of GPTAs for young selection candidates that lack phenotypes of their own are significantly higher than parental average breeding values, and the reliabilities of GPTAs for young bulls can approach those of pedigree-based PTAs of older progeny-tested bulls. GPTAs revolutionized procurement and marketing of bulls, as they allowed widespread marketing of elite young bulls at 2 yr of age, reduced the generation interval by half,

and doubled the rate of genetic gain (Schaeffer, 2006; Hayes et al., 2009; García-Ruiz et al., 2016).

Physiologically speaking, a bull can enter puberty and be used for breeding by 1 year old. GPTAs allowed for this generation interval threshold to be realized, by providing a mechanism to obtain an accurate assessment of a bull's genetic worth at a very young age – previously, the low accuracy of pedigree-based PTAs could not justify collection and widespread marketing of semen from young dairy bulls.

As the cost of genotyping was reduced by the introduction of inexpensive low-density DNA microarrays (Vazquez et al., 2010), farmers obtained the power to genotype heifer calves and select the most profitable replacements very early in life, and sire acquisition teams pushed the AI studs to house bulls prior to 1 yr old and start collecting semen as early as possible. A simulation study suggested that AI companies could avoid nearly 92% of their costs by avoiding progeny testing (Schaeffer, 2006), although it is likely that realized cost reductions have been much more modest.

Progeny testing still exists, in a sense, because phenotypic data of offspring produced from semen of widely marketed young bulls still enter the national genetic evaluation system. This provides a progeny-based (or progeny-enhanced) breeding value prediction later in life that can validate the early genomic prediction and capture any genetic effects not yet flagged by an identified gene or haplotype.

Traditionally, AI companies acquired bulls through partnerships or contracts with elite dairy herds. Schaeffer (2006) foreshadowed the use of nucleus herds at AI companies, where elite animals are raised "in-house", and this trend has become widespread as AI companies seek to

reduce generation interval, reduce potential exposure of young bulls to infectious diseases, and more tightly manage their growth and nutrition.

1.5.1   Global Focus, Markets, Indexes

Complete utilization of global data records in bull evaluations would capture the bull's performance across many environments and potentially increase the reliability of his predictions. Previous studies (Weigel et al., 2001; Mulder et al., 2006; Berry et al., 2014a) have considered this possibility, and the International Bull Evaluation Service (INTERBULL) provides international sire comparisons for many traits, based on meta-analysis of genetic and genomic predictions from its member countries..

Multiple genetic rankings are needed to reflect the climate and management difference seen globally, as performance of important traits can differ due to genotype by environment or genotype by management system interactions (Zwald et al., 2003; VanRaden, 2004). Although the US has four merit indexes (CM$, GM$, FM$, and NM$) in an attempt to capture the different production practices and milk markets associated with herds that serve the fluid, cheese, and grazing (perhaps also organic) markets, other countries also tailor their national indexes according to their environments, management practices, and selection objectives.

The following is a short synopsis of how selection objectives differ around the world. In Saudi Arabia, for example, the selection emphasis remains on high yield traits to accommodate the increased dairy demand in the Middle East (Alqaisi et al., 2010), and farmers tend to select similar profiles to that of the US commercial farms. China's primary breed is the Chinese Holstein, which was developed from crossbreeding of Chinese Yellow Cattle with European Holstein-Friesians (Olasege et al., 2019). Their breeding goal had been increased milk production, without compromising milk components, but conformation traits and heat tolerance

have received attention recently in an attempt to increase longevity of dairy cattle in southern

China (Olasege et al., 2019).

Like China, South American countries are shifting their focus away from high milk production.

South American's breeding objectives emphasize on milk composition, udder health, fertility,

workability (e.g., milking temperament in Zebu-descendant dairy breeds), and conformation

traits. Researchers are also focused on adaptation and environmental resilience for cattle raised in

the tropical regions, with main indicator traits of heat tolerance, survival, and parasite resistance

(Ventura et al., 2020).

The European Union (**EU**) is faced with milk quotas and strict environmental regulations. This

contributes to breeding objectives that tend to be centered around health, conformation, and

efficiency, especially for dairy cattle in confinement housing systems (Berry et al., 2014a).

Ireland and New Zealand primarily graze their cattle (Berry et al., 2014a). New Zealand's

primary dairy market is dry milk export, so their breeding goals emphasize on milk components

and mobility traits, whereas the United Kingdom puts greater emphasis on productive life and

feed efficiency (Shook, 2006).

There is extensive research literature on genetic and genomic evaluations of bulls for various

traits, but the primary focus is on the genetic profile of a bull's offspring and the economic

benefits these offspring can generate for the dairy farm, as opposed to forecasting the financial

contribution a bull can make to the AI stud. The next section discusses analyses of tools for cow

valuation and replacement decisions could be adapted to bulls in an AI stud.

1.5.2 Dairy Ranking and Replacement Analyses

As detailed in the prior section, selection criterion and valuation of bulls are directly related to

the contribution that bull can bring to offspring performance and farm profitability in the

following generation. To the author's knowledge, a ranking or replacement policy for bulls has not yet been established. Each AI company has its own way of identifying young bulls as prospective replacements, and this can be a very subjective process. This section highlights the current strategies for ranking and culling bulls at one leading bovine AI company, as well as cow replacement policies and models published in the scientific literature.

Replacement policies, net present value (**NPV**) calculators, and decision-support tools are well-established for dairy cows. These analyses use either Markov Chains (**MC**) or Markovian Decision Processes (**MDP**), a specific kind of Dynamic Programming (**DP**) that is most often used in herd replacement problems. The biggest difference between MDP and MC is that MDP has the goal of optimization, finding an optimal policy by maximizing profit, whereas MC simulates an already predefined policy. Because of this predefined policy, an MC is computationally faster, less complex, and can be easily implemented into a decision-support tool. Additionally, MCs allow greater flexibility, as they run on a user-defined policy. They can also allow introduction of external parameters to interact with the model. Although they may not always achieve an optimal solution to a problem, such as maximizing profit, they are more realistic and forgiving in modeling replacement policies than MDP (Nielsen and Kristensen, 2015).

MDPs suffer from the curse of dimensionality, and due to the iterative nature of the approach, MDPs can be computationally burdensome if the state space is large. Although an MDP finds the optimal policy, it may not be practical for the user to use often due to the large computational time (Cabrera, 2012). It is also hard to adjust MDP to find suboptimal solutions that are more realistic for the user, and a user cannot introduce external parameters to interact with the model through recursive solutions (Nielsen and Kristensen, 2015).

MDPs do have advantages over MCs, however. They give a full spectrum of cow value results

for all potential cow states (e.g., parity, days in milk, reproductive status). This can be

advantageous if we have a wide range of animals, or want to analyze the full spectrum of values.

However, with a large state-set, the results of an MDP can overwhelming and of little practical

value to a manager, as they may have direct goals in mind and will not be able to scan a huge

matrix and tease out useful information efficiently. On the other hand, an MC provides clear

results for animals, such as NPV, and these can be ranked and easily interpreted by managers.

If the correct policy is defined, and the overall goal of the program is to find maximum profit,

MC can perform similarly to MDP. In livestock replacement problems (e.g. De Vries, 2004,

2006), a MDP is often used to define the optimal policy, and then an MC is used to take that

policy and define herd performance summaries.

Both algorithms share some downfalls. For example, MDP and MC assume there is always a

replacement available. This is not always the case for livestock, but there is not yet an algorithm

that can account for the lack of a replacement. Also, these algorithms do not adapt well to

biological variation (Nielsen and Kristensen, 2015).

One such model (De Vries, 2004, 2006) contained three modules to predict the economic value

of delayed replacement of cows with new heifers, while considering the value of pregnancy.

These included a bioeconomic module (for entering and calculating cow performance data and

prices), a replacement policy module (using DP to optimize culling decisions for individual cows

and enter decisions for replacement heifers), and a herd performance module (using a MC model

to compute summary results). The study focused on management and environmental conditions

in Florida and considered many factors, including: milk production, body weights, feed intake,

reproduction (pregnancy rate, voluntary waiting period), involuntary culling, salvage value, milk

price, cost of insemination, heifer price, calves sold at birth, feed cost, vet cost, labor costs (milking and dry periods), involuntary culling losses, variable costs, and fixed costs. The original model was subsequently modified to consider the U.S. dairy population more broadly, while computing the value of a pregnancy based on lactation number, stage of lactation, and milk yield (De Vries, 2006).

A replacement tool developed more recently by Cabrera (2012) considered value of the cow, value of a potential pregnancy, and cost of a lost pregnancy, all contained in an easy spreadsheet for use by dairy farmers. This tool relied on a MC model internally, and user-provided data included months in milk, months of pregnancy, current and expected future milk production, reproductive factors, body weight, and current prices of replacement heifers, culled cows, calves, milk, and feed, as well as the interest rate (Cabrera, 2012).

A recent study investigated the potential benefits and opportunity costs of using beef semen to mate animals of low predicted genetic merit in dairy herds (De Vries, 2020)). This herd simulation considered several different breeding strategies, including conventional, sexed, and beef semen, as well as recipient and donor cow strategies. The author provided several models that considered opportunity costs and evaluated competing breeding programs based on genetic merit and future milk production, using an MDP (De Vries, 2020).

Given previous literature, a MC to model a bull's NPV would be desirable, as the end user could enter their policy of choice. The MC's further advantage of computational speed and easy integration would be advantageous for an AI company to use routinely, and this could make replacement decisions involving AI bulls more objective while also allowing some diagnostics (e.g., "what if" analyses based on changes in prices, management factors, or policies).

1.6   Product Allocation Analyses

1.6.1   AI Company Example of Current Practices

At least one leading AI company has expressed interest in a decision-support tool that would make their product allocation process more objective and, perhaps, more nearly optimal. At present, the Council on Dairy Cattle Breeding (CDCB; Bowie, MD) releases official genetic evaluations of U.S. dairy cattle three times per year, in April, August, and December. Next, AI companies meet with their global regional branch managers or independent distributors to plan the next trimester's allocation of semen from individual bulls or groups of bulls. Many factors feed into this subjective process, and the following sections outline the biological and logistical constraints that influence global product allocation for an AI company.

1.6.2   Biological constraints influencing allocation

Several factors affect allocation that result directly from a bull's biology, such as semen production capacity, health status, genetic traits, and pedigree. To forecast the number of units available for the next trimester, a company needs to have an accurate prediction of a bull's production capability. As mentioned in previous sections, many factors affect sperm production. A simple, but common, method used to identify potential product availability is to take the bull's sperm production in the most recent trimester as a base, then guarantee that 90% of that product will be available during the next marketing period. However, this method does not consider factors that are known to influence TSp, such as age of bull, which would change the number of units available for bulls that are still maturing. Furthermore, allocating only 90% of every bull's production capacity can conflict with logistical constraints, such as inventory capacity, because 10% of units from a potentially large number of bulls will be produced but not allocated and sold in the next trimester, and the excess product must be stored or destroyed.

Another biological factor constraining product allocation is health of the bull. In the United States, it is standard practice to vaccinate dairy calves. However, the EU does not allow products from animals carrying titers to specific pathogens into their countries. To fulfill EU requirements, bulls must undergo a quarantine before entering the production herd and test negative for bovine tuberculosis, brucellosis, enzootic leukosis virus (BLV), infectious bovine rhinotracheitis/infectious pustular vulvovaginitis (IBR/IPV), Bovine viral diarrhea-mucosal disease (BVD-MD), *Campylobacter fetus* ssp. *venerealis*, and *Trichomonas foetus* (European Commission, 2016). Countries that allow IBR-positive bulls but not leukosis-positive bulls include China, United Kingdom, and Turkey. In addition, Canada and most countries in the Middle East do not allow importation of semen from bulls that test leukosis-positive. As such, sales of semen from bulls that are pathogen-positive are often limited to the Latin America and domestic markets. As AI companies bring dairy bull calves into the stud at younger ages, or produce their own bull calves through nucleus breeding programs, fewer bulls are impacted by these restrictions. These restrictions are a major challenge for the beef industry, however, as most beef bulls are purchased or leased by AI studs after weaning. At the time of weaning, it is standard for U.S. beef calves to be vaccinated. Because of this, 90% of beef bulls are vaccinated against IBR, preventing the sale of their semen to the EU. Nationwide, nearly 52% of beef operations vaccinate calves age 22d through weaning against IBR, and 63% being vaccinated against multiple pathogens (United States Department of Agriculture, 2020).

Inbreeding is a concern among the dairy cattle industry, as the Holstein breed has a 9.1% inbreeding coefficient and expected future inbreeding of 8.8% (Council on Dairy Cattle Breeding, 2021). These values are even higher for young genome-tested bulls, at 12.3%, 14.1%

and 10.1% for pedigree, genomic, and genomic future inbreeding, respectively (Council on Dairy

Cattle Breeding, 2021).
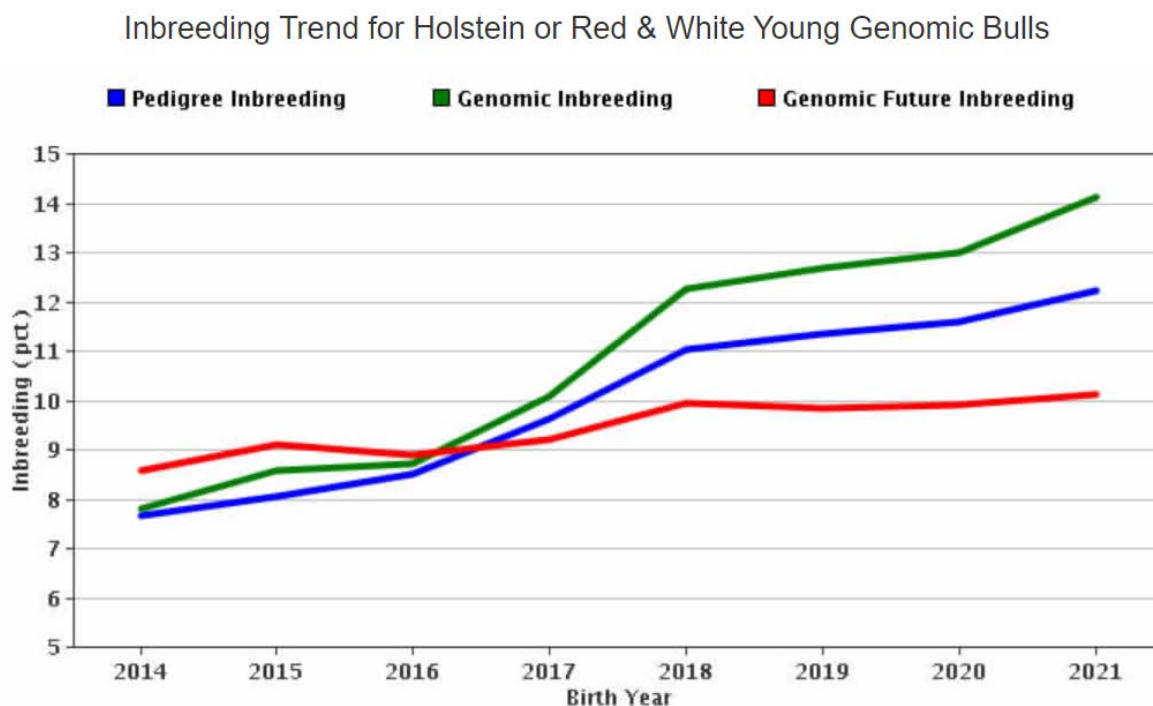
Figure 1.2. Inbreeding trend (pedigree, genomic, and genomic future) for Holstein or Red and White young genomic bulls. Figure from Council on Dairy Cattle Breeding (2021).

There is a desire to control inbreeding, as an increase in homozygosity causes decreased fertility,

production, and survivability (Bjelland et al., 2013). To control inbreeding, AI companies try to

increase the availability of "outcross bulls" to their customers. To maintain genetic diversity in

the long term, it may be advantageous to consider the relatedness of bulls whose semen is

exported to specific countries or regions, such that customers are not purchasing semen from

bulls that are closely related to each other.

1.6.3 Logistical constraints influencing allocation

Some logistical constraints influencing product allocation are inventory capacity, collection

scheduling, country preferences and seasonality, and treaties or contracts. Many of these

constraints interact with each other, as well as the biological constraints. To maintain its quality and shelf-life, semen is stored in cryopreservation tanks. Without it, the semen (with diluent) has a shelf-life of 2-4 days (Vishwanath and Shannon, 2000). Storage in dry ice at −79°C or liquid nitrogen at −196°C can extend shelf life and retain fertilizing potential indefinitely (Vishwanath and Shannon, 2000). Undoubtedly, the essential storage of product prior to shipment plays a role in product allocation, as the available space for semen storage is limited. For an AI company to meet their goal of having 6 months' of product on-hand for distribution, they need storage capacity for 8 million or more units.

Scheduling of bull semen collection also plays a role in meeting allocation needs. Many factors affect the weekly collection schedule, such as special or research orders and the gap between the current inventory and allocation target for an individual bull. The number of saleable units is a direct function of collection frequency and interval (the AI industry typically strives for 2 collections/wk/bull); however, if a bull's collection does not meet quality standards during processing this could also change the collection schedule. Research is crucial for an AI organization, and any special requests for research trials are typically considered first. Also, certain markets have preference over others when attempting to meet product needs (e.g., up to 40% of saleable semen may be reserved for the EU).

Other market preferences may play a role in the allocation process. For instance, emerging dairy markets, such as Saudi Arabia, may get preferential status at reduced costs to foster a promising long-lasting relationship. In 2019, Saudi Arabia had about 700,000 dairy cows and expected 7% growth by 2024 (UAE Dairy Products Market, By Type (Dairy Milk, Ghee & Butter, Ice Cream & Milk Cream, Cheese & Spread, Yogurt, Others), By Distribution Channel

(Supermarket/Hypermarket, Grocery Stores, Online & Others), By Region, Competition Forecast & Opportunities, 2027, 2021).

Seasonality of dairy production in certain regions also plays a part in the allocation problem. Many countries with predominantly pasture-based systems breed for spring or autumn calving (Garcia and Holmes, 1999). For example, many pasture-based countries in the southern hemisphere (e.g., Australia, Argentina, Colombia) breed the majority of their cattle in August. Historically, such countries bought most of their semen during those time periods, but recently some have transitioned to year-round purchasing to ensure access to more semen from high-value sires, particularly during the COVID-19 pandemic.

1.6.4   Allocation studies in the animal and dairy sciences

Allocation studies have many potential applications in the dairy industry. Linear programs (**LP**) are used to optimize decisions, such as replacement policies and resource allocation, and they are sometimes used in place of dynamic programming (Hillier and Lieberman, 1986; Cabrera and Hildebrand, 2012). Cabrera and Hildebrand (2012) described four advantages of LPs relative to DPs: 1) standard LP algorithms ensure consistent solutions; 2) LPs allow sub-optimal solutions; 3) different time spans can be modeled in MC dimensions of a DP problem, 4) interactions of herdmates can be supported in an LP formulation (Cabrera and Hildebrand, 2012).

Cabrera (2010) used a Markovian LP to optimize dairy farmer-defined goals under different decision schemes regarding replacement policies and herd net income and the impacts of diet and nitrogen excretion. An LP algorithm was used to find the maximum net return for the decision of keeping or replacing a cow in each state under a specified diet. Cabrera concluded that, "the implementation of a Markovian LP for dairy decision making provides both robustness and versatility in operations research" (Cabrera, 2010).

Another dairy feeding management optimization problem was solved using LP as the baseline

for comparison with another method, Differential Evolution (**DE**). Pareto-based multi-objective

optimization using evolutionary algorithms can help address challenges and show the trade-offs

among various and conflicting objectives. DE was found to address complex objectives and

performed similarly to LP (Notte et al., 2020). However, some LP solvers allow a sensitivity

analysis to evaluate shadow prices and reduced costs of constraints (e.g., Analytic Solver®).

Beyond LP, other algorithms that can be used in optimizing livestock management scenarios.

Villalba et al. (2019) used a multi-objective genetic algorithm at the farm level to explore

economic and environmental trade-offs.

 In the dairy products realm, Banaszewska et al. (2013) introduced an LP-based dairy

valorization model to identify the optimal product portfolio composition for raw milk inputs.

Their model improved the value of milk utilization and provided an understanding of prevailing

production processes (Banaszewska et al., 2013).

An earlier dairy production planning study used a time-staged LP to find the most profitable

daily production schedule for powder, casein, cheese, and butter products (Benseman, 1986).

Using a graphical networking process, an interacting planning model was developed to maximize

revenue based on dairy product prices in New Zealand, variable processing and transportation

costs, and constraints of factory capacity, product demand, and raw material supply (Mellalieu

and Hall, 1983).

Allocation of milk resources for cheese making was modeled with an LP to maximize net returns

and cheese yield while minimizing costs (Kerrigan and Norback, 1986).

The nature of dairy product allocation and resource optimization is comparable to that of semen

product allocation from dairy bulls. Bulls' semen can be directed towards conventional or

gender-selected products; and these products are exported globally, and their production is subject to constraints in labor, processing, and inventory capacity.

In the AI industry, LP and mixed-integer programs (**MIP**) have been used to model the optimal portfolio of sires for dairy herds (McGilliard and Clay, 1983a; b; Erba et al., 1991; McConnel and Galligan, 2004). McConnel and Galligan (2004) used three different selection programs (two traditional and one integer method) to model the effects of semen quantity price discounts on the lowest cost portfolio of sires from three AI companies. The MIP resulted in the lowest cost portfolio for dairy farmers when genetic trait goals were changed to be more or less stringent. An earlier study used a 450-cow commercial herd to model the optimal bull profile using a LP to reduce costs by selecting genetically similar (but cheaper) bulls (Galligan and Ferguson, 1995) and concluded that this approach could be generalized and implemented on different dairy herds. The MAXBULL model was one of the first LP formulations to consider sire selection for dairy herds (McGilliard and Clay, 1983a; b). The model aimed to maximize weighted average Predicted Difference (**PD**) for milk while meeting minimum average goals for PD fat percent, final score, and six linear type traits, subject to a maximum average semen price. (McGilliard and Clay, 1983a; b). Erba et al. (1991) proposed an IP sire selection model (IPSIRE) using an optimization software. Like MAXBULL, the objective was to select a group of sires that maximized PD milk subject to various constraints (Erba et al., 1991). Both models were tested on large and small test sets, and IPSIRE achieved a slightly greater optimal objective value than MAXBULL, with higher PD milk (4.1 and 7.3 kg), albeit with greater computation time (Erba et al., 1991).

In 1982, Schneeberger et al. applied portfolio theory to dairy herd sire selection. They used a quadratic program (**QP**) to obtain the combination of sires that gave the smallest variance of

income for expected income (variance frontier). Expected income was defined as an index of the sire's PD$ and semen price. As variance of income increased, so did expected income, and "fewer bulls remained in the efficient set of portfolios as expected income and variance increased," (Schneeberger et al., 1982). They proposed this QP could aid dairy farmers in sire selection by using their individual weightings of expected income and variance of income (Schneeberger et al., 1982).

Weigel and Lin (2000) investigated inbreeding and NM$ consequences with various mating scenarios using an LP model. The model minimized inbreeding, maximized NM$ subject to a fixed inbreeding threshold, and maximized expected lifetime profit after adjustment for inbreeding depression (Weigel and Lin, 2000). Another study modeled multiple goals of the sire selection problem with a multi-objective program that was built and compared with the integer programs considering the interactions of the objectives (Tozer and Stokes, 2001). The three objectives were to maximize NM$, minimize inbreeding, and minimize total semen expenditures. The authors concluded that it was feasible to obtain a solution with multiple objectives, but that optimal solution suffered compared with a single-objective solution. They suggest that the multi-objective program be used, "in conjunction with selection indexes to allow a dairy producer to assign higher weights to those traits that are more desirable for the producer and to select sires that may be more suited to the goals of the breeder," (Tozer and Stokes, 2001). Although LP and MIP have been used in the AI industry, to the authors' knowledge, there has not been an analysis of global product allocation considering differing regional demands and bull production capacities. If all constraints and functions considered in the allocation problem are linear, an LP would be the appropriate and efficient model to implement in a decision support tool.

1.7   Conclusions

Although ML algorithms within the dairy farming and dairy genetics industries are not novel,

published research on their usage in the dairy sire and semen supply chain contexts is lacking.

Previous studies have established the genetic and management factors influencing mainly proven

bulls' TSp and semen traits. Young sires are lesser characterized, and the era of genomics has

increased pressure to collect young bulls as early as possible. There is an opportunity to leverage

ML algorithms to predict TSp and identify the management factors most influential on semen

production in young bulls. Such tools and knowledge could aid in better management of bulls

while improving collection scheduling and product allocation. There is also a desire to

objectively value bulls based on their genetic merit, production capability, and market potential

relative to other herd mates, to aid in replacement decisions. There are plenty of studies and

indexes valuing bulls' contributions to their offspring, but none of these consider semen

production capacity and the actual profit individual bulls can bring to an AI company. Prior MC

replacement policies for dairy herds provide a framework to build a tool to value bulls and model

a replacement policy. Lastly, LPs have provided the dairy industry with ample optimization

solutions to problems concerning resource allocation and sire selection for dairy herds. Current

global allocation practices in the dairy sire semen distribution are subjective and intensive, and

there is an opportunity to use LP for semen product allocation. The following chapters aim to

leverage dairy genetics company data across the supply chain and provide ML algorithms to aid

in decision-making.

1.8   References

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CHAPTER 2: PREDICTING SPERM PRODUCTION OF YOUNG DAIRY BULLS USING COLLECTION HISTORY AND MANAGEMENT FACTORS

2.1   Abstract

Selection of elite young dairy bulls by using genomic data shortened the generation interval and increased pressure to collect and market germplasm at an early age. The objectives of this study were (1) develop prediction models for daily, weekly, and monthly total sperm (TSp) production from collection history, health status, and management factors, and (2) assess the ability of these models to forecast future TSp production, as well as differences in prediction accuracy by seasonality or age of bull. Data consisted of 43,918 daily processing records from 1,037 Holstein and Jersey bulls between 10 and 28 mo of age at collection. Potential explanatory variables included year and season of collection, barn location, collection frequency, breed, scrotal circumference, TSp in previous months, health events, and age at arrival, first collection, and current collection. Linear regression, random forest (RF), Bayesian regularized neural network, model tree, multilayer perceptron neural network with multiple layers, and extreme learning machine were used to predict daily, weekly, and monthly TSp (R v3.5.1, https://www.r-project.org/). In the additive approach, all prior data were used for training; however, in the fixed-window approach, records from 3 previous months were used for age-based prediction, records from 4 previous months or 1 yr were used for the monthly date-based analyses, and records from 1 previous month or year were used for the weekly date-based analyses. Model performance was measured by root mean squared error (RMSE) and the correlation (r) between actual and predicted TSp in testing sets. In monthly analyses, RF with additive training performed best in age-based (RMSE = 13.6 billion cells, r = 0.93) and date-based (RMSE = 11.9, r = 0.94) prediction, compared with linear regression (age-based RMSE = 16.6, r = 0.89; date-

based RMSE = 15.5, r = 0.90) and Bayesian regularized neural network (age-based RMSE = 14.1, r = 0.92). On average, RMSE was 0.93 or 0.14 billion cells greater with fixed 4-mo or 1-yr training windows, respectively, than in the additive analyses. The most important management variables affecting TSp were collection frequency, TSp in previous months, and age at collection. Results indicate RF models with additive training can predict TSp output of individual bulls with ≥85% accuracy up to 4 mo into the future. Spikes in accuracy were associated with sire summary times and company processing changes, and accuracy tended to stabilize when bulls reached 19 to 20 mo of age.

2.2 Introduction

Selection of elite young bulls using genomic data has shortened the generation interval and increased pressure to collect large quantities of semen at an early age (García-Ruiz et al., 2016). However, these young bulls vary greatly in their production capabilities, making it difficult for the AI companies to accurately predict the quantity of semen that will be collected from each bull, schedule processing of sexed and conventional semen, manage inventories, and allocate product to customers. The general processes for semen collection are as follows. A bull can either be collected from using electro-ejaculation (least common), a mounting or teaser steer, or a mounting dummy. Bull preference plays a big role in deciding which stimulation or mounting method is used for collection. Ejaculates are collected using an artificial vagina. Bulls are typically collected 2 to 3 times per week, with 2 to 3 ejaculates per collection. After an ejaculate has been collected, it undergoes initial quality control checks before going to the processing laboratory for further quality testing and packaging into units.

Selecting bulls for collection is based on priority listings of demand and allocations, inventory, special orders for in vitro fertilization, research, and workload balance between barns and processing centers. In choosing which bulls to collect on a given day, there are considerations about whether the bull should be collected for sexed or conventional units at the same time as trying to achieve and a balance of seminal quantities for processing (i.e., not exceed processing capabilities). An andrologist determines when a bull is ready for collection. Collection begins when a bull is approximately 8 to 10 mo of age.

Previous research has established effects of management and environmental factors on sperm production of mature bulls that have completed progeny testing (Amann and Almquist, 1976; Everett et al., 1978; Mathevon et al., 1998). Amann et al. (1974) found that total sperm (TSp) per ejaculate increased until bulls were 7.5 yr of age and then decreased, whereas Everett and Bean (1982) reported the peak TSp was achieved at 4 yr of age. Another study identified season, collection team, and collection frequency as influential factors in TSp production (Mathevon et al., 1998). The authors identified the ideal collection interval, in terms of achieving the maximum number of motile sperm per ejaculate, as between 4 and 5 d. Everett et al. (1978) suggested that increasing the collection interval from 2 d to >6 d would yield more semen per ejaculate, but daily sperm output would be greater if bulls were collected more frequently. The authors concluded that frequency of ejaculation was the most important factor in TSp harvested per year (Everett et al., 1978). A more recent study (Fuerst-Waltl et al., 2006) reported that TSp produced on a given collection day increased with age of bull and collection interval, and the authors noted that the first ejaculate on a given day yielded more sperm than subsequent ejaculates.

With the pressure to collect and market large quantities of semen at an earlier age in the past decade, Murphy et al. (2018) evaluated the effects of age of bull, ejaculate number, and season of collection on sperm production in Holstein-Friesian bulls. The authors confirmed that TSp increased with age of bull, up to 4 yr, and noted that bulls <1 yr of age produced less TSp than bulls >1 yr of age. As in previous studies, the first ejaculate yielded more TSp and higher prefreeze motility than the second ejaculate. However, the ejaculates did not differ in postthaw motility, and the authors concluded that collecting second ejaculates in young genome-tested bulls would be a useful strategy (Murphy et al., 2018).

Previous studies of TSp production have relied on linear models to identify important management and environmental factors (Taylor et al., 1985; Mathevon et al., 1998; Murphy et al., 2018). However, the association between TSp production and factors such as age at collection is often nonlinear. Machine learning algorithms offer greater flexibility than linear models; therefore, they may be able to capture nonlinear relationships between outputs and potential explanatory variables with fewer assumptions about the distributions of variables or restrictions on missing values (Kuhn and Johnson, 2013). The popularity of machine learning methods has increased rapidly in recent years within the fields of animal and dairy sciences, with applications including prediction of genomic breeding values (Yao et al., 2016), prediction of early postpartum health disorders (Pralle et al., 2018), prediction of insemination outcomes (Shahinfar et al., 2014), forecasting of future milk yield (Murphy et al., 2014), and analysis of images to determine BCS (Rodríguez Alvarez et al., 2018).

Despite rapid increases in the usage of semen from young genome-tested bulls in leading dairy countries, published research focused on forecasting TSp production of such bulls is lacking. The objectives of this study were (1) develop prediction models for daily, weekly, and monthly TSp

production from collection history, health status, and management factors to compare their performance, and (2) assess the ability of these prediction models to forecast future TSp production, as well as differences in prediction accuracy by seasonality or age of bull.

2.3   Materials and Methods

Ejaculate-level semen production data, bull demographic information, and health events of Holstein and Jersey bulls collected from 2015 to 2019 at 2 collection facilities of a commercial AI company (ABS Global Inc.) were used in this study. Data were filtered to include collections at 10 to 28 mo of age to ensure at least 150 unique bulls were collected at each age. Collections for research studies or in vitro fertilization protocols were excluded, as were collections reporting >45 billion cells per day, collections following an interval >31 d since the previous collection, and collections from bulls with missing age at arrival. After filtering, 92,211 ejaculate records from 1,118 bulls were available for analysis.

Before October of 2018, following collection, neat semen was initially diluted, and a sample was removed. The sample was then further diluted, and the concentration was determined using a DU800 spectrophotometer (Beckman Coulter). The standard curve for the spectrophotometer was established using absorbance data compared directly to cell counts using a hemocytometer counting chamber and a NucleoCounter (SP-100, ChemoMetec). More recently, (post October 2018) ejaculate concentrations were measured using computer-aided sperm analysis and validated to the NucleoCounter as well. Following initial dilution, a sample was retained and analyzed in a Leji counting chamber with the IVOS II (IMV International). Absorbance readings and cell counts were used with ejaculate volume to determine the concentration of TSp (concentration $\times$ volume) from each ejaculate, and the final results were recorded into a central database for each method respectfully.

Ejaculate records were then aggregated to create daily, weekly, and monthly records—note that a daily record would correspond to a single collection (bulls are not collected more than once per day), but 1 collection could include 2 or more ejaculates. A bull's TSp counts from all ejaculates in a given day were summed to determine his daily TSp, whereas weekly TSp represented the sum of daily TSp for the bull in a given week, and monthly TSp represented the sum of daily TSp for a bull in a given month. The TSp per day, week, or month was the dependent variable. Potential explanatory variables included the following: age at collection, age at first successful collection, age at arrival to the AI stud, collection frequency (ejaculates/collection, ejaculates/week, collections/week, or collections/month), collection interval (days since previous collection), breed of bull, barn where housed and collected (8 barns, with 28–1,038 animals per barn), year-season of collection, scrotal circumference (SC) at 10 to 11 mo of age (5 evenly spaced categories from 26.5–36 cm, available for 355 bulls), health events (described below), and TSp on the 3 most recent collection dates.

Health events, including routine procedures and examinations, were grouped into 16 categories (with number of events ≤6 mo before collection) as follows: dehorning (688), gastrointestinal system (210), hoof trim (21,469), integumentary system (300), musculoskeletal system (1,255), respiratory system (986), urogenital abnormality (207), or other (3,492), as well as any 2- or 3-way interactions with at least 100 events. To determine if timing of health events relative to collection affected TSp, health events were classified into 3 categories, corresponding to date of event ≤1, ≤3, or ≤6 mo before collection.

2.3.1 Model Selection

Algorithms were chosen based on their ability to accommodate continuous phenotypes, with preference given to newer methods and those used previously in the animal sciences, as well as

accessibility in the train function of the Caret 6.0–85 software (Kuhn, 2020). Methods used in

this study included linear regression (LM), random forest (RF), Bayesian regularized neural

networks (BRNN), model tree, multilayer perceptron neural network (MLP), and extreme

learning machine (ELM); LM was used as the baseline method, as it is most widely used as a

baseline in prediction of continuous outcomes in our field, and it allows a detailed understanding

of how various explanatory variables affect the outcome. The RF is an ensemble method

comprising decision trees that tend to provide robust predictions and resist bias in the presence of

messy data and missing values (Breiman, 2001). Random forest is known to be extremely

successful in prediction, due to performing a very large number of iterations across all possible

tree configurations, and it provides a variable importance ranking. Model tree is a tree-based

algorithm where the leaf nodes contain linear regression models. Model trees handle missing

data effectively and capture nonlinear relationships through tree-building, and end nodes can

capture linear relationships. The specific algorithm used in this study was M5P, in which the

model tree is constructed, pruned, and smoothed, allowing efficient learning and computational

feasibility in high-dimensional tasks (Quinlan, 1992). The M5P was run using rWeka, a group of

machine learning algorithms for data preprocessing, classification, regression, clustering,

association rules, and visualization (Hornik et al., 2009). The popularity of neural networks (NN)

has increased exponentially in animal sciences and many other fields in recent years, as they are

able to accommodate highly complex and nonlinear relationships (Kuhn and Johnson, 2013). The

most basic of NN algorithms, MLP, is a feed-forward NN with 1 or more hidden layers, trained

using back-propagation (Reed and Marks, 1999). In this study, MLP was used as a baseline for

comparison with more complex NN and the baseline (LM). The ELM is a basis function method

that is often used in time-series analyses, including applications in soil science (Liakos et al.,

2018), and it is known for computational efficiency and resistance to overfitting due to its simple

structure and no need for tuning (Huang et al., 2012). The BRNN is a back-propagation network

that uses ridge regression in the objective function and a Bayesian decision framework to end

training (Burden and Winkler, 2008); it is robust and resistant to overfitting, but computational

time can be a limitation (Burden and Winkler, 2008; Pérez-Rodríguez et al., 2013). The main

factors considered when selecting algorithms were the ability for the model to provide

predictions for a continuous outcome, computational feasibility, ease of implementation (as the

chosen models may later be applied in a commercial setting by users that are not data scientists),

robustness to missing data and outliers, and resistance to overfitting.

Daily, weekly, and monthly data sets were split randomly, with 75% of observations allocated to

the training set and the remaining 25% assigned to the testing set. Five-fold cross validation was

used to optimize model parameters within the training set. Tuning parameters were determined in

a 2-step process: (1) run a given model in which tuning length is based on number of variables in

the model, and (2) use a grid search to optimize parameters within a range determined in the

previous step.

Prediction accuracy was measured in 2 ways: root mean squared error (RMSE) in the testing set

and correlation (r) between predicted and actual values in the testing set. Models were run with

TSp in the previous 3 records (3 collections for daily, 3 wk for weekly, and 3 mo for monthly),

as lag variables or without lag variables, to evaluate the importance of knowledge regarding a

bull's recent collection history. Health events from the most recent 1-, 3-, or 6-mo period were

included or excluded as binary (presence vs. absence) explanatory variables, depending on

goodness of fit.

Variable importance was determined based on caret's variable importance function, varImp, which ranks explanatory variables based on the influence of each variable on TSp predictions. For NN, variable importance was based on the absolute value of the weight each variable had within the network. For RF, the varImp function tracked changes in model statistics for each predictor and computed the reduction in these statistics when each predictor's features were added to the model (Kuhn, 2020). Variables were verified as important based on high correlations with TSp as compared with other variables.

2.3.2   Age-Based Forecasting

To quantify our ability to predict TSp output for bulls of differing ages, from 10 to 28 mo at time of collection, a rolling age-based analysis was implemented. Monthly TSp was forecasted using age at current collection, age at first successful collection, age at arrival, collection frequency, year, season, breed, barn, SC (when available), and standardized lag variables (when available). Standardized lag TSp was computed as TSp collected 1, 2, or 3 mo previously divided by the number of collections in that month. Health data were excluded from the final age-based analysis because these variables did not improve model performance.

Algorithms used in age-based analyses were LM (as baseline), RF, and BRNN, with parameters as determined in the aforementioned model selection. The RF and BRNN were selected due to their performance in model selection (lowest RMSE and highest correlation) compared with the other models. The LM was selected as a baseline approach for comparison. Training and testing sets were split by age at collection. In the additive approach, all cumulative prior data were used as the training set, whereas in the fixed-window approach, only records from the 3 most recent months were used as the training set. Each training set had 4 testing sets that contained the next 4 mo of TSp records. In the additive approach, the number of records (bulls) in the training sets

ranged from 115 (115) at 13 mo of age to 4,859 (666) at 27 mo of age. Conversely, in the fixed-window approach, the number of records (bulls) in the training sets ranged from 115 (115) at 13 mo of age to 1,253 (558) at 17 mo of age, and the number of records (bulls) in the testing sets ranged from 232 (232) at 28 mo of age to 428 (428) at 15 and 16 mo of age. Models were trained using 5-fold cross validation, and model performance was based on RMSE and correlation of predicted and actual TSp in the testing set.

2.3.3   Date-Based Forecasting

To quantify our ability to predict future TSp output of individual bulls throughout the calendar year, date-based forecasting was also implemented. Monthly and weekly TSp were predicted using age at collection, age at first successful collection, age at arrival, collection frequency, year, season, breed, barn, SC (when available), and standardized lag TSp variables from the previous 3 records (when available). As previously mentioned, health data were not included in the final models, as these variables did not improve model prediction. The TSp production records from January 2015 through November 2019 were used for date-based analyses. Models used for date-based monthly TSp forecasting included LM and RF. Disadvantages of BRNN in the age-based analyses were long computational time and inability to handle missing or sparse factors that may have differed in the training and testing sets. The RF accommodated missing values and categories, and RF performed better than BRNN in age-based analyses. Monthly TSp was forecasted for each month beginning in 2017. As previously discussed, training sets were constructed with the additive approach using all available TSp records to date, or with the fixed-window approach using TSp records from the previous 1 yr or 4 mo only. The TSp records for each of the next 4 subsequent months comprised the testing sets.

Models used for date-based weekly TSp forecasting included LM (as baseline) and RF. The TSp

records corresponding to each week from January 2017 to November 2019 were analyzed.

Additive training sets were used for LM. The RF and LM were run on fixed training sets based

on all records from the previous year or all records from the previous month to determine the

effect of the quantity of retrospective data. Testing sets comprised TSp records for the 4

subsequent weeks.

2.4 Results and Discussion

2.4.1 Descriptive Statistics

Mean age at arrival was 6.1 ± 1.9 mo, whereas mean age at first collection was 11.3 ± 1.1 mo.

Output of TSp for individual bulls was analyzed on a daily, weekly, and monthly basis. Daily

data consisted of 43,918 records from 1,037 bulls, including 39,172 records from 900 Holstein

bulls and 4,746 records from 137 Jersey bulls. Mean daily TSp was 8.81 ± 4.77 billion cells,

from 2.00 ± 0.28 ejaculates. Weekly data consisted of 23,404 records from 1,003 bulls, including

20,661 records from 872 Holsteins and 2,743 records from 131 Jersey bulls. Mean weekly TSp

was 15.09 ± 8.97 billion cells from 1.80 ± 0.56 collections and 3.54 ± 1.26 ejaculates. Monthly

data consisted of 5,127 records from 664 bulls, including 4,441 records from 570 Holstein bulls

and 686 records from 94 Jersey bulls. Mean monthly TSp was 48.89 ± 34.82 billion cells from

5.85 ± 2.97 collections and 11.7 ± 6.21 ejaculates. The mean TSp of 5.41 billion cells per

ejaculate in the present study agrees with estimates of Hering et al. (2014; 4.97 ± 2.15 billion

cells) and Druet et al. (2009; 4.38 ± 2.45 billion cells).

2.4.2 Model Selection

The 3 most important variables in prediction of TSp output were collection frequency, lag TSp

production, and age at collection. These variables were also identified as most important in the

age- and date-based analyses. Collection frequency had the greatest effect on weekly and monthly TSp predictions, as the correlation between number of collections per month and TSp output was 0.77. Collection frequency and collection interval are interdependent. Although it has been established that more ejaculates yield more TSp over time (Everett et al., 1978), a longer collection interval yields more TSp at the subsequent collection (Everett and Bean, 1982; Mathevon et al., 1998; Fuerst-Waltl et al., 2006).

The second most important variable was lag TSp production. The TSp at previous collections were moderately correlated with TSp at the current collection. For example, TSp production on the current collection day had a 0.57 correlation with TSp output on the previous collection day (lag 1), a 0.62 correlation with TSp output 2 collections ago (lag 2), and a 0.56 correlation with TSp production 3 collections ago (lag 3). Lag TSp from 2 collections earlier (lag 2) not only had the highest correlation with TSp output on the current day, but it was also the most important of the 3 lag variables in almost all of the analyses carried out in this study; however, prediction accuracy was greatest when 3 lags were included in the model simultaneously. Presumably, the strong relationship between current TSp and lag 2 TSp reflected the fact that most bulls were collected twice weekly, in which case lag 2 TSp corresponded to the same day in the previous week.

Last, TSp production increased with age at collection. This relationship is well established in literature, and it is one of the critical challenges facing AI companies in the age of genomic selection. Customer demand is greatest for young bulls that are identified as having elite genetic merit through genomic testing, but their semen-producing capacity is poorer and more variable than that of older bulls. Amann et al. (1974) reported that TSp per ejaculate of Holstein-Friesian bulls increased with age at collection until 7.5 yr, after which it began to decrease (Amann et al.,

1974). More recently, Murphy et al. (2018) found that TSp increased until bulls reached 4 yr at age of collection, which agreed with Everett and Bean (1982).

Average prediction accuracy from the model selection process is shown in Table 1. Based on RMSE in the testing set, performance of RF (daily, weekly, and monthly values of 3.0, 4.7, and 14.5 billion cells, respectively) was similar to that of BRNN (3.0, 4.8, and 15.6, respectively) and M5P (3.1, 4.9, and 15.7, respectively). Performance of the baseline LM (3.3, 5.1, and 16.9, respectively) was somewhat poorer than BRNN, RF, and M5P, but superior to that of ELM (3.4, 5.7, and 18.2, respectively) and MLP (3.6, 7.7, and 28.7, respectively). To give perspective, the testing set RMSE for daily TSp production was roughly equivalent to the amount of TSp produced in a single ejaculate, whereas the RMSE of weekly TSp predictions was roughly equivalent to the TSp from a typical collection, and the RMSE of monthly TSp predictions was approximately that of an average weekly TSp for a typical bull.

The RF models performed better than the others considered in this study. This advantage can be attributed to the nature of RF, in which many random iterations consider all possible configurations of variables, capture any complex relationships within the data, and reduce variation and overfitting through random feature selection (Herrera et al., 2019). It was expected that LM would perform poorly, as LM are unable to capture complex, nonlinear relationships. As a generalized network, BRNN minimizes a linear combination of squared errors and weights during training and prevents overfitting by rewarding simpler models (Dongre et al., 2012). We expected the performance of BRNN to be similar to that of RF, despite complications with computational time and inability to work with missing data or categories. Performance of M5P lies between RF and LM because M5P combines nonlinear relationships through the tree structure and linear relationships in the nodes. The MLP performed most poorly on the training

and testing data. This can be attributed to MLP's simplicity and early stopping criterion. The models may have identified local minima, rather than globally optimal solutions, despite cross validation. The ELM performed similarly to LM, but was not comparable with RF and BRNN. This could be due to the use of a single hidden layer, which randomly selects node parameters from continuous distributions and estimates output weights via least squares (Huang et al., 2012; Milačić et al., 2017). Although it is fast, the ELM algorithm may not be suitable for the data structure and variables of the present study.

Health data did not improve predictive performance of the models. A potential explanation is that 1, 3, and 6-mo incidences of health events were not precise enough to identify the true effects of health problems on TSp production. However, we can conclude that, despite the momentary decrease in TSp a bull might experience during or shortly following a health event, common health events do not seem to affect the long-term predictive performance of TSp.

2.4.3 Age-Based Forecasting

Table 2 shows results for age-based TSp predictions 1, 2, 3, or 4 mo into the future, using LM, RF, and BRNN. Based on RMSE and correlations between predicted and actual values in the testing sets, prediction accuracy was greatest for RF and BRNN with lag variables and additive training sets that contained all previous TSp collection data. Correlations between actual and predicted values were 0.93 when predicting 1 mo into the future, and remained at 0.92 (RF) and 0.91 (BRNN) as far as 4 mo into the future, when lag variables were included. Correlations from the baseline LM ranged from 0.89 (4 mo into the future) to 0.90 (1 mo in the future). Prediction accuracy was compromised only slightly when using a fixed-window training set comprised of TSp data from the most recent 3 mo, and this could be a useful option for data reduction if computational feasibility becomes an issue. Prediction accuracy deteriorated substantially when

lag variables were excluded, with correlations between predicted and actual TSp production for additive and fixed 3-mo analyses, ranging from 0.78 to 0.83 for 4 mo into the future, and 0.83 to 0.93 for 1 mo into the future. In this study, models excluding the lag variables would best reflect the expected accuracy of predictions 3 and 4 mo into the future because, in a real-time application, we would not yet know a bull's TSp output 1 or 2 mo into the future when predicting his TSp performance 3 or 4 mo into the future.

Figure 1 shows the effect of age at collection on prediction accuracy. The relative accuracies of RF and BRNN predictions tended to be very similar from 16 to 27 mo of age; however, RF provided greater prediction accuracy at early ages of 14 and 15 mo. Performance of the baseline LM was consistently poorer than that of RF and BRNN, as measured by RMSE and correlation.

2.4.4   Date-Based Forecasting

For the date-based prediction exercise, results from the monthly analyses tended to be quite similar to those of the age-based analyses (Table 3). Prediction accuracy was greatest for RF, with RMSE ranging from 4.5 to 17.7 billion cells per month, and correlations ranging from 0.89 to 0.99 for predictions 1 to 4 mo into the future, when lag variables were included and an additive training set was used. The baseline LM performed inferiorly, with RMSE from 11.3 to 21.0 billion cells and correlations from 0.84 to 0.94. Model performance using fixed-window 1-yr training sets performed similar to additive windows, with a 0.2 billion cell difference at most in RMSE and no difference in correlation. Using fixed training sets containing the most recent 4 mo of TSp data, but excluding lag variables, was detrimental to prediction accuracy, with correlations as low as 0.73 and RMSE as high as 26.7 billion cells per month. Again, models excluding lag variables are most reflective of the accuracy one would expect when predicting TSp several months into the future, without knowledge of the bull's TSp for collections in the

interim. Another situation where prediction models without lag variables would be used is when making predictions for young bulls with no prior collection data.

The trajectories of prediction accuracy over time when using an additive training set to predict TSp 1 mo into the future are shown in Figure 2. Performance of LM was consistently poorer than RF over time. We speculate that spikes in RMSE and correlation in December associate with Council on Dairy Cattle Breeding (Bowie, MD) sire summaries and the pressure to collect new bulls that rank highly for traits such as Lifetime Net Merit. When comparing November 2018 and December 2018, November had 26 unique bulls with an average age at collection of 20.5 mo, and December had 35 unique bulls with an average age at collection of 13.2 mo. When these new, younger bulls are added, LM models and models without lags suffer, whereas lag RF models do well. Additionally, a spike was observed in August 2017 when predicting 1 mo into the future. The following month was when a new semen sorting program was introduced. As with any big changes that occur in supply chain management, semen collection was affected and differed from what was predicted.

Results from the weekly analyses using LM and RF are shown in Table 4. As previously discussed, RF tended to provide TSp predictions with smaller RMSE and higher correlations between actual and predicted values than LM across all scenarios. Correlations for weekly predictions were slightly poorer than those of monthly values, ranging from 0.85 to 0.86 for RF when predicting 1 to 4 wk into the future with lag variables included and fixed-window training sets comprising TSp data from the most recent month or year.

2.5   CONCLUSIONS

Total sperm production can be predicted with >90% accuracy up to 4 mo into the future. Sperm production is highly repeatable, so lag variables corresponding to recent collections can enhance

prediction accuracy. Machine learning algorithms provide greater flexibility and robustness to messy data than linear models, which improves prediction accuracy. Management factors, such as age at collection, frequency of collection, breed, barn, year, season, and scrotal circumference contribute to prediction accuracy, but health events did not improve predictions in this study. In practice, weekly total sperm predictions could enhance the operational efficiency of semen processing, scheduling, and inventory control, whereas monthly predictions could be used to forecast product availability for specific markets. Future studies should identify management, environmental, and genetic factors that could further improve prediction accuracy for individuals or groups of bulls whose semen is destined for specific markets and develop decision support tools to incorporate this information into standard operating procedures and inventory management decisions.

2.6   ACKNOWLEDGMENTS

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2.8   Tables and Figures

Table 2.1 Prediction accuracy1 of the best performing model within each method for daily, weekly, or monthly total sperm (TSp) production using randomly constructed training and testing sets.

Method[2]	Daily TSp		Weekly TSp		Monthly TSp	
	RMSE	r	RMSE	r	RMSE	r
LM	3.3	0.73	5.1	0.82	16.9	0.87
RF	3.0	0.77	4.7	0.84	14.5	0.90
BRNN	3.0	0.77	4.8	0.84	15.6	0.91
M5P	3.1	0.76	4.9	0.84	15.7	0.91
MLP	3.6	0.65	7.7	0.73	28.7	0.69
ELM	3.4	0.71	5.7	0.78	18.2	0.84

[1] Measures of accuracy included root mean squared error (RMSE; billions of cells) and correlation (r) in the testing set.
[2] Methods included linear regression (LM), random forest (RF), Bayesian regularized neural network (BRNN), model tree (M5P), multilayer perceptron neural network (MLP), and extreme learning machine (ELM).

Table 2.2 Prediction accuracy1 for monthly total sperm (TSp) production using training and testing sets defined by age of bull, and using additive (cumulative) or fixed (most recent 3 mo) training windows, with or without lag variables.

Method[2]	Training set	Lag	Age + 1 mo		Age + 2 mo		Age + 3 mo		Age + 4 mo	
			RMSE (SD)	r (SD)	RMSE (SD)	r (SD)	RMSE (SD)	r (SD)	RMSE (SD)	r (SD)
LM	Additive	Yes	15.7 (2.4)	0.90 (0.02)	16.4 (2.0)	0.89 (0.02)	17.0 (1.8)	0.89 (0.02)	17.7 (1.6)	0.89 (0.02)
RF	Additive	Yes	12.7 (1.8)	0.93 (0.01)	13.4 (1.4)	0.93 (0.01)	14.0 (1.3)	0.92 (0.01)	14.5 (1.2)	0.92 (0.02)
BRNN	Additive	Yes	13.0 (1.4)	0.93 (0.02)	13.7 (1.0)	0.92 (0.02)	14.6 (1.6)	0.92 (0.03)	15.3 (1.7)	0.91 (0.03)
LM	Fixed 3 mo	Yes	15.1 (2.0)	0.90 (0.01)	15.7 (1.6)	0.90 (0.02)	16.3 (1.5)	0.90 (0.02)	17.0 (1.3)	0.89 (0.02)
RF	Fixed 3 mo	Yes	12.9 (1.8)	0.93 (0.01)	13.5 (1.5)	0.93 (0.01)	14.2 (1.4)	0.92 (0.01)	14.7 (1.2)	0.92 (0.01)
BRNN	Fixed 3 mo	Yes	13.5 (1.9)	0.92 (0.02)	14.5 (1.9)	0.91 (0.02)	15.5 (2.4)	0.91 (0.03)	16.3 (3.4)	0.91 (0.03)
LM	Additive	No	19.6 (2.8)	0.93 (0.03)	20.9 (2.2)	0.83 (0.03)	22.6 (1.5)	0.83 (0.02)	25.9 (4.6)	0.83 (0.02)
RF	Additive	No	18.0 (1.6)	0.85 (0.04)	20.2 (1.0)	0.84 (0.03)	22.3 (1.6)	0.84 (0.02)	24.4 (2.6)	0.83 (0.02)
BRNN	Additive	No	18.4 (1.8)	0.84 (0.03)	20.2 (1.6)	0.82 (0.03)	21.7 (1.4)	0.80 (0.04)	23.3 (1.8)	0.78 (0.06)
LM	Fixed 3 mo	No	18.6 (2.2)	0.83 (0.03)	19.7 (1.6)	0.83 (0.03)	21.0 (1.4)	0.83 (0.02)	23.8 (5.5)	0.83 (0.02)
RF	Fixed 3 mo	No	18.0 (1.5)	0.85 (0.04)	20.1 (0.9)	0.84 (0.03)	22.0 (1.7)	0.84 (0.02)	24.1 (2.7)	0.83 (0.03)
BRNN	Fixed 3 mo	No	18.3 (1.9)	0.84 (0.03)	19.9 (1.3)	0.83 (0.03)	21.5 (1.2)	0.81 (0.05)	23.2 (2.4)	0.79 (0.08)

[1] Measures of accuracy included root mean squared error of prediction (RMSE; billions of cells) and correlation between predicted and actual TSp (r) in the testing set, when predicting TSp output 1, 2, 3, or 4 mo into the future.
[2] Methods included linear regression (LM), random forest (RF), and Bayesian regularized neural network (BRNN).

Table 2.3 Prediction accuracy[1] for monthly total sperm (TSp) production using training and testing sets defined by calendar date, and using additive (cumulative) or fixed (most recent 1 yr or 4 mo) training windows, with or without lag variables.

Method[2]	Training set	Lag	Date + 1 mo		Date + 2 mo		Date + 3 mo		Date + 4 mo	
			RMSE (SD)	r (SD)	RMSE (SD)	r (SD)	RMSE (SD)	r (SD)	RMSE (SD)	r (SD)
LM	Additive	Yes	15.3 (2.2)	0.90 (0.02)	15.4 (2.0)	0.90 (0.02)	15.5 (2.1)	0.90 (0.02)	15.6 (2.1)	0.90 (0.02)
RF	Additive	Yes	11.9 (2.4)	0.94 (0.02)	12.0 (2.5)	0.94 (0.02)	11.8 (2.3)	0.94 (0.02)	11.8 (2.4)	0.94 (0.02)
LM	Fixed 1 yr	Yes	15.3 (2.2)	0.90 (0.02)	15.6 (2.0)	0.90 (0.02)	15.8 (2.1)	0.90 (0.02)	15.9 (2.0)	0.89 (0.02)
RF	Fixed 1 yr	Yes	12.1 (2.5)	0.94 (0.02)	12.2 (2.5)	0.94 (0.02)	11.9 (2.2)	0.94 (0.02)	11.9 (2.3)	0.94 (0.02)
LM	Fixed 4 mo	Yes	15.6 (2.5)	0.90 (0.03)	15.8 (2.6)	0.89 (0.02)	15.9 (2.6)	0.89 (0.02)	16.3 (2.9)	0.89 (0.03)
RF	Fixed 4 mo	Yes	13.1 (2.2)	0.93 (0.02)	13.1 (2.0)	0.93 (0.02)	13.0 (1.9)	0.93 (0.01)	13.1 (1.7)	0.93 (0.01)
LM	Additive	No	19.7 (1.9)	0.83 (0.03)	20.4 (2.3)	0.83 (0.03)	20.6 (2.1)	0.83 (0.02)	20.8 (2.1)	0.83 (0.02)
RF	Additive	No	17.3 (2.5)	0.87 (0.03)	18.3 (2.9)	0.86 (0.03)	18.5 (3.0)	0.85 (0.04)	19.0 (3.3)	0.85 (0.04)
LM	Fixed 1 yr	No	19.5 (2.0)	0.83 (0.03)	19.9 (1.9)	0.83 (0.3)	20.0 (1.9)	0.83 (0.03)	20.1 (1.9)	0.82 (0.03)
RF	Fixed 1 yr	No	17.3 (2.5)	0.87 (0.03)	18.4 (2.9)	0.85 (0.04)	18.6 (3.2)	0.85 (0.04)	19.1 (3.4)	0.84 (0.05)
LM	Fixed 4 mo	No	19.6 (2.3)	0.83 (0.03)	20.1 (2.2)	0.82 (0.03)	20.2 (2.2)	0.82 (0.03)	20.7 (2.3)	0.82 (0.03)
RF	Fixed 4 mo	No	17.9 (2.7)	0.86 (0.03)	18.8 (2.4)	0.84 (0.03)	19.4 (2.5)	0.83 (0.03)	20.1 (2.5)	0.82 (0.03)

[1] Measures of accuracy included root mean squared error of prediction (RMSE; billions of cells) and correlation between predicted and actual TSp (r) in the testing set, when predicting TSp output 1, 2, 3, or 4 mo into the future.

[2] Methods included linear regression (LM) and random forest (RF).

Table 2.4 Prediction accuracy[1] for weekly total sperm (TSp) production using training and testing sets defined by calendar date, and using additive (cumulative) or fixed (most recent year or month) training windows, with or without lag variables.

Method[2]	Training set	Lag	Date + 1 wk		Date + 2 wk		Date + 3 wk		Date + 4 wk	
			RMSE (SD)	r (SD)	RMSE (SD)	r (SD)	RMSE (SD)	r (SD)	RMSE (SD)	r (SD)
LM	Additive	Yes	4.8 (0.6)	0.84 (0.04)	4.8 (0.6)	0.84 (0.04)	4.8 (0.6)	0.84 (0.04)	4.8 (0.6)	0.84 (0.04)
LM	Fixed 1 year	Yes	4.8 (0.6)	0.84 (0.04)	4.8 (0.6)	0.84 (0.04)	4.8 (0.6)	0.84 (0.04)	4.8 (0.6)	0.84 (0.04)
RF	Fixed 1 year	Yes	4.4 (0.6)	0.86 (0.04)	4.4 (0.6)	0.86 (0.04)	4.4 (0.6)	0.86 (0.04)	4.5 (0.6)	0.86 (0.04)
LM	Fixed 1 mo	Yes	4.9 (0.6)	0.84 (0.04)	4.9 (0.6)	0.84 (0.04)	4.9 (0.6)	0.84 (0.04)	4.9 (0.7)	0.83 (0.04)
RF	Fixed 1 mo	Yes	4.7 (0.6)	0.85 (0.04)	4.7 (0.6)	0.85 (0.04)	4.7 (0.6)	0.85 (0.04)	4.7 (0.6)	0.85 (0.04)
LM	Additive	No	5.9 (0.7)	0.74 (0.06)	6.0 (0.7)	0.74 (0.06)	6.0 (0.7)	0.74 (0.06)	6.0 (0.7)	0.74 (0.06)
LM	Fixed 1 yr	No	5.9 (0.7)	0.74 (0.06)	5.9 (0.7)	0.74 (0.05)	5.9 (0.7)	0.74 (0.05)	6.0 (0.7)	0.74 (0.06)
RF	Fixed 1 yr	No	5.1 (0.6)	0.82 (0.05)	5.3 (0.6)	0.80 (0.05)	5.4 (0.6)	0.79 (0.05)	5.5 (0.7)	0.78 (0.05)
LM	Fixed 1 mo	No	5.8 (0.7)	0.75 (0.05)	5.9 (0.7)	0.75 (0.05)	5.9 (0.7)	0.74 (0.05)	6.0 (0.7)	0.74 (0.05)
RF	Fixed 1 mo	No	5.1 (0.7)	0.81 (0.06)	5.3 (0.7)	0.80 (0.05)	5.4 (0.6)	0.79 (0.05)	5.6 (0.7)	0.77 (0.05)

[1] Measures of accuracy included root mean squared error of prediction (RMSE; billions of cells) and correlation between predicted and actual TSp (r) in the testing set, when predicting TSp output 1, 2, 3, or 4 wk into the future.
[2] Methods included linear regression (LM) and random forest (RF).
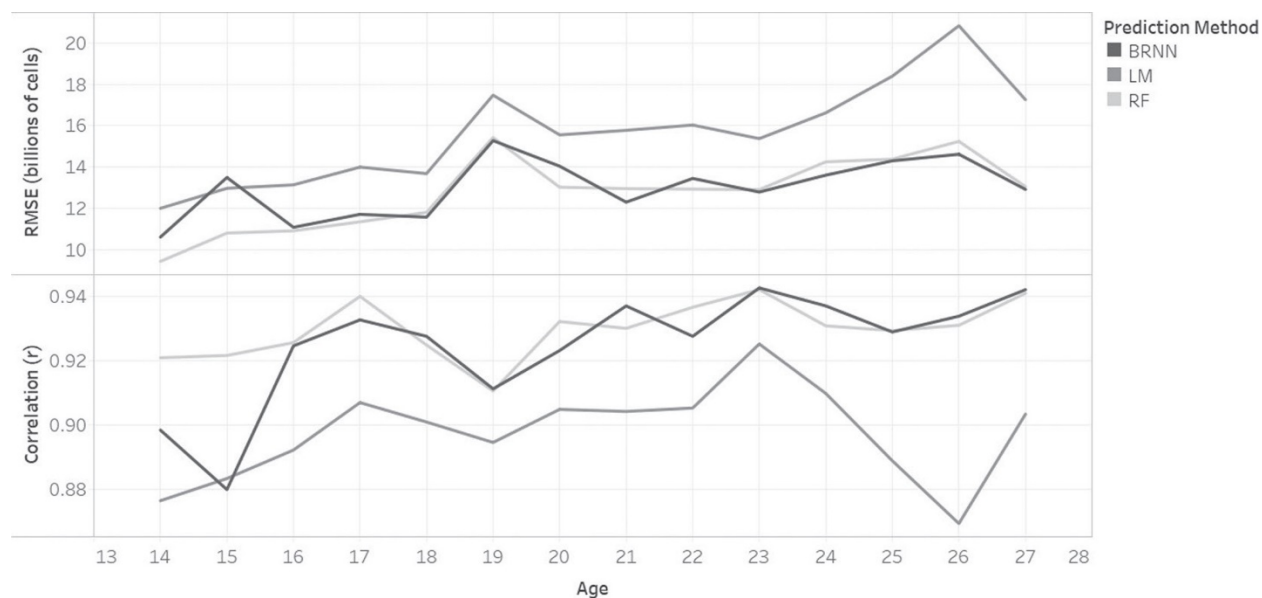
Figure 2.1 Comparison of prediction accuracy for monthly total sperm (TSp) production using linear regression (LM), random forest (RF), and Bayesian regularized neural network (BRNN) on additive training sets defined by age of bull, and with lag variables in the prediction model. Shown is the root mean squared error (RMSE; billions of cells) in the testing set 1 mo out (top), and correlation (r) between actual and predicted TSp production records of the same bulls 1 mo into the future (bottom).

Figure 2.2 Comparison of predictive ability for monthly total sperm (TSp) production using linear regression (LM) and random forest (RF) using additive training sets defined by calendar date (year-month, where M01 = month 1, etc.), using lag variables in the prediction model. Shown is the root mean squared error (RMSE; billions of cells) in the testing set 1 mo out (top), and correlation (r) between actual and predicted TSp production records of the same bulls 1 mo into the future (bottom).

CHAPTER 3: BULLVAL$: AN INTEGRATED DECISION-SUPPORT TOOL FOR PREDICTING THE NET PRESENT VALUE OF A DAIRY BULL BASED ON PREDICTED GENETIC MERIT, SEMEN PRODUCTION POTENTIAL, AND DEMOGRAPHIC FACTORS

3.1   Abstract

Most Artificial Insemination (**AI**) companies have well-established protocols for acquiring and rearing young bulls and collecting, processing, and selling their semen. However, the decision of when to replace a bull with a new selection candidate can be influenced by many factors and their interactions. This study aimed to provide a user-friendly Markov Chain (MC) model for economic valuation of dairy bulls based on the most important factors contributing to replacement decisions, such as age, predicted semen production, and predicted genetic merit, and to describe the features and outcomes associated with applying this model to data from a leading AI company. A bull's net present value (NPV) was calculated based on costs and revenues associated with housing, collecting, and marketing the bull's semen as well as its probability of staying in the herd until the next age bin. Production, sales, and bull demographic data from 2018 to 2020 from one AI company were used to establish base values. Within the MC, a bull's state was assigned based on his age, in 4-mo bins (AGE) from 10 to 85 mo. Involuntary culling percentages defined transition probabilities from one AGE to the next. The MC modeled the steady state proportion of bulls within a herd across 330 iterations, with aggregated NPV calculated after each time point, and steady state was reached at 310 iterations. Data needed to calculate NPV include: age at arrival, housing cost, depreciation cost and term, replacement cost, salvage value, total sperm production (TSp), TSp per straw unit (packing rate), genetic prediction for lifetime Net Merit (NM$; binned by decile (NM bin)), market distribution and price per unit

(by AGE and NM bin), and interest rate. The difference between a bull's NPV and that of a young replacement bull is the bull's valuation (BullVal$). A replacement bull was defined as entering the production herd at AGE =1, arrival age = 6 mo, NM bin = 9, and TSp deviation = 0%, resulting in an NPV of $250,951. The range of BullVal$ encountered was -$316,748 to $497,710, with 49% of bulls recommended for culling based on negative BullVal$. A bull's NPV was influenced primarily by market allocation and pricing, as well as the interaction of sperm production with genetic merit.

Key Words: Markov chain, herd simulation, bull valuation

3.2   Introduction

Dairy genetics companies seek to provide top genetics from elite bulls to accelerate genetic progress and enhance farm profitability of their customers. Most companies have well-established protocols for acquiring and raising young bulls and collecting, processing, and selling their semen. However, the decision of if and when to replace a bull with a new selection candidate can be subjective and may be influenced by many factors and their interactions. Currently, replacement decisions typically involve many individuals, with competing interests, within a given artificial insemination (**AI**) company, including sire analysts (who acquire the bulls), veterinarians, inventory managers, sales and marketing staff, and barn managers. These individuals must use data regarding genetic potential, semen production, health, temperament, and other factors to decide whether a given bull is likely to: 1) achieve "premium" status in the marketplace and generate millions of dollars in revenue and tens of thousands of offspring; 2) reach (or remain in) "cash cow" status and contribute a modest revenue stream for the foreseeable future, or 3) lag behind its herd mates in revenue-generating potential due to poor semen production and/or a genetic profile that is no longer competitive or marketable. Each bull

must be evaluated relative to its existing herd mates at the AI company, as well as potential replacement bulls that may be younger and have higher genetic merit (i.e., opportunity cost), while simultaneously considering the fixed and variable costs associated with keeping the bull or acquiring a replacement.

While objective methods to combine semen production, genetic potential, age, and other factors for valuation of dairy bulls in an AI company context are lacking, such methodologies and decision-support tools are well-established for dairy cows (De Vries, 2004, 2006; Cabrera, 2012). These methods combine data regarding age, parity, milk production, pregnancy status, genetic potential, and the inventories of lactating cows and replacement heifers to formulate an estimate of the future income that will be generated by an individual cow, relative to her current and potential herd mates, such that the farmer can decide when to replace a specific cow in an objective and optimal manner (e.g., CowVal$). To our knowledge, this framework has not been extended to the monetization or ranking of dairy bulls based on income-generating potential for an AI company. Focus has been entirely on ranking bulls based on their potential to generate profit for the dairy farmer by producing offspring of greater or lesser genetic potential for individual traits or an overall profit index (e.g., Schroeder et al., 1992; VanRaden et al., 2018). The most common index used for ranking dairy cattle today is lifetime net merit (**NM$**), which considers the predicted genetic merit of cows, bulls, heifers, and calves for production, type, health, longevity, fertility, and calving traits relative to an average animal of the same breed (Van Raden et al., 2021). However, the NM$ index does not consider the semen production characteristics of a bull, only the traits he will transmit to his female offspring. As such, NM$ can be considered as an optimal tool by which dairy farmers can rank bulls when purchasing semen, but expected semen production for a specific bull at a given time varies widely (Quick et

al., 2021), and NM$ is not sufficient for making replacement decisions regarding individual bulls based on their likely contributions to the future net profit of an AI company.

Another, possibly most important, defining factor of a bull's profitability for an AI company is his market appeal. Globally, even within a country, farmers' needs for genetics and types of bulls differ (Cole et al., 2021).

Therefore, the objectives of this study are: 1) provide a user-friendly Markov Chains (**MC**) model of economic valuation for dairy bulls, focusing on the most important factors contributing to replacement decisions, and 2) describe the features and outcomes of this model when applied to data from a leading AI company.

3.3   Materials and Methods

The replacement problem of a bull was solved by MC as the difference between net present value (**NPV**) of a bull (**NPV bull**) and its replacement (**NPV replacement**), hence:

$$BullVal\$ = NPV\ bull - NPV\ replacement.$$

This simple algorithm is the aggregation of a MC model, in which a user can define parameters of a bull and compare with those of a potential replacement, with considerations of age, total sperm production (**TSp**), and genetic merit.

3.3.1   3.3.1 Markov Chain Bull Model

A dairy bull herd was represented by a 4-mo age bin MC model as a matrix. Four months was chosen to model three rounds of replacement decisions per year, based on the current frequency of Council on Dairy Cattle Breeding (CDCB; Bowie, MD) genetic evaluations of US dairy cattle. One state defines potential bull ages: **AGE** (19 bins of 4-mo duration, spanning the period from 10 to 85 mo of age).

In a MC simulation, each bull is decomposed through time in all possible states dictated by the transition probabilities, which are then referred to as resulting fractions or proportions of a bull in each iteration. The proportions of a bull represented over time (**BULL$_{AGE}$**) were simulated through MC following Cabrera (2012). A vector of transition probabilities represented the probabilities of a bull leaving the herd (**CULL**) while in a given age bin. The proportions of a given bull explains the probability in which a bull in AGE bin i will remain in the herd until the AGE bin i+1. Then, the proportions of a bull remaining in herd until the next age bin are calculated as:

$$(BULL_{AGE+1}) = (BULL_{AGE})(1\text{-}CULL_{AGE});$$

and the replacement bulls enter the herd as AGE=1, (BULL$_1$) as:

$$(BULL_1) = \sum_1^{19} BULL_{AGE}(CULL_{AGE}),$$ which assures the herd size remains constant.

A bull's (or replacement's) probabilistic life was represented from the time the bull entered the analysis (Age Start) until a point in the future when the bull and its potential replacements had reached the MC condition of steady state (Cabrera and Giordano, 2010). The MC condition of steady state is realized when the proportions of animals in each state no longer change with an increase in time (iteration), regardless of the current state of the bull or replacement in the first iteration (Hillier and Lieberman, 1986).

The model was solved through recursive iterations until the probability distribution of a bull across all states of model reached steady state. In each iteration, aggregated discounted net returns of all probabilities of the bull were estimated for the given 4-mo time period. Steady state was reached after 310 iterations, and the model parameter was set to 330 iterations to ensure bull and replacement were consistent.

Assumptions. To create the MC, assumptions were made to establish a base herd of bulls. Bulls were assumed to enter production at 10 mo of age. Once they entered collection status, bulls were collected eight times per mo until culled. In practice, bulls removed from collection rarely return; exceptions include injury, illness, or bulls that have not yet reached puberty. In the model, any remaining bulls were culled at age 85 months (7 yr 1 mo). TSp for a given bull in a 4-mo period was treated as a deviation from the mean sperm production for bulls of that age. In a production setting, many factors may impact predicted and actual TSp, including collection frequency, barn personnel, temperament, environmental conditions, semen quality, and processing regimen.

3.3.2   Economic Module

NPV of a Bull or a Replacement. The NPV of a Bull or a Replacement was the aggregated 4-mo discounted (∂) net value over 330 iterations (330 4-mo, *i*) that resulted in NPV bull (value of keeping the bull) or NPV replacement (value of replacing the bull). Economic factors used in this calculation were the incomes and revenues incurred in the maintenance, production, and culling of a bull: 1) income from straw units produced (*Si*) according to the bulls' age, predicted TSp deviation, genetic merit, and market; 2) maintenance cost (*Mc*), including housing, veterinary care, labor, and feed; 3) costs associated with involuntary culling (*Cc*), including cost of replacement and depreciation, and 4) income generated from involuntary culling a bull (*Ci*) and salvage value.

Therefore,

$$NPV\ bull\ or\ NPV\ replacement\ =\ \sum_{i=1}^{330}\left[\partial \sum_{AGE=age}^{AGE+1}(Si - Mc - Cc + Ci)_{age}(BULL_{age})\right];$$

where *i* marked the 4-mo time iteration of aggregated NPV calculations, up to 330 iterations. Age defined the bull being analyzed and ranged from 1 to 19. A replacement bull started at AGE = 1, assuming a bull was replaced with a new young sire entering production.

Table 1 is a list of minimum variables required to calculate bull value and base values for bull replacement, herd, and economic variables.

Bull Variables

AGE. Age bin (AGE) defined age of bull at the starting point (iteration =1) in the MC model. As explained previously, AGE contained 19 four-month bins, from 10 to 85 mo of age.

Age Class. To obtain price per unit in the income equation (explained below), age bins were grouped into 3 classes: young (1-4 AGE), in-waiting (5-12 AGE), and proven (12-19 AGE). In-waiting signified a bull that is older than genomic (young) bulls who entered the AI stud recently and younger than proven (old) bulls that already have offspring with performance data. This was done to reduce dimensionality, allow more samples within each grouping, and achieve a more stable price.

Arrival Age (mo). Age at which a bull arrived at the AI stud. Used to calculate Depreciation value within culling cost variable of NPV (Depreciation calculation is defined in herd variables section). A bull could arrive to the AI stud at 1 to 15 mo of age and might not enter the production herd immediately. Costs associated with rearing bulls prior to production were assumed to be constant across all bulls and are not considered within the NPV calculation.

Expected TSp percent deviation from mean (Pdev; %). The NPV bull could be calculated assuming a bull's average TSp production. A bull's expected production capability, Pdev, was the percent deviation from mean TSp, and was multiplied by the aggregated income generated (Inc) based on average TSp production.

Net Merit Decile bin. The genetic contribution of a bull was considered using the decile of NM$ for the bull, compared with the herd's distribution of NM$ values. This value was used to find the price per unit, which was a function of age, market, and genetic merit, in the income calculation.

Economic Variables

Aggregated discount. The aggregated discount was defined as: $\partial = \frac{1}{(1+int)^{i+1}}/n$ where *int* was the interest rate and *n* was the number of bulls in the herd.

Income from Straws produced. Income generated by unit sales was defined as:

$$Si = (1 + Pdev) * \sum_{MKT=mkt}^{6} \left(Inc_{mkt,NM,age}\right);$$

Where:

Pdev: Bull's sperm production deviation from herd mean, based on the average TSp deviation of a bull for the three most recent trimesters

Mkt: Product market (1-6, explained below)

Inc: money generated with the sale of product destined to different markets, based on age, TSp production, and NM bin.

Market Pricing, Distribution of product. Bulls (and units) were valued differently depending where the semen was sold. The income equation had the capability to calculate Inc based on the amount of product distributed to each market group (market share).

TSp per straw unit (packing rate). Average number of cells packaged into a unit. The value divided TSp expected per bull into units, which was then multiplied by price per unit to get income from straw units produced.

Income generated from unit sales. Money generated with the sale of product destined to different markets, based on age, TSp production, and genetic merit was the product of price per unit (PU), market share percentage (MS), and number of units produced (U):

$$Inc_{mkt,NM} = (PU_{age\ class,NM}) * (MS_{age,NM}) * (U_{age}).$$

Maintenance Cost. The maintenance cost variable incorporated prices for housing, maintenance, and veterinary costs for a bull.

Culling Cost. Cost of culling a bull $Cc = CR + CULL_{age} * Depr_{age}, where$:

CR: Cost of Replacement, which was the purchase price of a new bull

Depr: Depreciation cost, which was an aggregated price based on depreciation term and value.

Depreciation. Value assigned to a bull for insurance purposes, based on age of bull, arrival age, and term length. Depreciation cost (Depr) within the NPV was calculated as:

Depr = Depreciation Value – [Depreciation Value /(Depreciation term – ArrivalAge)*(age-ArrivalAge)],

Where Depreciation Value is the original value assessed for a bull, Depreciation term is the length of depreciation realization, and age is the age that is currently being evaluated within the aggregated NPV.

Depreciation term. The length for depreciation realization, based on age (mo). Depreciation was the remaining cost that must be paid if a bull was culled prior to the depreciation term.

Culling Income. Income generated from culling the bull, which was simply the product of salvage value (SV, constant across all ages) and proportion of culled animals: $Ci = SV * CULL_{age}$.

Culling Percentage (%). Involuntary culling percentage (**CULL**) per age bin. It was assumed that all bulls were culled at the end of AGE 19.

3.3.3 Data Required for Application

Table 1 contains base values of user-defined variables, along with explanations in the following sections. The model's base values were defined using data from the case study described below.

3.3.4 Case Study

Model performance was demonstrated using production data, sales records, health events, and bull demographics of Holstein bulls at two collection facilities of a commercial AI company (ABS Global Inc., DeForest, WI). Bulls in production from April through November 2020 were used in this illustration (reflective of two trimesters). The MC model for each bull was calculated using age of the bull in April 2020. Genetic predictions for NM$ from the December 2020 CDCB genetic evaluation were used to classify each bull into a decile, and its arrival age was used to calculate depreciation. Each bull's valuation was relative to a replacement animal of AGE = 1, Arrival age = 6, and NM = 9. It was assumed that a replacement bull would be a young bull at the beginning of its productive life, with the average arrival age, and NM just below that of the most elite bulls used to create the next generation (i.e., NM = 9).

Involuntary Culling Percentage. Involuntary culling percentages, used as transition probabilities, were derived from health records of bull deaths, recommended culling decisions, or actual culls (Table 2).

Expected TSp percent deviation from mean (Pdev; %). This was derived using company collection records from 2018 to 2020, aggregated to an average TSp per age bin, such that each month a bull was collected 8 times (Table 2). For the decision support tool, the user could enter

the deviation from this mean. In the herd case study, a bull's TSp deviation was calculated by averaging deviations from the last 3 (at most) collection months.

Market Share and Pricing. Twenty-nine countries that received more than 200,000 semen units according to 2018 to 2020 sales records were split into 6 market classes. To identify trends in types of products used in each country, PTAs of bulls sold in each country were averaged. The countries were then ranked for each PTA value, providing an estimate of importance that trait has on overall selection by country. Similar countries were grouped together manually. Market A contained 6 countries, in which fertility traits had high importance and milk composition traits had low importance. Market B contained 3 countries, in which milk production traits were of high importance and fertility and type traits had low importance. Market B contains the domestic market. Market C contained 5 countries, in which milk yield and type composites were of moderately high importance. Market D contained 3 countries with high importance for type composites. Market E contained 6 countries, in which PTA Milk, Productive Life, SCS, and Net Merit were of high importance. Lastly, Market F contained 6 countries that did not fit into above groupings and lacked a discernable pattern in traits of high importance.

Once grouped, average price per group was calculated per age bin. A smoothing function was applied to each market to limit the influence of outliers (see below). Market share was calculated as the percentage of total units per age group directed to each market. Supplemental Figure S1 contains box plots of market percentages across age bins. Supplemental Table S1 contains prices by NM bin, market, and age class.

Unit Price Smoothing Function. Price per unit of semen was estimated based on age class (young, in-waiting and proven), market class, and NM$ decile (Supplemental Table S1). Age class was used to decrease dimensionality of ages, while capturing price differences between

young, in-waiting, and proven bulls. Sales data obtained from the company did not include the

actual price received for each unit of each bull in a specific country. Rather, a blended price was

available for all bulls sold to the country in that transaction, which reflected the average price per

unit across all bulls in the order; this tended to dilute variation in prices per unit of different

bulls, especially when high-value and low-value bulls were grouped in the same order. 2018 to

2020 sales records and were filtered to remove outliers. Bulls were classified into age class,

market, and NM bin groupings at the time of sale. Empirical Bayes was used to smooth the price

estimates (Martin, 2018). The empirical Bayes method provides a balance between group

estimates and the population mean, such that population mean carries more weight for groups

with limited information. In this case, prices within age class and NM decile were blended with

population means for prices in a given market, as shown below:

$$\beta_i = \frac{\tau^2}{\tau^2 + \varepsilon_i^2};$$

$B_i = interpolation\ factor$

$\tau^2 =$ population variance

$\varepsilon_i^2 =$ standard error in the price of group i, which is $\sigma^2{}_i/n_i$

$shrunk\ price = \beta_i \bar{x}_i + (1 - \beta_i)\mu;$

$\mu =$ population mean

$\bar{x}_i =$ average price per group i

Maintenance Cost. The AI company used in this case study assigns an estimate of $30/bull/d for

covering all physical maintenance costs, such as feeding, housing, and veterinary costs. This

value was adjusted to fit 4-mo age bin and remains the same across all bulls in the herd.

Depreciation value and term length. The company insured bulls at $54,000 for 36 months

(depreciation term).

3.3.5 Model and Figure Creation

The MC model and tool were created in an Excel Workbook, and figures were generated using Tableau (2020 4.13).

3.4 Results and Discussion

3.4.1 Performance of the Model and Results of Base Scenario at Steady State

The base scenario was derived from the case study, subsequently all results pertain to the case study. Across 330 iterations, steady state was reached around the 310th iteration, based on $BULL_{AGE=1}$. The SD between the 310th and 330th iterations for AGE =1 was 0.137%, showing that there was minimal variability in the proportions between iterations. The replacement bull (AGE = 1, NM Bin = 9, Arrival Age = 6) had a discounted NPV of $250,951. This was broken down into maintenance cost of $63,600, culling cost of $7,264, income from culling of $532, and income from semen sales of $321,283. Adjusting any input values of a replacement bull would change his NPV and the BullVal$ of the herd, but it would not change the overall ranking of bulls within the herd.

Market prices (Supplemental Table S1) were established using an empirical Bayes smoothing function. Contrary to intuitive thinking, the NM Bin 10 reflected average market price. We speculate that this may be due to pairing of elite bulls with lower-demand bulls as "blend" packages, where fewer units from elite bulls are sold with greater numbers of units from inexpensive bulls that are more readily available; this would reduce the valuation of genetically elite bulls in our case study analysis. We chose to use semen prices derived in this manner for the case study, despite the aforementioned limitations in data clarity, but future users may have access to more precise pricing data at the individual bull level for specific markets.

3.4.2   Case Study

A total of 396 Holstein bulls collected from April to November 2020 made up the herd. Table 3 shows the distribution of bulls in each NM bin, with an average of 7.9. With the knowledge that the deciles were established using bulls collected from 2018 to 2020, the company's herd had a higher NM than previous trimesters or years, a trend that was expected. The genetic trend can be observed in Supplemental Figure S2, a plot of the herd bulls' raw NM$ with their ages in April 2020. As age decreased, NM$ increased, showing that younger bulls had higher NM, except those that were chosen for specialty markets, like high genetic merit for type conformation. The average arrival age was 6 mo, and average age bin of these bulls at the start of the MC was 5, ranging from 81 in AGE= 1 and 2 in AGE = 15 at i=1 (Figure 1). The herd distribution by age at steady state (Figure 1), ranged from 16 bulls in AGE=19 to 23 bulls in AGE=1. The drastic difference in herd distribution between i= 1 and i=310 demonstrates decisions that cannot be captured due to data limitations.

Supplemental Figure S1 describes the percentage of product sold to each market by age. Market B dominated the market share in young bulls, whereas other markets increased their share as bulls aged. International sales relied more heavily on older, proven bulls.

The herd's BullVal$ ranged from -$316,748 to $497,710. Deviations from mean TSp ranged from -94% to 139% (Figure 2). For TSp deviation bins with more than 1 observation, wide ranges of BullVal$ were realized. As expected, with an increase in TSp, the overall trend of BullVal$ increased. Bulls with high BullVal$ did not have the highest TSp, but most tended to be above the mean.

A previous study showed that TSp forecasts up to 4 months into the future were reliable (Quick et al., 2021). It would be feasible for a company to incorporate TSp forecasts as opposed to deviations from mean TSp, but this would not drastically change the BullVal$ ranking.

To explore the relationship between NM$ and BullVal$, Figure 3 plots NM bin with BullVal$. The expected relationship between BullVal$ increasing with NM bin was not observed across all bins (Figure 3). In the first 5 NM bins, there was an increase in value, with the lowest BullVal$ in lowest NM bins. However, there was a decrease in average BullVal$ from NM bin 6 to 10. A possible explanation for this decrease is that higher NM bins have younger bulls, with Age Start mean of 2.26 for NM bin 10; very little production data was available for these bulls, so a TSp deviation might not be an accurate portrait of the bull's lifetime potential. For NM bin 10, TSp deviation was 3.55±41.58% and NM bins 7 and 8 had TSp deviations below mean (Table 3). Young bulls beginning the production process have varying performance, as they are new to the collection process and have yet to reach maturity. Other possible reasons why the average BullVal$ was lower than expected for higher NM$ bulls are reservations of elite bulls for contract matings, or package deals where high value bulls' units are sold in limited quantities with large quantities of lower NM$ bulls' units. The first example highlights rare cases which elite bulls' semen may not be immediately available for sale, or if a sale is allowed, a contract is bound to the offspring, which would skew the price of units. The latter, more probable, reason would lead to skewed blended prices within sales records, driving down the apparent market price for elite bulls. The sales data provided assigned a blended price across the whole order, so the high-valued units were recorded at a lower price, heavily influenced by the mass lower-priced units. To establish market prices, empirical Bayes smoothing function was used in attempt to smooth outliers and blended prices. With so few records of elite bull unit sales, the smoothing

function set the market prices to average, which decreased elite bulls' values. If actual bull-level sales data was attainable, one would expect a bull of higher NM$ to have a higher BullVal$, as long as his TSp was above average. TSp and NM$ contribute to BullVal$, but there are also other intangible factors, such as market distribution and pricing, that contribute to a bull's potential net revenue.

 BullVal$ would be a beneficial tool in culling decisions as well as determining early on if a bull would be worth adding to the herd (if his predicted TSp and NM$ would jointly be beneficial in a profitable market). Figure 4 shows the number of bulls per each $50,000 BullVal$ bin added, involuntarily culled, and voluntarily culled between the August and December 2020 trimesters. Logistically, we would like to see bulls added to the herd with positive BullVal$ bins and conversely, culled bulls with negative BullVal$; however, this did not hold true with the case study herd. Out of the 20 new bulls added to the collection herd, all bulls had negative BullVal$. Out of 41 voluntary-culled bulls, 17 (41%) bulls had a BullVal$ below $0.

This model and case study had limitations and challenges. First, the sales data available for this study were average sales prices for orders, which could contain multiple bulls, all averaging to the same price. This does not accurately portray the actual sales price of the bull. Moreover, a company may sacrifice on sales price to foster a budding relationship with a new market, undervaluing bulls and losing present revenue for (hopeful) future gain. Additional business relationships, contracts, and government regulations, among other constraints are not considered in this study, but would play significant roles in pricing and market distribution. Lastly, the adoption of an objective tool can be a challenge when competing interests exist. It would be beneficial for the tool to be modified or updated to reflect market changes and bull herd demographics.

The authors suggest that this tool would be most beneficial in culling decisions as well as being tied into the product allocation and collection scheduling process. Bulls with negative BullVal$ should be culled before high BullVal$ bulls (barring any health issues), to make way for more profitable replacements. An example of how this may fit into a collection scheduling process is in a situation where collection spots are limited, we would prioritize higher BullVal$ bulls for those spots. A similar case can be made with product allocation: assigning higher BullVal$ bulls to markets would capitalize on the potential net revenue. Again, this model would need to be updated routinely (2-3 times/yr) to reflect the current bull population and market characteristics.

3.5   Conclusion

The present study demonstrated that a Markov chain model can be used to provide economic valuation of dairy bulls, while focusing on the most important factors contributing to replacement decisions, such as age, predicted semen production, and predicted genetic merit. The Markov chain model allows for user-defined input based on current replacement policy and bull demographics. This model provides a new metric of ranking and valuing bulls based on their actual contribution to revenue of the company. A negative bull value indicates that the chosen bull is less profitable than the predicted discounted lifetime profit of a new young sire of average production capabilities, suggesting the bull should be culled. A case study demonstrated the tool's feasibility of valuing and ranking a herd and highlighted pitfalls with data availability. The range of BullVal$ encountered were -$316,748 to $497,710, with 49% of bulls recommended for culling based on negative BullVal. A bull's NPV was influenced primarily by market allocation and pricing, as well as the interaction of sperm production with genetic merit. This decision support tool is contained within an Excel workbook, allowing individual bull valuation and whole-herd assessment.

3.6   Acknowledgements

3.7   References

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3.8   Tables and Figures

Table 3.1 List of minimum variables required to calculate bull value using MC model, and base values used in model illustration.

Variable	Base Value
Bull Variable evaluated	
Current age bin	Bull-Specific (1 to 19)
Replacement bull variable	
Age bin	1
Net Merit bin	9
TSp Deviation	0
Arrival age (mo)	6
Herd variable	
bulls in herd	396
Economic variable	
Maintenance cost ($/bull/mo)	900
Depreciation cost ($)	54,000
Depreciation term (mo)	36
Cost of replacement ($)	10,000
Salvage value ($)	850
Packing rate (TSp/straw unit)	15,000,000
Interest rate (%/yr)	6.00
Market price	See Supplemental Figure S1 for distribution, Supplemental Table S1 for price

Table 3.2. Average Total Sperm (TSp) production per 4-mo age bin, generated using production records from 2018 to 2020. Involuntary culling proportions across the 4-mo age bins. It is assumed all animals are culled after AGE 19. bins. It is assumed all animals are culled after AGE 19.

Age (mo)	AgeBin (4 mo)	TSpBin Ave (Billion Cells)	Involuntary Culling Proportion (%)
10 to 13	1	99.6	0.0067
14 to 17	2	229.3	0.0040
18 to 21	3	296.0	0.0014
22 to 25	4	342.9	0.0041
26 to 29	5	366.3	0.0030
30 to 33	6	386.7	0.0063
34 to 37	7	403.8	0.0104
38 to 41	8	399.8	0.0162
42 to 45	9	415.2	0.0100
46 to 49	10	398.1	0.0148
50 to 53	11	406.5	0.0088
54 to 57	12	422.8	0.0215
58 to 61	13	450.6	0.0202
62 to 65	14	489.2	0.0094
66 to 69	15	485.6	0.0250
70 to 73	16	486.0	0.0200
74 to 77	17	469.2	0.0571
78 to 81	18	433.7	0.0789
82 to 85	19	259.4	1.0000

Table 3.3. Lifetime Net Merit (NM$), number of bulls, mean TSp deviation % (and standard deviation; SD), and mean bull valuation (BullVal$) and SD per net merit (NM) decile bin for the modeled herd.

NM decile bin	NM$ range	Number of bulls	TSp mean deviation % (SD)	Mean BullVal$ (SD)
1	-151 to 152	8	4.2 (31.7)	-257,759 (21,280)
2	205 to 286	3	-29.9 (26.9)	-235,546 (38,630)
3	298 to 351	4	-3.5 (33.7)	-40,291 (120,230)
4	361 to 418	9	5.0 (32.5)	7,151 (103,780)
5	423 to 474	15	-0.3 (26.8)	210,924 (142,140)
6	479 to 559	40	1.7 (29.3)	16,8307 (147,720)
7	560 to 636	55	-3.0 (21.0)	30,979 (83,700)
8	637 to 692	76	-6.9 (22.4)	64,302 (93,650)
9	693 to 756	87	4.8 (28.8)	3,953 (94,440)
10	757 to 950	99	3.6 (41.6)	-151,324 (-71,390)
Total		396	0.3 (30.9)	-2,565 (148,450)
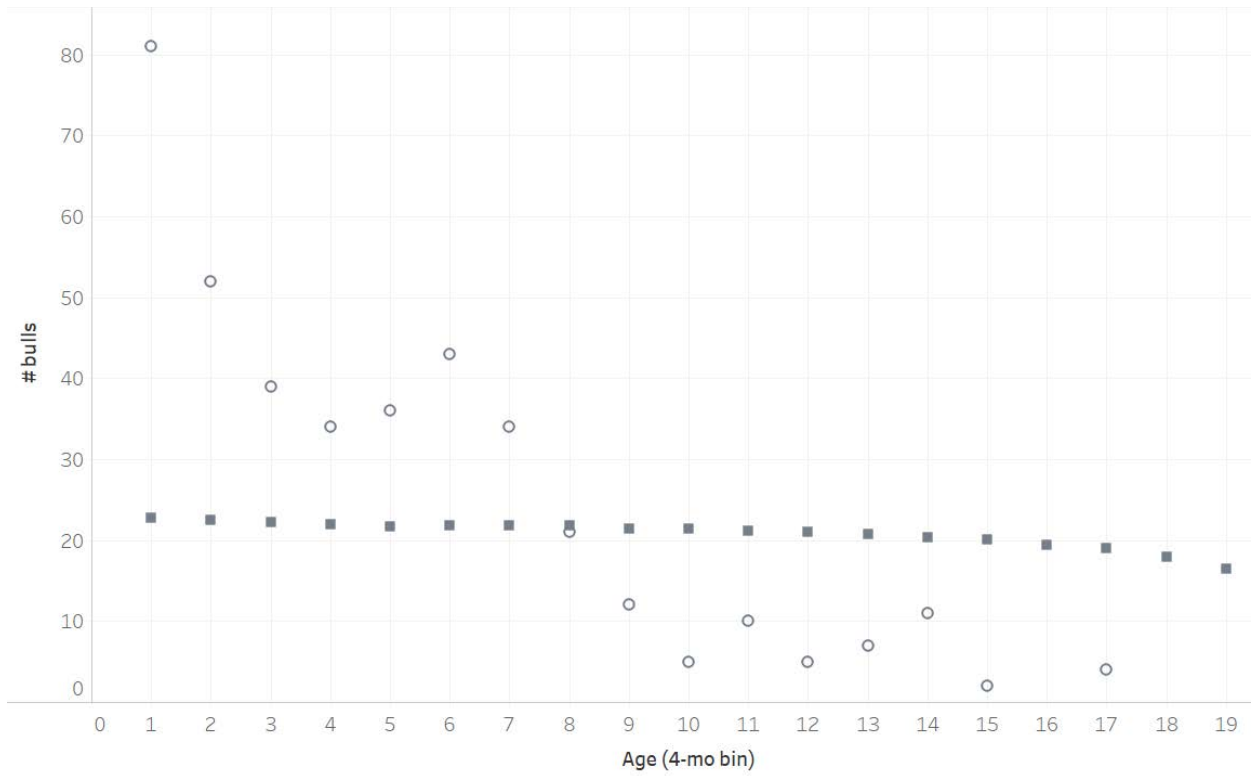
Figure 3.1. Distribution of herd demonstration bulls across the AGE bins in which they start the MC model in (i=0, open circles) and at steady state (i=310, closed squares).
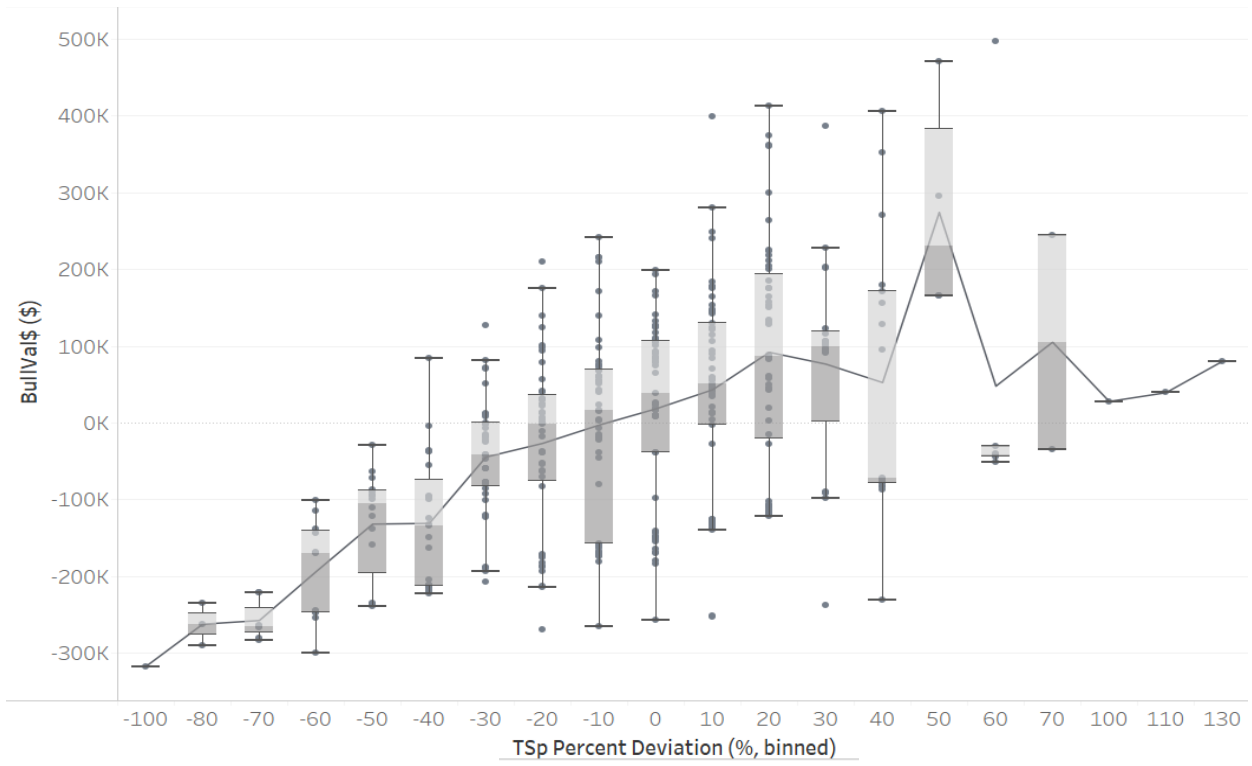
Figure 3.2. Boxplot of herd bulls' total sperm (TSp) deviation from mean (%) and their bull valuation (BullVal$).
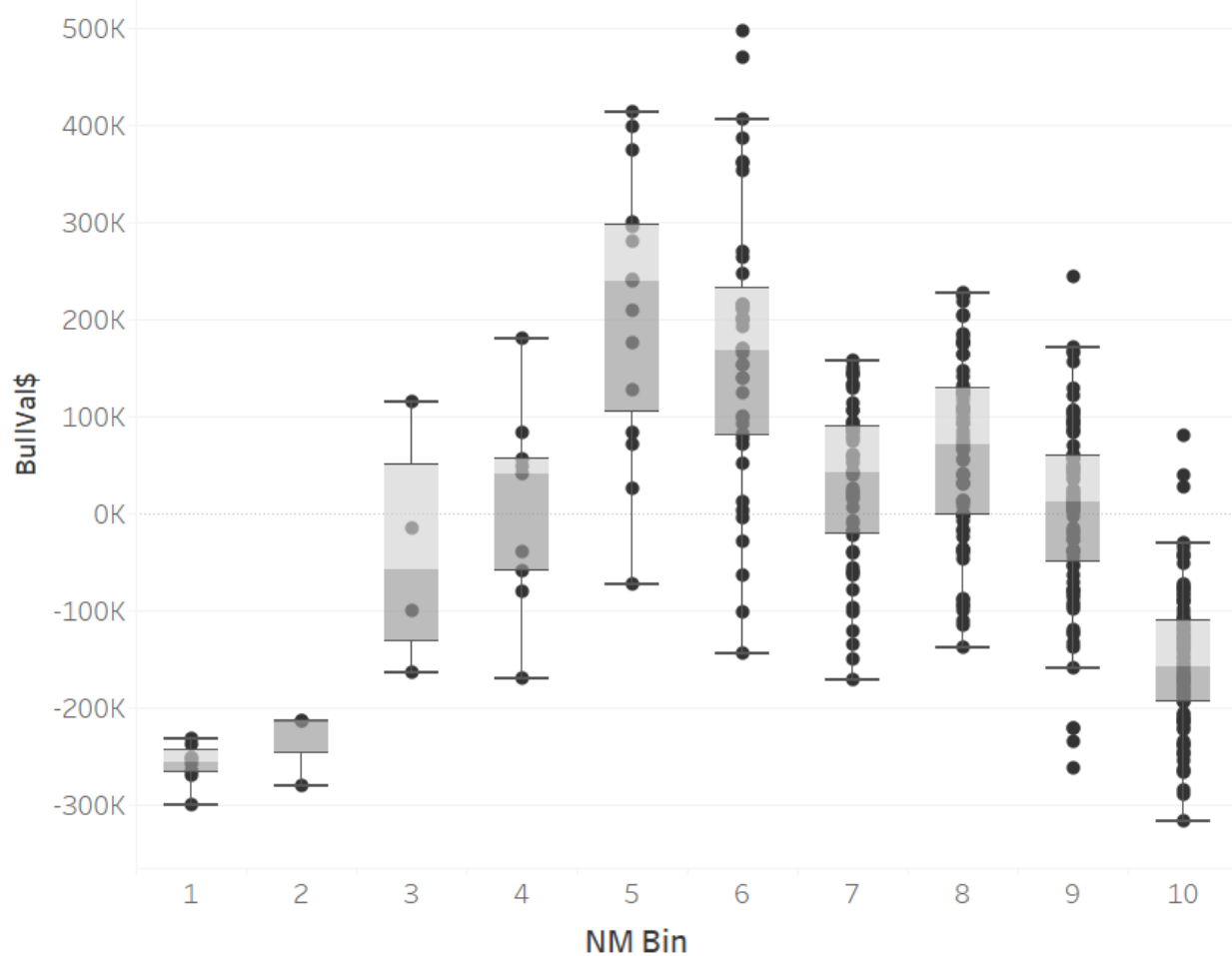
Figure 3.3. Boxplot of herd's bull valuations across different net merit (NM) decile bins.
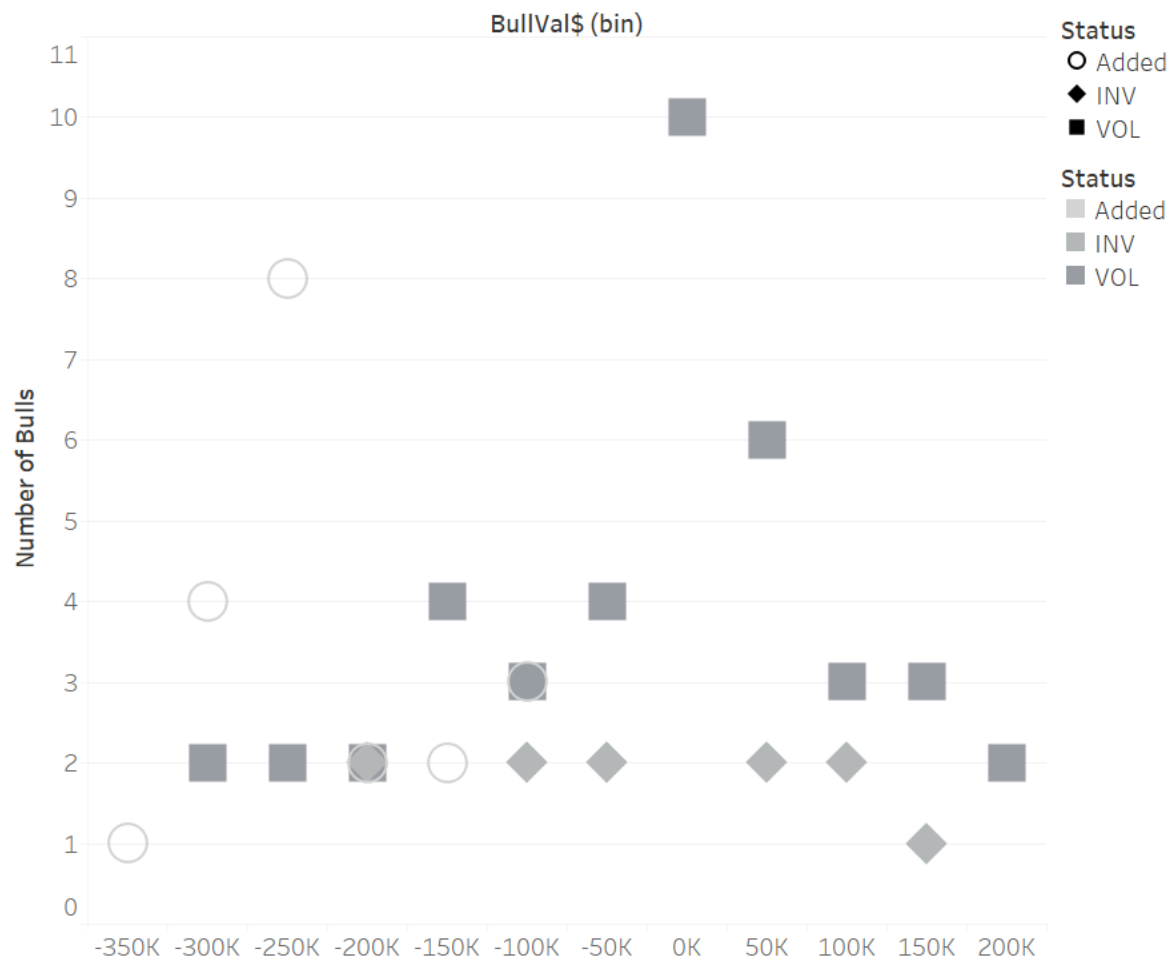
Figure 3.4. Histogram of bulls added (light grey circle), involuntarily culled (medium grey square), and voluntarily culled (dark grey diamond) from April 2020 through November 2020 in herd demonstration with their assigned bull valuations (BullVal$).

Supplemental Table 1: Prices assigned to each market based on age class and NM Bin using empirical Bayes smoothing function.

AgeClass	NMBin	Market Price (USD/dose)					
		A	B	C	D	E	F
Young	1	8.96	7.10	14.65	7.10	7.10	9.81
In-waiting		7.39	7.08	8.94	15.29	6.87	8.48
Proven		4.18	6.04	7.07	5.54	5.00	5.74
Young	2	8.84	7.10	14.81	7.10	7.10	9.43
In-waiting		7.45	7.30	8.02	12.74	3.52	6.52
Proven		3.81	6.52	5.35	5.94	3.82	6.69
Young	3	7.60	5.00	9.10	7.10	7.10	9.39
In-waiting		9.08	4.47	6.71	8.92	4.93	5.12
Proven		6.89	5.66	6.33	15.67	2.31	5.25
Young	4	7.89	4.15	11.52	7.10	9.52	7.24
In-waiting		5.90	6.21	6.67	9.97	2.40	6.81
Proven		9.03	6.24	7.84	7.10	3.38	3.48
Young	5	7.09	4.50	9.19	7.10	5.68	9.59
In-waiting		9.24	5.03	5.56	7.10	3.21	5.03
Proven		7.10	8.46	5.98	7.10	9.06	3.73
Young	6	9.19	6.37	10.51	7.10	8.49	9.62
In-waiting		9.06	9.04	7.74	10.31	7.37	6.66
Proven		4.67	7.19	3.10	7.10	7.10	4.44
Young	7	8.99	6.72	5.14	9.34	8.83	7.74
In-waiting		8.31	7.16	5.99	7.10	7.10	6.48
Proven		7.10	7.10	3.59	7.10	7.10	4.30
Young	8	8.43	5.91	7.97	8.23	14.01	7.87
In-waiting		8.71	7.50	2.82	9.30	7.10	3.71
Proven		7.10	7.10	7.62	7.10	7.10	3.41
Young	9	9.53	5.16	8.02	8.15	7.10	9.41
In-waiting		9.38	7.00	4.96	7.10	7.10	6.56
Proven		7.10	7.10	7.10	7.10	7.10	7.10
Young	10	8.55	5.64	12.37	9.47	7.10	8.43
In-waiting		8.26	7.00	8.21	10.30	7.10	8.70
Proven		7.10	7.10	7.10	7.10	7.10	7.10

Supplemental Figure S1: Percentage of product sold to each market A through F across 4-mo age bins.
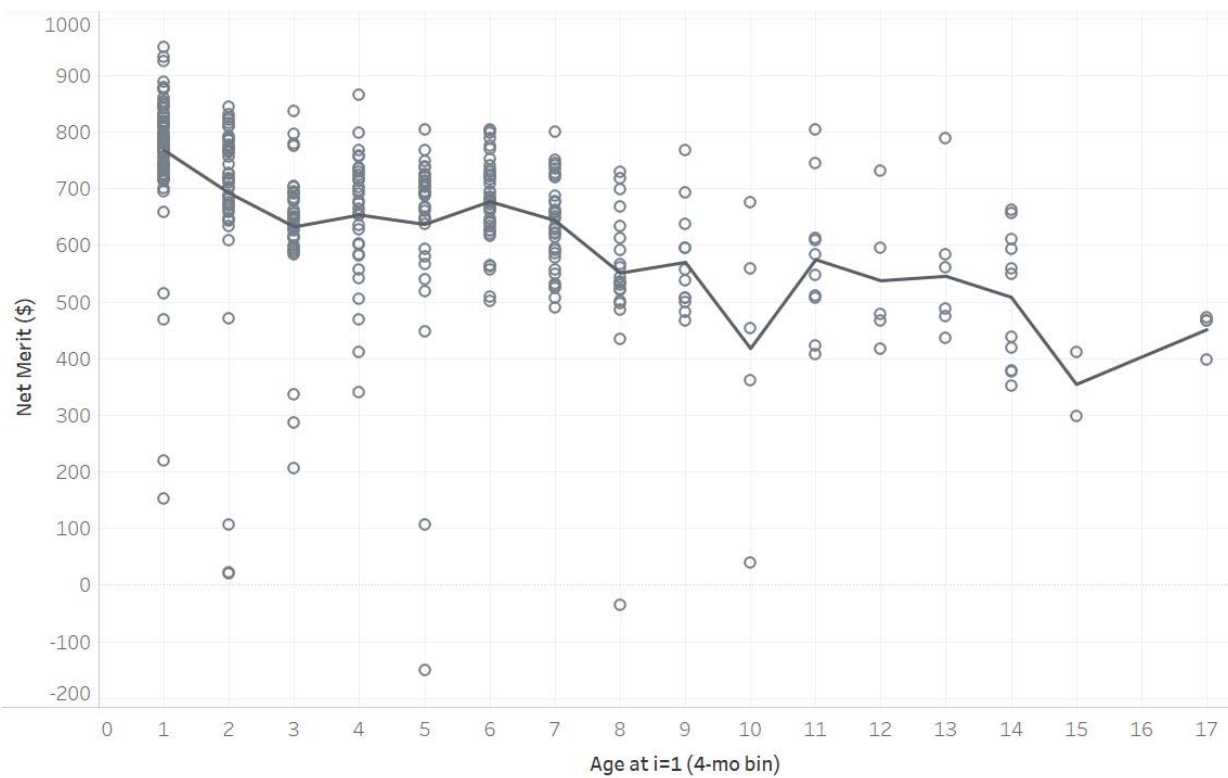
Supplemental Figure S2. Raw NM$ values of case study bulls by age bin they were in April 2020.

CHAPTER 4: DECISION-SUPPORT TOOL FOR GLOBAL ALLOCATION OF DAIRY SIRE SEMEN BASED ON REGIONAL DEMAND, SUPPLY CONSTRAINTS, AND GENETIC PROFILES

4.1   Abstract

Currently an arduous subjective process, an artificial insemination (AI) company seeks to allocate semen units globally by balancing perceived demand with uncertain product supply. This study aims to objectivize this process by providing a user-friendly linear programming (LP) model to allocate bulls' units to regions for the next trimester sales period based on maximum revenue, and to describe the features and outcomes of this model when applied to a sample bull herd and global demand scenario that are reflective of a leading AI company. The objective function of maximizing revenue was calculated by summing the product of units allocated by bull and region with purchase prices assigned by bull and region. Constraints considered were regional demand for overall units, regional preferences for specific genetic traits, bulls' production capacity, and percentage of bulls' units allocated to a single region. A sensitivity analysis was performed to identify the impact of variables and constraints on total revenue. Production, sales, and bull demographic data from 2018 to 2021 from a leading AI company were used to establish base values and build a sample herd of 61 bulls and 5 global regions. The case study provided a maximum revenue of \$8,287,197 in semen sales per trimester, with 634,700 units allocated. Of the 61 bulls in the case study, 9 were not allocated to any region. The most limiting constraint was regional demand, which resulted in a surplus of 274,564 units not allocated. A sensitivity analysis confirmed this finding, with largest shadow prices assigned to regional demands, and indicated that a single unit increase in regional demand would add up to \$14.84 to total revenue.

Key Words: Linear program, allocation, sperm production

4.2   Introduction

Global dairy genetics companies seek to allocate product globally to balance customers'

demands with uncertainty in product availability. The process of allocating future product is

subject to factors such as regional demand (total quantity and genetic profile preferences),

quantity of bulls' units produced or available from inventory, bulls' health status and countries'

import regulations, and the company's supply and inventory constraints. Many internal and

external factors and competing interests create a highly subjective and complicated allocation

problem, which US AI companies struggle with 3 times per year, coinciding with Council on

Dairy Cattle Breeding (CDCB; Bowie, MD) genetic evaluations of US dairy cattle. There is

potential benefit among AI companies to make this process more objective and streamlined, such

as with a decision-support tool.

Allocation problems are not new to the dairy industry. Linear programs (**LP**) have been used to

model allocation problems involving dairy farms (Cabrera, 2010; Wu et al., 2019; Bellingeri et

al., 2020) and dairy processing plants (Kerrigan and Norback, 1986; Banaszewska et al., 2013).

For example, Benseman (1986) developed a time-staged LP to find the most profitable daily

production schedule of powder, casein, cheese, and butter products. The nature of dairy product

allocation and resource optimization is comparable to dairy bulls' semen product allocation, with

raw biological products from cattle that can be destined for different end products and markets.

In the AI industry, LP and mixed-integer programs (**MIP**) have been used to model the optimal

portfolio of sires for dairy herds (McGilliard and Clay, 1983a; b; Erba et al., 1991; McConnel

and Galligan, 2004). McConnel and Galligan (2004) used an MIP to model the effects of semen

quantity price discounts on the lowest cost portfolio of sires from three AI companies. Although

LP and MIP have been used in the AI industry, to the authors' knowledge, there has not been an analysis of global product allocation considering differing regional demands and bulls' semen production capacities.

Therefore, the objectives of this study are: 1) provide a user-friendly LP model to allocate bulls' semen units to global regions for the next trimester sales period based on maximum revenue, and 2) describe the features and outcomes of this model when applied to a sample herd and global demand scenario that are reflective of a leading AI company.

4.3 Materials and Methods

4.3.1 Programming Approach

The LP optimization model is defined as:

$$\max_{X} Z = C'X$$

$$\text{subject to: } AX \geq, =, or \leq B$$

$$X \geq 0,$$

where Z = maximum revenue generated from the sale of semen units to regions; C' = matrix of objective function coefficients (e.g., price of unit by bull (b), region (r)); A = matrix of technical coefficients; B = vector of constraints (e.g., units available, demand); and X = decision variables (e.g., bulls' units per region). A MIP has the added constraint that all variables in X (number of units) are integers:

$$X \in \mathbb{Z}.$$

The revenue is calculated as the summed product of bulls' units per region by price per bull and region:

$$Revenue = \sum_{region} (\sum_{bull} (units_{r,b} * price_{r,b}))$$

4.3.2 Model and Figure Creation

The problem was set in an Excel Workbook and the model solved using the Analytic Solver®

platform with a standard LP/quadratic engine (Frontline Systems Inc.). Figures were generated

using Tableau (2020 4.13).

4.3.3 Case Study, Data Description

Production data, sales records, health events, and bull demographics of Holstein bulls at two

collection facilities were obtained from a commercial AI company (ABS Global Inc., DeForest,

WI).

Regions. Five global regions were designated based on the company's recommendation

regarding geographic location, production type, and current regional marketing practices.

Regions were classified as A through E. Country-level sales data from 2018-2021 were

aggregated at the regional level. Sales data obtained from the company did not include the actual

per unit price received for each bull's semen in a specific country. Rather, a blended price was

available for all bulls sold to the country in that bulk order transaction, which reflected the

average price per unit across all bulls in the order; this tended to dilute variation in prices per unit

of different bulls, especially when high-value and low-value bulls were grouped in the same

order.

Bull Herd. A sample herd was selected from bulls available for sale between April and

December. To ensure each region was represented in the sample herd, 15 bulls from each region

with the highest number of units sold were chosen. Once duplicate bulls were removed, 56

unique bulls remained.

An important consideration to the allocation problem is country-specific regulations preventing

the sale of semen from specific bulls in certain locations. For example, roughly 10% of US

Holstein bulls do not meet health standards for importation into the European Union (European Commission, 2016). Of the 56 bulls originally chosen for the case study, only 1 did not meet EU health standards. Therefore, to make the case study more realistic, 5 additional bulls with the most units sold that failed EU health standards (**HT bulls**) were added, resulting in 61 total bulls for the case study.

Bull Units Available. Assuming bulls would be collected twice weekly, an aggregated Total Sperm (**TSp**) was calculated for the trimester of August-November 2020. An average TSp packing rate of 15×10^6 was used to convert TSp to units available for the trimester.

Regional Demand. Regional demand was considered in two ways: 1) demand for total units; 2) desired genetic trait profile of selected bulls. Total unit quantity demand by region was assigned using actual unit quantity sold for the August to November 2020 trimester. The level of sales data does not allow differentiation between company's supply and demand; for example, we do not know if a given region would have purchased an additional 10% of product if it had been offered. Therefore, upper and lower bounds were added to the regional demands to provide flexibility in demand and supply. For the 61 bulls considered, demand was 44,000 units in region A, 149,000 units in region B, 145,000 units in region C, 131,000 units in region D, and 108,000 units in region E.

To determine the genetic trait profiles associated with these regional demands, the top five bulls (highest units sold) for each region were identified, and their trait profiles were averaged within region. The average values for each trait were compared with those of other regions, and one trait per region was selected based on the trait for which those five bulls excelled. The traits that were selected for each region's strengths were PTA type for region A, dairy composite for region B, PTA milk for region C, feet and legs composite (**FL**) for region D, and cheese yield for region E.

Using 2020 sales data, the percentage of total units each region needed from bulls in top 25%

and bottom 25% for each trait are shown in Table 1. The top 25% serves as a lower bound (i.e., a

region can receive more units from bulls ranking among the top 25% for the trait), and the

bottom 25% serves as an upper bound (i.e., a region can receive fewer units from bulls ranking

among the bottom 25% for the trait).

Market Pricing. Sales data from 2018-2020 for the 61 sample bulls were summarized as price

per unit by region and averaged by bins corresponding to 50-points in lifetime net merit (**NM$**)

(Supplemental Table S1).

Company-Imposed Supply Constraint. To restrict one region from receiving all available units

from a given bull, a company may impose a constraint on the percentage of a bull's total units

allowed to a single region. In this case study, individual regions were limited to 50% of a bull's

total units, except for HT bulls, which were limited to 90% of total units for an eligible region.

To model the supply range on the overall units obtained by a region, upper and lower bounds of

the regional demand were modeled. In the base scenario, a region could receive between 90 and

110% of demanded units.

4.3.4   Decision Variables and Constraints

The problem is made up of 299 integer decision variables, $Units_{r,b}$, which is the number of units

per bull per region. There are 61 bulls, with 5 regions (305 possible variables) minus 6 HT bulls

that were not eligible for one region and were automatically set to 0.

Table 2 summarizes the constraints. The problem consists of 122 functions (including constraints

and objectives), 1,991 dependencies (whenever a constraint or objective depends on the decision

variable), and 593 simple bounds on the decision variables. To prevent all units from a bull being

allocated to a single region, the user can define a percentage (z) of units available per bull that

can be allocated to a single region (Table 2, constraint 4). The base scenario's $z = 50\%$ for non-HT bulls and 90% for HT bulls. Accommodating potential deviations from regional demand (uDemand), constraints 5 and 6 provide lower and upper bounds based on percentages (lt and ut) defined by the user. These bounds, beyond demand, reflect the potential variation in supply, allowing for under- and over-supply relative to demand, such as would occur if the company were unable to meet the region's demand or the region was willing to accept product beyond their original demand. The base scenario values were $lt = 90\%$ and $ut = 110\%$. Lastly, to meet the desired genetic trait profile of bulls for a given region, the number of units a region demanded from bulls ranking in the top 25% and bottom 25% for a given trait were considered as lower and upper bounds, respectively (Table 2; constraints 7 and 8). A region can obtain more units from the top 25% than demanded, and on the contrary, they can receive fewer units from bulls in the bottom 25% than demanded.

4.3.5   Sensitivity Analysis

To obtain a sensitivity report from Analytic Solver®, the constraint of integer decision variables was removed. Decision variables' and constraints' influences on the objective function were tested. Reduced costs measure the change in objective function per unit increase in a decision variable; nonzero values occur when the variable value is equivalent to a lower or upper bound. Shadow price measures change in objective function per unit increase in the constraint's bound. If the shadow price is zero, the constraint is non-binding. Allowable ranges which reduced costs and shadow prices remain constant were examined.

4.4   Results and Discussion

4.4.1   Base-Case Herd Statistics

Units available per bull ranged from 1,368 to 33,672, with an average of 14,906. Total units

available for allocation was 909,264. The total unit demand across the five regions was 577,000.

The 90 to 110% bounds on demand created a supply range from 519,300 to 634,700 units.

Price per unit was assigned based on bull's NM$. Distribution of the herd's NM$ and price by

NM$ is shown in Supplemental Table S1.

4.4.2   Base-Case Model Results

The revenue achieved in the optimal solution was $8,287,197.15. Total number of units allocated

was 634,700, leaving 274,564 units not allocated. The unit quantities supplied to specific regions

reached the upper bounds of regional demand constraints and were: 48,400 units for region A,

163,900 for B, 159,500 for C, 144,100 for D, and 118,800 for region E (Table 3). Based on the

sensitivity analysis, it would take an upper bound of 140% above the regional demand to activate

other constraints. In this example, an upper bound of 140% above regional demand would keep

region B from reaching the upper bound, as the trait constraint of bottom 25% of sires for the

desired trait profile would become the limiting constraint.

The numbers of bulls assigned to each region under the optimal solution were 11, 26, 27, 20, and

21, for regions A through E respectively (Table 3). Of the bulls allocated, the average (SD) of

units allocated per region was highest for market D, at 7,205 (6,721), and lowest for market A, at

4,400 (3,757). Despite the large differences in demand between regions, the numbers of units

allocated per bull by region were similar, and the numbers of bulls per region drove differences

in total units allocated.

There were 9 bulls not allocated to any region, 14 bulls assigned to one region, 26 bulls assigned to two regions, 9 bulls assigned to three regions, and 3 bulls assigned to four of the five available regions. In other words, 9 bulls would be collected but not needed to meet demand. Beyond this example, Gorr et al. (under review, 2022) showed that 49% of bulls would be recommended for culling based on negative net present value (NPV) relative to others in the herd. The current and previous studies suggest that opportunities exist within the AI stud to reduce the number of bulls collected, thereby decreasing production costs without losing revenue, while still meeting market demands. The present study also supports the transition of AI companies' marketing campaigns to those based on promotion types of bulls (i.e., groups of bulls with similar genetic trait profiles) rather than individual bulls. Genomic evaluations enabled the selection and marketing of young bulls, shortening the generation interval faster than in the pre-genomic era (Ruiz-López et al., 2018). This selection pressure has shortened the productive life of bulls, as newer and genetically superior bulls replace them, perhaps solidifying the relevance of marketing teams of bulls rather than the bull itself. The NM$ bins of bulls not allocated were 550 (5 bulls) or 450 (4 bulls). These bulls tended to be in the lowest 25% or middle 50% for nearly every trait except PTA milk (4 bulls were among the top 25% for PTA milk), and they had an average of 19,023 (5,741) units available for allocation. In summary, bulls not selected for allocation were of average or below average genetic merit but were above average for semen production.

Figure 1 shows the demand (dark lines) of unit quantity for semen from top 25% and bottom 25% of bulls for each trait, as well as the quantity assigned from the optimal solution (lighter grey bars). Demand for the top 25% served as a lower bound, whereas demand for the bottom 25% served as a lower bound. For 11 of the 25 region/trait combinations for top and bottom 25%, the bounds were met and not exceeded. Region B received 20,207 ± 22,850 (mean ± SD)

more units beyond the top 25% demand constraint across all traits considered. For the top 25% constraint, every region exceeded demand for Dairy composite units, whereas the minimal demands for PTA milk, cheese yield, and FL composite trait profiles were met for 3 regions each. Region D received $19,090 \pm 15,605$ units below trait demand for bottom 25%, consequently receiving more units from higher trait profile bulls to fill regional demand. All but one trait, cheese yield with 3,062 units below, were capped at the upper bound for Region B's bottom 25% demand versus allocated.

4.4.3 Sensitivity Analysis

The relaxed LP solution (removal of integer decision variables) received nearly the same optimal revenue, $8,287,197.19. Rounding differences made up the change in units allocated, with 1 unit removed from a bull in market A.

Among the 299 total decision variables, 145 were not bound by a constraint, resulting in a reduced cost of 0. The average reduced cost of the decision variables was -0.76 ± 1.85, indicating that a one unit increase would reduce revenue by $0.76. Of the 121 constraints, 77 were not binding. The range of shadow prices was -$2.34 to $14.84. The constraints with the largest shadow prices were regional upper bounds for total units demanded (Table 3). For an example of the influence of shadow prices on the objective function, an increase in the final value of region C's total units by 100 units would result in an increase in revenue of $1,484.

Thirty-one bulls were limited by their semen production capabilities, and more units could have been marketed if available. The number of bulls bound by the percentage of bulls' units allowed to each region was actively constrained 63 times (twice for region A, 18 times in B, 17 times in C, 11 times in D, and 15 times in E).

Figure 2 provides a visual of the allowable value range compared its final value, as well as the shadow price for all trait/region combinations. When the shadow price is zero, the constraint is non-binding. Of the 50 regional/trait (top and bottom) constraints, 19 were binding. The upper and lower bounds of these non-binding constraints demonstrate the number of units needed for that category to change into a binding constraint. When the shadow price is less than 0, adding units will negatively impacts the objective function. Top 25% trait demand constraint acted as lower bounds, leading to negative shadow prices. The legend of Figure 2 provides a detailed example from Figure 2. Decreasing the unit quantity of Region A in cheese yield would add $2.34 to the revenue, with an allowable increase of 1,118 units (Figure 2). When the shadow price is greater than 0, that constraint positively impacts the objective function value; adding units above the final value will increase revenue. Bottom 25% had positive shadow prices, as they acted as upper bounds (Figure 3). Adding one unit within lower-tiered FL bulls for Region B would add $2.67/unit to the objective function, with an allowed increase of 776 units. Generally, the final values were close to upper and lower bounds, demonstrating that moderate to large changes in unit quantity for the constraints will change the shadow price and the manner in which the objective function is subsequently impacted.

We suggest this tool would be most useful during product allocation discussions if used in tandem with the semen production forecasts of individual bulls (as proposed by Quick et al., 2021) and developing collection schedules for the coming trimester. For instance, the 9 bulls not allocated could potentially be culled, if they are not needed to fulfill market demand. The sensitivity analysis would be beneficial for an AI company to negotiate bounds and constraints. For example, a region could request more units from a particular trait profile, and the company could provide the (shadow) price needed for the transaction to be profitable. The tool can be

modified to meet company's goals and marketing schemes, such as allocating groups of bulls to regions rather than specific bulls. Computational time should also be considered in the decision-support tool's practicality. The speed of the LP/MIP solver provided results in less than 1 second, making it an efficient tool to utilize during decision-making.

4.5   Conclusions

The present study demonstrated that an LP/MIP can be used to allocate semen units regionally, given demand and supply constraints. The LP model allowed for user-defined bounds based on regional demand and bulls' individual semen production capabilities. This model provides unit quantities by bull provided to each region. Results from the case study demonstrate the feasibility and efficiency of this decision support tool. A sensitivity analysis confirmed that the case study's most limiting to the solution were regional demand. This decision-support tool was contained in an Excel workbook, with the Analytic Solver® Add-in to model the LP and sensitivity analysis.

4.6   Acknowledgements

4.7   References

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4.8   Tables and Figures

Table 4.1 Percentage of units each trait regions demand for five traits, PTA milk, cheese yield, type, feet and legs composite (FLComp), dairy composite (DairyComp).

Traits	**Region % of units needed**				
	Region A	Region B	Region C	Region D	Region E
Top 25%					
Milk	0.00	0.18	0.41	0.37	0.29
Cheese Yield	0.17	0.29	0.37	0.26	0.39
Type	0.35	0.33	0.23	0.25	0.23
FLComp	0.26	0.21	0.25	0.23	0.24
DairyComp	0.28	0.32	0.24	0.17	0.21
Bottom 25%					
Milk	0.43	0.22	0.24	0.18	0.18
Cheese Yield	0.28	0.22	0.26	0.37	0.19
Type	0.25	0.23	0.22	0.34	0.28
FLComp	0.18	0.22	0.31	0.31	0.30
DairyComp	0.24	0.17	0.28	0.43	0.33

Table 4.2 Summary of constraints within the LP model.

Constraint Description	Constraint	Constraint Type
(1) Integer decision variables	$Units_{r,b} = int$ $\forall$ region, bull	Value type
(2) Positive decision variables	$Units_{r,b} \geq 0$ $\forall$ region, bull	Lower bound
(3) Bulls' total units cannot exceed production capability	$\sum_r Units_{r,b} \leq uAvail_b \forall$ bull	Upper bound
(4) Bull's units per region cannot exceed user-defined percent (z)	$Units_{r,b} \geq z*uAvail_b$ $\forall$ region, bull	Upper bound
(5) Region's total units above lower threshold (lt) based on demand	$\sum_b Units_{r,b} \geq lt*uDemand_b \forall$ region	Lower bound
(6) Region's total below upper threshold (ut) based on demand	$\sum_b Units_{r,b} \leq ut*uDemand_b \forall$ region	Upper bound
(7) # units region needs of bulls in top 25% each trait	$\sum_b Units_{r,b,t} \geq t75Demand_{r,t} \forall$ region, trait	Lower bound
(8) # units region needs of bulls in bottom 25% each trait	$\sum_b Units_{r,b,t} \leq t25Demand_{r,t} \forall$ region, trait	Upper bound

Table 4.3. Number of bulls and units per bull allocated to each region in the optimized solution in the base scenario and sensitivity report of the upper-bound constraints on regional total demand. Final Value is the assigned value for the optimized solution, shadow price is the change in objective function per unit increase in constraint's bound. Constraint right-hand (R.H.) side is the value of the constraint's bound. Allowable increase and decrease are the values for which the final value can be altered without changing the shadow price.

Constraint Name (n = # bulls)	Average (SD) units from assigned bulls	Final Value	Shadow Price	Constraint R.H. Side	Allowable Increase	Allowable Decrease
region total A (n = 11)	4,400 (3,757)	48,400	10.86	48,400	306	1,270
region total B (n = 26)	6,304 (4,103)	163,900	6.20	163,900	7,003	1,270
region total C (n = 27)	5,907 (3,537)	159,500	14.84	159,500	126	475
region total D (n = 20)	7,205 (6,721)	144,100	10.77	144,100	915	1,717
region total E (n = 11)	5,657 (3,276)	118,800	10.85	118,800	915	5,582

Supplemental Table S1: Price assigned to each market by Net Merit (NM$) binned by 50.

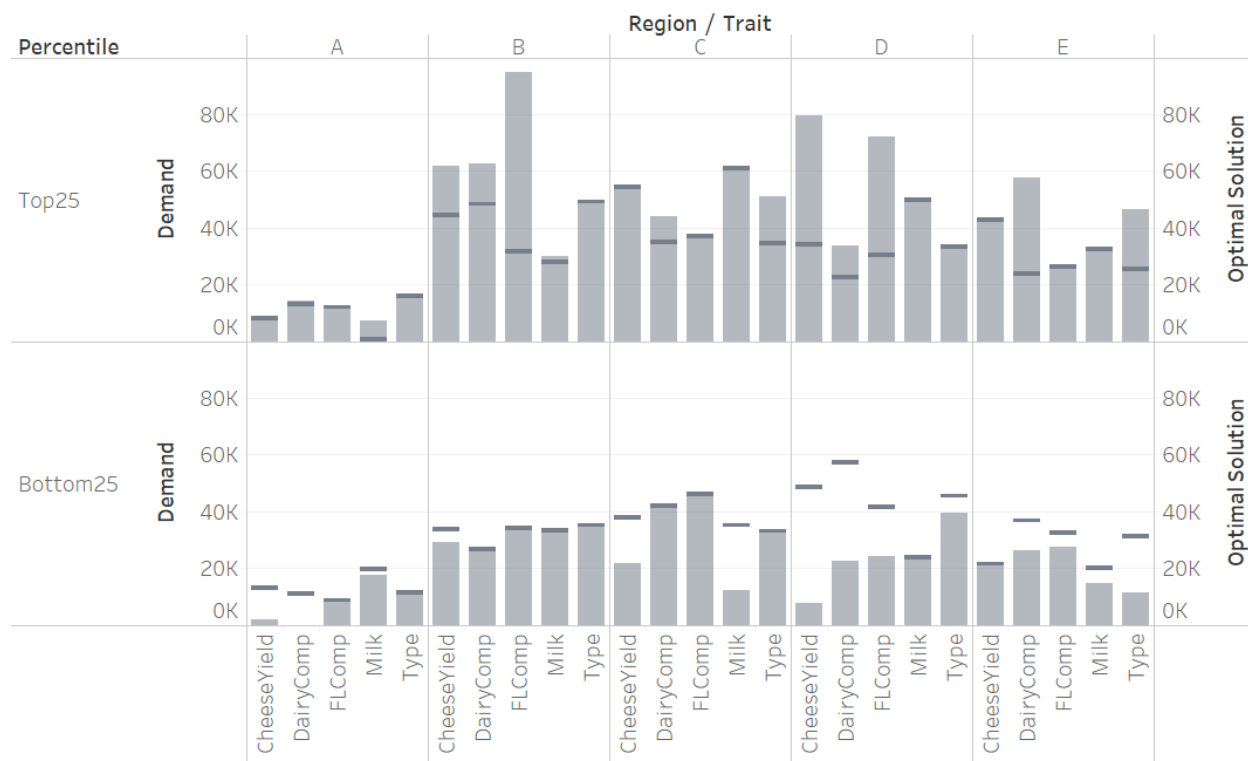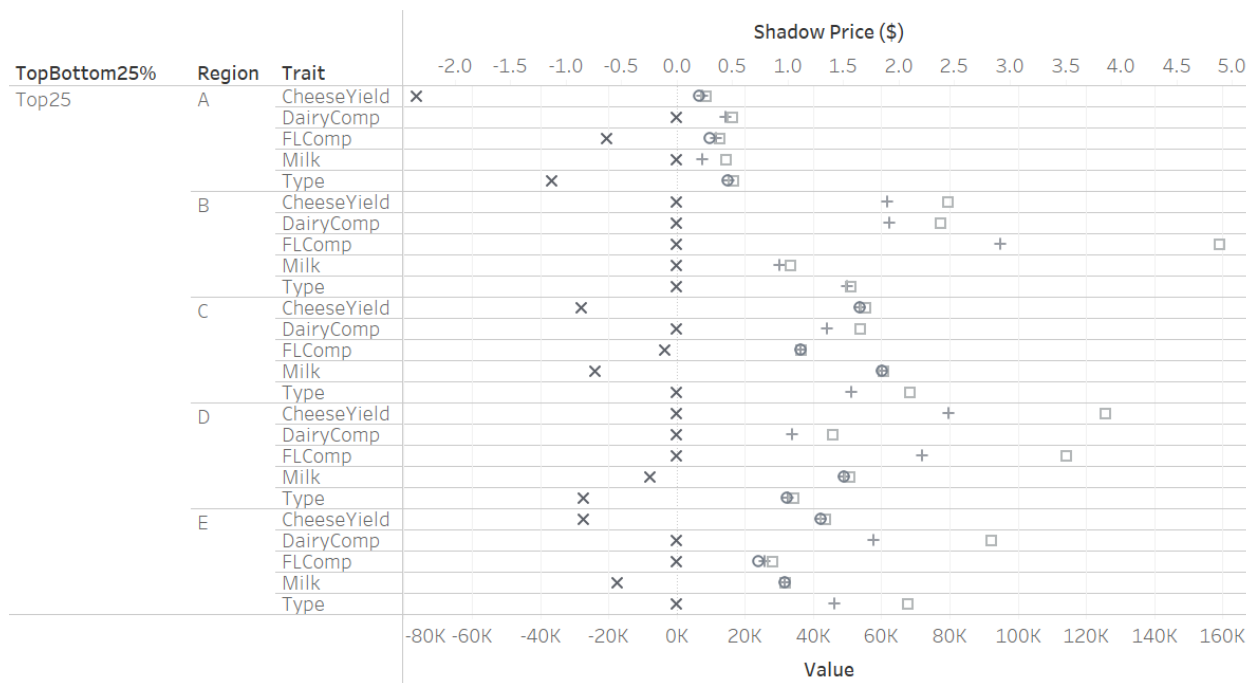| Region	Net Merit binned								Grand Total
	≤400	450	500	550	600	650	700	≥750	
A	9.38	9.11	8.45	9.74	12.00	8.38	7.58	7.19	**9.06**
B	10.22	7.89	6.20	5.70	7.34	8.87	5.74	12.20	**7.56**
C	14.95	11.81	13.60	14.10	15.59	15.33	17.03	17.87	**15.11**
D	7.69	8.53	8.50	8.74	13.34	10.53	10.77	20.61	**10.77**
E	11.78	9.07	12.84	10.58	10.10	9.48	10.85	13.40	**10.62**
Grand Total	11.23	9.26	10.41	10.15	11.94	10.88	11.47	15.60	**11.13**
# bulls	**2**	**5**	**5**	**9**	**5**	**17**	**14**	**4**	**61**

Figure 4.1 Demand (dark line) of unit quantity for Top 25% and bottom 25% of each trait and the amount assigned from optimal solution (lighter grey bars).

Shadow Price ($)

TopBottom25%	Region	Trait	-2.0	-1.5	-1.0	-0.5	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
Top25	A	CheeseYield	×					⊕□									
		DairyComp					×	+□									
		FLComp			×			⊕□									
		Milk					× + □										
		Type				×		⊕□									
	B	CheeseYield					×				+	□					
		DairyComp					×				+ □						
		FLComp					×						+				□
		Milk					×	+□									
		Type					×		+□								
	C	CheeseYield			×				⊕□								
		DairyComp					×		+ □								
		FLComp				×		⊕									
		Milk			×				⊕								
		Type					×		+ □								
	D	CheeseYield					×			+			□				
		DairyComp					×	+□									
		FLComp					×			+	□						
		Milk			×			⊕□									
		Type			×			⊕□									
	E	CheeseYield			×				⊕□								
		DairyComp					×		+		□						
		FLComp					×	⊕□									
		Milk			×			⊕									
		Type					×		+□								

-80K -60K -40K -20K 0K 20K 40K 60K 80K 100K 120K 140K 160K

Value

Measure Names
- ○ Lower
- □ Upper
- + Final Value
- × Shadow Price

TopBottom25%	Region	Trait	-2.0	-1.5	-1.0	-0.5	0.0	0.5	1.0	1.5	2.0
Top25	A	CheeseYield	× -2.339								○ + □ 6,603 7,535 8,653

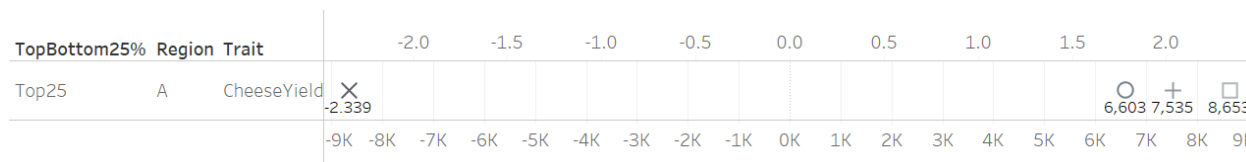-9K -8K -7K -6K -5K -4K -3K -2K -1K 0K 1K 2K 3K 4K 5K 6K 7K 8K 9K

Figure 4.2 Allowable ranges (lower (circle), upper (square)) with final values (plus) and shadow prices (x) assigned to each constraint within the Top 25% trait and region combinations. Example of Figure 2: Shadow price, final value, and bounds for the constraint of units of top 25% cheese yield for region A. An increase of one unit to region A for top 25% cheese yield will result in the objective function decreasing by $2.34. The constraint's final value assigned at optimal solution was 7,535, and the shadow price is held constant if the units stay within 6,603 and 8,653. In this example, barring any other changes, it would be beneficial to decrease the value to the lower bound to increase revenue.
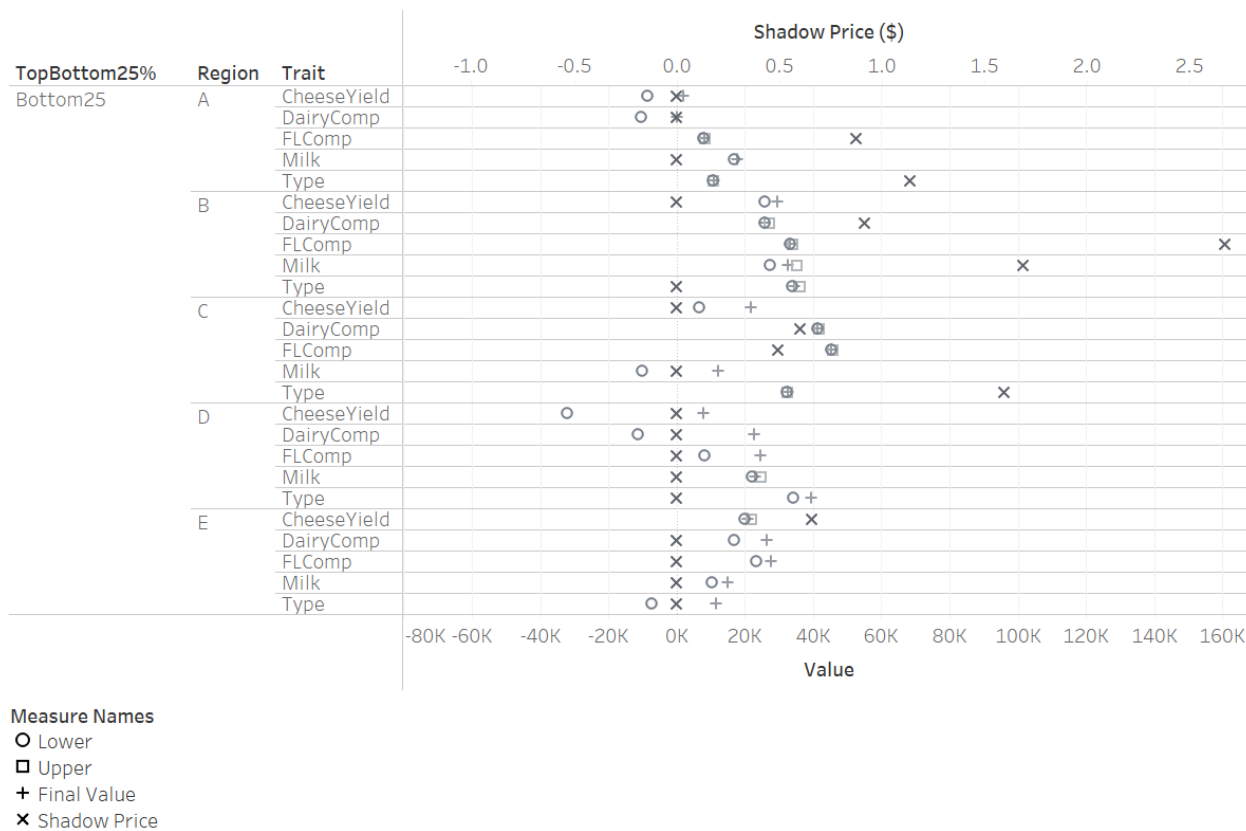
Figure 4.3 Allowable ranges (lower (circle), upper (square)) with final values (plus) and shadow prices (x) assigned to each constraint within the Bottom 25% trait and region combinations.

CONCLUDING REMARKS

This dissertation investigated several areas along the AI supply chain, focusing on product forecasting and the development and optimization of objective decision-support tools. Specifically, it 1) evaluated ML algorithms' performance in forecasting TSp using management factors and bull demographics and identified important factors in predicting young bulls' TSp; 2) provided a decision-support tool framework for bull valuation and herd ranking; 3) developed and evaluated an optimization tool for global allocation of semen product.

Starting at the bull level of the supply chain, we wanted to leverage the power of ML algorithms in forecasting bulls' TSp. In chapter 2, a variety of ML algorithms were tested in forecasting daily, weekly, and monthly TSp when using management factors and bull demographics as predictors. Random forest (RF) and Bayesian regularization neural networks (BRNN) performed the best in the model selection portion. When these two models and linear regression were evaluated in age-based analyses, RF and BRNN performed similarly, however RF was computationally faster and handled missing values better than BRNN. In the date-based analyses, RF out-performed linear regression. Another consideration of this study was the length of training sets needed for accurate predictions. We found that a fixed training set of four months did not sacrifice prediction accuracy of monthly TSp compared to using all prior data available. The most important management factors in predicting TSp were collection frequency, previous TSp records, and age at collection. We suggest that, in practice, a RF model be used in forecasting TSp to aid in supply chain and management decisions. There is an opportunity to improve the predictive ability by adding additional predictors such as genes related to TSp and bull-handler data.

Herd replacement decisions for an AI company are highly subjective with many factors and competing interests involved. The third chapter aimed at utilizing a Markov chain (MC) framework, formerly used in dairy cow herd replacements to provide a bull valuation and ranking system. Considering bull's age, the MC modeled the state set with involuntary culling percentage as transition probabilities. An aggregated net present value (NPV) was calculated at each time iteration, considering the bull's age, potential TSp, genetic merit, and market potential. A bull's valuation (BullVal$) was obtained by subtracting a replacement bull's NPV by his NPV. A case study demonstrated the tool's feasibility of valuing and ranking a herd. A bull's NPV was influenced primarily by market allocation and pricing, as well as the interaction of sperm production with genetic merit. The case study further highlighted the tool's pitfalls with data availability. For implementation in an AI company, precise price data would aid the decision-support tool in providing more realistic BullVal$.

Moving towards the end of the supply chain, the fourth chapter aimed to optimize the global allocation of semen units. Utilizing a linear program (LP) framework, the model provided optimal unit quantity by bull destined to each global region when maximizing revenue. The LP model allowed for user-defined bounds based on regional demand and bulls' individual semen production capabilities. Results from a case study demonstrated the feasibility and efficiency of this decision-support tool. A sensitivity analysis assessed the influence of constraints and decision variables on the objective function; it verified that the most limiting constraint to the revenue was regional demand. We suggested this tool would be most useful during product allocation discussions and developing collection schedules for the coming trimester as well as culling decisions. Furthermore, the sensitivity analysis would be beneficial for an AI company to negotiate bounds and constraints.

We demonstrated that ML, simulation, and optimization models can add value to the AI supply chain by providing objective decision-support tools. We envision that the TSp forecast can be integrated into both the herd valuation and global allocation tools. Although this dissertation focused on applying algorithms commonly used outside animal and dairy sciences, we demonstrate opportunities to leverage these models in the AI, animal, and dairy industries when creating decision-support tools. Production and sales data obtained from industry need to be cautiously examined and considered when modeling, as real-life data (specifically when dealing with animals) is messy, containing missing values, outliers, or averaged data that do not portray actual practices.