Teaching Statistics at Google Scale*

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Abstract

Modern data and applications pose very different challenges from those of the 1950s or even the 1980s. Students contemplating a career in statistics or data science need to have the tools to tackle problems involving massive, heavy-tailed data, often interacting with live, complex systems. However, despite the deepening connections between engineering and modern data science, we argue that training in classical statistical concepts plays a central role in preparing students to solve Google-scale problems. To this end, we present three industrial applications where significant modern data challenges were overcome by statistical thinking.

1 Introduction

Technology companies like Google generate and consume data on a staggering scale. Massive, distributed data present novel and interesting challenges for the statistician, and have spurred much excitement among students, and even a new discipline: Data Science. Hal Varian famously quipped in 2009 that Statistician would be “the sexy job in the next 10 years” (Lohr, 2009), a claim seemingly backed up by the proliferation of job postings for data scientists in high-tech. The McKinsey Global Institute took a more urgent tone in their 2011 report examining the explosion of big data in industry (Manyika et al., 2011). While extolling the huge productivity gains that untapping such data would bring, they predicted a shortage of hundreds of thousand of “people with deep analytical skills”, and millions of data-savvy managers, over the next few years.

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Massive data present great opportunities for a statistician. Estimating tiny experimental effect sizes becomes routine, and practical significance is often more elusive than mere statistical significance. Moreover, the power of approaches that pool data across observations can be fully realized. But these exciting opportunities come with strings attached. The data sources and structures that a graduating statistician (or data scientist) faces are unlike those of the 1950s, or even the 1980s. Statistical models we take for granted are sometimes out of reach: constructing a matrix of dimensions $n$ by $p$ can be pure fantasy, and outliers are the rule, not the exception. Moreover, powerful computing tools have become a prerequisite to even reading the data. Modern data are in general unwieldy and raw, often contaminated by ‘spammy’ or machine-generated observations. More than ever, data checking and sanitization are the domain of the statistician.

In this context, some might think that the future of data science education lies in engineering departments, with a focus on building ever more sophisticated data-analysis systems. Indeed, the American Statistical Association Guidelines Workgroup noted the “increased importance of data science” as the leading Key Point of its 2014 Curriculum Guidelines (ASA, 2014). As Diane Lambert and others have commented, it is vital that today’s statisticians have the ability to “think with data” (Hardin et al., 2014). We agree wholeheartedly with the notion that students must be fluent in modern computational paradigms and data manipulation techniques. We present a counter-balance to this narrative, however, in the form of three data analysis challenges inspired by an industrial ‘big data’ problem: click cost estimation. We illustrate how each example can be tackled not with fancy computation, but with new twists on standard statistical methods, yielding solutions that are not only principled, but also practical.

Our message is not at odds with the ASA’s recent recommendations; indeed, the guidelines highlight statistical theory, “flexible problem solving skills”, and “problems with a substantive context” as core components of the curriculum (ASA, 2014). The methodological tweaks presented in this article are not particularly advanced, touching on well-known results in the domains of resampling, shrinkage, randomization and causal inference. Their contributions are more conceptual than theoretical. As such, we believe that each example and solution would be accessible to an undergraduate student in a statistics or data science program. In relaying this message to such a student, it is not the specific examples or solutions presented here that should be stressed. Rather, we wish to emphasize the value of a solid understanding of classical statistical ideas as they apply to modern problems in preparing tomorrow’s students for large-scale data science challenges.

In many cases, the modern statistician acts as an interface between the raw data and the consumer of those data. The term ‘consumer’ is used rather broadly here. Traditionally
it would include the key decision-makers of a business, and perhaps the scientific research community at large. Increasingly, computerized ‘production’ systems—automated decision engines that are critical to a company’s success—may also be counted among the consumers. Leaning on this framing, we see that difficulties may arise in all three phases of data science: the input phase, the inference phase, and the output phase.

Section 2 highlights some challenges posed by the input or data retrieval phase. We describe a common paradigm for data reduction and some of the constraints it imposes, and then show how we can overcome the resulting engineering difficulties with a targeted use of the bootstrap. In Section 3 we present a concrete modeling problem made more difficult by the scale of the data, and discuss how to judiciously simplify the problem to alleviate the computational burden without needlessly reducing the quality of inference. Section 4 considers the output phase—specifically, the situation where the output of a statistical model is piped directly into a production system. We frame this in terms of a causal inference paradigm, highlight a problem which may result, and propose a remedy. In addition to providing evidence for the value of statistical analysis in modern data science, we also hope that these examples can provide students with an idea of the kind of problems that modern industrial statisticians may be confronted with.

2 Sharding, MapReduce, and the Data Cube

Many new challenges in statistics arise from the size and structure of modern data sources. Here we focus on difficulties caused by a sharded architecture, where pieces of the data are stored on many different machines (or shards), often in a manner determined by system efficiency rather than ease of analysis. Such architectures usually arise when we need to work with data sources that are too large to be practically handled on a single machine. In practice, the sharding happens far upstream of any data analysis; the statistician typically has no control over which pieces of data are stored on which machines.

One common procedure for reducing massive data to a smaller form amenable to inference is the MapReduce framework (Dean and Ghemawat, 2004). A detailed description of MapReduce is beyond the scope of this paper; however we give a brief overview in Section 2.1 below.

At a high level, MapReduce lets us create (multi-way) histograms of our data. This computational architecture makes computing some functionals of the data easy, while other functionals are more difficult to get. For example, if $x \in \mathbb{R}^{100}$, then computing $\mathbb{E}[x]$ is easy, but computing the number of pairs of observations that are exact duplicates of
Uncertainty in massive streams

Motivating the problem

A cartoon Google data stream

User population

Server 3

Server 2

Server 1

···

Server K

Server logs (raw data)

···

Map phase

Mapper 1

Mapper 2

···

Mapper M

Reduce phase

Reducer 1

···

Reducer J

Statistician

queries

many-to-1

many-to-many

data dump

Figure 1: A stylized example of a Google data stream. Every user-generated query is processed by one of \( K \) servers, with different queries from the same user possibly hitting different servers. The servers write raw data to logs, one record per query. These records are first processed by \( M \) mapper machines, whose output is shuffled along the key of interest \( k \) and mapped in order to \( J \) reducer machines. The data are further processed by the reducers into a single summary tuple for each unique value of \( k \). These data are finally analyzed by the statistician. Typically, \( K \gg M \gg J \).

each other is hard. As statisticians, we need to express the primitives on which we base our inferential procedures in terms of queries that are feasible with MapReduce.

2.1 Computing with Map Reduce

Here, we follow the exposition of Chamandy et al. (2012), who consider a basic instance of MapReduce; reproduction of a stylized diagram of the system is provided in Figure 1. The internals of MapReduce are less important to this discussion than the sort of data that the program takes as input and spits out at the other end as output. The input can in general be petabytes \((10^{15}\text{B})\) of sharded, unstructured or hierarchical data objects (such as machine-generated log files). The output is typically a flattened table of key-value tuples of aggregated statistics.

Most MapReduce jobs run in just a few hours (or less). In its simplest form, the MapReduce network consists of a single master machine, which coordinates the process, and
many mapper and reducer machines. The system is fully parallel in that there is no communication among mappers nor among reducers (though there is some limited communication between the two groups, and both communicate with the master).

During the map phase, each mapper processes its set of input records, which may themselves be complex non-vector objects, and produces an intermediate tuple by applying some aggregation function. The tuples are different from the final output because they have been computed from only a subset of the data, and must be further combined. These intermediate data are then sorted by their key and sent as input to the reducers, a process known as shuffling. In the reduce phase, each reducer machine further aggregates its own input tuples to produce a final statistic for every unique key. The resulting data, which are of a manageable size, can then be downloaded from the MapReduce network and interrogated using R, SQL, and other such tools. Their final structure is what is known as a data cube: a set of key-value pairs where the key is a possibly high-cardinality categorical vector, and the value is a highly aggregated numeric vector. For example, in a Google Search application, the key might be the cartesian product of all countries, languages, web browser versions, types of computing device, and hours of day. The value might contain aggregated statistics like the number of queries and clicks in each bin.

2.2 Example: Variance estimation with big data

In the context of MapReduce, uncertainty estimation can be challenging, even for relatively rudimentary statistics. The reason is that the record used for sharding and storing the data rarely coincides with the unit of analysis, i.e., the smallest unit for which an independence assumption can be made. Therefore, computing exact second-order statistics like sums of squares is impossible without expensive communication between machines in the network.

Consider the following example. We work for a pay-per-click advertising platform (such as Google), and wish to estimate the average cost per ad click paid by advertisers over some collection of search queries in different countries. We get to measure the cost of clicks, each of which can be attributed to a user who is in one of the countries of interest. Specifically, let $Y_{iuc}$ denote the cost of the $i$-th click of the $u$-th user in the country $c$. Finally, suppose that the “record units” are clicks, meaning that each click is stored separately, and there are no guarantees about whether any pair of clicks may or may not be on the same shard. All clicks are not, in general, independent.

Although the data may be massive, obtaining a simple point estimator for the mean country-wise cost per click is easily accomplished using MapReduce, with sums as the
aggregation functions, clicks and spend as the values, and country as the key. Writing \( N_c \) for the total number of clicks in country \( c \), we can estimate our parameter of interest as

\[
\hat{\theta}_c = Y_{-c}/N_c, \quad \text{where } Y_{-c} = \sum_{i,u} Y_{iuc}.
\]

As statisticians, however, we are rarely satisfied with a simple point estimate \( \hat{\theta} \), and also want a measure of the stability of this estimator. And this is where the details of the MapReduce implementation become important.

Given that the data are stored at the click-level, we can easily compute a naïve variance estimate using MapReduce,

\[
S^2_c = \frac{1}{N_c} \left( \frac{1}{N_c} \sum_{i,u} Y^2_{ijc} - \hat{\theta}^2_c \right),
\]

by simply tacking on a sum of squared click costs, \( Y^2_{iuc} \), to the value tuple. More explicitly, when mapping over a given click, the MapReduce program first determines its country, say \( c \), followed by its cost \( Y_{iuc} \), and then emits the tuple \((1, Y_{iuc}, Y^2_{iuc})\) to the entry of a summation aggregator with country key \( c \). The variance estimator \( S^2_c \) would be justified under the assumption that all click records in the data are independent.

In general, however, the estimator \( S^2_c \) is biased, because the true “experimental unit” is something coarser than the click. In particular, \( S^2_c \) will fail to account for the (usually positive) correlation between the cost of successive clicks from the same user. In a typical computing architecture, we can easily get around this issue by computing user-level variances:

\[
V^2_c = \frac{1}{M_c} \left\{ \left( \frac{M_c}{N_c} \right)^2 \frac{1}{M_c} \left( \sum_u Z^2_{uc} \right) - \hat{\theta}^2_c \right\}; \quad \text{where } Z_{uc} = \sum_i Y_{iuc}
\]

and \( M_c \) is the number of unique users in country \( c \). The problem is, the individual \( Y_{iuc} \) comprising user \( u \)’s total cost \( Z_{uc} \) are not usually on the same shard, and so we need to compute a separate MapReduce query to get each \( Z_{uc} \) (or key our aggregators by \( u \)). Thus, to compute (3), the size of the output returned by MapReduce would need to scale as the number of users in the system. As the number of users is almost as large as the number of clicks, this is computationally prohibitive.
2.3 The Poisson bootstrap

Perhaps surprisingly, however, it turns out that we can side-step the engineering problem of how to compute $V_c^2$ with a statistical idea. Although $V_c^2$ itself is difficult to compute, we can produce a MapReduce-friendly alternative to it using a variation of the bootstrap (Efron and Tibshirani, 1993). The key trick is to replace multinomial bootstrap sampling with Poisson sampling, which can be implemented while streaming over the data.

More specifically, recall that bootstrap procedures draw a sequence of resamples which can be viewed as weighted versions of the original sample. The idea behind the Poisson bootstrap is to use Poisson weight vectors instead of multinomial weight vectors, since the former can be generated on-the-fly without knowing the sample size, while the latter cannot. The method works as follows. To construct $B$ replicates of the output tuple from a MapReduce, $B$ independent Poisson(1) random variables are drawn for each record in the data, as the record is processed. Given a record belonging to a statistical unit with the unique identifier $u$, the random number generator for replicate $b$ is seeded with $g(h(u) + b)$, where $g$ and $h$ are two fingerprint functions. This procedure ensures that any two records originating from the same unit will have identical Poisson vectors. The $b$-th Poisson variable represents a count of how many times the unit is to appear in replicate $b$.

If there are $n$ total units, the sample size of any Poisson bootstrap replicate is not fixed, but rather a random variable distributed as Poisson($n$). Nevertheless, the Poisson bootstrap is asymptotically equivalent to the traditional multinomial bootstrap, and to streaming analogues of related resampling techniques (Chamandy et al., 2012). These ideas have been studied by, among others, Hanley and MacGibbon (2006), Lee and Clyde (2004), and Politis et al. (1999).

2.4 Illustration with Google data

Figure 2 illustrates this problem with Google data, by showing standard errors for average click cost in 234 countries. The data are normalized so that estimates are displayed relative to $V_c$ (3), which is based on an i.i.d. user assumption. As we might have feared, the naïve variance estimates $S_c^2$ (2), which assume that clicks are i.i.d., are badly biased downwards. We also include an intermediate estimator computed from an i.i.d. query

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1 A fingerprint function $f$, as used here, is a mapping of arbitrary data into the space of 64-bit integers. It is virtually 1-to-1, so that collisions are extremely rare (but not impossible). Moreover, knowing $f(x_1), f(x_2), \ldots, f(x_n)$, for some arbitrary collection of points $x_1, \ldots, x_n$, gives no information about the relationship between those data points.

2 Computing $V_c$ for this problem required using a very expensive data join, which would not be feasible as a part of a routine data-processing pipeline.
Figure 2: Estimated standard deviation of average click cost in 234 countries. Standard errors are computed relative to the computationally prohibitive independent-user estimator $V_c$ (gold line and x-axis, on a log scale). Assuming that all clicks are i.i.d. leads to $S_c$, which underestimates uncertainty (green dots). So does, to a lesser extent, assuming that all queries are i.i.d. (pink squares). The gold standard $V_c$ is fairly well-approximated in this example by applying the Poisson bootstrap with 1000 replicates (purple triangles).

model; in general, a query should be thought of as a set of actions comprising a single task that may include many clicks. Such a model is tractable in certain applications; query-level sharding, as depicted in Figure 1, is not uncommon. Accounting for the within-query correlation helps, but the i.i.d. query estimator still underestimates uncertainty on the standard error scale by about 10%.

Poisson bootstrap standard errors using $B = 1000$ replicates are also displayed in Figure 2. They are quite close, at least in expectation, to the gold standard $V_c$, computed from a “random user” model—that is, using between-user sums of squares. This is as expected, since the bootstrap procedure assumes that users are the independent units of analysis. Thus, the Poisson bootstrap has successfully provided us with a computationally efficient...
way of estimating the variance of $\hat{\theta}_c$ using MapReduce.

3 The Long Tail

Large data sets are notorious for having long-tailed occurrence distributions: many units occur infrequently, but together, these infrequent units account for a large fraction of total events. For example, Google advertisers have collectively input millions of keywords into their advertising campaigns. These keywords are a targeting mechanism—they allow the advertiser to indicate a desire to show an ad when the user’s search query contains the specified terms. But most Google ad keywords are only seen a small number of times. Because of this, when doing statistical analysis of such long-tailed data, the number of units of interest scales with the amount of data collected. This creates computational challenges for traditional statistical methods.

3.1 Example: Cost per click modeling

Suppose we are interested in predicting the average cost per ad click on each keyword. Such a prediction model might serve a number of purposes: classifying query strings into commerciality bins, estimating the revenue that will be generated by a new ad campaign, etc. Some of these uses may entail memory or computational constraints, for example if the model will be used as part of an online serving system.

As a simple version of this, we might want to fit a linear mixed effects model of the form

$$\log(\text{ad click cost}) \sim \text{country} + \text{query category} + (1|\text{keyword}),$$

where ‘query category’ refers to some coarse classification of query strings into topics like *Home and Garden, Finance, Arts and Entertainment*, and so on. Here we have expressed the model using an R *lme4*-style model formula (Bates et al., 2014). The response variable is ad click cost on the log scale. The last term on the right-hand-side denotes a simple keyword random effect, i.e., a different mean 0 random offset for every keyword. The fixed effects of country and query category are assumed to be constant across all keywords. This may be overly simplistic if a query category encompasses a diverse set of products, but is a reasonable first attempt. More sophisticated random effects models are of course possible but don’t fundamentally change the problem.

For convenience, we can fit the model in two stages: first, fit a coarse model without the keyword effect; and second, analyze the residuals to estimate keyword-level random
effects. Fitting the coarse model is easy—a straightforward regression on categorical predictors with which any undergraduate statistician should be familiar. The sufficient statistics are also particularly simple: total clicks and log cost for each combination of country and query category. These statistics are not only easy to compute using MapReduce, but also easy to work with afterward, fitting nicely in memory (as long as there aren’t too many query categories).

Next, we need to analyze the keyword-level residuals. This is where the challenge lies. There are many keywords, most of which are extremely rare. Intuitively, though, the rare keywords are not completely useless. Ideally, we would like to be able to ‘borrow strength’ from the distribution of keyword effects when estimating parameters for any given keyword. This is the key idea behind shrinkage estimators. In a second MapReduce step, one can easily apply the first stage model and even collect keyword-level residual statistics; for simplicity, a count, mean and sample variance.

Ignoring the uncertainty in the variances, the random effects problem then reduces to that of estimating a vector of normal means. Suppose each keyword $k$ has a true effect $\mu_k$. We observe a noisy sample mean residual $R_k$, with true variance $\sigma_k^2$ inversely proportional to its frequency:

$$\mu_k \sim N(0, \eta^2)$$
$$\sigma_k \sim G$$
$$R_k | \mu_k, \sigma_k \sim N(\mu_k, \sigma_k^2),$$

where $G$ is an unspecified prior on the keyword-level standard deviations. We want to estimate $\mu_k$ based on $R_k$ and $\sigma_k$.

We could choose to treat all keywords equally. But for most applications, it is more important to perform well on frequent keywords. Therefore, our loss function must be weighted by frequency (or inverse variance). This is no different from treating every unique instance of a keyword as a separate observation. The appropriate squared-error loss is then

$$L(\mu, \hat{\mu}) = \sum_k L_k(\mu, \hat{\mu}) = \sum_k (\mu_k - \hat{\mu}_k)^2 / \sigma_k^2.$$  \hspace{1cm} (4)

We wish to minimize risk, that is the expected loss $E[L(\mu, \hat{\mu})]$ averaged over the priors. Assuming known $\eta$ and $\sigma_k^2$’s, this is achieved by using the Bayes estimator (Lehmann and Casella, 1998), i.e. the posterior mean

$$E(\mu_k | R_k, \sigma_k) = \frac{\eta^2}{\sigma_k^2 + \eta^2} R_k.$$
This estimator shrinks the observed average residuals towards 0 (the prior mean). For the \( k \)-th keyword, the Bayes estimator has risk

\[
R_{\text{Bayes}} = \mathbb{E} \left[ (\mu_k - \mathbb{E}(\mu_k|R_k, \sigma_k))^2 / \sigma_k^2 \right] = \mathbb{E} \left[ \mathbb{E} \left[ \text{Var}(\mu_k|R_k, \sigma_k) / \sigma_k^2 \right] \right] = \mathbb{E} \left[ \eta^2 / (\sigma_k^2 + \eta^2) \right] = \mathbb{E} \left[ \tau_k / (1 + \tau_k) \right],
\]

where \( \tau_k = \eta^2 / \sigma_k^2 \) is the signal to noise ratio, and the last expectation is taken over \( G \). This estimator minimizes our loss function, but it is computationally expensive. Not only does it require computing statistics for all keywords, but more importantly storing a coefficient for each keyword if we wish to make predictions from the model. The latter would be especially problematic in an online setting, where speed and memory are at a premium. Nevertheless, this ‘long tail’ problem gives a hint as to how we might proceed. In practice, we often wish to make predictions for examples we have never before seen, corresponding to \( \tau_k = 0 \) and therefore \( \hat{\mu}_k = 0 \) (there is no signal, only noise). Intuitively, making a prediction for cases we have only observed once or twice, of which there may be millions, is a qualitatively similar task.

### 3.2 Pruning rare units

The Bayes-optimal approach described above spends its computational resources unwisely—it uses the same amount of memory (one coefficient) for each keyword. This is wasteful since the rare keywords are less important in the loss function, and their effects are harder to estimate anyway. Nevertheless, the Bayes estimator is a clear improvement on our prior knowledge. Compared to simply plugging \( \hat{\mu} \equiv \mathbb{E}(\mu_k) = 0 \) into (4), it reduces the \( k \)-th term in our risk by

\[
\mathbb{E}[\mathcal{L}_k(\mu, 0)] - \mathbb{E}[\mathcal{L}_k(\mu, \mathbb{E}(\mu_k|R_k, \sigma_k))] = \mathbb{E} \left[ \frac{\text{Var}(\mu_k) - \text{Var}(\mu_k|R_k, \sigma_k)}{\sigma_k^2} \right] = \mathbb{E} \left[ \frac{\eta^2}{\sigma_k^2} \left( \frac{\eta^2}{\eta^2 + \sigma_k^2} \right) \right] = \mathbb{E} \left[ \tau_k \left( \frac{\tau_k}{1 + \tau_k} \right) \right].
\]

Recall that \( \tau_k \) is proportional to the frequency of keyword \( k \). For rare keywords, \( \tau_k \) is small, so the Bayes estimator is only a small improvement over the prior in such cases.

This suggests an obvious strategy: compute the Bayes estimate for common keywords, and use the prior for rare keywords. This can be implemented by running a MapReduce
to find keywords for which $\tau_k$ is bigger than some threshold $T$, gathering data for these keywords (either in the same MapReduce or in another one), and using the truncated estimator

$$\hat{\mu}_k = \begin{cases} \frac{\eta^2}{\sigma_k^2 + \eta^2} R_k & \tau_k \geq T \\ 0 & \tau_k < T \end{cases}. \quad (5)$$

A similar calculation shows that for keyword $k$, the risk of this estimator is

$$R_{\text{Trunc}} = \mathbb{E}\left(\frac{\tau_k}{1 + \tau_k} (1 + \tau_k \mathbb{1}\{\tau_k < T\})\right).$$

The truncated estimator is often nearly as good as the Bayes estimator. Clearly, $R_{\text{Trunc}} \leq (1 + T) R_{\text{Bayes}}$. If most keywords are rare and only a few occur frequently, $\tau$ is concentrated near 0, making $\tau_k \mathbb{1}\{\tau_k < T\}$ small and $R_{\text{Trunc}}$ close to $R_{\text{Bayes}}$. Also, since even a small $T$ is usually enough to eliminate a huge number of keywords, the truncated estimator can perform nearly as well as the Bayes estimator while using a small fraction of the keywords. A nice side-benefit in online applications is that (5) provides us with an initial click cost estimate even for keywords that we have never before observed.

Extensions of similar pruning ideas to more general contexts such as regression and optimization have been considered by, among others, Duchi et al. (2010), Langford et al. (2009), and McMahan et al. (2013). Of course, in a real application $\eta$ and $G$, and even perhaps the prior mean, would be unknown. While a classical Bayesian might hazard an educated guess at these, perhaps bolstered by diagnostic checks, in the big data regime one can do better. *Empirical Bayes* provides a framework for estimating these parameters from the data (Casella, 1985; Efron, 2010). While these ideas are especially powerful in a big data setting, they are surprisingly underrepresented in typical undergraduate curricula.

### 3.3 Simulation study

Figure 3 illustrates with a simulation study how the truncated estimator described in the previous section can offer attractive performance-computation tradeoffs. We generated $\sigma_k^2$ from a log-normal distribution $G$ with sd $(\log (\sigma_k)) = 1.5$, and set $\eta = \mathbb{E}\left(1/\sigma_k^2\right) = 1$. The far right shows that if we keep all the data, the truncated and Bayes estimators are the same, so $R_{\text{Trunc}}/R_{\text{Bayes}} = 1$. As we increase the threshold $T$, we start filtering out keywords, and move left on the plot. $R_{\text{Trunc}}/R_{\text{Bayes}}$ rises, but slowly—we can keep just 10% of the data and perform only 7.5% worse than the Bayes estimator. Finally, as we start discarding informative keywords, $R_{\text{Trunc}}/R_{\text{Bayes}}$ explodes and we perform much
Figure 3: Simulated loss incurred by the truncated estimator in the rare keyword example, relative to Bayes loss, for different occurrence thresholds $T$. The $x$-axis indicates the fraction of all keyword effects estimated (i.e., $P[\tau \geq T]$). By estimating only 10% of the random effects, and discarding the rest of the keywords, we perform about 7.5% worse than optimal while obtaining an order-of-magnitude computational savings.

worse than the Bayes estimator.

4 Statistical Feedback

In traditional applications, both academic and industrial, statistical models or inference procedures tend to be of a ‘throw-away’ nature. A model is fit and a parameter estimated, or a decision is made under uncertainty, and the result is communicated to the relevant stakeholders. Typically, the statistician’s job ends there, and the model or inference is unlikely to be revisited except if improvements to the methodology are desired, or in rare follow-up or meta analyses.

In this section we describe a scenario where the output of a sequentially-run statistical procedure is at risk of being used by one or more of its consumers in a way that could be damaging to the inference itself. Such use is typically not malicious, nor can it really be termed abuse; nonetheless it may have unintended side-effects.
4.1 Example: Query classification in ads serving

Suppose that we have built a statistical classifier to predict whether a search query has commercial intent. Our goal is to use the predictions from our “commerciality” classifier for stratified data analysis, forecasting query growth, or some other such offline application. These predictions are updated by periodically collecting feature data over some time window, but not by retraining the model itself (or by retraining it only very rarely); the reason for this is that fitting our commerciality model is costly as it requires collecting hand-labeled training data and curation by a statistician.

In this example, we chose to use expected click cost, i.e., the output from the model in Section 3, as a feature in our classifier. If we were operating in isolation, this choice would be completely innocuous. However, if we share the output of our classifier with other teams, feedback loops can emerge. For example, suppose that another team—the ads serving engineering team—hears of the existence of our model for predicting commercial intent, and wants to exploit that signal in their own algorithms. Perhaps, for example, they wish to search for more candidate ads on queries that they deem to be highly commercial. If our model is logistic regression and produces probabilities \( \hat{Y}_i = \hat{p}[\text{query } i \text{ is commercial}] \), this may correspond to situations where \( \hat{Y}_i > p \), for some threshold \( p \). Alternatively they may wish to fetch a set of candidates whose size is proportional to the odds of \( \hat{Y} \).

On the surface, such uses of our model are entirely reasonable. The problem is, if the other engineering team uses our signal in a way that changes the expected click cost, then our model may get biased by feedback. For example, take a query for which our model predicts a large probability, either correctly or because of some prediction error. The serving system may suddenly begin to fetch more candidate ads for this query, increasing auction pressure and leading to higher average click costs. Since we haven’t retrained our classifier in the interim, this increase in click cost will be taken by the model as evidence that the query is even more likely to be commercial than previously thought. This effect can worsen in successive time periods. On the other hand, a query for which we erroneously predict a small \( \hat{Y} \) may be disfavoured in serving, pushing down click cost and reinforcing our misguided belief that the query lacks commercial intent.

4.2 Detecting feedback with noise injection

Although feedback itself is an engineering problem, detecting feedback is a statistics problem. Perhaps the most difficult part of getting a handle on statistical feedback is to define precisely and quantitatively what we mean by feedback. Here, we follow the
approach of Wager et al. (2014), and frame the problem in terms of the Rubin Causal Model (Rubin, 2005) and counterfactual model predictions.

More specifically, let $\hat{Y}^t_i[\emptyset]$ denote the predictions we would have made for the $i$-th item (query, say) in time period $t$ if there hadn’t been any feedback, i.e., the prediction that our model would make if the engineering team never began using it in production. Other counterfactual predictions are indexed by the prediction deployed in the previous period: $\hat{Y}^{t+1}_i[\hat{Y}^t_i]$ denotes the time $t+1$ model prediction, in a system with feedback, given that $\hat{Y}^t_i$ was the prediction for item $i$ produced at time $t$. Given this notation, we define the feedback at time $t+1$ on item $i$ as a difference in potential outcomes,

$$\text{feedback}^t_i = \hat{Y}^{t+1}_i[\hat{Y}^t_i] - \hat{Y}^{t+1}_i[\emptyset],$$

i.e., the difference between the prediction the system in fact made, and the prediction it would have made were there no feedback.

In order to use the formalism (6) in practice, we need to restrict the kinds of feedback we seek to detect. Our first assumption is that feedback is Markovian, i.e., that feedback $\hat{Y}^t_i$ is conditionally independent of $\hat{Y}^1_i, ..., \hat{Y}^{t-1}_i$ given $\hat{Y}^t_i$. Second, we assume that the feedback is additive, i.e., that it does not depend on $\hat{Y}^{t+1}_i[\emptyset]$ conditional on $\hat{Y}^t_i$.

Given these two assumptions, we can define a feedback function

$$f(y) = \mathbb{E} \left[ \hat{Y}^{t+1}_i[\hat{Y}^t_i] - \hat{Y}^{t+1}_i[\emptyset] \mid \hat{Y}^t_i = y \right]$$

and so

$$f(y) = \theta y.$$  

The goal of our analysis is to estimate this feedback function $f(\cdot)$. The principal challenge in doing so is that it is not possible to simultaneously observe the two sets of predictions represented by the two terms on the right-hand side of (7), namely $\hat{Y}^{t+1}_i[\hat{Y}^t_i]$ and $\hat{Y}^{t+1}_i[\emptyset]$.

The solution we proposed in Wager et al. (2014) involves secretly injecting a noise term $\nu^t_i$ into the prediction at time $t$. The intuition behind this approach is that it creates a sort of synthetic randomized experiment, allowing us to estimate the average causal effect $f(y)$ of feedback. Noise injection is related to the idea of instrumental variables (Angrist et al., 1996) in the sense that, once we have injected this artificial noise into the system, we analyze its effect on the system just like we would in an instrumental variables regression.

For simplicity, consider the case where feedback enters into the model linearly

$$\hat{Y}^{t+1}_i[\hat{Y}^t_i] = \hat{Y}^{t+1}_i[\emptyset] + \theta \hat{Y}^t_i,$$

and so $f(y) = \theta y$.  

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This model is rather unlikely to hold in reality, but it admits a simple analysis. Note that the formulation (9) implicitly assumes that all the randomness in the system has been absorbed into $\hat{Y}_{i}^{t+1}[\emptyset]$.

Now, in order to detect the feedback, suppose that we start secretly deploying noisy predictions $\hat{Y}_{i}^{t} + \nu_{i}^{t}$ instead of $\hat{Y}_{i}^{t}$ in serving at time $t$. In other words, we never tell other engineering teams what the raw value $\hat{Y}_{i}^{t}$ produced by our predictor is, and only give them access to the noised-up quantity $\hat{Y}_{i}^{t} + \nu_{i}^{t}$. Any feedback mechanism must now act through these noisy predictions, and so the relationship (9) becomes

$$\hat{Y}_{i}^{t+1}[\hat{Y}_{i}^{t} + \nu_{i}^{t}] = \hat{Y}_{i}^{t+1}[\emptyset] + f(\hat{Y}_{i}^{t} + \nu_{i}^{t})$$

(10)

$$= \hat{Y}_{i}^{t+1}[\emptyset] + \theta \hat{Y}_{i}^{t} + \theta \nu_{i}^{t}.$$  

(11)

Here, both the new model predictions $\hat{Y}_{i}^{t+1}[\hat{Y}_{i}^{t} + \nu_{i}^{t}]$ and the noise terms $\nu_{i}^{t}$ are observed. Thus, since $\nu_{i}^{t}$ is independent of all other quantities on the right-hand side of (11) by construction, we can estimate $\theta$ from (11) using simple linear regression of $\hat{Y}_{i}^{t+1}[\hat{Y}_{i}^{t} + \nu_{i}^{t}]$ on $\nu_{i}^{t}$.

Under this recipe, the precision with which we estimate the feedback slope is a ratio of the variance of the noise we have injected to the variance of the noise inherent in our prediction model:

$$n \text{Var}(\hat{\theta}) = \frac{\text{Var}\left(\hat{Y}_{i}^{t+1}[\hat{Y}_{i}^{t}]\right)}{\text{Var}(\nu_{i}^{t})}. \quad (12)$$

There is a clear tradeoff. Adding more noise improves our ability to measure feedback, but of course it degrades the quality of the published predictions that will be used in production. More details pertaining to (12), and extensions of this idea to general non-linear feedback functions, are considered in Wager et al. (2014).

Having an estimate of $\theta$ or, more generally, $f(\cdot)$, can be useful in several ways. First, merely detecting non-zero feedback can alert us to emerging problems and help us identify “rogue” uses of our published signals $\hat{Y}_{i}^{t}$. More ambitiously, we could also try to do a post hoc feedback correction. For example, in the case of linear feedback, we could use an estimate $\hat{\theta}$ to generate sanitized predictions $\hat{Y}_{i}^{t+1} \overset{\text{def}}{=} \hat{Y}_{i}^{t+1}[\hat{Y}_{i}^{t} + \nu_{i}^{t}] - \hat{\theta}(\hat{Y}_{i}^{t} + \nu_{i}^{t})$; our simulation experiments below use this correction.

### 4.3 Simulation study

To illustrate this technique, we simulate from a simplistic setting: linear feedback in a linear model. This allows us to demonstrate concretely how the randomization procedure might be carried out in ideal circumstances, and even to approximately remove the
offending feedback once we’ve detected it.

We start with the following true underlying model:

$$Y_t^i = \alpha + \beta X_t^i + \epsilon_t^i, \quad \epsilon_t^i \sim N(0, \sigma^2).$$

(13)

We assume that enough data is collected when we train the model at \( t = 0 \) so that \( \alpha \) and \( \beta \) can be taken as known (since the interesting source of error is in the feedback, not in the estimation itself). We imagine that we must make \( n \) weekly predictions for a full year before our next opportunity to retrain the model; i.e., \( T = 52 \). The predictors \( X \) are generated as follows:

$$X_{t+1}^i[H_i] = X_{t+1}[0] + \gamma \hat{Y}_t^i,$$

(14)

where

$$X_{t+1}[0] = X_t[0] + \delta Y_t^i + \xi_t^i, \quad \xi_t^i \sim N(0, \tau^2).$$

(15)

Thus the predictors vary across time even before the feedback occurs, in a way that may depend on the true value of \( Y \). Combining (13) and (14), it can be seen that the feedback function is \( f(y) = \theta y \) with \( \theta = \gamma \beta \).

Given a set of simulated predictions \( \hat{Y}_t^i \) at time \( t \), we first add noise \( \nu_t^i \sim N(0, \omega^2) \). We then generate a new set of \( X \)s from (14), but with \( \hat{Y}_t^i + \nu_t^i \) in place of \( \hat{Y}_t^i \). Next we perform the regression of \( X_{t+1}[\hat{Y}_t^i + \nu_t^i] \) on \( \nu_t^i \). The coefficient of \( \nu_t^i \) from this regression is our estimate of \( \gamma \), call it \( \hat{\gamma}_{t+1} \). We then compute the corrected prediction

$$\hat{Y}_{t+1}^i = \beta \left( X_{t+1}[\hat{Y}_t^i + \nu_t^i] - \hat{\gamma}_{t+1}(\hat{Y}_t^i + \nu_t^i) \right),$$

(16)

again ‘deploy’ the noised-up version \( \hat{Y}_{t+1}^i + \nu_{t+1}^i \), and iterate until \( t = T \).

Note that in this example the variables and predictions grow in expectation across time. Therefore, in Figure 4 we plot the relative root-mean squared error of our estimator, defined as

$$R(t) = \left( \frac{\mathbb{E}[(\hat{Y}_t^i - Y_t^i)^2]}{\mathbb{E}[Y_t^i]^2} \right)^{1/2},$$

(17)

as a function of time. We allowed the standard deviation of the injected noise, \( \omega \), to vary, while fixing the remaining parameter values: \( \beta = 1, \sigma = 1, \gamma = 0.3, \delta = 0.15, \tau = 1, n = 10^5 \).

The general effectiveness of the procedure, along with the tradeoff inherent in the choice of \( \omega \), is evident from the curves in Figure 4. With \( \omega = 0.1 \), early predictions have about as much error as naïve predictions; this error decays quickly but rather noisily.
Figure 4: Simulated relative root-mean square error across 52 time points for linear feedback in a 1-predictor linear model. If no adjustment to our predictor is made, feedback causes an asymptotically (in time) constant amount of error in our predictions (green dashed line). The remaining lines show the error obtained by injecting normal noise of different standard deviations $\omega$, and then using it to remove an estimate of the feedback from $X$ before making a new prediction.

with $\omega = 0.7$ seems about right for this problem. When we inject too much noise, e.g. $\omega = 1.3$, we begin with poor predictions and don’t really make up for it with more stability at larger $t$.

5 Conclusions

In this paper, we described three sub-problems within the broader context of click cost estimation for paid web search. By no means have we presented an exhaustive list of methodological challenges awaiting the modern industrial statistician. Rather, we have chosen the problems to highlight a few distinct ways in which modern data and applications differ from traditional statistical applications, yet can benefit from careful statistical analysis.

In the first problem, uncertainty estimation was nontrivial because the types of second-
order statistics that statisticians normally take for granted can be prohibitively expensive in large data streams. The second problem, which centered around building a fine-grained prediction model, explored the gains that are possible by judiciously chopping off the long tail of a massive data set. Finally, Example 3 highlighted the importance of protecting one’s methods from unexpected uses, in an environment where product decisions driven by statistical models can feed back inconspicuously into the inference procedure. All three problems initially appeared to be straightforward and amenable to standard methods, until a technical wrinkle presented itself. In each case, it was primarily through careful statistical reasoning, and not by designing some heavyweight engineering machinery, that we were able to arrive at a solution.

In doing so, we drew upon ideas that have been around for at least four decades—and in some cases much longer. Over that time, these methods have been taught to undergraduate students with an eye to small data problems. It is increasingly important, in light of the rapid growth of available data sources, to modernize classroom examples so that graduating students are not shell-shocked by their first encounter with big data. Likewise, data-based simulation techniques should be emphasized as a proving-ground for methodology before applying it naively to a billion data points. Early exposure to tools like MapReduce can help build confidence, but frankly, a newly-minted statistician with “deep analytical skills” should have no trouble learning such things on the job. As we have argued, it remains as critical as ever that we continue to equip students with classical techniques, and that we teach each and every one of them to think like a statistician.

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