An Open-source Bayesian Atmospheric Radiative Transfer (BART) Code. I. Design, Tests, and Application to Exoplanet HD 189733b

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Received 2019 November 10; revised 2021 April 21; accepted 2021 July 13; published 2022 April 18

Abstract

We present the open-source Bayesian Atmospheric Radiative Transfer (BART) retrieval package, which produces estimates and uncertainties for an atmosphere’s thermal profile and chemical abundances from observations. Several BART components are also stand-alone packages, including the parallel Multi-Core Markov-chain Monte Carlo (MC3), which implements several Bayesian samplers; a line-by-line radiative-transfer model, transit; a code that calculates Thermochemical Equilibrium Abundances (TEA), and a test suite for verifying radiative-transfer and retrieval codes, BARTTEST. The codes are in Python and C. BART and TEA are under a Reproducible Research (RR) license, which requires reviewed-paper authors to publish a compendium of all inputs, codes, and outputs supporting the paper’s scientific claims. BART and TEA produce the compendium’s content. Otherwise, these codes are under permissive open-source terms, as are MC3 and BARTTEST, for any purpose. This paper presents an overview of the code, BARTTEST, and an application to eclipse data for exoplanet HD 189733b. Appendices address RR methodology for accelerating science, a reporting checklist for retrieval papers, the spectral resolution required for synthetic tests, and a derivation of the effective sample size required to estimate any Bayesian posterior distribution to a given precision, which determines how many iterations to run. Paper II, by Cubillos et al., presents the underlying radiative-transfer scheme and an application to transit data for exoplanet HAT-P-11b. Paper III, by Blecic et al., discusses the initialization and post-processing routines, with an application to eclipse data for exoplanet WASP-43b. We invite the community to use and improve BART and its components at http://GitHub.com/ExOSPORTS/BART/.

Unified Astronomy Thesaurus concepts: Exoplanet atmospheric composition (2021); Exoplanet systems (484); Open source software (1866); Astrostatistics techniques (1886); Uncertainty bounds (1917); Planetary atmospheres (1244)

1. Introduction

Fitting an atmospheric spectrum model to remotely sensed data is the main way we learn the composition and thermal structure of planetary atmospheres and is the only technique viable for exoplanets for the foreseeable future. Inferring, or “retrieving,” gas properties from spectral data dates to 1859 (Kirchhoff & Bunsen 1860; Becker 2017). The line-by-line approach to calculating an atmospheric spectrum requires a computer and dates to the early 1970s or before (Anderson et al. 1994).

Atmospheric retrievals for solar system planets typically fit, either with a minimizer or by eye, a synthetic spectrum to high-resolution data (Δλ/λ ~ 1000–100,000, where λ is wavelength) with signal-to-noise ratio (S/N) > 100 per wavelength channel. In contrast, exoplanet data often have S/N ~ 10 per point and may have just a few points representing bandwidths larger than 1 μm. A simple atmospheric model with just nine free parameters (four for chemical abundances and five for the temperature structure) might fit six or even fewer broadband photometric fluxes observed at different times and loosely called a spectrum. The question then becomes, what kinds of atmospheres are consistent with the data, and how confidently? The stakes for answering this question reliably are high, as the search for life outside our solar system will likely have its first potential positive result in spectroscopic data, and those data will be as relatively crude to the problem of life detection as the exoplanet example above was to the first exoplanet atmospheric characterizations.

Thus, it is not surprising that atmospheric radiative transfer (RT) met Bayesian inference. Early grid-sampling approaches for exoplanet retrievals (Madhusudhan & Seager 2009) led
quickly to Markov-chain Monte Carlo (MCMC; Madhusudhan & Seager 2010). Madhusudhan et al. (2011) published the first fully Bayesian approach, with integrals over the posterior distribution to estimate the relative probabilities of two classes of models, C-rich and O-rich.

There are now over a dozen such codes, with more in development. Madhusudhan (2018) provides a review, and his Table 1 lists current codes, including references. Retrieval is computationally expensive, involving a full RT calculation per Bayesian iteration. The codes differ in their statistical approaches, with newer MCMC sampling algorithms reducing the number of iterations required to converge from tens of millions to hundreds of thousands and Bayesian nested sampling showing promise of even faster computation, at least for models with fewer than 10 parameters (Buchner 2016). Most of the codes use parallel processing, with Graphical Processing Units coming into play as well (Malik et al. 2017, 2018; Zhang et al. 2019, 2020). The latter makes sufficient simplifying assumptions (e.g., an isothermal atmosphere in chemical equilibrium) to run in minutes to an hour, much faster than the more general approaches of most codes. With the inclusion of high-temperature opacities, including those for ions present at such temperatures, this approach may be suitable for transits of very hot planets.

Earth’s variable atmosphere makes decontamination of ground-based spectra at the level required for exoplanet characterization challenging. Early high-resolution cross-correlation spectroscopy approaches aimed at simple detection (e.g., Wiedemann et al. 2001; Deming et al. 2005a) were ill-suited to retrieving altitude-dependent abundances and temperatures, although Snellen et al. (2010) did obtain a bulk CO abundance for HD 209458b in their landmark detection. Brogi et al. (2017) described and Brogi & Line (2019) detailed a Bayesian framework for altitude-dependent retrievals using both high-resolution ground-based and low-resolution space-based data. A concern for high-resolution spectroscopy is that wavelengths listed for spectral lines in line lists must be precise at the level of the data, which is not always the case for theoretically derived lists.

Machine learning promises dramatic speedups. Waldmann (2016) uses machine learning to identify the molecules of interest, which can otherwise take several full retrieval runs. Márquez-Neila et al. (2018) and Zingales & Waldmann (2018) have both utilized machine learning as a surrogate for retrieval modeling and found comparable results, while reducing computing time from hundreds of CPU hours to seconds and minutes, respectively, although the match of posterior distributions was not perfect (a well-known issue in machine learning). Among others, two attempts to improve on these approaches involve an RT surrogate model demonstrated using BART’s RT code (Himes et al. 2022) and a direct-to-retrieval approach using a variable number of random-forest trees (Nixon & Madhusudhan 2020).

Different retrieval codes address different observing geometries, depths in the atmosphere, and spectral regions. Mid-IR data taken around secondary eclipse, for example, include both the star’s spectrum and a planetary spectrum deriving primarily from the atmosphere’s own dayside thermal emission and subsequent self-absorption. They yield the planet-to-star flux ratio, derived from the disappearance of the planetary spectrum during the eclipse. The reflected stellar component in the mid-IR is weak, due both to the rapidly falling stellar emission at these wavelengths for all types of stars and to low planetary albedos in the mid-IR. In the near-IR and optical, the stellar emission and planetary albedo are both larger, and the planetary emission decreases, leading to a mostly reflective planetary spectrum in the optical, except possibly for the hottest planets.

However, the flux ratio to the stellar spectrum, and thus data quality, is quite poor in the optical, by comparison to longer wavelengths. For example, the Spitzer Space Telescope detected the first exoplanet-derived photons in eclipse observations for TrES-1 (Charbonneau et al. 2005) and HD 209458b (Deming et al. 2005b). For TrES-1, the 4.5 and 8 μm planet—star flux ratios were 0.094% ± 0.024% and 0.213% ± 0.042%, respectively, in a reanalysis by Cubillos et al. (2014). For HD 209458b, the 24 μm ratio was 0.26% ± 0.046%. The optical reflected ratio of Jupiter at opposition (just before eclipse) is about 4 × 10⁻²⁹. A hot-Jupiter planet with a 5% albedo and 10-solar-radius orbit radius has an optical reflected contrast to the Sun near 5 × 10⁻⁶. The main natural noise source in all such observations is the Poisson statistics of the unwanted stellar photons.

Phase-curve data sense varying degrees of both the dayside and the nightside, with no reflected component from the latter. This allows signal disentanglement to relatively narrow planetary sectors, which can be identified with longitudes, if the subobserver latitude is low, as is generally presumed for close-in, transiting planets.

In transit, the planetary atmosphere modulates the small component of the stellar radiation that passes through a significant atmospheric path length around the planetary limb. It is the only geometry with no reflected component. Disentangling what may be quite different atmospheric compositions and cloud structures at the morning, evening, and polar limb sectors is a challenge. In addition, Rayleigh scattering and, for small planets, refraction (Bétrémieux & Swain 2018) around the planetary limb on the side away from the star complicate attempts to resolve the event in time to separate the different limb sectors, as does the unknown pole orientation.

However, resolving eclipses in time to locate the signal sources on the planetary dayside has had initial success for at least one planet. Majeau et al. (2012) and de Wit et al. (2012) both analyzed multiple Spitzer 8 μm eclipses of HD 189733b and localized the peak emission. HD 189733b provides the best eclipse signal of any planet, by far. The promise of this approach, with much more and better data and combined with the retrieval technique that is the subject of this paper, is a full 3D reconstruction of the atmosphere’s thermal and condensation structure and at least 2D recovery of the chemical composition. Doing so independently for multiple eclipses would yield a time-resolved view of an exoplanet’s atmosphere and is the holy grail of exoplanet atmospheric retrieval.

Given the demand for the method, the high impact of some of the application papers (e.g., Line et al. 2014; Madhusudhan et al. 2011), and the prospect that this might be the method that discovers the effects of life on another planet, one might wonder why there were only three established implementations in the first five years after the method matured (Madhusudhan & Seager 2009, 2010; Madhusudhan et al. 2011; Benneke & Seager 2012; Line et al. 2013).

The answer, of course, is that the calculation is challenging to implement. RT depends on molecular line lists containing...
billions of lines that change shape with temperature and pressure, and Markov chains require thousands to millions of function evaluations. Hence, both memory and processor demands are high. Implementing the calculation requires expertise in both atmospheric RT and Bayesian statistics, two disciplines rarely taught to the same people before about 2015. The coding effort itself is involved, with practical application requiring parallel programming and attention to both memory and computational efficiency, again at a level not typically taught to scientists.

Demands on the calculation are evolving. For example, Oreshenko et al. (2017), noting that WASP-12b is hot enough for thermochemical equilibrium to dominate, retrieve atomic abundances and compute the approximate molecular chemistry at each step. Fraine et al. (2014) add an arbitrary shift in the spectrum between data from different instruments. Extensive code alterations require good software design and change management, including version control, if the code is not to become tangled and unusable over time, yet, historically, few astronomers have been trained in software engineering.

Further, the science itself poses challenges. With the data quality now available for exoplanets, solutions can be degenerate or indeterminate (Deming & Seager 2017). Data are still noisy, sparse, coarse in wavelength space, and spatially unresolved. Nonsimultaneous observations introduce biases (e.g., stars vary over time). The 3D atmospheric dynamics are unknown and are difficult to infer. The addition of even modest amounts of data can substantially change a solution, leading one to wonder whether even that solution is valid. Nonetheless, Bayesian retrieval is the state of the art and can at least be used to determine what future observations and physical data will most constrain an atmospheric model.

In this paper and companion works by Cubillos et al. (2022, hereafter BART2) and Blecic et al. (2022, hereafter BART3), we describe our open-source retrieval code, called Bayesian Atmospheric Radiative Transfer (BART). Our code was designed from the outset to be used and extended by others. A hybrid of user-friendly Python and fast C, there are both user and developer documents in addition to these technical papers. The code has been tested against both hypothetical problems with known answers and against the results of other codes on real data.

Exoplanet characterization results are famously difficult to reproduce, due to the brevity and sometimes the outright inaccuracy of published reports. As analyses become increasingly complex, describing the hundreds of decisions in them becomes impossible in a paper of reasonable length and would be uninteresting to most readers. Further, it is frequently impossible to know which decisions are important. We recently discovered significant differences between two supposedly identical calculations, one in Python and one in the Interactive Data Language, due to differences in their native median and standard deviation routines. With some calculations (such as retrieval) taking years to implement correctly, even with a published description in hand, checking or building on the work of others becomes impractical without access to the source code, input data, and configuration information used to support a scientific claim.

The Reproducible Research (RR) movement promotes the rapid advance of science by requiring that these be included in a compendium published with each paper. Producing the compendium should be easy, if codes are written to support it and if researchers keep good records. While such sharing undoubtedly accelerates science, it carries a burden and some risks for the researcher, particularly if done openly before publication.

In our development of a new kind of software license for science, we attempt to raise awareness of the problems that proprietary computer codes create with respect to research reproducibility and efficiency and that open development creates with respect to quality, priority, and credit (National Academies of Sciences, Engineering, and Medicine 2018). By restricting others’ use before publication and requiring citation and the full disclosure of code and data that support published scientific claims, our Reproducible Research Software License resolves these issues.

This paper gives an overview of BART’s design goals and our approaches in achieving them, describes its high-level design, and discusses performance optimizations and the convergence of Bayesian samplers. It presents the BARTTEST test suite and its application to BART, demonstrating BART on data for HD 189733b. Appendices discuss reproducible research and how BART’s license promotes better science, provide a checklist for users and reviewers of items to include in published retrieval reports, derive the number of Monte Carlo iterations required to determine Bayesian credible regions to a given precision, and address the resolution required in synthetic retrieval spectra.

The paper series includes full derivations of some well-known equations because, in writing BART, we found disagreements or incompatible conventions in the literature, equations expressed as proportionalities, and other impediments to implementing a quantitative code correctly. Likewise, we explain some topics in more detail than needed merely to justify our claims to existing experts, in hopes that BART will be used by students (and senior researchers!) not already expert in all of the disparate topics involved. Our goal is not merely to present a code but to improve the practice and understanding of retrieval.

The two companion papers describe BART’s calculations and present additional applications. BART2 presents transit, the RT code originally written by Rojo (2006) and heavily modified for use in BART, and its application to eclipse and transit geometry. The paper applies BART to transit data for HAT-P-11b. BART3 describes the inputs, user configuration, and initialization; two modules from the optimization loop, the atmospheric profile generator and the spectrum integrator; and the outputs and post-processing routines, including the calculation of contribution functions. The paper applies BART to eclipse data for WASP-43b. Prior papers describe BART’s Thermochemical Equilibrium Abundances (TEA; Blecic et al. 2016) code, used in the initialization, and BART’s Multi-Core Markov Chain Monte-Carlo statistical package (MC3; Cubillos et al. 2017), which drives the main loop.

2. Goals and Implementation Approach
BART’s main goal is to infer atmospheric properties from particularly noisy observations, including data from multiple observatories and, eventually, simultaneous fits to different types of observations (e.g., eclipses, transits, and phase curves). A second goal is to be a platform for comparing different approaches to the retrieval problem, to assess the effects of different inputs (such as different line lists for the same
molecule), and to compare multiple algorithms. Third, it should be flexible enough to implement future calculations, whatever they may be. Rather than just contributing yet another algorithm to the comparison, BART aims for the flexibility to implement any applicable physics and be a venue for conducting comparisons by varying only one part of the calculation at a time.

Thus, we designed a modular, object-oriented framework capable of such flexibility and implemented a straightforward, one-dimensional (1D) retrieval scheme with a modest variety of thermal and chemical profiles for the initial release described here and in the two companion papers. The framework allows BART to incorporate the full panoply of physical, chemical, and biological effects on planetary observations, as well as a variety of statistical and observational approaches, as code modules contributed by interested experts.

Also, we have endeavored to give the user control over every physically relevant parameter of the calculation. RT output-grid resolution and starting point, parameter ranges, Voigt-profile resolution and extent, number of Voigt profiles in each dimension of the Voigt-profile grid, reference pressure, layer pressures, limiting optical depth, and many others are all user choices, with reasonable defaults set for hot-Jupiter exoplanets.

The version of BART described here models the atmosphere as a 1D vertical grid of temperatures and chemical abundances. BART’s design makes it possible to implement a 3D atmospheric grid, including wavelength-dependent scattering by clouds and hazes, or to feed the RT calculation with data from global circulation or active chemical models.

To enable such contributions, we have adopted an open-source development model, provided documents for both users and developers, and implemented a variety of tests. The tests verify the code’s correctness and make it more difficult for future modifications to introduce bugs.

Since the portions most likely to be altered are also those least requiring computational speed, most BART modules are written in Python and its NumPy array mathematics package, which are popular and free. They expose the planet’s physical description to the user, allowing user-written routines to alter or add to the description before the RT calculation. The routines that process the modeled spectra afterward are likewise exposed. We supply both the source distribution and pre-compiled binaries in containers that make installation singularly easy.

### 3. High-level Design

Fundamentally, BART is an optimizer and parameter-space explorer. That is, it finds the class of model atmospheres that produce the simulated spectroscopic observations and that are most similar to some measured spectrum, within its uncertainties. This is true even for problems with fewer measurements than free model parameters, although in this case a single best fit cannot be determined. Thus, the entire RT apparatus is merely an elaborate function being fit to data. Setting up (reasonably) self-consistent initial conditions, providing the initial data for the RT calculation, and producing plots and tabulated spectra are substantial tasks that surround the fitting procedure.

Figure 1 presents the execution flow of BART. The optimization loop is in the upper right (connected by thick arrows). The initialization and support routines surround the main loop (blue boxes). BART requires numerous inputs, including planetary system parameters, the observations being modeled, initial values and limits of free model parameters, line lists, filter or spectrometer bandpass functions, the list of atmospheric layers in the model, elemental abundances for the initial atmosphere, and the list of chemical species to model. In the chart, many of these appear as blue “data files” with wavy bottoms.

The initialization (BART3) evaluates the starting temperature–pressure profile, $T(p)$, in each layer. It uses BART’s TEA code (Blecic et al. 2016) to calculate molecular abundances in each layer. The user can choose to use these profiles, an arbitrary set of abundance profiles, or constant vertical abundances.

At the top of the main loop, our optimization and statistics package, MC3 (aqua box in Figure 1; Cubillos et al. 2017; see below), produces sets of atmospheric parameters from its walk through the parameter space. The three green boxes at the bottom of the optimization loop are together the function being fit to the data. An atmospheric profile generator turns sets of parameters from MC3 into a grid of temperatures and chemical abundances. The transit RT code uses that grid to calculate an emission spectrum or transmission spectrum modulation for the model atmosphere. The spectrum integrator/checker produces per-channel measurement predictions from the spectrum (BART3). MC3 then calculates $\chi^2$ and iterates.

MC3 implements both a simple Metropolis–Hastings (MH) sampler and the differential-evolution Markov-chain algorithms of ter Braak (2006) and ter Braak & Vrugt (2008, added to MC3 since its publication). Each MCMC chain has one transit program attached to it, just one of which is illustrated in Figure 1.

The profile generator (BART3) parameterizes $T(p)$ several different ways. Currently, it scales the abundance profiles it receives from the initialization by a constant parameter per profile. With better data than currently available for exoplanets, the profile generator could apply abundance profiles with free parameters, as it now does for thermal profiles. As very hot planets are thought always to be in thermochemical equilibrium, a faster TEA could enable recalculating equilibrium abundances at each iteration and using atomic abundances as free parameters (e.g., Oreshenko et al. 2017).

BART2 details transit/BART’s RT code. Initially a PhD dissertation project under JH (Rojo 2006), it implemented the tangent geometry of a transiting exoplanet observation. We modified it to handle multiple similar calculations without restarting and reinitializing, feeding it different model atmospheres via the Message Passing Interface (MPI). We also implemented the emergent-ray geometry of an transit observation and optimized many of its calculations, either removing them from transit’s main loop or pre-calculating them before the BART run entirely. Transit implements a gray cloud deck and Rayleigh scattering; parameterized scattering is a planned extension. Even with observations much coarser than the width of a line, the nonlinearity of the radiation integral requires reasonably accurate and highly resolved line shapes, sampling those opacities onto an output grid that resolves the lines in the RT forward model, and then integrating over observational bandpasses to compare to data.

The RT is complex and must execute quickly, so transit is a C program, written in an object-oriented style, and wrapped for Python with the Simplified Wrapper Interface Generator (SWIG). It was also designed to be altered, although with
spectrum or an emission spectrum. The spectrum integrator boxes are initialization and support (free parameters to the RT machinery in the upper right and processing the data into opacities in each layer and at each opacity table in shared memory, to avoid duplicating it for each BART is implemented. It stores the large, static, pre-calculated code modules; white boxes name the information being transferred black silhouetted space telescope represents the observations. See Section 3.

The Planetary Science Journal, 3:80 (31pp), 2022 April Harrington et al.

necessarily greater effort than the Python in which the rest of BART is implemented. It stores the large, static, pre-calculated opacity table in shared memory, to avoid duplicating it for each MCMC chain.

Transit accepts an atmospheric description that specifies the temperature and molecular composition (including isotopologues) at each of a given set of atmospheric layers. It either computes the opacities on the spot for a given atmospheric model or interpolates from a pre-calculated table. For forward models, it can use either approach, but retrieval requires the pre-calculated grid, for efficiency. The four-dimensional grid is calculated for each molecule on the wavenumber grid of the output spectrum and over the range of temperatures and pressures present in the atmosphere. One stand-alone run of transit pre-computes this grid, which can be used for many related calculations by BART, or for stand-alone transit runs.

The output of transit is either a transmission modulation spectrum or an emission spectrum. The spectrum integrator integrates these over filter or spectrometer bandpass transmission functions, for comparison to data by MC3.

Once MC3 produces a sufficient number of samples (Section 5), it calculates relevant statistics and produces plots for the spectrum and all the individual and pairwise parameter histograms by marginalizing the posterior distribution.

The post-processing routines (BART3) identify the best-fit transit run, calculate contribution functions for each bandpass, calculate the credible regions of the thermal profile, and make retrieval-specific plots. Synthetic and real examples, with sample inputs and outputs, appear below.

4. Optimizing the Calculation

The original Rojo (2006) transit is a single-pass RT program that takes minutes to hours to run, depending on the number of lines, layers, and wavelength channels. Optimization is thus critical for a Bayesian approach involving $10^9$–$10^7$ iterations. Most of the calculation involves reading the line lists and processing the data into opacities in each layer and at each wavelength. These became transit’s first pass, which produces an opacity file useful for many runs. This pass runs before BART, as a stand-alone program, and can take several hours on its own (days if using modern $10^{10}$+ line lists for multiple molecules without pre-processing), so even this initialization required optimization.

The second pass, used in BART, reads that file, receives a set of atmospheric profiles, and produces either an emission spectrum or a transmission spectrum modulation. This pass must run in under a few seconds, regardless of the number of lines.

Here are our most significant optimizations over a single-pass RT solver (we refer to BART2 and BART3 for details of the calculations):

1. Define separate initialization and spectrum calculation steps.
2. Put a loop around the spectrum calculation, removing as much as possible from the loop.
3. Precalculate and save the opacity table, so the RT just interpolates the opacities in a given atmosphere.
4. Precalculate a 3D table of Voigt profiles, covering the range of expected Voigt line peaks and Lorentz widths over a wavenumber range reaching well into the distribution’s broad tails.
5. Sum the strengths of lines with the same profiles in the 3D Voigt table before broadening.
6. Set a user-defined line-strength lower bound, relative to the strongest line at each temperature–pressure combination in the opacity table. Ignore lines below this threshold.
7. Only calculate to a user-defined optical depth at each wavenumber.
8. Use long-lived, initialized instances of transit’s second pass (“workers” or “servers”) that receive atmospheric profiles from the Bayesian sampler and communicate spectra to them, to avoid the overhead of restarting them.
9. Use shared memory, so all MCMC workers access one copy of the opacity table.
10. Use reliable Bayesian samplers that require few separate workers and converge quickly.

For items 3 and 4, transit computes the Voigt profiles in the 3D table at very high resolution (thousands of samples per output grid interval) and aligned to the output grid. When filling the opacity array, for each line, it shifts the appropriate profile by an integer number of profile samples to best match the line peak and samples its values at the output grid wavenumbers. Due to the nonlinearity of the RT calculation, this produces more consistent and accurate spectra than averaging opacity over bins. Appendix D, BART2, and our tests against spectra calculated with other methods in Section 6.2.1 demonstrate the robustness of this approach. Users must select output grids that sample a few times per line width or risk missing entire lines, although sampling other lines at their peaks mitigates this somewhat. Many others have studied efficient Voigt calculations, notably with the correlated-k approach (Fu & Liou 1992).

The final item also bears some discussion. BART currently offers three Bayesian samplers. Since the parameter space is rarely Gaussian and often shows nonlinear parameter correlations, the MH algorithm converges slowly, and often not at all.
The ter Braak (2006) differential-evolution Monte Carlo algorithm (DEMC) requires twice as many chains as free parameters. Although it generally converges much faster and more reliably than MH, DEMC still sometimes has a few chains that refuse to converge for strongly correlated parameter posteriors. The ter Braak & Vrugt (2008) Snooker DEMC algorithm (DEMCzs) converges well with as few as three chains, and typically converges faster with more (total samples matter, not just samples per chain). It converges reliably in our tests.

We attempted to parallelize pylineread, the program that ingests line lists of various formats, but found that it ran in the same time, regardless of the number of cores. The limiting factor is the time to read and write the files, which parallelization cannot straightforwardly improve (using fast storage would help).

5. Bayesian Samplers and Convergence

Although written with respect to BART, this section, as with much of this paper, applies to all Bayesian retrievals, and in this case all Monte Carlo Bayesian analyses, whether using MCMC or another sampler.

BART is fundamentally a model—the atmospheric profile generator, transit, and the spectrum integrator, taken as a unit—being compared to data by a Bayesian parameter-space explorer. As such, it has all the benefits and liabilities of the Bayesian approach.

Our Monte Carlo convergence goals are to forget the initial conditions and to produce enough samples to estimate posterior summaries, such as credible regions, with sufficient precision. BART uses two separate approaches to accomplish these tasks.

First, we ask, how many iterations convince us that the parameter-space sample resembles the unknowable posterior distribution well enough to begin sampling from it, i.e., that the initial conditions are forgotten? This is a subtle topic in the literature, with no perfect answer. We have implemented one of the best-known tests, that of Gelman & Rubin (1992; GR), requiring that all parameters achieve a GR statistic within 1% of unity. Unfortunately, simply discarding the run prior to GR convergence violates the Markov assumption, introducing bias into the results. BART thus allows the user to specify a number of burn-in steps to ignore and computes the GR statistic for the kept samples as a convergence diagnostic.

Second, we ask how many steps (MCMC iterations) are needed to find credible regions with a given accuracy. In Appendix C, we show that the effective sample size (ESS) needed to ensure that a credible region contains estimated probability \( \hat{C} \) with accuracy \( s_\hat{C} \) is

\[
\text{ESS} \approx \frac{\hat{C}(1 - \hat{C})}{s_\hat{C}^2}.
\]

In most MCMC samplers, steps are small, and thus the samples are correlated. For BART, there may be \( 10^2 \) to \( 10^4 \) (or more) steps per effectively independent sample (SPEIS), depending on the sampler and the problem, and the number can vary a great deal between the parameters. There are many methods to estimate SPEIS. BART does it for each parameter by summing the autocorrelation function from zero lag to some small, positive threshold of autocorrelation value and using the largest value among the parameters. The number of steps required is the product of SPEIS and ESS. For example, if one calculates a 95.45% credible region with ESS \( \approx 1700 \), the 1σ uncertainty on the probability content of this credible region is 0.5%. If SPEIS \( = 1000 \), one must run \( 1.7 \times 10^6 \) iterations.

BART runs a user-specified number of iterations. Good MCMC practice is to do trial runs to determine SPEIS and the GR convergence length, calculate the required ESS, and run a number of iterations larger than the sum of the required steps and GR convergence length and many times the GR convergence length. BART will discard a user-specified number of burn-in steps, which can be set to the GR convergence length calculated from trial runs. Every 10% of the run BART saves data. After the burn-in steps, BART also calculates GR convergence when saving. At the end of the run, it computes SPEIS and ESS for that run. We determine \( s_\hat{C} \) for a given \( \hat{C} \) (usually 68.27%, 95.45%, and 99.73%) from the calculated ESS.

It is possible for runs started in a high-probability region not to reach GR convergence in practical run lengths (e.g., \( 10^7 \) iterations, which might take many days on 10 cores, depending on many factors). Often, one can solve such problems by choice of sampler, parameters, and priors.

A parameter-space sampler seeks the most probable location and explores around it to ascertain the credible region. What if there is no information in one or more parameters? That is, what if the posterior histogram for that parameter is basically flat, or flat up/down to some level, and then zero? The sampler will run back and forth over the flat range for that parameter while trying different combinations of the remaining parameters, searching for some improvement in \( \chi^2 \). For many samplers, this introduces a high computational cost.

The first thing to do in such cases is to widen the allowed range of all such parameters dramatically, to ensure that good fits are not excluded by the range. If a good fit appears in the new range, subsequent runs might use a narrower range that includes it.

If no good fits emerge, the two cases are still informative, but in a negative way. Fairly flat posterior histograms suggest that the data may have nothing to say about that parameter. One should eliminate the parameter, rerun the fit, and compare Bayes factors (or approximations like the Bayesian Information Criterion) to see whether the parameter is useful. If not, reports should say that the data were uninformative regarding that parameter. An example is an atmospheric fit including CH\(_4\) in a spectral region where CH\(_4\) has very low opacity, such that no matter how high the abundance, there would be no measurable effect on the spectrum.

Posterior histograms that are flat up/down to a cutoff indicate limits. In our HD 189733b retrieval (Section 7), the spectral range includes CO lines, but none were detected. The cutoff gives the maximum allowed abundance. In the case of absorption, a lower limit with a flat region at higher values indicates a saturated spectrum. Increasing the abundance changes nothing significant in the region with data; all lines/bands are already saturated. In such cases, after exploring a wide abundance range, it is legitimate to reduce the range to a small region containing the cutoff and report the limit. This may speed up convergence in the final runs, depending on the sampler.

As a final check on run quality, trace plots (parameter value versus iteration number) should show each parameter running...
over the entire allowed parameter range many times, and not sticking too long in one region, nor avoiding any.

We may hope, at some future point, to automate the selection of parameters to include in a run. While this would certainly make things easier for the user, there is always the risk that peculiar posteriors might fool an algorithm into improperly keeping or removing a parameter. For the time being, then, the user must be as diligent in checking the posterior plots, trace plots, and run time as in selecting the input settings, choosing the line lists, and even analyzing the input data. BART is not intended as a black box.

6. Tests and BARTTEST

At the level required for most retrievals, calculating RT is sufficiently complicated that one cannot verify the correctness of efficient codes by inspection. Codes calculating it are, therefore, subject to numerous types of errors (“bugs”), including subtle changes of values that produce plots that look correct but are wrong. We have thus developed BARTTEST, an independent package of quantitative and qualitative tests for both RT and retrieval codes. This section presents an initial set of tests, using transit and BART as the first test subjects.

BARTTEST has four kinds of tests: analytic RT, comparison RT, synthetic retrieval, and real-data retrieval. The analytic and synthetic tests quantitatively assess correctness against known results. Several tests developed to catch file-reading and data-combining bugs also appear in the analytic group. The comparison and real-data retrieval tests compare complex, real-world calculations among multiple codes. The reliability of these tests depends on the strength of the consensus result. The analytic RT tests can be useful in diagnosing differences between results if a comparison test does not match the consensus.

Given the number of variables and setup parameters, this text focuses on general description and important points. The transit and BART configuration files for each test appear in the BARTTEST package as a reference for users to configure their own RT and retrieval codes to run these tests. The version of BARTTEST described here appears in the compendium. These detailed configurations and their meanings in our codes are the official versions of these tests, not the high-level descriptions in this paper. Others performing these tests should thus configure their codes to mimic the configurations, including the specific line lists, wavelengths computed, layer boundaries, thermal profile, included species, etc. For retrievals, it is important to use the same observations and uncertainties, even if better results appear in the literature in the future.

We encourage RT- and retrieval-code authors to validate their codes with BARTTEST’s analytic tests, to contribute their results to build the consensus for comparison tests, and to add new tests, especially to handle calculations not yet found in transit or BART, such as those involving hazes and clouds. For example, in Section 6.2.1, we compare transit to the hot-Jupiter cases of Barstow et al. (2020). Results and new tests may be submitted via pull requests at the code’s development repository on GitHub.

Table 1 summarizes the tests. Subsequent subsections expand on some of them and define terminology in the table.

6.1. Analytic RT Tests

Our simple RT code, miniRT, performs BARTTEST’s analytic calculations for eclipse geometry (Equations (14)–(18) of BART2). Written in Python, its goal is verifiability by inspection, not efficiency. It follows how a human thinks about RT. Additional BARTTEST routines accept the output of the code being tested in human-readable form, compare these to the output from miniRT, and make comparison plots.

Many tests use a set of fictional gases with line lists constructed to facilitate the tests (see Table 2). Otherwise, these gases behave like the common molecules given in the table. To make mathematical confirmation straightforward, there is no continuum opacity in most tests, and there are just a few lines in each list.

All tests have an emission (eclipse geometry) version. BARTTEST includes transmission (transit geometry) cases only where it makes sense. For example, in f0isololine, the emission case is simply the product of the line strength, a Voigt curve, density, and layer thickness, which verifies by inspection. The transmission case entails calculating the slanted path length through the single layer of LG1 of rays at multiple altitudes, calculating the optical depth and transmission as above, multiplying by 2πr, where r is layer distance from the planet center, and integrating over altitude. Further, the slant path may hit the layer twice or only partially. This loses the inspection-level simplicity of the emission case and combines these calculations with the Voigt function, making the test less diagnostic. Broadening is the same calculation for eclipse and transit geometries, so well-written codes will have one routine for it and will not require two tests. The transmission case for test f05abundance would require assessing a linear change in τ = 1 altitude, where τ is optical depth, which has the issues outlined above and also requires many tightly spaced layers.

Next, we expand on selected tests.

6.1.1. f04broadening: Line Broadening

At least theoretically, spectral lines broaden into Voigt profiles, V. These are the convolution of Gaussian (G) and Lorentzian (L) functions. The Gaussian derives from Doppler broadening due to the Maxwell-Boltzmann distribution of velocities in a gas. The Lorentzian derives from Heisenberg uncertainty in the transition energy due to short state lifetimes, especially at high pressures and temperatures. As a function of wavenumber, ν,

\[ G(\nu; \sigma) = \frac{1}{\sigma \sqrt{2\pi}} e^{-\nu^2/2\sigma^2}, \]  

\[ L(\nu; \gamma) = \frac{\gamma}{\pi(\nu^2 + \gamma^2)}, \]

where \( \sigma \) and \( \gamma \) are the Gaussian width and Lorentzian half width, respectively (see BART2 for a more detailed description).

The Voigt profile can be constructed from the Faddeeva function:

\[ w(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-\eta^2}}{z - \eta} d\eta \]

\[ z = \frac{\nu + i\gamma}{\sigma \sqrt{2}} \]
### Table 1
Summary of Tests

| Name               | Purpose                                                                 | Atmospheric Composition                                                                 | Notes                                                                                      |
|--------------------|-------------------------------------------------------------------------|------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| **RT Analytic Tests**                                                                 |                                                                                           |                                                                                           |                                                                                            |
| f01oneline         | Location, width, shape, and strength of a single, known line.           | One layer of LG1 at ∼40 mbar, rest CG1 (see Table 2). Calculating the line shape in transmission is nontrivial, so that case is not tested. |                                                                                            |
| f02fewline         | Combination of multiple, separate lines from one molecule.              | Same as f01oneline, but with LG2.                                                         |                                                                                            |
| f03multiline       | Combination of lines from multiple molecules and line lists.            | Three layers each have a different gas with three lines (LG2, LG3, LG4). Others have a gas with no lines (CG1). |                                                                                            |
| f04broadening      | Broadening line shape in opacity, isolating the broadening calculation from the radiation integral. | One layer of LG1, rest CG3. This test produces an opacity table sampled every 0.005 cm⁻¹ over a short range, in addition to an intensity spectrum. All other tests produce only intensity spectra. |                                                                                            |
| f05abundance       | (Near) linear relationship between abundance and line depth at low optical depth. | Based on f01oneline, but abundance varies in 10 steps uniformly from 10⁻⁹ to 10⁻³, with CG1 filling in. | LG1 trades off against CG1 to keep line broadening constant. Line is optically thin for near-linear absorption increase. Two lines in LG1 and LG2 are ∼0.04 cm⁻¹ apart at ∼2.29 μm. The wavenumber sampling interval is 0.005 cm⁻¹. One of the following: no CIAs, H₂-He CIAs, both H₂-H₂ and H₂-He CIAs (some codes may also require LG1). |                                                                                            |
| f06blending        | Line blending from different molecules in the same layer.              | The ~9 mbar layer has 1% LG1, 9% LG2, and 90% CG1; others have 85% CG1 and 15% CG2.       |                                                                                            |
| f07multicia        | Multiple collision-induced absorption (CIA) sources, similar to f03multiline. | Uniform 85% H₂, 15% He. 10⁻₉⁻₈% LG1, if code requires a line list. CIA line lists. |                                                                                            |
| f08isothermal      | Background emission and emission-absorption cancellation for the isothermal case. | Uniform composition of 60% H₂, 10% each CO, CO₂, CH₄, and H₂O, using their full line lists, but no CIAs. Constant background and atmosphere temperatures. | Full line lists for all species. Result is a Planck spectrum. Uses just Sharp & Burrows (2007) gases, as some codes only have these, but users may configure many more. Not offered in transmission, as the result is not a Planck spectrum. |                                                                                            |
| **RT Comparison Tests**                                                                 |                                                                                           |                                                                                           |                                                                                            |
| c01hjcleariso      | Forward model of cloudless HD 189733b-like planet.                      | Isothermal T(p) profile in emission and transmission. Mean temperature ~1100 K. Full line lists for CH₄, CO, CO₂, H₂O, NH₃, and H₂, H₂-H₂ and H₂-He CIAs. | Test of all code features on realistic cases. Validated by comparison to others. |                                                                                            |
| c02hjclearnoinv    | Forward model of cloudless HD 189733b-like planet.                      | Same as c01hjcleariso, except non-inverted T(p) profile in emission and transmission.     | Same.                                                                                      |                                                                                            |
| c03hjclearinv      | Forward model of cloudless HD 189733b-like planet.                      | Same as c01hjcleariso, except inverted T(p) profile in emission and transmission.        | Same.                                                                                      |                                                                                            |
| c04hjclearisoBarstowEtal | Forward model of cloudless HD 189733b-like planet.                     | Follows models of Barstow et al. (2020). Includes some CO-only models (1.0 Rₑ, 1.0 Mₚ, 1.0 Rₑ, 1.162 Mₚ, 1.138 Rₑ, 0.85 H₂-O, 0.15 He, 1500 K, 300 ppmv CO at 1500 K; 100 ppmv CO at 1000 K and 1500 K) and Model 0 (0.781 Rₑ, 1.162 Mₚ, 1.138 Rₑ, 0.85 H₂-O, 0.15 He, 1500 K, 300 ppmv CO at 1500 K; 100 ppmv CO at 1000 K and 1500 K). | Same.                                                                                      |                                                                                            |
| c05hjcloudisoBarstowEtal | Forward model of cloudy HD 189733b-like planet.                         | Follows Model 1 of Barstow et al. (2020) (0.781 Rₑ, 1.162 Mₚ, 1.138 Rₑ, 0.85 H₂-O, 0.15 He, 1500 K, 300 ppmv CO at 1500 K; 100 ppmv CO at 1000 K and 1500 K). | Same.                                                                                      |                                                                                            |
Table 1 (Continued)

| Name                      | Purpose                                      | Atmospheric Composition                                                                 | Notes |
|---------------------------|----------------------------------------------|----------------------------------------------------------------------------------------|-------|
|                           |                                              | $\text{H}_2:0.15 \text{ He, 1500 K, 300 ppmv H}_2\text{O, 350 ppmv CO, cloud deck at 10 mbar)}$. |       |

| Name                      | Purpose                                      | Atmospheric Composition                                                                 | Notes |
|---------------------------|----------------------------------------------|----------------------------------------------------------------------------------------|-------|
| s01hjc\text{cleariso}     | Can we retrieve what we put in?              | Model from c01hjc\text{cleariso}.                                                      |       |
| s02hjc\text{clearnoinv}   | Same.                                        | Model from c02hjc\text{clearnoinv}.                                                   |       |
| s03hjc\text{clearinv}     | Same.                                        | Model from c03hjc\text{clearinv}.                                                     |       |
| s04hjc\text{clearisoBarstowEtal} | Same.                                  | Model 0 from c04hjc\text{clearisoBarstowEtal}.                                         |       |
| s05hjc\text{cloudisoBarstowEtal} | Same.                                         | Model 1 from c05hjc\text{cloudisoBarstowEtal}.                                       |       |

Retrieval Real-data Test

| Name                      | Purpose                                      | Data                                                                                   | Notes |
|---------------------------|----------------------------------------------|----------------------------------------------------------------------------------------|-------|
| r01hd189733b              | Reality check                                | Photometry: Spitzer IRAC channels 1$-$4, IRS $16 \mu \text{m},$ MIPS $24 \mu \text{m}$. Spectra: Spitzer IRS, HST NICMOS G206 grism.$^b$ |       |
|                           |                                              | Multiple reductions of these data exist. Tests must use the same eclipse depths and uncertainties as BARTTEST to be accurate comparisons. |       |

Notes.

$^a$ Barstow et al. (2020) report the planetary radii in terms of the volumetric mean radius of Jupiter (69,911 km), rather than the IAU-defined value of RJ (71,492 km; Prša et al. 2016). For codes that use the IAU value, the radii must be converted accordingly.

$^b$ IRAC is the InfraRed Array Camera. IRS is the InfraRed Spectrograph. MIPS is the Multiband Imaging Photometer for Spitzer. HST is the Hubble Space Telescope. NICMOS is the Near Infrared Camera and Multi-Object Spectrograph.
Table 2
Test Line Lists and Fictitious Test Gases

| Name  | Like | No. of Lines | \( \lambda \) |
|-------|------|--------------|--------------|
| CG1   | H\(_2\) | 0           |              |
| CG2   | He   | 0           |              |
| CG3   | N\(_2\) | 0         |              |
| LG1   | H\(_2\)O | 1     | 2.289 19     |
| LG2   | CH\(_4\) | 3     | 2.289 21, 2.15, 3.20 |
| LG3   | CO   | 3           | 2.38, 2.50, 2.54 |
| LG4   | CO\(_2\) | 3  | 2.86, 3.02, 3.78 |

Notes.

\(^a\) CG = Clear Gas; LG = Line Gas.

\(^b\) Properties (mass, isotopes, etc.) same as this molecule, except line list.

The Planetary Science Journal, 3:80 (31pp), 2022 April

Harrington et al.

At extremely high spectral resolution or at long wavelengths, one must configure transit’s pre-calculated Voigt table to ensure sufficient accuracy, which can be assessed by running a modified version of this test (set the resolution/wavelength range, move the fake line to that location).

6.1.2. \( f05\) abundance: Varying Abundance

This tripwire test relies on the property that, in the optically thin regime (optical depth \( \tau \ll 1 \)), the fraction of the interior (blackbody) radiation absorbed, \( A \), scales nearly linearly with the optical depth, since the linear term dominates in its Taylor-series expansion,

\[
A = 1 - \frac{F}{F_0} = 1 - e^{-\tau} \approx 1 - \sum_{n=0}^{\infty} \left(-\frac{\tau^n}{n!}\right)
\]

\[
\approx \tau - \frac{\tau^2}{2} + \frac{\tau^3}{6} - \ldots,
\]

where \( F \) is transmitted flux and \( F_0 \) is interior flux. \( \tau \) is linearly dependent on the density, which is proportional to the abundance. For two spectra of a gas with lower and higher abundance, each frequency channel should closely obey

\[
f = \frac{F_0 - F_h}{F_0 - F_l},
\]

where \( F_0 \) is the spectral flux without any lines, \( F_l \) is the flux in the low-abundance spectrum, \( F_h \) is the flux in the high-abundance spectrum, and \( f \) is the abundance ratio.

We test this using a noninverted atmospheric model uniformly composed of \( 0.00\%\)–\(10.0\%\) LG1, with the remainder CG1 (any CG species will do). The abundance of LG1 varies in steps of 0.01%. The 0.00 abundance case is \( F_0 \), the planetary interior blackbody without the LG1 spectral line. Taking \( F_l \) as the 0.01% abundance spectrum and starting \( F_h \) with the 0.02% case, \( f \) takes on the integers 2–10. Figure 3 shows the results of transit. Table 3 shows the output of BARTTEST.

6.1.3. \( f08\) isothermal: Isothermal Atmosphere

This tripwire test recognizes that, without scattering, line emission and absorption are equal in any optically thick, isothermal gas mixture. The mixture thus emits as a blackbody. The atmosphere for \( f08\) isothermal has many molecules uniformly present in all layers and a full line list for all of the species present. This should produce a blackbody emission spectrum peaking at the wavenumber corresponding to the atmospheric model’s temperature, according to Wien’s law. Deviations may arise from approximations or precision issues in the code. Figure 4 shows the theoretical Planck function plotted over transit’s result.

6.2. Comparison RT Test

To avoid aggregating working parts into an erroneous whole, one must validate the entire RT calculation. As the complexity is too great to verify reliably by inspection, \( c01\)hjcleariso, \( c02\)hjclearnoinv, and \( c03\)hjclearinv are tests inspired by the HD 189733 system. The strength of these tests rests on the number of participating codes, so we invite the community to perform these calculations in their own codes and to submit the results for inclusion in BARTTEST.

It is important to identify the sources of any differences without assuming that the tested codes are correct, as there is...
no assurance that several codes do not all share the same bug. With such honest testing, as the group of tested codes grows, so the likelihood of a groupthink bug decreases. The comparison of many codes implementing a single model also shows the range of outputs due to modeling approaches and assumptions, even with identical inputs.

Our model planet resembles HD 189733b. Tests must adopt the stellar radius of 0.756 solar radii, stellar temperature of 5000 K, planetary radius of 1.138 \( R_J \) (Torres et al. 2008), and planetary gravity of 2182.73 cm s\(^{-2}\), which corresponds to a mass of 1.14 \( M_J \). The reference pressure of 0.1 bars corresponds to this planetary radius. Tests must calculate spectra for the wavelength region between 1 and 11 \( \mu m \), as the most spectroscopically active species show features in this region. Tests should calculate both emission intensity spectra (secondary eclipse) and transmission modulation spectra (primary transit).

The common inputs are the isothermal, inverted, and noninverted \( T(p) \) profiles used for the RT model tests \( c01hjcleariso, c02hjclearnoinv, c03hjclearinv \), and their associated retrieval tests \( s01hjcleariso, s02hjclearnoinv, \) and \( s03hjclearinv \). The inverted and noninverted profiles use the \( T(p) \) parameterization of Line et al. (2013). The profiles have effective temperatures generally around 1100 K, to resemble HD 189733b.

### Table 3

| Abundance | \( f^a \) versus 0.01\% Case |
|-----------|-----------------------------|
| 0.02\%    | 1.999784                    |
| 0.03\%    | 2.999535                    |
| 0.04\%    | 3.999005                    |
| 0.05\%    | 4.998531                    |
| 0.06\%    | 5.997734                    |
| 0.07\%    | 6.996982                    |
| 0.08\%    | 7.995986                    |
| 0.09\%    | 8.994910                    |
| 0.1\%     | 9.993651                    |

*Note.*

\(^a\) Factor difference in line depth.

6.2.1. Barstow et al. (2020) Forward Models

To compare BART with additional peer-reviewed codes, we emulate some of the setups described in Barstow et al. (2020), which were executed using the NEMESIS (Irwin et al. 2008;...
Lee et al. (2012), CHIMERA (Line et al. 2013), and TAU-REX (Waldmann et al. 2015b) codes. These codes utilize the correlated-\(k\) method, whereas transit uses a line-by-line approach. (If the user-selected output resolution is low enough to miss some lines, it is properly called “line sampling” rather than “line-by-line,” but there is no difference in what the code does. As this is a user choice, we call it “line-by-line” below.) Specifically, we emulate the setups for the cloud-free Model 0, cloudy Model 1, and three of the CO-only cases. We summarize these setups in Table 1 (see c04hjclearisoBarstowEtal and c05hjcloudisoBarstowEtal, but we direct readers to Barstow et al. (2020) for more detailed descriptions of the tests and to BARTTEST for the exact setups. We note that Barstow et al. (2020) report planetary radii in terms of Jupiter’s mean volumetric radius (\(R_{J,\text{mean}}\), 69,911 km), rather than the IAU-defined value of \(R_J\) (71,492 km; Prša et al. 2016); not properly accounting for this will lead to a vertical offset in the transmission spectra.

Figure 6 shows comparisons between the spectra produced by transit, NEMESIS, CHIMERA, and TAU-REX. As in Barstow et al. (2020), we bin the CO spectra to steps of 0.01 \(\mu m\) and compute the residuals with respect to the average of the NEMESIS, CHIMERA, and TAU-REX spectra; for the Model 0 and 1 cases, we bin according to CHIMERA’s reported wavelengths. In general, there is close agreement between transit and the other codes. The differences are on the order of the differences between the other codes, despite transit’s opacity-sampling approach.
6.3. Synthetic Retrieval Tests

To test BART retrievals, we used the synthetic planets of the
\texttt{c01hjcleariso}, \texttt{c02hjclearnoinv}, \texttt{c03hjclearinv}, \texttt{c04hjclearisoBarstowEtal}, and \texttt{c05hjcloudisoBarstowEtal} tests. The tests are called
\texttt{s01hjcleariso}, \texttt{s02hjclearnoinv}, \texttt{s03hjclearinv}, \texttt{s04hjclearisoBarstowEtal}, and \texttt{s05hjcloudisoBarstowEtal}. We consider both eclipse and transit
gyrometry for each atmospheric model, except for the Barstow et al. (2020) cases, which are only in transmission.

To generate eclipse and transit depths for the \texttt{s01–s03} cases, we use 47 channels spanning 2–5\,\mu m that have perfect transmission over their spectral ranges. We use relatively high S/N synthetic data so that the retrieved credible regions will be relatively small and thus more likely to expose small coding errors when compared to inputs. We set uncertainties such that each channel has S/N = 50 for emission cases and 300 for transmission cases. For stellar emission, we use a K2 solar-abundance Kurucz stellar model (Castelli & Kurucz 2003). For the \texttt{s04} and \texttt{s05} cases, we consider each of the simulated spectra by NEMESIS, CHIMERA, and TAU-REX with noise levels of 60 parts per million.

We include opacities for the species as described in Section 6.2. The \texttt{s01–s03} retrievals each have five parameters for the \textit{T(p)} profile (Line et al. 2013); five for the scaling factors of the log abundances of H$_2$O, CO, CO$_2$, CH$_4$, and NH$_3$; and, for the transmission cases, a parameter for the planetary radius at 0.1 bars. The \texttt{s04} and \texttt{s05} retrievals have free parameters for the isothermal temperature, the planetary radius at 10 bars, the log mixing ratios of H$_2$O and CO, and the pressure corresponding to an opaque cloudtop. All cases feature uniform priors on the model parameters; parameters that are the logarithm of the true parameter therefore have log-uniform priors.

BART’s results for the \texttt{s01–s03} retrievals are similar in some respects (Figures 7, 8, and 9). The retrieved thermal profiles and molecular abundances generally match the inputs in the regions of the atmospheres probed by these synthetic observations (Figures 8 and 9, middle columns). The lower atmospheres are generally poorly constrained, as the spectrum is minimally influenced by those pressure levels at the wavelengths of the synthetic data. The emission cases provide better constraints than the transmission cases on the \textit{T(p)} profile and abundances, as expected (Griffith 2014; Heng & Kitzmann 2017; Madhusudhan 2018).

The isothermal emission case’s retrieved abundances and \textit{T(p)} profile demonstrate the inability to detect molecular features from an isothermal atmosphere. In the region with sensitivity, the best-fit thermal profile is isothermal; the inversion seen in the explored thermal profiles corresponds to regions with negligible or no contribution to the spectrum. We allow for any \textit{T(p)} profile rather than enforcing an isothermal condition because it would not be known a priori whether the atmosphere were isothermal. The 1D marginalized posteriors for the molecular abundances are poorly constrained and tend to favor a log mixing ratio $<-4$, with significant probability for log mixing ratios $<-8$, consistent with a lack of spectral features for an isothermal atmosphere.

Table 4 shows the SPEIS, ESS, and posterior accuracies for these retrievals. The large SPEIS (and small ESS) is due to a combination of factors. We choose the highest SPEIS value among all chains and all parameters as a conservative estimate; the noninverted eclipse case has a SPEIS $>15,000$ with a median SPEIS of $\sim$2730. Compared to the Barstow et al. (2020) cases and the HD 189733b retrieval, these SPEIS values are significantly greater. This may be related to a numerical effect seen in synthetic retrievals tests (see Appendix D).

6.3.1. Barstow et al. (2020) Synthetic Retrievals

Figures 10 and 11 show the best-fit spectra and marginalized posteriors for the retrievals on the Barstow et al. (2020) synthetic spectra produced by NEMESIS, CHIMERA, and TAU-REX for Models 0 and 1, respectively, with an uncertainty of 60 ppm. Tables 5 and 6 summarize the retrieved credible regions for each of the retrievals. The true parameters are contained within the 95.45% credible regions, with most also being contained within the 68.27% regions.

Comparing the reported 1$\sigma$ credible regions for each retrieval shows minor differences. For most cases, BART finds narrower credible regions for temperature than the other codes. In the case of Model 0, the upper bounds of the 1$\sigma$ temperature regions are consistently just below the known 1500 K temperature, while the true radius falls at the lower bound of the 2$\sigma$ region of the BART retrieval on the TAU-REX forward model. For the Model 0 cases, BART favors high cloudtop pressures, consistent with the absence of clouds; slightly greater radii; and narrower credible regions for CO than the other codes. The CO retrieval on the NEMESIS spectrum falls in the 2$\sigma$ region. For H$_2$O in the Model 0 cases, BART finds similar values, but with narrower credible regions compared to TAU-REX and CHIMERA. For the Model 1 cases, BART favors similar radii and lower cloudtop pressures. Compared to NEMESIS, BART finds narrower credible regions for CO and H$_2$O when retrieving on TAU-REX and wider credible regions when retrieving on CHIMERA. Compared to TAU-REX, BART finds a similar amount of H$_2$O but with greater uncertainty; BART also favors greater CO with similar or slightly smaller uncertainties. Compared to CHIMERA, BART favors greater CO and H$_2$O when retrieving on NEMESIS, favors similar CO and less H$_2$O when retrieving on TAU-REX, and generally finds narrower credible regions. For all cases except NEMESIS on CHIMERA, BART agrees with the other codes at 1$\sigma$ or less. The single exception agrees at just greater than 1$\sigma$.

Together with the tests in Section 6.3, this demonstrates BART’s ability to retrieve parameters accurately from synthetic data produced by various RT codes.

6.4. Real-data Retrieval Test

In a synthetic test, we may or may not know the answer as we work (e.g., in blind testing), but we know in principle what could have gone into the test. A test on real data is a full analysis, including concerns for unknown systematic errors, time variability of the star and planet, the 3D structure of the atmosphere, physics and chemistry not included in the model, errors and incompleteness in line lists, and even the unknown existence of background sources within the point-spread function of the target star. Given the state of exoplanet data today, we chose HD 189733b, a system with a high planetary S/N, a relatively large number of observations in the literature, and little controversy over their interpretation. Those implementing this test for comparison to our result must configure their codes as we have, in one dimension, without clouds, using the same line lists, and using exactly the same observations.
The value of any comparison test lies in the number of comparisons, so we reiterate our invitation to those willing to contribute results of their own application of this test.

In designing this test, we must mimic one of the two Bayesian models (discussed more in Section 7) by Line et al. (2014) and Waldmann et al. (2015a). Further, we wish the test to be accessible on a modest computer. We chose to emulate the analysis of Line et al. (2014) with CHIMERA, for two reasons. First, CHIMERA has been applied more broadly than the Waldmann et al. (2015a) TAU-REX. Second, the TAU-REX analysis uses the Yurchenko & Tennyson (2014) CH₄ line list, which is so complete that it exceeds the storage capacity of many modest computers. Although transit can use this line list either directly or digested into a continuum opacity table and a separate list of the strongest lines (Cubillos 2017), not all codes can, and the TAU-REX test did not. Additionally, Hargreaves et al. (2020) showed that ExoMol’s CH₄ list does not match laboratory studies.

This first test on real data is thus deliberately simple, as appropriate for a test suite, as it ignores clouds and the largest line lists. Applications with greater completeness, including clouds, the ExoMol lists, numerous variations, and comparison to multiple other works, appear in BART2 and BART3. As this test evaluates whether algorithms consistently fit data not produced by, and unlikely to be fit perfectly by, their respective underlying RT codes, the metric of success is not $\chi^2$ to the data but similarity among retrievals.

Of course, as future observations and models improve, it may be desirable to add additional real-data tests, with more recent observations, line lists, physics, and code configurations.
Given the length and complexity of the analysis, we present our test, including discussion of the literature for this planet, in its own section.

7. Application to HD 189733b

Due to both its proximity to Earth and its high S/N, the atmosphere of HD 189733b has been extensively studied since its discovery (Bouchy et al. 2005). Being one of the most analyzed hot Jupiters to date, HD 189733b is a prime candidate for a real-data retrieval test using published secondary-eclipse data. Here we discuss previous retrieval analyses of HD 189733b (Madhusudhan & Seager 2009; Lee et al. 2012; Line et al. 2012; Moses et al. 2013; Line et al. 2014; Waldmann et al. 2015a) and BART’s retrieved atmospheric profiles and dayside emission spectra in the context of these prior analyses.

Figure 8. Comparison between input and retrieved $T(p)$ profiles (left column), the normalized contribution functions (middle column, BART3), and best-fit molecular abundances (right column) for the isothermal (top row), noninverted (middle row), and inverted (bottom row) emission cases of the s01hjcleariso, s02hjclearnoinv, and s03hjclearinv tests. Dark- and light-blue shadings in $T(p)$ profile plots designate the 68.27% and 95.45% credible regions, respectively. These regions and the median derive from all the fits on a per-pressure-level basis. They do not follow the functional form of the individual profiles. Few, if any, individual $T(p)$ profiles, including the best fit, stay confined to these regions, especially where the contribution functions indicate low sensitivity. BART accurately retrieves the $T(p)$ profile and abundances wherever they contribute to the spectra. However, isothermal, nonscattering emission spectra are blackbodies, insensitive to abundances. Most MCMC-proposed spectra in those cases are not isothermal. Those with detectable structure (high abundances) are rarely accepted, creating the artificially low upper limits. This affects all Monte Carlo Bayesian retrievals.
At an orbital semimajor axis of $0.0312 \pm 0.00037$ AU and with an eccentricity of $0.0041 \pm 0.0025$, it takes $2.21857312 \pm 0.00000076$ days for HD 189733b to orbit its $5052 \pm 16$ K, K-type host star (Triaud et al. 2009; Stassun et al. 2018). In Jovian units, its mass is $1.130 \pm 0.025$ and its radius is $1.178 \pm 0.023$ (Triaud et al. 2009), making its bulk density just over three-quarters of Jupiter’s (Southworth 2010). Previous studies on HD 189733b use data from NICMOS (Swain et al. 2009), IRAC (Charbonneau et al. 2008; Knutson et al. 2009; Agol et al. 2010; Knutson et al. 2012), IRS (Deming et al. 2006; Grillmair et al. 2007), and MIPS (Charbonneau et al. 2008; Knutson et al. 2009).

When Madhusudhan & Seager (2009) published the first exoplanet retrieval via a parametric grid search, they derived that the atmospheric composition of HD 189733b was high in CO and CO$_2$, had a moderate abundance of H$_2$O, and had minimal CH$_4$. Further studies by Lee et al. (2012) and Line et al. (2012) confirm these abundances, though Moses et al. (2013) indicate that the comparatively large abundance of CO$_2$ is somewhat of an anomaly. Barstow et al. (2014) included clouds. These studies used optimal estimation rather than a Bayesian sampler. The upper limit on the CH$_4$ abundances presented by Line et al. (2012) is higher than previous results, such as Madhusudhan & Seager (2009) and Swain et al. (2009).

Figure 9. Same as Figure 8, but for transmission cases of the s01hjcleariso, s02hjclearnoinv, and s03hjclearinv tests. (Recall that low-resolution transmission spectra are relatively insensitive to temperature structure.)
Table 4

| Test            | Geometry | SPEIS | ESS* | Credible Region Uncertainty |
|-----------------|----------|-------|------|-----------------------------|
|                 |          |       |      | 68.27% ("1σ")b | 95.45% ("2σ")b | 99.73% ("3σ")b |
| s01hjcleariso   | Eclipse  | 5131  | 97   | 4.65% | 2.08% | 0.52% |
|                 | Transit  | 9204  | 162  | 3.62% | 1.62% | 0.40% |
| s02hjclearninv  | Eclipse  | 15506 | 96   | 4.68% | 2.09% | 0.52% |
|                 | Transit  | 8129  | 184  | 3.40% | 1.52% | 0.38% |
| s03hjclearninv  | Eclipse  | 14485 | 103  | 4.32% | 2.02% | 0.50% |
| s04hjcleariso   | Transit  | 4553  | 329  | 2.55% | 1.14% | 0.28% |
| s04hjcleariso   | Transit  | 54    | 1851 | 1.08% | 0.48% | 0.12% |
| s05hjcloudiso   | Transit  | 65    | 769  | 1.68% | 0.75% | 0.19% |
| s05hjcloudiso   | Transit  | 511   | 978  | 1.49% | 0.67% | 0.17% |
| s05hjcloudiso   | Transit  | 412   | 970  | 1.49% | 0.67% | 0.17% |
| s05hjcloudiso   | Transit  | 812   | 862  | 1.58% | 0.71% | 0.18% |
| r01hd189733b    | Eclipse  | 2084  | 959  | 1.50% | 0.67% | 0.17% |

Notes.
* Computed from the nonburned iterations for each case.
b Here and in the literature, these credible regions are labeled in analogy to the Gaussian, although they are not, generally, multiples of the posterior’s standard deviation.

Line et al. (2014) attribute the discrepancy to non-Gaussian posterior distributions under Gaussian-assuming optimal estimation.

We adopt the following data set: NICMOS data from Swain et al. (2009), with the four shortest-wavelength channels omitted; IRS data from Grillmair et al. (2008); IRAC 5.8 μm, IRS 16 μm photometric, and MIPS 24 μm data of Charbonneau et al. (2008); and IRAC 8.0 μm data of Agol et al. (2010). IRAC 3.6 and 4.5 μm data are adopted as 0.1533 ± 0.0029% and 0.1886 ± 0.0017%, consistent with Line et al. (2014).

While newer data (e.g., the secondary-eclipse measurements of Knutson et al. 2012) and analyses (e.g., the IRS reanalysis by Todorov et al. 2014) are available, this setup is meant as a real-data retrieval test to benchmark BART and future retrieval codes. This data set exactly matches that of Line et al. (2014), allowing a direct comparison of results. We note that Line et al. (2014) cite the IRS data as coming from Grillmair et al. (2007) but use data from Grillmair et al. (2008). The IRAC 5.8 μm data are cited as coming from Agol et al. (2010), who did not publish 5.8 μm data. Rather, they use the 5.8 μm data of Charbonneau et al. (2008). Similarly, the IRAC 3.6 and 4.5 μm data are cited as Knutson et al. (2012), but the data used do not appear to match any published data (M. Line, private communication).

The retrieval model has nine free parameters: five for the T(p) profile (Line et al. 2013) and four scaling factors for the vertically constant log abundances of CO, CO2, CH4, and H2O. All priors are uniform, with the log parameters therefore having a log-uniform prior. The model atmosphere has 100 layers spanning 10−8 to 100 bars, evenly spaced in log pressure. We include HITRAN opacities for CO, CO2, and H2O (Rothman et al. 2010; valid at the temperature of HD 189733b), and HITRAN opacities for CH4 (Rothman et al. 2013; measured at 296 K with some hot bands). We also include H2-H2 and H2-He collision-induced absorptions (CIAs; Richard et al. 2012). For compatibility with the initial comparison studies, we do not include opacities for minor species whose abundances are not sought, although this is a good practice.

We also consider two additional models that are identical in setup except for line lists, to explore their effect on the retrieval results. To match the setup of Line et al. (2014), one model only differs for CH4, using the theoretically derived Spherical Top Database System (STDS; Wenger & Champion 1998) at wavelengths greater than 1.7 μm and HITRAN 2008 (Rothman et al. 2009) at shorter wavelengths. The other model uses the latest HITEMP CH4 (Hargreaves et al. 2020) and CO lists, as well as ExoMol lists for H2O (Polyansky et al. 2018) and CO2 (Yurchenko et al. 2020) processed via REPACK (Cubillos 2017). While both these fits are better, the setups are more complex, involving the relatively obscure STDS list and the large ExoMol database. Since none of these come close to a perfect spectrum fit, the test in BARTTEST is the simplest of the three, using just HITRAN 2012 and HITRAN 2010. Those interested in reproducing the STDS and ExoMol runs can find the relevant lists, setup details, and plots in this article’s electronic compendium (see below).

Figure 12 shows BART’s retrieved results for HD 189733b. Except for Line et al. (2014), each of the studies from the literature differs from BART in several fundamental ways, including data, line lists, and modeling approach. Figure 13 and Table 7 show the effect of these differences among the studies.

In the BARTTEST run, except for the IRAC channel 2 data point, the best-fit spectrum qualitatively agrees with that of Line et al. (2014), and the retrieved abundances agree at 1σ, as shown in Table 7 and Figure 13. While Line et al. (2014) find no evidence of a thermal inversion, BART favors a slight inversion in all three models, with retrieved T(p) parameters closely agreeing. Except for CO2, the retrieved molecular-abundance credible regions for the three models agree at 1σ. For CO2, the ExoMol model agrees with the BARTTEST and STDS models at 1σ, while the BARTTEST and STDS models differ by less than 2σ. When restricting BART to noninverted thermal profiles, χ2 increases significantly, favoring the inverted model by a maximum likelihood ratio of 30–90, depending on the forward-model gridding (0.1 versus 1 cm−1, respectively).

We demonstrated 1σ agreement between BART and the modern CHIMERA in Section 6.3.1, using synthetic cases. In those tests, the forward model used in the retrieval, or one very similar to it, generated the test data, so a (near-)perfect match
exists in the retrieval phase space. Yet, despite similar spectra and mostly consistent posteriors, $\chi^2$ values in Table 7 differ substantially. The reduced $\chi^2$ values are greater than 2, indicating model misspecification. Real planets will always have physics that are not in any model, in this case including additional opacity sources, more sophisticated and varied clouds, some reflected stellar spectrum, and 3D temperature and compositional variation. There are also well-known, uncorrected systematics in the NICMOS data (e.g., Gibson et al. 2011; Crouzet et al. 2012). The error from such misspecification must distribute somehow among the parameters, but model differences could distribute it differently.

Figure 10. Summary of retrieval results for the s04hjc/eras/Barstowetal test, which retrieve on the spectra of Barstow et al. (2020) Model 0 cases with 60 ppm uncertainties. Best-fit spectra (left column) and marginalized posteriors (right column) for the NEMESIS (top row), CHIMERA (middle row), and TAU-REX (bottom row) data sets.
There are some modest model differences. BART’s Bayesian sampler was DEMCzs versus DEMC for CHIMERA. All Bayesian methods should converge to the same posterior, within the noise of random sampling (see Appendix C). For example, we find similar results to CHIMERA’s PyMultiNest with our DEMCzs in Section 6.3.1, and these algorithms are less similar than DEMCzs and the DEMC of Line et al. (2014). So, we do not blame the samplers for the discrepancy among models. BART uses Kurucz stellar models, while Line et al. (2014) use PHOENIX, but Martins & Coelho (2007) found that Kurucz and PHOENIX models are comparable in the near-infrared for stars with effective temperatures greater than 4250 K, like HD 189733. The pre-computed opacity grid of Line et al. (2014) used 20 temperatures ranging from 500 to 3000 K.
Note. For each data set, we report the 68.27%, 95.45%, and 99.73% credible regions, from top to bottom per model.

### Table 5

| Forward Model | $T$ (K) | $R_p$ (km) | H$_2$O (ppmv) | CO (ppmv) | log $P_{\text{cloud}}$ |
|---------------|---------|------------|---------------|-----------|-----------------------|
| True          | 1500    | 79 558.718 | 300           | 350       | n/a                   |
| NEMESIS       | [1455, 1492] | 79549, 79588 | [265, 369]    | [548, 1372] | [0.17, 1.38]         |
| [1440, 1513] | 79527, 79608 | [223, 436]    | [325, 2126]   | [−0.12, 1.50]        |
| CHIMERA       | [1421, 1531] | 79477, 79626 | [190, 522]    | [178, 3476] | [−0.40, 1.50]        |
| TAU-Rex       | [1457, 1497] | 79581, 79621 | [286, 395]    | [282, 783]  | [0.24, 1.35]         |
| [1437, 1516] | 79557, 79643 | [242, 469]    | [153, 1289]   | [−0.15, 1.49]        |
| [1421, 1539] | 79471, 79660 | [204, 542]    | [76, 2094]    | [−0.38, 1.50]        |

### Table 6

| Forward Model | $T$ (K) | $R_p$ (km) | H$_2$O (ppmv) | CO (ppmv) | log $P_{\text{cloud}}$ |
|---------------|---------|------------|---------------|-----------|-----------------------|
| True          | 1500    | 79 558.718 | 300           | 350       | −2.0                  |
| NEMESIS       | [1416, 1524] | 79122, 79666 | [214, 5198]   | [584, 10750] | [−3.13, −1.87]      |
| [1344, 1578] | 79019, 80024 | [82, 7905]   | [110, 15241]  | [−3.32, −1.30]        |
| [1270, 1630] | 78869, 80204 | [52, 14246]  | [38, 2065]    | [−3.55, −1.06]        |
| CHIMERA       | [1402, 1512] | 79221, 79947 | [104, 2418]   | [96, 2678]  | [−2.82, −1.36]       |
| [1342, 1564] | 79024, 80866 | [75, 7096]   | [36, 6025]    | [−3.22, −1.17]        |
| [1291, 1618] | 78865, 80195 | [52, 13029]  | [11, 9897]    | [−3.50, −1.03]        |
| TAU-Rex       | [1399, 1520] | 79062, 79946 | [98, 568]     | [100, 391]  | [−3.21, −1.38]       |
| [1330, 1573] | 78929, 80888 | [69, 1068]   | [24, 891]     | [−3.43, −1.19]        |
| [1273, 1633] | 78774, 80206 | [47, 2006]   | [3, 1448]     | [−3.70, −1.02]        |

Note. For each data set, we report the 68.27%, 95.45%, and 99.73% credible regions, from top to bottom per model.

and 20 pressures ranging from 20 to $10^{-6}$ bars, while BART used 25 temperatures spanning 600–3000 K and 100 pressures ranging from 100 to $10^{-8}$ bars. This may explain BART’s slight improvement in reduced $\chi^2$ for the STDS case, but not likely the inversion, as the contribution plots indicate little sensitivity in the extended regions and the pressure gridding should be sufficient for interpolation in both cases. Priors on thermal profile parameters differed (uniform versus Gaussian), which could have kept Line et al. (2014) from finding a $\chi^2$ minimum with an inverted profile.

The model differences above lead to a $\chi^2$ improvement of 10.29 from Line et al. (2014) to our STDS case, which uses the same line lists, for a maximum likelihood ratio of 172. One might expect even more improvement using the much more complete HITTEMP and ExoMol line lists. Instead, $\chi^2$ deteriorates to just 2.28 better than Line et al. (2014; maximum likelihood ratio of 3.1). Evidently, the need to distribute the misspecification error dominates the improvement in the modern line lists.

The next-closest study, and the only other Bayesian approach, used TAU-REX 2’s Stage 1 MCMC (Waldmann et al. 2015a). With the release of version 3 (Al-Refaie et al. 2021), many new results from TAU-REX 2’s Stage 1 MCMC are not anticipated, so we have not emulated it directly, but we can discuss it.

They omit the IRAC 5.8 μm point, which is quite constraining, due to its smaller uncertainties than the IRS spectrum at those wavelengths. At 10 bars, their uncertainties on $T(p)$ are small (their Figure 15), despite the data not probing to that depth. This may be due to conditioning $T(p)$. Our Figure 12 and similar plots elsewhere show the lack of contribution from that level and the resultant broadening of the $T(p)$ credible region there.

They used the CH$_4$ line list of Yurchenko & Tennyson (2014). Its higher limiting temperature yields many times the lines of the test’s HITRAN list, and thus greater overall opacity. This tends to reduce the abundance of CH$_4$ and could also reduce other species’ abundances, if CH$_4$ opacity appeared where there had been none previously. This may explain their usually lower retrieved abundances (Table 7 and Figure 13). BART’s retrieved $T(p)$ profile (all three cases) differs substantially, with a lower temperature in the upper atmosphere and a lower tropopause pressure ($10^{-2}$ versus $10^{-1}$ bar) than TAU-REX’s. Like Line et al. (2014), they also find no inversion.

In Table 7 and Figure 13, we also provide the fitted ranges for pre-Bayesian-retrieval abundances reported by Madhusudhan & Seager (2009), Swain et al. (2009), Lee et al. (2012), and Line et al. (2012). We find agreement within 3σ for most molecular abundances. BART’s results differ at 3σ for CO$_2$ and H$_2$O reported by Swain et al. (2009) and CO$_2$ reported by Madhusudhan & Seager (2009). Like Lee et al. (2012), we similarly find that CO is poorly constrained. In the case of $T(p)$ profiles, Lee et al. (2012) found the upper atmosphere to be isothermal (~1100 K) down to ~0.1 bars. Line et al. (2012) find a variety of potential $T(p)$ profiles, some of which are consistent with Lee et al. (2012), and some of which are consistent with the results of BART and Line et al. (2014). The $T(p)$ profiles explored by Madhusudhan & Seager (2009) generally agree with these other analyses, with the exception of...
the upper atmosphere, which is cooler. Swain et al. (2009) did not publish a \( T(p) \) profile. These investigations used either a grid search or optimal estimation rather than a Bayesian method, and they used a different data set from that used here. Both of these differences could explain discrepancies in retrieved parameters.
The level of disagreement among studies using different modeling approaches, and sometimes different data, for the same planet indicates what we might expect going forward, when better instruments make similar-quality 1D measurements of potentially habitable planets. Thus, when a discovery analysis enters the literature, we should ask whether the conclusion about habitability would change if $T(p)$ or abundances changed by $3\sigma$ or even more, due to the impact of the inevitable model misspecifications on parameter estimates and even on the interpretations of the parameters.

Given the high temperatures of the most easily observed exoplanets, it is critical to have lists that include lines excited by those high temperatures. By extension, given the high opacities of radicals and ions, it is likely important to include those species as well, when the temperatures warrant it.

Conversely, it is important not to include species above the temperatures at which they dissociate, although we have seen this in the literature. So, although we have supplied a free tool that allows anyone to perform a retrieval, care is necessary to do so correctly.

Much of what we have learned in creating, testing, and using BART applies to retrieval analyses generally, and even well beyond that scope, giving rise to the four appendices that follow.

We have not found a satisfactory stopping condition (sufficient number of iterations) for Monte Carlo Bayesian analysis in the literature. The decision of when to stop has varied among practitioners of exoplanet retrieval and light-curve fitting and has never been justified statistically, to our knowledge. Many practitioners incorrectly stop at Gelman–Rubin convergence (this is when the statistical posterior may mimic the true posterior sufficiently that we can start using samples). Credible regions and other quantities derived from a sampled posterior become more accurate with more accepted steps. Appendix C derives a new expression relating credible-region accuracy to the number of steps, allowing practitioners to run until they have achieved a desired accuracy.

While developing synthetic-data tests, we obtained poor reproducibility until we discovered that such spectra must be created at extremely high resolution, much higher than needed in the retrieval spectra. As others may run afoul of this requirement, we demonstrate the effect and experimentally derive the needed resolution in Appendix D.

In reproducing the work of others to validate BART, we have found inconsistencies between things as basic as the data cited and those actually used. Frequently, published descriptions are inadequate to reproduce retrieval work without extensive direct conversations with and even data requests of their investigators. As time passes, such conversations become much more difficult: old research records are lost, and people leave the field. By providing a checklist for authors and reviewers in Appendix B, we hope that future retrieval reports from all codes will be more complete and reproducible.

By releasing BART under a license that requires full disclosure and archiving of a retrieval calculation, including any code modifications, we ensure that BART’s body of work, at least, will be reproducible in the long term. See Appendix A to learn why this accelerates science and how to manage it without undue additional work. We hope others will embrace reproducible research in their own work, and we look forward to a deeper conversation on openness and reproducibility in astrophysics and planetary science.

The description of BART’s algorithms, initialization, and post-processing routines continues in Papers II and III.

A compendium of this paper’s software and analyses is available at https://doi.org/10.5281/zenodo.5585645.

We thank J. Fortney for co-advancing the dissertations of J.B. and P.E.C., and for discussions. We also thank M. Line for helpful clarification on the HD 189733b data used in Line et al. (2014). We appreciate references to historical sources provided by J. Pasachoff. We appreciate feedback and feature requests provided by members of the BART mailing lists and others who tried out early versions. We thank contributors to NumPy, SciPy, Matplotlib, AstroPy, the Python Programming Language, GitHub.io, the NASA Astrophysics Data System, and the free and open-source software communities for software communities.

8. Conclusions

In this paper, we present an open-source code, BART, that makes atmospheric retrieval accessible to the entire community. It has separate user and code documents and is intended for use and improvement by others. Its modular, high-level code enables the examination of assumptions by allowing the user to swap out line lists, thermal profiles, and other aspects of the calculation. The code passed the four categories of tests included in the new BARTTEST package, including analytic and comparison RT tests and synthetic and real-data retrieval tests. The comparison and real-data tests depend on multiple codes implementing them and contributing the results to a central repository, which we invite the community to do.

In applying BART to HD 189733b, we attempt to validate it by comparing to six retrievals in the literature, one of which we conducted, we find that physics modeled, line lists, and data can each have a significant effect on the results. While synthetic tests may match very well when utilizing the same line lists and data, if there is model misspecification (and there always is, on a real planet), its impact on parameter estimates will differ for even slightly different codes. Figure 13 offers some comfort, in that models with significantly different best-fit $\chi^2$, and thus degrees of misspecification, can still give consistent parameter estimates.

Figure 13. Comparison of best-fit retrieved log abundances for HD 189733b: BART’s retrieved 68% credible region, TAU-REX’s Stage 1 result, CHIMERA’s best fit and 68% interval, the best fit and possible fit range reported by Lee et al. (2012), and the range of values reported by Line et al. (2012), Madhusudhan & Seager (2009), and Swain et al. (2009).

The Planetary Science Journal, 3:80 (31pp), 2022 April

Harrington et al.
Table 7
Comparison of Fitted Log Abundances for HD 189733b

| Item   | This Work, HH | This Work, STDS | This Work, EM | Waldmann et al. (2015a) | Line et al. (2014) | Lee et al. (2012) | Line et al. (2012) | Madhusudhan & Seager (2009) | Swain et al. (2009) |
|--------|---------------|-----------------|---------------|-------------------------|-------------------|-----------------|-------------------|-----------------------------|---------------------|
|        |               |                 |               | Stage I                 |                   |                 |                   |                             |                     |
| H₂O    | [−3.1, −2.4]  | [−3.4, −2.6]    | [−3.4, −2.7]  | −3.9 ± 0.2              | [−3.5, −2.9]      | [−4.5, −2.0]    | [−4.3, −3.5]      | [−5.0, −3.0]               | [−5.0, −4.0]         |
|        | [−3.4, −1.9]  | [−3.8, −2.2]    | [−3.7, −2.3]  |                         |                   |                 |                   |                             |                     |
|        | [−3.6, −1.4]  | [−4.2, −1.6]    | [−3.9, −1.8]  |                         |                   |                 |                   |                             |                     |
|        | [−4.7, −3.7]  | [−4.5, −3.9]    | [−5.1, −4.5]  | −6.7 ± 0.7              | [−5.0, −4.6]      | <−4.0           | <−2.0             | <−5.2                      | <−5.0               |
|        | [−10.5, −3.1] | [−4.8, −3.5]    | [−5.2, −4.2]  |                         |                   |                 |                   |                             |                     |
|        | [−12.7, −3.1] | [−5.1, −3.1]    | [−5.5, −3.7]  |                         |                   |                 |                   |                             |                     |
| CH₄    | [−6.6, −0.5]  | [−4.8, −0.5]    | [−4.8, −0.5]  | −2.7 ± 1.4              | [−4.6, −1.5]      |                 |                   |                             |                     |
|        | [−12.5, −0.5] | [−12.4, −0.5]   | [−12.5, −0.5] |                         |                   |                 |                   |                             |                     |
|        | [−12.9, −0.5] | [−12.7, −0.5]   | [−12.9, −0.5] |                         |                   |                 |                   |                             |                     |
| CO     | [−6.6, −0.5]  | [−4.8, −0.5]    | [−4.8, −0.5]  | −2.7 ± 1.4              | [−4.6, −1.5]      |                 |                   |                             |                     |
|        | [−12.5, −0.5] | [−12.4, −0.5]   | [−12.5, −0.5] |                         |                   |                 |                   |                             |                     |
|        | [−12.9, −0.5] | [−12.7, −0.5]   | [−12.9, −0.5] |                         |                   |                 |                   |                             |                     |
|        | [−3.3, −2.7]  | [−2.6, −1.8]    | [−2.9, −2.3]  | −3.7 ± 0.5              | [−2.9, −2.4]      | [−3.8, −1.5]    | [−2.8, −2.2]      | ∼−1.2                      | [−7.0, −6.0]         |
|        | [−3.7, −2.3]  | [−2.9, −1.4]    | [−3.2, −2.0]  |                         |                   |                 |                   |                             |                     |
|        | [−4.0, −2.0]  | [−3.2, −0.9]    | [−3.5, −1.6]  |                         |                   |                 |                   |                             |                     |
| CO₂    | [−6.6, −0.5]  | [−4.8, −0.5]    | [−4.8, −0.5]  | −2.7 ± 1.4              | [−4.6, −1.5]      |                 |                   |                             |                     |
|        | [−12.5, −0.5] | [−12.4, −0.5]   | [−12.5, −0.5] |                         |                   |                 |                   |                             |                     |
|        | [−12.9, −0.5] | [−12.7, −0.5]   | [−12.9, −0.5] |                         |                   |                 |                   |                             |                     |
|        | [−3.3, −2.7]  | [−2.6, −1.8]    | [−2.9, −2.3]  | −3.7 ± 0.5              | [−2.9, −2.4]      | [−3.8, −1.5]    | [−2.8, −2.2]      | ∼−1.2                      | [−7.0, −6.0]         |
|        | [−3.7, −2.3]  | [−2.9, −1.4]    | [−3.2, −2.0]  |                         |                   |                 |                   |                             |                     |
|        | [−4.0, −2.0]  | [−3.2, −0.9]    | [−3.5, −1.6]  |                         |                   |                 |                   |                             |                     |
|        | [169.60]      | [139.53]        | [147.54]      | ...                      | [149.82]          | ...             | ...               | ...                        | ...                 |
| Red. χ² | 2.98          | 2.45            | 2.59          | ...                      | 2.63              | ...             | ...               | ...                        | ...                 |

Notes.

a 68.27%, 95.45%, and 99.73% credible regions, stacked vertically.
b Main BARTTEST model, which uses HITRAN 2012 and HITEMP 2010 line lists.
c Same as HH, but using the STDS CH₄ line list at wavelengths >1.7 μm and HITRAN 2008 at wavelengths <1.7 μm.
d Model using most recent ExoMol line lists for H₂O and CO₂ and HITEMP line lists for CO and CH₄.
e Reported 68.27% interval.
f Possible fit range for Δχ²/N < 1.0 case, with n/a indicating no constraint.
g Reported range of model abundances.
h Comparing χ² between different models fitting different data does not tell which model is better, so we do not report the χ² of other studies besides Line et al. (2014).
i Calculated from their reported statistic of χ²/N_data.
j 57 degrees of freedom, though the independence of adjacent spectral channels is questionable if they sense the same molecular band.
and services. Part of this work is based on observations made with the Spitzer Space Telescope, which is operated by the Jet Propulsion Laboratory, California Institute of Technology, under a contract with NASA. This work was supported by NASA Planetary Atmospheres grant NNX12Af69G, NASA Astrophysics Data Analysis Program grant NNX13AF38G, and NASA Exoplanets Research Program grant NNX17AB62G, held by J.H. M.D.H. held NASA Fellowship Activity fellowship 80NSSC20K0682. J.B. held NASA Earth and Space Science Fellowship NNX12AL83H. I.D.-D. and J.B. held NASA Exoplanets Research Program grant NNX17AC03G. P. E.C. was supported by the Fulbright Program for Foreign Students. P.M.R. acknowledges support from CONICYT project Basal AFB-170002.

Software: BART (This work; BART2; BART3), MC3 (Cubillos et al. 2017), TEA (Blecic et al. 2016), REPACK (Cubillos 2017), NumPy (Oliphant 2015; van der Walt et al. 2011), SciPy (Jones et al. 2001; Virtanen et al. 2020), SymPy (Meurer et al. 2017), Matplotlib (Hunter 2007), and AAS-TeX6.3.1 (AAS Journals Team & Hendrickson 2018).

Facilities: HST(NICMOS), Spitzer(IRAC), Spitzer(IRS), Spitzer(MIPS).

HD 189733b.

Appendix A

Methods for Reproducible Research

In this appendix, we discuss research methods, applied herein, that, if widely adopted, could (and in other fields do) accelerate the progress of science, by making it easier to find out exactly what was done in a numerical study and by making efforts at reproducing work more straightforward. Reproducibility distinguishes science from all other knowledge systems. The first question we should ask of a new discovery is whether it could just be a fluke. Before the advent of computers, research reports carried all the information needed to reproduce an experiment or observation. They detailed experimental setups and presented all the raw data. Observatories kept extensive archives of sketches, photographic plates, and astronomers’ original notes. Visits to access original data were common.

With the advent of computers, studies became much more complex, and the barriers to reproducing them rose dramatically. It is now challenging, and often impossible, to learn the exact methods applied in a numerical study, because the number of settings, implementation choices, and input data is too large to describe in any reasonable paper. Even if one could, writing the code for a significant investigation from scratch can take person-years of effort. This means that most studies are never independently checked, even to the extent of simply running the same code to confirm that it indeed produces the reported output.

This is particularly worrisome at the cutting edge of discovery, where signal is low, systematics abound, the physical situation under observation is not well understood, and the quantity of independent data points is insufficient to constrain a complete physical model. This describes the field of exoplanet characterization for the foreseeable future. As demonstrated in the main text, modest differences in methods or data can lead to significantly different results. It is often entirely opaque why two different studies obtained different results on the same data until someone methodically reproduces both studies and other possible variants to determine which differences explain the disparity. Without access to original codes and data, this rarely happens.

The Reproducible Research (RR; Fomel & Claerbout 2009; Stodden 2009; Donoho 2010; Barba 2018) movement simply proposes that all reports based on computation include a compendium of the codes, data, settings, and output that support each scientific claim in a paper. This allows full transparency without bloating the report. Readers can answer a host of methodological questions just by looking at the code. They can reprocess the output, plotting it differently or comparing it to the output of similar studies. They can even rerun the code, adjusting parameters to determine how the results change under different assumptions.

Further, in any computational analysis, the code and inputs, not a text written about them, are the most complete, detailed, and accurate record of what was actually done. While the written description is critical, its main function is summary, informing those using the result and providing a guide to any subsequent reproduction effort. No one would want to skip the written description, but only the code is authoritative.

RR also benefits science directly by improving practice.

Being human, and under significant pressure to publish quickly and frequently, investigators sometimes take shortcuts or even hide inconvenient details that could impede publication. When others attempt replication from their insufficiently detailed reports, it may be impossible to identify why the results do not match. This can lead to months of fruitless work on the part of the second investigator, often a junior scientist just trying to understand and build on prior work.

Also, by nature, computer codes evolve as investigators add features to handle new situations. Thus, the code used for the first-run cases in a report may differ from that used later, even though there is only one description. Worse, if an author receives a question years after publication, the code as published may no longer exist. The investigators may even no longer be available.

At first glance, RR looks much more time-consuming than current practice. It is, if compendium assembly is done retroactively, especially if corners have been cut. We argue that good codes should build their own compendia, and careful workers thus spend little additional time. BART, for example, makes a directory for each run, copies the configuration files to it, and puts all the output there. It also records the software version. As there are many files, BART includes a guide to the file structure that helps readers find the most-sought items. To build the compendium, the investigator simply collects these run directories and adds a top-level text file mapping the runs to the claims in the paper (e.g., “Figure 7 comes from run 9”). In conducting the work, the investigator logs the purpose of each run and keeps a list of the best runs for each claim, to locate the right directories later among what could be many trial runs. Careful investigators already do this, so there is little extra burden.

Upon submission, the investigators upload the compendium, usually as a single, compressed file, to one of many RR archive services, provides the permanent identifier in the paper, and never touches it again.

12 https://github.com/exosports/BART
13 https://github.com/pcubillos/mc3
14 https://github.com/dzesmin/TEA
Why not continue with the status quo? The purest replication would not even look at the original code. If code access is really needed, the authors can propose a collaboration with the original authors, or just ask for access.

Unfortunately, the time required to implement many computational analyses from scratch strongly deters reproduction, and often we just want to answer a question, rather than fully rerun an analysis. If little is reproduced or even questioned, science strays from its founding strength. Also, authors often consider their codes to be proprietary, a sort of moat against competition. This attitude, time since the original work’s publication, and simple busyness can reduce the level of cooperation below that needed for a successful confirmation.

On the other hand, with access to the full investigation, readers can ask, “What did they really do?” “How did they do that?” and even, “What happens if we do this instead?” Most of these questions are too small to merit bothering original authors with, but they could easily be answered with a look at the compendium. This quickly builds trust in the work (and citations) or identifies errors before they mislead the field. RR makes hiding dishonesty and cutting corners much harder too.

RR is different from open-source software (OSS). A proprietary code could appear in an RR compendium with a license that allows reading and even running the code but prohibits redistribution, modification, or publishing new calculations without permission from and even coauthorship with the code owners. We promote the OSS approach, as it allows others to stand on our shoulders, as we have stood on the shoulders of those who came before us.

We have released BART under the same Reproducible Research Software License (RRSL) used for TEA (Blecic et al. 2016). This license ensures that all work produced by BART and its derivatives is subject to confirmation. It also addresses concerns often raised about openness. When publishing, code users are required to cite the papers describing the code. Investigators can develop the code in the open without fear of others publishing with it, or portions of it, before they finish it and publish, as this is forbidden. Those improving the code must share their improvements if they publish results from them. This prevents “casting,” where investigators privatize a public code they did not write by improving it but not sharing. Authors may still write less-restrictive licenses to specific parties, possibly in exchange for compensation. For commercial or other nonscientific purposes, the RRSL acts as a permissive OSS license.

The RR approach produces a higher quality of work in original papers without unduly greater effort and makes evident exactly what was done without longer papers. There are also abundant political, social, financial, and access benefits of RR, which we leave to white papers and national studies (references above and National Academies of Sciences, Engineering, and Medicine 2018). The RRSL eliminates barriers to openness that do not exist in the commercial world of conventional software licenses, but softer solutions might be better received. Ideally, funders, journals, and peers would provide incentives, and researchers could choose whether and when to participate. Our main hope is thus to raise a conversation and propose norms on how we conduct and report computational work.

Appendix B
What to Include in Published Reports

Above, and elsewhere, we have attempted to demonstrate BART’s correctness and flexibility by duplicating several studies in the literature. There are many inputs and settings in a BART analysis (observations and their uncertainties, filter functions, line lists, atmospheric profiles). Only in a few cases (and none in this paper) have we been able to set up runs to reproduce another’s work based on published reports alone. While we are grateful to the authors of the original papers, communicating with an author should never be required to reproduce a study. We thus offer the following minimal checklist of items that authors and reviewers should ensure are in all retrieval papers and/or their compendia, ideally in machine-readable form, whether from BART or any other code, and whether following RR or not:

1. Input data, including uncertainties and filter transmission functions.
2. Atmospheric pressure/altitude limits and gridding.
3. Analytic form(s) (possibly by reference) and initial values of all retrieved vertical profiles.
4. Line lists (including CIAs), including statement of their temperature limits.
5. Statement that the atmosphere was thick enough that no rays reached the abyssal layer, or the properties of a surface or thick cloud with realistic reflectance/scattering.
6. Discussion of molecular stability under the retrieved $T(p)$ conditions, if relevant.
7. List of retrieval parameters and any conditioning (e.g., smoothing), allowed ranges (can be shown on histograms), and initial values. If there is conditioning, any reduction in the number of effective free parameters must be stated.
8. How initial values were chosen (e.g., thermochemical equilibrium at a given pressure and temperature).
9. List of nonretrieval values that affected the spectrum (e.g., a constant abundance of $C_2H_4$).
10. Publication reference for retrieval code.
11. Any modifications to the code since the publication.
12. Statement of convergence and how it was tested.
13. Number of iterations, SPEIS, and ESS; SPEIS calculation method; and precision of confidence intervals.
14. Values and uncertainties and/or confidence intervals of all retrieved parameters, including any nuisance parameters.
15. Plots (at least in an electronic supplement or compendium) of posterior histograms, pairwise parameter correlations, and parameter traces.
16. $\chi^2$ and reduced $\chi^2$ values.
17. Retrieved vertical profile and filter contribution functions on same or shared-axis, two-panel plot (uniform profiles excepted).

This is a long list. It combines what is needed to reproduce and to validate a run. It also includes the answers to most questions that readers will have. Users of proprietary codes that cannot be included in a Reproducible Research Compendium (RRC), and those unwilling to share one, can still provide these details in their texts and electronic supplements, greatly improving reproducibility.

Per BART’s license (above), users must publish all of this information in reviewed reports of BART runs in an RRC. To make this easier, BART saves nearly all of this information in its output directory. In addition to the points above, a full RRC includes the code or access to it, full configuration information.
(including command line) of each reported run, and the scripts that produced all plots and tables. If the user takes proper scientific care to document runs as they execute, including recording their command lines and the general purpose and features of each run, then making the RRC is a matter of collecting the BART output directories for the runs in the paper into one directory and writing a README file. That file should give the command line for each run and identify the specific runs that support the claims in the paper (e.g., table entries, plots, and statements in the text). BART’s user manual is useful for locating specific information in the compendium, as it documents the inputs and outputs in detail. We warn that compendium assembly can be quite time-consuming if the user is sloppy and does not later recall which figure or table entry came from which run.

Appendix C
Required MCMC Effective Sample Size

MCMC-based posterior sampling uses a finite set of dependent random samples from a posterior distribution to approximate the values of integrals that summarize the posterior. We address here the question of how large a set of posterior samples one should collect to compute common posterior summaries with sufficient precision.

For a problem with a parameter, \( \theta \), and posterior distribution, \( p(\theta) \), common summaries we might want to compute include the posterior mean,

\[
\mu \equiv \int \theta \ p(\theta) \ d\theta,
\]

the posterior standard deviation, \( \sigma \), with

\[
\sigma^2 \equiv \int (\theta - \mu)^2 \ p(\theta) \ d\theta,
\]

and the probability content, \( C \), of a credible region \( \mathcal{R} \),

\[
C \equiv \int I_{\mathcal{R}}(\theta) p(\theta) \ d\theta,
\]

where \( I_{\mathcal{R}}(\theta) \) is the indicator function for the region, taking the value 1 inside the region and 0 outside it.

Note that the last two summaries are quantifications of uncertainty. We are computing them with a Monte Carlo algorithm, so estimates of these uncertainty quantities will themselves have uncertainties (due to use of a finite and random Monte Carlo sample). This leads to some awkward but necessary linguistic constructions, e.g., “the standard error of the estimate of the standard deviation.” Note further that the reason we use MCMC algorithms is that \( p(\theta) \) is not a simple distribution like a Gaussian, which would be amenable to analytic computation. As a result, there is no general relationship between \( \sigma \) and \( C \) (e.g., the \( \mu \pm \sigma \) interval will not in general have \( C \approx 0.683 \)), so, even if we have a precise estimate of \( \sigma \), we still must separately compute \( C \). Similarly, if we find a region with \( C \approx 0.683 \), it does not follow that expanding that region by a factor of two produces a region with \( C \approx 0.954 \) (as it would for a one-dimensional Gaussian). If we want to report credible regions of different sizes, each one needs its own computation and will have its own Monte Carlo uncertainty.

We here estimate how large a Monte Carlo sample we need to compute these summaries with usefully small uncertainty. We present guidelines for the number of samples from an algorithm that produces independent, identically distributed (IID) samples from \( p(\theta) \). For MCMC algorithms, the samples are dependent; these guidelines should be interpreted in terms of the effective sample size (ESS) for the MCMC output (which may be estimated with various standard techniques that quantify the strength of dependence in the Markov chain output).

We use hats to denote a Monte Carlo estimate of a posterior summary that replaces the integral over \( p(\theta) \) with an average over IID posterior samples. Using a Monte Carlo sample size of \( N \), \( \{ \theta_i \} \), the estimate of the posterior mean, \( \mu \), is

\[
\hat{\mu} = \frac{1}{N} \sum_{i=1}^{N} \theta_i.
\]

An analogous expression holds for \( \hat{\sigma} \), based on Equation (2), and substituting \( \hat{\mu} \) for \( \mu \):

\[
\hat{\sigma}^2 = \frac{1}{N} \sum_{i} [\theta_i - \hat{\mu}]^2.
\]

(An unbiased estimator for \( \sigma^2 \) would divide by \( (N - 1) \), but we are interested in cases with large \( N \), so we ignore the difference between \( N \) and \( N - 1 \); in any case, the slightly biased estimator using \( N \) has slightly smaller standard error; also, we are interested in estimating \( \sigma \) rather than \( \sigma^2 \).) For \( \hat{C} \), the sum is over values of the indicator function; this amounts to simply counting the number of samples in \( \mathcal{R} \), which we denote \( N_{\mathcal{R}} \), so

\[
\hat{C} = \frac{N_{\mathcal{R}}}{N}.
\]

We will use the standard error (rms variability) as a measure of the uncertainty in one of these estimates. For \( \hat{\mu} \), the standard error is the standard deviation of the \( p(\theta) \) distribution, divided by \( \sqrt{N} \). Of course, that standard deviation is unknown, but we can estimate it using Equation (C2). So, an estimate of the standard error for \( \hat{\mu} \) is

\[
s_{\hat{\mu}} = \frac{\hat{\sigma}}{\sqrt{N}}.
\]

The standard error for the \( \hat{\sigma} \) estimate is trickier to compute. Booth & Sarkar (1998) give a simple approximation, suitable for ballpark estimates of the required sample size. Their calculation is in the context of bootstrap resampling; we adapt it to our purposes as follows. Divide Equation (C5) by the (unknown) true value of \( \sigma^2 \), giving

\[
\frac{\hat{\sigma}^2}{\sigma^2} = \frac{1}{N} \sum_{i} \frac{[\theta_i - \hat{\mu}]^2}{\sigma^2}.
\]

Adopt a Gaussian approximation for the distribution of \( (\theta_i - \hat{\mu}) \). Then, the distribution for the sum will be approximately \( \chi^2 \) with \( N - 1 \) degrees of freedom (since \( \mu \) is estimated by \( \hat{\mu} \)). Recall that a \( \chi^2 \) random variable with \( N \) degrees of freedom has expectation value \( N \) and standard deviation \( \sqrt{2N} \). Thus (again ignoring the difference between \( N \) and \( N - 1 \)), we expect

\[
\frac{\hat{\sigma}^2}{\sigma^2} \approx 1 \pm \frac{\sqrt{2}}{\sqrt{N}}.
\]
The relative error of the $\hat{\sigma}^2$ (variance) estimate is

$$\delta = \left| \frac{\hat{\sigma}^2 - \sigma^2}{\sigma^2} \right| = \left| \frac{\hat{\sigma}^2}{\sigma^2} - 1 \right|. \quad (C10)$$

Using Equation (C9), the expected relative error in the variance is thus

$$\langle \delta \rangle \approx \frac{2}{\sqrt{N}}. \quad (C11)$$

Let $s_\delta$ denote the standard error in $\hat{\delta}$. By propagation of errors (the delta method), the expected relative error in the standard deviation is half of $\langle \delta \rangle$, giving

$$\frac{s_\delta}{\sigma} \approx \frac{1}{2\sqrt{N}}. \quad (C12)$$

Hence, if we are aiming for 5% relative error in $\sigma$ (say), we need $N \approx 200$ IID samples.

Turning now to the error in $\hat{C}$, note that estimating $C$ corresponds to estimating the probability parameter for a binomial distribution, based on $N_R$ successes in $N$ trials. We can treat this as a basic Bayesian inference problem. Adopting a flat prior on $C$ and a binomial sampling distribution, the posterior distribution for $C$ is a beta distribution, $\text{Beta}(N_R + 1, N + 1)$. The posterior mode is $\hat{C}$, and the posterior standard deviation is

$$s_{\hat{C}} = \sqrt{\frac{\hat{C}(1 - \hat{C})}{N + 3}}. \quad (C13)$$

If we specify target values for $\hat{C}$ and $s_{\hat{C}}$, the necessary sample size (ignoring the insignificant + 3) is

$$N \approx \frac{\hat{C}(1 - \hat{C})}{s_{\hat{C}}^2}. \quad (C14)$$

Some useful examples:

1. Targeting a 68.27% credible region ("1σ") for a Gaussian with 2% (absolute) error requires $N \approx 500$.
2. Targeting a 95.45% credible region ("2σ") with 0.5% error requires $N \approx 1700$.
3. Targeting a 99.73% credible region ("3σ") with 0.1% error requires $N \approx 2700$.

The latter two sample sizes are fairly large because accurately estimating the probability content of larger regions requires adequate sampling of the tail of the posterior distribution. A "4σ" region extends far into the tail, with $C = 0.999994$; to capture its first non-nine digit accurately would require $N \approx 250, 000$.

Given the prevalence and usefulness of "2σ" and "3σ" intervals, it is a good practice to generate an ESS of 3000, when computationally feasible. Flegal et al. (2008) advocate a more detailed approach; they use a batch means algorithm to estimate the standard errors for every quantity of interest as an MCMC calculation proceeds, stopping the run when target values are achieved.

During the preparation of this manuscript, Vehtari et al. (2021) introduced an improvement on the convergence criteria of Gelman & Rubin (1992) by considering both the within-chain and between-chain variances to determine when all chains have converged to the same stationary distribution. They also present a related method to estimate SPEIS (and from it, ESS) via combining the autocorrelation estimates of each chain by similarly considering the within- and between-chain variances, which they describe as a conservative estimate. Their accepted article appeared during final review of this article.

We have elected to use the convergence metric of Gelman & Rubin (1992) and the SPEIS method described in this manuscript rather than their methods for a few reasons. First, our SPEIS method is more conservative. It yields a greater SPEIS and correspondingly lower ESS, ensuring that our credible-region uncertainties are not smaller than they would be if estimated using the Vehtari et al. (2021) criterion. Second, for our runs, we find similar values for both convergence criteria. Additionally, their recommendation regarding posterior draws ("only using the sample if $\hat{R} < 1.01$") would require significantly more MCMC iterations for a negligible change in the results shown in this paper. We highlight that their recommended cutoff of 1.01 is consistent with some papers in the literature (including here), although many others use greater values (see Table 1 of Vats & Knudson 2021).

Recognizing the likely emergence of a new criterion from recognized experts, we recommend, for the time being, evaluating both criteria and using the more conservative estimate. A true convergence determination is theoretically impossible. Other studies, especially with the legacy MCMC explorers still included in BART, may find that either criterion may be more conservative.

**Appendix D**

**Retrieval Errors due to Wavenumber Sampling Grid Mismatch**

When performing the synthetic retrievals described in Section 6.3, we observed a numerical effect that can bias the Bayesian sampler toward slightly incorrect answers when the forward and retrieval models use differing wavenumber grids. Here we describe this effect and how to minimize it. We note that this error most strongly manifests when the RT code that produced the synthetic spectrum matches the RT code used when retrieving on the synthetic spectrum, and the error appears to be negligible when retrieving on real data at current resolutions.

Line-by-line calculations necessitate a discrete sampling of the resulting spectrum. Yet spectra are continuous, and this discrete sampling will therefore introduce error when, e.g., band integrating a spectrum during a retrieval. At commonly used grid spacings (e.g., 1.0 cm$^{-1}$) for current- and next-generation telescope resolutions, these errors can drive the Bayesian sampler to an incorrect part of the phase space.

We consider forward models with four different grid spacings: 0.025, 0.1, 0.25, and 1.0 cm$^{-1}$. For each grid spacing, we also consider a horizontal shift of all values by $\mu$ and $\sigma$; with 0.1 cm$^{-1}$ grid spacings, there is disagreement in the 2.5–3.5 μm and >4.5μm regions. By comparison, when only considering the 0.025 and 0.1 cm$^{-1}$ grid spacings, the differences tend to be comparable to the width of the plotted lines.

We further investigate this effect by simulating a spectrum at 0.1 cm$^{-1}$, band integrating according to some filters, and retrieving with wavenumber grids that only differ in their spacing. The retrieval models use grid spacings of 0.1, 0.25, 0.5, and 1.0 cm$^{-1}$. We ensure that all wavenumbers in the...
retrieval model grids exactly overlap with wavenumbers from the forward-model grid. Figure 15 shows that choosing coarser griddings than that of the forward model leads to a reduction in accuracy: the 0.1 cm$^{-1}$ gridding recovers all of the parameters within 1$\sigma$, while the 0.25 and 0.5 cm$^{-1}$ griddings recover most parameters at $>1\sigma$. The 1.0 cm$^{-1}$ gridding entirely misses four out of the five parameters.

This effect would be expected to be most pronounced in the case where the same RT code is used for the forward and retrieval models, since the retrieval RT model can, in theory, exactly match the forward RT model. To test whether this effect arises when the forward and retrieval RT codes differ, we ran the Barstow et al. (2020) cases at two different resolutions (0.1 and 1.0 cm$^{-1}$; Figure 16). The inferred
temperatures and radii are generally insensitive to the grid selection, though the retrieved molecular abundances only slightly overlap, with the lower/upper credible-region boundaries varying by around an order of magnitude. On the other hand, when retrieving using the real data of HD 189733b at the aforementioned grid resolutions, we find only minor differences (Figure 17). The posteriors of thermal profiles (calculated via the $\kappa$, $\gamma_1$, and $\beta$ parameters) are nearly identical, and H$_2$O and CO$_2$ are essentially unaffected. CO and CH$_4$ are minorly affected, with the coarser grid preferring slightly higher CO and lower CH$_4$ abundances. These minor differences are not significant enough to change the interpretation of the results in the case of current-resolution data for HD 189733b. However, the numerical effect described in this section may manifest in real-data retrievals as resolution improves.
Figure 17. Comparison of retrieved posteriors for HD 189733b at two different wavenumber-grid resolutions. In general, the posteriors match; only CO and CH₄ show minor differences, though they are not significant enough to affect conclusions drawn from the posterior.

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