EMPIRICAL BAYES FOR LARGE-SCALE RANDOMIZED EXPERIMENTS: A SPECTRAL APPROACH

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Large-scale randomized experiments, sometimes called A/B tests, are increasingly prevalent in many industries. Though such experiments are often analyzed via frequentist t-tests, arguably such analyses are deficient: p-values are hard to interpret and not easily incorporated into decision-making. As an alternative, we propose an empirical Bayes approach, which assumes that the treatment effects are realizations from a “true prior”. This requires inferring the prior from previous experiments. Following Robbins, we estimate a family of marginal densities of empirical effects, indexed by the noise scale. We show that this family is characterized by the heat equation. We develop a spectral maximum likelihood estimate based on a Fourier series representation, which can be efficiently computed via convex optimization. In order to select hyperparameters and compare models, we describe two model selection criteria. We demonstrate our method on simulated and real data, and compare posterior inference to that under a Gaussian mixture model of the prior.

1. Introduction. Consider a randomized experiment with a binary treatment and a continuous outcome. We use c and t to denote the control and treatment groups respectively. We wish to estimate the (true) average treatment effect (ATE) \( \Delta := \mu_t - \mu_c \), the difference in the population means. Subjects are randomly assigned: \( n_c \) to control and \( n_t \) to treatment. An unbiased estimator for \( \Delta \) is the difference in the empirical means

\[
\hat{\Delta} = \bar{X}_t - \bar{X}_c
\]

which we will call the “observed effect”.

Suppose \( n = n_t + n_c \to \infty \) and \( n_t/n \to \gamma \in (0, 1) \). By the central limit theorem, one can show that

\[
T := \frac{(\bar{X}_t - \mu_t) - (\bar{X}_c - \mu_c)}{\sqrt{s_t^2/n_t + s_c^2/n_c}} = \frac{\bar{X}_t - \bar{X}_c}{\sqrt{s_t^2/n_t + s_c^2/n_c}} \overset{d}{\to} N(0, 1),
\]

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where $s^2_t$, $s^2_c$ are treatment/control group variances, and \( \Rightarrow \) denotes convergence in distribution. If the observations from treatment/control groups are further assumed to be normally distributed, then under finite $n$, approximately $T \sim t_{\nu}$, which is known as an unequal-variance or Welch’s $t$-test (Welch, 1947). Formulae are available for approximating the degrees of freedom $\nu$ from data, e.g., those proposed by Satterthwaite (1946) and Welch (1947). $t$-tests are routinely used for the analysis of randomized experiments. In this paper, we focus on the setting where $n$ is typically very large. Note that $\nu \to \infty$ as $n \to \infty$, so the normal limit in Eq. (2) is recovered.

For the analysis of a single experiment, it is common to compute a $p$-value from the $t$-statistic. However, in modern technological and industrial settings, a large number of randomized experiments are run every day. In this setting, continuing to use the $t$-test for each experiment separately is inefficient. As we will see, doing so essentially ignores the information from the population of experiments, even though two experiments may seem unrelated. A similar phenomenon, where estimation benefits from sharing information across seemingly unrelated data, is known as Stein’s paradox; the reader is referred to Stein (1956) and Efron and Morris (1977) for more discussions. Also, while the $t$-test is proper for testing whether the true effect is below or above zero, it is inconvenient for industrial decision making, which may be targeted at a specified function that maps the decision and the true effect to a loss/utility. Lastly, it is often difficult to communicate the precise interpretation of the $p$-value to a wider audience; see Amrhein et al. (2019) for a recent debate. In the following, we argue that an empirical Bayes approach is a more appealing framework for the analysis of large-scale experiments that overcomes these issues.

The rest of this paper is organized as follows. In Section 2, we review the foundational idea of Robbins and illustrate how an empirical Bayes analysis of experiments can be conducted and its benefits. In Section 3, we briefly review parametric estimation of the prior with normal mixtures. In Section 4, we show that the estimation problem is characterized by a heat equation and develop a nonparametric maximum likelihood estimate based on a spectral representation. We present an efficient algorithm, consider two model selection criteria, and prove consistency in terms of the method of sieves. In Section 5, we compare the performance of our spectral estimator with the mixture-of-Gaussian estimator on simulated and real data. Finally, discussion and bibliographic remarks are presented in Section 6.

2. An empirical Bayes framework.
2.1. The basic idea. The study of empirical Bayes was pioneered by Herbert Robbins (Robbins, 1956, 1964, 1983). The motivation was to estimate parameters associated with “many structurally similar problems” (Lai and Siegmund, 1986). For example, in Robbins (1977), he considered predicting the number of accidents in the upcoming year based on the number of accidents from the current year for a population of \( n \) taxi drivers. Suppose driver \( i \) is associated with the rate of accidents \( \lambda_i \), and we model the number of accidents \( X_i \mid \lambda_i \sim \text{Pois}(\lambda_i) \) independently for each driver. Further, suppose that the rate of accidents is the same from year to year, then the expected number of accidents in the coming year is \( \mathbb{E}[X_i^* \mid \lambda_i] = \lambda_i \), for which \( X_i^* \) is the maximum likelihood estimate that treats each driver separately. The idea of Robbins is to assume that \( \lambda_i \)'s are drawn independently from some unknown distribution \( G \), which we will call the “true prior”. By doing so, he further showed that the posterior mean for \( \lambda_i \) can be estimated nonparametrically by the formula

\[
\hat{\mathbb{E}}[\lambda_i \mid X_i = x] = \frac{(x + 1)n_{x+1}}{n_x},
\]

where \( n_{x+1} \) is the number of drivers in the sample with \( x + 1 \) accidents in the current year. As we can see, the formula utilizes information from other “seemingly unrelated” drivers.

The idea has been recently applied to large-scale hypothesis testing for microarray data; see Efron (2003) for an overview. In the context of large-scale experimentation, the idea seems readily applicable if we assume that the true treatment effects \( \Delta_i \) are realized independently from some unknown distribution \( G \). True effects \( \Delta_i \) should be comparable across experiments for the population distribution \( G \) to be meaningful. For the rest of the paper, we will assume that the true effects are measured in the same unit and are normalized to the same time duration.

The actual data generating process for the outcome of an experiment also involves several nuisance parameters, for which we would like to refrain from assuming an (even unknown) prior. For example, it seems unnatural to specify priors on the means and variances of treatment and control groups; and as we will see, it is also unnecessary if our goal is to infer the posterior over the true effect. Note that this deviates from the usual “fully Bayesian” analysis where priors are typically specified for nuisance parameters.

2.2. Nuisance-free asymptotic likelihood. We now consider a likelihood for the true effect that does not involve nuisance parameters, and hence frees us from specifying prior on the nuisance. Observe that Eq. (2) can be turned into an asymptotically efficient likelihood on \( \Delta \), given by

\[
L(\Delta; \hat{\Delta}, \hat{s}) = \phi_{\hat{s}}(\Delta - \hat{\Delta}), \quad \hat{s} = \sqrt{s_t^2/n_t + s_c^2/n_c},
\]
where \( \hat{s} \) is the estimated asymptotic scale and \( \phi_s(\cdot) = s^{-1}\phi(\cdot/s) \) is the Gaussian density function with variance \( s^2 \). In other words, the observational model relative to \( \Delta \) is asymptotically a normal experiment; see van der Vaart (2000, Chap 9) for more on limits of experiments. Since the sample size in large-scale experimentation is typically very large, we make no distinction between \( \hat{s} \) and the true scale \( s := \sqrt{\sigma_t^2/n_t + \sigma_c^2/n_c} \), with \( \sigma_t^2, \sigma_c^2 \) being the population variances. In the following, we will treat the scale \( s_i \) for an experiment \( i \) as fixed and given.

An experiment \( i \) is represented by the tuple \( (\Delta_i, \hat{\Delta}_i, s_i) \). Following the idea of Robbins, we make the following assumption.

**Assumption 1.** \( \Delta_i \overset{\text{iid}}{\sim} G \) for some distribution \( G \).

This supposes an underlying population of experiments from which the experiments performed are randomly sampled. Then under the empirical Bayes framework, the observational model for an experiment is asymptotically an additive Gaussian noise model with heterogeneous scales

\[
\Delta_i \overset{\text{iid}}{\sim} G, \quad \hat{\Delta}_i = \Delta_i + s_i Z_i,
\]

where \( Z_i \) is a standard normal variable that is independent of \( \Delta_i \) and independent across experiments. The prior \( G \) is an unknown distribution on \( \mathbb{R} \). Since the true effects \( \{\Delta_i\} \) are unobserved, estimating \( G \) from \( \{(\hat{\Delta}_i, s_i)\} \) is a problem of deconvolution (Delaigle and Meister, 2008).

We comment that this asymptotic treatment is also adopted by several authors, including Deng (2015); Goldberg and Johndrow (2017); Azevedo et al. (2019). Among others, we note that Deng (2015) specifies the true prior on \( \Delta_i/\hat{s}_i \) instead of \( \Delta_i \), with \( \hat{s}_i := \sqrt{\sigma_t^2(1+n_t/n_c) + \sigma_c^2(1+n_c/n_t)} \). We find this specification not the most natural, since \( \Delta_i/\hat{s}_i \) is not an objective truth because \( \hat{s}_i \) depends on \( n_t/n_c \) and hence the design of experiment. In our model Eq. (4), the prior is only assumed on the objective quantity \( \Delta_i \), while \( s_i \) is treated as given.

2.3. Posterior analysis of experiments. It follows from Eq. (4) that if the prior \( G \) is known, we can find the posterior distribution of the true effect \( \Delta_i \). If \( G \) has density \( g \) (with respect to Lebesgue), then the posterior density is given by Bayes’ rule

\[
p_{s_i}(\Delta_i \mid \hat{\Delta}_i) = \frac{g(\Delta_i)\phi_{s_i}(\Delta_i - \hat{\Delta}_i)}{p_{s_i}(\hat{\Delta}_i)},
\]

\(^1\)Here the term “experiment” is a statistical experiment in the sense of van der Vaart (2000).
where

\begin{equation}
ps_i(\hat{\Delta}_i) = \int g(u)\phi_{s_i}(\hat{\Delta}_i - u) \, du
\end{equation}

is the marginal density for \(\hat{\Delta}_i\). Technically, \(s\) is not treated as random, but rather as a fixed covariate. Therefore, we write \(s\) in the subscript.

Before going into the estimation of \(G\), we briefly discuss what one should do if \(G\) is known. In short, we will show that if the true prior is employed in computing the posterior, then (i) the posterior has an exact frequency calibration over the sampling distribution of true effects, and (ii) the Bayes optimal decision for a loss function minimizes the expected loss with respect to that sampling distribution. Therefore, if a loss function is well-specified, then the standard Bayesian decision theory may be applied directly. The properties (i) and (ii) exactly address the issues raised in the Introduction against \(t\)-tests.

\subsection{2.3.1. Frequency calibration of the posterior.}

Using the true prior, the posterior probability \(P_{s_i}(\Delta_i \in A \mid \hat{\Delta}_i)\) for a measurable set \(A \subset \mathbb{R}\) possesses a frequency interpretation. In the following, we fix \(s_i\). With \(A\) also fixed, \(G_A(x) := P_{s_i}(\Delta_i \in A \mid \hat{\Delta}_i = x) : \mathbb{R} \to [0, 1]\) is a measurable map from the observable to a posterior probability.

**Theorem 1.** Given any \(\varphi \in [0, 1]\) and any measurable \(A \subset \mathbb{R}\), if \(P(G_A(\hat{\Delta}_i) = \varphi) > 0\), then it holds that

\begin{equation}
P\left(\Delta_i \in A \mid G_A(\hat{\Delta}_i) = \varphi\right) = \varphi.
\end{equation}

Suppose \(\varphi = 40\%\), this says that with respect to hypothetical replications over \((\Delta_i, \hat{\Delta}_i)\), out of those instances whose posterior probabilities of hypothesis \(A\) is 40\%, exactly 40\% of them actually have their associated \(\Delta_i\) satisfying the hypothesis. We leave the proof to Appendix A. When \(P(G_A(\hat{\Delta}_i) = \varphi) = 0\), by integrating the density over an infinitesimal interval and taking the limit, the statement can be generalized to the following. Note that the quantity should be interpreted as a conditional expectation.

**Corollary 1.** Given any \(\varphi \in [0, 1]\) and any measurable \(A \subset \mathbb{R}\), it holds that

\begin{equation}
P\left(\Delta_i \in A \mid G_A(\hat{\Delta}_i) = \varphi\right) = \varphi.
\end{equation}
2.3.2. Bayes optimal decision making. When the true prior is used, the Bayes rule \( d_B \) is optimal with respect to the sampling distribution. That is, if \( d_B \) is used throughout, it will minimize the expected loss accumulated over future experiments; see Appendix A for a brief review of Bayesian decision theory. More concretely, as in Azevedo et al. (2019), consider the decision over whether to “launch” a change/feature based on an experiment. The action space is \( \mathcal{A} = \{0, 1\} \), respectively denoting launching and not launching. Suppose in this context \( \Delta \) denotes the gain in launching the treatment. Consider the following loss function

\[
l(\Delta, a) = \begin{cases} 
-(\Delta - C), & a = 1 \\
0, & a = 0
\end{cases},
\]

where \( C \geq 0 \) is the cost for implementing the treatment. Then the Bayes optimal decision \( d_B(\hat{\Delta}) \) should minimize the posterior risk

\[
\mathbb{E}[l(\Delta, a) | \hat{\Delta}] = \begin{cases} 
-(\mathbb{E}[\Delta | \hat{\Delta}] - C), & a = 1 \\
0, & a = 0
\end{cases}.
\]

Clearly, we have

\[
d_B(\hat{\Delta}) = \mathbb{I}\{\mathbb{E}[\Delta | \hat{\Delta}] > C\},
\]

which says that the change/feature should be launched whenever the posterior mean effect exceeds the cost.

3. Parametric estimation. As we have seen, the key to implementing the framework is to estimate the underlying true prior \( G \) with data \( \{(\hat{\Delta}_i, s_i)\} \) from past experiments. A straightforward approach would be to estimate \( G \) within a parametric family, which has been considered in the literature: Goldberg and Johndrow (2017) and Azevedo et al. (2019) considered estimating \( G \) as a scaled, shifted \( t \)-distribution with unknown degrees of freedom; Deng (2015) modeled \( G \) as a mixture of Gaussian densities with a point mass at zero.

For completeness, in Appendix D we describe an expectation-maximization (EM) algorithm (Dempster et al., 1977) for estimating \( G \) with a mixture of \( K \) Gaussian components, where \( K \) is pre-specified or selected in some manner. However, we should emphasize that estimating \( G \) within a parametric family is inevitably subject to model misspecification, which motivates the development of nonparametric methods that make much weaker assumptions on the prior. It should be noted that fitting a parametric prior under additive noise is essentially fitting a latent variable model, and hence the
log-likelihood is usually non-convex. The EM algorithm is often used, but it only converges to a local maximum, can have an extremely slow rate of convergence (when $K$ is over-specified) (Dwivedi et al., 2018), and can be numerically unstable as well (Archambeau et al., 2003). In the next Section, we propose a nonparametric estimator based on convex optimization, which is free from these issues.

4. Nonparametric spectral estimation. In this Section, we develop a nonparametric estimation strategy based on a spectral characterization of the problem. Before describing the characterization, we first review empirical Bayes formulae that relate posterior cumulants to the derivatives of marginal densities.

4.1. Tweedie’s formula. Certain posterior quantities are of special interest to a decision maker. For example, as we saw from Eq. (8), the Bayes optimal decision rule for launching was determined by the posterior mean. Under our modeling assumption $\Delta \sim G$, $\hat{\Delta} \mid \Delta \sim \mathcal{N}(\Delta, s^2)$, Robbins (1956) presented the following formula due to Maurice Tweedie

$$E[\Delta \mid \hat{\Delta}] = \hat{\Delta} + s^2 \ell_s'(\hat{\Delta}),$$

where $\ell_s(\hat{\Delta}) := \log p_s(\hat{\Delta})$ is the logarithmic marginal density for the observed effect under a given scale $s$. The two terms on the RHS are, respectively, the unbiased estimate of $\Delta$ and a Bayesian shrinkage term that pulls the estimate towards a marginal mode ($\ell_s'(\hat{\Delta}) > 0$ if $\hat{\Delta}$ is on the left of a mode). Moreover, the formula only depends on the prior $G$ implicitly through the score (with respect to location) of the marginal density. As a result, one can estimate the posterior mean by directly estimating the marginal density, which circumvents estimating $G$ in the first place — this strategy is called “$f$-modeling” by Efron (2014), as opposed to “$g$-modeling” that starts with estimating the prior.

Robbins generalized Equation (11) to exponential families.

**Lemma 1 (Robbins (1956)).** Suppose $\eta \sim G$ with density $g$ and

$$X \mid \eta \sim f_\eta(x) = e^{\eta x - \psi(\eta)} f_0(x),$$

where $f_0(x)$ is the conditional density $f_\eta(x)$ when $\eta = 0$, and $\psi(\eta)$ the cumulant generating function that ensures normalization. Let $f(x) = \int f_\eta(x) g(\eta) \, d\eta$ be the marginal density for $X$, and define $\lambda(x) = \log(f(x)/f_0(x))$. Then for $k = 1, 2, \ldots$, the $k$-th posterior cumulant of $\eta$ given $X$ is the $k$-th derivative of $\lambda(x)$ evaluated at $X$. 
Specifically for $k = 1, 2$, it follows that

\begin{equation}
\mathbb{E}[\eta \mid X] = \lambda'(X), \quad \text{var}[\eta \mid X] = \lambda''(X).
\end{equation}

We specialize this result to the Gaussian case.

**Lemma 2 (Tweedie’s formulae).** Under the additive Gaussian noise model Eq. (4), we have

\begin{equation}
\mathbb{E}_s[\Delta \mid \hat{\Delta}] = \hat{\Delta} + s^2 \ell_s'(\hat{\Delta}),
\end{equation}

and

\begin{equation}
\text{var}_s[\Delta \mid \hat{\Delta}] = s^2 \left(1 + s^2 \ell_s''(\hat{\Delta})\right).
\end{equation}

**Proof.** In the context of Lemma 1, let $\eta = \Delta/s^2$. $G$ in the lemma becomes our “$G$” scaled by $s^{-2}$. The conditional density for $\hat{\Delta} \mid \eta$ can be expressed as

\[ f_\eta(\hat{\Delta}) = \phi_s(\hat{\Delta} - \Delta) = \exp(\eta \hat{\Delta} - \eta^2 s^2/2) f_0(\hat{\Delta}), \quad f_0(\hat{\Delta}) = \phi_s(\hat{\Delta}). \]

Therefore,

\[ \lambda(\hat{\Delta}) = \log f(\hat{\Delta}) - \log f_0(\hat{\Delta}) = \ell_s(\hat{\Delta}) + \hat{\Delta}^2/(2s^2) + \text{const}, \]

where $\ell_s(\hat{\Delta}) = \log p_s(\hat{\Delta})$ from Eq. (6). It follows from Eq. (10) that

\[ \mathbb{E}[\Delta \mid \hat{\Delta}] = s^2 \mathbb{E}[\eta \mid \hat{\Delta}] = s^2 \lambda'(\hat{\Delta}) = \hat{\Delta} + s^2 \ell_s(\hat{\Delta}), \]

and

\[ \text{var}[\Delta \mid \hat{\Delta}] = \text{var}[s^2 \eta \mid \hat{\Delta}] = s^4 \lambda''(\hat{\Delta}) = s^2 \left(1 + s^2 \ell_s''(\hat{\Delta})\right). \]

\[ \square \]

Tweedie’s formulae suggest that the family of marginal densities \( \{ p_s(\hat{\Delta}) : s \geq 0 \} \) is a natural estimand, from which we can obtain estimates for the posterior mean and variance. This $f$-modeling (marginal-modeling) strategy is adopted by Efron (2003, 2011, 2014), where he modeled $\log p(x)$ as a linear function of polynomials in $x$, fitted with a simple Poisson regression via Lindsey’s method (Efron and Tibshirani, 1996). However, his strategy is not applicable here since we have a density $p_s$ to be estimated for every $s \geq 0$. The heterogeneity in the likelihood poses a new challenge to $f$-modeling, which, to our knowledge, has not been addressed previously. Besides, as noted by Wager (2014), Efron’s method does not constrain the modeled marginal densities to those representable under Eq. (4), and hence is subject to misspecification and inefficiency.
4.2. Characterization via the heat equation. Estimating the density family \( \{p_s : s \geq 0\} \) subject to our modeling assumption is equivalent to estimating the prior, since the prior density \( g = p_0 \). In the literature, recovering \( G \) from observations with additive noise, with known or unknown heterogenous scales has been considered by Delaigle and Meister (2008), who proposed a deconvolution kernel estimate based on inverting an empirical characteristic function (Carroll and Hall, 1988; Stefanski and Carroll, 1990; Fan, 1991a,b). In addition to the usual problem of bandwidth selection, inverting an empirical estimate is not the most efficient. To improve efficiency, we consider estimating \( \{p_s : s \geq 0\} \) based on maximum likelihood. In the following, we first answer a prerequisite question — what is the space of all density families representable under the additive Gaussian noise model?

For ease of exposition, we make a change of variable \( s = \sqrt{t} \) for \( t \geq 0 \), and reindex \( p_t := p_{s = \sqrt{t}} \) whenever the letter \( t \) is used. The modeling assumption poses non-trivial constraints on the density family \( \{p_t : t \geq 0\} \). For example, the first two moments are related by

\[
E_t \Delta = \text{const}, \quad \text{var}_t \Delta = \text{var} \Delta + t.
\]

More generally, we have the following characterization.

**Theorem 2.** The density family \( \{p_t : t \geq 0\} \) on \( \mathbb{R} \) can be represented as

\[
p_t(x) = \int \phi_{\sqrt{t}}(x - u)g(u) \, du
\]

for a probability density \( g \) on \( \mathbb{R} \) if and only if

\[
\frac{\partial}{\partial t} p_t(x) = \frac{1}{2} \frac{\partial^2}{\partial x^2} p_t(x), \quad t \geq 0, \ x \in \mathbb{R},
\]

and \( p_0 = g \).

Equation (14) is the heat equation with thermal diffusivity constant \( 1/2 \), which describes how heat diffuses on \( \mathbb{R} \) as time \( t \) elapses from zero; see Fig. 1 for an example. As a result, \( p_t(x) \) obeys the maximum principle (Evans, 1998, page 54), which says that the maximum of \( p_t(x) \) within any interval will not exceed the maximum value previously encountered; and as a consequence, the number of local maxima in \( p_t(x) \) is non-increasing in \( t \). Eq. (13) is the solution to the heat equation with initial condition \( p_0 = g \). The solution is based on convolving the initial condition with a Gaussian kernel with variance \( t \), which is the Green function (also called the fundamental solution) to the heat equation, i.e., the solution when the initial condition is a delta function.
proof. We need to show that Eq. (13) is the unique solution to Eq. (14) with initial condition $p_0 = g$. We first verify that it is a solution. Fix $u \in \mathbb{R}$, consider $\varphi_u(x, t) := \phi_{\sqrt{t}}(x - u)$. We check that $\varphi_u(x, t)$ satisfies Eq. (14). We have

\[
\frac{\partial}{\partial t} \varphi_u(x, t) = \frac{1}{2} \varphi_u(x, t) \left\{ \left( \frac{x - u}{t} \right)^2 - \frac{1}{t} \right\},
\]

\[
\frac{\partial}{\partial x} \varphi_u(x, t) = -\varphi_u(x, t) \left( \frac{x - u}{t} \right),
\]

and it follows that

\[
\frac{\partial^2}{\partial x^2} \varphi_u(x, t) = \varphi_u(x, t) \left\{ \left( \frac{x - u}{t} \right)^2 - \frac{1}{t} \right\} = 2 \frac{\partial}{\partial t} \varphi_u(x, t).
\]

Then by linearity, $p_t(x) = \int \varphi_u(x, t) g(u) \, du$ also satisfies Eq. (14). Also, $p_0(x) = \lim_{t \to 0^+} p_t(x) = g(x)$. Further, by Evans (1998, Theorem 7, Sec. 2.3) $p_t(x) = \int \varphi_u(x, t) g(u) \, du$ is the unique solution such that $p_t(x)$ is a density for every $t \geq 0$. \qed

The general solution to the heat equation Eq. (14) can be characterized with Fourier transforms; see Appendix B for details. However, since the Fourier transform is infinite dimensional, representing the transform is as difficult as representing the density $g$ itself. To proceed, we need to truncate the domain from $\mathbb{R}$ to a compact interval, upon which the Fourier transform becomes a Fourier series.

We remark that the connection between density estimation and the heat equation is also made by Botev et al. (2010) and previously by Chaudhuri...
and Marron (2000). Contrary to our case, where $t$ corresponds to the variance of an additive noise, their consideration of $t$ is to optimize the amount of smoothing applied to the empirical measure for constructing a density estimator.

4.3. Toric formulation. For tractability, we consider Fourier series representations, which are only associated with periodic functions with a fixed period. By Theorem 2, $p_0$ equals the prior density $g$.

**Assumption 2.** The prior $G$ has a uniformly continuous density $p_0(x)$ with respect to Lebesgue, supported on a subset of $[-L, L]$ for $0 < L < \infty$.

Recall that $p_0(x)$ is uniformly continuous if for every $\varepsilon > 0$, there exists $\delta > 0$ such that for all $x, y \in [-L, L]$ such that $|x - y| < \delta$, we have $|p_0(x) - p_0(y)| < \varepsilon$. Uniform continuity is a weak smoothness condition, which is implied by Lipschitz or Hölder continuity, and some smoothness assumption is usually required to establish consistency. Compact support is assumed for technical convenience (e.g., Stefanski and Carroll (1990) and Meister (2007)), although it can be relaxed by letting $L$ grow with $n$. The domain is assumed to be symmetric about zero, which can be ensured by translation. Since we work with Fourier series, let us introduce $\tilde{p}_0$ as the periodicized version of $p_0$:

\begin{align}
(15) \quad \tilde{p}_0(x) &= p_0(x) \text{ for } x \in [-L, L], \\
&\quad \tilde{p}_0(x + 2L) = p_0(x) \text{ for all } x \in \mathbb{R}.
\end{align}

Hence, any interval of length $2L$ is a torus, and for convenience we will mostly use the torus $[-L, L]$. Next, we introduce an assumption that reduces the data generating process from $\mathbb{R}$ to the torus.

**Assumption 3.** The data is generated from $x_i \sim p_{t_i}$ independently, where $p_t$ is a probability density on $[-L, L]$

\begin{align}
(16) \quad p_t(x) := \int_{-\infty}^{\infty} \tilde{p}_0(u) \phi_{\sqrt{t}}(x - u) \, du.
\end{align}

This a simplifying assumption on the data generating mechanism, such that a heat diffusion on $\mathbb{R}$ is reduced to a heat diffusion on a compact domain with periodic boundary conditions. Note that the true data generating mechanism is $x_i \sim p^*_t$, with the following density on $\mathbb{R}$

\begin{align}
(17) \quad p^*_t(x) = \int_{-L}^{L} p_0(u) \phi_{\sqrt{t}}(x - u) \, du.
\end{align}
Notice that \( p_t \) and \( p_t^* \) differ in terms of their domain of integration. It is easy to check that \( p_t(x) \geq 0 \), has period \( 2L \), and integrates to one on \([-L, L]\):

\[
\int_{-L}^{L} p_t(x) \, dx = \int_{-L}^{L} \left\{ \int_{-\infty}^{+\infty} \bar{p}_0(u) \phi_t(x - u) \, du \right\} \, dx
= \int_{-L}^{L} \left\{ \int_{-\infty}^{+\infty} \bar{p}_0(x - u) \phi_t(u) \, du \right\} \, dx
= \int_{-\infty}^{+\infty} \left( \int_{-L}^{L} \bar{p}_0(x - u) \, dx \right) \phi_t(u) \, du = 1.
\]

Further, the difference between \( p_t \) and \( p_t^* \) becomes negligible with a large enough \( L \). Let \( t_{\text{max}} \) be an upper bound on the variance \( t \).

**Lemma 3.** Given \( t_{\text{max}} < \infty \), for all \( x \in [-L, L] \) and \( t \in [0, t_{\text{max}}] \) it holds that

\[
0 < p_t(x) - p_t^*(x) < \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt{t_{\text{max}}} \{ \exp(2L^2/t_{\text{max}}) - 1 \}}.
\]

**Proof.** By breaking the integral in Eq. (16) into intervals of length \( 2L \), we have

\[
\begin{align*}
p_t(x) &= \sum_{k=-\infty}^{+\infty} \int_{-L}^{L} \bar{p}_0(u - 2kL) \phi_t(x - u - 2kL) \, du \\
&= \sum_{k=-\infty}^{+\infty} \int_{-L}^{L} p_0(u) \phi_t(x - u - 2kL) \, du \\
&= p_t^*(x) + \int_{-L}^{L} p_0(u) \left\{ \sum_{k\neq 0} \frac{1}{\sqrt{t}} \phi \left( \frac{x - u - 2kL}{\sqrt{t}} \right) \right\} \, du,
\end{align*}
\]

where we used the fact that \( \bar{p}_0(u) \) has period \( 2L \). Define \( H_r(x) := \sum_{k \neq 0} \phi(x - kr) \). Clearly for all \( x \in \mathbb{R} \), we have

\[
H_r(x) \leq H_r(0) = 2 \sum_{k=1}^{\infty} \phi(kr) = \sqrt{\frac{2}{\pi}} \sum_{k=1}^{\infty} \exp(-k^2r^2/2)
< \sqrt{\frac{2}{\pi}} \sum_{k=1}^{\infty} \exp(-kr^2/2)
= \sqrt{\frac{2}{\pi}} \frac{1}{\exp(r^2/2) - 1}.
\]
Applying this to Eq. (19) with \( r = 2L/\sqrt{t} \) and using \( \int_{-L}^{L} p_0(u) \, du = 1 \), we have
\[
0 < p_t(x) - p^*_t(x) < \frac{1}{\sqrt{\pi \sqrt{t} \left( \exp(2L^2/t) - 1 \right)}}.
\]

Let \( \gamma(t) := \sqrt{t \left( \exp(2L^2/t) - 1 \right)} \). We claim that \( \gamma(t) \) is decreasing in \( t \geq 0 \).

To see this, note that \( \gamma'(t) = \frac{2}{\sqrt{t}} \left( \exp(2L^2/t) - 1 \right) \). By rearranging, \( \gamma'(t) < 0 \) iff \( e^{-2L^2/t} > 1 - 4L^2/t \), which is true by \( e^{-2L^2/t} \geq 1 - 2L^2/t \).

Therefore, for \( t \in [0, t_{\text{max}}] \) the RHS of the previous display is lower bounded by its value at \( t_{\text{max}} \).

By Lemma 3, one can always use a large enough \( L \) such that Assumption 3 approximately holds for the data at hand. In the following, we will work under Assumptions 1 to 3. Furthermore, since a rescaling \( x \leftarrow \pi x/L \) can be applied, without loss of generality, we suppose \( L = \pi \) for convenience.

Under Assumptions 2 and 3, Theorem 2 still holds if we replace the domain \( \mathbb{R} \) with the torus \([0, \pi] \) (or any torus of length \( 2\pi \)).

**Lemma 4.** The set of solutions, in the form of periodic functions in \( x \) with period \( 2\pi \), to the heat equation Eq. (14) with initial condition \( \bar{p}_0 \), has the following trigonometric series representation
\[
(20) \quad p_t(x) \sim \sum_{k=-\infty}^{\infty} c_k e^{-k^2 t/2} e^{ikx}, \quad c_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} p_0(x) e^{-ikx} \, dx.
\]

The symbol \( \sim \) means “associated with”, since one needs to specify in what sense the series converges to the function \( p_t(x) \). For example, a usual notion is the convergence in \( L^2 \); besides, in a pointwise sense, if \( p_0(x) \) is continuous and the series converges uniformly in \( x \), then \( \sim \) can be replaced by “=”; see Zygmund (2002, Theorem 6.3, Chapter I).

\( \{c_k\} \) are complex Fourier coefficients of \( p_0(x) \) satisfying complex conjugacy \( c_{-k} = \overline{c_k} \), which holds since \( p_0(x) \) is real. With \( a_k := 2 \text{Re} \, c_k \) and \( b_k := -2 \text{Im} \, c_k \), the series in the previous display can be rewritten as
\[
(21) \quad p_t(x) \sim \frac{1}{2} a_0 + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx) e^{-k^2 t/2}.
\]

**4.4. Modeling with trigonometric polynomials.** Now we consider modeling \( p_0(x) \), and hence \( p_t(x) \) by Lemma 4, in terms of a partial sum of trigonometric polynomials. A trigonometric polynomial of order \( N \) takes the form
for \((2N + 1)\) complex Fourier coefficients \(\{c_k\}\) satisfying \(c_{-k} = \overline{c_k}\). In fact, \(\{c_k\}\) are the Fourier coefficients associated with function \(S_N(x)\), and are hence uniquely determined from \(S_N(x)\).

Let us fix an order \(N\). Suppose \(p_0(x) = S_N(x)\), by Lemma 4, the entire density family remains within trigonometric polynomials with order \(N\), given by the closed form expression

\[
S_N(x; t) := \sum_{k=-N}^{N} c_k e^{-k^2 t / 2} e^{ikx}, \quad t \geq 0,
\]

where \(S_N(x; 0) = S_N(x)\). In addition to \(c_{-k} = \overline{c_k}\) for \(k = 1, \ldots, N\), the coefficients are further subject to an equality constraint due to normalization

\[
1 = \int_{-\pi}^{\pi} S_N(x) \, dx = (2\pi)c_0.
\]

Taking the normalization constraint into account, \(S_N\) has \(2N\) degrees of freedom. \(S_N\) can also be uniquely parametrized by \((2N + 1)\) interpolating nodes \(\{(x_\nu, f_\nu) : \nu = 0, \pm 1, \ldots, \pm N\}\) such that \(S_N(x_\nu) = f_\nu\) for every \(\nu\). In particular, we focus on equidistant nodes

\[
x_\nu = \frac{2\pi \nu}{2N + 1}, \quad \nu = 0, \pm 1, \ldots, \pm N
\]
on the torus \([-\pi, \pi]\). Given any real-valued \(\{f_\nu\}\), there is a unique \(S_N(x)\) that passes through every \((x_\nu, f_\nu)\), given by

\[
S_N(x) = \frac{1}{2N + 1} \sum_{\nu=-N}^{N} f_\nu D_N(x - x_\nu),
\]

where \(D_N(u)\) is the Dirichlet kernel of order \(N\)

\[
D_N(u) = \sum_{k=-N}^{N} e^{iku} = 1 + 2 \sum_{k=1}^{N} \cos ku = \frac{\sin((N + 1/2)u)}{\sin u / 2},
\]

with \(D_0(u) \equiv 1\). From these two expressions, one can easily check that \(S_N(x)\) is an order-\(N\) trigonometric polynomial. To see that \(S_N(x)\) passes through
every interpolating point, observe that $D_N(0) = 2N + 1$ and $D_N(x_\nu) = 0$ for $\nu \neq 0$. By comparing the trigonometric terms between Eq. (26) and Eq. (22), the Fourier coefficients are recovered as

$$c_k = \frac{1}{2N + 1} \sum_{\nu = -N}^{N} f_\nu e^{-\frac{2\pi i}{2N + 1} k \nu}, \quad k = 0, \pm 1, \ldots, \pm N.$$  

In particular, the normalization constraint Eq. (24) translates to

$$\frac{1}{2\pi} = c_0 = \frac{1}{2N + 1} \sum_{\nu = -N}^{N} f_\nu.$$  

The full-rank linear transform Eq. (28) is known as the discrete Fourier transform (DFT), which we will denote with shorthand $\{c_k\} = \text{DFT}_N(\{f_\nu\})$. DFT$_N$ and its inverse transform can be computed in $O((2N+1)\log(2N+1))$ time with fast Fourier transform (FFT) algorithms. To sum up, an order-$N$ trigonometric polynomial model of the density family $\{S_N(x; t) : t \geq 0\}$ can be parametrized by $(2N+1)$ real-valued $\{f_\nu\}$ such that $\frac{2\pi}{2N+1} \sum_{\nu = -N}^{N} f_\nu = 1$.

We remark that among other orthogonal polynomials, the trigonometric polynomials are the most natural choice for our problem. They are the eigenfunctions of the heat equation Eq. (14) and provide an orthogonal basis for representing $p_t(x)$ in closed form. Estimating a density with trigonometric polynomials/series was proposed by Kronmal and Tarter (1968) and has since been extensively studied; see also Wahba (1975); Walter and Blum (1979); Hall (1981, 1986). The estimator considered by these authors is primarily a Fourier partial sum sequence with $\{\hat{c}_k : k = \pm 1, \ldots, \pm N\}$ unbiasedly estimated by the sample average of the corresponding $e^{ikx}$. The performance of the estimator, as $N$ grows with $n$ properly, is analyzed in terms of the mean integrated square error relative to the true density. In the following, we show that maximum likelihood estimation can be performed on $S_N$ to improve efficiency.

4.4.1. Non-negativity. An obvious drawback of this type of model is that an estimated $S_N(x)$ is not guaranteed to be non-negative for a finite $N$, even if one places constraints $f_k \geq 0$. In the literature, the non-negativity constraint is sometimes relaxed to obtain a faster rate of convergence (Terrell and Scott, 1980), or dismissed by arguing that the estimate will stay positive “most of the time” (Kronmal and Tarter, 1968). Post-processing of an estimator to ensure non-negativity is also proposed; see Kronmal and Tarter (1968); Hall (1981); Gajek (1986).
In the context of ours, we find this issue particularly disturbing: (i) a negative value in Eq. (23) yields an invalid objective for maximum-likelihood estimation; (ii) $S_N(x; t)$ can have up to $2N$ zeros in $[-\pi, \pi]$ (Zygmund, 2002, Theorem 10.1.7), and the posterior mean, by Tweedie’s formula Eq. (11), will shoot to infinity at these zeros because $\ell'(x) = S'_N(x; t)/S_N(x; t)$; (iii) $S_N(\Delta; t)$ is the normalizing constant, when computing the posterior density of the true effect is desired. In the following, we present a simple parametrization that ensures a bona fide density.

Consider the Cesàro sum of trigonometric polynomials

\begin{equation}
C_N(x) := \frac{S_0(x) + S_1(x) + \cdots + S_N(x)}{N+1},
\end{equation}

which is the arithmetic mean of the first $N+1$ partial sums given by Eq. (22) ($S_0(x) \equiv 1/2a_0$). The Cesàro sum $C_N(x)$ has stronger convergence guarantee compared to the symmetric partial sum $S_N(x)$. Feké’s theorem (Zygmund, 2002, Section 3.3) states that as $N \to \infty$, $C_N(x)$ converges uniformly to $p_0(x)$ if $p_0$ is continuous. By definition, $C_N(x)$ is also a trigonometric polynomial of order $N$

\begin{equation}
C_N(x) = \sum_{k=-N}^{N} \left(1 - \frac{|k|}{N+1}\right) c_k e^{ikx},
\end{equation}

with complex Fourier coefficients reweighted by $1 - |k|/(N+1)$ accordingly. Similarly, let $C_N(x; t)$ be the arithmetic mean of $\{S_m(x; t) : m = 0, \ldots, N\}$ given by Eq. (23). By linearity, $C_N(x; t)$ satisfies the heat equation Eq. (14).

**Definition 1.** The Fejér kernel is

\begin{equation}
K_N(u) := \frac{1}{N+1} \sum_{k=0}^{N} D_k(u),
\end{equation}

where $D_k(\cdot)$ is the Dirichlet kernel given by Eq. (27).

**Lemma 5** (Zygmund (2002, Sec. 3, Chapter III)). The Fejér kernel has the following properties.

(a) It holds that

\begin{equation}
K_N(u) = \frac{1}{N+1} \left(\frac{\sin (N+1/2)u}{\sin u/2}\right)^2,
\end{equation}

where in particular $K_N(0) := \lim_{u \to 0} K_N(u) = N + 1$. 

(b) $K_N(u) \geq 0$.
(c) $\int_{-\pi}^{\pi} K_N(u) \, dx = 2\pi$.
(d) For $u \in [-\pi, \pi]$, $K_N(u)$ vanishes iff $u = \frac{2\pi m}{N+1}$ for $m = \pm 1, \ldots, \pm \lfloor \frac{N+1}{2} \rfloor$.

**Lemma 6.** With $\{(x_\nu, f_\nu)\}_{\nu = -N}^N$ given by Eqs. (25) and (26), $C_N(x)$ in Eq. (30) can be expressed as

\[ C_N(x) = \frac{1}{2N+1} \sum_{\nu = -N}^N f_\nu K_N(x - x_\nu). \]

**Proof.** Using $S_N(x) = \sum_{k=-N}^N c_k e^{-ikx}$ with $\{c_k\}$ given by Eq. (28), $C_N(x)$ in Eq. (30) can be expressed as

\[
C_N(x) = \frac{1}{2N+1} \sum_{k=-N}^N \left( 1 - \frac{|k|}{N+1} \right) \sum_{\nu = -N}^N f_\nu e^{\frac{2\pi k}{2N+1} i k x}
\]

\[
= \frac{1}{2N+1} \sum_{\nu = -N}^N f_\nu \left\{ 1 + \sum_{k=1}^N \left( 1 - \frac{k}{N+1} \right) \left( e^{ik(x-x_\nu)} + e^{-ik(x-x_\nu)} \right) \right\}
\]

\[
= \frac{1}{2N+1} \sum_{\nu = -N}^N f_\nu \left\{ 1 + 2 \sum_{k=1}^N \left( 1 - \frac{k}{N+1} \right) \cos k(x - x_\nu) \right\},
\]

where $x_\nu = \frac{2\pi \nu}{2N+1}$. By Definition 1, we also have

\[
K_N(u) = \frac{1}{N+1} \sum_{k=0}^N D_k(u) = \frac{1}{N+1} \left( N + 2 \sum_{k=1}^N (N + 1 - k) \cos ku \right),
\]

where we used Eq. (27) for $D_k(u)$. The lemma is proven by comparing the previous two displays.

**Theorem 3.** Suppose $S_N(x)$ is parametrized by $\{f_\nu\}$ satisfying $f_\nu \geq 0$ and $\frac{2\pi}{2N+1} \sum_{\nu = -N}^N f_\nu = 1$, then $C_N(x)$ in Eq. (30) is a valid density on $[-\pi, \pi]$. Further, if there exist $\nu \neq \nu'$ with $f_\nu, f_{\nu'} > 0$, then $C_N(x)$ is strictly positive.

**Proof.** From (b) and (c) of Lemma 5, we know $\frac{1}{2\pi} K_N(u)$ is a density on $[-\pi, \pi]$. It follows from Lemma 6 that $C_N(x)$ is a mixture of $\{K_N(u - x_\nu)\}$ with corresponding weights $\{\frac{2\pi}{2N+1} f_\nu\}$. Given $f_\nu \geq 0$ and $\frac{2\pi}{2N+1} \sum_{\nu = -N}^N f_\nu = 1$, $C_N(x)$ is a density on $[-\pi, \pi]$. Further, suppose $f_\nu, f_{\nu'} > 0$ for $\nu \neq \nu'$. We prove by contradiction that $C_N(x)$ is positive. Suppose $C_N(y) = 0$. By
Lemma 5(b), $K_N(y-x_\nu)$ and $K_N(y-x_{\nu'})$ must both vanish. By Lemma 5(d), we have $y-x_\nu = \frac{2\pi m}{N+1}$ and $y-x_{\nu'} = \frac{2\pi m'}{N+1}$ for some non-zero integers $m, m'$. By taking the difference on Eq. (25), we have $y-x_\nu = \frac{2\pi m}{N+1}$ and $y-x_{\nu'} = \frac{2\pi m'}{N+1}$ for some non-zero integers $m, m'$. We observe that $N + 1$ and $2N + 1$ are co-prime. Given that $\nu' \neq \nu$, the only possibility is that $\nu' - \nu$ cancels with $2N + 1$. However, $|\nu' - \nu| \leq 2N$. By contradiction we conclude that $C_N(x)$ stays positive.

**Remark 1.** $C_N(x)$ is a generalized form of Jackson polynomial $J_{N,2N+1}(x)$ based on “nodes” $\{(x_\nu, f_\nu)\}$; see Zygmund (2002, Sec. 6, Chapter X). However, unlike $S_N(x)$, $C_N(x)$ does not pass through these “nodes”.

To summarize, we have shown that a valid density family can be modeled by a family of trigonometric polynomials of order $N$

$$C_N(x; t) = \sum_{k=-N}^{N} \left(1 - \frac{|k|}{N+1}\right) c_k e^{-k^2 t/2} e^{ikx}, \quad \{c_k\} = \text{DFT}_N(\{f_\nu\})$$

subject to $f_\nu \geq 0$ ($\nu = 0, \pm 1, \ldots, \pm N$) and $\frac{2\pi}{2N+1} \sum_{\nu=-N}^{N} f_\nu = 1$. This density family satisfies the heat equation in Theorem 2 with the domain replaced by the torus $[-\pi, \pi]$.

### 4.5. Maximum likelihood estimation.

We are now ready to estimate the density family with trigonometric polynomials. For the sake of efficiency, we consider maximum likelihood estimation for the model in Equation (34). Let $f := \{f_\nu\}_{\nu=-N}^{N}$ be the parameter vector and let $C_{N,f}(x; t)$ be $C_N(x; t)$ defined through $f$. The log-likelihood of the dataset is

$$\ell_n(f) = \sum_{i=1}^{n} \log C_{N,f}(\hat{\Delta}_i; s_i^2).$$

Since (i) $-\log(\cdot)$ is convex, (ii) $C_{N,f}(x; t)$ is linear in $\{c_k\}$, and (iii) $\{c_k\} = \text{DFT}_N(f)$ is linear and full-rank, indeed $(-\ell_n)$ is convex in $f$. Let $S_{2N} \subset \mathbb{R}^{2N+1}$ denote the $2N$-dimensional unit simplex. The MLE can thus be obtained from the following convex optimization

$$\min \left\{ -\sum_{i=1}^{n} \log C_{N,f}(\hat{\Delta}_i; s_i^2) : \kappa_N f \in S_{2N} \right\},$$

where $\kappa_N := 2\pi/(2N + 1)$ is a constant.
4.5.1. Accelerated projected gradient. The log-likelihood is continuously differentiable in \( f \). The constrained convex optimization can be solved by the more general proximal gradient method, formulated as

\[
\min_{f \in \mathbb{R}^{2N+1}} \ell_n(f) + \delta_{\kappa_N^{-1}S_{2N}} (f),
\]

where the indicator \( \delta_A(x) \) takes \(+\infty\) when \( x \notin A \) and zero otherwise.

We use the Fast Iterative-Shrinkage Thresholding Algorithm (FISTA) of Beck and Teboulle (2009), which solves unconstrained convex optimization of the form \( \min_x h(x) + g(x) \) for a smooth convex function \( h \) and a non-smooth convex function \( g \). In each iteration, the algorithm executes Nesterov’s accelerated gradient step with \( \nabla h \), followed by a proximal operator acting on the updated coordinate. In our case, \( h = \ell_n \) and \( g = \delta_{\kappa_N^{-1}S_{2N}} \), and the proximal operator becomes a projection.

**Algorithm 1:** Accelerated Projected Gradient for MLE

**Data:** \((s_i, \hat{\Delta}_i)_{i=1}^n\)

**Input:** order of trigonometric polynomial \( N \), domain half-length \( L \), step size \( \gamma_t > 0 \)

1. \( x_0 \leftarrow \text{median}(\{\hat{\Delta}_i\}) \);
2. \( \hat{\Delta}_i \leftarrow (\hat{\Delta}_i - x_0)\pi/L, s_i \leftarrow s_i\pi/L \) for all \( i \);
3. \( f^{(0)} \leftarrow f^{(-1)} \leftarrow (1, \ldots, 1)^\top/\kappa_N \);
4. For \( m = 1, 2, \ldots \) until convergence do

5. \( y \leftarrow f^{(m-1)} + \frac{m-2}{m+1}(f^{(m-1)} - f^{(m-2)}) \);
6. \( f^{(m)} \leftarrow (\kappa_N)^{-1} \text{Proj}_{S_{2N}} (\kappa_N \{y + \gamma_m \nabla \ell_n(y)\}) \);

**Output:** MLE \( \hat{f} = f^{(m)} \)

The step-size should be either set as a constant that is no greater than the inverse of a Lipschitz constant of \( \ell_n \), or determined by a line search; see Beck and Teboulle (2009) for more details. The resulting algorithm achieves \( \ell_n^* - \ell_n(f^{(m)}) \leq O(1/m^2) \), where \( \ell_n^* \) denotes the maximum of \( \ell_n \). The iterates \( \ell_n(f^{(m)}) \) are not monotonic in general, and a simple restarting trick from O’Donoghue and Candes (2015) can be employed to suppress oscillation. We implemented the algorithm with automatic differentiation from Autograd (Maclaurin et al., 2015) for computing \( \nabla \ell_n(f) \), which is able to differentiate through the FFT. The log-likelihood is can be efficiently evaluated with matrix-vector multiplications.

The operator \( \text{Proj}_{S_{2N}} (\cdot) \) in Algorithm 1 is the Euclidean projection of a vector onto the unit simplex. We implement it with the following algorithm from Duchi et al. (2008); see also Wang and Carreira-Perpiñán (2013) for
an exposition.

**Algorithm 2:** Projection of a vector onto the unit simplex

Input: $y \in \mathbb{R}^N$

1. Order $y$ as $y^{(1)} \geq \cdots \geq y^{(N)}$;
2. $\rho \leftarrow \max \left\{ 1 \leq j \leq N : y^{(j)} + \frac{1}{j} (1 - \sum_{i=1}^{j} y^{(i)}) > 0 \right\}$;
3. $\lambda \leftarrow \frac{(1 - \sum_{i=1}^{\rho} y^{(i)})}{\rho}$;

Output: $x$ with $x_i = \max \{ y^{(i)} + \lambda, 0 \}$ for $i = 1, \ldots, N$.

We remark that Wager (2014) also used DFT for a related problem, which, in our terms, is to estimate the marginal density $p_{s=1}$ when $s_i \equiv 1$ in the dataset (no heterogeneity in $s$). His approach is geometric, namely to find the $L^2$ projection of the empirical measure $P_n$ onto the space of possible marginal densities under $t = 1$. By Parseval’s identity, the $L^2$ distance becomes the $\ell_2$ norm in the space of Fourier coefficients. Therefore, the projection can formulated as a quadratic program that can be efficiently solved. Besides, Wager (2014) also uses simplex constraints on node points, but its effect is only approximate since his parametrization does not guarantee $\hat{p}_1$ to be non-negative. In contrast to our approach, Wager (2014) does not consider heterogeneity in the error scale, and his estimator is not an MLE.

4.6. **Model selection.** In practice, the order $N$ of trigonometric polynomial $C_N$ should be chosen empirically. This is a classical bias-variance trade-off: $N$ being too small introduces bias from missing high-frequency components; $N$ being too big introduces spurious oscillations in the estimate. This phenomenon is illustrated by simulation studies in Section 5. In the following, we discuss two criteria for model selection: (i) the predicted log-likelihood, which is typically used for evaluating probabilistic models, and (ii) a square loss that is targeted at the accuracy of the estimated posterior mean, which exploits Hyvärinen’s (2005) score matching technique.

4.6.1. **Predicted log-likelihood.** One model selection criterion common to probabilistic modeling is the predicted log-likelihood on the held-out data.

**Lemma 7.** Fix any $s \geq 0$, $g$ is uniquely identifiable (up to Lebesgue almost everywhere) from the marginal $p_s(\cdot) = \int \phi_s(\cdot - u)g(u) \, du$.

**Proof.** By Eq. (43), the characteristic function of $G$ is determined by $\mathcal{F}(g)(\xi) = e^{\frac{i}{2} \xi^2 s^2} \mathcal{F}(p_s)(\xi)$, where $\mathcal{F}(p_s)$ is the characteristic function of $p_s$. $g$ is uniquely determined (up to Lebesgue almost everywhere) by $\mathcal{F}^{-1} \mathcal{F}(g)$. \qed
Suppose \( p_s \) and \( \hat{p}_s \) are the marginal densities under \( G \) and \( \hat{G} \) respectively. It follows that the Kullback-Leibler divergence

\[
0 \leq D_{\text{KL}}(p_s \| \hat{p}_s) = \int p_s(x) \log \frac{p_s(x)}{\hat{p}_s(x)} \, dx = C_G - \mathbb{E}_{p_s} \log \hat{p}_s(\Delta),
\]

where the equality holds if and only if \( G = \hat{G} \), the constant \( C_G \) does not depend on \( \hat{G} \). This motivates model selection with the averaged predictive log-likelihood

\begin{equation}
\mathbb{E}_{s \sim Q} \mathbb{E}_{p_s} \log \hat{p}_s(\Delta^s) = \frac{1}{n^*} \sum_{i=1}^{n^*} \log \hat{p}_{s^* i}(\Delta^s_i) + O_p(1/\sqrt{n^*}),
\end{equation}

which is uniquely maximized when \( \hat{G} =_d G \). Samples \((\Delta^s_i, s^*_i)\) come from a held-out dataset of size \( n^* \). \( Q \) is either the population distribution or simply an empirical distribution for \( s \). A model with a higher predictive log-likelihood is preferred.

4.6.2. Score-matching for the posterior mean. As we have seen in Section 2.3.2, the posterior mean is crucial to deciding whether one should launch a change. We consider a particular loss targeted at accurately approximating the true posterior mean based on the score matching technique. The following lemma is adapted from Hyvärinen (2005).

**Lemma 8.** Suppose \( p, \hat{p} \) are periodic functions with period \( 2\pi \) and are densities on \([-\pi, \pi]\). Suppose \( p \) is continuously differentiable and \( \hat{p} \) is twice continuously differentiable. Let \( \ell = \log p \) and \( \hat{\ell} = \log \hat{p} \). It holds that

\begin{equation}
\mathbb{E}_p (\ell' - \hat{\ell}')^2 = \mathbb{E}_p \left\{ (\hat{\ell}')^2 + 2\hat{\ell}'' \right\} + C_p,
\end{equation}

when all the terms on the RHS are finite, where the constant \( C_p = \int_{-\pi}^{\pi} p(x)(\ell'(x))^2 \, dx \) only depends on \( p \).

**Proof.** We have

\[
\mathbb{E}_p (\ell' - \hat{\ell}')^2 = \int_{-\pi}^{\pi} \left( \frac{p'(x)}{p(x)} - \frac{\hat{p}'(x)}{\hat{p}(x)} \right)^2 p(x) \, dx
\]

\[
= \int_{-\pi}^{\pi} p(x)(\ell'(x))^2 \, dx + \int_{-\pi}^{\pi} p(x)(\hat{\ell}'(x))^2 \, dx - 2 \int_{-\pi}^{\pi} \frac{p'(x)}{\hat{p}(x)} p(x) \, dx,
\]
where via integration by parts we obtain
\[
\int_{-\pi}^{\pi} \frac{p'(x)\hat{p}(x)}{\hat{p}(x)} \, dx = \int_{-\pi}^{\pi} \frac{\hat{p}(x)}{\hat{p}(x)} \, dp(x) = p(x)\hat{\ell}'(x)|^{+\pi}_{-\pi} - \int_{-\pi}^{\pi} p(x)\hat{\ell}''(x) \, dx
\]
\[= -\int_{-\pi}^{\pi} p(x)\hat{\ell}''(x) \, dx,
\]
where the boundary difference term vanishes due to the periodicity of \(2\pi\).

It follows that
\[
E_p(\ell' - \hat{\ell}')^2 = E_p \left\{ (\hat{\ell}')^2 + 2\hat{\ell}'' \right\} + E_p(\ell'_p)^2.
\]

**Lemma 9.** Fix any \(s > 0\). Suppose \(p_0\) is the true prior and \(E_s[\Delta | \hat{\Delta}]\) is the posterior mean under \(p_0\). Suppose \(\hat{p}_0\) is the estimated prior, and \(\hat{E}_s[\Delta | \hat{\Delta}]\) is the posterior mean under \(\hat{p}_0\). Under Assumptions 1 to 3, it holds that
\[
E_{\hat{\Delta} \sim \hat{p}_s} \left( E_s[\Delta | \hat{\Delta}] - \hat{E}_s[\Delta | \hat{\Delta}] \right)^2 = s^4 E_s \left\{ (\hat{\ell}'_s(\hat{\Delta}))^2 + 2\hat{\ell}''_s(\hat{\Delta}) \right\} + C_{p_0,s},
\]
when every term on the RHS is finite. \(C_{p_0,s}\) does not depend on \(\hat{p}_0\).

**Proof.** Suppose \(\ell_s\) and \(\hat{\ell}_s\) are the logarithmic marginal densities under \(p_0\) and \(\hat{p}_0\) respectively. By Tweedie’s formula Eq. (11), the square loss in approximating the posterior mean is
\[
\left( E_s[\Delta | \hat{\Delta}] - \hat{E}_s[\Delta | \hat{\Delta}] \right)^2 = s^4 \left( \ell'_s(\hat{\Delta}) - \hat{\ell}'_s(\hat{\Delta}) \right)^2.
\]
For \(s > 0\), \(p_s(x)\) and \(\hat{p}_s(x)\) are infinitely many times differentiable by the property of Gaussian convolution. Further, under Assumptions 2 and 3, \(p_s\) and \(\hat{p}_s\) have period \(2\pi\) and are densities on the torus \([-\pi, \pi]\). Hence, we can apply Lemma 8 and obtain
\[
E_{\hat{\Delta} \sim \hat{p}_s} \left( E_s[\Delta | \hat{\Delta}] - \hat{E}_s[\Delta | \hat{\Delta}] \right)^2 = s^4 E_{p_s} \left( \ell'_s(\hat{\Delta}) - \hat{\ell}'_s(\hat{\Delta}) \right)^2
\]
\[= s^4 \left\{ (\hat{\ell}'_s(\hat{\Delta}))^2 + 2\hat{\ell}''_s(\hat{\Delta}) \right\} + C_{p_0,s},
\]
where \(C_{p_0,s} = s^4 E_{p_0}(\ell'_s(\Delta))^2\) does not depend on \(\hat{p}_0\). \(\square\)
Since the $E_s[\Delta | \hat{\Delta}]$ has the same unit as $s$, we scale the square loss at $s$ by $s^{-2}$ to make it dimensionless. Dropping the irrelevant constant, we use the following averaged loss for model selection

$$
E_{s \sim Q} E_{\Delta \sim p_s} s^{-2} \left( E_s[\Delta | \hat{\Delta}] - \hat{E}_s[\Delta | \hat{\Delta}] \right)^2 - C_{Q,p_0}
$$

(40)

$$
= E_{s \sim Q} s^2 \mathbb{E}_{p_s} \left\{ \left( \frac{s^2}{s^2} \right)^2 \left[ \frac{2s^2}{s^2} \right] \right\} + O_p(1/\sqrt{n^*}).
$$

4.7. Consistency. Let $\hat{p}_0 := \hat{C}_N(x; t = 0)$ be the MLE for the prior density from solving Eq. (36). To achieve consistency, we have to enlarge the class of densities optimized over by letting $N \to \infty$ as $n \to \infty$. This type of estimation is called Grenander’s method of sieves (Grenander, 1981). For maximum likelihood, when the class of functions (“sieves”) is dense relative to the space of true density functions, the resulting estimator is consistent under weak conditions. One condition that we require is that $t$ is upper-bounded in data.

**Assumption 4.** $t \leq t_{\text{max}}$ almost surely for some $t_{\text{max}} < \infty$.

Let $\| \hat{p} - p \|_{\infty} := \sup_x \| \hat{p}(x) - p(x) \|$.

**Theorem 4.** Under Assumptions 1 to 4, for $N \to \infty$ as $n \to \infty$, it holds that $\| \hat{p}_0 - p_0 \|_{\infty} \to_p 0$.

The consistency can be shown by verifying the generic conditions from Chen (2007, Page 5590). We delegate the proof to Appendix C. It is worth mentioning that the sieve MLE is also in general asymptotically efficient in the Fisher sense; see Shen (1997).

Despite the fact that uniform convergence of $\hat{p}_0$ need not imply the convergence of $\hat{p}_0$ as $n \to \infty$ (see Rudin (1964, Example 7.5)), by the property of Gaussian convolution, we in fact have uniform convergence of the estimated posterior mean functions.

**Corollary 2.** Given any $t > 0$, $\| \hat{p}_t - p_t \|_{\infty} \to_p 0$ and $\| \hat{p}_t' - p_t' \|_{\infty} \to_p 0$. 
Proof. With $s = \sqrt{t}$, we have

$$\|\hat{p}_t - p_t\|_\infty = \sup_x \left| \int (\hat{p}_0(u) - p_0(u)) \phi_s(x - u) \, du \right|$$

$$\leq \|\hat{p}_0 - p_0\|_\infty \sup_x \left| \int \phi_t(x - u) \, du \right| = \|\hat{p}_0 - p_0\|_\infty \to_p 0,$$

and

$$\|\hat{p}_t' - p_t'\|_\infty = \sup_x \left| \int (\hat{p}_0(u) - p_0(u)) \phi'_s(x - u) \, du \right|$$

$$\leq \|\hat{p}_0 - p_0\|_\infty \sup_x s^{-2} \int \phi_s(x - u)|x - u| \, du$$

$$= \|\hat{p}_0 - p_0\|_\infty s^{-2} \int \phi_s(z)|z| \, dz \to_p 0.$$

Recall that $E_t(\Delta \mid \hat{\Delta} = \cdot)$ and $\hat{E}_t(\Delta \mid \hat{\Delta} = \cdot)$ are posterior mean functions $[-L, L] \to [-L, L]$ under $p_0$ and $\hat{p}_0$ respectively.

**Lemma 10.** Given any $t > 0$, under the same conditions as Theorem 4, $\|\hat{E}_t(\Delta \mid \hat{\Delta} = \cdot) - E_t(\Delta \mid \hat{\Delta} = \cdot)\|_\infty \to_p 0$.

Proof. By Lemma 2, it suffices to show

$$\sup_{x \in [-L, L]} \left| \frac{\hat{p}_t'(x)}{\hat{p}_t(x)} - \frac{p_t'(x)}{p_t(x)} \right| \to_p 0.$$

For any $x \in [-L, L]$, by Taylor expansion on $f(a, b) = a/b$ we have

$$\left| \frac{\hat{p}_t'(x)}{\hat{p}_t(x)} - \frac{p_t'(x)}{p_t(x)} \right| = \left| \frac{1}{\hat{p}_t(x)} (\hat{p}_t'(x) - p_t'(x)) - \frac{p_t'(x)}{p_t^2(x)} (\hat{p}_t(x) - p_t(x)) \right|$$

$$+ o \left( \|\hat{p}_t' - p_t'\|_\infty + \|\hat{p}_t - p_t\|_\infty \right).$$

Note that on $[-L, L]$, $p_t$ is lower-bounded by a positive constant (see Eq. (51) in Appendix C), and $|p_t'|$ is upper bounded by a positive constant (a computation similar to Eq. (41)). The previous display is thus upper bounded by

$$\left\| \frac{\hat{p}_t'(x)}{\hat{p}_t(x)} - \frac{p_t'(x)}{p_t(x)} \right\|_\infty \leq c_1 \|\hat{p}_t' - p_t'\|_\infty + c_2 \|\hat{p}_t - p_t\|_\infty + o \left( \|\hat{p}_t' - p_t'\|_\infty + \|\hat{p}_t - p_t\|_\infty \right)$$

for $0 < c_1, c_2 < \infty$. The result then follows from Corollary 2. \qed
5. Numerical results. We present some results on simulated examples and real large-scale experiments.

5.1. Simulations. In the following we consider several simulation studies where $p_0$ is chosen to be a known prior.

5.1.1. Uniform distribution. We set $p_0 = \text{unif}(-4, 4)$. The domain half-length is chosen to be $L = 8$. We simulate $n = 2,000$ data points $(\Delta_i, s_i)$ with $s_i \sim \text{unif}(0, 1)$. The reader is referred to Wager (2014) for a similar example where $s_i$ is fixed to 1. To select $N$, we use Monte Carlo cross-validation that randomly splits between the training set (90% of data) and the test set (10% of data). The random split is repeated 100 times. We select $N$ from options $\{4, 6, 12, 16, 24, 32, 48, 64\}$. See Table 1 for the results based on the two model-selection criteria proposed in Section 4.6; $N = 32$ is selected by both criteria (the highest predicted log-likelihood and the lowest score-matching loss).

| Dataset          | Method | $N$ 4  | 6   | 12  | 16  | 24  | 32  | 48  | 64  |
|------------------|--------|--------|-----|-----|-----|-----|-----|-----|-----|
| Uniform          | Spectral log-likelihood | -2.264 | -2.240 | -2.213 | -2.205 | -2.197 | -2.193 | -2.197 | -2.199 |
|                  |        | (0.002) | (0.002) | (0.002) | (0.003) | (0.003) | (0.003) | (0.003) | (0.003) |
|                  | score-matching       | -0.082 | -0.090 | -0.101 | -0.105 | -0.107 | -0.114 | -0.108 | -0.101 |
|                  |        | (0.002) | (0.002) | (0.002) | (0.002) | (0.003) | (0.002) | (0.002) | (0.003) |
| Mixture of 2 Gaussians | Spectral log-likelihood | -2.149 | -2.075 | -1.992 | -1.980 | -1.973 | -1.962 | -1.955 | -1.967 |
|                  |        | (0.003) | (0.003) | (0.003) | (0.003) | (0.003) | (0.004) | (0.004) | (0.004) |
|                  | score-matching       | -0.139 | -0.205 | -0.261 | -0.261 | -0.261 | -0.273 | -0.286 | -0.294 |
|                  |        | (0.004) | (0.002) | (0.004) | (0.004) | (0.004) | (0.004) | (0.004) | (0.005) |

Figure 2 compares the estimates from $N = 32$ (chosen by cross-validation) and from a larger $N = 64$. Choosing $N = 64$ introduces more high-frequency oscillations in the estimate for $p_0$ (under-smoothed). The difference between the two estimates diminishes as we compare $\hat{p}_s$ for a larger $s$. The high-frequency errors are damped very quickly; see Lemma 4.
5.1.2. Mixture of Two Gaussians. We consider a mixture of two Gaussians
\[ p_0 = 0.3 N(-1.5, 0.2^2) + 0.7 N(2, 1.0^2) \]
and set \( L = 8 \). We simulate 1,000 samples with \( s_i \sim \text{unif}(0, 1.5) \). See Fig. 3 for the marginal densities and the scatterplot of a simulated dataset. Again we cross-validate on the order of trigonometric polynomials \( N \). Table 1 shows the predicted log-likelihood and the score-matching loss computed from held-out data (10% of samples), based on 200 random splits of the same dataset. \( N = 48 \) is selected in terms of both criteria. In Fig. 4, we compare the estimates from \( N = 6 \) (too small, over-smoothed) and from \( N = 48 \) (selected by cross-validation) from 50 realizations of the sampling distribution. As a reference, we also include estimates from fitting the true model.

5.2. Large-scale experimentation at Amazon. We apply our method to large-scale A/B tests run at Amazon. Fig. 5 shows a subset of 680 past experiments coming from the same population, where \( \hat{\Delta}_i \) is the empirical estimate of some effect measured in some standardized duration and unit. We choose an appropriately large \( L \), which leaves 8 data points off the domain; those data points are approximately projected to the boundary via \((\hat{\Delta}, s) \leftarrow (\text{sign}(\hat{\Delta})L, Ls/|\hat{\Delta}|)\) (the transform is exact if the associated true effect is zero).

Fig 2: Comparison of estimates under \( p_0 = \text{unif}(-4, 4) \). Estimated (blue) versus true densities (red) \( p_s(\cdot) \) for \( s = 0, 0.5, 1 \) are shown (top: using \( N = 32 \) as selected from cross validation, bottom: using a larger \( N = 64 \)). The grey curves are 50 bootstrap estimates. The error in high-frequency components diminishes quickly as \( s \) grows.
We select \(N\) from \(\{512, 1024, 1536, 2048, 3072, 4096\}\). We ran cross-validation 400 times randomly holding out 10% of data. Table 1 shows the two model selection criteria. Both the predicted log-likelihood and the score-matching loss prefer \(N = 2,048\) from the list of options. We fit the full dataset with this selected \(N\). Figure 6 displays the estimated prior density. The pointwise 95% confidence bands are estimated from 500 bootstrap replicates.

**Comparison.** We compare to fitting the prior with a mixture of \(K\) Gaussian distributions; see Appendix D for the fitting algorithm. We select \(K\) using the same cross-validated criteria. As shown in Table 1, \(K = 3\) is selected. The prior density fitted is shown in Fig. E.2 in the Appendix. The difference between our method and the mixture of Gaussians is apparent when plotting on the logarithmic scale — our method fits heavier tails (areas with large

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![Fig 3: The marginal densities \(p_s(\hat{\Delta})\) (left) and the simulated data points \((s_i, \hat{\Delta}_i)\), where \(p_0\) is a mixture of two Gaussians.](image)

![Fig 4: Estimates compared to the true density when \(p_0\) is a mixture of two Gaussians. The first two plots come from our method with \(N = 6\) (over-smoothed) and \(N = 48\) (selected by cross-validation). The last plot corresponds to fitting the true model. To illustrate the performance of the estimators over hypothetical replications, the blue curves are estimated from 50 simulated datasets, each consisting of 1,000 data points.](image)
Observed effect

Fig 5: 680 experiments ($\hat{\Delta}_i, s_i$) from the same population run at Amazon.

Fig 6: The prior over the true effect estimated from a set of experiments run at Amazon. The pointwise confidence bands are estimated from bootstrap. The density is drawn in the logarithmic scale; see Fig. E.1 in the Appendix for the linear scale. Also compare to Fig. E.2, which is fitted with a mixture of Gaussians.

$|\Delta|$; compare Fig. 6 and Fig. E.2.

As a consequence of the heavier tails in the estimated prior, our method imposes milder shrinkage when making posterior inference. To illustrate this effect, in Fig. 7 we plot the amount of shrinkage in the posterior mean corresponding to different noise scales $s$. By Tweedie’s formula Eq. (11), the amount of shrinkage upon observing $\hat{\Delta} = x$ and $\hat{s} = s$ is

$$\tilde{E}_s[\Delta \mid \hat{\Delta} = x] - x = s^2 \hat{p}'_s(x) = s^2 \hat{p}'_s(x)/\hat{p}_s(x).$$
Note that strict positivity of \( \hat{p}_s(x) \) proved in Theorem 3 guarantees that the estimated posterior mean is finite. Also, Lemma 10 guarantees that the shrinkage curves will uniformly converge to the corresponding true curves as \( n \to \infty \). In the bottom panel of Fig. 7, we compare to the shrinkage functions from estimating the prior as a mixture of three Gaussians. We can see that the mixture-of-Gaussian model imposes much stronger shrinkage compared to our method (the dashed diagonal lines in the plots represent the strongest possible shrinkage that always shrinks the posterior mean to exactly zero).

Additionally, the posterior density of \( \Delta \) upon observing \( s \) and \( \hat{\Delta} = x \) can be computed via

\[
\hat{p}_s(\Delta \mid \hat\Delta = x) = \hat{p}_0(\Delta) \phi_s(\Delta - x) / \hat{p}_s(x).
\]

See Fig. 8 for an example of the estimated posterior density. Again, we can observe that the prior fitted with mixture of Gaussians implies stronger shrinkage; note that under the mixture of Gaussian model, little mass accumulates around \( \hat{\Delta} \) for any of the noise scales considered.

6. Concluding remarks. We have developed a new, principled and intuitive framework for the analysis of large-scale randomized experiments. We first characterized the density family arising from the problem with a PDE (the heat equation), which unifies “f-modeling” (marginal) and “g-modeling” (prior) approaches towards empirical Bayes (Efron, 2014) under (asymptotic) Gaussian likelihood. Second, we estimated the density family with trigonometric polynomials, which are eigenfunctions of the heat equation. Third, we introduced a novel parametrization of non-negative trigonometric polynomials that ensures a bona fide probability density, which further guarantees that the implied posterior mean is finite. Fourth, we presented an efficient convex optimization algorithm for maximum likelihood estimation. Moreover, towards model selection, we connected the square loss in estimating the posterior mean to Hyvärinen’s (2005) score-matching via Tweedie’s formula. Lastly, we showed that our estimator, as a sieve MLE, is uniformly consistent in estimating the prior density and the posterior mean functions. Our methodology provides a simple and scalable approach to analyzing large-scale randomized experiments, that offers many advantages relative to commonly used \( t \)-tests or fitting the prior to a parametric mixture model with the EM algorithm.

It is worth mentioning that the methodology developed here is applicable to more general settings, where one wants to estimate the prior distribution for some parameter \( \theta \in \mathbb{R} \) from many asymptotically normal estimators.
Fig 7: The amount of shrinkage in the posterior mean function $\mathbb{E}_s[\Delta | \hat{\Delta}] - \hat{\Delta} = s^2 \ell_s(\hat{\Delta})$ estimated from Amazon data (top: our spectral method, bottom: prior fitted with a mixture of three Gaussians). Colors correspond to different values of $s$. The strongest shrinkage is $y = -\hat{\Delta}$ as $s \to \infty$ (dashed diagonal line), which always sets the posterior mean to zero. See also Figure E.3 for a wider range of $\hat{\Delta}$.

$\hat{\theta}_i$, which correspond to the parameters $\theta_i$ realized independently from the prior. Here is an example.

**Example 1.** Suppose an urn is filled with an infinite number of coins, and the probability of heads for a random coin is $\theta \in [0, 1]$. For each experiment $i$, one can draw a coin from the urn, flip $n_i$ times and observe the number of heads $m_i$. The MLE for $\theta_i$ is $\hat{\theta}_i = m_i/n_i$, which is asymptotically normal when $n_i \to \infty$. Under a large number of coin tosses for each exper-
Fig 8: Estimated posterior density $p_s(\Delta | \hat{\Delta})$ for Amazon data under different $s$ (top: our spectral method, bottom: prior fitted with a mixture of three Gaussians). The observed $\hat{\Delta}$ is marked as dashed. As the error scale $s$ decreases from 0.1 (corresponding to increasing experimental sample size), the posterior is initially concentrated at zero, but then gradually shifts towards $a$ (a prior mode near $\hat{\Delta}$), and should finally concentrate around $\hat{\Delta}$. It is clear that the mixture-of-Gaussian prior imposes stronger shrinkage.

We conclude with a few remarks. First, closely related to our work, Walter (1981); Walter and Hamedani (1991) and Carrasco and Florens (2011) considered estimating the prior with orthogonal polynomials chosen with respect to the Gaussian convolution/integration kernel, which are Hermite...
polynomials; see Carrasco and Florens (2011, Example 1) and Walter and Hamedani (1991, Appendix B.1). Here we take a differential perspective instead of an integral one, and the resulting polynomials are trigonometric. Second, in terms of nonparametric maximum likelihood, Laird (1978) and Leonard (1984) considered estimating the prior in the form of a mixture of delta functions, fitted with some iterative schemes such as the EM. Third, we leave the removal or relaxation of our technical assumptions to further studies, such as the toric simplification of the domain (Assumption 3).

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APPENDIX A: BAYESIAN ANALYSIS OF EXPERIMENTS

A.1. Proof of Theorem 1.

PROOF. By Bayes’ theorem,

\[
P \left( \Delta_i \in A \ \mid G_A(\hat{\Delta}_i) = \varphi \right) = \frac{P(\Delta_i \in A, G_A(\hat{\Delta}_i) = \varphi)}{P(G_A(\Delta_i) = \varphi)},
\]

where the denominator is positive by assumption. By the law of total probability, the numerator becomes

\[
P(\Delta_i \in A, G_A(\hat{\Delta}_i) = \varphi) = \int_A P \left( G_A(\hat{\Delta}_i) = \varphi \mid \Delta_i = u \right) g(u) \, du
\]

\[
= \int_A \left( \int_{\{x : G_A(x) = \varphi\}} \phi_{s_i}(x - u) \, dx \right) g(u) \, du
\]

\[
= \int_A \int_{\{x : G_A(x) = \varphi\}} \phi_{s_i}(x - u) g(u) \frac{p_{s_i}(x)}{p_{s_i}(x)} \, du \, dx
\]

\[
\overset{(i)}{=} \int_{\{x : G_A(x) = \varphi\}} \left( \int_A \frac{\phi_{s_i}(x - u) g(u)}{p_{s_i}(x)} \, du \right) p_{s_i}(x) \, dx
\]

\[
\overset{(ii)}{=} \int_{\{x : G_A(x) = \varphi\}} G_A(x) p_{s_i}(x) \, dx
\]

\[
= \varphi \int_{\{x : G_A(x) = \varphi\}} p_{s_i}(x) \, dx
\]

\[
= \varphi P(G_A(\hat{\Delta}_i) = \varphi),
\]

where (i) uses Fubini’s theorem, and (ii) uses Eq. (5). The result is proven by noting that \( P(G_A(\Delta_i) = \varphi) \) cancels with the denominator. □
A.2. Bayes optimal decision making. In the context of Section 2.3.2, suppose \( A \) is the collection of possible actions, and we have a loss function \( l(\Delta, a) : \mathbb{R} \times A \to \mathbb{R} \). Without loss of generality, consider a deterministic decision function \( d(\hat{\Delta}) : \mathbb{R} \to A \). The expected loss, with respect to the sampling distribution of future experiments, of making decision \( d \) is

\[
\mathbb{E} l(\Delta, d(\hat{\Delta})) = \int g(\Delta) \left[ \int l(\Delta, d(\hat{\Delta})) p(\Delta \mid \hat{\Delta}) d\hat{\Delta} \right] d\Delta \\
= \int p(\Delta) \left[ \int l(\Delta, d(\hat{\Delta})) p(\Delta \mid \hat{\Delta}) d\hat{\Delta} \right] d\Delta \\
\geq \int p(\Delta) \left[ \int l(\Delta, d_B(\hat{\Delta})) p(\Delta \mid \hat{\Delta}) d\hat{\Delta} \right] d\hat{\Delta},
\]

where the Bayes decision rule \( d_B(\hat{\Delta}) \) minimizes the posterior risk \( \int l(\Delta, d(\hat{\Delta})) p(\Delta \mid \hat{\Delta}) d\Delta \) for every \( \hat{\Delta} \).

APPENDIX B: GENERAL SOLUTION TO THE HEAT EQUATION

For a function \( h : \mathbb{R} \to \mathbb{C} \) and \( h \in L^1(\mathbb{R}) \), the Fourier transform \( \mathcal{F} h : \mathbb{R} \to \mathbb{C} \) is defined as

\[
\mathcal{F} h(\xi) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ix\xi} h(x) \, dx.
\]

And its inverse Fourier transform is defined as

\[
\mathcal{F}^{-1} h(\xi) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ix\xi} h(x) \, dx.
\]

It holds that \( h = \mathcal{F}^{-1} \mathcal{F} h \). The Fourier transform for \( p_t(x) \) is therefore

\[
(\mathcal{F} p_t)(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ix\xi} p_t(x) \, dx,
\]

which is also called the characteristic function of \( p_t \) in statistics. Taking Fourier transform on both sides of Eq. (14) with respect to \( x \), we have

\[
\mathcal{F} \left( \frac{\partial p_t(x)}{\partial t} \right)(\xi) = \frac{1}{2} \mathcal{F} \left( \frac{\partial^2 p_t(x)}{\partial x^2} \right)(\xi).
\]

Using the property that \( \mathcal{F} \left( \frac{\partial^m h(x)}{\partial x^m} \right)(\xi) = (i\xi)^m \mathcal{F} h(\xi) \), the previous display becomes

\[
\frac{\partial}{\partial t} \mathcal{F}(p_t)(\xi) = -\frac{1}{2} \xi^2 \mathcal{F}(p_t)(\xi),
\]

which is an ordinary differential equation in \( t \). The solution is

\[
(43) \quad \mathcal{F}(p_t)(\xi) = \mathcal{F}(p_0)(\xi) e^{-\frac{1}{2} \xi^2 t} = \mathcal{F}(g)(\xi) e^{-\frac{1}{2} \xi^2 t},
\]
where $F(g)$ is the Fourier transform of the prior density. The factor $e^{-\frac{1}{2}\xi^2 t}$ describes how components corresponding to different $\xi$ are damped over time. The inverse Fourier transform of Eq. (43) leads to the solution Eq. (13) in terms of Green function. From the previous display, it becomes clear that we can evaluate the density family $p_t(x) = (F^{-1}Fp_t)(x)$ at any $x \in \mathbb{R}$, $t > 0$ if we can represent $F(g)(\xi)$ for $\xi \in \mathbb{R}$; and the density family can be approximated if we can approximate $F(g)$.

**APPENDIX C: PROOF OF CONSISTENCY**

Our proof of consistency will be based on the following result.

**Lemma C.1 (Chen (2007, Page 5590)).** Let $(\Theta, d)$ be a metric space. Let $\{\Theta_N\}$ be a sequence of sieves such that $\Theta_N \subseteq \Theta$. Let $\hat{\theta}_n$ be an (approximate) maximizer of the sample criterion function within sieve $\Theta_N$, namely one that satisfies

\[(44) \quad Q_n(\hat{\theta}_n) \geq \sup_{\theta \in \Theta_N} Q_n(\theta) - o_p(1),\]

for some $N \to \infty$ as $n \to \infty$. Then $d(\hat{\theta}_n, \theta_0) \to_p 0$ under the following conditions.

(a) (i) $Q(\theta)$ is continuous at $\theta_0$ in $\Theta$, $Q(\theta_0) > -\infty$; (ii) for all $\varepsilon > 0$, $Q(\theta_0) > \sup_{\theta \in \Theta, d(\theta, \theta_0) \geq \varepsilon} Q(\theta)$.
(b) For any $\theta \in \Theta$ there exists $\theta_N \in \Theta_N$ such that $d(\theta, \theta_N) \to 0$ as $N \to \infty$.
(c) For each $k \geq 1$, (i) $Q_n(\theta)$ is measurable for all $\theta \in \Theta$, and (ii) $Q_n(\theta)$ is upper semicontinuous on $\Theta_k$ under metric $d(\cdot, \cdot)$.
(d) $\Theta_k$ is compact under $d(\cdot, \cdot)$ for every $k \geq 1$.
(e) For every $k \geq 1$, $\sup_{\theta \in \Theta_k} \| Q_n(\theta) - Q(\theta) \| \to_p 0$.

**Remark 2.** Chen (2007) also requires that $\Theta_N \subseteq \Theta_{N+1}$ for every $N$. But establishing consistency does not require the nestedness of sieves; see also Newey and Powell (2003, Lemma A1) and Shen (1997, Conditions (A-D)).

For the ease of presentation, we will adopt the standard notations from Chen (2007). Without loss of generality, let us assume $L = \pi$. Let $\Theta$ denote the parameter space under Assumption 2, namely

\[(45) \quad \Theta := \{ \theta(x) : \theta \text{ is a uniformly continuous density on } [-\pi, \pi] \}.

For $\theta \in \Theta$,

\[(46) \quad p_{\theta, t} := \int_{-\infty}^{\infty} \bar{\theta}(u)\phi_{\sqrt{t}}(x-u) \, du\]
is the implied marginal density on \([-\pi, \pi]\), where \(\tilde{\theta}: \mathbb{R} \to \mathbb{R}\) is the periodized version of \(\theta\) satisfying \(\tilde{\theta}(x + 2\pi) = \tilde{\theta}(x)\). Let us define the population “criterion function” as the expected log-likelihood \(Q(\theta): \Theta \to \mathbb{R}\), given by

\[
Q(\theta) := \mathbb{E}_t \mathbb{E}_{X|t} \log p_{\theta,t}(X).
\]

**Lemma C.2.** Under \(\theta_0\), \(Q(\theta)\) is uniquely maximized at \(\theta_0\).

**Proof.** It suffices to show that for any fixed \(t \geq 0\), \(Q(\theta; t) := \mathbb{E}_X \log p_{\theta,t}(X)\) is uniquely maximized at \(\theta = \theta_0\). Note that, \(-Q(\theta; t) = D_{KL}(p_{\theta_0,t} || p_{\theta,t}) + \text{const}\), which is uniquely minimized when \(p_{\theta,t} = p_{\theta_0,t}\). By Lemma 7, \(p_{\theta,t} = p_{\theta_0,t}\) iff \(\theta_0 = \theta\) Lebesgue almost everywhere. Further, since \(\theta, \theta_0\) are continuous by definition of \(\Theta\), \(\theta_0 = \theta\) Lebesgue almost everywhere iff \(\theta_0 = \theta\).

The sample version of the criterion function is defined as

\[
Q_n(\theta) := \mathbb{P}_n \log p_{\theta,t}(X),
\]

where \(\mathbb{P}_n\) is the empirical measure over \((t, X)\). The maximum likelihood estimator \(\hat{\theta}_n(\mathbb{P}_n)\) of the prior density can be written as

\[
\hat{\theta}_n = \arg \max_{\theta \in \Theta_N} Q_n(\theta),
\]

where \(N\) grows with \(n\) and \(\Theta_N\) is the class of densities representable under our parametrization. More precisely, by Eq. (33) and the conditions \(f_\nu \geq 0\), \(\frac{2\pi}{2N+1} \sum_{\nu=-N}^N f_\nu = 1\), the class can be expressed as

\[
\Theta_N = \left\{ \sum_{\nu=-N}^N \gamma_\nu \tilde{K}_N(x - x_\nu) : \gamma \in \mathcal{S}_{2N} \right\},
\]

where \(\gamma_\nu = 2\pi f_\nu/(2N + 1)\), \(\tilde{K}_N(\cdot) = K_N(\cdot)/(2\pi)\) and \(x_\nu = \frac{2\nu}{2N+1}\). Recall that \(\mathcal{S}_{2N}\) is the \(2N\)-dimensional unit simplex.

**Lemma C.3.** \(\Theta_N\) is compact in \(\| \cdot \|_\infty\) for every \(N \geq 1\).

**Proof.** The metric space \((\Theta_N, \| \cdot \|_\infty)\) is compact iff it is sequentially compact (Kumaresan, 2005, Theorem 4.3.14). Now we show sequential compactness. Since \(\mathcal{S}_{2N}\) is compact, for any sequence \(\gamma^{(n)}\) in \(\mathcal{S}_{2N}\) there exists a subsequence \(\gamma^{(m_n)} \to \gamma \in \mathcal{S}_{2N}\). Let \(\gamma\) be the density that corresponds to \(\gamma\). We have

\[
\|\theta^{(m_n)} - \theta\|_\infty = \left\| \sum_{\nu} \left( \gamma^{(m_n)}_\nu - \gamma_\nu \right) \tilde{K}_N(x - x_\nu) \right\|_\infty \leq \tilde{K}_N \|\gamma^{(m_n)} - \gamma\|_\infty \to 0,
\]

where \(\tilde{K}_N := \tilde{K}_N(0) = \frac{N+1}{2\pi} < \infty\); see Lemma 5(a).
\{\Theta_N\} is a sequence of sieves in the sense of Grenander (1981). We show that the sieves are dense in \(\Theta\) with respect to \(|\cdot|_\infty\).

**Lemma C.4.** For every \(\theta \in \Theta\), there exists \(\theta_N \in \Theta_N\) such that \(|\theta_N - \theta|_\infty \to 0\).

**Proof.** Let us first consider the sieves without the simplex constraint. Define
\[
\tilde{\Theta}_N := \left\{ \sum_{\nu=-N}^{N} \gamma_\nu K_N(x-x_\nu) : \gamma \in \mathbb{R}^{2N+1} \right\}.
\]
Consider \(\tilde{\theta}_N := \tilde{\theta}_N(\gamma) \in \tilde{\Theta}_N\) determined by \(\gamma_\nu(\gamma) = \frac{2\pi}{2N+1}\theta(x_\nu) \geq 0\). Zygmund (2002, Theorem 6.3, Chapter X) shows that (i) \(|\tilde{\theta}_N - \theta|_\infty \to 0\), and (ii) \(\tilde{\theta}_N\) remains within the same bounds as \(\theta\). Now let us consider \(\theta_N := \theta_N(\gamma) \in \Theta_N\) with normalized weights \(\gamma(\gamma) \in S_2\). Using (ii), we have
\[
|\tilde{\theta}_N - \theta_N|_\infty \leq \left| 1 - \frac{\|\gamma(\gamma)\|_1}{\|\tilde{\gamma}(\gamma)\|_1} \right| c,
\]
where \(c\) is the maximum density of \(\theta\). Clearly, \(c < \infty\) since \(\theta\) is a continuous density on \([-\pi, \pi]\). Note that
\[
1 = \int_{-\pi}^{\pi} \theta(x) \, dx = \sum_{\nu=-N}^{N} \int_{x_\nu}^{x_{\nu+1}} \theta(x) \, dx = \frac{2\pi}{2N+1} \sum_{\nu=-N}^{N} \theta(x_\nu')
\]
for \(x_\nu' \in [x_\nu, x_{\nu+1}]\) by the mean value theorem. We have
\[
\left| \|\tilde{\gamma}(\gamma)\|_1 - 1 \right| = \left| \frac{2\pi}{2N+1} \sum_{\nu=-N}^{N} (\theta(x_\nu) - \theta(x_\nu')) \right|
\leq 2\pi \sup_{|x-x'| \leq 2\pi/(2N+1)} |\theta(x) - \theta(x')| \to 0,
\]
by uniform continuity of \(\theta\). It follows that \(|\tilde{\theta}_N - \theta_N|_\infty \to 0\). Finally, \(|\theta_N - \theta|_\infty \leq |\theta_N - \tilde{\theta}_N|_\infty + |\tilde{\theta}_N - \theta|_\infty \to 0\), using (i) above. \(\square\)

Next, we show a uniform law of large numbers for \(\Theta_N\) using the following lemma.

**Lemma C.5 (Theorem 19.4 of van der Vaart (2000)).** Every class \(\mathcal{F}\) of measurable functions such that \(N(\varepsilon, \mathcal{F}, L_1(P)) < \infty\) for every \(\varepsilon > 0\) is \(P\)-Glivenko-Cantelli.
A function class \( \mathcal{F} \) is called \( P \)-Glivenko-Cantelli if \( \sup_{f \in \mathcal{F}} |(\mathbb{P}_n - P)f| \to_p 0 \), where \( \mathbb{P}_n \) is the empirical measure of \( P \) under \( n \) iid samples. Given two functions \( l \) and \( u \), let \([l, u] := \{ f : l(x) \leq f(x) \leq u(x) \} \). \([l, u] \) is called an \( \varepsilon \)-bracket in \( L_1(P) \) if \( |l - u| \leq \varepsilon \). The bracketing number \( N_{\varepsilon}(\mathcal{F}, L_1(P)) \) is the smallest cardinality \(|I|\) of a set of \( \varepsilon \)-brackets that covers \( \mathcal{F} \), i.e., \( \mathcal{F} \subseteq \bigcup_{i \in I} [l_i, u_i] \). Similarly, we use \( N(\varepsilon, \mathcal{F}, \| \cdot \|) \) to denote the covering number of \( \mathcal{F} \), namely the smallest cardinality of \( \{ f_i : i \in I \} \) such that \( \mathcal{F} \subseteq \bigcup_{i \in I} \{ f : \| f - f_i \| \leq \varepsilon \} \). See van der Vaart (2000, Chapter 19) for more background.

**Lemma C.6.** Under Assumption 4, \( \sup_{\theta \in \Theta_N} |Q_n(\theta) - Q(\theta)| \to_p 0 \) as \( n \to \infty \) for every \( N \geq 1 \).

**Proof.** By Assumption 4, let
\[
\mathcal{F}_N := \{ p_0(x, t) : [-\pi, \pi] \times [0, t_{\text{max}}] \to \mathbb{R} \mid \theta \in \Theta_N \},
\]
where \( p_0(x, t) \) is defined by Eq. (46). By definition of \( Q \) and \( Q_n \) (see Eqs. (47) and (48)), to show the lemma is to show that \( \log \mathcal{F}_N := \{ \log f : f \in \mathcal{F}_N \} \) is \( P \)-Glivenko-Cantelli for every \( N \geq 1 \).

Fix any \( N \geq 1 \). By Lemma C.5, we can show the result by showing finite bracketing number for \( \log \mathcal{F}_N \) for every \( \varepsilon > 0 \). First, we show finite bracketing number for \( \mathcal{F}_N \). Note that \( N(\varepsilon, \Theta_N, \| \cdot \|_\infty) < \infty \) for every \( \varepsilon > 0 \) by Lemma C.3. Take \( \{ \theta_i : i \in I \} \) to be an \( \varepsilon/2 \)-cover of \( \Theta_N \) in \( \| \cdot \|_\infty \). For any \( p_{\theta_1}, p_{\theta_2} \in \mathcal{F}_N \), it holds that
\[
\| p_{\theta_1} - p_{\theta_2} \|_\infty = \left\| \int_{-\infty}^{+\infty} (\tilde{\theta}_1(u) - \tilde{\theta}_2(u)) \phi_{\sqrt{T}}(x - u) \, du \right\|_\infty \leq \| \tilde{\theta}_1(u) - \tilde{\theta}_2(u) \|_\infty \int_{-\infty}^{+\infty} \phi_{\sqrt{T}}(x - u) \, du = \| \tilde{\theta}_1(u) - \tilde{\theta}_2(u) \|_\infty.
\]
Hence, for any \( p_0 \in \mathcal{F}_N \), there exists some \( i \in I \) such that \( \| p_0 - p_{\theta_i} \|_\infty \leq \varepsilon/2 \).

Under Assumption 4, we claim that \( \mathcal{F}_N \) is bounded from above and below by positive constants. The upper bound is given by
\[
\int_{-\infty}^{+\infty} \tilde{\theta}(u) \phi_{\sqrt{T}}(x - u) \, du \leq \| \tilde{\theta} \|_\infty \leq K_N,
\]
where \( K_N \) appeared in the proof of Lemma C.3. And the lower bound comes from
\[
\int_{-\infty}^{+\infty} \tilde{\theta}(u) \phi_{\sqrt{T}}(x - u) \, du \geq \int_{-\pi}^{+\pi} \tilde{\theta}(u) \phi_{\sqrt{T}}(x - u) \, du \geq \inf \{ \phi_{\sqrt{T}}(x) : t \in [0, t_{\text{max}}], x \in [-\pi, \pi] \} \geq \phi_{\sqrt{t_{\text{max}}}}(2\pi) > 0.
\]
For every \( \theta_i \) in the cover, we construct a pair of brackets

\[
l_i(x,t) := \left( \int_{-\infty}^{+\infty} \tilde{\theta}_i(u) \phi \sqrt{t}(x-u) \, du - \varepsilon/2 \right) \vee \phi \sqrt{t_{\max}}(2\pi),
\]

\[
u_i(x,t) := \left( \int_{-\infty}^{+\infty} \tilde{\theta}_i(u) \phi \sqrt{t}(x-u) \, du + \varepsilon/2 \right) \wedge \bar{K}_N.
\]

By construction, \( F_N \subseteq \bigcup_{i \in I} [l_i, u_i] \) and \( P|u_i - l_i| \leq \varepsilon \). Therefore, we have

\[
N[\varepsilon, F_N, L_1(P)] \leq N(\varepsilon, \Theta_k, \| \cdot \|_{\infty}) < \infty.
\]

Further, since \( 0 < \phi \sqrt{t_{\max}}(2\pi) \leq F_N \leq \bar{K}_N < \infty \), \( \log F_N \) is a Lipschitz transform on \( F_N \) and it follows that \( N[\varepsilon, \log F_N, L_1(P)] < \infty \). By Lemma C.5, \( \log F_N \) is \( P \)-Glivenko-Cantelli.

Finally, consistency is established as follows.

**Proof of Theorem 4.** We prove consistency by verifying the conditions in Lemma C.1, with \( \Theta \) defined in Eq. (45) and metric \( d(f,g) := \| f - g \|_{\infty} \). Clearly, \( \hat{\theta}_n \) as defined in Eq. (49) satisfies Eq. (44). Condition (a) is satisfied due to (i) the continuity of \( Q \) and (ii) Lemma C.2. By Lemma C.4, Condition (b) is satisfied. Condition (c) is clearly satisfied by the definition of \( Q_n \) in Eq. (48). Finally, Condition (d) and (e) are verified by Lemma C.3 and Lemma C.6 respectively. \( \square \)

**APPENDIX D: GAUSSIAN MIXTURE MODEL OF THE PRIOR**

**D.1. The EM algorithm.** We first consider a parametric model by assuming that the prior \( G \) is a mixture of \( K \) Gaussians, namely

\[
G(\Delta) = \sum_{k=1}^{K} \alpha_k N(\Delta; \mu_k, V_k),
\]

where \( \alpha_k \geq 0, \sum_{k=1}^{K} \alpha_k = 1 \) and \( V_k \geq 0 \).

The induced marginal likelihood on \( \bar{\Delta} \) is again a mixture of Gaussians

\[
\bar{\Delta} \sim \sum_{k=1}^{K} \alpha_k N(\mu_k, V_k + s^2).
\]

And the marginal log-likelihood is

\[
\ell_n = \sum_{i=1}^{N} \log \left\{ \sum_{k=1}^{K} \alpha_k N(\bar{\Delta}_i; \mu_k, V_k + s^2) \right\}.
\]

Note that \( \ell_n \) is not concave in \( \{(\alpha_k, \mu_k, V_k^{-1})\} \).
$K = 1$. In the simplest case of fitting one Gaussian, setting $\nabla\ell_n = 0$ yields
\[
\hat{\mu} = \frac{\sum_{i=1}^N (\hat{\mu} + s_i^2)^{-1} \hat{\Delta}_i}{\sum_{i=1}^N (\hat{\mu} + s_i^2)^{-1}}, \quad \hat{V} = \frac{1}{N} \sum_{i=1}^N (\hat{\Delta}_i - \hat{\mu})^2 - \frac{1}{N} \sum_{i=1}^N s_i^2.
\]
A fixed-point can be found by iterating the two equations. Note the estimates are different from naively fitting a normal from $\{\hat{\Delta}_i\}$.

$K > 1$. It is not straightforward to optimize Eq. (52) due to non-convexity. Instead, an EM algorithm (Dempster et al., 1977) can be constructed by imputing latent component indicators $z_{ik}$ and unobserved true effects $\Delta_i$, such that we can iteratively maximize a lower-bound for $\ell_n$. This algorithm, in the more general multivariate setting, was derived by Bovy et al. (2011).

The E-step entails updating the following $N \times K$ matrices
\[
q_{ik} \leftarrow -\frac{\alpha_k \mathcal{N}(\hat{\Delta}_i; \mu_k, V_k + s_i^2)}{K \sum_{l=1}^K \alpha_l \mathcal{N}(\hat{\Delta}_i; \mu_l, V_l + s_i^2)},
\]
\[
b_{ik} \leftarrow \frac{s_i^2 \mu_k + V_k \hat{\Delta}_i}{s_i^2 + V_k}, \quad B_{ik} \leftarrow \frac{s_i^2 V_k}{s_i^2 + V_k}.
\]

The M-step updates the estimates for $k = 1, \ldots, K$ by
\[
\alpha_k \leftarrow \frac{1}{N} \sum_{i=1}^N q_{ik}, \quad \mu_k \leftarrow \frac{\sum_{i=1}^N q_{ik} b_{ik}}{\sum_{i=1}^N q_{ik}}, \quad V_k \leftarrow \frac{\sum_{i=1}^N q_{ik} \{(\mu_k - b_{ik})^2 + B_{ik}\}}{\sum_{i=1}^N q_{ik}}.
\]

The EM algorithm converges to a local maximum of $\ell_n$. To approach the global maximum, one can run the algorithm multiple times with random initializations.

D.2. Posterior inference. Under a mixture of Gaussian prior, the posterior for $\Delta$ is also a mixture of Gaussians
\[
\Delta \mid \hat{\Delta}, s \sim \sum_{k=1}^K \alpha'_k \mathcal{N}(\mu'_k, V'_k),
\]
where the updated parameters are given by
\[
\alpha'_k \propto \frac{\alpha_k}{\sqrt{s^2 + V_k}} \exp \left\{ -\frac{(\mu_k - \hat{\Delta})^2}{2(s^2 + V_k)} \right\}, \quad \sum_{k=1}^K \alpha'_k = 1
\]
and
\[
\mu'_k = \frac{s^2 \mu_k + V_k \hat{\Delta}}{s^2 + V_k}, \quad V'_k = \frac{V_k s^2}{s^2 + V_k}.
\]
Suppose $\mu_1 = V_1 = 0$, i.e., the first component is a point mass at zero. Then $\alpha'_1$ can be interpreted as the posterior probability that the true effect is zero.
APPENDIX E: ADDITIONAL PLOTS

We provide additional plots Figs. E.1 to E.3.

Fig E.1: The prior over the true effect estimated from a set of experiments run at Amazon using the spectral method developed in this paper. The pointwise confidence bands are estimated from bootstrap replications. See also Fig. 6 in the main text for the logarithmic scale.

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Fig E.2: The prior over the true effect estimated from a set of experiments run at Amazon fitted with a mixture of three Gaussians (top: in linear scale; bottom: in logarithmic scale). Compare to Fig. 6 and Fig. E.1 estimated by the spectral method.

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Fig E.3: The amount of shrinkage in the estimated posterior mean function $E_s[\Delta \mid \hat{\Delta}] - \hat{\Delta} = s^2 \ell_s'(\hat{\Delta})$ for different $s$ (top: our spectral method, bottom: fitting the prior with a mixture of three Gaussians). The strongest shrinkage is $y = -\hat{\Delta}$ as $s \to \infty$ (dashed diagonal line), which always sets the posterior mean to zero. See also Fig. 7 for more details around zero.

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