

**ebnm: An R Package for Solving the Empirical Bayes Normal Means Problem Using a Variety of Prior Families**

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**Abstract**

The empirical Bayes normal means (EBNM) model is important to many areas of statistics, including (but not limited to) multiple testing, wavelet denoising, and gene expression analysis. There are several existing software packages that can fit EBNM models under different prior assumptions and using different algorithms; however, the differences across interfaces complicate direct comparisons. Further, a number of important prior assumptions do not yet have implementations. Motivated by these issues, we developed the R package *ebnm*, which provides a unified interface for efficiently fitting EBNM models using a variety of prior assumptions, including nonparametric approaches. In some cases, we incorporated existing implementations into *ebnm*; in others, we implemented new fitting procedures with a focus on speed and numerical stability. We illustrate the use of *ebnm* in a detailed analysis of baseball statistics. By providing a unified and easily extensible interface, the *ebnm* package can facilitate development of new methods in statistics, genetics, and other areas; as an example, we briefly discuss the R package *flashier*, which harnesses methods in *ebnm* to provide a flexible and robust approach to matrix factorization.

*Keywords*: empirical Bayes, normal means, shrinkage estimation, mixture models, NPMLE, maximum likelihood.

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**1. Introduction**

Given *n* observations $x_i \in \mathbb{R}$ with known standard deviations $s_i > 0$, $i = 1, \ldots, n$, the normal means model (Robbins 1951; Efron and Morris 1972; Stephens 2017; Bhadra *et al.* 2019; Johnstone 2019; Sun 2020) has

$$
  x_i \overset{\text{ind.}}{\sim} \mathcal{N}(\theta_i, s_i^2),
$$

where the unknown (“true”) means $\theta_i \in \mathbb{R}$ are the quantities to be estimated. Here and throughout, we use $\mathcal{N}(\mu, \sigma^2)$ to denote the normal distribution with mean $\mu$ and variance $\sigma^2$.

The empirical Bayes (EB) approach to inferring $\theta_i$ — which we refer to as “solving the empirical Bayes normal means problem” — attempts to improve upon the maximum-likelihood estimate $\hat{\theta}_i = x_i$ by “borrowing information” across observations, exploiting the fact that each observation contains information not only about its respective mean, but also about how the means are collectively distributed (Robbins 1956; Morris 1983; Efron 2010; Stephens 2017).
Specifically, the empirical Bayes normal means (EBNM) approach assumes that
\[ \theta_i \overset{\text{ind.}}{\sim} g \in \mathcal{G}, \]  
where \( \mathcal{G} \) is some family of probability distributions that is specified in advance and \( g \in \mathcal{G} \) is estimated using the data (typically, via maximum likelihood). Given \( \hat{g} \in \mathcal{G} \), estimates of \( \theta_i \) can be obtained using, for example, posterior means:
\[ \hat{\theta}_i := \mathbb{E}(\theta_i \mid x_i, \hat{g}). \]  

See Figure 1 for an illustration.

Applications in which the EBNM model plays an important role include wavelet denoising (Clyde and George 2000; Johnstone and Silverman 2004, 2005b); multiple testing (Efron 2010; Stephens 2017); gene expression analysis (Love et al. 2014; Zhu et al. 2019; Smyth 2004); multiple linear regression (Kim et al. 2022; Mukherjee et al. 2023); and matrix factorization (Wang and Stephens 2021).

This versatility has motivated the development of a number of software packages using different choices of prior family \( \mathcal{G} \); for a review, see Section 2. Still, important gaps in the software
remain. For example, we are not aware of any package that fits the EBNM model in the simple case where \( G \) is taken to be the family of all univariate normal distributions. Further, each existing package has a different interface and outputs, which hinders comparisons as well as making it difficult to develop software packages that flexibly build upon EBNM methods. Motivated by these issues, we developed the ebnm software package, which provides a unified interface for efficiently solving the EBNM problem using a wide variety of prior families.

We wrote the ebnm package in R (R Core Team 2023), which is free, open source, and highly interoperable — for example, with Python via package rpy2 (Gautier 2023); with MATLAB via R-link (Henson 2024); and with Julia via RCall (Bates et al. 2024). The ebnm package can be downloaded from the Comprehensive R Archive Network (CRAN), and the latest development branch is available on GitHub (https://github.com/stephenslab/ebnm). The package’s website, which includes detailed documentation and package vignettes, is available at https://stephenslab.github.io/ebnm/. Code for reproducing results and figures in the text is available on GitHub at https://github.com/willwerscheid/ebnm-paper.

The paper is organized as follows. In Section 2, we give a brief history of the EBNM problem and review existing approaches. Section 3 gives an overview of the ebnm package, including the unified interface and the newly implemented prior families. In Section 4, we compare different choices of prior family and illustrate how this choice of prior family can impact performance. This section also includes a runtime benchmark for implemented prior families. Section 5 illustrates usage of the ebnm package in an analysis of baseball statistics. In Section 6, we outline a matrix factorization approach, implemented in the R package flashier, which builds on the methods in ebnm. Here, the EBNM problem arises as a subproblem that must be solved many times, so that the speed and flexibility of the ebnm methods prove critical. Finally, Section 7 summarizes the key contributions of this work.

2. Background and existing software

In this section we review existing approaches to the EBNM problem within a common modeling framework.

2.1. Normal priors

Stein (1956) famously discovered that under quadratic loss, the maximum-likelihood estimate (MLE) \( \hat{\theta}_i = x_i, i = 1, \ldots, n \), is an inadmissible solution to the homoskedastic normal means problem

\[
x_i \overset{\text{ind.}}{\sim} \mathcal{N}(\theta_i, s^2), \quad i = 1, \ldots, n,
\]

when \( n \geq 3 \). James and Stein (1961) subsequently gave an explicit formula for a shrinkage estimator that dominates the MLE. As Efron and Morris (1973) showed, a lightly modified version of the James-Stein estimator can be derived via an EB approach that assumes

\[
\theta_i \overset{\text{ind.}}{\sim} g \in \mathcal{G},
\]

where the prior family \( \mathcal{G} \) is taken to be the family of zero-mean normal distributions,

\[
\mathcal{G}_{\text{norm0}} := \{ g : g(x) = \mathcal{N}(x; 0, \sigma^2), \sigma^2 \geq 0 \}.
\]
Here, we use $\mathcal{N}(x; \mu, \sigma^2)$ to denote the normal probability density function at $x$ with mean $\mu$ and variance $\sigma^2$.

In many applications, the mean of the $\theta_i$’s may be non-zero, and so a natural generalization takes $\mathcal{G}$ to be the family of normal distributions
\[
\mathcal{G}_{\text{norm}} := \{ g : g(x) = \mathcal{N}(x; \mu, \sigma^2), \sigma^2 \geq 0 \text{ and } \mu \in \mathbb{R} \}. \tag{7}
\]
Estimating $g \in \mathcal{G}_{\text{norm}}$ reduces to estimating $\sigma^2$ and $\mu$. For the homoskedastic case (4), the maximum-likelihood estimates have simple, closed-form solutions:
\[
\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} x_i, \quad \hat{\sigma}^2 = \max \left\{ 0, \frac{1}{n} \sum_{i=1}^{n} (x_i - \hat{\mu})^2 - s^2 \right\}. \tag{8}
\]
When $\mu$ is fixed at zero, this solution is similar to the one implied by the positive-part James-Stein estimator, with the difference that it divides $\sum_{i=1}^{n} x_i^2$ by $n$ rather than by $n - 2$ (Efron and Morris 1973). For the heteroskedastic case (1), the likelihood $L(\mu, \sigma^2)$ has a closed form but must be maximized numerically.

In both the homoskedastic and heteroskedastic cases, the posterior distributions
\[
p(\theta_i \mid x_i, s_i, \hat{g}) \propto \hat{g}(\theta_i) p(x_i \mid \theta_i, s_i) \tag{10}
\]
are normal distributions which are available analytically.

### 2.2. Sparse priors

Although the normal prior family has the advantage of simplicity, in practice more flexible priors are usually preferred. In particular, one would often like the prior to be able to capture sparsity in $\theta := \{\theta_1, \ldots, \theta_n\}$. One approach is to use a “spike-and-slab” prior; that is, a mixture consisting of two components, one a point-mass at zero (the “spike”) and the other (the “slab”) belonging to some family of continuous distributions, usually symmetric and centered at zero. A common choice is the “point-normal” family,
\[
\mathcal{G}_{\text{pn}} := \{ g : g(x) = \pi_0 \delta_0(x) + (1 - \pi_0)\mathcal{N}(x; 0, \sigma^2), 0 \leq \pi_0 \leq 1, \sigma^2 > 0 \}, \tag{11}
\]
in which $\delta_y(x)$ denotes the density function at $x$ for the delta-Dirac mass centered at $y$.

With this choice, estimating $g$ reduces to estimating two parameters, $\pi_0$ and $\sigma$. Similar to the family of normal distributions, the likelihood for the point-normal prior family has a closed form, and standard numerical optimization methods can be used to efficiently find the maximum-likelihood solution. Given $\hat{g} \in \mathcal{G}_{\text{pn}}$, the posterior distributions (10) are mixtures of a point-mass at zero and a normal distribution, and are available analytically.

As Johnstone and Silverman (2005b) showed, replacing the normal slab with a “heavy-tailed” distribution generally improves accuracy. Their EbayesThresh software, available in R and S-PLUS (Johnstone and Silverman 2005a), implements two such priors: the point-Laplace prior,
\[
\mathcal{G}_{\text{pl}} := \{ g : g(x) = \pi_0 \delta_0(x) + (1 - \pi_0)\text{Laplace}(x; 0, a), 0 \leq \pi_0 \leq 1, a \geq 0 \}, \tag{12}
\]
in which \( \text{Laplace}(x; \mu, a) \) denotes the probability density of the Laplace distribution \( \text{(Gelman et al. 2014)} \) at \( x \) with mean \( \mu \) and scale \( a \), and a family of priors in which the slab has “Cauchy-like” tails. Again, maximum-likelihood estimates \( \hat{g} \in G \) can be found using numerical methods.

Another parametric prior that is well-suited for capturing sparse signals is the horseshoe prior \( \text{(Carvalho et al. 2010)} \), which models sparsity by having appreciable mass near zero rather than exactly at zero. The R package \texttt{horseshoe} \( \text{(Van der Pas et al. 2019)} \) solves the homoskedastic EBNM problem with \( G \) the family of horseshoe distributions. See Bhadra et al. \( \text{(2019)} \) for a review of other implementations of the horseshoe prior.

### 2.3. Nonparametric approaches

The estimate of \( g \) when \( G \) is the unconstrained family of all distributions is called the nonparametric maximum-likelihood estimate (NPMLE) \( \text{(Kiefer and Wolfowitz 1956; Laird 1978; Lindsay 1983; Jiang and Zhang 2009; Koenker and Mizera 2014; Dicker and Zhao 2016)} \). In practice, most nonparametric methods approximate this family, which we denote as \( \tilde{G}_{\text{npmle}} \), by a dense but finite mixture of point masses,

\[
\tilde{G}_{\text{npmle}} := \left\{ g : g(x) = \sum_{k=1}^{K} \pi_k \delta_{\mu_k}(x) \mid \pi_1, \ldots, \pi_K \geq 0, \sum_{k=1}^{K} \pi_k = 1 \right\},
\]

where \( \mu_1, \ldots, \mu_K \) is a fixed, dense grid of values spanning the range of the observations. Estimating \( g \in \tilde{G}_{\text{npmle}} \) amounts to solving the constrained optimization problem,

\[
\begin{align*}
\text{maximize} & \quad L\pi \\
\text{subject to} & \quad 0 \preceq \pi \preceq 1_K \\
& \quad \pi^\top 1_K = 1,
\end{align*}
\]

where \( \pi := (\pi_1, \ldots, \pi_K)^\top \), \( 1_K \) is a column vector of ones of length \( K \), and \( L \in \mathbb{R}^{n \times K} \) is the matrix with entries \( L_{ik} = \mathcal{N}(x_i; \mu_k, \sigma_k^2) \). This is a convex optimization problem \( \text{(Koenker and Mizera 2014)} \). The R package \texttt{REBayes} \( \text{(Koenker and Gu 2017)} \) implements an efficient solution based on interior point optimization methods \( \text{(MOSEK ApS 2019)} \), but see Kim et al. \( \text{(2020)} \) and Zhang et al. \( \text{(2022)} \) for other approaches.

Although the fully nonparametric approach is the most flexible, the NPMLE is a discrete distribution \( \text{(Laird 1978)} \), so posterior distributions \( \text{(10)} \) are discrete as well. While the posterior mean from a discrete prior may be perfectly adequate for point estimation, interval estimates can be unsatisfactory. The R package \texttt{deconvolveR} \( \text{(Narasimhan and Efron 2020)} \) uses a natural spline basis to obtain a smoothed nonparametric estimate of \( g \), which yields sensible interval estimates and can outperform the NPMLE in certain respects when the true prior is smooth \( \text{(Koenker 2017)} \).

### 2.4. Constrained nonparametric approaches

Constrained nonparametric approaches can offer a middle ground, retaining much of the flexibility of fully nonparametric approaches while avoiding the potential perils of “overfitting” \( \text{(Hastie et al. 2009)} \). Stephens \( \text{(2017)} \) argued that the set of all distributions that are unimodal at zero can be a particularly good choice for \( G \) in the context of multiple testing. If it is
reasonable to assume that the prior \( g \) is symmetric, one can instead take \( \mathcal{G} \) to be the family of scale mixtures of normals,

\[
\mathcal{G}_{\text{smn}} := \{ g : g(x) = \int_0^\infty \mathcal{N}(x; 0, \sigma^2) \, dh(\sigma^2) \text{ for some } h \},
\]

or, for slightly more flexibility, the family of all symmetric distributions that are unimodal at zero, which can be represented by scale mixtures of uniform distributions,

\[
\mathcal{G}_{\text{symm-u}} := \{ g : g(x) = \int_0^\infty \text{Unif}(x; -a, a) \, dh(a) \text{ for some } h \},
\]

in which \( \text{Unif}(x; a, b) \) denotes the probability density function at \( x \) of the uniform distribution on the interval \([a, b]\).

When these families are approximated by finite mixtures, estimating \( g \) reduces to the same convex optimization problem that arises from the NPMLE, and can again be solved using fast algorithms for convex optimization. This approach is implemented in the \texttt{R} package \texttt{ashr} (Stephens et al. 2023), which, by default, uses \texttt{mixsqp} (Kim et al. 2020) to solve the optimization problem (14).

### 3. The \texttt{ebnm} package: implementation and usage

The \texttt{ebnm} package provides a unified interface for solving the EBNM problem using a wide variety of prior assumptions, including all of the choices of prior family discussed above in Section 2. In addition to making available existing implementations via a shared interface, the package provides new implementations for several simple but useful prior families that, to our knowledge, have not previously been implemented, such as the normal and point-normal prior families \( \mathcal{G}_{\text{norm}} \) and \( \mathcal{G}_{\text{pn}} \). The underlying computations for all prior families have been carefully optimized (see Section 3.2 below). The implemented prior families are summarized in Table 1. Note, also, that \texttt{ebnm} was designed to be easily extensible to other prior families; to facilitate and encourage such extensions, we have written a vignette, “Extending \texttt{ebnm} with custom \texttt{ebnm}-style functions,” available on the \texttt{ebnm} package website.

#### 3.1. The \texttt{ebnm()} function

The \texttt{ebnm()} function is the main interface to the EBNM methods. It has the following input arguments, which, apart from the first argument \( x \), are all optional:

- \( x \): The vector of observations, \( x = \{x_1, \ldots, x_n\} \).
- \( s \): The vector of standard errors, \( s = \{s_1, \ldots, s_n\} \). (\( s \) may be a scalar for the homoskedastic case.)
- \texttt{prior\_family}: The choice of prior family \( \mathcal{G} \) (see Table 1).
- \texttt{mode}: For prior families that are unimodal, this argument specifies the location of the mode. The mode may also be estimated by setting \texttt{mode} = "estimate".
- \texttt{scale}: This is either the scale parameter (for parametric priors) or the grid of parameters used to approximate the nonparametric prior. By default it is \texttt{scale} = "estimate", which directs \texttt{ebnm} either to estimate the scale or to automatically select the grid using grid selection strategies described in Willwerscheid (2021).
- **g_init**: An initial estimate \( \hat{g} \) which can be used to improve the search for a maximum-likelihood estimate.

- **fix_g**: A boolean value, which when TRUE causes the prior to be fixed to \( g_{\text{init}} \) (which must be provided) so that the posterior distributions are computed at this initial estimate.

- **output**: A character vector indicating which quantities should be output.

- **optmethod**: The name of the optimization method to use. (Currently, this option is only relevant for parametric prior families; see Section 3.2 below.)

- **control**: A list of control parameters to be passed to the optimization function.

The `ebnm()` outputs include:

- **fitted_g**: The estimated prior \( \hat{g} \).

- **log_likelihood**: The log-likelihood at \( \hat{g} \), which can be used to compare quality of fit across different priors or prior families:

  \[
  \log p(x_1, \ldots, x_n \mid s, \hat{g}) = \sum_{i=1}^{n} \log \int p(x_i \mid \theta_i, s_i) \hat{g}(\theta_i) \, d\theta_i. \tag{17}
  \]

- **posterior**: Summaries of the posterior distributions \( p(\theta_i \mid x_i, s_i, \hat{g}) \), including posterior means, posterior standard deviations and local false sign rates (Stephens 2017),

  \[
  lfsr(i) := \min \{ p(\theta_i \leq 0 \mid x_i, s_i, \hat{g}), p(\theta_i \geq 0 \mid x_i, s_i, \hat{g})\}. \tag{18}
  \]

- **posterior_sampler**: A function that can be used to generate random samples from the posterior distributions.

The return value is an object of class "ebnm". Many of the S3 methods that are typically associated with model fits in R also work for objects of class "ebnm", including:

- **summary()**: Gives an overview of the fitted model.

- **plot()**: Produces a scatterplot comparing the observations \( x_i \) against posterior estimates of the true means \( \theta_i \) and, optionally, a visualization of the prior cumulative density function.

- **nobs()**: Returns the number of observations \( n \) used to fit the model.

- **coef()**: Returns the posterior means from the fitted model, \( \hat{\theta}_i := \mathbb{E}(\theta_i \mid x_i, s_i, \hat{g}) \).

- **vcov()**: Returns the posterior variances, \( \text{Var}(\theta_i \mid x_i, s_i, \hat{g}) \).

- **fitted()**: Returns a data frame that includes various posterior summary statistics for the unknowns means \( \theta_i \) such as posterior means and variances.

- **residuals()**: Returns the “residuals”, which we define as the differences \( x_i - \hat{\theta}_i \).

- **logLik()**: Returns the log-likelihood at \( \hat{g} \).
• `simulate()`: Generates random draws of each $\theta_i$ from their posterior distributions.

• `quantile()`: Uses the sampler to compute posterior quantiles for each $\theta_i$.

• `confint()`: Uses the sampler to compute posterior “credible intervals” for each $\theta_i$. We define the $(1 - \alpha)\%$ credible interval for $\theta_i$ as the narrowest continuous interval $[a_i, b_i]$ such that $\theta_i \in [a_i, b_i]$ with posterior probability at least $1 - \alpha$, where $\alpha \in (0, 1)$. We estimate these credible intervals using Monte Carlo methods. The proportion $1 - \alpha$ is specified by the `level` argument to `confint()`, and is 0.95 by default.

• `predict()`: Uses the fitted prior $\hat{g}$ to compute posterior mean estimates $\hat{\theta}_i^{\text{new}}$ for a different set of observations $x_i^{\text{new}}$ (with standard deviations $s_i^{\text{new}}$). This could be used, for example, to provide a more reliable measure of the model fit’s quality by computing the accuracy of predictions over a test set.

We illustrate several of these methods in Section 5 and in the package vignettes.

3.2. Details of the optimization

The `ebnm()` function involves two key computations:

1. **Estimate the prior.** Specifically, compute $\hat{g} := \arg\max_{g \in \mathcal{G}} L(g)$, where $L(g)$ denotes the marginal likelihood,

   $$L(g) := p(x \mid g, s) = \prod_{i=1}^{n} \int p(x_i \mid \theta_i, s_i) g(\theta_i) \, d\theta_i,$$

   where $x := (x_1, \ldots, x_n)$ and $s := (s_1, \ldots, s_n)$.

2. **Compute posterior quantities.** `ebnm()` outputs various summaries from the posterior distributions (means, variances, etc.) obtained using the estimated prior $\hat{g}$,

   $$p(\theta_i \mid x_i, s_i, \hat{g}) \propto \hat{g}(\theta_i) p(x_i \mid \theta_i, s_i).$$

The complexity of both steps depends upon the choice of prior family $\mathcal{G}$ (see Table 1), but in most cases estimating the prior is the most difficult and computationally intensive step; for all but the simplest prior families, it involves the use of numerical optimization algorithms to compute $\hat{g}$.

**Parametric priors**

Parametric priors available in `ebnm` include the normal, point-normal, point-Laplace, point-exponential, and horseshoe prior families. For normal, point-normal, and point-Laplace priors, the prior mode can either be estimated or fixed at zero. We developed special implementations for each of these prior families with the exception of the horseshoe, for which we relied on the `horseshoe` package (Van der Pas et al. 2019).

A closed-form solution is available only for the normal prior with homoskedastic errors. In all other cases we use numerical methods to search for parameter estimates maximizing the
Table 1: Prior families implemented in ebnm. The “prior_family” column gives the corresponding prior_family argument to ebnm(). The “Source” column gives the name of the R package that implements the model fitting routines. “Support” indicates whether the prior has support for only positive realizations of $\theta_i$ (+) or all real numbers (±). A “yes” in the “Sym?” column means that the prior is symmetric about its mode. The “flat” prior, which is mainly intended for use as a point of comparison with other prior families, is a special case with no parameters, and recovers the maximum-likelihood estimates $\hat{\theta}_i = x_i$. Note that some specialized priors such as the “generalized binary prior” (Liu et al. 2023) are not included in this table; run help(ebnm) for information on such priors.

For parametric prior families, this involves searching for at most three parameters: the scale of the slab component, the mixture weight for the spike, and, when mode = "estimate", the mode.

We found that several off-the-shelf optimizers worked well for fitting parametric priors, although care was needed in implementing the underlying objective and gradient computations to avoid numerical issues. In particular, we found that the quasi-Newton method nlm() from the stats package worked very reliably in our tests across a range of parametric prior families. Therefore, we chose this method to be the default for estimating the prior in all cases except the horseshoe, which uses the stats function optimize() (this was the choice made by the authors of the horseshoe package).
Since other optimization methods might be preferred in some circumstances — say, when dealing with large or complex data sets, or to refine the estimation of the prior — we have designed the package to allow for the use of other off-the-shelf optimization methods. Further, we allow the user to specify whether to use analytical gradients and Hessians, or whether gradients and/or Hessians are be estimated numerically (which is often faster, especially when the analytical calculations are complex). These options are controlled by the `optmethod` argument to `ebnm()`. The default for most parametric priors, "nohess_nlm", uses `nlm()` with gradients calculated analytically and Hessians estimated numerically. Alternatives include "nlm" (both gradients and Hessians are calculated analytically); "nograd_nlm" (both gradients and Hessians are estimated numerically); "lbfgsb" and "nograd_lbfgsb", which use the L-BFGS-B algorithm as implemented in the `stats` function `optim()` (L-BFGS-B always estimates Hessians numerically, so the two options use, respectively, analytical and numerical gradients); and the trust region method from the `trust` package (Geyer 2020), which requires analytical gradients and Hessians (`optmethod = "trust"`).

In our benchmarking experiments (Appendix A.1), "nohess_nlm" was either the fastest method or differed from the fastest by less than a factor of two. All of the other `nlm()` methods reliably converged to a solution, as did the `trust()` method, but these other methods tended to be somewhat slower than "nohess_nlm". The L-BFGS-B methods were the least reliable; they occasionally failed to find a solution, particularly in the “null” setting where the true prior was a point mass at zero.

**Constrained nonparametric priors**

The constrained nonparametric families — scale mixtures of normals and the unimodal, symmetric unimodal, and nonnegative unimodal families — are all implemented in package `ashr` (Stephens et al. 2023), which uses the mix-SQP algorithm (Kim et al. 2020) as its default optimization method. Different optimization methods can again be specified via the `optmethod` argument to `ebnm()`: for details on these different optimization methods, see the documentation in the `ashr` package. The only constrained nonparametric family that does not rely on `ashr` is the family of scale mixtures of normals. For this family, we re-implemented the `ashr` algorithm with the aim of improving efficiency. Our implementation improved the runtime over `ashr` by a full order of magnitude for data sets with $n \approx 1,000$ (Appendix A.2).

**Nonparametric priors**

The NPMLE can, in principle, be computed using `ashr`, but this computation is cumbersome since `ashr` requires the user to specify the grid of point masses in advance. Further, we have found that, as with scale mixtures of normals, `ashr` can be slow for large data sets. The `REBayes` package (Koenker and Gu 2017) was developed specifically for the NPMLE, and is typically very fast, but it relies on the commercial interior-point solver MOSEK (MOSEK ApS 2019). Therefore, in order to provide a fully open-source toolkit that does not require installation of commercial software, we re-implemented estimation of the NPMLE in `ebnm` using the open-source package `mixsqp` (Kim et al. 2020). As with the constrained nonparametric prior families, `optmethod = "mixsqp"` is the default setting. If desired, however, the `REBayes` algorithm can be used by setting `optmethod = "REBayes"`. In our tests, `mixsqp` was typically faster than `REBayes` for smaller $K$ (the number of mixture components in the prior; see eq. 13), whereas `REBayes` was often faster than `mixsqp` when $K$ approached or
Figure 2: Results of fitting EBNM models with different prior families to “Normal”, “Point-t” and “Asymmetric tophat” data sets. For each prior family, the table gives the following quantities averaged across EBNM analyses of 20 data sets with $n = 1,000$ observed means, with “better” results highlighted using darker shades of green: the log-likelihood at $\hat{g}$ relative to the log-likelihood attained by the NPMLE (higher log-likelihoods are better); the root mean-squared error (lower RMSEs are better); and the proportion of 90% posterior credible intervals containing the true mean (CI coverage values closer to 0.9 are better).

exceeded 80 (see Appendix A.2).

4. Numerical comparisons of prior families

To test our implementations and to compare prior families, we simulated data sets from three different data-generating distributions:

1. Normal. In this simplest case, we simulated from a normal prior, $\theta_i \sim \mathcal{N}(0, 2^2)$.

2. Point-t. In this second, more challenging scenario, the prior was both sparse and heavy-tailed, yet still symmetric: $\theta_i \sim 0.8\delta_0 + 0.2t_5(0, 1.5)$, where $t_\nu(\mu, \sigma)$ denotes the Student-t distribution with location $\mu$, scale $\sigma$, and $\nu$ degrees of freedom.

3. Asymmetric Tophat. In the third simulation scenario, we simulated data with uniformly-distributed means, $\theta_i \sim \text{Unif}(-5, 10)$. Although this scenario is perhaps less realistic than the other simulations, it yields data sets that are best modeled with nonparametric or constrained nonparametric priors.

In all simulations, we generated the observations as $x_i \sim \mathcal{N}(\theta_i, 1)$. 
Figure 2 summarizes results from running EBNM analyses on 10 data sets in each of the three simulation scenarios, with $n = 1,000$ observations in each data set. We used the following three measures to evaluate the EBNM model fits:

a. The log-likelihood, which, for ease of interpretation, is shown relative to the log-likelihood attained at the NPMLE estimate. (In theory, the NPMLE estimate should always give the highest likelihood because the family of all distributions includes all other prior families as proper subsets.) These log-likelihoods were obtained by calling `logLik()` on the `ebnm()` return value.

b. The root mean-squared error, $\text{RMSE} := \sqrt{\frac{\sum_{i=1}^{n}(\hat{\theta}_i - \theta_i)^2}{n}}$, where $\hat{\theta}_i$ denotes the posterior mean estimate, $\hat{\theta}_i := \mathbb{E}(\theta_i \mid x_i, s_i, \hat{g})$. These estimates were obtained by calling `coef()` on the `ebnm()` return value.

c. The proportion of true means $\theta_i$ that are contained within the 90% posterior credible intervals, which were obtained by calling `confint()` on the `ebnm()` return value. (For our method for computing credible intervals, see Section 3.1 above.)

As expected, the model fit returned by `ebnm()` with `prior_family = "npmle"` always attained the largest log-likelihood. More generally, log-likelihoods were largely (though not exactly) aligned with the orderings implied by nestings of prior families, such as, for example,

$$\mathcal{G}_{\text{norm0}} \subset \mathcal{G}_{\text{pn}} \subset \mathcal{G}_{\text{smn}} \subset \mathcal{G}_{\text{symm-u}} \subset \mathcal{G}_{\text{npmle}}.$$  \hspace{1cm} (21)

Prior families that were a poor match with the distribution used to simulate the data typically had worse log-likelihoods.

The RMSE evaluates the quality of the posterior estimates $\hat{\theta}_i$ generated by an EBNM analysis. Reassuringly, nearly all prior families improved upon the maximum-likelihood estimates $\hat{\theta}_i = x_i$ returned by the “flat” prior, which we included as a baseline. However, the improvement was sometimes small, particularly when the prior family was a poor match with the true distribution (e.g., symmetric prior families in the asymmetric tophat scenario). In general, higher log-likelihoods were indicative of better accuracy in estimates of $\theta_i$. Exceptions are suggestive of overfitting; for example, the RMSE for the NPMLE was typically worse than for prior families that better matched the true distribution.

The “CI coverage” measures how well posterior credible intervals are calibrated. A known limitation of empirical Bayes methods is that they often underestimate uncertainty in the posteriors, since uncertainty in the estimate of $g$ is not taken into account (see, for example, Ignatiadis and Wager 2022). Indeed, the credible intervals tended to be too small (i.e., less than 90%) for most prior families and simulation scenarios (Figure 2). Still, the intervals were usually not far off the target coverage of 90%, showing a surprising robustness to modeling assumptions. The lone exception was the NPMLE, which tended to have much poorer coverage because, as noted in Section 2.3, it results in a discrete prior that can greatly underestimate uncertainty.

Finally, to assess the ability of our implementation to handle large data sets, we recorded runtimes for simulated (point-t) data sets ranging in size from $n = 200$ to $n = 1,000,000$. These analyses were performed in R 4.2.2 on a desktop running Windows 11 Pro with an Intel Core i9-13900KF multicore processor and 32 GB of memory. Results are summarized in
Figure 3: Runtimes for fitting EBNM models with different prior families to data sets ranging in size from \( n = 100 \) to \( n = 1,000,000 \). For each combination of sample size \( (n) \) and prior family, an EBNM model was fit to 20 data sets simulated using the Point-\( t \) distribution. Each point in the plot gives the average runtime over all 20 simulations; the error bars depict 10% and 90% quantiles.

As expected, the less flexible priors with the fewest parameters tended to also be the fastest, whereas the most complex methods (e.g., unimodal prior, NPMLE) were slower than the fastest methods by multiple orders of magnitude. Most importantly, all prior families implemented in \texttt{ebnm} scaled well to large data sets; the computational effort grew linearly or close to linearly in \( n \).

5. An analysis of weighted on-base averages with \texttt{ebnm}

In this section, we illustrate the key features of \texttt{ebnm} in an analysis of baseball statistics. See the package vignette for an expanded version of this example.

5.1. The “wOBA” data set

We begin by loading and inspecting the \texttt{wOBA} data set, which consists of wOBAs (“weighted on-base averages”) and standard errors for the 2022 MLB regular season:

\begin{verbatim}
R> library("ebnm")
R> data("wOBA")
R> nrow(wOBA)

[1] 688

R> head(wOBA)
\end{verbatim}
| FanGraphsID | Name       | Team | PA | x     | s     |
|------------|------------|------|----|-------|-------|
| 1          | Khalil Lee | NYM  | 2  | 1.036 | 0.733 |
| 2          | Chadwick Tromp | ATL | 4  | 0.852 | 0.258 |
| 3          | Otto Lopez  | TOR  | 10 | 0.599 | 0.162 |
| 4          | James Outman | LAD | 16 | 0.584 | 0.151 |
| 5          | Matt Carpenter | NYY | 154| 0.472 | 0.054 |
| 6          | Aaron Judge  | NYY  | 696| 0.458 | 0.024 |

Column “x” contains observed wOBAs, which we interpret as estimates of a player’s hitting ability. Column “s” gives standard errors. See Appendix B for background on the wOBA statistic and details on how standard errors were calculated.

Most players finished the season with a wOBA between .200 and .400. A few had very high wOBAs (> .500), while others had wOBAs at or near zero. A casual inspection of the data suggests that players with these extreme wOBAs were simply lucky (or unlucky). For example, the 4 players with the highest wOBAs (included in the code output above) each had fewer than 20 plate appearances. (The number of plate appearances, or PAs, is the sample size over which wOBA is measured for each hitter, so smaller numbers of PAs are generally associated with larger standard errors.)

In contrast, Aaron Judge’s production — which included a record-breaking number of home runs — appears to be “real,” since it was sustained over nearly 700 PAs. Other cases are more ambiguous: how, for example, are we to assess Matt Carpenter, who had several exceptional seasons between 2013 and 2018 but whose output steeply declined in 2019–2021 before his surprising “comeback” in 2022? An empirical Bayes analysis can help to answer this and other questions.

5.2. The “ebnm” function

Function `ebnm()` is the main interface for fitting the empirical Bayes normal means model (1–2); it is a “Swiss army knife” that allows for various choices of prior family \( \mathcal{G} \) as well as multiple options for fitting and tuning models. For example, we can fit a normal means model with \( \mathcal{G} \) taken to be the family of normal distributions as follows:

```r
R> x <- wOBA$x
R> s <- wOBA$s
R> names(x) <- wOBA$Name
R> names(s) <- wOBA$Name
R> fit_normal <- ebnm(x, s, prior_family = "normal", mode = "estimate")
```

(The default behavior is to fix the prior mode at zero. Since we certainly do not expect the distribution of true hitting ability to be centered at zero, we set `mode = "estimate"`.)

The `ebnm` package has a second model-fitting interface in which each prior family gets its own function:

```r
R> fit_normal <- ebnm_normal(x, s, mode = "estimate")
```

Textual and graphical overviews of results can be obtained using the `summary()` and `plot()` methods. The `plot()` method returns a "ggplot" object (Wickham 2016), so that the plot
Figure 4: Initial wOBA estimates ("observations") vs. posterior mean wOBA estimates, in which the posterior estimates were obtained by fitting a prior from the family of normal distributions. The color of the points is varied by the number of plate appearances. The dashed line shows the diagonal \((x = y)\) line.

can be conveniently customized using \texttt{ggplot2}. For example, we can vary the color of points by the number of plate appearances:

\begin{verbatim}
R> plot(fit_normal) +
+ geom_point(aes(color = sqrt(wOBA$PA))) +
+ labs(x = "wOBA", y = "EB estimate of true wOBA skill",
+ color = expression(sqrt(PA))) +
+ scale_color_gradient(low = "blue", high = "red")
\end{verbatim}

The resulting plot, shown in Figure 4, compares the initial wOBA estimates — that is, the first input in the \texttt{ebnm()} call — against the posterior estimates returned by \texttt{ebnm()}. The plot tells us that wOBAs associated with fewer plate appearances (blue points) were shrunk toward the league average (near .300) much more strongly than wOBAs for hitters with many plate appearances (red points).

Let us revisit the first 6 hitters in the data set to see what the EBNM model suggests about their true hitting ability. The \texttt{fitted()} method returns a posterior summary for each hitter (by default, the posterior mean and standard deviation):

\begin{verbatim}
> print(head(fitted(fit_normal)), digits = 3)

 mean  sd
Khalil Lee    0.303 0.0287
Chadwick Tromp 0.308 0.0286
Otto Lopez    0.310 0.0283
James Outman  0.311 0.0282
Matt Carpenter 0.339 0.0254
Aaron Judge   0.394 0.0184
\end{verbatim}
Estimates for the first four ballplayers are shrunk strongly toward the league average, reflecting the fact that these players had very few plate appearances. Carpenter had many more plate appearances (154) than these other four players, but according to this model we should remain skeptical about his strong performance; after factoring in the prior, we judge his “true” talent to be much closer to the league average, downgrading an observed wOBA of .472 to the posterior mean estimate of .339.

5.3. Comparing different priors

Judge’s “true” talent is also estimated to be much lower (.394) than his observed wOBA (.458) despite sustaining this high level of production over a full season (696 PAs). For this reason, one might ask whether a prior that is more flexible than the normal prior — that is, a prior that can better adapt to “outliers” like Judge — might produce a different result. The \texttt{ebnm} package is very well suited to answering this question. For example, to obtain results using the family of all unimodal priors rather than a normal prior, we need only update the argument to \texttt{prior\_family}:

\begin{verbatim}
R> fit_unimodal <- ebnm(x, s, prior\_family = "unimodal", mode = "estimate")
\end{verbatim}

Using this prior, estimates for players with many plate appearances and outlying performances (very high or very low wOBAs) are not adjusted quite so strongly toward the league average. Judge’s estimated “true” talent, for example, remains much closer to his observed wOBA:

\begin{verbatim}
R> dat <- cbind(wOBA[, c("PA","x")],
+       fitted(fit_normal),
+       fitted(fit_unimodal))
R> names(dat) <- c("PA", "x", "mean\_n", "sd\_n", "mean\_u", "sd\_u")
R> print(head(dat), digits = 3)
\end{verbatim}

\begin{tabular}{lcccccc}
PA & x & mean\_n & sd\_n & mean\_u & sd\_u \\
Khalil Lee & 2 & 1.036 & 0.303 & 0.302 & 0.0277 \\
Chadwick Tromp & 4 & 0.852 & 0.308 & 0.307 & 0.0306 \\
Otto Lopez & 10 & 0.599 & 0.310 & 0.310 & 0.0315 \\
James Outman & 16 & 0.584 & 0.311 & 0.311 & 0.0318 \\
Matt Carpenter & 154 & 0.472 & 0.339 & 0.355 & 0.0430 \\
Aaron Judge & 696 & 0.458 & 0.394 & 0.439 & 0.0155 \\
\end{tabular}

Carpenter’s estimated “true” talent is also higher, but is still adjusted much more than Judge’s in light of Carpenter’s smaller sample size. Interestingly, the unimodal prior also assigns greater uncertainty (the “sd\_u” column) to Carpenter’s estimate than does the normal prior.

5.4. Reanalysis using a nonparametric prior

An alternative to prior families that make specific assumptions about the data is to use the prior family that contains all distributions \(G_{npmle}\), which is in a sense “assumption free” (see Section 2.3 for background). Note that although nonparametric priors require specialized computational techniques, switching to a nonparametric prior is seamless in \texttt{ebnm}, as these
Figure 5: The CDFs for priors fitted to the 2022 MLB wOBA data: the normal prior (prior_family = "normal"), the unimodal prior (prior_family = "unimodal"), and the NPMLE (prior_family = "npmle").

imputation details are hidden. Similar to above, we need only make a single change to the prior_family argument:

\texttt{R} > fit\_npmle <- ebnm(x, s, prior\_family = "npmle")

(Note that because the family \( G_{\text{npmle}} \) is not unimodal, the mode = "estimate" option is not relevant here.)

We visually compare the three fits obtained so far using the \texttt{plot()} method. We use the subset argument to focus on results for Judge and other players with a large number of plate appearances, and we include argument incl\_cdf = TRUE to also show the cumulative distribution functions (CDFs) of the fitted priors \( \hat{g} \):

\texttt{top50 <- order(wOBA$PA, decreasing = TRUE)}
\texttt{top50 <- top50[1:50]}
\texttt{plot(fit\_normal, fit\_unimodal, fit\_npmle, incl\_cdf = TRUE, subset = top50)}

The plots generated by this call are shown in Figures 5 and 6. Estimates largely agree, differing primarily at the tails (e.g., Judge), where both the unimodal prior family and the NPMLE are sufficiently flexible to avoid the strong shrinkage behavior of the normal prior family.

Fits can be compared quantitatively using the \texttt{logLik()} method, which, in addition to the log likelihood for each model, usefully reports the number of free parameters or “degrees of freedom” (note that Wilks’ theorem does not apply to these nonparametric comparisons):

\texttt{R} > logLik(fit\_unimodal)
Figure 6: Initial wOBA estimates (“Observations”) vs. posterior mean wOBA estimates for priors fitted to the 2022 MLB wOBA data: the normal prior (prior_family = "normal"), the unimodal prior (prior_family = "unimodal"), and the NPMLE (prior_family = "npmle"). Results are shown only for the top 50 ballplayers by number of plate appearances.

'R' log Lik.' 992.6578 (df=40)

R> logLik(fit_npmle)
'R' log Lik.' 994.193 (df=94)

A nonparametric prior \(G\) is approximated by \(K\) mixture components on a fixed grid, with mixture proportions to be estimated (see Section 2.4). We can infer from the above output that the family of unimodal priors has been approximated by a family of mixtures over \(K = 41\) fixed components, while \(G_{npmle}\) has been approximated as a family of mixtures over a grid of \(K = 95\) point masses spanning the range of the data. (The number of degrees of freedom is one fewer than \(K\) because the mixture proportions must always sum to 1, which removes one degree of freedom from the estimation of \(\pi\).)

One potential issue with the NPMLE is that, since it is discrete (as Figure 5 makes apparent), observations are variously shrunk toward one of the support points, which can result in poor interval estimates. For illustration, we calculate 80% posterior credible intervals (since credible intervals are obtained using Monte Carlo methods, we set a seed for reproducibility):

R> fit_npmle <- ebnm_add_sampler(fit_npmle)
R> set.seed(123)
R> print(head(confint(fit_npmle, level = 0.8)), digits = 3)

|          | CI.lower | CI.upper |
|----------|----------|----------|
| Khalil Lee | 0.265    | 0.309    |
Each credible interval endpoint is constrained to lie at one of the support points of the NPMLE \( \hat{g} \). Note in particular that the NPMLE yields a degenerate interval estimate for Judge.

To address this and other issues, the \texttt{deconvolveR} package (Narasimhan and Efron 2020) uses a penalized likelihood that encourages “smooth” priors \( \hat{g} \); that is, priors \( \hat{g} \) for which few of the mixture proportions are zero:

\[
R> \text{fit_deconv <- ebnm_deconvolver(x / s, output = ebnm_output_all())}
\]

Note however that since package \texttt{deconvolveR} fits a model to \( z \)-scores rather than observations and associated standard errors, the “true” means \( \theta \) being estimated are \( z \)-scores rather than raw wOBA skill. While this may be reasonable in many settings, it does not seem appropriate for the wOBA data:

\[
R> \text{set.seed(123)}
R> \text{print(head(confint(fit_deconv, level = 0.8) * s), digits = 3)}
\]

|       | CI.lower | CI.upper |
|-------|----------|----------|
| Khalil Lee | 0.000    | 1.600    |
| Chadwick Tromp | 0.563    | 1.127    |
| Otto Lopez | 0.442    | 0.796    |
| James Outman | 0.412    | 0.742    |
| Matt Carpenter | 0.413    | 0.531    |
| Aaron Judge | 0.406    | 0.459    |

These interval estimates do not match our basic intuitions; for example, a wOBA over .600 has never been sustained over a full season.

### 6. Building on \texttt{ebnm} for new matrix factorization methods

As mentioned above in the introduction, the EBNM model underlies other well-studied statistical problems, and so there is the potential for \texttt{ebnm} to aid in the development of other software tools. One such example is matrix factorization: as Wang and Stephens (2021) showed, fitting an empirical Bayes matrix factorization (EBMF) model can be reduced to solving a sequence of EBNM problems (typically very many of them). Therefore, the aspects that we have emphasized in developing \texttt{ebnm} — the unified interface, the variety of prior families and fitting options, and the speed and robustness of the numerical optimization — have greatly facilitated the creation of a flexible software framework for EBMF in the R package \texttt{flashier} (Willwerscheid et al. 2023), available on CRAN and GitHub (https://github.com/willwerscheid/flashier/)
In matrix factorization, we attempt to approximate a data matrix $X$ by a low-rank matrix product, $X \approx LF^\top$. The EBMF approach introduces priors on the low-rank matrices $L$ and $F$:

$$X = LF^\top + E$$
$$e_{ij} \sim \mathcal{N}(0, \sigma^2)$$
$$\ell_{ik} \sim g_{\ell}^{(k)} \in G_\ell$$
$$f_{jk} \sim g_{f}^{(k)} \in G_f,$$

where $X$, $L$, $F$, and $E$ are, respectively, matrices of dimension $n \times p$, $n \times K$, $p \times K$, and $n \times p$ storing real-valued elements $x_{ij}$, $l_{ik}$, $f_{jk}$, and $e_{ij}$, and $G_\ell, G_f$ are specified prior families. In brief, each iteration of the EBMF model-fitting algorithm involves solving an EBNM problem separately for each column of $L$ (using the prior family $G_\ell$) and each column of $F$ (using the prior family $G_f$). The solutions to these EBNM problems yield fitted priors $\hat{g}_{\ell}^{(k)}$, $\hat{g}_{f}^{(k)}$ and posterior estimates of $\ell_{ik}$ and $f_{jk}$. See Wang and Stephens (2021) for details.

The EBMF framework is highly flexible in that different choices of prior families $G_\ell$ and $G_f$ can give very different factorizations. For example, the use of normal priors yields factorizations similar to the truncated singular value decomposition (SVD) (Nakajima and Sugiyama 2011). The use of sparse priors (e.g., the point-normal prior family) can yield sparse matrix factorizations, which in many settings are more interpretable than an SVD (Engelhardt and Stephens 2010; Yang et al. 2014; Witten et al. 2009). By choosing priors with nonnegative support (e.g., the point-exponential family), one can obtain nonnegative factorizations (Lee and Seung 1999). More novel combinations are also possible: for example, one can obtain a semi-nonnegative matrix factorization (Ding et al. 2010; Wang et al. 2019; He et al. 2020) by choosing a prior family with nonnegative support for $G_\ell$ and a prior family without constraints for $G_f$; and Liu et al. (2023) proposed the family of “generalized binary” priors to encourage binary-valued $l_{ik}$.

By building on the fast and reliable methods in ebnm, the flashier package makes it straightforward to obtain any of these kinds of matrix factorization (and many more). For example, a sparse factorization can be obtained by calling the flashier function `flash()` with argument `ebnm_fn = ebnm_point_normal`, which specifies point-normal distributions for all priors $g_{\ell}^{(k)}$ and $g_{f}^{(k)}$. To obtain a sparse, semi-nonnegative factorization, one need only update the argument as `ebnm_fn = c(ebnm_point_exponential, ebnm_point_normal)`, which specifies point-normal priors for all $g_{f}^{(k)}$ and point-exponential priors for all $g_{\ell}^{(k)}$. In general, any of the prior families discussed above can be used (see Table 1), and if some other option is desired, it is not difficult to implement a new “ebnm-style” function (see the ebnm package vignette for details).

We provide a detailed illustration of these ideas in the flashier package vignette, “Introduction to flashier,” available on the package’s website (https://willwerscheid.github.io/flashier/).

### 7. Summary

The ebnm package provides a comprehensive toolkit for solving the empirical Bayes normal means (EBNM) problem under a variety of prior assumptions. In many situations — as in our analysis of baseball statistics in Section 5 — the “best” choice of prior family is not
known in advance. The \texttt{ebnm} package is especially well-suited to handling such situations by providing a large set of prior families to choose from (Table 1), and an interface that allows for convenient comparison of different prior families. When deciding which prior family to proceed with, our general recommendation is to weigh prior assumptions about the data against empirical measures of fit. The best prior will very often depend on the context, and for this reason we have designed \texttt{ebnm} to be easily extensible so that researchers are not limited by the existing options. Our ultimate hope is that experts in other research areas will consider contributing to our package and help expand the use of EBNM methods to other domains.

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### A. Supplementary benchmarking results

#### A.1. Optimization methods for parametric families

We first compare the performance of six optimization methods, all of which are implemented in *ebmm* via parameter `optmethod`. In each case, parameters are transformed so that the optimization problem is unconstrained (specifically, a log transformation is used for scale parameters, which are constrained to be nonnegative, while a logit transformation is used for mixture proportions, which are constrained to lie between zero and one).

Three choices of `optmethod` call into function `nlm()`, a Newton-type algorithm included in the base `stats` package. Gradient and Hessian functions can be provided; if they are not, `nlm()` estimates them numerically. Option `optmethod = "nlm"` provides both the gradient and Hessian functions; `optmethod = "nohess_nlm"` provides the gradient but not the Hessian; `optmethod = "nograd_nlm"` provides neither. Options `optmethod = "lbfgsb"` and `optmethod = "nograd_lbfgsb"` call into function `optim()`, also in the `stats` package, with argument `method = "L-BFGS-B"`. The former provides the gradient function; the second does not. By definition, L-BFGS-B does not accept a Hessian. Finally, `optmethod = "trust"` calls
into function `trust()`, a trust-region algorithm implemented in the `trust` package (Geyer 2020). Since `trust()` requires both a gradient and Hessian function, there is only one corresponding `optmethod`. In sum, then, there are two methods that use both gradients and Hessians ("nlm" and "trust"); two that use only gradients ("nohess_nlm" and "lbfgsb"); and two that estimate all derivatives numerically ("nograd_nlm" and "nograd_lbfgsb").

For both `ebnm_point_normal()` and `ebnm_point_laplace()`, we ran tests for $2 \times 3 \times 2 \times 3 = 36$ scenarios:

- The mode is either fixed at zero via argument `mode = 0` or estimated (via `mode = "estimate"`).
- The data-generating prior distribution $g$ is: i) a true member of the prior family, $\pi_0 \delta_\mu + (1-\pi_0)N(\mu, a^2)$ or $\pi_0 \delta_\mu + (1-\pi_0)\text{Laplace}(\mu, a)$, with $\pi_0 \sim \text{Beta}(10, 2)$, $a \sim \text{Gamma}(4, 1)$, and either $\mu = 0$ or $\mu \sim \text{Unif}(-10, 10)$; ii) the null distribution $\delta_0$; or iii) a distribution not in the prior family, so that $G$ is misspecified. When `mode = 0`, the misspecified prior is a point-normal prior as above but with $\mu \sim \text{Unif}(-10, 10)$; when `mode = "estimate"`, the misspecified prior is the point-$t_5$ distribution $\pi_0 \delta_0 + (1-\pi_0)t_5(0, a)$, with $\pi_0$ and $a$ distributed as above.
- The $N(0, s_i^2)$ noise added to the true means $\theta_i \sim g$ is either homoskedastic, with $s_i = 1$ for all $i$, or heteroskedastic, with $s_i^2 - 1 \sim \text{Exp}(1)$.
- The number of observations $n$ is 1000, 10000, or 100000.

For each scenario, we ran $10^6/n$ simulations (so, depending on $n$, 1000, 100, or 10 simulations) and compared runtimes using package `microbenchmark` (Mersmann 2019). All experiments were performed on a 2021 MacBook Pro with an Apple M1 Max processor and 64 GB of unified memory. Results are displayed in Figures 7 and 8.

In general, the methods that supplied the gradient function outperformed the methods that required all derivatives to be estimated numerically. Timing was similar among the four methods that do supply the gradient. However, method "lbfgsb" failed to converge in several of the `prior_null` simulations (in some scenarios, up to 7% of simulations resulted in an error). Further, the methods that supply Hessians ("nlm" and "trust") occasionally struggled when the data-generating prior was the null distribution $\delta_0$. We thus recommend the default setting `optmethod = "nohess_nlm"`.

### A.2. Comparisons with existing packages

Next we compare the performance of `ebnm` against three packages with directly comparable functions: function `ebnm_point_laplace()` is closely related to function `ebayesthresh()` in the `EbayesThresh` package (Silverman et al. 2017); function `ebnm_normal_scale_mixture()` is modelled on function `ash()` in the `ashr` package (with option `mixcompdist = "normal"`; Stephens et al. (2023)) but is implemented in a much simpler manner; and function `ebnm_npmle()` performs a similar task to function `GLmix()` in the `REBayes` package (Koenker and Gu 2017).

We ran tests for the same scenarios as Section A.1, with the difference that the mode is always fixed at zero (mode estimation is not possible with `EbayesThresh`). Further, since
Figure 7: Timing comparisons for `ebnm_point_normal()`. Tests in the top figure fix the mode at zero (by setting argument `mode = 0`) while those in the bottom estimate the mode (by setting `mode = "estimate"`). Different columns correspond to different data-generating priors: a true member of the point-normal prior family; the null distribution $\delta_0$; or a distribution from outside the prior family. Different rows correspond to different noise models, with the noise added to the “true” observations either homoskedastic (with $s_i = 1$ for all $i$) or heteroskedastic (with $s_i^2 \sim \text{Exp}(1)$). Plotted is the time as a multiple of the fastest time for a given combination of mode, prior, noise, and value of $n$. Shades of blue indicate optimization methods that are within a factor of 2 of the fastest method for that mode, prior, noise, and value of $n$, while shades of red indicate slower methods.
Figure 8: Timing comparisons for `ebm_point_laplace()`. See Figure 7 caption and text for details.
it is not possible to "misspecify" the prior for the family of all distributions $G_{npmle}$, we only considered a single data-generating distribution (the point-Laplace), but we varied the number of grid points (mixture components) from 10 to 300. The number of simulations, microbenchmark settings, and hardware were as described in Section A.1. We set parameters to make outputs as similar as possible. For EBayesThresh, we set $threshrule = "mean"$ and $universalthresh = FALSE$; for ash(), we set $prior = "uniform"$. Results are given in Figures 9–11.

In some scenarios, EBayesThresh was nearly as fast as $ebnm_point_laplace()$, but in others it was outperformed by a full order of magnitude. Further, $ebnm$ regularly found significantly better solutions than EBayesThresh (in terms of the final objective attained) except when the data-generating prior was the null distribution, in which cases the packages found solutions of similar quality.

When the number of observations was small, $ebnm$ was faster than ashr by a factor of around 2 to 4, but ash performed comparably to $ebnm_normal_scale_mixture()$ for large problems.

Results in the comparison between $ebnm_npmle()$ and REBayes were mixed. $ebnm$ was regularly faster when the number of mixture components was small (fewer than 80), while REBayes was consistently faster when a dense grid was used (80 or more components). According to the theory developed in Willwerscheid (2021), 80 components should be “good enough” for homoskedastic observations when

$$n^{1/4} \left( \frac{\text{range}(x)}{s} \right) \leq 80\sqrt{8}.$$  \hspace{1cm} (23)

For example, if the number of observations $n = 10^4$, then 80 components should suffice as
Figure 10: Timing comparisons: `ebnm_normal_scale_mixture` vs. `ash`. See Figure 7 caption and text for details.

Figure 11: Timing comparisons: `ebnm_npmle` vs. `REBayes`. Column headers indicate the number of grid points (mixture components) that were used to estimate the NPMLE. All simulations were from a point-Laplace distribution; the noise models (homoskedastic and heteroskedastic) are as above (see Figure 7 caption for details). The sample sizes used were \( n = 10^3 \), \( n = 10^4 \), and \( n = 10^5 \).
long as the studentized range
\[
\frac{\max(x) - \min(x)}{s} \leq 8\sqrt{8} \approx 22.6.
\] (24)

**B. Background on “weighted on-base averages”**

A longstanding tradition in empirical Bayes research is to include an analysis of batting averages using data from Major League Baseball (see, for example, Brown 2008; Jiang and Zhang 2010; Gu and Koenker 2017). Until recently, batting averages were the most important measurement of a hitter’s performance, with the prestigious yearly “batting title” going to the hitter with the highest average. However, with the rise of baseball analytics, metrics that better correlate to teams’ overall run production have become increasingly preferred. One such metric is wOBA (“weighted on-base average”), which is both an excellent measure of a hitter’s offensive production and, unlike competing metrics such as MLB’s xwOBA (Sharpe 2019) or Baseball Prospectus’s DRC+ (Judge 2019), can be calculated using publicly available data and methods.

Initially proposed by Tango et al. (2006), wOBA assigns values (“weights”) to hitting outcomes according to how much the outcome contributes on average to run production. For example, while batting average treats singles identically to home runs, wOBA gives a hitter more than twice as much credit for a home run.\(^1\)

Given a vector of wOBA weights \(w\), hitter \(i\)’s wOBA is the weighted average
\[
x_i := w^\top z^{(i)}/n_i, \tag{25}
\]
where \(z^{(i)} = (z_1^{(i)}, \ldots, z_7^{(i)})\) tallies outcomes (singles, doubles, triples, home runs, walks, hit-by-pitches and outs) over the hitter’s \(n_i\) plate appearances (PAs). Modeling hitting outcomes as i.i.d.
\[
z^{(i)} \sim \text{Multinomial}(n_i, \pi^{(i)}), \tag{26}
\]
where \(\pi^{(i)} = (\pi_1^{(i)}, \ldots, \pi_7^{(i)})\) is the vector of “true” outcome probabilities for hitter \(i\), we can regard \(x_i\) as a point estimate for the hitter’s “true wOBA skill”,
\[
\theta_i := w^\top \pi^{(i)}. \tag{27}
\]

Standard errors for the \(x_i\)’s can be estimated as
\[
s_i^2 = w^\top \hat{\Sigma}^{(i)} w/n_i, \tag{28}
\]
where \(\hat{\Sigma}^{(i)}\) is the estimate of the covariance matrix for the multinomial model (26) obtained by setting \(\pi = \hat{\pi}\),\(^2\) where
\[
\hat{\pi}^{(i)} = z^{(i)}/n_i. \tag{29}
\]

\(^1\)Weights are updated from year to year, but wOBA weights for singles have remained near 0.9 for the last several decades, while weights for home runs have hovered around 2.0 (FanGraphs 2023).

\(^2\)To deal with small sample sizes, we conservatively lower bound each standard error by the standard error that would be obtained by plugging in league-average event probabilities \(\hat{\pi}_l = \sum_{i=1}^N z^{(i)}/\sum_{i=1}^N n_i\), where \(N\) is the number of hitters in the data set.
The relative complexity of wOBA makes it well suited for analysis via **ebnm**. With batting average, a common approach is to obtain empirical Bayes estimates using a beta-binomial model (see, for example, Robinson 2017). With wOBA, one can estimate hitting outcome probabilities by way of a Dirichlet-multinomial model; alternatively, one can approximate the likelihood as normal and fit an EBNM model directly to the observed wOBAs. We take the latter approach.

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